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Development of a Novel Method for Deriving Thresholds of Toxicological Concern (TTCs) for Vaccine Constituents

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Development of a Novel Method for Deriving Thresholds of Toxicological Concern (TTCs) for Vaccine Constituents

by

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Abstract

Safety assessment relating to the presence of impurities, residual materials and contaminants in vaccines is a focus area of research at the United States Food and Drug Administration (FDA). Sponsors who submit Investigational New Drug (IND) applications for new vaccine products must report the results of safety assessments to the Division of Vaccines and Related Products Applications (DVRPA). Scientifically defining thresholds of toxicological concern (TTCs) as they apply to vaccine constituents will provide a useful aid to the sponsors and public regarding safety assessments of compounds for which there is little or no toxicity data. TTCs are mathematically modeled and extrapolated levels, below which adverse human health effects are not expected to occur (Kroes, 2004). In this project, we accessed DVRPA's submission databases and open source data to yield an initial chemical test set. Using INCHEM, RepDose, RTECS and TOXNET, we gathered LD50 and TDLo data.

Using a structure-based decision tree, provided in the ToxTree software package, (3) different algorithms (The Cramer extended, the In vivo Rodent Micronucleus assay, and the Benigni-Bossa rule base for Carcinogenicity by ISS) were applied to assign the initial test set (n= 197) of chemicals into structural families based on structural alerts (SAs). This resulted in six (6) potential methods for elucidating TTCs: In Vivo Rodent Micronucleus assay/ LD50, Benigni-Bossa/ LD50, Cramer extended/ LD50, In Vivo Rodent Micronucleus assay/ TDLo, Benigni-Bossa/ TDLo, and the Cramer extended/ TDLo.

After each algorithm designated two structural families each, the distribution of TDLo's and LD50's for each structural family was subjected to a preliminary data analysis using JMP statistical software version 9. Based on an analysis of quantiles, skew, and kurtosis, it was concluded that the TDLo dataset was of poor quality and was dropped from further analysis, and that the In vivo rodent micronucleus assay algorithm failed to partition the initial test set in a meaningful way, so it too was culled from further consideration. This resulted in (2) remaining TTC methods for further consideration: Benigni-Bossa/ LD50 and the Cramer extended/ LD50.

The remaining methods were subjected to internal validation based on Gene-Tox, CCRIS, CPDB, IARC, and EPA classifications for genotoxic mutagenicity and carcinogenicity. Validation parameters were calculated for both methods and it was determined that the Benigni-Bossa/ LD50 method outperformed the Cramer extended/ LD50 method in terms of specificity (87.2 vs. 48.1%), accuracy (65.2 vs. 52.94%), positive predictivity (66.6 vs. 50%), negative predictivity (64.8 vs. 56.5%), ROC+ (2 vs. 1) and ROC- (1.84 vs. 1.3). These results indicated that the Benigni-Bossa/ LD50 were the most appropriate for calculating TTCs for vaccine constituents.

For each class, the lower 2.5^{th} percentile LD50 was extrapolated to a TTC value using safety estimates derived using uncertainty factors (UF) and adjusting for adult human weight. Final TTCs were designated as 18.06 μg/ person and 20.616 μg/ person for the Benigni-Bossa positive and negative structural families.

Introduction

Since the federal government passed the Biologics Control Act in 1902, it has been responsible for ensuring the safety and efficacy of all vaccine products licensed in this country. Throughout the 20th century, the federal government's regulatory capacity has increased by leaps and bounds, often in response to public health tragedies such as the diphtheria vaccine contamination of 1901 and the Cutter Polio Vaccine Incident of 1955. Today, the Center for Biologics Evaluation and Research (CBER) within the FDA is responsible for "ensuring the safety, purity, potency, and efficacy of biological and related products (biologics) intended for use in the diagnosis, prevention, treatment, or cure of diseases in humans, and for ensuring the safety of the nation's supply of blood and blood products".

Public health concerns relating to the presence of leachables, extractables, impurities, and contaminants in vaccines has been a focus area of research at the CBER. Sponsors who submit IND applications for new vaccines need to conduct a safety assessment for any new vaccine formulation or delivery system and report the results to the DVRPA. TTCs, also called 'thresholds of regulation' are mathematically modeled and extrapolated levels below which adverse human health effects are not expected to occur (Kroes, et. al.. 2004). Currently, TTCs are not scientifically defined with respect to vaccine

constituents. If a TTC method is developed and validated for vaccines, it may provide a useful screening aid for compounds of unknown toxicity.

The concept of the TTC is still evolving, some of the more well established TTC methods include those that have been adopted by regulatory authorities, including oral reproductive toxicity TTCs, developed by the European Union's (EU) existing chemicals program, derived by Bernauer et. al. (2008). The TTC values were based on 91 chemicals assessed in 50 fertility studies and 62 developmental studies (Hennes, 2012). The first regulatory body to formally adopt TTCs was the FDA for food packaging and contact materials at 0.5 parts per billion; that is "a substance present in the daily diet for a lifetime at 0.5 parts per billion (ppb) would pose only negligible risk even if it were later shown to be a carcinogen" (FDA, 1995). The value of 0.5 ppb was derived by A.M. Rulis (1986) via the extrapolation of carcinogenic potency data (TD50's) and the application of the EPA's lifetime excess cancer risk threshold of 1×10-6 (this level is arbitrary; not based on any scientific analysis). The adopted blanket level TTC of 0.5 ppb per day, equivalent to 1.5 μg/ person/ day, assuming a daily consumption of 3000g (Munro et. al, 1996) was stringently conservative and intended for use with any chemical of unknown toxicity (Hennes, 2012). The level was so conservative it covered virtually all non-carcinogenic potentially sensitive biological endpoints, with the exception of allergenicity (International Life Sciences Institute (ILSI), 1999). TD50's[1] for carcinogenic endpoints were used in this process because carcinogenicity was considered the most sensitive toxic

[1] TD50: "that chronic dose rate in mg/kg body weight/ day which would induce tumors in half the test animals at the end of a standard lifespan for the species." (National Institute of Health, 2007, http://toxnet.nlm.nih.gov/cpdb/td50.html)

endpoint (Cheeseman, et. al 1999). Furthermore, TD50's, when plotted on a semi-logarithmic scale, were found to follow a Gaussian distribution, which allowed for a better extrapolation to a reference value.

The FDA's adoption of the blanket TTC of 0.5 ppb per day for food contact substances was followed by the Joint FAO/WHO Expert Committee on Food Additives (JECFA). JECFA employed TTCs in the risk assessment of food flavoring compounds and set an exposure threshold of 1.5 μg/person/ day (Hennes, 2012).

Traditionally, TTCs have been restricted primarily to oral exposure pathways, and that trend continues even today. Although there are a few oral vaccines that are currently approved (and a few more on the horizon), most vaccines are still administered via intramuscular (IM) injection.

In 1999, Cheeseman et. al. built upon Rulis' work, and endorsed the 'tiered' approach to TTCs, which not only validated Rulis' result of 0.5 ppb, but also provided a method of classifying chemicals into structural groups or 'families' that is generally preferred today as a refinement over the earlier blanket value TTCs when dealing with large chemical sets (this method was not, however, adopted by the FDA). The Cheeseman group utilized lethal dose 50% data (LD50's[2]), TD50's and identified the structural features in the most potent chemicals within their set, and sorted their chemicals into classes based

[2] LD50: also called median lethal dose, is the dose which induces lethality in half of the test animals within a specified time frame. An analogue to the TD50.

on the absence or presence of such toxicophores, provided a certain minimum LD50/ TD50 and Ames mutagenicity criteria was met.

In 1996, Munro et. al. employed the Cramer decision tree (1978) to develop a TTC methodology for noncarcinogenic endpoints along oral exposure pathways. The Cramer algorithm (1978) divides chemicals into (3) classes:

Class I: Substances [with] a simple chemical structure and efficient modes of metabolism that would suggest a low order of oral toxicity.

Class II: Substances [with] a chemical structure [in] which there is little knowledge of metabolism, pharmacology, and toxicology, but with no clear indication of oral toxicity.

Class III: Substances [with] a chemical structure that permit no strong presumption of safety, or suggestive of significant oral toxicity.

The Cramer tree divided the test set of chemicals into three structural groups that were classified as having low, intermediate, or high presumed oral toxicity, with recommended human exposure thresholds of 1800, 540, and 90 μg/person/day; respectively. These exposure thresholds were derived by identifying the lower 5^{th} percentile NOEL[3] (no observable effect level) for each structural group and applying a safety factor of 100, assuming an adult human body weight of 60 kg (Munro et. al.., 1996). In 2003, the ILSI

[3] NOEL: the highest dose at which no observable effect (beneficial or detrimental) is elicited in a group of experimental animals.

expert group endorsed the use of the Cramer tree for assessing neurotoxicants, immunotoxicants, and teratogens.

In 2004, the ILSI Europe Expert Group examined all the currently validated TTC methodologies and decided that a separate algorithm was needed to assess for organophosphate contaminants in food products. Unlike the previous decision trees, the new algorithm they developed was not wholly based on the structural features, but also incorporated estimated daily intakes and chemical classifications to determine whether or not a substance "would not be expected to be a safety concern" (European Commission, 2008). The ILSI group recommended this algorithm for low level food contaminants which lacked toxicity data, but for which exposure data was readily available. The working group adopted a separate TTC for organophosphates of 18-μg/ person/ day. For certain chemical groups (heavy metals, polyhalogenated biphenyls, endocrine disruptors, polymers, proteins, and lipophilic substances) and certain endpoints (allergic reactions, intolerance, and hypersensitivity) the TTC's of 1800, 540, and 90 μg/person/day have not been proven valid (Kroes et. al, 2004).

In addition to safety assessments, the TTC approach can also be applied to risk assessment, in which exposure data is critical, as many TTC algorithms within the risk assessment paradigm classify chemicals based on absorption, bioaccumulation, target tissues, and magnitudes of exposure (Bernauer et. al., 2008).

A common theme among many TTC methodologies is the use of a structure based decision tree to sort chemicals into classes based on the presence or absence of toxicophores, or structural alerts. Structural alerts are functional groups within a compound's physical structure that may be associated with an adverse effect on a living system; common examples include aromatic rings, vinyl amides, or nitro groups. This is, essentially, a formalization of the process that has been applied to chemicals of unknown toxicity for decades—in the absence of reliable human or animal data, the structure of the chemical and the opportunity for human exposure is evaluated to elucidate any potentially toxic effects. TTC values have been validated and applied to flavoring substances (1.5 μg/person/day) (JECFA, EFSA), food contact substances, migrants, and impurities (0.5 ppb, by the FDA) and genotoxic impurities in pharmaceuticals (also, 1.5 μg/person/day EMA, 2006). Validated methodologies represent a formalized procedure for integrating structure-activity relationships (SARs) into the safety assessment and risk-benefit assessment paradigms (Munro, 1996).

Table 1. List of Published TTC Values.

Endpoint/ Route of Exposure	Reported TTC value, in μg/ person/ day	Reference	Application
Repeat-dose/ oral	1800 (Cramer I) 540 (Cramer II) 90 (Cramer III)	Munro et. al. (1996, 1999), Cramer et. al. (1978)	Industrial organic substances
Carcinogenicity/ oral	1.5 (compounds with positive genotoxicity testing and/ or no nitroso, bezidine, hydrazine, azo, endocrine disruptor SAs, or no testing data available 15 (no SAs or negative Ames) 45 (no SAs, or negative	Cheeseman et. al. (1999)	Food packaging migrants, contact materials, flavoring substances and unintended chemicals in food

Table 1 Continued

	Ames, and appropriate minimum LD50 of 1000 mg/kg)		
Noncarcinogenics/ inhalation	Systemic effects: 980 (Cramer I), 170 (Cramer III), 300 (blanket value for all compounds not assigned to class I or III) Local effects (respiratory tract): 1400 (Cramer I), 470 (Cramer III), 1000 (blanket value for all compounds not assigned to class I or III)	Carthew et. al. (2009), Cramer et. al. (1978)	Airborne toxics
Genotoxicity/ oral	18 (organophosphates) 1.5 (Cramer class I) 9 (Cramer class II 30 (Cramer class III)	Rulis (1986, 1989, Gold et. al. (1984, 1989), Kroes et. al. (2004)	Food packaging migrants, contact materials, flavoring substances and unintended chemicals in food
Genotoxicity/ oral	0.15 (chemicals with SAs for genotoxicity, as determined by the Kroes decision tree) 1.5 (chemicals with SAs for genotoxicity, but negative Ames data)	Cheeseman et. al. (1999). Felter et. al. (2009)	Food packaging migrants, contact materials, flavoring substances and unintended chemicals in food
Repeat-dose/ oral	54 (sub-acute exposures) 84 (sub-chronic exposures) 38 (chronic exposures) All are based on pooled data from the Munro and Repdose databases.	Tluczkiewicz et. al. (2009), Munro et. al. (1996, 1999)	Industrial organics
Reproductive toxicity/ oral	1.5 (fertility specific endpoints) 1.0 (developmental endpoints) Endpoint specific TTCs are derived from lowest oral value (NOAEL/ LOAEL) found in the	Bernauer et. al. (2008)	Industrial organics

Table 1 Continued

	European Union database and divided by a safety factor.		
Genotoxicity/ oral	1.5 (allowable daily intake for exposures >12 mo.) 10 (allowable daily intake for exposures > 6-12 mo.) 20 (allowable daily intake for exposures >3-6 mo.) 40 (allowable daily intake for exposures > 1-3 mo.) 120 (allowable daily intake for exposures ≤ 1 mo.) For genotoxic pharmaceutical impurities of unknown carcinogenicity. This method does not utilize a structure based decision tree.	Müller et. al. (2006)	Pharmaceutical impurities
Multiple endpoints (carcinogenicity, neurotoxicity, developmental toxicity)/ oral	1 (for substances likely to be carcinogenic) 10 (for substances likely to be potent or highly toxic) 100 (for substances not likely to be potent, highly toxic or carcinogenic) Carcinogenic potential in humans assesses via presence of genotoxic SAs, in vitro mutagenicity, and an accepted in vivo test (such as the micronucleus test). Based on cancer potency estimates of regulated carcinogens.	Dolan et. al. (2005)	Pharmaceutical impurities
Repeat-dose	88 µg/person/day (sub-	Tluczkiewicz	Airborne toxics

Table 1 Continued

toxicity endpoints/inhalation	acute exposures) 12 µg/person/day (sub-chronic exposures) 17 µg/person/day (chronic exposures) All are based on pooled data from the Munro and Repdose databases.	et. al. (2009), Bitsch et. al. (2006), Munro et. al. (1996, 1999)	
Repeat-dose toxicity endpoints/inhalation	180 (Cramer class I compounds) 4 (Cramer class III compounds) Applied NOEC values to the Munro approach (5^{th} percentile NOECs as point of departure for extrapolation) for industrial compounds.	Escher et. al. (2010), Cramer et. al. (1978)	Airborne toxics
Reproductive toxicity/inhalation	1.0 µg/m3 (fertility) 0.5 µg/m3 (developmental) Endpoint specific TTCs are derived from lowest oral value (NOAEL/ LOAEL) found in the European Union database and divided by a safety factor.	Bernauer et. al. (2008)	Airborne toxics
Acute toxicity/inhalation	4 µg/m3 (Cat.1) 20 µg/m3 (Cat.2) 125 µg/m3 (Cat.3) 125 µg/m3 (Cat.4) 1000 µg/m3 (Cat.5) Did not utilize a structure based decision tree; applied the Global Harmonized System of Classification and Labeling of Chemicals proposed by the United Nations (acute toxicity categories 1-5) to the chemical set, identified the 10^{th} percentile NOEL for each category and applied a safety factor to	Grant et. al. (2007)	Airborne toxics

Table 1 Continued

	extrapolate to a TTC.		
Skin sensitization/dermal	900 μg/cm2 "Non-reactive" chemicals 1.64 μg/cm2 for rinse-off products; 0.55 μg/cm2 for leave-on products Classified chemicals in the local lymph node assay dataset according to mechanistic chemistry domains. Assigned to domains based on the presence or absence of a few SAs for sensitization: micheal acceptors, Schiff-base formers, certain electrophiles, or acetylating agents. Benchmarked against human potency data (no expected sensitization levels) gathered for 58 known fragrance allergens.	Safford et. al. (2011), Safford (2008)	Topical substances
Skin sensitization/dermal	0.91 μg/cm2 for typical exposure conditions 0.30 μg/cm2 for unfavorable exposure conditions (e.g. penetration enhancement). Did not use a structure based decision tree, conducted a meta-analysis of no expected sensitization induction levels for fragrance ingredients in to International Fragrance Association database, applied safety factors for account for variability and difference exposure	Keller et. al. (2009)	Topical substances

Table 1 Continued

	conditions, compounds grouped according to contact area of skin.		

Table 1 indicates that TTCs have been developed for a diverse range of endpoints, from reproductive toxicity to skin sensitization and have been derived using a variety of methods: some have reused the Cramer algorithm, some have developed new endpoint-specific algorithms, and others have not used any algorithm, but calculated a blanket (one size fits all) TTC. Since this method will be subjected to validation, the selection of endpoints must be carefully considered to ensure that assay and/ or epidemiological data will be available for validation procedures. Although the ToxTree software program offers algorithms for several endpoints, only the three that allowed for validation were selected: the Benigni-Bossa rule base for Carcinogenicity by ISS, the Cramer Extended decision tree, and the In Vivo Rodent Micronucleus Assay algorithm. These algorithms, coupled with two separate datasets, both the LD50 and TDLo, will comprise the six different methods that will be evaluated in this project: 1) Rodent Micronucleus/LD50, 2) Benigni-Bossa/LD50, 3) Cramer/LD50, 4) Rodent Micronucleus /TDLo, 5) Benigni-Bossa/TDLo, and 6) Cramer/TDLo. The TDLo data, which is generated in a very similar manner to the traditional NOELs, will serve as a control for the more unorthodox LD50 dataset.

The In Vivo Rodent Micronucleus Assay algorithm (hereafter referred to as the Microassay) was developed as a coarse grain filter to predict potential mutagens based on SAs for a positive in vivo micronucleus assay result in rodents. The micronucleus rodent assay has long been the standard follow-up for positive in vitro mutagenicity tests (such

as the Ames reverse mutation test). This algorithm includes SAs for carcinogenicity and mutagenicity previously included in ToxTree and additional substructures found in micronucleus positive compounds through data mining efforts of ISSCAN, Gene-Tox, and CCRIS. It should be noted that, despite an exhaustive search for new SAs by the authors of this algorithm, the positive predictivity of this algorithm is quite inferior to those for carcinogenicity and salmonella mutagenicity, which may reflect the low sensitivity of the micronucleus assay. It was recorded that mutagenic toxicophores that exerted themselves in other assays (such as in vitro clastogenicity) were not activated by the micronucleus assay (Benigni, et. al., 2009).

The Benigni-Bossa ISS rule base for Carcinogenicity and Mutagenicity (hereafter referred to as Benigni-Bossa) utilizes 30 SAs for genotoxic carcinogenicity and 5 SAs for nongenotoxic carcinogenicity. The module recognizes genotoxic carcinogens as electrophiles or activated electrophilic intermediates causing DNA damage, and putative mutagens (Benigni, 2008). Alternatively, nongenotoxic or epigenetic carcinogens cause no direct damage to DNA and are generally not recognized mutagens. Nongenotoxic carcinogens act through diverse mechanisms; a common example is oxidative stress.

Possible outcomes of the Benigni-Bossa algorithm are as follows: 1) no structural alerts for carcinogenicity, or, 2) at least one structural alert for genotoxic carcinogenicity, and/or 3) at least one structural alert for nongenotoxic carcinogenicity. Additionally, if a structural alert for aromatic amines or α, β- unsaturated aldehydes (congeneric classes) is fired, the quantitative structure- activity relationship (QSAR) protocol is initiated, which

offers four possible outcomes: 1) potential S. typhimurium TA100 mutagen based on QSAR, 2) unlikely to be S. typhimurium TA100 mutagen based on QSAR, 3) potential carcinogen based on QSAR, or, 4) unlikely to be carcinogen based on QSAR.

The Cramer Extended rule base is, by far, the oldest available algorithm, originally published in 1978 and validated with NOEL data gathered from 82 carcinogenic compounds (Cramer, et. Al, 1978; and Patlewicz, et. al, 2008). In 1996, Munro, et. al. extended the rule base to alleviate the misclassification of certain class I and II compounds with very low NOEL observations (Munro et. al., 1996). The extensions reclassify 'harmless' phosphates (anionic) as harmless (class I) substances, benzenes with single aromatic rings with zero to six single atom substituents as class III (harmful) substances, unnatural divalent sulfur moieties as class III, and α, β- unsaturated heteroatom moieties as class III. Most importantly, the extension rules recognize over 400 unique compounds that naturally occur in the human body (except hormones) as class I (the original Cramer rule base identified only 67) (Burenhof, 2009).

These algorithms were selected because they all offer endpoints that can be easily validated with external data: genotoxicity, mutagenicity, and carcinogenicity. Genotoxicity is the broadest of the three endpoints, and is often used interchangeably with mutagenicity, although such generalization is often incorrect. A genotoxic agent is one that can alter the structure or sequence of DNA (Aardema, 2013), and such damage may be induced at the nucleotide level or the chromosome level. Additionally, genotoxicity may be induced directly, in which the agent or its metabolite interacts with

DNA; or indirectly, in which the chemical or metabolite interacts with a macromolecule such as a mitotic spindle fiber (Aardema, 2013). Within the living system, genotoxic induced DNA damage can be successfully repaired, incorrectly repaired, or not repaired. The former option (error free repair or apoptosis) will eliminate the genotoxic pathway of toxicity. The latter two options may result in chromosomal mutation, duplication, cleavage, or aberration.

A mutagenic compound is one that elicits a specific genotoxic pathway that results in chromosomal mutation—therefore, all mutagens are genotoxics, but not all genotoxics are mutagenic. Alternative to a mutagenic classification, genotoxics may be clastogenic (inducing a break in chromosome structure, or cleavage) or aneugenic (inducing a change in the number of chromosomes via duplication or deletion). Any of these chromosome aberrations may evoke carcinogenesis, but usually will not, as immune processes within a living system may suppress such mechanisms. Additionally, there are nongenotoxic carcinogens that induce carcinogenesis via oxidative stress, heavy metals being an example. From a mechanistic standpoint, it is clear that these three endpoints are similar but certainly not identical, as such, the three algorithms used in this project may overlap somewhat. Mutagenicity may be seen as an intermediary endpoint, as all mutagens are genotoxic, some mutagens are carcinogenic, and many carcinogens are mutagenic (Miller, J., and Miller, E., 1971). We may infer that a compound that returns positive for carcinogenicity may also return positive for mutagenicity or genotoxicity, but this will not always be the case. Most importantly, mutagenicity and genotoxicity are reversible

endpoints, whereas carcinogenicity generally requires therapeutic intervention if the living system is going to return to homeostatic function.

In front-end toxicity testing and hazard identification, genotoxicity and mutagenicity have often been used as a stand-in for carcinogenicity, since DNA damage may lead to numerous pertinent human health endpoints. DNA damage to germ cells may result in heritable diseases to the exposed offspring or infertility; damage to somatic cells may lead to cancer. Germ cell damage is qualified as a change in chromosome structure or number; currently, there are no known human germ cell mutagens (Aardema, 2013).

Genotoxicity testing procedures have been used by regulatory authorities (such as EPA's ToxCast program) and private industries to prioritize chemicals on which to spend additional resources. If a chemical is a confirmed or suspected carcinogen, genotoxic testing may indicate if the carcinogen's mechanism of action is genotoxic or nongenotoxic.

Many, but not all carcinogens are genotoxic, and preliminary *in silico* and *in vitro* toxicity testing helps to save precious resources and reduce the number of animals used in biomedical research. In the past 100 years, a diverse array of analytical techniques have been developed to suit this purpose: rodent bioassays, developed around 1915, in vivo and in vitro assays in the 1970s, and in silico QSAR/ SAR, and physiology-based pharmacokinetic (PBPK) modeling in the 1990s, which offer the possibility of toxicogenomic studies which may be integrated into personalized medicine. Today, there

are literally hundreds of assays in existence that measure DNA damage, and such assays are often categorized based on endpoint: DNA mutation, repair, damage, or chromosome aberration; additionally, there are assays that detect biomarkers of DNA damage based on numerous test organisms: yeast, fungus, plants, invertebrates, mammalian cell lines, etc.

Though a plethora of assays exist, only a few are favored for inclusion within the standard battery of toxicity tests. Regulatory expert groups such as the Organization for Economic Cooperation and Development (OECD) and the International Congress on Harmonization (ICH) have published guidelines that recommend certain assays for specific endpoints and consumer products. These recommendations are the product of rigorous analyses on assay performance, such as internal and external validity testing to calculate sensitivity, specificity, and positive and negative predictivity. A popular choice for mutagenicity testing in the Ames reverse mutation assay, with a sensitivity of 59%, specificity of 74%, positive predictivity of 87%, and negative predictivity of 34% (Kirkland, 2005). In keeping with this regulatory standard, the algorithm that is selected for this project will be subjected to validation testing.

In the past decade, there has been an increased emphasis on animal free toxicology, as the traditional animal bioassay to human epidemiology approach includes numerous drawbacks, such as long latency periods (particularly for carcinogenicity studies), excessive financial burdens, and ethical human rights and animal welfare considerations (Basketter, et. al. 2012). These issues, coupled with an increase in previously untested novel compounds in consumer products, such as nanoparticles and cell therapies, and the

limited predictive capacity and external validity of animal and epidemiological studies, has given rise to integrative testing strategies, which utilizes numerous analytical components: in silico modeling, in vitro and in vivo assay data, and human epidemiological data. In keeping with the FDA's objectives to reduce the numbers of animals in biomedical research and incorporate computational techniques in safety assessments, this project will integrate the following components: in silico modeling to fill in missing data (QSAR) and categorize compounds into structural families (SAR), animal and human LD50's and TDLo's for database construction and extrapolation, and epidemiological and bioassay data for internal validation.

Statement of the problem

The objectives of this study are 1) to scientifically define thresholds of toxicological concern (TTCs) as they apply to vaccine constituents, 2) to determine whether statistically distinct classes of chemicals are created by applying a novel method for deriving TTCs for vaccine constituents, and, 3) to investigate the feasibility of using LD50 data as a point of departure when extrapolating reference levels.

Hypothesis

This study will attempt to verify the following hypothesis:

1. The hypothesis of this project will be toxicity of structural family 1 ≠ toxicity of structural family 2. Testing this hypothesis will determine whether statistically distinct groups of chemicals are created as a result of the algorithm.

Materials and Methods

Currently, there is no scientifically validated method for applying TTCs to vaccine safety assessments. TTCs are levels below which adverse human health effects are not expected to occur, similar to a reference dose. The project will be conducted in (4) phases: 1) database construction, 2) chemical classification and preliminary data analysis, 3) algorithm validation and selection, and 4) TTC calculations and hypothesis testing.

Database Construction

To compile an initial chemical test set, submission databases at the Division of Vaccines and Related Products Applications (DVRPA) were mined to determine which chemicals (such as contaminants, extractables and leachables, adjuvants, and preservatives) have been detected in currently approved vaccines. Biologicals (such as immunogens and antigens) and structurally undefined components (resins, gelatins, and oils) were excluded from the analysis, since the validated chemical structures are necessary to predict carcinogenicity, mutagenicity, and genotoxicity. Chemical Abstract Service registry numbers (CASRNs) and SMILES strings are also listed.

The primary focus of the extrapolation dataset will be toxicity measurements: LD50's and TDLo data, with corresponding test species and route of administration (RoA) by chemical. Only acute mammalian studies are included in the database, in addition to

teratology and reproduction studies. Chronic TDLo's were excluded, since they are not representative of exposure to vaccines. This data has been gathered from industry material safety datasheets (Sigma-Aldrich), the TOXNET database, the INCHEM database, RepDose, and the RTECS database.

For chemicals without published LD50's, T.E.S.T. (Toxicity Estimation Software Tool) version 4.1 was used to derive predicted LD50's (oral, rat) based on QSARs. This software program comes with a preloaded training set for providing external predictions and is available open source via the EPA's website. Values were generated via the Consensus and FDA methodologies and were included in the database. For certain chemicals and compounds, T.E.S.T. software was unable to generate any results, usually because there were no compounds in the training set that were structurally similar enough to the test compound to provide a reasonably accurate prediction of toxicity. T.E.S.T. software has been particularly useful in deriving LD50's for amino acids. The FDA and Consensus models were selected because the FDA model generated results based on the closest analogs to the compound's structure, and the Consensus model was reported to achieve the most accurate results according to external validation (EPA, 2012).

The FDA method was based on the work of Contrera et. al. (2002), and is unique among QSAR models in that it creates a structurally similar training cluster for each test compound during runtime. This method has been used by the FDA's Center for Drug Evaluation and Research (CDER) for regulatory and scientific decision making purposes. The program uses parameters such as electropological E-state indices and connectivity,

and boasts a specificity of 72%, sensitivity of 74%; positive predictivity of 69% and negative predictivity of 76% when using pharmaceutical compounds in the external validation set (Contrera, et. al, 2002). Other methodologies, such as the hierarchal method, can only produce clusters prior to runtime. Generally, the training cluster must contain a minimum of 15-20 compounds, ideally with a cosine similarity coefficient not less than 75% (to the test compound). Oral toxicity for the test compound is then predicted via multiple regression and genetic algorithm. The obvious advantage of this method is that each training cluster is custom built for the test compound in question, and, since the test compound is never included in the cluster, toxicity predictions are always external. If a cluster approaches 75 compounds and a valid prediction cannot be made, then the software aborts the run and no prediction is rendered. The program declares a model invalid if the multiple regression yields a coefficient of multiple determination (leave one-out-cross validation, also called "LOO q2", with q2 being the leave one out correlation coefficient) below 0.5, which indicates that the regression model is improperly fitted. The program also required a correlation coefficient (R^2) of at least 0.6 to proceed, since the q2 has been reported 'necessary but not sufficient' to determine a models predictive performance (Golbraikh and Tropsha, 2002).

The Consensus method generates the predicted oral toxicity of a test compound based upon the average of the predicted toxicities rendered by all other methods, and may include descriptors such as connectivity matrices, ionization potential, molecular composition and structure, and number of atoms. The applicability domain for each method still applies, and if only a single methodology is able to render a prediction, the

toxicity value is invalid. Since this method inherently stifles erroneous predictions by using an arithmetic mean, it frequently provides the most accurate prediction of toxicity (Zhu et. al., 2008). A recent validation study reported that the T.E.S.T. consensus (hierarchal, nearest neighbor, and FDA) method out performed all other QSAR prediction models for acute rat toxicity with 100% coverage and a correlation coefficient (R^2) of 0.62 (Lagunin, et. al. 2011).

Of the 197 compounds in the initial test set (pre-validation), the following compounds were analyzed by the T.E.S.T. program for oral rat LD50's:

Table 2. QSAR Derived Oral Rat LD50's

Chemical	CASRN	Method	Predicted LD50 (Oral, Rat, mg/kg)
1,2-Polybutadiene	9003-17-2	Consensus	4652.85
		FDA	3303.29
2,2 dimethyl pentane	590-35-2	Consensus	8161.59
		FDA	3003.36
2,6-Di-tert-butyl-4-methylene-2,5-cyclohexadiene-1-one	2607-52-5	Consensus	741.13
		FDA	1143.81
2'Deoxycytidine		Consensus	1039.08
		FDA	394.33
3-methylpentane	96-14-0	Consensus	4998.55
		FDA	14521.22
5-Methyldeoxycytidine	838-07-3	Consensus	1103.21
		FDA	512.45
alpha- tocopherol phosphate disodium	60934-46-5	Consensus	566.44
		FDA	866.57
carbonate	3812-32-6	Consensus	2277.33
		FDA	3392.99
cholesterol	57-88-5	Consensus	5711.38
		FDA	1879.56
DL-glutamic acid	56-86-0	Consensus	3577.2
		FDA	4554.83

D-ribose Table 2 Continued	50-69-1	Consensus	14541.36
		FDA	13204.41
ferrous succinate (butanedioic acid)	56-14-4	Consensus	1547.53
		FDA	1081.9
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	7365-45-9	Consensus	6470.74
		FDA	No Prediction Made
hydroxy L proline	51-35-4	Consensus	1848.13
		FDA	2057.6
hydroxylysine	28902-93-4	Consensus	5787.08
		FDA	6251.79
L-alanine	56-41-7	Consensus	2530.81
		FDA	8154.06
L-asparagine	70-47-3	Consensus	2487.87
		FDA	5712.62
L-lysine	56-87-1	Consensus	2471
		FDA	5373.5
L-proline	147-85-3	Consensus	1642.91
		FDA	2892.54
n-hexadecane	544-76-3	Consensus	8156.82
		FDA	5430.51
n-octadecane	593-45-3	Consensus	8269.52
		FDA	6442.2
tetrafluoroethylene	116-14-3	Consensus	621.59
		FDA	895.89
sodium glucuronate	14984-34-0	Consensus	4369.26
		FDA	5183.07
sodium pyruvate	113-24-6	Consensus	1604.07
		FDA	1068.15
Triphosphopyridine Nucleotide (NADP)		Consensus	24039.83
		FDA	31255.95
Uridine 5'- triphosphate	63-39-8	Consensus	1158.05
		FDA	2659.45
Xanthine	69-89-6	Consensus	642.49
		FDA	758.16

Unfortunately, no such software was available for elucidating TDLo's, and the lack of available TDLo data was a hindrance when constructing the initial test set. Within the

initial test set, there were 68 chemicals for which LD50 data could be gathered or generated for which TDLo data was unavailable, as a result, the TDLo dataset was considerably smaller (n=818) than the LD50 dataset (n=1008).

The database also included data for validation purposes. Databases that offered classifications with respect to carcinogenicity or mutagenicity, such as the Cancer Potency Database (CPDB), the Chemical Carcinogenesis Research Information System (CCRIS, a component of TOXNET), the Gene-Tox system for mutagenicity (also a component of TOXNET), the International Agency for Research on Cancer (IARC) monographs, and the Environmental Protection Agency (EPA) 2005 Cancer Guidelines database were mined for classifications. All chemicals with published classifications were included in the initial internal validation chemical set. Chemicals with a rating of 'equivocal' were not included in the internal validation analysis.

Chemical Classification and Preliminary Data Analysis

The initial test set was subjected to partitioning by the following algorithms: the Cramer extended rules, the Benigni- Bossa ISS rule base for genotoxicity, mutagenicity, and carcinogenicity, and structural alerts for the In Vivo Micronucleus Assay in Rodents (a mutagenicity algorithm). One limitation of the ToxTree software is that user developed algorithms can only incorporate certain structural alerts; therefore, using a well-validated decision tree (such as Cramer) may produce better results than a user designed algorithm. For the purpose of this study, Cramer class II compounds (those that were classified as intermediate, marginal or equivocal for toxicity) were folded into class III, so as to keep

all three algorithms on equal footing by providing "binary results", so each algorithm could classify a chemical as being "positive" (high presumed toxicity, due to the presence of one or more structural alerts) or "negative" (low presumed toxicity, due to the absence of structural alerts or presence of protective structural elements).

The hypothesis of this project is: toxicity of structural family 1 ≠ toxicity of structural family 2. Testing this hypothesis will determine whether statistically distinct groups of chemicals are created as a result of the algorithm. After the initial test set was run through each of the algorithms, the distribution of LD50's and TDLo's for each structural family as determined by each algorithm was analyzed using the JMP v9.0.2 statistical package to determine whether the algorithms were successfully able to sort the initial test set into meaningful structural families-- that is, chemicals with the lower LD50's and TDLo's were classified as positive for mutagenicity, carcinogenicity, or genotoxicity by the selected algorithm, and chemicals with higher LD50's or TDLo's were generally classify as negative. Any unsuccessful algorithms will be culled from further analysis. For the purposes of this study a comparison of the quantiles between the 'positive' and 'negative' structural families will be used to determine if an algorithm is successful, that is, negative families should consistently exhibit higher toxicity measurements than families that are positive for structural alerts. To maintain a conservative dataset, all LD50 and TDLo values in excess of 25,000 mg/kg/body weight were excluded from analysis. The quality of TDLo versus LD50 data was evaluated via markers of distribution—skew, kurtosis, and the points of departure—PODs that were deemed excessively conservative (those that yield TTCs so stringently conservative that industry

could not possibly meet them) or overly liberal (those that might place public safety at risk) will indicate a data set of poor quality. The goal of this research is to eliminate at least three of the six possible methods, but more or less may be culled depending on the results of the analysis.

Algorithm Validation and Selection

The final method was selected by calculating the sensitivity, specificity, accuracy, and positive and negative predictive values for each of the remaining algorithms, based on a ~10% internal group leave-out validation based on the CPDB, CCRIS, Gene-Tox, EPA, and IARC carcinogenicity and mutagenicity data. The CPDB, EPA, and IARC systems were used for carcinogenicity validation, the CCRIS database were used for both carcinogenicity and mutagenicity validation, and the Gene-Tox was used solely for mutagenicity validation.

Since the primary goal of the project was to screen out compounds that are definitely negative as opposed to those that are decidedly positive, specificity was considered the most important parameter when making a final decision. This is typical in the regulatory setting, since chemicals that are screened as 'negative' or 'low priority' are excused from detailed individual chemical risk assessment, whereas chemicals that are decidedly highly toxic or marginally toxic require a more detailed review process.

The CPDB, CCRIS, and Gene-Tox systems provide results based primarily on animal studies. If the database in question reported even a single study with positive results, that

chemical was labeled as positive for mutagenicity or carcinogenicity for validation purposes. The EPA and IARC databases are a little more complex, as they attempt to synthesize both epidemiological and animal data into a hierarchy of evidence, and are thus more sophisticated than the TOXNET systems. The EPA and IARC systems are tiered, and a chemical may be labeled as 'carcinogenic', 'likely carcinogenic', 'possibly/ suggestively carcinogenic', 'equivocal', or 'not carcinogenic'; or some qualitative variation thereof. Since this protocol was designed with regulatory applications in mind, a worst case scenario will be assumed with respect to mutagenicity and carcinogenicity, therefore, chemicals that are reported as 'carcinogenic', 'likely carcinogenic', and 'possibly/ suggestively carcinogenic' will be considered positive for validation purposes.

Since the EPA and IARC classifications are the result of a systematic risk assessment that takes many types of evidence into account—epidemiological, mechanistic, and animal—they will be favored over the TOXNET results, which only report animal data. Chemicals that are labeled as 'equivocal' or having 'inadequate information to assess carcinogenic potential' by the EPA or IARC databases will be excluded from internal validation, regardless of the TOXNET ruling.

The IARC characterizes the categories of carcinogenicity as follows: group 1 is described as agents that are carcinogenic to humans; this label is applied when there is "sufficient evidence of carcinogenicity in humans". In rare cases, a compound may be placed in group 1 when evidence of human carcinogenicity is insufficient but evidence of carcinogenicity in animal is sufficient and there is strong evidence of a mechanism of

carcinogenicity in humans. Group 2 is further divided into two subgroups, 2A and 2B, compounds that are probably carcinogenic to humans and agents that are possibly carcinogenic to humans, respectively. According to IARC guidelines, the qualifications of possibly carcinogenic and probably carcinogenic have no quantitative significance and are simply delimiters used to further tier the magnitude of evidence for human carcinogenicity. To be placed in group 2A, an agent must produce sufficient evidence of carcinogenicity in animals but only limited evidence in humans. In exceptional cases, an agent may be placed in this category based solely on limited evidence of carcinogenicity in humans. To be assigned to group 2B, an agent must display limited evidence of carcinogenicity in humans and less than sufficient evidence of carcinogenicity in animals, or, alternatively, if there is inadequate evidence of carcinogenicity in humans but sufficient evidence of carcinogenicity in animals. A chemical may also be placed in this group solely on the basis of strong mechanistic evidence. IARC group 3 agents are considered not classifiable with respect to human carcinogenicity, and as such, will not be included in the internal validation scheme. Chemicals assigned to this group display inadequate evidence of carcinogenicity in humans and inadequate or limited evidence of carcinogenicity in animals. In rare cases, a chemical may be placed in this group if there is sufficient evidence of carcinogenicity in animals, but there is sufficient evidence that the mechanism of carcinogenicity is not present in humans. Placement in this group is considered neutral and is not an endorsement of safety or carcinogenicity, rather a recommendation for further carcinogenicity studies of the chemical in question. Chemicals placed in group 4 are probably not carcinogenic to humans based on evidence that suggests a lack of carcinogenicity in humans and animals, and, exceptionally, when

there is inadequate evidence of carcinogenicity in humans but evidence that suggests a lack of carcinogenicity in animals, supported by strong mechanistic data (IARC, 1996).

The USEPA's hazard identification for carcinogens is similar to that of IARC in that it considers a wide variety of evidence. The EPA guidelines for carcinogenic risk assessment recognizes three tiers of data: human epidemiological evidence, long term animal bioassays, and supporting data which may include short term genotoxicity tests, pharmacokinetic studies, and SARs (EPA, 2005). The categories are defined as follows: group A, carcinogenic to humans, includes compounds with adequate human data to support a causal relationship between the compound and human cancer (generally, this requires human epidemiological evidence), group B includes compounds that are probably carcinogenic to humans, those that display sufficient evidence from animal studies to infer a causal relationship and limited supporting human evidence (subgroup B1) or no human evidence (subgroup B2). Chemicals assigned to group C are considered possible carcinogenic to humans, they demonstrate limited animal evidence and little or no human data. Compounds in group D are considered not classifiable as to human carcinogenicity, that is, there is little or no evidence to confirm or refute carcinogenicity in humans or animals. This group is comparable to IARC group 3, and will also be excluded from internal validation procedures. Lastly, compounds in group E, evidence of non-carcinogenicity in humans, display through human and or animal evidence to be non-carcinogenic. Generally, at least two animal studies are required, with two different species, or adequate epidemiological evidence in humans (EPA, 2005).

Internal validation will also serve as a guide for making recommendations on the limitations of the methodology, since many other structure-based algorithms require the exclusion of certain classes of compounds (such as organophosphates and heavy metals). Since this project is being conducted within the regulatory paradigm, it is important to be aware of any limitations and shortcomings inherent in the methodology. Such recommendations will be reported with the internal validation results. The results will report the following parameters: sensitivity, specificity, accuracy, positive predictivity, negative predictivity, ROC positive and ROC negative.

TTC Calculations and Hypothesis Testing

To maintain a conservative dataset, all observations in excess of 25,000 mg/kg will be excluded from analysis. TTC derivation will be probabilistic, rather than deterministic, since a distribution of data points are gathered for each class, which eliminates the need to rely on a single point estimate during extrapolation.

The application of LD50's and TDLo's as points of departure for calculating TTC's is a novel approach; traditionally, NOELs have been used. There is one publication (Rulis, 1986), in which LD50's were extrapolated to TTCs; however, this publication is not currently available. The decision to use LD50's and TDLo's as opposed to NOELs is threefold: 1) LD50 data focuses on a single endpoint, death, which is a certain, irreversible, and dichotomous outcome, as opposed to many of the endpoints measured by NOEL studies; 2) NOEL studies are fixed-dose, and therefore, do not provide true dose response data; and 3) NOEL data does not appear to be widely available for many of

the chemicals present in vaccines, however, TDLo's are widely available in the RTECS database. The use of TDLo's in calculating TTC's is not documented, however, extrapolation techniques that have been traditionally used for NOELS and LOELs may be adapted to suit.

Traditionally, when calculating TTC's from NOELs for noncancer endpoints the lower fifth percentile value NOEL is identified for each of the structural families, multiplied by 60 (conversion from mg/kg body weight to mg/person body weight), and divided by 100 (margin of safety), resulting in a different TTC for each class (three separate threshold values corresponding to low and high presumed toxicity). This methodology was originally devised for oral genotoxics (a different route of exposure than typical vaccines) and included chronic, sub chronic, and acute NOELs. Currently, there is only a scientific precedent for deriving TTC's from NOELs and TD50 (carcinogenic potency) data and one of the objectives of this study is to determine whether LD50 or TDLo data can provide TTC values for vaccine constituents. Different sources have suggested using margins of safety up to 100,000 as a starting point, others have suggested using logistic or probit analysis, however, since LD50 data tells the researcher nothing about the shape of the slope—homogeneity or otherwise (unlike NOEL and TDLo data), this type of extrapolation may not be appropriate if the selected methodology is based upon LD50's. Unlike LD50 data, TDLo data is based on a single recorded mortality or morbidity, and carries less confidence than the LD50, which is calculated by statistical analysis.

Although there is no published method for extrapolating TDLo's or LD50's to TTC's, the methodology published by DeSosso for extrapolating Acceptable Daily Intake (ADI) from TDLo's [ADI = TDLo/ margin of safety (MOS), where the MOS is some factor of 10 adjusting for human variability and species extrapolation] may be adapted (TDLo/ 100 = NOEL). Similar techniques have been published for LD50 and LDLo data (DeSosso, 1987), where an uncertainty factor of 100,000 is applied to some LD50. Additionally, the FDA CDER utilizes TD50 (carcinogen potency data from rodent bioassays) data extrapolated with an uncertainty factor of 50,000 when calculating TTCs for potentially genotoxic and carcinogenic impurities in drug products. The lower uncertainty factor is justified because drug products confer considerable therapeutic benefits, impurities notwithstanding. This logic certainly extends to vaccines, and therefore, this approach may offer the best balance of risk and benefit when conducting risk assessments for therapeutics, it will be given first priority and will be eliminated only if it yields excessively liberal TTCs. According to the CDER's guidance document ICH M7: Impurity Limits, the default TTC should be applied only when chemical specific carcinogenicity data is not available. If such data is available, a chemical specific TTC is indicated, extrapolated from the lowest TD50 value. Chemical specific TTCs may be higher or lower than the default TTC (1.5 μg/ day) depending on the TD50 value. The guidance document indicates that the default TTC method overestimates risks and exposures in excess of the default TTC are often acceptable, as determined by chemical specific risk assessment.

Results and Discussion

Database Construction

After mining the DVRPA database for leachable and extractable reports, excipient studies, safety assessments, biological license applications, and open source publications, a list of 215 compounds was compiled. Each compound was subjected to the ToxTree QSAR/SAR program to ensure that a validated structure was available. Inclusion in the study also required that either an acute mammalian TDLo or LD50 data was available as well, either from the TOXNET database or via QSAR in the T.E.S.T. software program. Of the 215 chemicals found in vaccines, 18 compounds were excluded, either because they were structurally undefined (resins or gels) or lacked TDLo and LD50 data. This effort yielded an initial test set of 197 chemicals for entry into the ToxTree program (see appendix III).

Although the T.E.S.T. program proved useful in generating LD50's, there was, unfortunately, no such software available for elucidating TDLo's, and the lack of available TDLo data was a hindrance when constructing the initial test set. Within the initial test set, there were 68 chemicals for which LD50 data could be gathered or generated for which TDLo data was unavailable, and as a result, the TDLo dataset was considerably smaller (n=818) than the LD50 dataset (n=1008).

Of note in the initial test set is the presence of polychlorinated biphenyls (PCBs); which are a relatively new impurity in vaccine products. The presence of PCBs can be attributed to novel adjuvants containing squalene (shark liver oil), and, as lipophilic endocrine disruptors, this family of chemicals may require special considerations in the risk assessment process. PCBs, commercially known as Aroclors, are, from a metabolic prospective, very inert, and resistant to metabolism by oxidation, reduction, and electrophilic substitution. Being fat soluble, they are also difficult for mammals to eliminate. Other properties may vary widely from compound to compound, but, generally, as chlorination increases, so does lipophilicity. From a SAR standpoint, PCBs can be sorted into two groups: coplanar or ortho-substituted congeners. Coplanar molecules generally act as aryl hydrocarbon receptor (AhR) agonists, and are often qualified as being "dioxin-like", and have the distinction of altering gene transcription (since AhR is a transcription factor) (Safe, et. al, 1984; Safe, et. al., 1985). AhR receptor mediated toxicity is not the only avenue through which PCBs exert toxic effects, noncoplanar PCBs that feature chlorine atoms at the ortho positions are notably not AhR agonists, but may illicit some neurotoxic or immunotoxic tendencies, however, only at much higher concentrations than the dioxin-like PCBs (Winneke, et. al, 1998). One such example is the ability of di-ortho-substituted non-coplanar PCBs to interfere with calcium dependent signal transduction within cells, leading to neurotoxic effects (Simon, et. al., 2007), and the disruption of thyroid hormone transport via transthyretin competition (Chauhan, et. al. 2000).

Chemical Classification and Preliminary Data Analysis

The initial test set was partitioned by three different algorithms that were available in the ToxTree version 2.5.4 program: the Cramer Extended decision tree (designated as Cramer), the Benigni-Bossa Carcinogenicity (genotoxic and nongenotoxic) and Mutagenicity rule base by ISS (designated as Benigni-Bossa), and the In vivo Micronucleus assay in Rodents (designated Microassay). For the purposes of data entry, a chemical sorted into a structural family that was positive for at least one structural alert were designated as "1", and chemicals sorted into the negative structural family were designated as "0".

The Cramer algorithm identified structural alerts for genotoxicity, irrespective of mutagenicity or carcinogenicity. A notable limitation of the Cramer algorithm with respect to this project is that it only makes predictions for oral toxicity—although there are a few vaccines that are administered orally, most are administered via the intramuscular route—therefore, owing to the lack of first pass metabolism in these cases, the Cramer system may have underestimated the toxicity of vaccine constituents, an undesirable shortcoming within the regulatory paradigm. Among the algorithms used in this project, the Cramer method has the distinction of producing (3) structural families of chemicals (whereas the others produce only two). Class II, the 'marginal class' was populated so sparsely that it was folded into class III in order to uphold the worst-case scenario that is consistently assumed in regulatory toxicology. This resulted in the reassignment of the following compounds from class II to class III:

List 1. Compounds Reassigned to Cramer class III from class II

Compound	CASRN
2-phenoxyethanol	122-99-6
butylated hydroxytoluene (BHT)	128-37-0
L-cystine	56-89-3
nicotinic acid	59-67-6
octoxynol 9	9002-93-1
polyethylene glycol nonylphenyl ether	9016-45-9

The initial test set was assigned by the Cramer algorithm (see also Appendix III) as follows: 82 compounds sorted in class I (presumed low order of oral toxicity, the negative structural family) and 113 compounds class III (presumed high order of oral toxicity, the positive structural family).

The Microassay algorithm sorted chemicals into positive and negative structural families based on whether they would be expected to produce a positive or negative result in the in vivo rodent micronucleus mutagenicity assay. This algorithm sorted 105 chemicals positive and 90 negative, however, as previously discussed, this assay has an unfavorable sensitivity rating compared to the Ames mutagenicity assay—therefore, there may be a high number of false positives within the Microassay sorting scheme.

The Benigni-Bossa is by far the least conservative algorithm used in this project; it produced a positive structural family of only 39 chemicals and a negative structural family of 155. To a certain extent, this is expected, since carcinogenicity is after all, a far rarer outcome than mutagenicity and genotoxicity. Internal validation with a specificity measurement will determine if there is an unacceptable level of false negatives within this sorting scheme.

Table 3. Classification Schemes by Algorithm

Algorithm	No. of Chemicals Labeled Positive	No. of Chemicals Labeled Negative
Microassay	105	90
Benigni-Bossa	39	155
Cramer Extended	113	82

The primary objectives of the preliminary data analysis were to determine the quality of both the TDLo and LD50 datasets and to determine which algorithm was most appropriate for sorting vaccine constituents into high and low toxicity groups. The final selection of the dataset (TDLo or LD50) and algorithm (Cramer, Microassay, or Benigni-Bossa) was partially dependent on the results of this initial analysis, as part of the purpose of this exercise was to eliminate those methods that would yield obviously invalid TTCs. A final selection was based upon the results of internal validation parameters. The final dataset was subjected to a more rigorous summary analysis.

To maintain a conservative dataset, all TDLo and LD50 values above 25,000 mg/kg were culled. For the LD50 analysis, 1,008 data points were initially included, however, since the upper limit was set at 25,000 mg/kg, 34 data points were culled from analysis. This resulted in the exclusion of some or all LD50 values for the following compounds:

List 2. Compounds with LD50 Data Points Excluded from Final Analysis Due to Cap of 25,000 mg/kg

Compound	CASRN
aluminum silicate	1335-30-4
Cyclohexane	110-82-7
D-galactose	59-23-4
d-sorbitol	50-70-4
dextran	9004-54-0
Glycerin	56-81-5
hemin chloride	16009-13-5
hexamethyldisiloxane	9006-65-9
Indigo	482-89-3

List 2 Continued

Iron	7439-89-6
L-ascorbic acid	50-81-7
L-glutamic acid	56-85-9
L-methionine	63-68-3
monosodium L glutamate	142-47-2
n-Hexane	110-54-3
polyethylene glycol nonylphenyl ether	9016-45-9
Polypropylene	9003-07-0
polysorbate 20	9005-64-5
polysorbate 80	9005-65-6
sorbitan monoleate	1338-43-8
Sucrose	57-50-1
titanium dioxide	13463-67-7
vinyl acetate chloroethene	

For the TDLo analysis, initially 818 data points were included. Constraining to 25,000 mg/kg resulted in the exclusion of some or all data points (n=70) for the following compounds:

List 3. Compounds with TDLo Data Points Excluded from Final Analysis Due to Cap of 25,000 mg/kg.

Compound	**CASRN**
adenosine	58-61-7
aluminum hydroxide	21645-51-2
aluminum sulfate	7783-20-2
butylated hydroxytoluene (BHT)	128-37-0
calcium carbonate	471-34-1
citric acid	77-92-9
D-galactose	59-23-4
folic acid	59-30-3
formaldehyde	50-00-0
glutaral	111-30-8
glycine	56-40-6
hexamethyldisiloxane	9006-65-9
L-cysteine	52-90-4
L-lysine	56-87-1
L-methionine	63-68-3
L-phenylalanine	63-91-2
monosodium glutamate	142-47-2
n-Hexane	110-54-3
nicotinic acid	59-67-6
octoxynol 9	9002-93-1

List 3 Continued

polysorbate 80	9005-65-6
sodium borate	1303-96-4
sodium chloride	7647-14-5
sodium metabisulphite	7681-57-4
sucrose	57-50-1
titanium dioxide	13463-67-7
vinyl acetate-chloroethene	

A basic distribution analysis was performed using JMP statistical software with the following output:

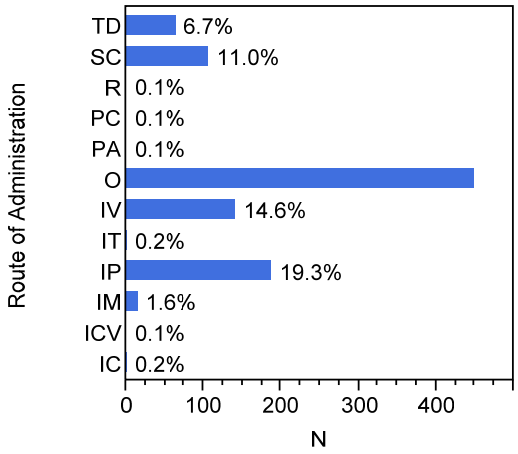


Figure 1. Relative Frequencies of Route of Administration (RoA) in the LD50 Data

As seen in figures 1-2, the toxicity data included in both the TDLo and LD50 datasets primarily include oral rodent data. Since most vaccines are not oral, and the oral route of exposure features a first pass effect that is not included in the typical intramuscular exposure scenario, this may lead to some overly liberal points of departure. Fortunately, the subcutaneous, intravenous, and intraperitoneal routes of administration are the second, third, and fourth most frequently observed data types present in both the TDLo and LD50 datasets. These exposure scenarios are, from a mechanistic standpoint, much more similar to the intramuscular route of exposure that is typical in vaccine administration.

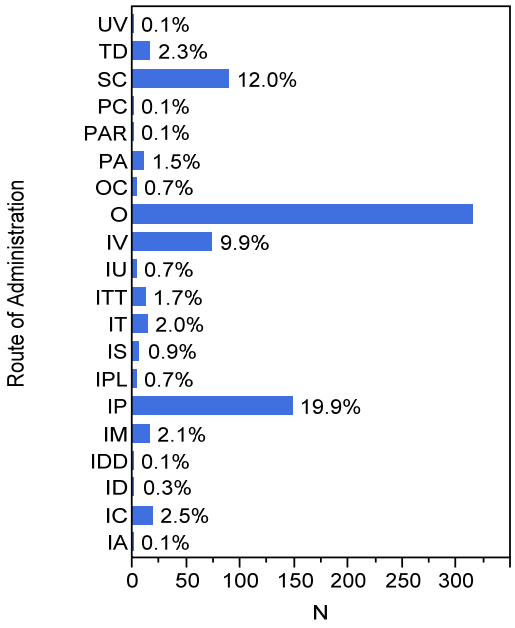


Figure 2. Relative Frequencies of Route of Administration (RoA) in the TDLo Data

One major variable that comes into play with an injection route is the presence of catabolism at the injection site, which is obviously not a feature of the oral route of exposure (Richter, et. al.. 2012), however, the mechanics of this "first-pass" catabolism process are poorly understood, and even when controlling for route of administration and molecular weight, there is a considerable degree of interspecies variability. It is generally believed that catabolism occurs at the hypodermal level and/or in the draining lymphatics. Other variables that are associated with injections include endocytosis prior to reaching systemic circulation and disposition after reaching circulation. The inclusion of a wide range of exposure routes will hopefully ameliorate any overly liberal effects of using oral data alone.

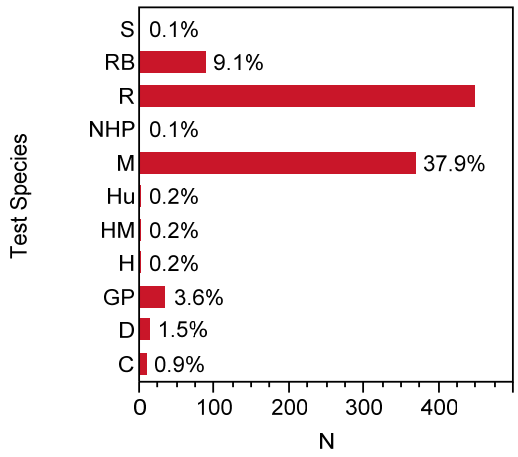


Figure 3. Relative Frequencies of Test Species in the LD50 Data

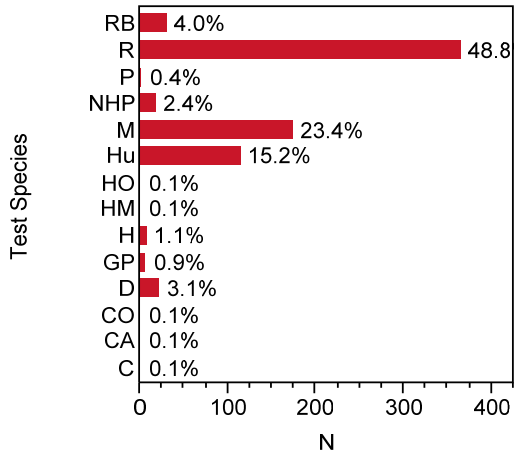
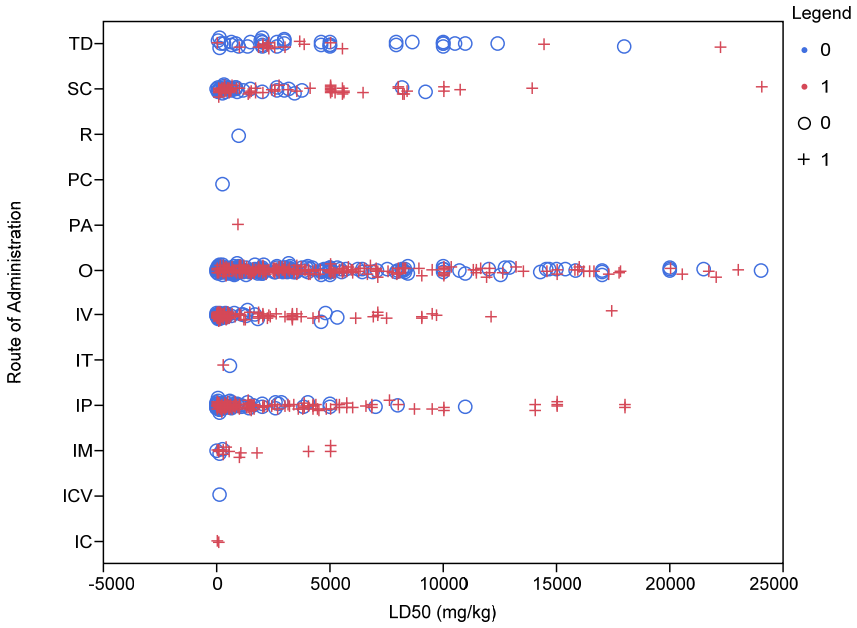


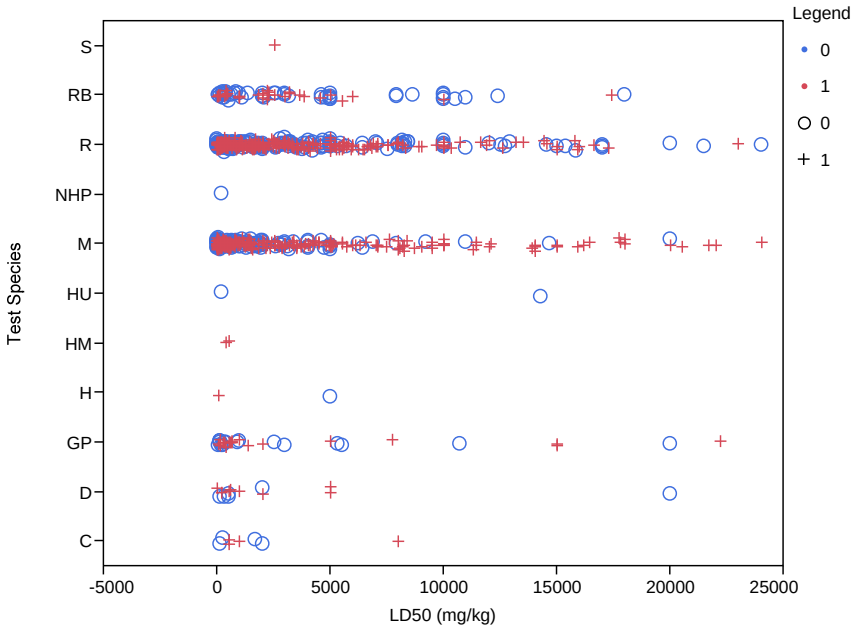
Figure 4. Relative Frequencies of Test Species in the TDLo Data

There is a relative paucity of non-rodent toxicity data, which is expected, given that the chemical industry overwhelmingly favors rats for range finding toxicity studies. Within the TDLo dataset, the percentage of human data (15.2) is of interest; this dataset may provide a TTC estimate that is more applicable to humans. A prime example of interspecies variability is illustrated by the subcutaneous administration of insulin, which displays a wide range of bioavailability depending upon species: 81.5% for rats, 31.5% for sheep, 100% for dogs, and 84% for humans (Richter et. al., 2012). For ethical reasons, animal models are used in pre-clinical studies to assess for any possible human hazards, but depending on the compound in question, there may be a marked difference

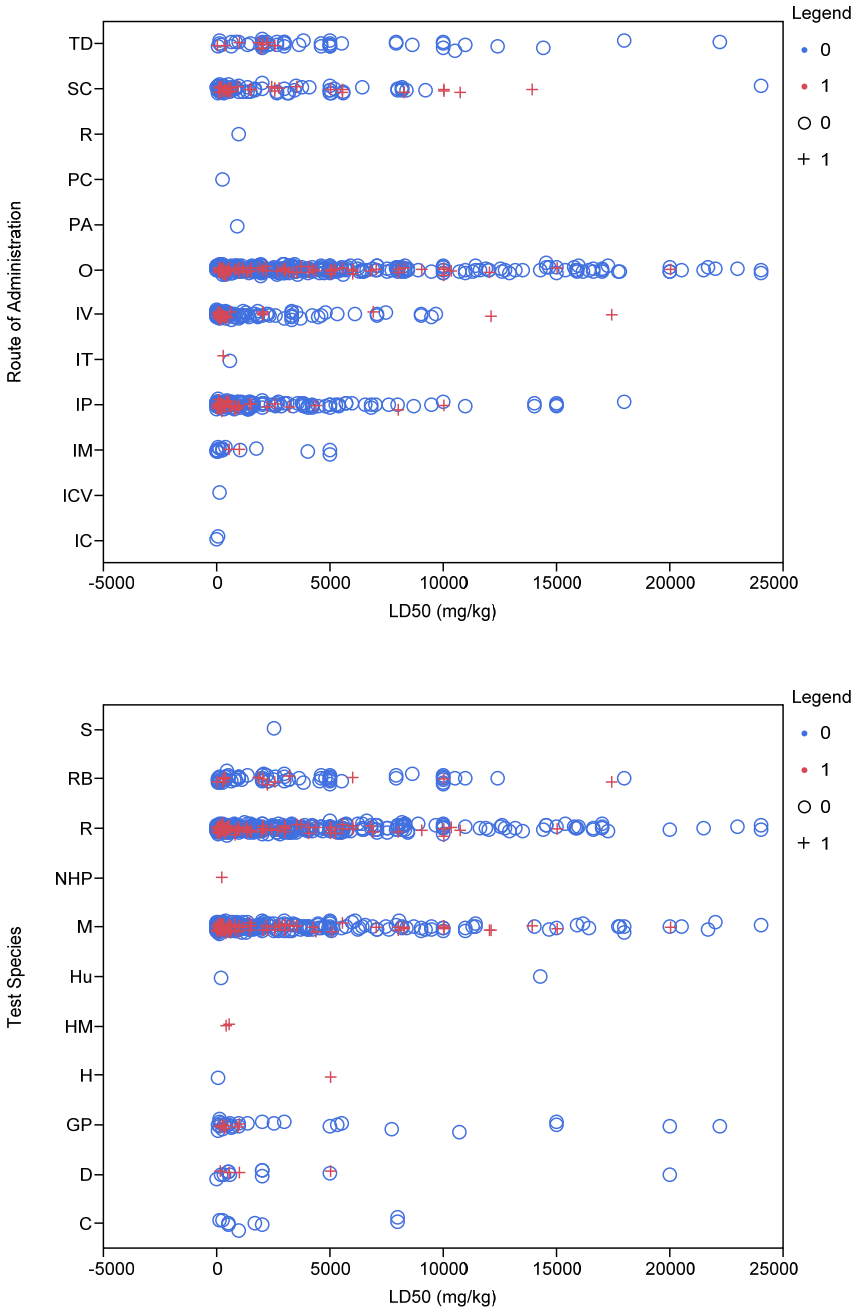
in the disposition of a compound from one species to the other. Such differences can usually be elucidated via the comparison of CYP-mediated metabolism between species. The CYP family is the primary enzyme system responsible for the biotransformation of therapeutics. Depending on a drug's specific target enzyme, a compound may behave very consistently from one species to the next, or just the opposite. Mechanistic studies have found that CYP2E1 demonstrates a similar mode of action across all test species, and dose extrapolation from one species to the next is relatively straightforward. In contrast, chemicals that target the CYP1A -2C, -2D, and -3A may display a marked difference in catabolic susceptibility from one species to the next, and therefore, extrapolating to humans may be difficult (Martignoni, et. al. 2006).

Figures 9-10 shed the Benigni-Bossa algorithm in a particularly favorable light compared to the other two algorithms. There is a relative paucity of positive observations in the upper 50% of the LD50 distribution when the initial test set is subjected to partitioning by the Benigni-Bossa algorithm. This provides an early indication that the Benigni-Bossa/ LD50 method is a particularly attractive choice for calculating TTCs for this test set. Figures 15-16 also reflect positively upon the Benigni-Bossa algorithm, with very few positive observations found in the upper bounds of the TDLo distribution, however, a final decision cannot be made until internal validation results are calculated. The primary shortcoming in visualizing the dataset this way is the opportunity for signal loss at the lower end of the distribution, where the majority of the observations are found. This issue must be taken into account, since the point of departure will be the 2.5^{th} percentile observation for each structural family.

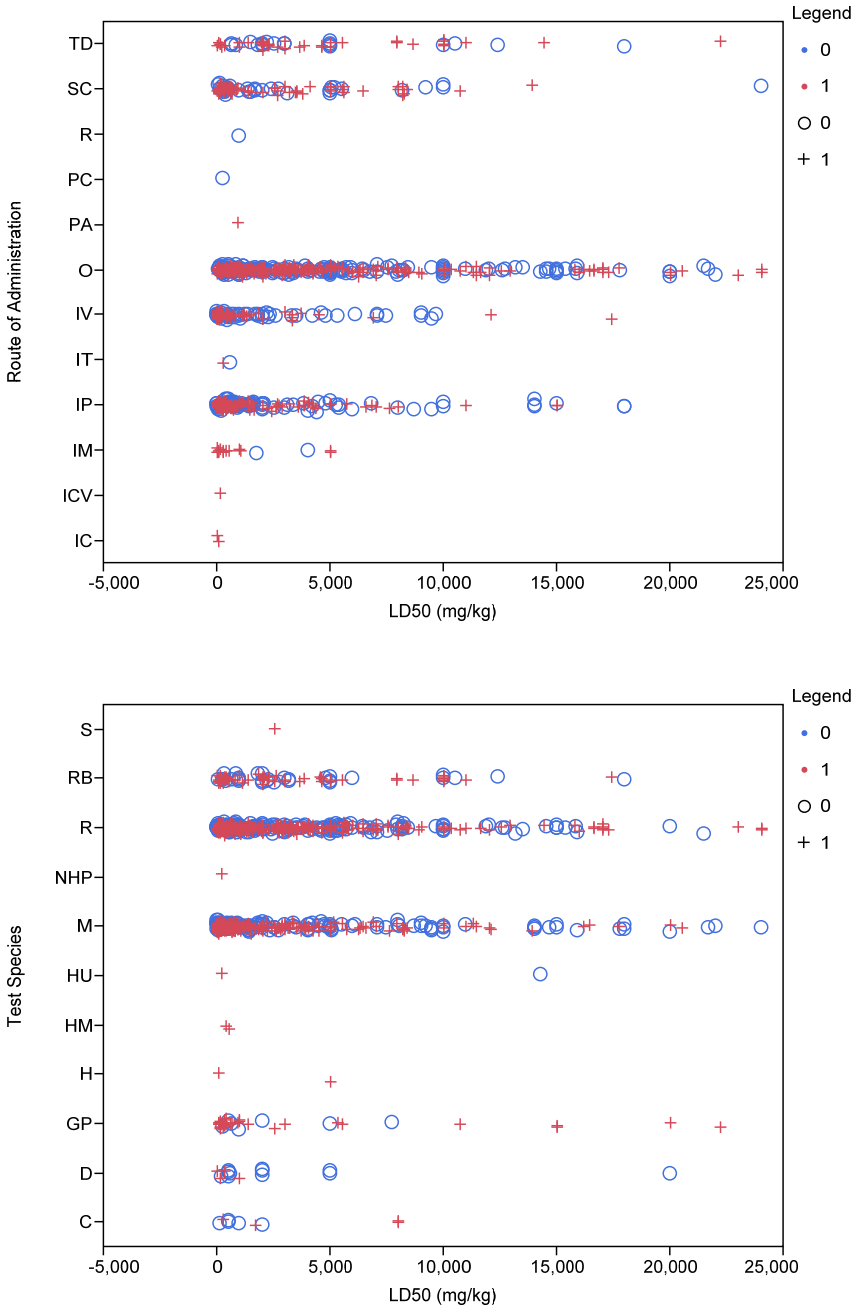




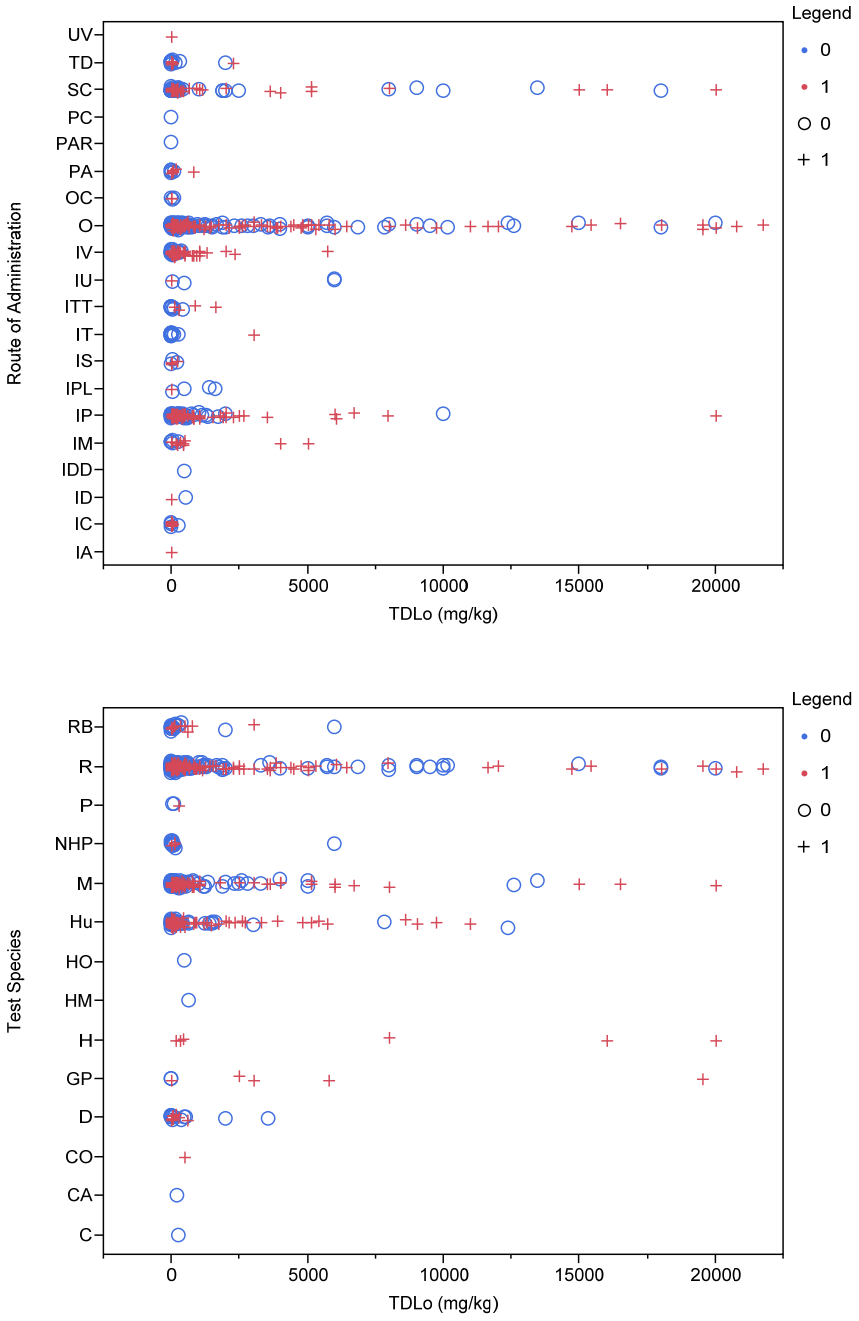
Figures 5-6. Route of Administration and Test Species vs. LD50 by Microassay Structural Family (1= Positive, 0= Negative)



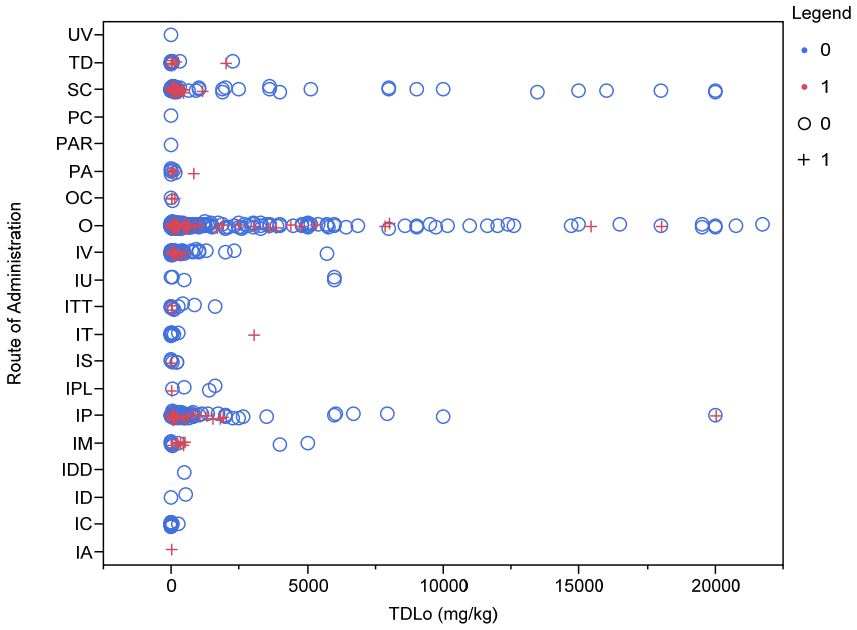
Figures 7-8. Route of Administration and Test Species vs. LD50 by Benigni-Bossa Structural Family (1= Positive, 0= Negative)

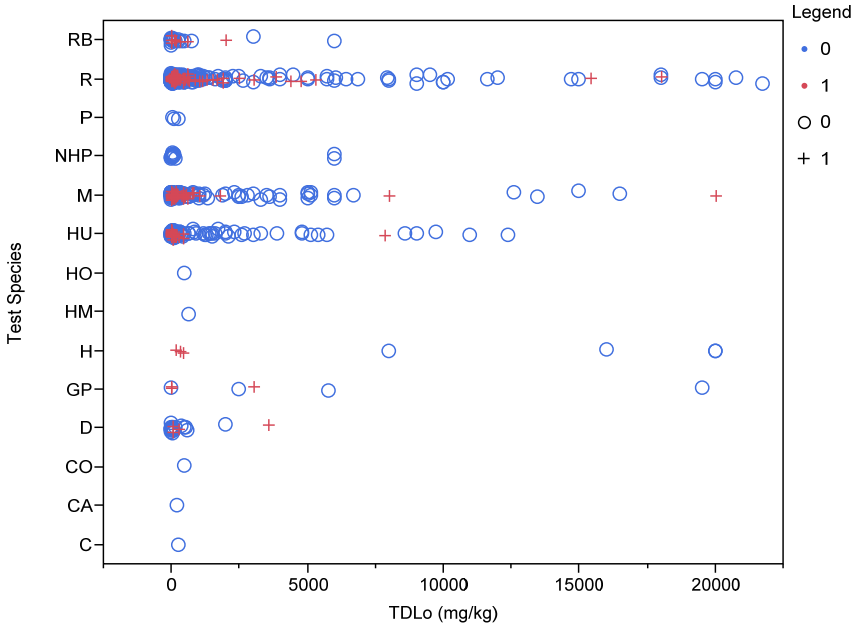


Figures 9-10. Route of Administration and Test Species vs. LD50 by Cramer Structural Family (1= Positive, 0= Negative)

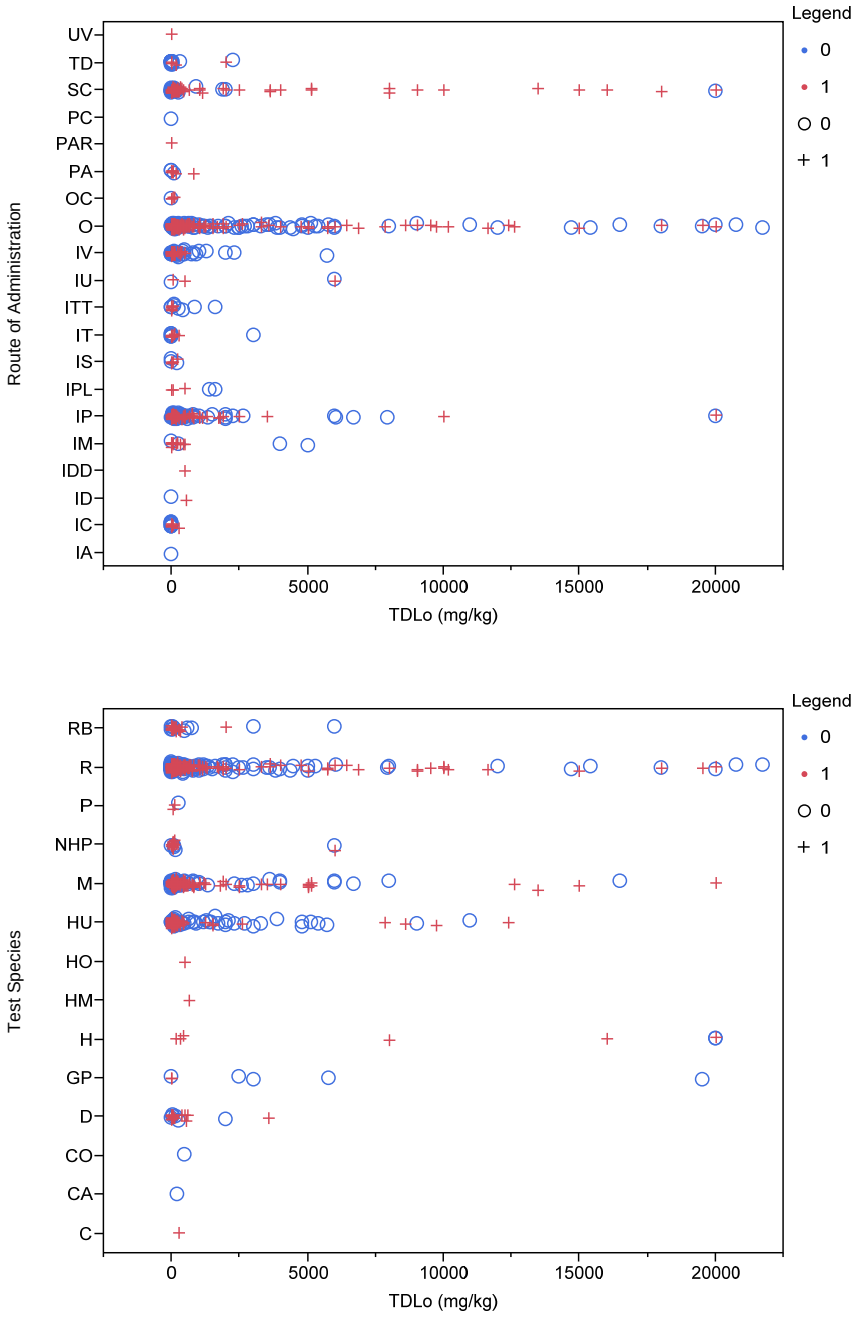


Figures 11-12. Route of Administration and Test Species vs. TDLo by Microassay Structural Family (1= Positive, 0= Negative)





Figures 13-14. Route of Administration and Test Species vs. TDLo by Benigni-Bossa Structural Family (1= Positive, 0= Negative)



Figures 15-16. Route of Administration and Test Species vs. TDLo by Cramer Structural Family (1= Positive, 0= Negative)

Table 4. Quantiles of LD50 Data by the Cramer, Microassay, and Benigni-Bossa Algorithms

Quantile (%)	Cramer Extended		Microassay		Benigni-Bossa	
	Positive	Negative	Positive	Negative	Positive	Negative
100 (maximum)	24000	24000	24000	24000	20000	24000
99.5	22975.4	22300	22307.1	23912.5	19870	23170
97.5	16600	18000	16600	17000	13450	17255
90.0	8266	10000	10000	10000	8000	10000
75 (quartile)	3990	5500	5000	4640	3000	5000
50 (median)	1200	2240	2000	1344	600	2000
25 (quartile)	250	684.5	401.25	316.75	175	495
10	60.64	246	92.72	87	85	95.6
2.5 (point of departure)	12.28	27.75	13.435	23.9275	13.5175	19.225
0.5	1.503	8.6975	1.4938	5.1435	1.675	2.3055
0 (minimum)	1.2	2.45	1.2	2.45	1.5	1.2

Table 5. Quantiles of TDLo (mg/kg) Data by the Cramer, Microassay, and Benigni-Bossa Algorithms

Quantile (%)	Cramer Extended		Microassay		Benigni-Bossa	
	Positive	Negative	Positive	Negative	Positive	Negative
100 (maximum)	20000	21750	21750	20000	20000	21750
99.5	20000	21280	20975	18050	20000	20101.2
97.5	12502.8	17475	19500	10000	7939.23	15000
90.0	2862.6	4920	5104	2000	1697.5	5000
75 (quartile)	462.5	1400	1000	422	400	900
50 (median)	100	250	200	111	98.5	168
25 (quartile)	18.056	36	25	17.875	10	26.8125
10	1.15	2	1	2.175	0.7128	2
2.5 (point of departure)	0.0698	0.00905	0.01275	0.0435	0.07138	0.02725
0.5	0.00383	0.002	.002	0.00141	0.002	0.002
0 (minimum)	0.0005	0.002	.002	0.0005	0.0005	0.0005

The evaluation of the quantiles indicated which algorithms were most appropriate for evaluating the test set. Quantiles that are highlighted in red exhibit a departure from the expected based on positive and negative structural families. Since the positive structural family is comprised of chemicals that feature structural alerts, it is expected that this group consistently produce lower LD50 and TDLo values at each quantile. This

departure from the expected is especially evident when the initial test set is sorted with the Microassay algorithm, which may indicate that the algorithm misclassifies a number of compounds in the test set with respect to mutagenicity.

Table 6. Moments from LD50 Distribution Analysis by the Cramer, Microassay, and Benigni-Bossa Algorithms

Moments	Cramer Extended		Microassay		Benigni-Bossa	
	Positive	Negative	Positive	Negative	Positive	Negative
Mean	2972.6761	4227.67	3609.5377	3222.32	2398.4269	3734.911
Std Deviation	4186.9456	4798.8122	4502.8489	4414.3875	3580.8644	4642.1194
Std Error Mean	170.22354	249.81618	188.93534	219.08238	247.69357	167.83618
Variance	17530513	23028598	20275648	19486817	12822590	21549272
Skew	2.3125777	1.6633727	1.9143206	2.1727405	2.2234009	1.9378618
Kurtosis	5.9578081	2.5294932	3.7241485	5.0410553	5.2643834	3.7867503
N	605	369	568	406	209	765

Table 7. Moments from TDLo Distribution Analysis by the Cramer, Microassay, and Benigni-Bossa Algorithms

Moments	Cramer Extended		Microassay		Benigni-Bossa	
	Positive	Negative	Positive	Negative	Positive	Negative
Mean	1135.8162	1684.964	1789.3389	957.01747	777.07867	1527.491
Std Deviation	3147.6573	3737.5043	4053.3741	2622.0268	2546.6718	3604.831
Std Error Mean	147.56445	218.34733	215.4344	132.0958	191.96261	150.7255
Variance	9907746.8	13968939	16429842	6875024.5	6485537.3	1299480
Skew	4.0463317	3.6231133	3.3355381	4.3520925	5.7074001	3.557804
Kurtosis	17.414808	13.941366	11.173659	21.382707	35.832349	13.38188
N	455	293	354	394	176	572

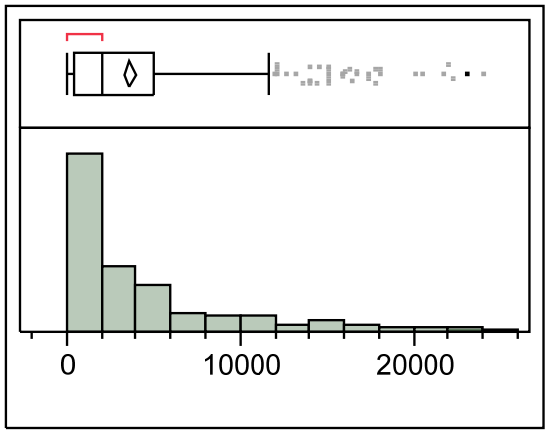
The examination of the skew and kurtosis indicated which datasets were most symmetric (skew approaching zero) and which had the greatest density of data points about the mean (kurtosis approaching zero). For all algorithms, the LD50 dataset consistently produced more desirable results (lesser skew and kurtosis) compared to the TDLo dataset. This is

likely due to two factors: TDLo data was gathered on multiple different endpoints, some of which are reversible and subject to different interpretations (notably behavioral endpoints), and TDLo data is based upon a single observation and therefore, more susceptible to error than LD50 data, which is calculated via statistical analysis. Although transformation techniques (such as Box-Cox) were considered to alleviate the distribution issues within the TDLo dataset, they were deemed superfluous since the LD50 dataset produced satisfactory results.

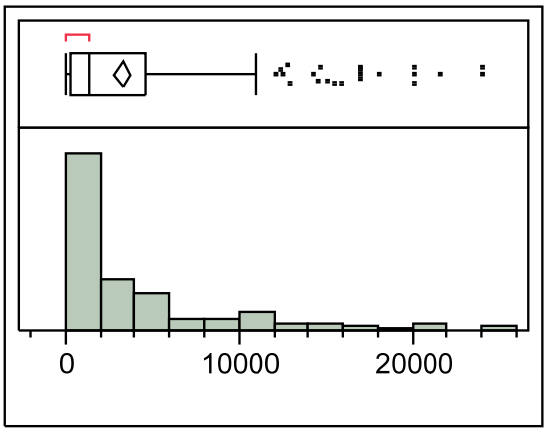
Also of note, the Microassay algorithm produced means that departed from the expected pattern for both the LD50 and TDLo dataset, with the positive group producing a higher mean than the negative group in both cases. No amount of data transformation will alleviate this problem, which would have resulted in a higher TTC for the positive structural family and a lower TTC for the negative structural family. Therefore, the Microassay algorithm was dropped from further analysis and not considered as a final candidate for inclusion within the TTC method. The most likely explanation for this failure is that the algorithm itself did not have appropriate coverage with respect to the initial test set, it is probable that important structural alerts for toxicity were missed, leading to a high rate of erroneous predictions for both the positive and negative families, since the Microassay algorithm created families that were very similar in size (105 positive and 90 negative). This division scheme is a juxtaposition to that of the remaining two algorithms: the Benigni-Bossa algorithm labeled far more compounds negative (155) than positive (39), whereas the Cramer extended algorithm labeled more compounds as positive (113) than negative (82). This trend is not altogether unexpected,

since carcinogenesis can be a downstream effect of mutagenicity and genotoxicity (however, not all carcinogens are mutagens), and mutagenicity and/or genotoxicity do not always result in carcinogenesis (fortunately). Therefore, it was expected that the mutagenicity and genotoxicity based algorithms (Microassay and Cramer extended) would return far more positives than the Benigni-Bossa algorithm-- in fact, only four Microassay negative compounds (arsenic, DDT (dichlorodiphenyltrichloroethane), mercury, and thimerosal) were returned as positive by the Benigni-Bossa. All four were also labeled as nongenotoxic carcinogens, which explains why the Microassay algorithm did not "catch" them—though they are certainly carcinogenic, they do not exert toxicity via mutagenic actions—the metals (arsenic, mercury, and thimerosal) via oxidative stress, and DDT is a suspected carcinogen via estrogenic effects (Jaga and Duwi, 2001), however, this hypothesis is not without conscientious objectors (Snedeker, 2001).

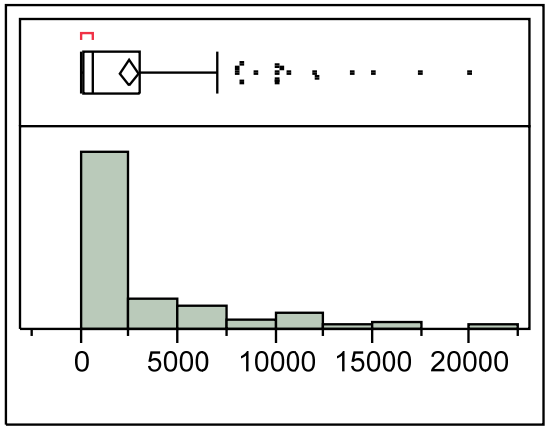
A one-way analysis was also performed to compare the distribution of LD50 and TDLo data across the positive and negative structural families as defined by each of the three algorithms. Cumulative distribution function (CDF) plots were generated to provide a visual clue as to how distinct the separation was between the positive and negative structural families with respect to measures of genotoxicity, mutagenicity and carcinogenicity. Investigating this relationship is central to the hypothesis of this project.



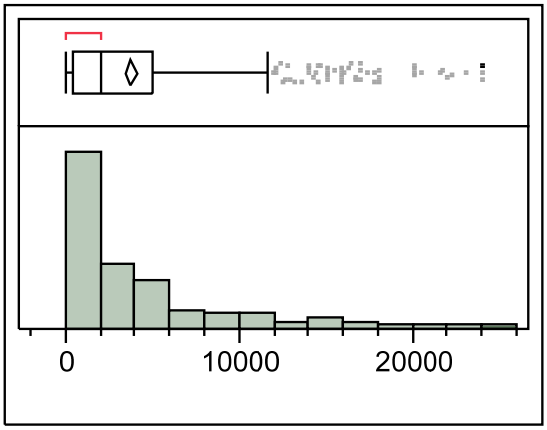
Microassay Positive LD50's (mg/kg)



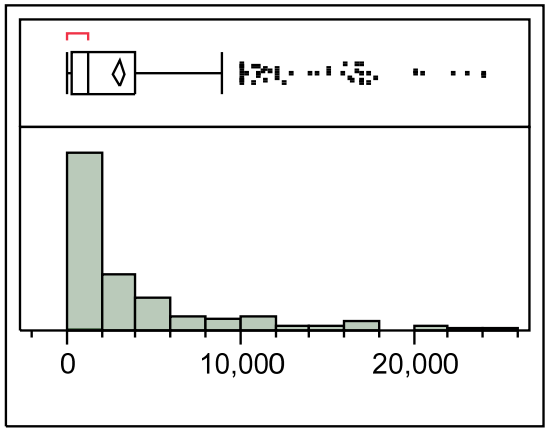
Microassay Negative LD50's (mg/kg)



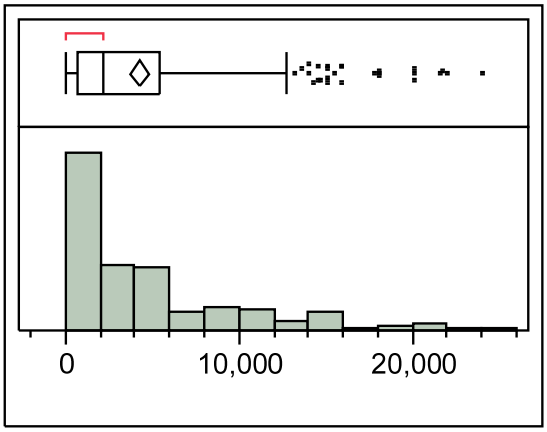
Benigni-Bossa Positive LD50's (mg/kg)



Benigni-Bossa Negative LD50's (mg/kg)

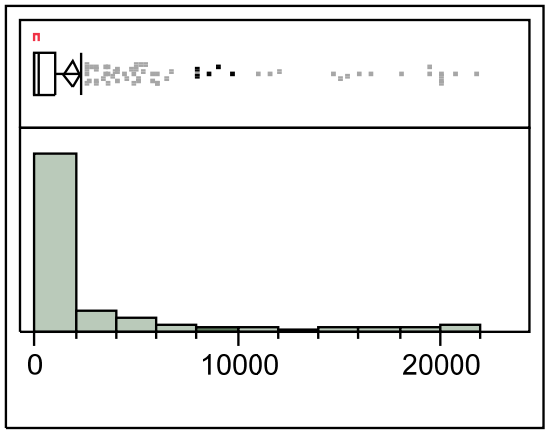


Cramer Positive LD50's (mg/kg)

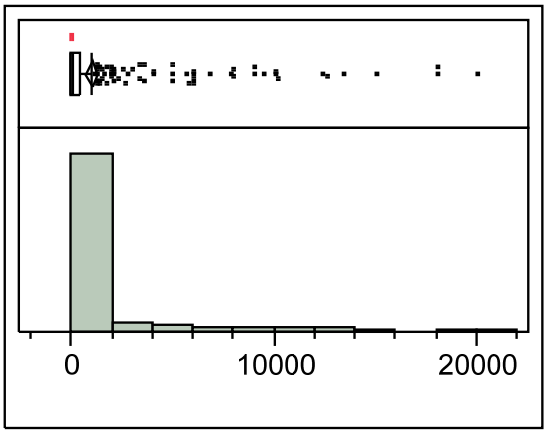


Cramer Negative LD50's (mg/kg)

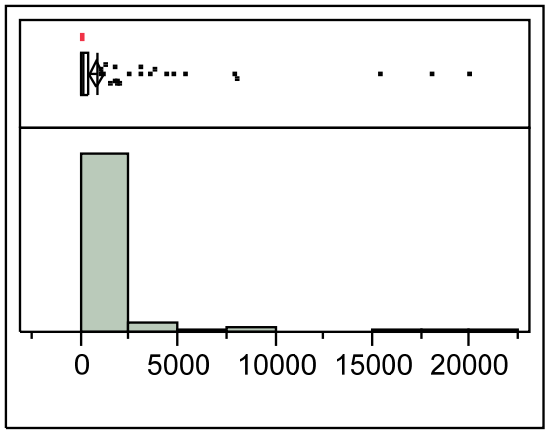
Figures 17-22. Distribution Histograms of LD50 Data by the Cramer, Microassay, and Benigni-Bossa Algorithms, With Box Plots



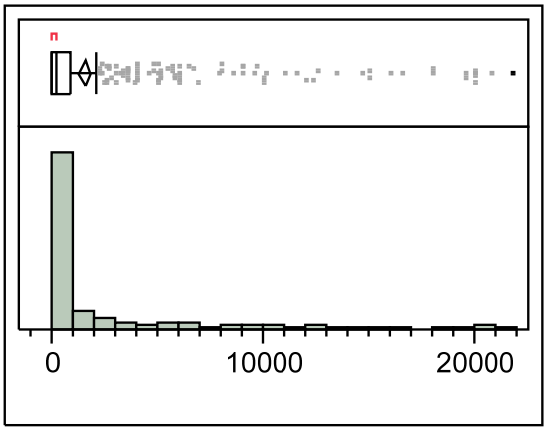
Microassay Positive TDLo's (mg/kg)



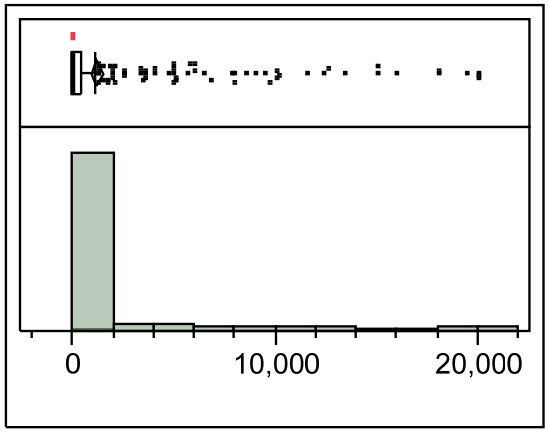
Microassay Negative TDLo's (mg/kg)



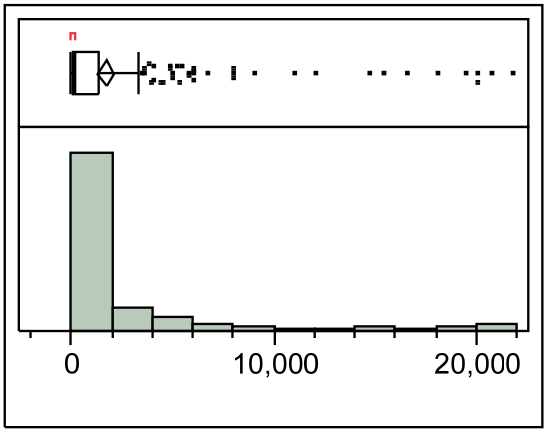
Benigni -Bossa Positive TDLo's (mg/kg)



Benigni -Bossa Negative TDLo's (mg/kg)

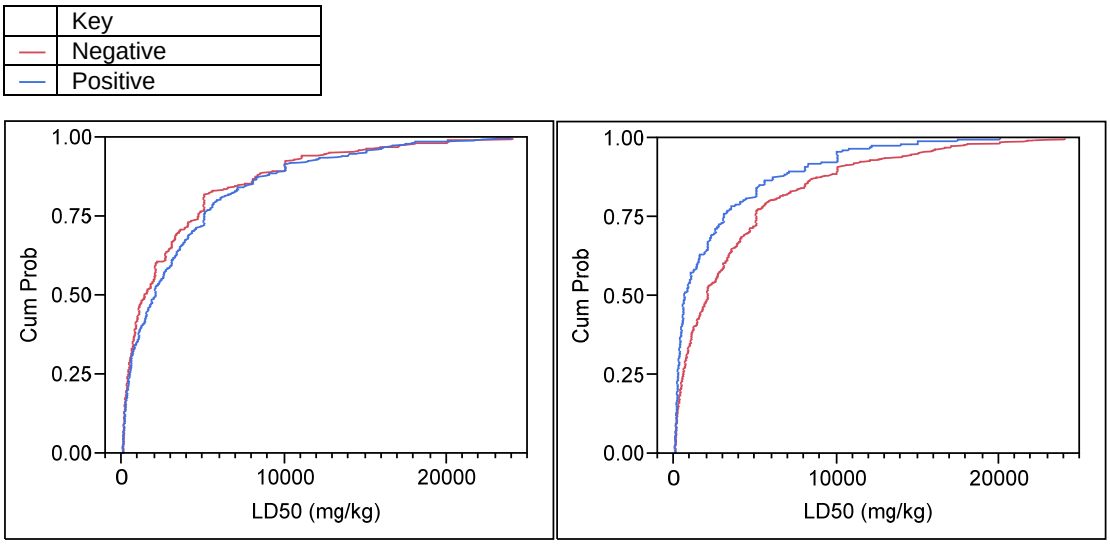


Cramer Positive TDLo's (mg/kg)



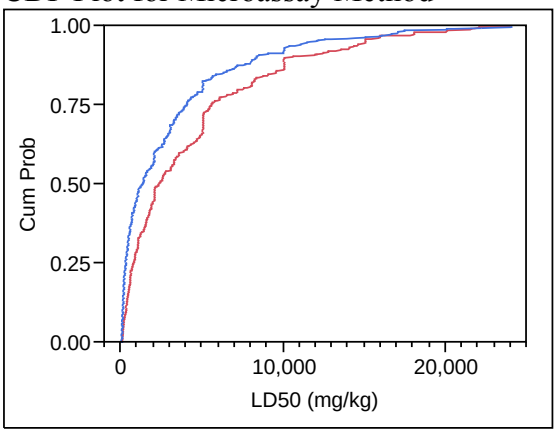
Cramer Negative TDLo's (mg/kg)

Figures 23-28. Distribution Histograms of TDLo Data by the Cramer, Microassay, and Benigni-Bossa Algorithms, With Box Plots.



CDF Plot for Microassay Method

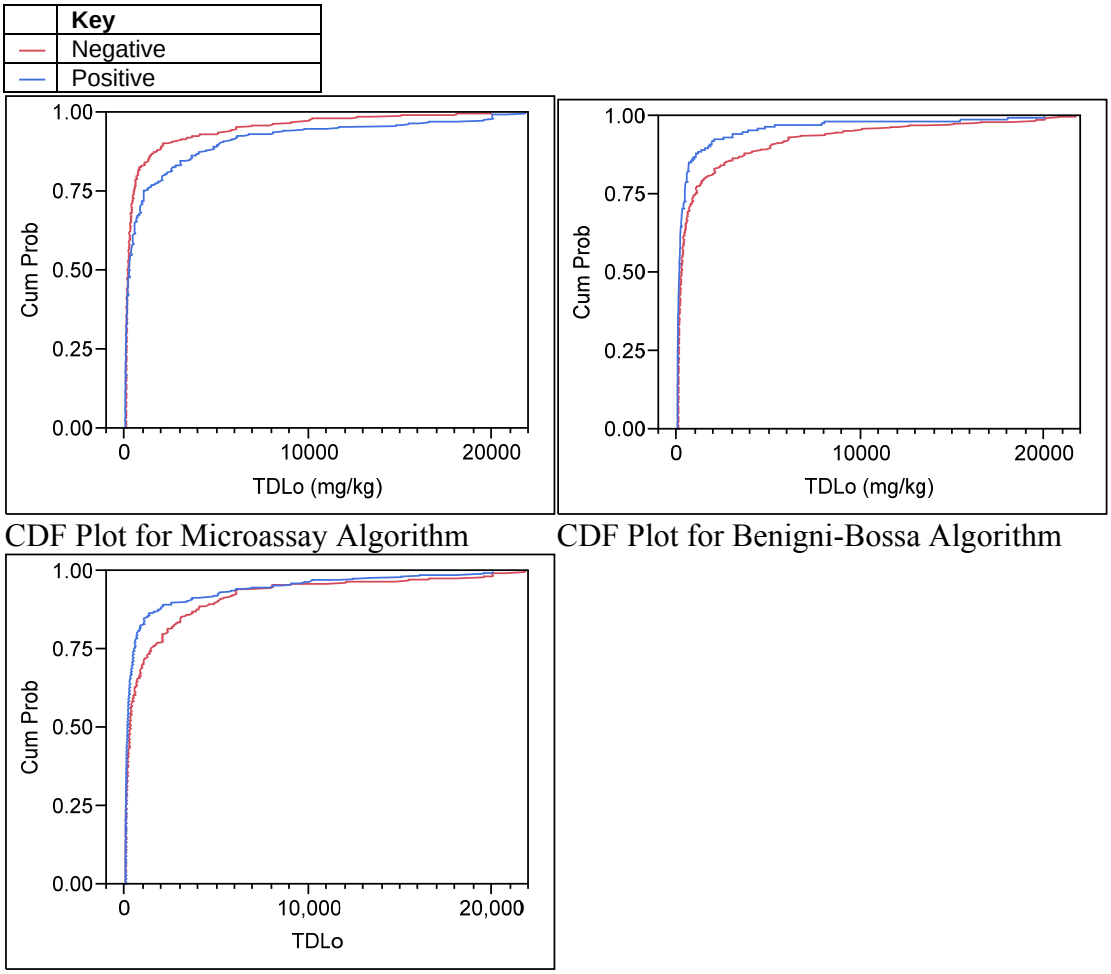
CDF Plot for Benigni-Bossa Method



CDF Plot for Cramer Method

Figures 29-31. CDF Plots of LD50 Data by the Cramer, Microassay, and Benigni-Bossa Algorithms

A comparison of the CDF plots further illustrates the quality issues inherent in the TDLo dataset—there is poor separation between the toxicity distributions of the positive and negative structural families throughout the majority of the distribution, regardless of algorithm. In contrast, the LD50 dataset shows excellent differentiation throughout the majority of the distribution when sorted by the Cramer and Benigni-Bossa algorithms.



CDF Plot for Microassay Algorithm

CDF Plot for Benigni-Bossa Algorithm

CDF Plot for Cramer Algorithm

Figures 32-34. CDF Plots of TDLo Data by the Cramer, Microassay, and Benigni-Bossa Algorithms

Selection of the Benigni-Bossa and Cramer methods in conjunction with the LD50 data is justified by the following observations: based upon skew and kurtosis, the LD50 dataset was of higher quality than the TDLo data set, additionally, TDLo data was not as widely available as LD50 data for this specific test set (Appendix III); also, based upon the points of departure, the TDLo dataset appeared overly conservative for the TTC approach. Based on the CDF plots and quantiles, it is apparent that the Benigni-Bossa and Cramer algorithms partitioned the LD50 data in a more meaningful way, with excellent separation throughout the distributions, consistent with what one would expect

when calculating reference values for chemical families with and without structural alerts, and as a result, it is expected that these algorithms will produce more valid TTCs than that of the Microassay algorithm. As a result of preliminary data analysis, all but two methods will be culled from further consideration: the Benigni-Bossa/ LD50 and the Cramer Extended/LD50. These final two methods will be subjected to internal validation to reach a final decision.

Algorithm Validation and Selection

Internal validation results were used to make a final algorithm selection. Both the Cramer and the Benigni-Bossa methods were validated against the same benchmarks. All compounds with carcinogenicity or mutagenicity rulings were included in the internal validation set (initially, n= 120). All chemicals that had a ruling of 'equivocal' either by the IARC or 'D' (unable to assess carcinogenicity) by the EPA were excluded from the validation set (resulting in an internal validation test set of n=105). Upon initial examination of the data, it was apparent that the Cramer algorithm incorrectly classified all vitamin-containing compounds in the test set, and the Benigni-Bossa algorithm incorrectly classified all polychlorinated biphenyls and most heavy metal compounds. Therefore, these compounds were excluded from their respective internal validation sets and will be considered inappropriate for TTC applications for their respective algorithms.

Figure 35 demonstrates the low level of agreement between the Cramer and the Benigni-Bossa algorithms. To a certain extent, this is to be expected, since many genotoxics are not carcinogens.

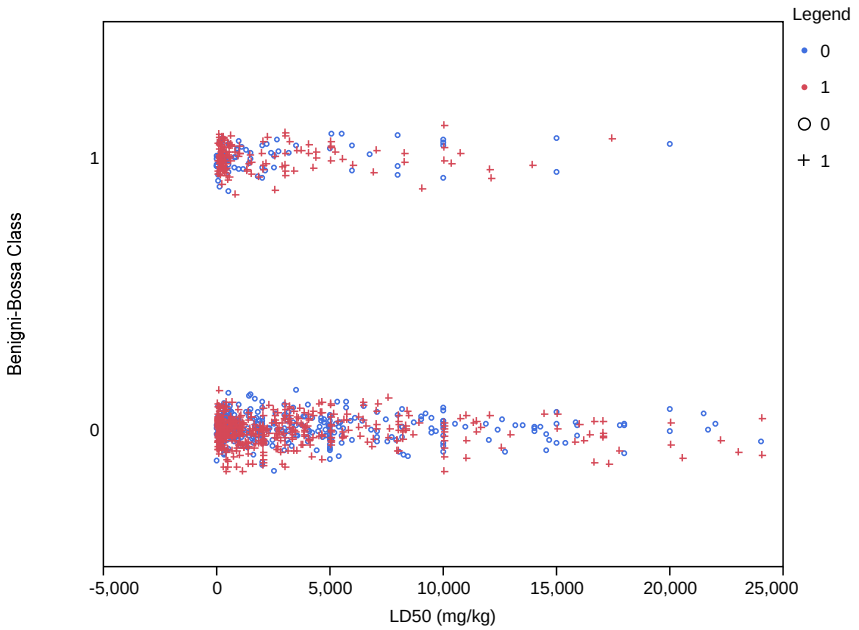


Figure 35. Agreement Between Benigni-Bossa and Extended Cramer Families (1= Positive, 0= Negative)

A difference in endpoint specific toxicophores may explain the heterogeneous clusters above, another possibility is that one method boasts a superior positive and negative predictivity compared to the other.

Table 8. Internal Validation Results

Result	Benigni-Bossa (n=95)	Cramer (n=102)
False Positives	7	28
False Negatives	26	20
True Positives	14	28
True Negatives	48	26

Table 9. Internal Validation Parameters

Parameter	Definition	Interpretation	Benigni-Bossa Result	Cramer Result
Sensitivity	=TP/ (TP+FN)	% of known positives that are correctly predicted	35%	58.3%
Specificity	=TN/(TN+FP)	% of known negatives that are	87.2%	48.1%

Table 9 Continued

		correctly predicted		
Accuracy	=(TP+TN)/(TP+TN+FP+FN)	Percent of chemicals in the training set which were correctly predicted by the model	62/95= 65.2%	54/102= 52.94%
Positive Predictivity	=TP/(TP+FP)	Positive predictions that are true positives (probability of a positive prediction being correct	66.6%	50%
Negative Predictivity	=TN/(TN+FN)	Negative predictions that are true negatives (probability of a negative prediction being correct)	64.8%	56.5%
ROC positive	=TP/FP	The ratio of true to false positives (discrimination of true versus false positives, significant when>2)	2	1
ROC negative	=TN/FN	The ratio of true to false negatives (discrimination of true versus false negatives, significant when>2)	1.84	1.3

With regulatory applications in mind for this method, it is far more desirable to see higher measurements of specificity, negative predictivity, and ROC negative curves, even at the expense of sensitivity and other positive centered parameters. When comparing these parameters of interest, it is apparent that the Benigni-Bossa outperforms the Cramer extended algorithm, with a ROC negative of 1.84, a negative predictivity of 64.8%, and a specificity of 87.2%, compared to the Cramer's results of 48.1%, 56.5%, and 1.3 for

specificity, negative predictivity, and ROC negative, respectively. This may be due in part to higher quality internal validation data—the carcinogen-based designations are based on a wide variety of data—animal, epidemiological, and mechanistic—as compared to the mutagenicity data that was used to validate the genotoxic-focused Cramer algorithm. Another possibility is that the Cramer Extended decision tree simply does not perform as well as the Benigni-Bossa algorithm, and misclassified far more compounds.

Since the Benigni-Bossa algorithm proved to be more robust to internal validation, it will provide the basis for calculating TTC's. All PCB's and metals will be dropped from the final test set, since, as a group, the Benigni-Bossa method generally fails to classify them accurately (see Appendix III).

Table 10. Benigni-Bossa Structural Alert Frequency in the Final Test Set

Structural Alert	Frequency	Compounds
Alkenylbenzenes	1	chlortetracycline
Alkyl halides (NG)	1	DDT (dichlorodiphenyltrichloroethane)
Aromatic amine without sulfonic group on the same ring	1	p-aminobenzoic acid
Dicarboximide (NG)	1	1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-
Epoxides and aziridines	2	1,2 propylene oxide, ethylene oxide
Halogenated polycyclic aromatic hydrocarbons (naphthalenes, biphenyls, diphenyls) (NG)	1	DDT (dichlorodiphenyltrichloroethane)
Heterocyclic poly aromatic hydrocarbons	1	hemin chloride
Imidazole and benzimidazole (NG)	6	diadenine sulfate, guanine hydrochloride, hypoxanthine, insulin, L-histidine, xanthine
Monohaloalkene	1	vinyl acetate
Polycyclic aromatic hydrocarbons	1	6,15-dihydroanthrazine-5,9,14,18-tetrone

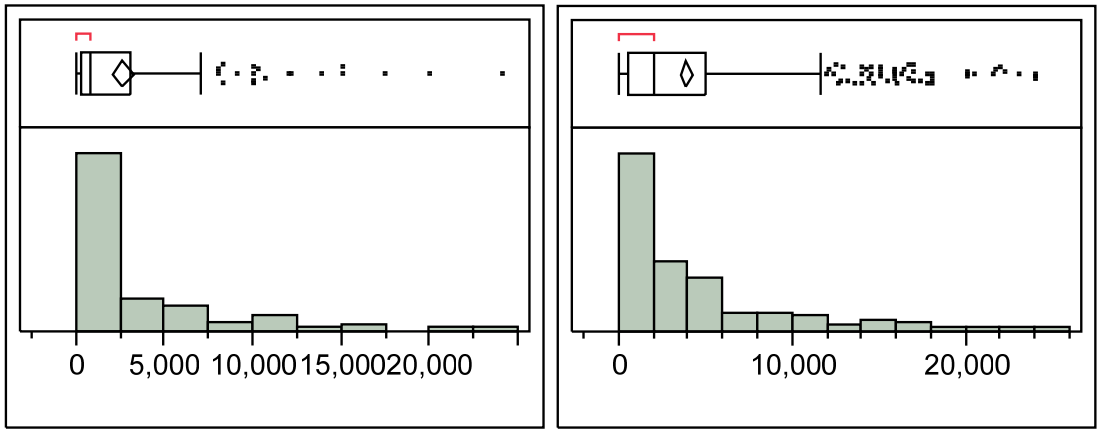
Table 10 Continued

Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)	9	2-deoxyadenosine, adenosine, co-carboxylase, diadenine sulfate, flavin adenine dinucleotide (FAD), nadide (NAD), p-aminobenzoic acid, thiamine, triphosphopyridine nucleotide (NADP)
Propiolactones and propiosultones	1	beta-propriolactone
Quinones	2	6,15-dihydroanthrazine-5,9,14,18-tetrone, menadione
Simple aldehyde	5	dextran, glutaral, pyridoxal, sodium glucuronate, streptomycin
Substituted n-alkylcarboxylic acids (NG)	2	calcium pantothenate (vitamin B5), citric acid
α,β unsaturated alkoxy	1	vinyl acetate
α,β unsaturated carbonyls	8	1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-, chlortetracycline, hydrocortisone, indigo, thymidine, thymine, uracil, uridine 5'- triphosphate

(NG)= Nongenotoxic mechanism

TTC Calculations and Hypothesis Testing

The final dataset (n=917) was characterized using JMP software to determine which method of hypothesis testing would be appropriate. A Shapiro Wilk W test for goodness of fit was executed to determine if the data distribution was normal enough for parametric testing.



Benigni-Bossa Positive LD50's Benigni-Bossa Negative LD50's

Figures 36-37. Distribution Histograms of Final LD50 Data by the Benigni-Bossa Algorithm

Table 11. Moments from Final LD50 Distribution Analysis by the Benigni-Bossa Algorithm

Parameters	Benigni-Bossa Positive LD50's	Benigni-Bossa Negative LD50's
N	204	713
Mean	2612.917	3853.379
Std Deviation	3900.445	4672.773
Minimum	1.5	1.2
Maximum	24039.83	24000
Range	24038.33	23998.8
% of Total	16.25%	83.75%
Variance	15213472.28	21834808.306
Std Error	273.0857	174.996
CV	149.27549	121.26427
Median	779.08	2000

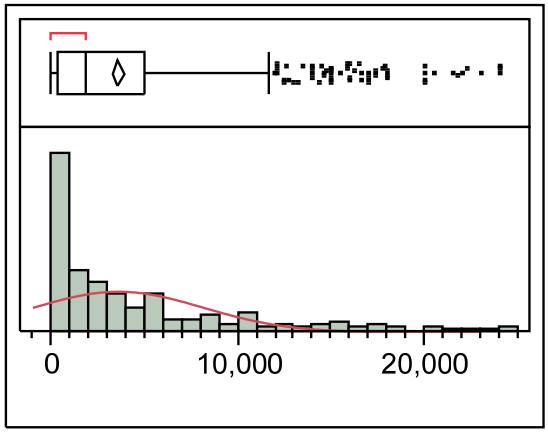


Figure 38. Distribution Histogram of Final Aggregate LD50 Data with Normal Curve

Table 12. Results of Shapiro Wilk-W Goodness-of-Fit Test

W	Prob <W
0.754033	<0.0001*

Note: Null Hypothesis (Ho) = The data is from the Normal distribution. Small p-values reject Ho.

Shapiro Wilk- W test results (p= <0.0001) indicated that the distribution was not normal and nonparametric hypothesis testing was indicated. For normal distributions, the Dunnett's T-test is favored when testing for significant differences in means, and has been used in numerous other studies in which TTCs were calculated. An acceptable non-

parametric equivalent is the Wilcoxon Rank sum test for statistical significance, which compares the median values of two datasets.

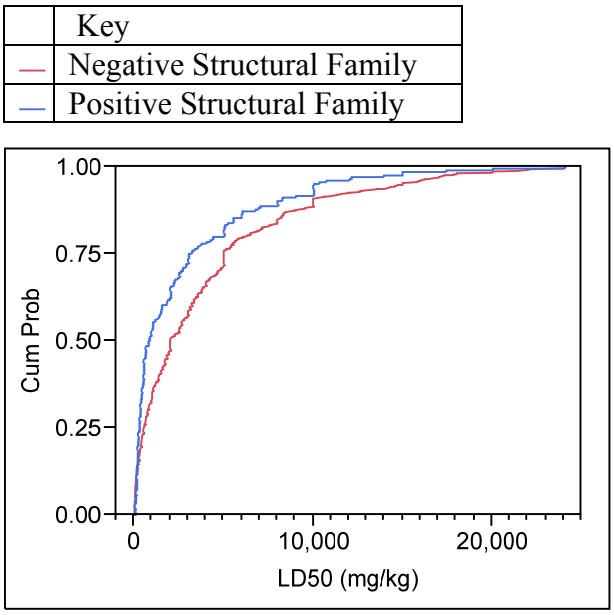


Figure 39. CDF Plot of Final LD50 Data by Benigni-Bossa Algorithm

Figures 39 and 40, the density plots, indicate that the further limitation of the LD50 dataset (as a result of internal validation) did not have a significant impact on separation or distribution. The Wilcoxon Rank Sums tests yielded statistically significant results (p= 0.0006 with the alpha set at 0.05).

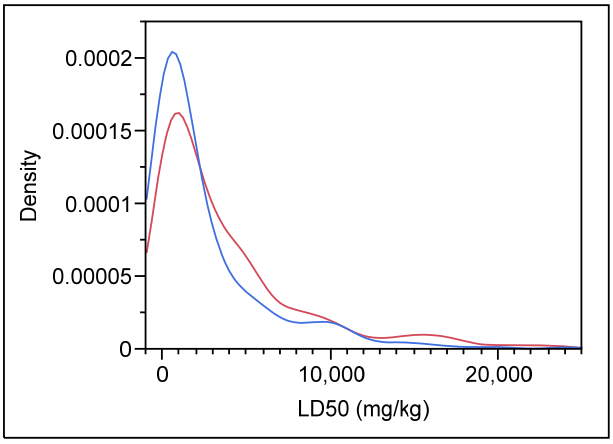


Figure 40. Comparison of LD50 Densities by Benigni-Bossa Algorithm

Tables 13. Wilcoxon / Kruskal-Wallis Tests Results

Rank Sums

Level	Count	Score Sum	Expected Score	Score Mean	(Mean-Mean0)/Std0
0	713	341973	327267	479.626	4.409
1	204	78930.0	93636.0	386.912	-4.409

2-Sample Test, Normal Approximation

S	Z	Prob>|Z|
78930	-4.40887	<.0001*

1-way Test, Chi-square Approximation

Chi-square	DF	Prob>ChiSq
19.4395	1	<.0001*

Table 14. TTC Calculations

Benigni-Bossa Structural Family	Point of Departure	Safety Factor	TTC (adjusted for adult human)
Positive (1)	15.05	50,000	18.06 µg/ person
Negative (0)	17.18	50,000	20.616 µg/ person

Within the final test set, the points of departure are quite similar, although the median toxicity measures are statistically significant in difference of magnitude—this may indicate that the positive structural family is not much more toxic than the negative structural family—which is reassuring, indicating that even the carcinogenic impurities in vaccines are not 'highly toxic', which is a credit to vaccines overall safety profile. It is important to consider that test set of vaccine impurities is quite narrow compared to that of food impurities or pharmaceutical impurities—most vaccines, regardless of the disease they are meant to prevent, contain a very homogenous profile of ingredients, since the basic manufacturing protocols are so similar.

The point of departure was extrapolated to a reference value using the relaxed uncertainty factors consistent with FDA recommendations for therapeutic impurities. After adjusting for the average adult human weight (60 kg), a safety factor of 50,000 was applied to each point of departure, yielding a TTC of 18.06 μg/ person for the positive structural family and 20.616 μg/ person for the negative structural family. These TTCs are comparable to many other published TTCs, and are likely to be protective of public health without inhibiting the manufacture and development of vaccine products.

Conclusions and Recommendations for Further Study

The objectives of this study were 1) to scientifically define thresholds of toxicological concern (TTCs) as they apply to vaccine constituents, 2) to determine whether statistically distinct classes of chemicals are created by applying a novel method for deriving TTCs for vaccine constituents, and, 3) to investigate the feasibility of using LD50 data as a point of departure when extrapolating reference levels. Additionally, this study also attempted to verify the following hypothesis:

1. The hypothesis of this project is toxicity of structural family 1 ≠ toxicity of structural family.

The Benigni-Bossa/ LD50 method defined TTCs for vaccine constituents as follows: 18.06 μg/ person for chemicals that are positive for at least (1) structural alert, and 20.616 μg/ person for chemicals that are negative for structural alerts.

The results indicate that, when using an LD50 dataset to extrapolate to TTC's, the Benigni-Bossa algorithm partitions the test set of vaccine constituents into structural families with toxicity distributions that are statistically significant from each other. The family that is positive for at least one structural alert for mutagenicity, genotoxicity, or carcinogenicity exhibits a distribution of LD50's that is significantly lower in magnitude than the structural family that lacks any structural alerts. This allows us to infer that LD50 data is an appropriate extrapolation basis for threshold of concern and the Benigni-Bossa rule base is able to sort the test set into meaningful structural families.

The Benigni-Bossa rule base has a distinct advantage over the other algorithms in that it predicts a more clinically relevant endpoint with respect to public health—living systems present immune-mediated mechanisms that may halt mutagenic and genotoxic pathways of toxicity, whereas carcinogenicity, which is often the result of irreversible mutagenicity or genotoxicity, typically requires therapeutic intervention. It is recommended that the Benigni-Bossa rule base be refined to vaccine constituents prior to implementation, specifically with an eye towards the correct classification of heavy metals and endocrine disruptors and lipophilics, since internal validation indicated a high rate of misclassifications of these compounds. Although the refinement of the algorithm is recommended, it is certainly not necessary, as the specificity of the method (89%) is already favorable. This parameter, as calculated by internal validation, is consistent with studies that have conducted external validation of popular predictive assays that have long been used as benchmarks for predictive toxicology (such as the Ames test).

Traditionally, front end toxicity assays that focus on mutagenicity (such as the Ames reverse mutagenicity test) were used an stand-ins for carcinogenicity, but as new in vitro and in vivo procedures are developed to test for carcinogenicity directly, we may see the Ames and comparable tests phased out, along with their in-silico counter parts (such as the Microassay algorithm). The CDER has already incorporated such tests, including the in vivo transgenic gene mutation assay and the transgenic mouse carcinogenicity assay for p53 or rasH2 into impurity safety assessment. The CDER has indeed postulated that, although a positive In vivo micronucleus assay result requires some follow-up (such as

the generation of mechanistic data to determine if clastogenicity or aneugenicity are present), the use of this test by sponsors is likely to be phased out within the next few years in favor of more sophisticated tests, such as the in vitro micronucleus, therefore, long term use of a micronucleus algorithm may not be efficient within the FDA's regulatory paradigm.

Although the inclusion of carcinogenicity is relevant to the FDA's aims with respect to safety assessment of vaccines, the method presented here would, ideally, apply to a broad range of endpoints, such as developmental and reproductive toxicity, neurotoxicity, immunotoxicity and others. Although carcinogenicity is considered a sensitive endpoint, this method should be validated against other endpoints prior to implementation. Another useful follow-up study, which would validate this method in a real world scenario, might be the correlation of structural alerts and adverse events in phase II or phase III clinical trials.

Within the Office of Vaccine Research and Review, the recommended implementation of this method is as follows: as a new compound is detected, it would be subjected to the Benigni-Bossa algorithm to determine which structural family it would be assigned to, either positive or negative for structural alerts. All that is required is the open source ToxTree software and a validated chemical structure. For chemicals that fall into the negative structural family, the detected quantity of the chemical in question would then be compared to the TTC for the negative family, 20.616 μg/ person. If the detected amount is at or below the designated TTC, the chemical would not be considered to pose

a significant threat to human health. For chemicals that fall into the positive family, a more judicious approach is indicated, owing to the low sensitivity of algorithm. The high specificity indicates that a chemical that returns negative can be reasonable expected to have a favorable safety profile. If the TTC is exceeded by the quantity detected, then the chemical should be subjected to chemical specific risk assessment, regardless of the structural family assignment. Most importantly, this system is not intended to replace evidence based expert knowledge, and the application of TTC's will always require a thoughtful scientific approach.

There are some notable limitations to this method. Internal validation has indicated that this method cannot reliably predict the carcinogenicity of many heavy metal and PCB containing compounds—therefore, if a novel constituent that either contains these chemicals or close analogs to these chemicals is detected in a vaccine, and chemical specific risk assessment will be necessary in the absence of pertinent human data. Additionally, the Benigni-Bossa does not take potentially toxic metabolites into account, it assesses each chemical as a stand-alone structure—therefore, pro-carcinogens should be subjected to a chemical-specific risk assessment (yet another example of how evidence-based expert knowledge is paramount in the application of TTCs). Furthermore, compounds that are returned as nongenotoxic carcinogens also require special attention. External validation testing by the algorithm's developers has indicated low sensitivity with respect to certain nongenotoxics, notably halogenated benzenes and thiocarbonyls (see appendix III).

TTCs yielded by this method (18.06 and 20.616 μg/person) compare favorably to those previously published for pharmaceutical impurities. In 2006, Müller et. al.. calculated TTCs ranging from 1.5 to 120 μg/person, depending on exposure duration; and Dolan et. al.. recommended TTCs ranging from 1- 100 μg/person depending on carcinogenic potency and general toxicity.

Finally, this project was conducted with regulatory applications in mind. When considering the application of TTCs specific to vaccines, one must not consider risk assessment, but benefit-risk assessment. Vaccines are potent tools within the arsenal of primary prevention, and the benefit that humanity has reaped from such therapeutics cannot be overstated, particularly with respect to infant and child mortality and morbidity. The epidemiologic shift away from communicable diseases in the early part of the 20th century can, in part, be attributed to advancements in vaccine science and the widespread administration of vaccines to the public.

List of References

Aardema, M. (2013). Introduction to Genetic Toxicology, Guidelines, Regulations, and the Impact of the 3Rs. 27th Annual Genotoxicity Workshop, Washington D.C., May 8-9, 2013. Sponsored by BioReliance, and affiliate of Sigma-Aldrich, LLC.

Basketter, D., Clewell, H., Kimber, I., Rossi, A., Blaauboer, B., Burrier, R. Daneshian, M., Eskes, C., Alan Goldberg, Nina Hasiwa, Sebastian Hoffmann, Joanna Jaworska, Thomas B. Knudsen, Robert Landsiedel, Marcel Leist, Paul Locke, Gavin Maxwell, James McKim, Emily A. McVey, Gladys Ouédraogo, Grace Patlewicz, Olavi Pelkonen, Erwin Roggen, Costanza Rovida, Irmela Ruhdel, Michael Schwarz, Andreas Schepky, Greet Schoeters, Nigel Skinner, Kerstin Trentz, Marian Turner, Philippe Vanparys, James Yager, Joanne Zurlo, and Thomas Hartung. (2012). "A roadmap for the development of alternative (non-animal) methods for systemic toxicity testing." *ALTEX* 29(1): 3-91.

The Benigni / Bossa rulebase for mutagenicity and carcinogenicity - a module of Toxtree, by R. Benigni, C. Bossa, N. Jeliazkova, T. Netzeva, and A. Worth. European Commission report EUR 23241 EN .

Benigni, B., Bossa, C., and Worth, A. (2009). "Structural analysis and predictive value of the rodent in vivo micronucleus assay results." *Mutagenesis* 25(4): 335-341.

Bernauer, U., Heinemeyer, G., Heinrich-Hirsch, B., Ulbrich, U., Gundert-Remy, U. (2008). "Exposure-triggered reproductive toxicity testing under the REACH legislation: A proposal to define significant/ relevant exposure." *Toxicology Letters* 176:68-76.

Blackburn, K., Bjerke, D., Daston, G., Felter, S., Mahoney, C., Naciff, J., Robison, S., and Wu., S. (2011). "Case studies to test: A framework for using structural, reactivity, metabolic and physiochemical similarity to evaluate the suitability of analogs for SAR-based toxicological assessments." *Regulatory Pharmacology and Toxicology* 60: 120-135.

Burenhof, A. (2009). Cramer Rules with Extensions: the Cramer rulebase with more human compounds and structural alerts. Curios-IT. Retrieved from: http://ihcp.jrc.ec.europa.eu/our_labs/predictive_toxicology/doc/Toxtree_Cramer_extensions.pdf

Carthew, P., Clapp, C., and Gutsell, S. (2009). "Exposure based waiving: The application of the toxicological threshold of concern (TTC) to the inhalation exposure for aerosol ingredients in consumer products." *Food and Chemical Toxicology* 47: 1287-1295.

Chauhan, K; Kodavanti, PR; McKinney, JD (2000). "Assessing the Role of ortho-Substitution on Polychlorinated Biphenyl Binding to Transthyretin, a Thyroxine Transport Protein". *Toxicology and Applied Pharmacology* 162(1): 10–21. doi:10.1006/taap.1999.8826. PMID 10631123.

Cheeseman, M.A., Machuga, E.J., and Bailey, A.B. (1999). "A Tiered Approach to Threshold of Regulation". *Food and Chemical Toxicology*. 37: 387- 412.

Contrera, J., Mattews, E., and Benz, R. (2002). "Predicting the carcinogenic potential of pharmaceuticals in rodents using molecular structural similar and E-state indices". *Regulatory Toxicology and Pharmacology* 38(2003): 243-259.

European Medicines Agency (EMA). Guideline on the Limits of Genotoxic Impurities. London, 28 June 2006. EMEA/CHMP/QWP/251344/2006

Escher, S.E., Tluczkiewicz, I., Batke, M., Bitsch, A., Melber, C., Kroese, E.D., Buist, H.E., and Mangelsdorf, I. (2010). "Evaluation of inhalation TTC values with the database RepDose." *Regulatory Toxicology and Pharmacology* 58(2): 259-274.

DeSesso. (1987). Hazard Ranking System Issue Analysis: Toxicity as a Ranking Factor. U.S. Environmental Protection Agency. pp. 44.

Dolan, D.G., Naumann, B.D., Sargent, E.V., Maier, A., Dourson, M. (2005). "Application of threshold of toxicological concern concept to pharmaceutical manufacturing operations." *Regulatory Toxicology and Pharmacology* 43(1): 1-9.

Felter, S., Lane, R., Latulippe, M., Llewellyn, G., Olin, S., Scimeca, J., and Trautman, T. (2009). "Refining the threshold of toxicological concern (TTC) for risk prioritization of trace chemicals in food." *Food and Chemical Toxicology* 47: 2236-2245.

Golbraikh, A., and Tropsha, A. (2002). "Beware of q2!" *J Mol Graph Model* 20(4): 269-76.

Grant, R., Kadlubar, B., Erraguntla, N., Honeycutt, M. (2007). "Evaluation of acute inhalation toxicity for chemicals with limited toxicity information." *Regulatory Toxicology and Pharmacology* 47: 261-273.

Hennes, E.C. (2012). "An overview of values for the threshold of toxicological concern." *Toxicology Letters* 211: 296-303.

ICH Expert Working Group. Assessment and Control of DNA Reactive (Mutagenic) Impurities in Pharmaceuticals to Limit Potential Carcinogenic Risk. 6 February 2013. Retrieved from: http://www.ich.org/fileadmin/Public_Web_Site/ICH_Products/Guidelines/Multidisciplinary/M7/M7_Step_2.pdf

International Agency for Research of Cancer (IARC). Preamble to the IARC Monographs: Scientific Review and Evaluation. Lyon, 23 January 2006. Retrieved from: http://monographs.iarc.fr/ENG/Preamble/CurrentPreamble.pdf

Jaga, K., and Duwi, H (2001). "Risk reduction for DDT toxicity and carcinogenesis through dietary modification." *J R Soc Promot Health* 121(2): 107-113.

Keller, D., Krauledat, M., Scheel, J. (2009). "Feasibility study to support a threshold of sensitization concern concept in risk assessment based on human data." *Archives of Toxicology* 83: 1049-1060.

Kirkland, D., Aardema, M., Henderson, L., and Muller, L. (2005). "Evaluation of the ability of a battery of three in vitro genotixicity tests to discriminate rodent carcinogencs and nont-carcinogens: Sensitivity, specificity, and relative predictivity." *Mutation Research* 584(1): 1-256.

Kroes, R., Renwick, A.G., Cheeseman, M., Kleiner, J., Mangelsdorf, I., Piersma, A., Schilter, B., Schlatter, J., van Schothorst, F., Vos, J.G., and Wurtzen, G. (2004). "Structure-based threshold of toxicological concern (TTC): guidance for application to substances present at low levels in the diet." *Food and Chemical Toxicology* 42: 65-83.

Lagunin, A., Zaakharov, A., Filimonov, D., and Poroikov, V. (2011). "QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction." *Molecular Informatics* 30: 241-250.

Martignoni, M., Groothuis, G., and de Kanter, R. (2006). "Species differences between mouse, rat, dog, monkey, and human CYP-mediated drug metabolism, inhibition, and induction." *Expert Opin. Drug Metab. Toxicol.* 2(6): 875-894.

McDonald, S. (2002). Science and the Regulation of Biological Products. The Center for Biologics Evaluation and Research. Dept. of Health and Human Services. Retrieved from: http://www.fda.gov/downloads/AboutFDA/WhatWeDo/History/ProductRegulation/100YearsofBiologicsRegulation/UCM070313.pdf

Miller, J., and Miller, E. (1971). The Mutagenicity of Chemical Carcinogens: Correlations, Problems, and Interpretations. Chemical Mutagens. Springer US, pp.83-119.

Muller, L., Mauthe, R., Riley, C., Andino, M., De Antonis, D., Beels, C., DeGeorge, J., De Knaep, A., Ellison, D., Fagerland, J., Frank, R., Fritschel, B., Galloway, S., Harpur, E., Humfrey, C., Jacks, A., Jagota, N., MacKinnon, J., Mohan, G., Ness, D., O'Donovan, M., Smith, M., Vudathala, G., and Yotti, L. (2006). "A rational for determining, testing, and controlling specific impurities in pharmaceuticals that possess potential for genotoxicity." *Regulatory Toxicology and Phmarmacology* 44: 198-211.

Munro, I.C., Ford, R.A., Kennepohl, E., and Sprenger, J.G. (1996). "Correlation of Structural Class with No-Observed-Effect-Levels: A Proposal for Establishing a Threshold of Concern." *Food and Chemical Toxicology* 34: 829-867.

Patlewicz, G., Jeliazkova, N., Safford, R.J., Worth, A.P., and Aleksiev, B. (2008). "An evaluation of the implementation of the Cramer classification scheme in the Toxtree software, SAR QSAR." *Environ. Res* 19(2008): 495–524.

Richter, W., Bhansali, S., and Morris, M. (2012). "Mechanistic Determinants of Biotherapeutics Absorption Following SC Administration." *The AAPS Journal.* 14(3): 559-570.

Safe, S, Hutzinger, O. (1984). "Polychlorinated Biphenyls (PCBs) and Polybrominated Biphenyls (PBBs): Biochemistry, Toxicology, and Mechanism of Action." *Critical Reviews in Toxicology* 13(4): 319–95. doi:10.3109/10408448409023762. PMID 6091997.

Safe, Stephen; Bandiera, Stelvio; Sawyer, Tom; Robertson, Larry; Safe, Lorna; Parkinson, Andrew; Thomas, Paul E.; Ryan, Dene E. et. al.. (1985). "PCBs: Structure-Function Relationships and Mechanism of Action." *Environmental Health Perspectives* 60: 47–56. JSTOR 3429944. PMC 1568577. PMID 2992927.

Safford, R.J., Aptula, N., Gilmour, N. (2011). "Refinement of the Dermal Sensitisation Threshold (DST) approach using a larger dataset and incorporating mechanistic chemistry domains." *Regulatory Toxicology and Pharmacol*ogy 60: 218-224.

Simon, Ted; Britt, Janice K.; James, Robert C. (2007). "Development of a neurotoxic equivalence scheme of relative potency for assessing the risk of PCB mixtures." *Regulatory Toxicology and Pharmacology* 48(2): 148–70. doi:10.1016/j.yrtph.2007.03.005. PMID 17475378.

Snedeker, SM. (2001). "Pesticides and breast cancer risk: a review of DDT, DDE, and dieldrin." *Environ Health Perspect* 109 Suppl 1: 35-47.

The European Commission. SCHER/SCCP/SCENIHR scientific opinion on the use of the Threshold of Toxicological Concern (TTC) approach for the safety assessment of chemical substances, 19 November 2008.

Tluczkiewicz, I., Escher, S., Bitsch, A., and Mngelsdorf, I. (2009). "Refinement of TTC values: Identificationm of outliers in Cramer class 1-3." *Toxicology Letters* 189 suppl S241.

USEPA. Guidelines for Carcinogen Risk Assessment (2005). U.S. Environmental Protection Agency, Washington, DC, EPA/630/P-03/001F, 2005.

USEPA. User's Guide for T.E.S.T. (version 4.1) (Toxicity Estimation Software Tool): A Program to Estimate Toxicity from Molecular Structure) (2012). Retrieved from: http://www.epa.gov/nrmrl/std/qsar/TEST-user-guide-v41.pdf

Valerio, L., and Cross, P. (2012). "Characterization and validation of an in silico toxicology model to predict the mutagenic potential of drug impurities." *Toxicology and Applied Pharmacology* 260: 209-221.

Winneke, G, Bucholski, A, Heinzow, B, Krämer, U, Schmidt, E, Walkowiak, J, Wiener, J, Steingrüber, H, (1998). "Developmental neurotoxicity of polychlorinated biphenyls (PCBS): Cognitive and psychomotor functions in 7-month old children." *Toxicology Letters* 423(8): 102-103. doi:10.1016/S0378-4274(98)00334-8. PMID 10022290.

IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: http://goldbook.iupac.org (2006) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. doi:10.1351/goldbook.

Zhu, H., Tropsha, A., Fourches, D., Varnek, A., Papa, E., GRamatica, P., Oberg, T., Dao, P., Cherkasov, A., and Tetko, IV. (2008). "Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyrifomris." *J Chem Inf Model* 48(4): 766-84.

Appendix I. Abbreviations and Acronyms

FDA	Food and Drug Administration
IND	Investigational New Drug
DVRPA	Division of Vaccines and Related Products Applications
TTC	Threshold of Toxicological Concern
RTECS	Registry of Toxic Effects of Chemical Substances
TOXNET	Toxicology Data Network
LD50	Median Lethal Dose
TDLo	Lowest Toxic Dose
SA	Structural Alert
JMP	Refers to JMP (pronounced "jump") statistical software developed by the SAS institute
Gene-Tox	Gene-Tox System for Mutagenicity
CCRIS	Chemical Carcinogenesis Research Information System
CPDB	Cancer Potency Database
IARC	International Agency for Research on Cancer
EPA	Environmental Protection Agency
ROC	Receiver Operating Characteristic
UF	Uncertainty Factor
CBER	Center for Biologics Evaluation and Research
EU	European Union
ppb	Parts Per Billion
TD50	Median Tumor Dose
ILSI	International Life Sciences Institute
JECFA	Joint FAO/WHO Expert Committee on Food Additives
IM	Intramuscular
NOEL	No Observable Effect Level
EFSA	European Food Safety Authority
EMA	European Medicines Agency
SAR	Structure-Activity Relationship
Microassay	In Vivo Rodent Micronucleus Assay Algorithm

Appendix I Continued

ISSCAN	Chemical Carcinogens: Structures and Experimental Data (based on Italian nomenclature)
DNA	Deoxyribonucleic Acid
QSAR	Quantitative Structure- Activity Relationship
ToxCast	Toxicity Forecaster
PBPK	Physiology- Based Pharmacokinetic
OECD	Organization for Economic Cooperation and Development
ICH	International Congress on Harmonization
CASRN	Chemical Abstract Service Registry Numbers
SMILES	Simplified Molecular-Input Line-Entry System
RoA	Route of Administration
T.E.S.T.	Toxicity Estimation Software Tool
CDER	Center for Drug Evaluation and Research
LOO q2	Leave-One Out Cross Validation
R^2	Correlation Coefficient
POD	Point of Departure
ADI	Acceptable Daily Intake
MOS	Margin of Safety
LDLo	Lowest Lethal Dose
PCB	Polychlorinated Biphenyl
DDT	Dichlorodiphenyltrichloroethane
CDF	Cumulative Distribution Function
AhR	Aryl Hydrocarbon Receptor
TD	Transdermal
SC	Subcutaneous
R	Rectal
PC	Percutaneous
PA	Parenteral
O	Oral
IV	Intravenous
IT	Intratracheal
IP	Intraperitoneal
IM	Intramuscular
ICV	Intracervical
IC	Intracerebral
PAR	Parenteral
OC	Ocular
IU	Intrauterine
ITT	Intratesticular
IS	Intraspinal
IPL	Intraplacental

Appendix I Continued

IDD	Intraduodenal
ID	Intradermal
IA	Intraarterial
S	Sheep
RB	Rabbit
R	Rat
NHP	Non-Human Primate
M	Mouse
HU	Human
H	Hamster
GP	Guinea Pig
D	Dog
C	Cat
P	Pig
HO	Horse
CO	Cow

Appendix II. Definitions

TTC	Mathematically modeled and extrapolated levels, below which adverse human health effects are not expected to occur.
LD50	Median lethal dose; is the dose which induces lethality in half of the test animals within a specified time frame. An analogue to the TD50.
TDLo	The lowest dose which elicits a toxic effect in the test animal population within a given time frame. Analogue to the lowest lethal dose (LDLo) but may be acute or chronic.
SA	Structural alerts (SAs) are functional groups within a compound's physical structure that may be associated with an adverse effect on a living system; common examples include aromatic rings, vinyl amides, or nitro groups. Also referred to as functional groups or toxicophores.
ROC	Receiver operating characteristic (ROC) curve: a measure of accuracy for a test, obtained by graphing the sensitivity vs. 1-specificity
UF	Generally, a 10- fold factor used to adjust for variability such as animal to human, LOEL to NOEL, et. Cetera, when calculating reference doses.
TD50	The chronic dose rate in mg/kg body weight/ day which would induce tumors in half the test animals at the end of a standard lifespan for the test species.
NOEL	The highest dose at which no observable effect (beneficial or detrimental) is elicited in a group of experimental animals
SAR	The relationship between the physical structure of a molecule and its biological activity.
QSAR	Multistep regression process for relating a set of predictor variables (physiochemical structure, theoretical molecular descriptors),

Appendix II Continued

	to the potency of a response variable. Basic mathematical model: Activity= f(physiochemical and structural properties)+ Error.
In Silico	Computer based.
R2	The coefficient of determination is the proportion of variability in a data set that is accounted for by a statistical model. Generally, variability is represented by the sum of squares.
ADI	The estimate of the amount of food additive, expressed on a body weight basis; that can be ingested daily over a lifetime without appreciable health risk (IUPAC Gold Book, 2006).

Appendix III. Supplementary Lists and Tables

List 4. Initial Test Set

CHEMICAL NAME	CASRN
1,2 polybutadiene	9003-17-2
1,2 propylene oxide	75-56-9
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	26115-70-8
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	3006-93-7
2,2 dimethyl-pentane	590-35-2
2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	2607-52-5
2-deoxyadenosine	958-09-8
2-deoxycytidine	951-77-9
2-deoxyguanosine	961-07-9
2-phenoxyethanol	122-99-6
3-methylpentane	96-14-0
5-methyldeoxycytidine	838-07-3
6,15-dihydroanthrazine-5,9,14,18-tetrone	81-77-6
acrylonitrile	107-13-1
adenosine	58-61-7
aluminum (used toxicity values for aluminum chloride)	7429-90-5
aluminum hydroxide	21645-51-2
aluminum phosphate	7784-30-7
aluminum silicate	1335-30-4
aluminum sulfate	10043-01-3
ammonium sulfate	7783-20-2
amphotericin B	1397-89-3
arsenic	7440-38-2
benzethonium chloride	121-54-0
benzoic acid	65-85-0
beta-propriolactone	57-57-8
biotin	58-85-5
boron	7440-42-8
bromine	7726-95-6
butylated hydroxytoluene (BHT)	128-37-0
calcium carbonate	471-34-1
calcium chloride	10043-52-4

List 4 Continued

calcium chloride dihydrate	10035-04-8
calcium pantothenate (vitamin B5)	137-08-6
carbon	7440-44-0
cesium hydroxide	21351-79-1
cetrimonium bromide (CTAB)	57-09-0
chlortetracycline	57-62-5
cholesterol	57-88-5
choline chloride	67-48-1
citric acid	77-92-9
co-carboxylase	154-87-0
cyclohexane	110-82-7
DDT (dichlorodiphenyltrichloroethane)	50-29-3
deoxycholic acid	83-44-3
dextran	9004-54-0
D-galactose	59-23-4
diadenine sulfate	321-30-2
disodium phosphate	7558-79-4
disodium phosphate dodecahydrate	10039-32-4
DL-aspartic acid	617-45-8
DL-glutamic acid	617-65-2
D-ribose	50-69-1
D-sorbitol	50-70-4
ydroxyl disodium (EDTA)	6381-92-6
ergocalciferol (vitamin D2)	50-14-6
ethanolamine	141-43-5
ethyl acrylate	140-88-5
ethylene oxide	75-21-8
ethylene-ethylidenenorbomene-propylene terpolymer	25038-36-2
ferric (III) nitrate	10421-48-4
ferrous succinate (butanedioic acid)	10030-90-7
flavin adenine dinucleotide (FAD)	146-14-5
folic acid	59-30-3
formaldehyde	50-00-0
gentamicin	1403-66-3
glutaral	111-30-8
glutathione	70-18-8
glycerin	56-81-5
glycine	56-40-6
guanine hydrochloride	33735-91-10
hemin chloride	16009-13-5
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	7365-45-9
heptakis(2,6-O-dimethyl)beta-cyclodextrin	51166-71-3
hexachlorobenzene	118-74-1

List 4 Continued

hexamethyldisiloxane	9006-65-9
hydrocortisone	50-23-7
hydroxyl L proline	51-35-4
hydroxylysine	28902-93-4
hypoxanthine	68-94-0
i-Inositol	87-89-8
indigo	482-89-3
insulin	11061-68-0
iron	7439-89-6
iron (II) sulfate heptahydrate	7782-63-0
iron ammonium citrate	1185-57-5
iron III nitrate	7782-61-8
kanamycin	59-01-8
lactose	63-42-3
L-alanine	56-41-7
L-arginine	74-79-3
L-ascorbic acid	50-81-7
L-asparagine	70-47-3
L-cysteine	52-90-4
L-cystine	56-89-3
L-glutamic acid	56-86-0
L-glutamine	56-85-9
L-histidine	71-00-1
L-isoleucine	73-32-5
L-leucine	61-90-5
L-lysine	56-87-1
L-methionine	63-68-3
L-phenylalanine	63-91-2
L-proline	147-85-3
L-serine	56-45-1
L-threonine	72-19-5
L-tryptophan	73-22-3
L-tyrosine	60-18-4
L-valine	72-18-4
magnesium	7439-95-4
magnesium chloride	7786-30-3
magnesium silicate (talc)	14807-96-6
magnesium stearate	557-04-0
magnesium sulfate	7487-88-9
menadione	58-27-5
mercury	7439-97-6
methylcyclopentane	96-37-7
methyltrimethoxysilane	1185-55-3
monobasic potassium phosphate	7778-77-0

List 4 Continued

monobasic sodium phosphate	7558-80-7
monosodium L glutamate	142-47-2
m-xylene	108-38-3
nadide (NAD)	53-84-9
n-dodecane	112-40-3
neomycin	1404-04-2
n-hexadecane	544-76-3
n-hexane	110-54-3
nicotinamide	98-92-0
nicotinic acid	59-67-6
n-octadecane	593-45-3
n-tetradecane	629-59-4
octoxynol 9	9002-93-1
palmitic acid	57-10-3
p-aminobenzoic acid	150-13-0
PCB 1221	11104-28-2
PCB 1242	53469-21-9
PCB 1248	12672-29-6
PCB 1254	11097-69-1
PCB 1260	11096-82-5
p-cymene	99-87-6
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	25155-25-3
phenol	108-95-2
phenol red (phenolsulfonphthalein)	143-74-8
polyethylene glycol nonylphenyl ether	9016-45-9
polymyxin B	1404-26-8
polypropylene	9003-07-0
polysorbate 20	9005-64-5
polysorbate 80 (tween 80)	9005-65-6
polystyrene	9003-53-6
polyvinyl alcohol	9002-89-5
potassium	7440-09-7
potassium chloride	7447-40-7
potassium glutamate	19473-49-5
p-xylene	106-42-3
pyridoxal	66-72-8
pyridoxine	65-23-6
retinyl acetate	127-47-9
riboflavin	83-88-5
silicon	7440-21-3
silicon dioxide	7631-86-9
sodium	7440-23-5
sodium acetate	127-09-3

List 4 Continued

sodium bicarbonate	144-55-8
sodium borate	1303-96-4
sodium chloride	7647-14-5
sodium citrate	68-04-2
sodium dihydrogen phosphate dihydrate	13472-35-0
sodium glucuronate	14984-34-0
sodium hydroxide	1310-73-2
sodium metabisulphite	7681-57-4
sodium phosphate	7632 05 5
sodium phosphate dibasic heptahydrate	7782-85-6
sodium pyruvate	113-24-6
sorbitan monoleate	1338-43-8
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	111-02-4
stearic acid	57-11-4
streptomycin	57-92-1
sucrose	57-50-1
sulfur	7704-34-9
tetrafluoroethylene	9002-84-0
thiamine	59-43-8
thimerosal	54-64-8
thymidine	50-89-5
thymine	65-71-4
titanium dioxide	13463-67-7
triphosphopyridine nucleotide (NADP)	53-59-8
tromethamine	77-86-1
uracil	66-22-8
urea	57-13-6
uridine 5’- triphosphate	63-39-8
vinyl acetate-chloroethene	
vitamin E succinate	4345-03-3
xanthine	69-89-6
zinc	7440-66-6
zinc oxide	1314-13-2

Table 15. LD50 Data

Chemical	LD50 (mg/kg/bw)	Test species	RoA
1,2 polybutadiene	4652.85	R	O
1,2 polybutadiene	3303.29	R	O
1,2 propylene oxide	380	R	O
1,2 propylene oxide	440	M	O
1,2 propylene oxide	1.5	RB	TD
1,2 propylene oxide	175	M	IP

Table 15 Continued

1,2 propylene oxide	150	R	IP
1,2 propylene oxide	660	GP	O
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	1708	R	O
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	1.46	R	O
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	250	M	O
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	1370	R	O
2,2 dimethyl pentane	8161.59	R	O
2,2 dimethyl pentane	3003.36	R	O
2,6-Di-tert-butyl-4-methylene-2,5-cyclohexadiene-1-one	741.13	R	O
2,6-Di-tert-butyl-4-methylene-2,5-cyclohexadiene-1-one	1143.81	R	O
2-deoxyadenosine	800	R	IP
2-deoxycytidine	1039.08	R	O
2-deoxycytidine	394.33	R	O
2-deoxyguanosine	800	R	IP
2-phenoxyethanol	872	M	IP
2-phenoxyethanol	333	M	IP
2-phenoxyethanol	22180	GP	TD
2-phenoxyethanol	5000	RB	TD
2-phenoxyethanol	2250	RB	TD
2-phenoxyethanol	3815	RB	TD
2-phenoxyethanol	3660	RB	TD
2-phenoxyethanol	5545	RB	TD
2-phenoxyethanol	2218	RB	TD
2-phenoxyethanol	2300	R	TD
2-phenoxyethanol	14422	R	TD
2-phenoxyethanol	2728	R	O
2-phenoxyethanol	7500	R	O
2-phenoxyethanol	4013	R	O
2-phenoxyethanol	2937	R	O
2-phenoxyethanol	2000	R	O
2-phenoxyethanol	2580	R	O
2-phenoxyethanol	2000	R	O
2-phenoxyethanol	1345	R	O
2-phenoxyethanol	3100	R	O
2-phenoxyethanol	1440	R	O
2-phenoxyethanol	3400	R	O
2-phenoxyethanol	1400	R	O
2-phenoxyethanol	5550	R	O
2-phenoxyethanol	1260	R	O
2-phenoxyethanol	5000	RB	TD

Table 15 Continued

3-methylpentane	4998.55	R	O
3-methylpentane	14521.2	R	O
5-Methyldeoxycytidine	512.45	R	O
5-Methyldeoxycytidine	1103.21	R	O
6,15-dihydroanthrazine-5,9,14,18-tetrone	250	R	IT
6,15-dihydroanthrazine-5,9,14,18-tetrone	2000	R	O
acrylonitrile	50	GP	O
acrylonitrile	202	GP	TD
acrylonitrile	130	GP	SC
acrylonitrile	46	M	IP
acrylonitrile	27	M	O
acrylonitrile	25	M	SC
acrylonitrile	69	RB	IV
acrylonitrile	63	RB	TD
acrylonitrile	65	R	IP
acrylonitrile	143.3	R	O
acrylonitrile	36	M	SC
acrylonitrile	78	R	O
acrylonitrile	148	R	TD
acrylonitrile	75	R	SC
adenosine	20000	M	O
adenosine	500	M	IP
alpha- tocopherol phosphate disodium	566.44	R	O
alpha- tocopherol phosphate disodium	866.57	R	O
aluminum chloride	1130	M	O
aluminum chloride	222	M	O
aluminum chloride	770	M	O
aluminum chloride	370	R	O
aluminum chloride	3450	R	O
aluminum chloride	400	GP	O
aluminum chloride	400	RB	O
aluminum chloride	390	M	O
aluminum chloride	333	R	IP
aluminum chloride	96	M	IP
aluminum chloride	2000	RB	TD
aluminum chloride	105	M	IP
aluminum chloride	81	R	IP
aluminum chloride	3450	R	SC
aluminum hydroxide	1100	R	IP
aluminum hydroxide	5000	R	O
aluminum phosphate	4640	R	O
aluminum phosphate	5000	M	O
aluminum phosphate	4640	RB	TD
aluminum silicate	160000	R	O

Table 15 Continued

aluminum sulfate	1930	R	O
aluminum sulfate	6207	M	O
aluminum sulfate	980	M	O
aluminum sulfate	730	M	O
aluminum sulfate	274	M	IP
aluminum sulfate	40	M	IP
aluminum sulfate	25	R	IP
ammonium sulfate	640	M	O
ammonium sulfate	720	R	O
ammonium sulfate	115	M	IM
ammonium sulfate	110	M	TD
ammonium sulfate	610	M	IP
ammonium sulfate	2840	R	O
ammonium sulfate	3000	R	O
ammonium sulfate	4600	R	O
ammonium sulfate	2000	R	O
ammonium sulfate	2000	R, M	TD
amphotericin B	5000	R	O
amphotericin B	1.6	R	IV
amphotericin B	5000	R	IP
amphotericin B	5000	R	IM
amphotericin B	1.2	M	IV
amphotericin B	27.74	M	IP
amphotericin B	5000	M	IM
amphotericin B	6	D	IV
amphotericin B	4	M	IV
amphotericin B	88	M	IP
arsenic	46.2	M	IP
arsenic	145	M	O
arsenic	13.39	R	IP
arsenic	763	R	O
benzethonium chloride	119	R	SC
benzethonium chloride	19	R	IV
benzethonium chloride	16.5	R	IP
benzethonium chloride	30	M	IV
benzethonium chloride	7.81	M	IP
benzethonium chloride	338	M	O
benzethonium chloride	368	R	O
benzoic acid	1700	R	O
benzoic acid	1940	M	O
benzoic acid	1700	R	IV
benzoic acid	1600	R	IP
benzoic acid	1460	M	IP
benzoic acid	2000	C	O

Table 15 Continued

benzoic acid	2000	D	O
benzoic acid	5000	RB	TD
benzoic acid	10000	RB	TD
beta-propriolactone	405	M	IP
beta-propriolactone	170	R	IV
biotin	10000	M	O
boron	7000	R	IP
boron	11000	M	IP
boron	310	GP	O
boron	310	D	O
boron	250	C	O
boron	650	R	O
boron	560	M	O
boron	310	RB	O
bromine	1700	R	O
bromine	2500	Rb	O
bromine	3100	M	O
bromine	5500	GP	O
butylated hydroxytoluene (BHT)	2930	R	O
butylated hydroxytoluene (BHT)	890	R	O
butylated hydroxytoluene (BHT)	180	M	IV
butylated hydroxytoluene (BHT)	138	M	IP
butylated hydroxytoluene (BHT)	650	M	O
butylated hydroxytoluene (BHT)	10700	GP	O
butylated hydroxytoluene (BHT)	2100	RB	O
butylated hydroxytoluene (BHT)	8000	R	IP
butylated hydroxytoluene (BHT)	1040	M	O
butylated hydroxytoluene (BHT)	650	M	SC
butylated hydroxytoluene (BHT) (128-37-0)	2000	R	TD
calcium carbonate (talc powder)	6450	M	O
calcium carbonate (talc powder)	6450	R	O
calcium chloride	755	RBm	O
calcium chloride	507	RBm	O
calcium chloride	5000	RB	TD
calcium chloride	25	R	IM
calcium chloride	867	Mf	SC
calcium chloride	823	Mm	SC
calcium chloride	3798	Rf	SC
calcium chloride	2630	Rm	SC
calcium chloride	245	M	IP
calcium chloride	402	Mf	IP
calcium chloride	382	Mm	IP
calcium chloride	342	Rf	IP
calcium chloride	264	Rm	IP

Table 15 Continued

calcium chloride	2630	R	TD
calcium chloride	1000	RB	O
calcium chloride	500	RB	O
calcium chloride	2045	Mm	O
calcium chloride	1940	Mf	O
calcium chloride	4179	Rf	O
calcium chloride	3798	Rm	O
calcium chloride	1000	R	O
calcium chloride	42	M	IV
calcium chloride dihydrate	1000	R	O
calcium chloride dihydrate	1950	M	O
calcium chloride dihydrate	264	R	IP
calcium chloride dihydrate	2630	R	SC
calcium chloride dihydrate	1940	M	O
calcium chloride dihydrate	823	M	SC
calcium chloride dihydrate	42	M	IV
calcium chloride dihydrate	1000	R	O
calcium chloride dihydrate	1000	R	O
calcium chloride dihydrate	2630	R	TD
calcium pantothenate (vitamin B5)	3500	R	SC
calcium pantothenate (vitamin B5)	2500	M	SC
calcium pantothenate (vitamin B5)	1443	M	IP
calcium pantothenate (vitamin B5)	10000	M	O
calcium pantothenate (vitamin B5)	10000	R	O
carbon	10000	R	O
carbon	440	M	IV
carbon	440	M	IV
carbon	10000	R	O
carbon	3000	RB	TD
carbon	8000	R	O
carbon	15400	R	O
cesium hydroxide	100	R	IP
cesium hydroxide	570	R	O
cesium hydroxide	100	R	IP
cesium hydroxide	800	M	O
cesium hydroxide	759	M	O
cetrimonium bromide (CTAB)	32	M	IV
cetrimonium bromide (CTAB)	44	R	IV
cetrimonium bromide (CTAB)	125	RB	SC
cetrimonium bromide (CTAB)	125	RB	IP
cetrimonium bromide (CTAB)	106	M	IP
cetrimonium bromide (CTAB)	100	GP	SC
cetrimonium bromide (CTAB)	430	R	O
cetrimonium bromide (CTAB)	410	R	O

Table 15 Continued

chlortetracycline	1500	M	O
chlortetracycline	118	R	IV
chlortetracycline	3000	R	O
chlortetracycline	3000	M	O
chlortetracycline	2150	Mf	O
chlortetracycline	3350	Mf	O
chlortetracycline	4200	Mm	O
chlortetracycline	3000	M	O
chlortetracycline	155	M	IV
chlortetracycline	93	Mf	IV
chlortetracycline	102	M	IV
chlortetracycline	134	M	IV
chlortetracycline	102	Mm	IV
chlortetracycline	108	Mf	IV
chlortetracycline	113	Mf	IV
chlortetracycline	600	M	SC
chlortetracycline	5500	Mm	SC
chlortetracycline	8250	Mf	SC
chlortetracycline	192	M	IP
chlortetracycline	128	Mm	IP
chlortetracycline	168	Mf	IP
chlortetracycline	214	Mf	IP
chlortetracycline	3000	R	O
chlortetracycline	4000	Rf	O
chlortetracycline	5500	R	O
chlortetracycline	10300	R	O
chlortetracycline	10000	Rf	O
chlortetracycline	5000	R	O
chlortetracycline	3000	R	O
chlortetracycline	160	R	IV
chlortetracycline	167	Rm	IV
chlortetracycline	118	R	IV
chlortetracycline	335	R	IP
chlortetracycline	100	GP	IV
chlortetracycline	300	GP	SC
cholesterol	5711.38	R	O
cholesterol	1879.56	R	O
choline chloride	400	R	IP
choline chloride	6640	R	O
choline chloride	3400	R	O
choline chloride	3900	M	O
choline chloride	53	M	IV
choline chloride	450	R	IP
choline chloride	320	M	IP

Table 15 Continued

citric acid	6730	R	O
citric acid	975	R	IP
citric acid	42	M	IV
citric acid	5040	M	O
citric acid	903	M	IP
citric acid	2700	M	SC
citric acid	883	R	IP
citric acid	5500	R	SC
citric acid	330	RB	IV
co-carboxylase	5000	R	SC
co-carboxylase	465	R	IV
co-carboxylase	500	R	IM
co-carboxylase	2500	M	SC
co-carboxylase	360	M	IV
co-carboxylase	1000	M	IM
cyclohexane	12705	R	O
cyclohexane	813	M	O
cyclohexane	18000	RB	TD
cyclohexane	29820	R	O
DDT (dichlorodiphenyltrichloroethane)	150	D	O
DDT (dichlorodiphenyltrichloroethane)	150	GP	O
DDT (dichlorodiphenyltrichloroethane)	1000	GP	TD
DDT (dichlorodiphenyltrichloroethane)	900	GP	SC
DDT (dichlorodiphenyltrichloroethane)	5000	H	O
DDT (dichlorodiphenyltrichloroethane)	200	NHP	O
DDT (dichlorodiphenyltrichloroethane)	32	M	IP
DDT (dichlorodiphenyltrichloroethane)	135	M	O
DDT (dichlorodiphenyltrichloroethane)	250	RB	O
DDT (dichlorodiphenyltrichloroethane)	300	RB	TD
DDT (dichlorodiphenyltrichloroethane)	250	RB	SC
DDT (dichlorodiphenyltrichloroethane)	9.1	R	IP
DDT (dichlorodiphenyltrichloroethane)	87	R	O
DDT (dichlorodiphenyltrichloroethane)	1931	R	TD
DDT (dichlorodiphenyltrichloroethane)	1500	R	SC
deoxycholic acid	1000	R	O
deoxycholic acid	1000	M	O
deoxycholic acid	130	M	IV
deoxycholic acid	999.99	R	O
dextran	10700	R	SC
dextran	6900	R	IV
dextran	208000	RB	IV
dextran	17400	RB	IV
dextran	13900	M	SC
dextran	12100	M	IV

Table 15 Continued

dextran	12000	M	O
dextran	3000	R	O
D-galactose	300	M	O
D-galactose	3200	RB	O
D-galactose	980	R	O
D-galactose	25800	R	O
D-galactose	9000	M	IV
D-galactose	18000	M	IP
D-galactose	35000	RB	IV
D-galactose	25800	R	O
D-galactose	9000	M	IV
D-galactose	18000	M	IP
diadenine sulfate	750	M	IP
diadenine sulfate	200	R	IP
disodium phosphate	17000	R	O
disodium phosphate	1075	RB	IV
disodium phosphate dodecahydrate	430	M	IP
DL-aspartic acid	6000	M	IP
DL-glutamic acid	4554.83	R	O
DL-glutamic acid	3577.2	R	O
D-ribose	14541.4	R	O
D-ribose	13204.4	R	O
d-sorbitol	13500	R	O
d-sorbitol	9690	R	IV
d-sorbitol	22000	M	O
d-sorbitol	14000	M	IP
d-sorbitol	7470	M	IV
d-sorbitol	15000	M	IP
d-sorbitol	7100	M	IV
d-sorbitol	9480	M	IV
d-sorbitol	17800	M	O
d-sorbitol	24000	M	SC
d-sorbitol	7100	R	IV
d-sorbitol	15900	R	O
d-sorbitol	29600	R	SC
d-sorbitol	26900	M	O
d-sorbitol	7100	M	O
d-sorbitol	15900	M	O
d-sorbitol	9480	M	O
edetate disodium (EDTA)	30	M	O
edetate disodium (EDTA)	28.5	M	IV
edetate disodium (EDTA)	397	R	IP
edetate disodium (EDTA)	250	M	IP
ergocalciferol (vitamin D2)	23.7	M	O

Table 15 Continued

ergocalciferol (vitamin D2)	10	R	O
ethanolamine	225	R	IV
ethanolamine	67	R	IP
ethanolamine	50	M	IP
ethanolamine	1750	R	IM
ethanolamine	700	M	O
ethanolamine	1500	R	SC
ethanolamine	620	GP	O
ethanolamine	1000	RB	O
ethanolamine	1720	R	O
ethyl acrylate	599	M	IP
ethyl acrylate	1799	M	O
ethyl acrylate	2997	M	TD
ethyl acrylate	370	RB	O
ethyl acrylate	450	R	IP
ethyl acrylate	800	R	O
ethylene oxide	330	Rm	O
ethylene oxide	72	R	O
ethylene oxide	280	Mm	O
ethylene oxide	365	Mf	O
ethylene oxide	270	GP	O
ethylene oxide	100	R	IP
ethylene oxide	175	M	IP
ethylene oxide	187	R	SC
ethylene oxide	290	R	IV
ethylene oxide	290	M	IV
ethylene; (5E)-5-ethylidenebicyclo[2.2.1]hept-2-ene; prop-1-ene	5000	R	O
ethylene; (5E)-5-ethylidenebicyclo[2.2.1]hept-2-ene; prop-1-ene	2000	RB	TD
ferric (III) nitrate	3250	R	O
ferrous succinate (butanedioic acid)	1547.53	R	O
ferrous succinate (butanedioic acid)	1081.9	R	O
flavin adenine dinucleotide (FAD)	589	M	IV
flavin adenine dinucleotide (FAD)	7000	M	O
folic acid	120	GP	IV
folic acid	85	M	IP
folic acid	282	M	IV
folic acid	10000	M	O
folic acid	410	RB	IV
folic acid	500	R	IV
Formaldehyde	2020	R	O
Formaldehyde	100	R	O
Formaldehyde	800	R	O

Table 15 Continued

Formaldehyde	420	R	SC
Formaldehyde	87	R	IV
Formaldehyde	42	M	O
Formaldehyde	300	M	SC
Formaldehyde	16	M	IP
Formaldehyde	260	GP	O
Formaldehyde	270	RB	PC
Formaldehyde	240	RB	SC
Formaldehyde	550	D	SC
gentamicin	600	GP	SC
gentamicin	17.3	M	IC
gentamicin	250	M	IM
gentamicin	245	M	IP
gentamicin	47	M	IV
gentamicin	11269	M	O
gentamicin	478	M	SC
gentamicin	384	R	IM
gentamicin	630	R	IP
gentamicin	96	R	IV
gentamicin	5000	R	O
gentamicin	873	R	SC
gentamicin	430	M	IP
gentamicin	490	M	IP
glutaral	134	R	O
glutaral	246	Rm	O
glutaral	154	Rf	O
glutaral	315	Rm	O
glutaral	285	Rf	O
glutaral	352	Rm	O
glutaral	418	Rf	O
glutaral	820	R	O
glutaral	1330	Rm	O
glutaral	1470	Rm	O
glutaral	17.9	R	IP
glutaral	2390	R	SC
glutaral	15	R	IV
glutaral	9.8	R	IV
glutaral	2000	R	TD
glutaral	100	M	O
glutaral	1430	Mm	SC
glutaral	13.9	M	IP
glutaral	15.4	M	IV
glutaral	2240	RB	TD
glutaral	1800	RB	TD

Table 15 Continued

glutaral	2560	RB	TD
glutathione	4000	M	IM
glutathione	4020	M	IP
glutathione	2238	M	IV
glutathione	2000	RB	IV
glutathione	5000	M	SC
glutathione	5000	M	O
glycerin	100	R	SC
glycerin	12600	R	O
glycerin	5570	R	O
glycerin	4420	R	IP
glycerin	27000	RB	O
glycerin	50	RB	IV
glycerin	90	M	SC
glycerin	4100	M	O
glycerin	4250	M	IV
glycerin	8700	M	IP
glycerin	7750	GP	O
glycine	7930	R	O
glycine	5200	R	SC
glycine	2600	R	IV
glycine	4920	M	O
glycine	4450	M	IP
glycine	5060	M	SC
glycine	2370	M	IV
guanine hydrochloride	200	M	IP
hemin chloride	30000	R	O
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	6470.74	R	O
heptakis(2,6-O-dimethyl)beta-cyclodextrin	350	R	SC
heptakis(2,6-O-dimethyl)beta-cyclodextrin	220	R	IV
hexachlorobenzene	1700	C	O
hexachlorobenzene	3000	GP	O
hexachlorobenzene	4000	M	O
hexachlorobenzene	2600	RB	O
hexachlorobenzene	10000	R	O
hexamethyldisiloxane	17000	R	O
hexamethyldisiloxane	2000	RB	TD
hexamethyldisiloxane	20000	M	O
hexamethyldisiloxane	24000	R	O
hexamethyldisiloxane	40000	R	O
hexamethyldisiloxane	2000	RB	TD
hexamethyldisiloxane	17000	R	O
hexamethyldisiloxane	17000	R	O

Table 15 Continued

hexamethyldisiloxane	24000	R	O
hydrocortisone	449	R	SC
hydrocortisone	150	R	IP
hydrocortisone	500	M	SC
hydrocortisone	5000	R	O
hydroxy L proline	2057.6	R	O
hydroxy L proline	1848.13	R	O
hydroxylysine	5787.08	R	O
hydroxylysine	6251.79	R	O
hypoxanthine	8000	M	O
hypoxanthine	6000	RB	O
hypoxanthine	500	R	O
hypoxanthine	750	M	IP
i-Inositol	10000	M	O
i-Inositol	3000	R	IP
i-Inositol	750	R	IV
indigo	2200	M	IP
indigo	32000	M	O
indigo	5000	R	O
iron	30000	R	O
iron	20000	GP	O
iron	200	Hu	O
iron	750	R	O
iron (II) sulfate heptahydrate	180	M	IP
iron (II) sulfate heptahydrate	51	M	IV
iron (II) sulfate heptahydrate	1520	M	O
iron ammonium citrate	2000	R	O
iron III nitrate	3250	R	O
kanamycin	1014	R	IM
kanamycin	150	RB	IV
kanamycin	4070	R	SC
kanamycin	10000	R	O
kanamycin	437	R	IV
kanamycin	1515	R	IP
kanamycin	1350	M	SC
kanamycin	21	M	O
kanamycin	115	M	IV
kanamycin	794	M	IP
kanamycin	54	M	IM
kanamycin	34	M	IC
kanamycin	1385	GP	IP
kanamycin	20500	M	O
lactose	5000	R	SC
lactose	10000	R	IP

Table 15 Continued

lactose	10000	R	O
L-alanine	8154.06	R	O
L-alanine	2530.81	R	O
L-arginine	12000	R	O
L-arginine	3793	R	IP
L-ascorbic acid	11900	R	O
L-ascorbic acid	5000	R	O
L-ascorbic acid	5000	R	SC
L-ascorbic acid	1000	R	IV
L-ascorbic acid	3367	M	O
L-ascorbic acid	8021	M	O
L-ascorbic acid	50518	M	IV
L-ascorbic acid	1058	M	IV
L-ascorbic acid	5000	M	SC
L-ascorbic acid	2000	M	IP
L-ascorbic acid	5000	GP	O
L-ascorbic acid	1000	GP	SC
L-ascorbic acid	500	GP	IV
L-ascorbic acid	2000	GP	IP
L-ascorbic acid	2000	RB	O
L-ascorbic acid	1000	RB	SC
L-ascorbic acid	1000	RB	IV
L-ascorbic acid	1000	RB	IP
L-ascorbic acid	1000	C	O
L-ascorbic acid	500	C	SC
L-ascorbic acid	500	C	IV
L-ascorbic acid	5000	D	O
L-ascorbic acid	2000	D	SC
L-ascorbic acid	200	D	IV
L-asparagine	2487.87	R	O
L-asparagine	5712.62	R	O
L-cysteine	1890	R	O
L-cysteine	1620	R	IP
L-cysteine	1550	M	O
L-cysteine	660	M	O
L-cysteine	1400	M	IP
L-cysteine	1360	M	SC
L-cystine	49	M	IP
L-cystine	156	M	O
L-cystine	961	M	IP
L-glutamic acid	2300	RB	O
L-glutamic acid	30000	R	O
L-glutamine	7500	R	O
L-glutamine	21700	M	O

Table 15 Continued

L-histidine	15000	R	O
L-histidine	15000	M	O
L-histidine	10000	M	IP
L-histidine	2000	M	IV
L-histidine	10000	M	SC
L-histidine	8000	R	IP
L-histidine	2000	R	IV
L-histidine	10000	R	SC
L-isoleucine	6822	R	IP
L-leucine	5379	R	IP
L-lysine	5373.5	R	O
L-lysine	2471	R	O
L-methionine	9500	M	IP
L-methionine	36000	R	O
L-methionine	4238	R	IP
L-phenylalanine	1322	M	IP
L-phenylalanine	5287	R	IP
L-proline	1642.91	R	O
L-proline	2892.54	R	O
L-serine	300	M	O
L-serine	3200	RB	O
L-serine	980	R	O
L-threonine	3098	R	IP
L-tryptophan	1634	R	IP
L-tryptophan	4800	M	IP
L-tyrosine	1450	M	IP
L-tyrosine	15000	R	O
L-valine	5390	R	IP
magnesium	230	R	O
magnesium chloride	2800	R	O
magnesium chloride	1338	M	IP
magnesium chloride	14	M	IV
magnesium silicate	10000	R	O
magnesium silicate	10000	RB	TD
magnesium stearate	10000	R	O
magnesium sulfate	645	M	SC
magnesium sulfate	1029	M	IP
magnesium sulfate	1200	R	SC
menadione	500	M	O
menadione	50	M	IP
menadione	75	R	IP
menadione	138	M	SC
mercury	5	M	IP
methylcyclopentane	5000	R	O

Table 15 Continued

methyltrimethoxysilane	12500	R	O
methyltrimethoxysilane	10000	RB	TD
monobasic potassium phosphate	7100	R	O
monobasic potassium phosphate	4640	R	O
monobasic potassium phosphate	4640	RB	TD
monobasic potassium phosphate	2820	M	O
monobasic potassium phosphate	3200	R	O
monobasic potassium phosphate	1700	M	O
monobasic potassium phosphate	500	R	O
monobasic potassium phosphate	2000	RB	TD
monobasic sodium phosphate	8290	R	O
monobasic sodium phosphate	250	R	IM
monosodium L glutamate	8000	C	SC
monosodium L glutamate	15000	GP	IP
monosodium L glutamate	3800	M	IP
monosodium L glutamate	30000	M	IV
monosodium L glutamate	11400	M	O
monosodium L glutamate	8200	M	SC
monosodium L glutamate	4253	R	IP
monosodium L glutamate	3300	R	IV
monosodium L glutamate	16600	R	O
monosodium L glutamate	5580	R	SC
monosodium L glutamate	15800	Rf	O
monosodium L glutamate	17300	Rm	O
monosodium L glutamate	17700	Mm	O
monosodium L glutamate	16400	Mf	O
monosodium L glutamate	16200	M	O
monosodium L glutamate	3600	R	IP
monosodium L glutamate	5700	Rm	IP
monosodium L glutamate	6570	Mm	IP
monosodium L glutamate	5700	Mf	IP
monosodium L glutamate	15000	GP	IP
monosodium L glutamate	6400	Rf	SC
monosodium L glutamate	5580	Rm	SC
monosodium L glutamate	8400	Mf	SC
monosodium L glutamate	8200	Mm	SC
monosodium L glutamate	3300	Rf	IV
monosodium L glutamate	3300	Rm	IV
monosodium L glutamate	3300	Mf	IV
monosodium L glutamate	3700	Mm	IV
monosodium L glutamate	8000	C	SC
monosodium L glutamate	16600	R	O
monosodium L glutamate	4253	R	IP
monosodium L glutamate	11400	M	O

Table 15 Continued

monosodium L glutamate	30000	M	IV
monosodium L glutamate	3800	M	IP
m-xylene	5000	R	O
m-xylene	4988	R	O
nadide (NAD)	4333	M	IP
n-dodecane	800	R	IP
neomycin	2750	R	O
neomycin	200	R	SC
neomycin	633	R	SC
neomycin	2880	M	O
neomycin	116	M	IP
neomycin	275	M	SC
neomycin	27.6	M	IV
neomycin	22.3	M	IV
neomycin	35	M	IV
n-hexadecane	8156.82	R	O
n-hexadecane	5430.51	R	O
n-Hexane	25000	R	O
n-Hexane	29700	R	O
n-Hexane	15840	R	O
nicotinamide	3500	R	O
nicotinamide	1680	R	SC
nicotinamide	2500	M	O
nicotinamide	3500	R	O
nicotinamide	1680	R	SC
nicotinamide	2500	M	O
nicotinamide	2050	M	IP
nicotinamide	2000	M	IP
nicotinamide	2000	RB	TD
nicotinamide	7100	Rm	O
nicotinamide	5500	Rf	O
nicotinamide	1800	M	IV
nicotinic acid	5000	R	SC
nicotinic acid	7000	R	O
nicotinic acid	730	R	IP
nicotinic acid	3720	M	O
nicotinic acid	358	M	IP
nicotinic acid	3500	M	SC
nicotinic acid	4550	RB	O
nicotinic acid	2000	R	TD
nicotinic acid	8900	Rf	O
nicotinic acid	11650	Rm	O
nicotinic acid	5100	Mm	O
nicotinic acid	6300	Mf	O

Table 15 Continued

nicotinic acid	5000	R	SC
n-octadecane	8269.52	R	O
n-octadecane	6442.2	R	O
n-tetradecane	5000	R	O
n-tetradecane	5000	RB	TD
octoxynol 9	1800	R	O
octoxynol 9	3800	R	O
octoxynol 9	1900	R	O
octoxynol 9	3000	RB	TD
octoxynol 9	1200	M	IV
palmitic acid	57	M	IV
palmitic acid	10000	R	O
p-aminobenzoic acid	2000	RB	IV
p-aminobenzoic acid	1830	RB	O
p-aminobenzoic acid	1000	D	O
p-aminobenzoic acid	2850	M	O
p-aminobenzoic acid	6000	R	O
PCB 1221	3980	R	O
PCB 1242	4250	R	O
PCB 1242	794	R	O
PCB 1242	8650	RB	TD
PCB 1248	11000	R	O
PCB 1248	11000	RB	TD
PCB 1254	880	M	IP
PCB 1254	358	R	IV
PCB 1254	1010	R	O
PCB 1254	400	R	IV
PCB 1254	2840	M	IP
PCB 1260	1315	R	O
PCB 1260	4000	R	O
PCB 1260	1300	R	O
p-cymene	10545	RB	TD
p-cymene	5000	RB	TD
p-cymene	1125	M	IP
p-cymene	1695	M	O
p-cymene	4750	M	O
p-cymene	3200	R	O
p-cymene	4750	R	O
p-cymene	1400	R	O
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	23000	R	O
phenol	530	R	O
phenol	100	C	O
phenol	500	D	O

Table 15 Continued

phenol	317	R	O
phenol	127	R	IP
phenol	1500	R	TD
phenol	669	R	TD
phenol	300	R	SC
phenol	460	R	SC
phenol	270	M	O
phenol	180	M	IP
phenol	344	M	SC
phenol	112	M	IV
phenol	630	RB	TD
phenol	850	RB	TD
phenol red (phenolsulfonphthalein)	1368	M	IV
phenol red (phenolsulfonphthalein)	752	R	IV
phenol red (phenolsulfonphthalein)	600	R	SC
phenol red (phenolsulfonphthalein)	300	M	O
phenol red (phenolsulfonphthalein)	3200	RB	O
phenol red (phenolsulfonphthalein)	980	R	O
polyethylene glycol nonylphenyl ether	50000	M	O
polyethylene glycol nonylphenyl ether	1310	R	O
polyethylene glycol nonylphenyl ether	3000	R	O
polyethylene glycol nonylphenyl ether	4000	R	O
polyethylene glycol nonylphenyl ether	4000	R	O
polyethylene glycol nonylphenyl ether	16000	R	O
polymyxin B	61.4	M	IM
polymyxin B	3.98	M	IV
polymyxin B	50	R	SC
polymyxin B	13.3	R	IM
polymyxin B	82.5	M	SC
polymyxin B	59.5	M	SC
polymyxin B	58	GP	SC
polymyxin B	1187	M	O
polymyxin B	790	M	O
polymyxin B	12.1	M	IP
polymyxin B	20.5	M	IP
polymyxin B	6.1	M	IV
polymyxin B	3.9	M	IV
polymyxin B	5.4	M	IV
polypropylene	110000	R	IP
polypropylene	99000	R	IV
polypropylene	8000	R	O
polysorbate 20	37000	R	O
polysorbate 20	3850	R	IP
polysorbate 20	770	R	IV

Table 15 Continued

polysorbate 20	25000	M	O
polysorbate 20	2640	M	IP
polysorbate 20	2970	M	IV
polysorbate 20	1420	M	IV
polysorbate 20	33000	M	O
polysorbate 80	6804	R	IP
polysorbate 80	1790	R	IV
polysorbate 80	25000	M	O
polysorbate 80	7600	M	IP
polysorbate 80	4500	M	IV
polysorbate 80	1790	M	IV
polysorbate 80	53840	R	O
polystyrene	660	M	IP
polystyrene	90	M	IV
polystyrene	316	M	O
polystyrene	898	R	IP
polystyrene	2650	R	O
polystyrene	5000	R	O
polyvinyl alcohol	300	M	SC
polyvinyl alcohol	1500	M	O
polyvinyl alcohol	2000	M	IP
polyvinyl alcohol	4000	M	O
polyvinyl alcohol	14700	M	O
polyvinyl alcohol	10000	Rm	O
polyvinyl alcohol	1000	M	R
polyvinyl alcohol	20000	R	O
polyvinyl alcohol	21500	Rm	O
polyvinyl alcohol	5000	R	O
polyvinyl alcohol	15000	R	O
polyvinyl alcohol	20000	D	O
potassium	700	M	IP
potassium chloride	620	M	IP
potassium chloride	2500	GP	O
potassium chloride	117	M	IV
potassium chloride	660	R	IP
potassium chloride	39	R	IV
potassium chloride	142	R	IV
potassium chloride	1500	M	O
potassium chloride	383	M	O
potassium chloride	2600	R	O
potassium glutamate	4500	M	O
potassium glutamate	2400	M	IP
p-xylene	5000	R	O
p-xylene	3910	R	O

Table 15 Continued

p-xylene	2.45	M	IP
p-xylene	3810	R	IP
p-xylene	12400	RB	TD
pyridoxal	540	R	IP
pyridoxal	1120	M	O
pyridoxal	480	M	IP
pyridoxal	2150	R	O
pyridoxal	501	D	O
pyridoxine	3100	R	SC
pyridoxine	4000	R	O
pyridoxine	657	R	IV
pyridoxine	1500	R	IP
pyridoxine	545	M	IV
pyridoxine	966	M	IP
retinyl acetate	432	M	IV
retinyl acetate	410	M	O
riboflavin	50	R	IV
riboflavin	560	R	IP
riboflavin	340	M	IP
riboflavin	10000	R	O
riboflavin	5000	R	SC
riboflavin	560	D	IP
riboflavin	2000	D	O
silicon	3160	R	O
silicon dioxide	3160	R	O
silicon dioxide	3000	RB	TD
silicon dioxide	1800	R	O
silicon dioxide	1200	M	IV
sodium	4000	M	IP
sodium acetate	3530	R	O
sodium acetate	10000	RB	TD
sodium acetate	3200	M	SC
sodium acetate	6891	M	O
sodium acetate	3500	R	O
sodium bicarbonate	3360	M	O
sodium bicarbonate	4220	R	O
sodium borate	2660	R	O
sodium borate	2000	M	O
sodium borate	2711	M	IP
sodium borate	1320	M	IV
sodium borate	5330	GP	O
sodium borate	10000	RB	TD
sodium chloride	2600	R	IP
sodium chloride	131	M	ICV

Table 15 Continued

sodium chloride	3000	R	O
sodium chloride	2602	M	IP
sodium chloride	645	M	IV
sodium chloride	3000	M	SC
sodium chloride	10000	RB	TD
sodium chloride	4000	M	O
sodium citrate	1635	M	IP
sodium citrate	1348	R	IP
sodium citrate	379	RB	IV
sodium citrate	49	M	IV
sodium citrate	1548	R	IP
sodium citrate	1364	M	IP
sodium citrate	170	M	IV
sodium citrate	449	RB	IV
sodium citrate	8000	R	O
sodium dihydrogen phosphate dihydrate	5008	M	IP
sodium dihydrogen phosphate dihydrate	8290	R	O
sodium dihydrogen phosphate dihydrate	7940	RB	TD
sodium glucuronate	4369.26	R	O
sodium glucuronate	5183.07	R	O
sodium hydroxide	1350	RB	TD
sodium hydroxide	140	R	O
sodium hydroxide	40	M	IP
sodium metabisulphite	2000	R	TD
sodium metabisulphite	95	H	IV
sodium metabisulphite	65	RB	IV
sodium metabisulphite	130	M	IV
sodium metabisulphite	560	M	IP
sodium metabisulphite	1000	GP	TD
sodium metabisulphite	1540	R	O
sodium metabisulphite	2480	R	O
sodium metabisulphite	3200	R	O
sodium metabisulphite	2515	S	O
sodium metabisulphite	1903	Rm	O
sodium metabisulphite	1131	R	O
sodium metabisulphite	115	R	IV
sodium metabisulphite	910	M	PA
sodium phosphate	250	R	IM
sodium phosphate	8290	R	O
sodium phosphate	2000	M	O
sodium phosphate	7940	RB	TD
sodium phosphate dibasic heptahydrate	12930	R	O
sodium pyruvate	1068.15	R	O
sodium pyruvate	1604.07	R	O

Table 15 Continued

sorbitan monoleate	39800	R	O
squalene	1800	M	IV
squalene	5000	M	O
stearic acid	23	M	IV
stearic acid	5000	RB	TD
stearic acid	21.5	R	IV
stearic acid	4600	R	O
stearic acid	14286	Hu	O
streptomycin	90.2	M	IV
streptomycin	85	M	IV
streptomycin	525	M	IP
streptomycin	500	M	O
streptomycin	575	M	IP
streptomycin	500	M	SC
streptomycin	600	M	SC
streptomycin	400	HM	O
streptomycin	500	HM	SC
streptomycin	400	GP	SC
streptomycin	9000	R	O
streptomycin	520	M	SC
streptomycin	600	M	SC
sucrose	14000	M	IP
sucrose	29700	R	O
sucrose	14000	M	IP
sucrose	29700	R	O
sulfur	5000	R	O
sulfur	8437	R	O
tetrafluoroethylene	895.89	R	O
tetrafluoroethylene	621.59	R	O
thiamine	8224	M	O
thiamine	3710	R	O
thiamine	301	M	SC
thimerosal	54	M	IP
thimerosal	66	M	SC
thimerosal	45	M	IV
thimerosal	91	M	O
thimerosal	98	R	SC
thimerosal	75	R	O
thymidine	2512	M	IP
thymine	3500	M	O
thymine	300	M	O
thymine	3200	RB	O
thymine	980	R	O
titanium dioxide	12000	R	O

Table 15 Continued

titanium dioxide	25000	R	O
titanium dioxide	10000	RB	TD
titanium dioxide	2000	R	IP
titanium dioxide	7500	R	O
titanium dioxide	2000	R	SC
triphosphopyridine nucleotide	3166	M	IP
tromethamine	1800	R	IV
tromethamine	3280	R	IV
tromethamine	2300	R	IV
tromethamine	3000	R	O
tromethamine	5900	R	O
tromethamine	3350	M	IP
tromethamine	6100	M	IV
tromethamine	1210	M	IV
tromethamine	5500	M	O
tromethamine	3500	M	IV
uracil	6000	R	O
uracil	8000	M	O
uracil	10000	RB	O
uracil	1513	M	IP
uracil	5000	D	O
urea	567	R	IT
urea	8471	R	O
urea	8200	R	SC
urea	5300	R	IV
urea	5000	R	IP
urea	11000	M	O
urea	9200	M	SC
urea	4800	RB	IV
urea	4600	M	IV
Uridine 5'- triphosphate	1158.05	R	O
Uridine 5'- triphosphate	2659.45	R	O
vinyl acetate-chloroethene	25000	R	O
vitamin E succinate	7000	R	O
xanthine	500	M	IP
zinc	630	R	O
Zinc oxide	240	R	IP
Zinc oxide	7950	M	O
Zinc oxide	5000	R	O

Table 16. TDLo Data

Chemical	TDLo (mg/kg/bw)	Test species	RoA
1,2 propylene oxide	47	R	IP
1,2 propylene oxide	1860	R	IP
2'-deoxycytidine	800	M	IP
acrylonitrile	641	HM	IP
acrylonitrile	32	M	IP
acrylonitrile	600	M	O
acrylonitrile	650	R	O
acrylonitrile	644	R	O
acrylonitrile	100	R	O
acrylonitrile	9500	R	O
acrylonitrile	5700	R	O
acrylonitrile	5727	R	O
acrylonitrile	13.8	R	O
acrylonitrile	2.5	M	O
acrylonitrile	40	R	O
acrylonitrile	18	M	SC
acrylonitrile	37.5	R	SC
acrylonitrile	115	R	SC
acrylonitrile	60	R	SC
adenosine	217100	R	IV
adenosine	542800	R	IV
adenosine	1266500	R	IV
aluminum	1260	M	O
aluminum hydroxide	15000	R	O
aluminum hydroxide	122000	Hu	O
aluminum hydroxide	84000	Hu	O
aluminum hydroxide	79000	Hu	O
aluminum silicate	400	M	O
aluminum sulfate	800	M	IP
aluminum sulfate	27.371	R	ITT
aluminum sulfate	27.371	R	SC
aluminum sulfate	1100	R	IP
aluminum sulfate	30	R	IP
aluminum sulfate	300000	M	O
aluminum sulfate	910000	M	O
aluminum sulfate	1400000	M	O
aluminum sulfate	10138	R	O
aluminum sulfate	186000	R	O
aluminum sulfate	564200	R	O
aluminum sulfate	29538	R	O
ammonium sulfate	1500	Hu	O

Table 16 Continued

amphotericin B	20	R	IV
amphotericin B	5.5	R	IV
amphotericin B	600	D	O
amphotericin B	1	D	IV
amphotericin B	15	Hu	IV
amphotericin B	0.02	Hu	IV
amphotericin B	1	Hu	UV
amphotericin B	490	R	IP
amphotericin B	16.5	D	IV
amphotericin B	6	D	IV
amphotericin B	37	D	IV
amphotericin B	55	D	IV
arsenic	187	M	O
arsenic	605	R	O
arsenic	580	R	O
arsenic	4	HU	O
arsenic	7857	HU	O
arsenic	5	R	O
arsenic	1	M	IP
benzoic acid	6	Hu	TD
biotin	200	R	SC
biotin	100	R	SC
biotin (58-85-5)	17	M	O
boron	4.95	R	O
butylated hydroxytoluene (BHT)	12600	M	O
butylated hydroxytoluene (BHT)	1200	M	O
butylated hydroxytoluene (BHT)	6000	R	O
butylated hydroxytoluene (BHT)	18000	R	O
butylated hydroxytoluene (BHT)	9000	R	O
butylated hydroxytoluene (BHT)	35000	R	O
butylated hydroxytoluene (BHT)	28000	R	O
butylated hydroxytoluene (BHT)	3300	R	O
butylated hydroxytoluene (BHT)	100	M	IP
butylated hydroxytoluene (BHT)	150	M	IP
butylated hydroxytoluene (BHT)	10	R	IP
butylated hydroxytoluene (BHT)	1	R	IP
butylated hydroxytoluene (BHT)	50	M	O
butylated hydroxytoluene (BHT)	25	R	O
butylated hydroxytoluene (BHT)	80	Huf	O
butylated hydroxytoluene (BHT) (128-37-0)	43800	M	O
calcium carbonate	10	R	O
calcium carbonate (471-34-1)	60000	R	O
calcium carbonate (talc powder)	60	R	O
calcium carbonate (talc powder)	10	R	O

Table 16 Continued

calcium chloride	555	D	ID
calcium chloride	399.5	M	IP
calcium chloride	249	C	IV
calcium chloride	39.95	D	IV
calcium chloride	300	R	IV
calcium chloride	20	Huf	IV
calcium chloride	0.2	R	PAR
calcium chloride (10043-52-4)	0.044	M	IC
calcium chloride dihydrate (10035-04-8)	5	D	ITT
calcium chloride dihydrate (10035-04-8)	10	D	ITT
carbon	167	R	SC
carbon	16	R	IT
carbon	15	R	IT
carbon	10	R	IT
carbon	10	R	IV
carbon	1	M	IT
cetrimonium bromide (CTAB)	35	M	IP
cetrimonium bromide (CTAB) (57-09-0)	10.5	M	IP
chlortetracycline	100	R	IV
chlortetracycline (57-62-5)	372	M	SC
cholesterol	175	R	SC
cholesterol	1900	R	SC
cholesterol (57-88-5)	6000	RB	O
choline chloride	0.1	R	IC
choline chloride	0.558	R	IC
choline chloride	120	R	IP
choline chloride (67-48-1)	0.3	R	IC
citric acid	3000	GP	IT
citric acid	64	D	IV
citric acid	63	D	IV
citric acid	256	D	IV
citric acid	42	M	IV
citric acid (77-92-9)	118000	GP	IT
coenzyme A (85-61-0)	0.08	R	IV
DDT (dichlorodiphenyltrichloroethane)	60	R	IP
DDT (dichlorodiphenyltrichloroethane)	21	R	IP
DDT (dichlorodiphenyltrichloroethane)	3540	D	O
DDT (dichlorodiphenyltrichloroethane)	504	M	O
DDT (dichlorodiphenyltrichloroethane)	81	M	O
DDT (dichlorodiphenyltrichloroethane)	124	M	O
DDT (dichlorodiphenyltrichloroethane)	148	M	O
DDT (dichlorodiphenyltrichloroethane)	150	RB	O
DDT (dichlorodiphenyltrichloroethane)	112	R	O
DDT (dichlorodiphenyltrichloroethane)	100	R	O

Table 16 Continued

DDT (dichlorodiphenyltrichloroethane)	430	R	O
DDT (dichlorodiphenyltrichloroethane)	1890	R	O
DDT (dichlorodiphenyltrichloroethane)	250	R	O
DDT (dichlorodiphenyltrichloroethane)	50	R	O
DDT (dichlorodiphenyltrichloroethane)	420	R	O
DDT (dichlorodiphenyltrichloroethane)	418	M	SC
DDT (dichlorodiphenyltrichloroethane)	143	M	SC
DDT (dichlorodiphenyltrichloroethane)	40	M	SC
DDT (dichlorodiphenyltrichloroethane)	15	GP	IP
DDT (dichlorodiphenyltrichloroethane)	5	M	IP
DDT (dichlorodiphenyltrichloroethane)	5	R	IP
DDT (dichlorodiphenyltrichloroethane)	5	Hu	O
DDT (dichlorodiphenyltrichloroethane)	16	Hu	O
DDT (dichlorodiphenyltrichloroethane)	3.57	Hu	O
DDT (dichlorodiphenyltrichloroethane)	10.71	Hu	O
DDT (dichlorodiphenyltrichloroethane)	21.43	Hu	O
DDT (dichlorodiphenyltrichloroethane)	6	Hu	O
DDT (dichlorodiphenyltrichloroethane)	71.43	Hu	O
DDT (dichlorodiphenyltrichloroethane)	4.29	Hu	O
DDT (dichlorodiphenyltrichloroethane)	0.5	M	O
DDT (dichlorodiphenyltrichloroethane)	100	R	O
DDT (dichlorodiphenyltrichloroethane)	0.1	R	O
DDT (dichlorodiphenyltrichloroethane)	600	R	O
DDT (dichlorodiphenyltrichloroethane)	12.5	R	O
DDT (dichlorodiphenyltrichloroethane)	60	R	O
DDT (dichlorodiphenyltrichloroethane)	5	R	O
DDT (dichlorodiphenyltrichloroethane)	3	R	O
DDT (dichlorodiphenyltrichloroethane)	106	R	O
DDT (dichlorodiphenyltrichloroethane)	97	R	O
DDT (dichlorodiphenyltrichloroethane)	25	R	O
DDT (dichlorodiphenyltrichloroethane)	160	R	SC
DDT (dichlorodiphenyltrichloroethane)	95	R	SC
DDT (dichlorodiphenyltrichloroethane) (50-29-3)	40	M	IP
deoxycholic acid	166	R	IP
dextran	0.526	R	SC
dextran	0.4	R	SC
D-galactose	1260000	M	O
D-galactose	630000	M	O
D-galactose	16500	M	O
D-galactose	840000	M	O
D-galactose	240000	R	O
D-galactose	188000	R	O
D-galactose	440000	R	O
D-galactose	475000	R	O

Table 16 Continued

D-galactose	1000000	R	O
D-galactose	209642	R	O
D-galactose	20000	H	IP
D-galactose	6000	M	IP
D-galactose	300000	R	IP
D-galactose	2000	Huf	IV
D-galactose	1.057	Huf	IV
D-galactose	1300	Huf	IV
D-galactose	2000	Huf	O
D-galactose	20000	H	SC
D-galactose	100	M	IP
D-galactose	365	M	IP
D-galactose	2000	R	IP
D-galactose	750	RB	IV
D-galactose	357	Hu	O
D-galactose	2	M	O
D-galactose	2000	R	O
D-galactose	500	Huf	O
DL-aspartic acid	500	R	IP
DL-aspartic acid	100	R	IP
DL-aspartic acid	10	R	IP
DL-glutamic acid	71	Hu	O
D-ribose	5.045	M	IU
d-sorbitol	5714	Hu	IV
d-sorbitol	1000	R	IV
d-sorbitol	1167	Hu	O
d-sorbitol	1700	Hu	O
ergocalciferol	1.75	RB	IM
ergocalciferol	9.375	RB	IM
ergocalciferol	17.5	RB	IM
ergocalciferol	35	RB	IM
ergocalciferol	200	M	O
ergocalciferol	45	R	O
ergocalciferol	30	R	O
ergocalciferol	55	R	O
ergocalciferol	33.75	R	O
ergocalciferol	22.5	R	O
ergocalciferol	17.5	R	SC
ethanolamine	2250	R	TD
ethanolamine	500	R	O
ethanolamine	4500	R	O
ethyl acrylate	8000	R	O
ethylene oxide	750	M	IP
ethylene oxide	150	M	IP

Table 16 Continued

ethylene oxide	125	M	IP
ethylene oxide	225	M	IV
ethylene oxide	450	M	IV
ethylene oxide	324	RB	IV
ethylene oxide	81	RB	IV
folic acid	720	M	IP
folic acid	450	M	IP
folic acid	96600	R	O
folic acid	150	R	PA
folic acid	150	R	SC
Formaldehyde	259	M	IM
Formaldehyde	240	M	IP
Formaldehyde	160	M	IP
Formaldehyde	500	M	IP
Formaldehyde	80	R	IP
Formaldehyde	7	D	ITT
Formaldehyde	4	NHP	ITT
Formaldehyde	400	R	ITT
Formaldehyde	168	R	O
Formaldehyde	200	R	O
Formaldehyde	168	R	O
Formaldehyde	10.5	R	O
Formaldehyde	46243	R	SC
Formaldehyde	2	R	TD
Formaldehyde	5.3	R	PC
Formaldehyde	643	Hu	O
Formaldehyde	646	Hu	O
Formaldehyde	0.05	RB	PA
Formaldehyde	10	R	PA
Formaldehyde	16	M	SC
Formaldehyde	18.18	M	SC
Formaldehyde	25	M	SC
Formaldehyde	3.76	R	SC
Formaldehyde	1.25	R	SC
Formaldehyde	0.83	R	SC
Formaldehyde	2.5	R	SC
Formaldehyde	1	R	SC
Formaldehyde	10	R	SC
Formaldehyde	0.014	R	SC
gentamicin	375	R	IP
gentamicin	660	R	SC
gentamicin	17.3	M	IC
gentamicin	21	Hu	IV
gentamicin	45	Huf	IV

Table 16 Continued

gentamicin	0.013	R	IS
glutaral	50000	M	O
glutaral	8000	M	O
glutaral	585	RB	O
glutaral	875	R	O
glutaral	4370	R	O
glutaral	1000	R	O
glutaral	5300	R	O
glutaral	167.4	R	O
glutaral	1.25	M	TD
glutathione	1250	R	O
glutathione	200	M	IV
glutathione	300	M	O
glycerin	119	NHP	ITT
glycerin	280	R	ITT
glycerin	1600	R	ITT
glycerin	862	R	ITT
glycerin	100	R	O
glycerin	5000	R	IM
glycerin	4000	R	IM
glycerin	1428	Hu	O
glycerin	3880	Hum	O
glycine	42000	R	O
glycine	200	R	IP
glycine	800	R	IP
glycine	201	Hu	IV
glycine	225	Hu	IV
glycine	254.5	P	IV
glycine	800	Hu	O
hemin chloride	0.652	R	SC
hemin chloride	1.304	M	TD
hemin chloride	19.6	R	IP
hemin chloride	19.559	R	IP
hemin chloride	10	R	IP
hexachlorobenzene	0.91	NHP	O
hexachlorobenzene	1000	M	O
hexachlorobenzene	600	M	O
hexachlorobenzene	625	M	O
hexachlorobenzene	556	R	O
hexachlorobenzene	40	R	O
hexachlorobenzene	6450	R	O
hexachlorobenzene	88	R	O
hexachlorobenzene	812	R	O
hexachlorobenzene	212	R	O

Table 16 Continued

hexachlorobenzene	100	R	O
hexachlorobenzene	100	M	IP
hexachlorobenzene	150	R	IP
hexachlorobenzene	85.4	R	IP
hexachlorobenzene	1000	R	O
hexachlorobenzene	100	R	O
hexamethyldisiloxane	260	RB	SC
hexamethyldisiloxane	10000	R	SC
hexamethyldisiloxane	8000	R	SC
hexamethyldisiloxane	420000	R	O
hydrocortisone	150	H	IM
hydrocortisone	333	H	IM
hydrocortisone	400	H	IM
hydrocortisone	400	M	IM
hydrocortisone	200	M	IM
hydrocortisone	500	R	IM
hydrocortisone	400	M	IP
hydrocortisone	80	R	IP
hydrocortisone	4	M	IPL
hydrocortisone	2.94	RB	OC
hydrocortisone	10	M	O
hydrocortisone	210	R	O
hydrocortisone	50	R	PA
hydrocortisone	35	R	PA
hydrocortisone	12	GP	SC
hydrocortisone	400	M	SC
hydrocortisone	156	M	SC
hydrocortisone	200	M	SC
hydrocortisone	100	M	SC
hydrocortisone	6	RB	SC
hydrocortisone	50	R	SC
hydrocortisone	330	R	SC
hydrocortisone	220	R	SC
hydrocortisone	8.7	M	TD
hydrocortisone	50	M	IP
hydrocortisone	25	M	IP
hydrocortisone	150	R	IP
hydrocortisone	50	R	IP
hydrocortisone	0.5	Hu	IV
hydrocortisone	1	Hu	IV
hydrocortisone	1.43	Hu	O
hydrocortisone	0.429	Hu	O
hydrocortisone	400	Hu	O
hydrocortisone	1.43	Hu	O

Table 16 Continued

hydrocortisone	1.4	Hu	O
hydrocortisone	0.71	Hu	O
hydrocortisone	0.29	Hu	O
hydrocortisone	20	M	O
hypoxanthine	600	M	IP
hypoxanthine	1000	M	IP
i-Inositol	4000	M	O
iron	37.5	R	OC
iron	0.0005	R	IC
iron	77	Hu	O
iron (II) sulfate heptahydrate	0.278	R	IT
kanamycin	3500	M	IP
kanamycin	3600	R	SC
kanamycin	3600	R	SC
kanamycin	100	NHP	IV
lactose	375	R	O
L-arginine	40	Rm	IP
L-arginine	0.696	M	IC
L-arginine	0.034	R	IC
L-arginine	20	M	IP
L-arginine	100	M	IP
L-arginine	1000	M	IP
L-arginine	400	R	IP
L-arginine	40	R	IP
L-arginine	250	R	IP
L-arginine	125	R	IP
L-arginine	300	R	IP
L-arginine	200	R	IP
L-arginine	800	R	IP
L-arginine	0.002	M	IS
L-arginine	220	R	IS
L-arginine	428.6	Hu	IV
L-arginine	250	R	IV
L-arginine	500	R	IV
L-arginine	400	R	IV
L-arginine	200	R	IV
L-arginine	0.008	RB	OC
L-arginine	0.349	R	SC
L-ascorbic acid	6680	M	IP
L-ascorbic acid	800	M	IV
L-ascorbic acid	19500	GP	O
L-ascorbic acid	5800	GP	O
L-ascorbic acid	2471	GP	O
L-ascorbic acid	2500	R	O

Table 16 Continued

L-ascorbic acid	50	M	TD
L-ascorbic acid	90	M	IP
L-ascorbic acid	500	CO	IV
L-ascorbic acid	2300	Hu	IV
L-ascorbic acid	900	Huf	IV
L-ascorbic acid	250	M	O
L-ascorbic acid	100	M	O
L-ascorbic acid	2000	R	SC
L-cysteine	100	R	IP
L-cysteine	1000	R	IV
L-cysteine	3600	M	O
L-cysteine	27600	M	O
L-cysteine	6000	M	O
L-cysteine	6.058	M	IC
L-cysteine	5	R	IM
L-cysteine	800	R	IP
L-cysteine	1000	R	IV
L-glutamic acid	0.002	R	IC
L-glutamic acid	0.005	R	IC
L-glutamic acid	0.011	R	IC
L-glutamic acid	1.471	R	IC
L-glutamic acid	0.049	R	IC
L-glutamic acid	0.5	R	IC
L-glutamic acid	0.002	R	IC
L-glutamic acid	0.003	R	IC
L-glutamic acid	500	R	IP
L-glutamic acid	20	R	IP
L-glutamic acid	117	Hu	IV
L-glutamic acid	71	Hu	O
L-glutamic acid	45.2	M	SC
L-glutamine	27	Hu	O
L-histidine	1500	R	IP
L-histidine	500	R	IP
L-histidine	100	R	IP
L-histidine	3840	R	O
L-isoleucine	300	M	O
L-leucine	90	R	IP
L-leucine	60	R	IP
L-leucine	90	R	IP
L-leucine	60	R	IP
L-leucine	138	R	O
L-lysine	44000	R	IP
L-lysine	138000	R	O
L-lysine	72450	R	O

Table 16 Continued

L-lysine	90450	R	O
L-lysine	81000	R	O
L-methionine	26100	R	O
L-methionine	14720	R	O
L-methionine	35000	R	O
L-phenylalanine	7930	R	IP
L-phenylalanine	1980	R	IP
L-phenylalanine	2640	R	IP
L-phenylalanine	6048	R	IP
L-phenylalanine	33600	NHP	O
L-phenylalanine	220000	R	O
L-phenylalanine	160000	R	O
L-phenylalanine	192000	R	O
L-phenylalanine	21750	R	O
L-phenylalanine	30000	R	O
L-phenylalanine	30000	M	SC
L-tryptophan	200	R	O
L-tryptophan	1400	R	O
L-tryptophan	900	R	SC
L-tryptophan	10	R	ID
L-tryptophan	50	R	IP
L-tryptophan	50	R	IP
L-tryptophan	100	R	IP
L-tryptophan	100	Hu	IV
L-tryptophan	100	Hu	IV
L-tryptophan	300	Hu	O
L-tryptophan	857	Hu	O
L-tryptophan	10960	Huf	O
L-tryptophan	2700	Huf	O
L-tryptophan	3276	Huf	O
L-tryptophan	9000	Huf	O
L-tryptophan	4800	Huf	O
L-tryptophan	5400	Huf	O
L-tryptophan	36	Huf	O
L-tyrosine	3000	RB	O
L-tyrosine	20750	R	O
L-tyrosine	5000	R	O
L-tyrosine	3500	R	O
L-tyrosine	150	M	SC
L-valine	200	R	IP
magnesium	250	R	IT
magnesium chloride	500	M	IP
magnesium chloride	30	R	IP
magnesium chloride	0.077	R	IS

Table 16 Continued

magnesium chloride	1	RB	SC
magnesium sulfate	750	R	IP
magnesium sulfate	320	Huf	IV
magnesium sulfate	9000	R	SC
magnesium sulfate	18000	R	SC
magnesium sulfate	482	D	IDD
magnesium sulfate	1000	M	IP
magnesium sulfate	500	R	IP
magnesium sulfate	20	Huf	IS
magnesium sulfate	200	Huf	IS
magnesium sulfate	30.1	D	IV
magnesium sulfate	5.754	D	IV
magnesium sulfate	12	D	IV
magnesium sulfate	120	D	IV
magnesium sulfate	18.056	P	IV
magnesium sulfate	428	Hum	O
magnesium sulfate	2000	M	O
magnesium sulfate	1000	R	O
magnesium sulfate	351	Huf	O
menadione	20	M	IV
menadione	3000	R	O
mercury	129	Hu	TD
mercury	0.571	Hu	IV
mercury	0.023	Hu	IV
mercury	43	Hu	O
mercury	254	Hu	SC
mercury	0.714	Hu	SC
mercury	120	Huf	SC
monosodium glutamate	1315000	R	O
monosodium glutamate	48000	R	O
monosodium glutamate	19500	R	O
monosodium glutamate	140000	R	O
monosodium glutamate	16000	H	SC
monosodium glutamate	8000	H	SC
monosodium glutamate	20000	H	SC
monosodium glutamate	5104	M	SC
monosodium glutamate	5104	M	SC
monosodium glutamate	15000	M	SC
monosodium glutamate	58000	M	SC
monosodium glutamate	40000	R	SC
monosodium glutamate	40000	R	SC
monosodium glutamate	1000	R	SC
monosodium glutamate	34100	R	SC
monosodium glutamate	0.714	Hu	IV

Table 16 Continued

monosodium glutamate	43	Hu	O
monosodium glutamate	0.14	Hu	O
monosodium glutamate	3.571	Hum	O
monosodium glutamate	500	R	O
monosodium glutamate	1000	R	O
monosodium glutamate	50	Huf	O
monosodium glutamate	4000	M	SC
m-xylene	12	M	O
m-xylene	30	M	O
m-xylene	5	GP	TD
m-xylene	0.92	R	TD
m-xylene	1.2	R	TD
m-xylene	8	R	TD
neomycin	220	Hu	O
n-Hexane	20000	R	O
n-Hexane	238000	M	O
nicotinamide	5.128	M	TD
nicotinamide	250	M	IP
nicotinamide	35.7	Hu	O
nicotinamide	62.5	M	SC
nicotinamide	62.5	RB	SC
nicotinic acid	100	M	IP
nicotinic acid	10	M	IP
nicotinic acid	24.75	R	IP
nicotinic acid	16.5	R	IP
nicotinic acid	0.357	Hum	IV
nicotinic acid	7.14	Hu	O
nicotinic acid	31200	Hu	O
nicotinic acid	2571	Hu	O
nicotinic acid	9713	Hu	O
nicotinic acid	157.1	Hu	O
nicotinic acid	7.143	Hu	O
nicotinic acid	0.175	Hu	SC
octoxynol 9	65500	R	O
octoxynol 9	11600	R	O
octoxynol 9	5.7	R	O
octoxynol 9	11.3	R	O
octoxynol 9	5	R	PA
palmitic acid	4.4	M	O
p-aminobenzoic acid	2500	R	O
PCB 1221	28	RB	O
PCB 1221	210	R	O
PCB 1221	1000	R	SC
PCB 1221	2000	R	SC

Table 16 Continued

PCB 1221	160	R	IP
PCB 1221	190	R	SC
PCB 1242	3300	M	O
PCB 1242	825	M	O
PCB 1242	93	P	O
PCB 1242	945	R	O
PCB 1242	1890	R	O
PCB 1242	1250	R	O
PCB 1242	300	M	SC
PCB 1242	160	R	IP
PCB 1242	5000	R	O
PCB 1242	190	R	SC
PCB 1248	32	NHP	O
PCB 1248	55	NHP	O
PCB 1248	17	NHP	O
PCB 1248	35	NHP	O
PCB 1248	24	NHP	O
PCB 1248	83	NHP	O
PCB 1248	26.75	NHP	O
PCB 1248	53.5	NHP	O
PCB 1248	26.75	NHP	O
PCB 1248	2.25	NHP	O
PCB 1248	165	RB	O
PCB 1248	190	R	SC
PCB 1254	250	R	IP
PCB 1254	59.4	M	O
PCB 1254	222	M	O
PCB 1254	252	M	O
PCB 1254	360	M	O
PCB 1254	90	M	O
PCB 1254	350	RB	O
PCB 1254	280	RB	O
PCB 1254	192	R	O
PCB 1254	148	R	O
PCB 1254	35	R	O
PCB 1254	90	R	O
PCB 1254	40	R	O
PCB 1254	750	R	O
PCB 1254	96	R	O
PCB 1254	304	R	O
PCB 1254	380	R	O
PCB 1254	38	R	O
PCB 1254	152	R	O
PCB 1254	38	R	O

Table 16 Continued

PCB 1254	35	R	O
PCB 1254	320	R	O
PCB 1254	160	R	O
PCB 1254	222	R	O
PCB 1254	462.5	R	O
PCB 1254	4000	R	O
PCB 1254	396	R	O
PCB 1254	228	R	O
PCB 1254	675	R	O
PCB 1254	43	R	O
PCB 1254	14	R	O
PCB 1254	125	R	O
PCB 1254	44	R	O
PCB 1254	138	R	O
PCB 1254	396	R	O
PCB 1254	138	R	O
PCB 1254	300	M	SC
PCB 1254	90	R	SC
PCB 1254	270	R	SC
PCB 1254	90	R	SC
PCB 1254	90	R	SC
PCB 1254	0.024	R	IC
PCB 1254	50	M	IP
PCB 1254	200	M	IP
PCB 1254	50	M	IP
PCB 1254	200	M	IP
PCB 1254	500	R	IP
PCB 1254	10	R	IP
PCB 1254	300	R	O
PCB 1254	330	R	O
PCB 1260	20	M	IP
PCB 1260	10	R	IP
PCB 1260	0.4	R	ITT
PCB 1260	74	M	O
PCB 1260	1675	R	O
PCB 1260	210	R	O
PCB 1260	143	M	SC
PCB 1260	2000	RB	TD
PCB 1260	10	R	IP
PCB 1260	160	R	IP
PCB 1260	0.4	R	ITT
PCB 1260	500	M	O
p-cymene	2000	D	IP
p-cymene	3000	Hu	O

Table 16 Continued

p-cymene	42.86	Hu	O
phenol	600	R	IP
phenol	2300	M	O
phenol	2600	M	O
phenol	4000	M	O
phenol	2800	M	O
phenol	300	R	O
phenol	1200	R	O
phenol	3600	R	O
phenol	1200	R	O
phenol	329	M	TD
phenol	0.008	M	TD
phenol	66.7	M	TD
phenol	300	M	IP
phenol	300	M	IP
phenol	265	M	O
phenol	105.3	Hu	PA
phenol red (phenolsulfonphthalein)	0.035	R	IV
polymyxin B	3	Hu	IM
polymyxin B	0.01	R	IV
polymyxin B	0.1	R	IV
polymyxin B	8570	Hu	O
polypropylene	5000	M	O
polysorbate 20	1000	M	IP
polysorbate 20	2500	M	IP
polysorbate 20	1000	M	IP
polysorbate 80	0.08	R	IP
polysorbate 80	635000	R	O
polysorbate 80	1270000	R	O
polysorbate 80	20	R	O
polystyrene	4	M	IT
polystyrene	10	M	IT
polyvinyl alcohol	108.7	R	ITT
potassium chloride	272.2	R	IC
potassium chloride	214.29	Hu	O
potassium chloride	60	Huf	O
potassium chloride	1500	Huf	O
potassium glutamate	57	Hu	O
p-xylene	12	M	O
pyridoxine	2268	R	IP
pyridoxine	5143	Hu	O
pyridoxine	2100	Huf	O
pyridoxine	4800	Huf	O
pyridoxine	139	Huf	O

Table 16 Continued

retinyl acetate	330	M	IP
retinyl acetate	28	M	IP
retinyl acetate	220	M	IP
retinyl acetate	330	M	IP
retinyl acetate	28	RB	IP
retinyl acetate	110	RB	IP
retinyl acetate	275	R	IP
retinyl acetate	82.5	R	IP
retinyl acetate	413	R	IP
retinyl acetate	1350	R	IP
retinyl acetate	144	NHP	O
retinyl acetate	72	NHP	O
retinyl acetate	262	M	O
retinyl acetate	1321	M	O
retinyl acetate	660	M	O
retinyl acetate	220	M	O
retinyl acetate	13.75	R	O
retinyl acetate	36	R	O
retinyl acetate	248	R	O
retinyl acetate	16.5	R	O
retinyl acetate	206	R	O
retinyl acetate	275	R	O
retinyl acetate	440	R	O
retinyl acetate	138	R	O
retinyl acetate	80	R	O
retinyl acetate	275	R	SC
riboflavin	50	M	IP
riboflavin	25	R	IP
riboflavin	50	R	IP
silicon dioxide	1	R	IT
sodium acetate	50	R	IP
sodium bicarbonate	40	M	IP
sodium bicarbonate	1260	Hu	O
sodium bicarbonate	20	Hu	O
sodium borate	70000	D	O
sodium borate	70000	R	O
sodium borate	70000	R	O
sodium borate	37000	R	O
sodium chloride	1710	R	IP
sodium chloride	10000	R	IP
sodium chloride	480	HO	IPL
sodium chloride	27	Hu	IPL
sodium chloride	6000	NHP	IU
sodium chloride	500	R	IU

Table 16 Continued

sodium chloride	50	R	IU
sodium chloride	145000	R	O
sodium chloride	56400	R	O
sodium chloride	10	R	PA
sodium chloride	1900	M	SC
sodium chloride	2500	M	SC
sodium chloride	13440	M	SC
sodium chloride	491	R	IP
sodium chloride	375	D	IV
sodium chloride	2.1	M	IV
sodium chloride	0.04	RB	IV
sodium chloride	12357	Hu	O
sodium chloride	1	R	O
sodium chloride	1.43	R	O
sodium chloride	0.04	RB	SC
sodium hydroxide	44	R	O
sodium metabisulphite	20000	R	O
sodium metabisulphite	40000	R	O
sodium phosphate	150	R	IP
streptomycin	1750	M	IP
streptomycin	65	R	IV
streptomycin	25	M	SC
streptomycin	22.5	R	SC
streptomycin	225	R	SC
streptomycin	1125	R	SC
streptomycin	143	Hu	IP
streptomycin	400	Hu	O
streptomycin	28	Hu	PA
sucrose	1548000	R	O
sucrose	683000	R	O
sucrose	683000	R	O
sucrose	2	M	O
thiamine	20	M	IV
thimerosal	130	R	IP
thimerosal	1300	R	IP
thimerosal	112	RB	OC
thimerosal	0.065	RB	OC
thimerosal	1.4	M	IM
thimerosal	83	Hu	O
thimerosal	28.571	Hu	O
thimerosal	0.00143	Hu	PA
thymidine	20000	M	IP
thymidine	400	M	O
thymidine	800	M	PA

Table 16 Continued

titanium	158	R	O
titanium dioxide	100	M	IT
titanium dioxide	1.25	R	IT
titanium dioxide	1.6	R	IT
titanium dioxide	5	R	IT
titanium dioxide	60000	R	O
tromethamine	12000	R	O
tromethamine	125	D	IV
tromethamine	500	RB	IV
tromethamine	3000	M	O
tromethamine	3000	R	O
uracil	18000	R	O
uracil	15400	R	O
uracil	616	R	O
urea	1400	HuF	IPL
urea	1600	HuF	IPL
urea	6000	NHP	IU
urea	200	CA	O
urea	750	R	O
uridine 5'- triphosphate	0.05	R	IS
vinyl acetate	500	R	O
vinyl acetate	91000	R	O
vinyl acetate	4770	R	O
vitamin E succinate	117	M	IP
xanthine	4.02	R	IA
zinc	25	R	IT
zinc	5000	M	O
zinc	5000	M	O
zinc oxide	6846	R	O

Table 17. Chemical Test Set with ToxTree Validated Structures

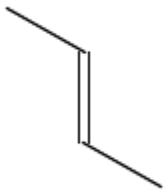
Chemical	CASRN	Toxtree Structure
1,2 polybutadiene	9003-17-2	

Table 17 Continued

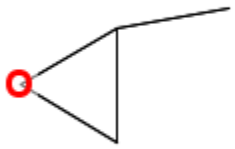
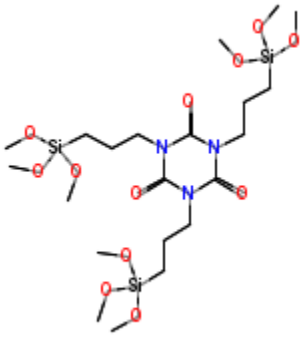
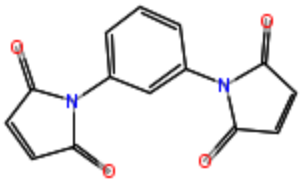
1,2 propylene oxide	75-56-9	
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	26115-70-8	
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	3006-93-7	
2,2 dimethyl-pentane	590-35-2	

Table 17 Continued

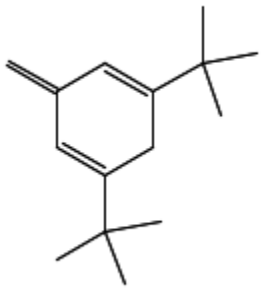
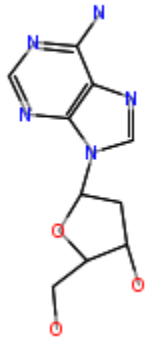
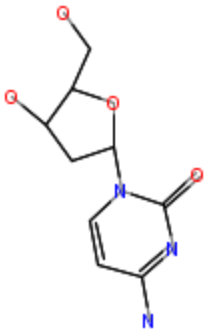
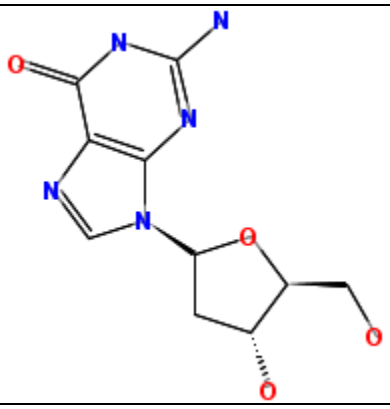
2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	2607-52-5	
2’-deoxyadenosine	958-09-8	
2’-deoxycytidine	951-77-9	
2’-deoxyguanosine	961-07-9	

Table 17 Continued

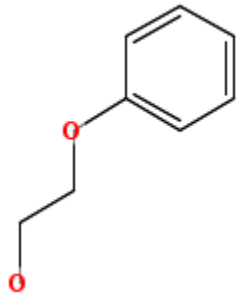
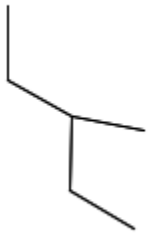
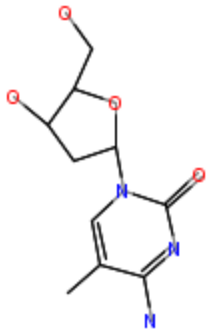
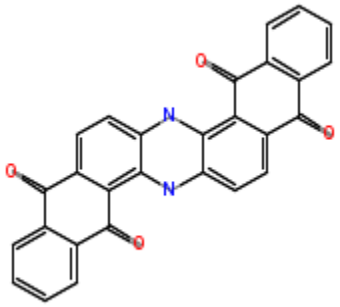
2-phenoxyethanol	122-99-6	
3-methylpentane	96-14-0	
5-methyldeoxycytidine	838-07-3	
6,15-dihydroanthrazine-5,9,14,18-tetrone	81-77-6	

Table 17 Continued

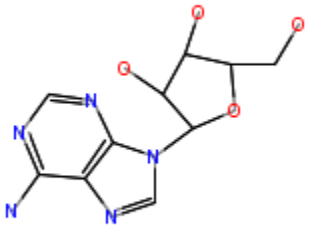
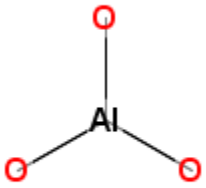
acrylonitrile	25014-41-9	
adenosine	58-61-7	
aluminum	7429-90-5	
aluminum hydroxide	21645-51-2	

Table 17 Continued

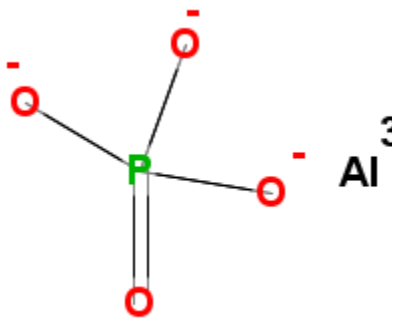
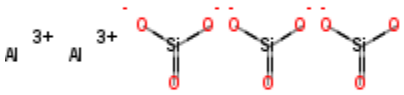
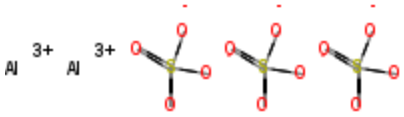
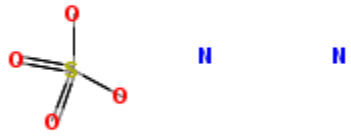
aluminum phosphate	7784-30-7	
aluminum silicate	1335-30-4	
aluminum sulfate	10043-01-3	
ammonium sulfate	7783-20-2	

Table 17 Continued

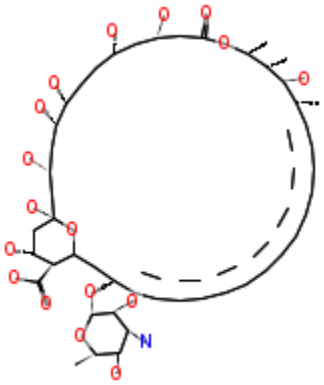
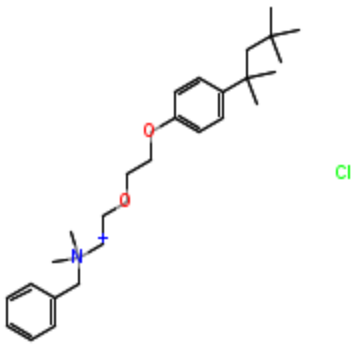
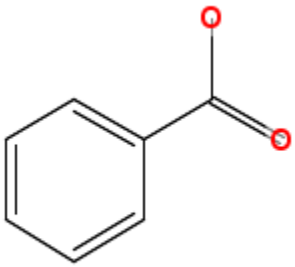
amphotericin B	1397-89-3	
arsenic	7440-38-2	
benzethonium chloride	121-54-0	
benzoic acid	65-85-0	

Table 17 Continued

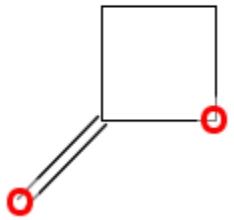
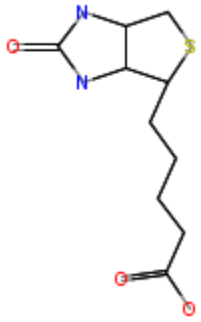
beta-propriolactone	57-57-8	
biotin	58-85-5	
boron	7440-42-8	
bromine	7726-95-6	

Table 17 Continued

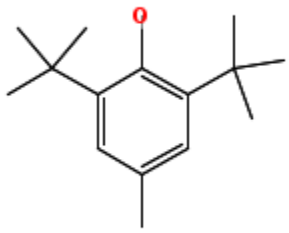
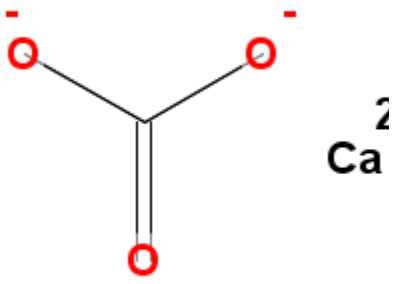
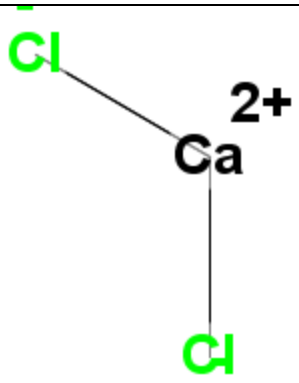
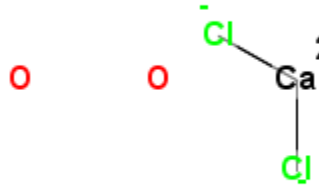
butylated hydroxytoluene (BHT)	128-37-0	
calcium carbonate	471-34-1	
calcium chloride	10043-52-4	
calcium chloride dihydrate	10035-04-8	

Table 17 Continued

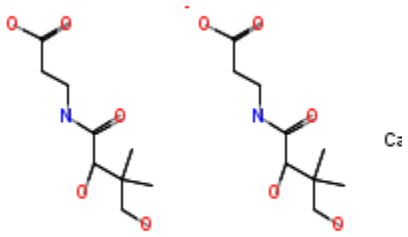
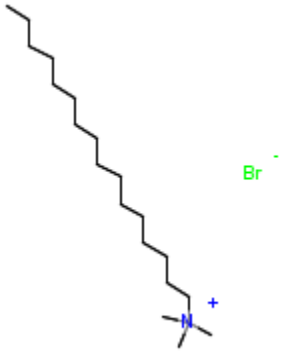
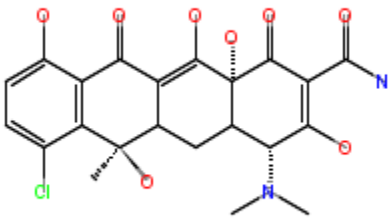
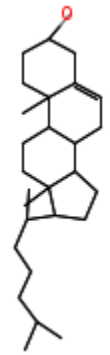
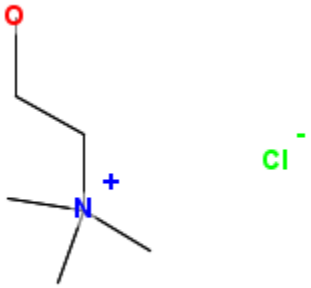
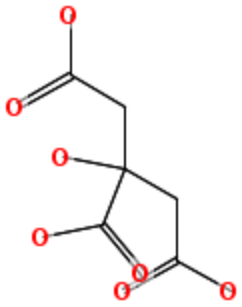
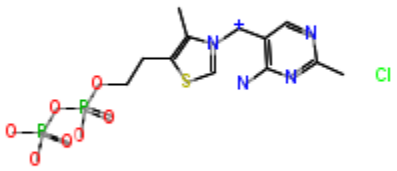
calcium pantothenate (vitamin B5)	137-08-6	
carbon	7440-44-0	C
cesium hydroxide	21351-79-1	
cetrimonium bromide (CTAB)	57-09-0	
chlortetracycline	57-62-5	

Table 17 Continued

cholesterol	57-88-5	
choline chloride	67-48-1	
citric acid	77-92-9	
co-carboxylase	154-87-0	

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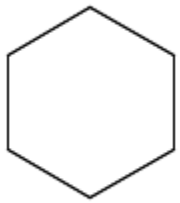
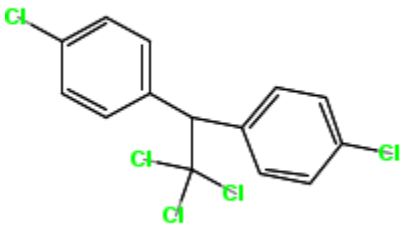
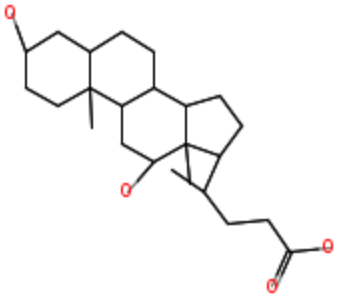
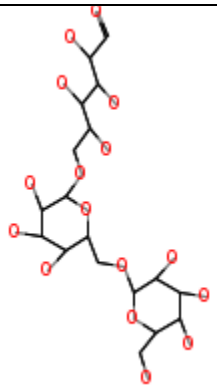
cyclohexane	110-82-7	
DDT (dichlorodiphenyltrichloroethane)	50-29-3	
deoxycholic acid	83-44-3	
dextran	9004-54-0	

Table 17 Continued

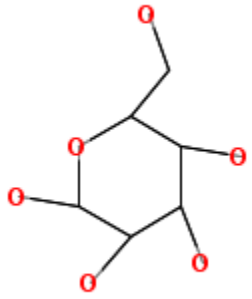
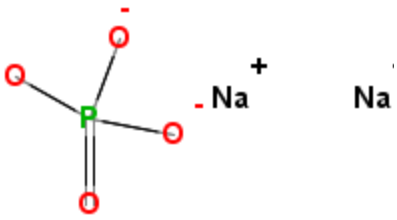
D-galactose	59-23-4	
diadenine sulfate	321-30-2	
disodium phosphate	7558-79-4	
disodium phosphate dodecahydrate	10039-32-4	

Table 17 Continued

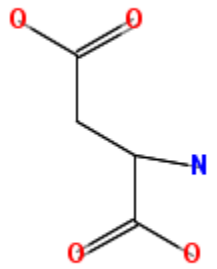
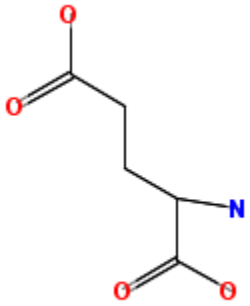
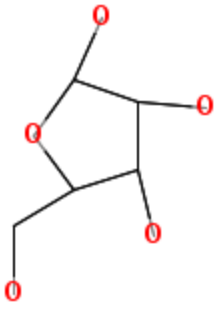
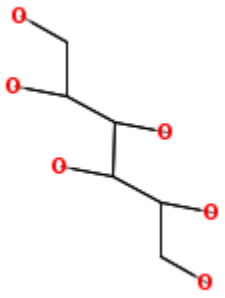
DL-aspartic acid	617-45-8	
DL-glutamic acid	617-65-2	
D-ribose	50-69-1	
D-sorbitol	50-70-4	

Table 17 Continued

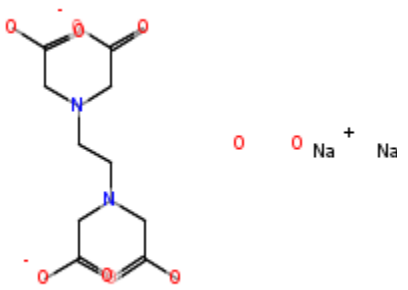
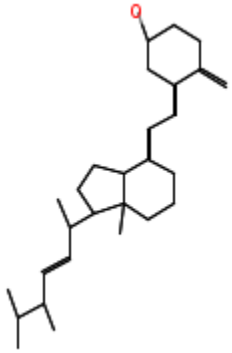
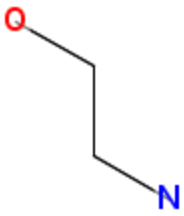
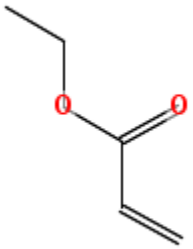
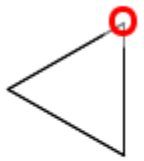
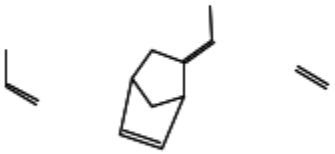
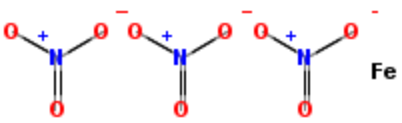
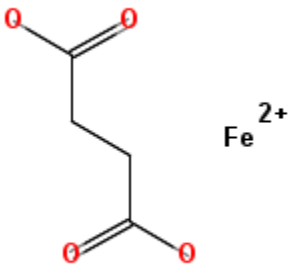
edetate disodium (EDTA)	6381-92-6	
ergocalciferol (vitamin D2)	50-14-6	
ethanolamine	141-43-5	
ethyl acrylate	140-88-5	

Table 17 Continued

ethylene oxide	75-21-8	
ethylene-ethylidenenorbomene-propylene terpolymer	25038-36-2	
ferric (III) nitrate	10421-48-4	
ferrous succinate (butanedioic acid)	10030-90-7	

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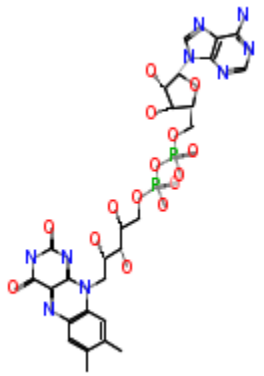
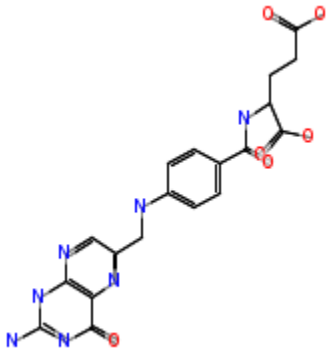
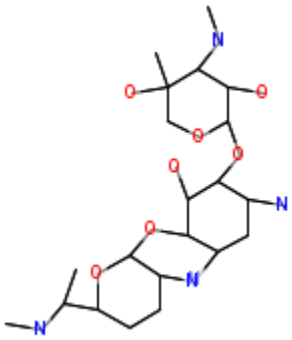
flavin adenine dinucleotide (FAD)	146-14-5	
folic acid	59-30-3	
formaldehyde	50-00-0	
gentamicin	1403-66-3	

Table 17 Continued

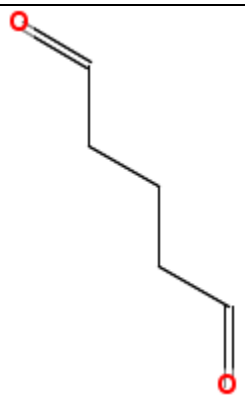
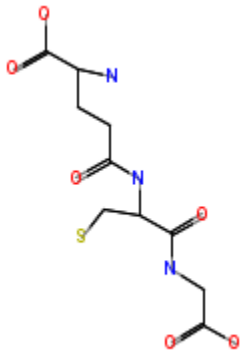
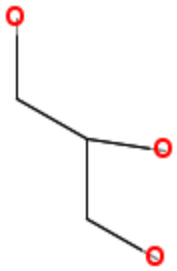
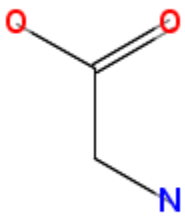
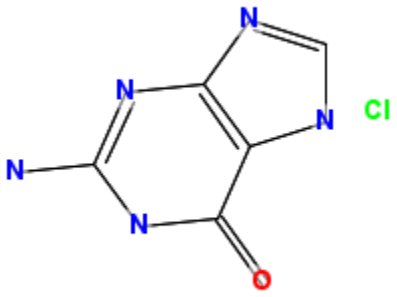
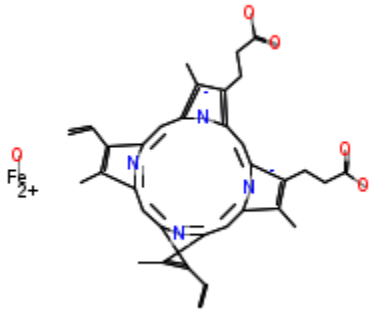
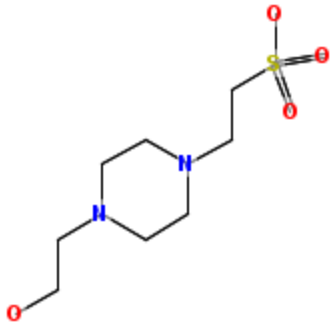
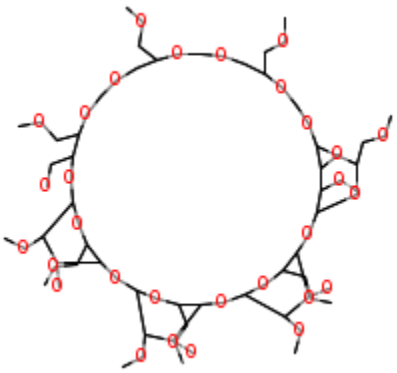
glutaral	111-30-8	
glutathione	70-18-8	
glycerin	56-81-5	
glycine	56-40-6	

Table 17 Continued

guanine hydrochloride	33735-91-0	
hemin chloride	16009-13-5	
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	7365-45-9	
heptakis(2,6-O-dimethyl)beta-cyclodextrin	51166-71-3	

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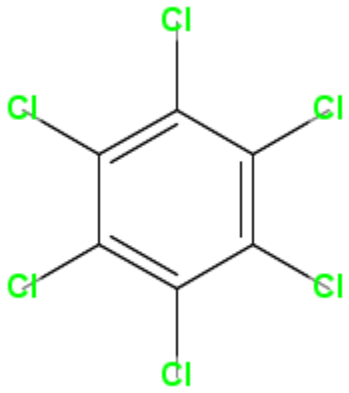
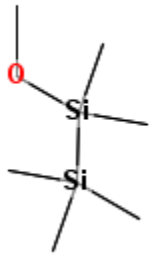
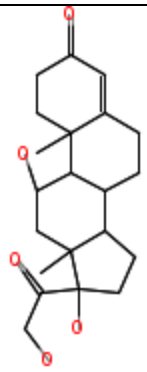
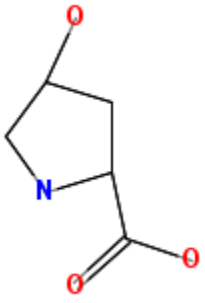
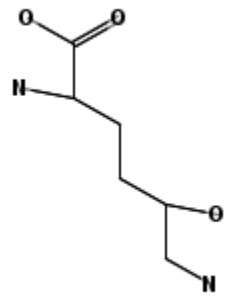
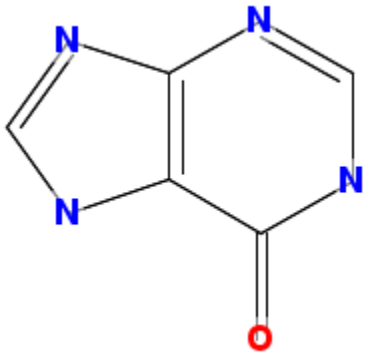
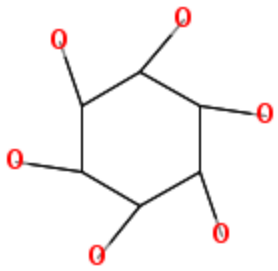
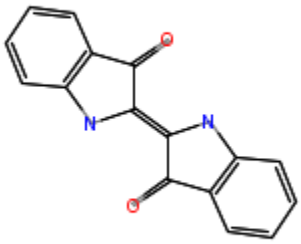
hexachlorobenzene	118-74-1	
hexamethyldisiloxane	9006-65-9	
hydrocortisone	50-23-7	
hydroxy L proline	51-35-4	

Table 17 Continued

hydroxylysine	28902-93-4	
hypoxanthine	68-94-0	
i-Inositol	87-89-8	
indigo	482-89-3	

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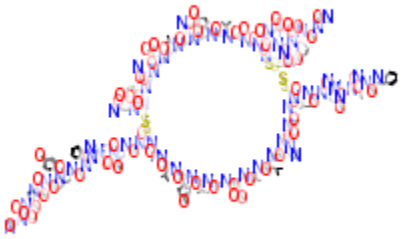
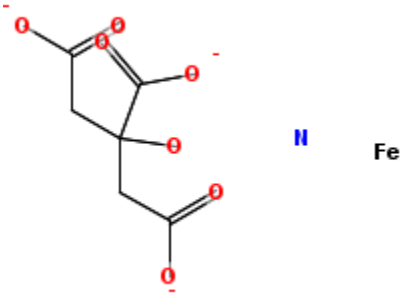
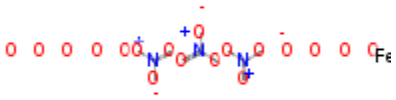
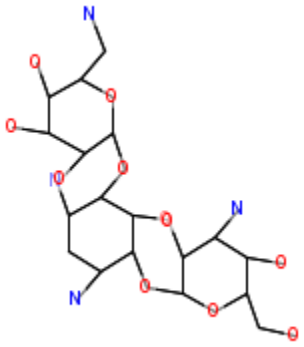
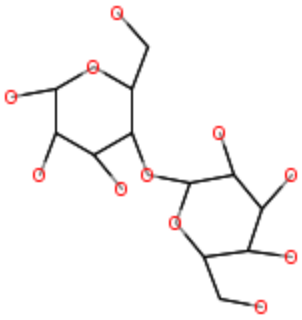
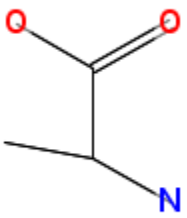
insulin	11061-68-0	
iron	7439-89-6	
iron (II) sulfate heptahydrate	7782-63-0	
iron ammonium citrate	1185-57-5	

Table 17 Continued

iron III nitrate	7782-61-8	
kanamycin	59-01-8	
lactose	63-42-3	
L-alanine	56-41-7	

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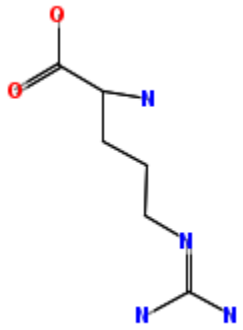
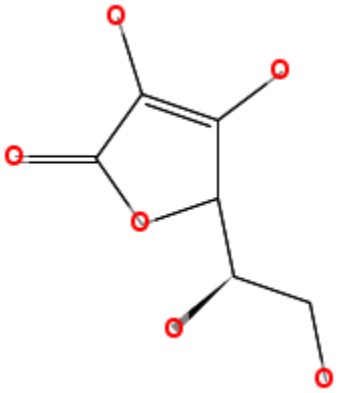
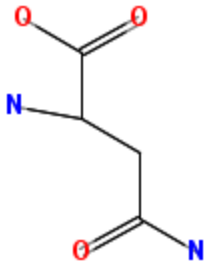
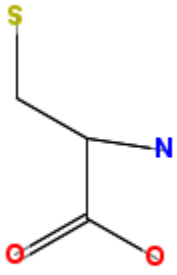
L-arginine	74-79-3	
L-ascorbic acid	50-81-7	
L-asparagine	70-47-3	
L-cysteine	52-90-4	

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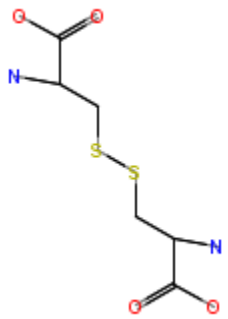
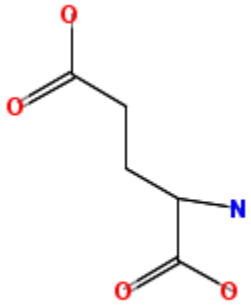
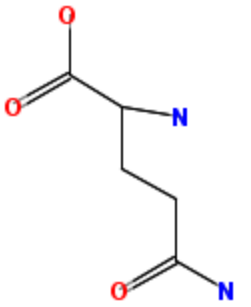
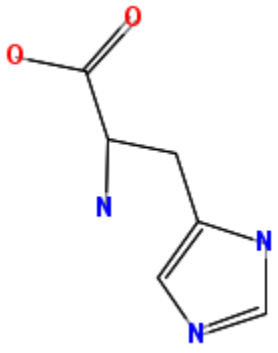
L-cystine	56-89-3	
L-glutamic acid	56-86-0	
L-glutamine	56-85-9	
L-histidine	71-00-1	

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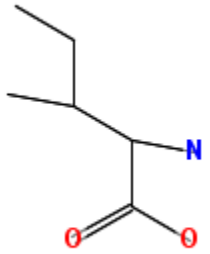
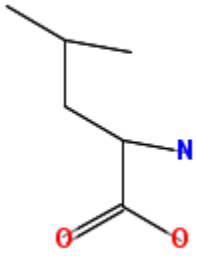
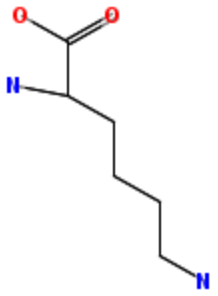
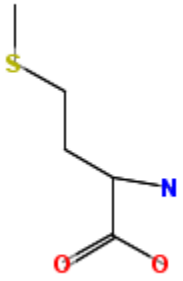
L-isoleucine	73-32-5	
L-leucine	61-90-5	
L-lysine	56-87-1	
L-methionine	63-68-3	

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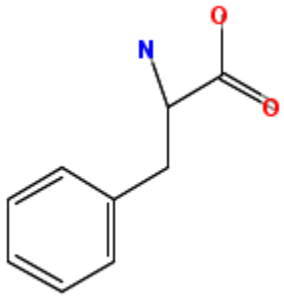
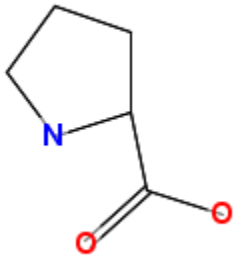
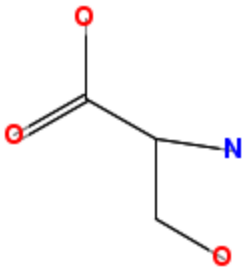
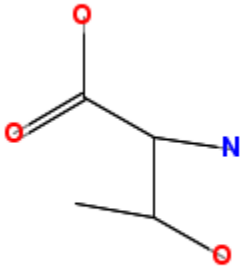
L-phenylalanine	63-91-2	
L-proline	147-85-3	
L-serine	56-45-1	
L-threonine	72-19-5	

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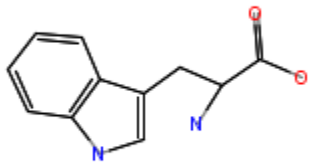
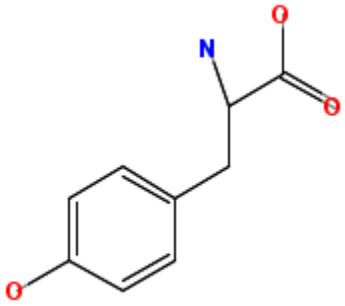
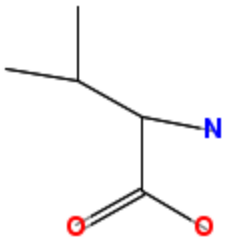
L-tryptophan	73-22-3	
L-tyrosine	60-18-4	
L-valine	72-18-4	
magnesium	7439-95-4	

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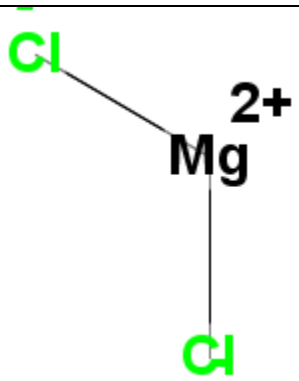
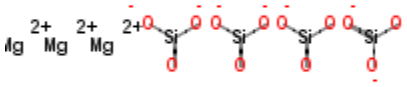
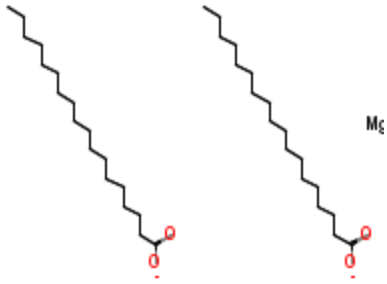
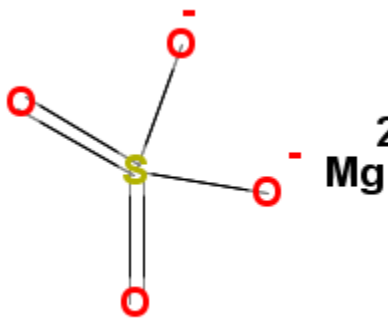
magnesium chloride	7786-30-3	
magnesium silicate (talc)	14807-96-6	
magnesium stearate	557-04-0	
magnesium sulfate	7487-88-9	

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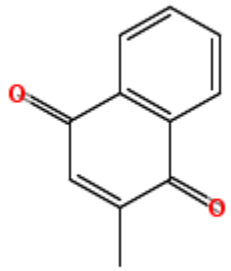
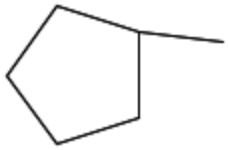
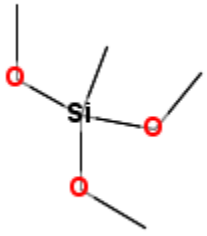
menadione	58-27-5	
mercury	7439-97-6	
methylcyclopentane	96-37-7	
methyltrimethoxysilane	1185-55-3	

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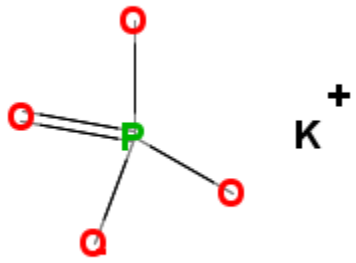
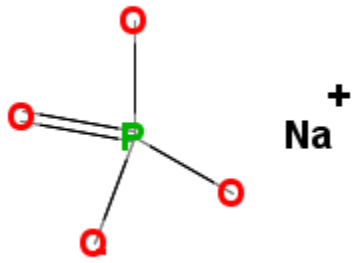
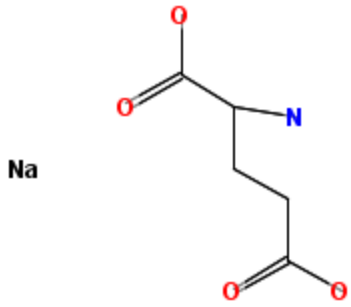
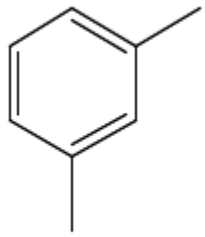
monobasic potassium phosphate	7778-77-0	
monobasic sodium phosphate	7558-80-7	
monosodium L glutamate	142-47-2	
m-xylene	108-38-3	

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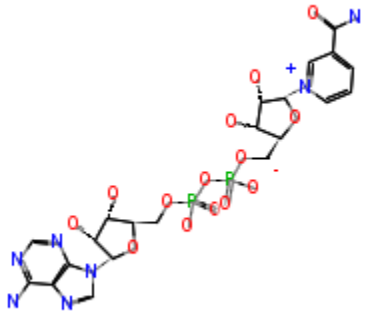
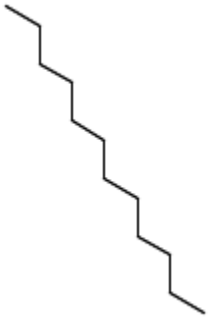
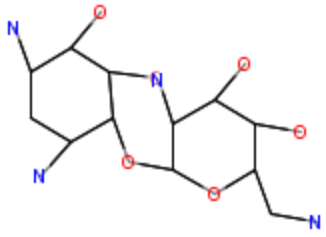
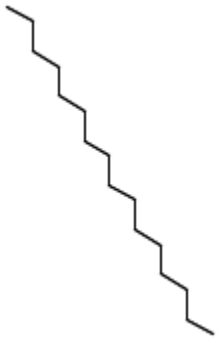
nadide (NAD)	53-84-9	
n-dodecane	112-40-3	
neomycin	1404-04-2	
n-hexadecane	544-76-3	

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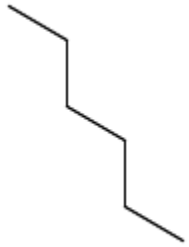
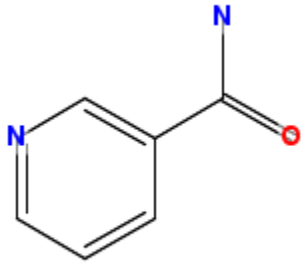
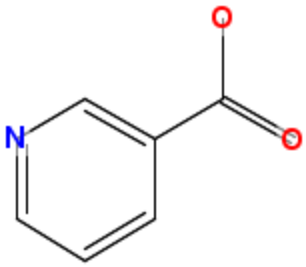
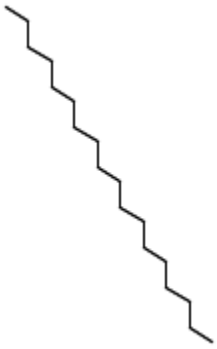
n-hexane	110-54-3	
nicotinamide	98-92-0	
nicotinic acid	59-67-6	
n-octadecane	593-45-3	

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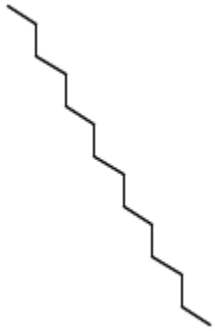
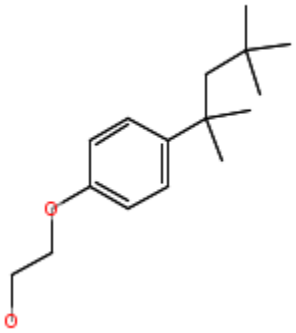
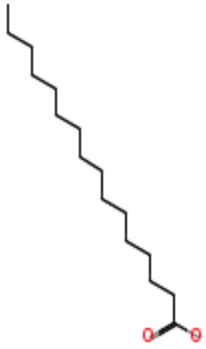
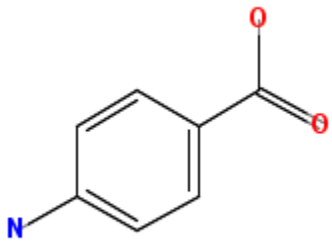
n-tetradecane	629-59-4	
octoxynol 9	9002-93-1	
palmitic acid	57-10-3	
p-aminobenzoic acid	150-13-0	

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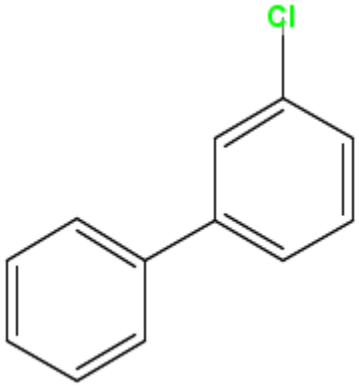
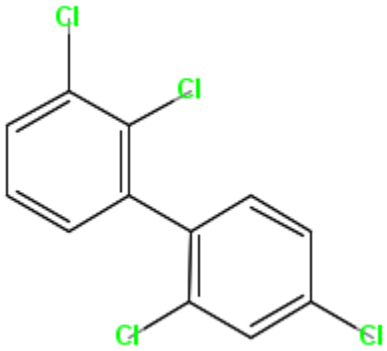
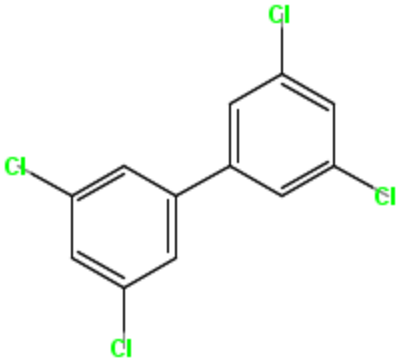
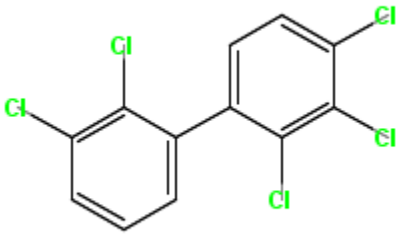
PCB 1221	11104-28-2	
PCB 1242	53469-21-9	
PCB 1248	12672-29-6	
PCB 1254	11097-69-1	

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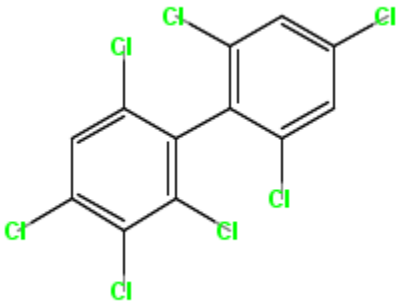
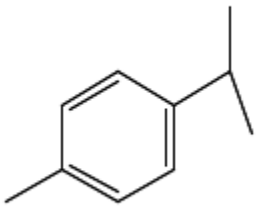
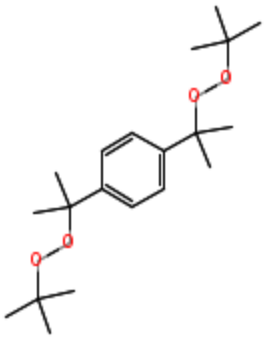
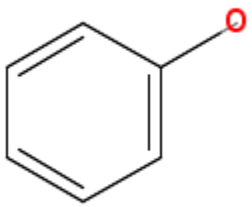
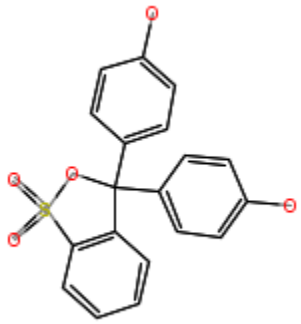
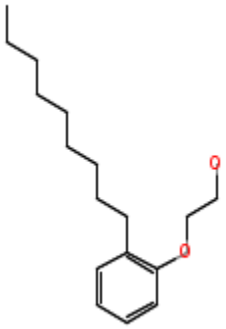
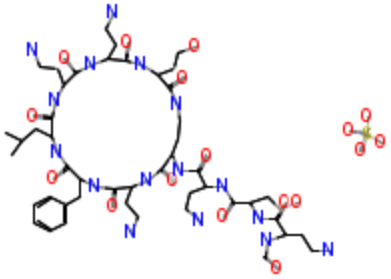
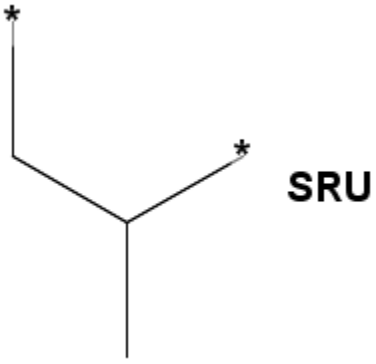
PCB 1260	11096-82-5	
p-cymene	99-87-6	
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	25155-25-3	
phenol	108-95-2	

Table 17 Continued

phenol red (phenolsulfonphthalein)	143-74-8	
polyethylene glycol nonylphenyl ether	9016-45-9	
polymyxin B	1404-26-8	
polypropylene	9003-07-0	

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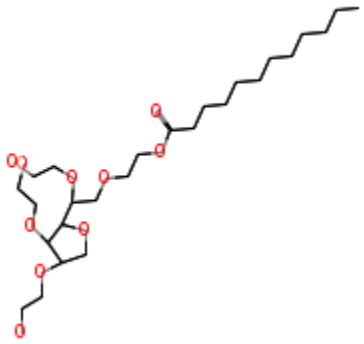
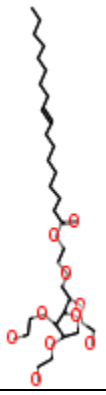
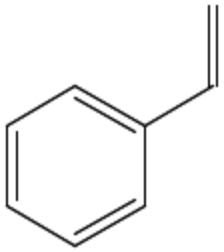
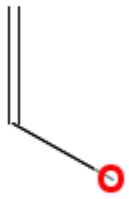
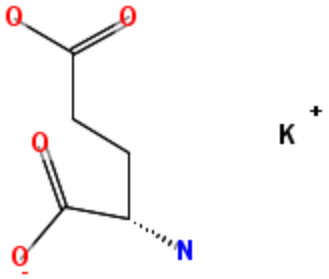
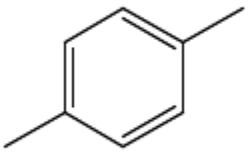
polysorbate 20	9005-64-5	
polysorbate 80	9005-65-6	
polystyrene	9003-53-6	
polyvinyl alcohol	9002-89-5	

Table 17 Continued

potassium	7440-09-7	
potassium chloride	7447-40-7	
potassium glutamate	19473-49-5	
p-xylene	106-42-3	

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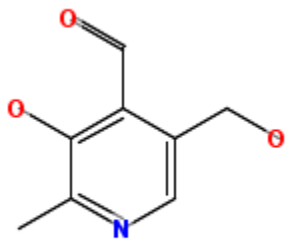
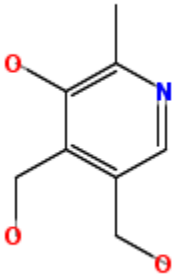
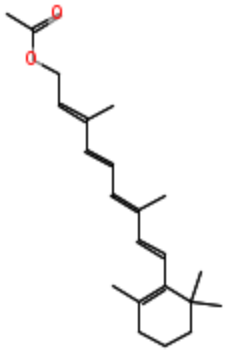
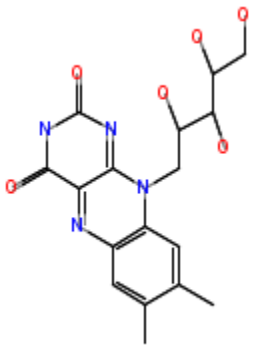
pyridoxal	66-72-8	
pyridoxine	65-23-6	
retinyl acetate	127-47-9	
riboflavin	83-88-5	

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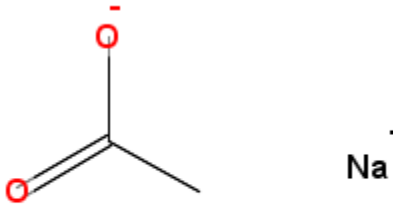
silicon	7440-21-3	
silicon dioxide	7631-86-9	
sodium	7440-23-5	
sodium acetate	127-09-3	

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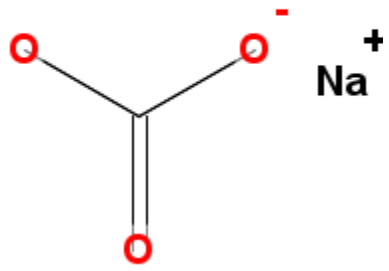
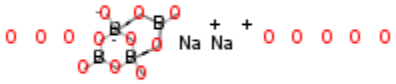
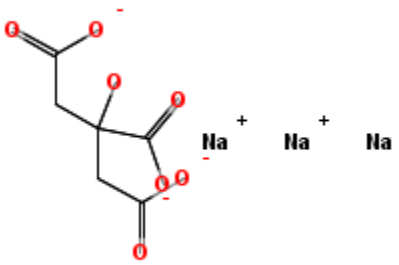
sodium bicarbonate	144-55-8	
sodium borate	1303-96-4	
sodium chloride	7647-14-5	
sodium citrate	68-04-2	

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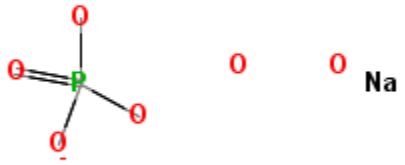
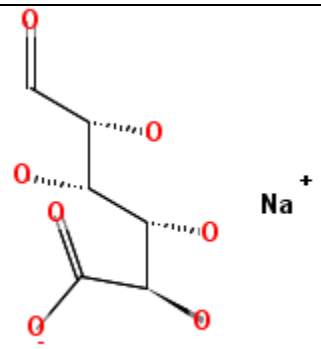
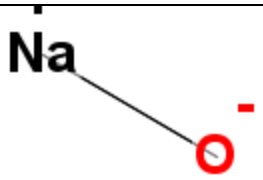
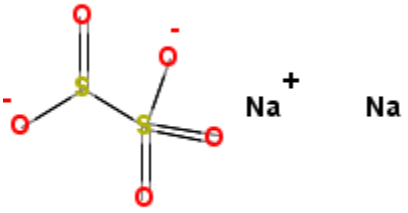
sodium dihydrogen phosphate dihydrate	13472-35-0	
sodium glucuronate	14984-34-0	
sodium hydroxide	1310-73-2	
sodium metabisulphite	7681-57-4	

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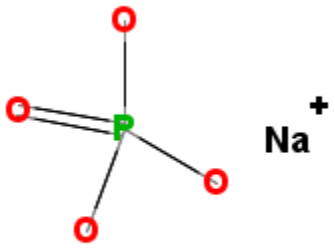
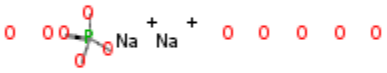
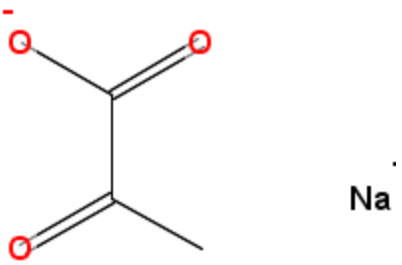
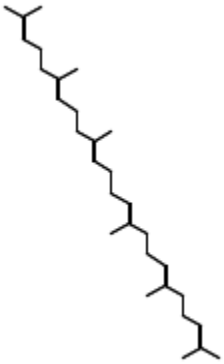
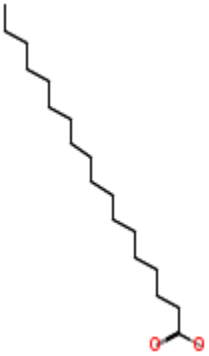
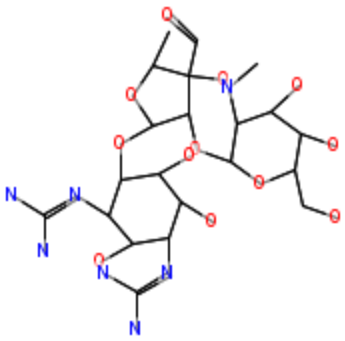
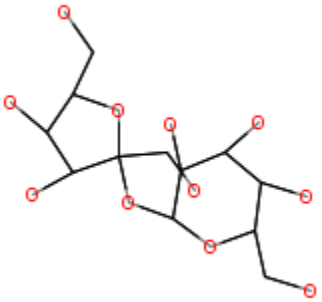
sodium phosphate	7632-05-5	
sodium phosphate dibasic heptahydrate	7782-85-6	
sodium pyruvate	113-24-6	
sorbitan monoleate	1338-43-8	
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	111-02-4	

Table 17 Continued

		
stearic acid	57-11-4	
streptomycin	57-92-1	
sucrose	57-50-1	

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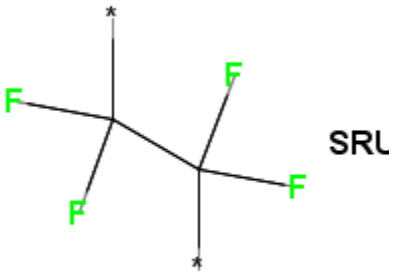
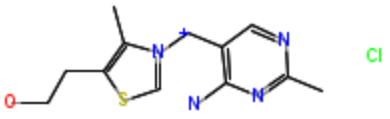
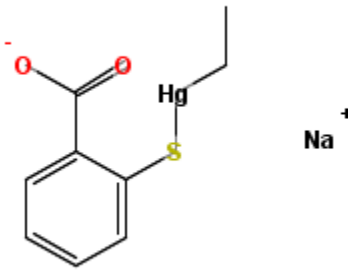
sulfur	7704-34-9	
tetrafluoroethylene	9002-84-0	
thiamine	59-43-8	
thimerosal	54-64-8	

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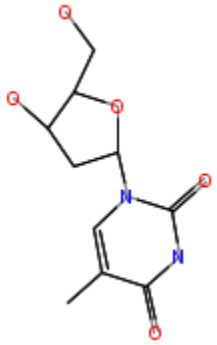
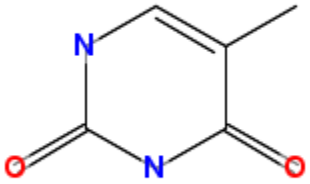
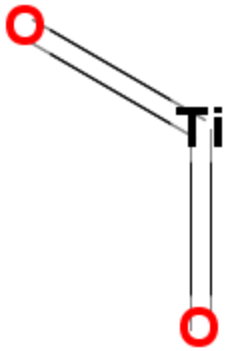
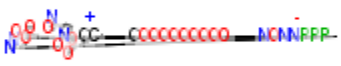
thymidine	50-89-5	
thymine	65-71-4	
titanium dioxide	13463-67-7	
triphosphopyridine nucleotide (NADP)	53-59-8	

Table 17 Continued

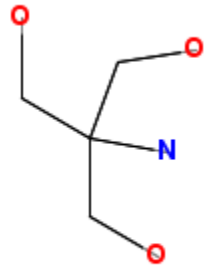
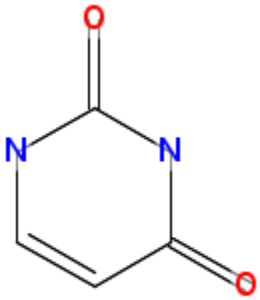
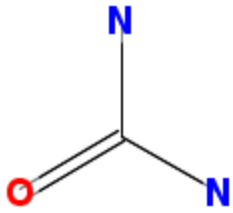
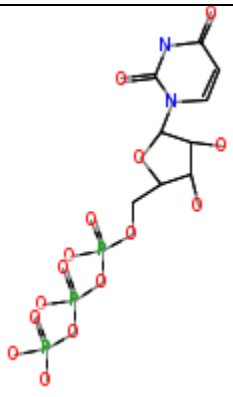
tromethamine	77-86-1	
uracil	66-22-8	
urea	57-13-6	
uridine 5'- triphosphate	63-39-8	

Table 17 Continued

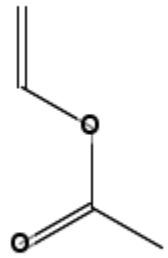
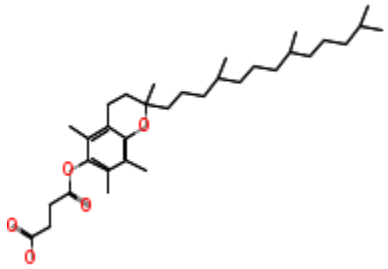
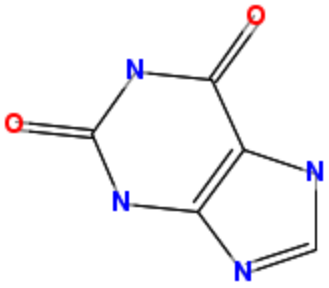
vinyl acetate		
vitamin E succinate	4345-03-3	
xanthine	69-89-6	
zinc	7440-66-6	

Table 17 Continued

zinc oxide	1314-13-2	

Table 18. Classification of the Test Set by Micronucleus Assay Algorithm

Chemical	Class	Verbose Explanation
1,2 propylene oxide	1	QSA1.Acyl halides No 75-56-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 75-56-9 QSA3.N-methylol derivatives No 75-56-9 QSA4.Monohaloalkene No 75-56-9 QSA5.S or N mustard No 75-56-9 QSA6.Propiolactones and propiosultones No 75-56-9 QSA7.Epoxides and aziridines Yes 75-56-9 QSA8.Aliphatic halogens No 75-56-9 QSA9.Alkyl nitrite No 75-56-9 QSA10.α,β unsaturated carbonyls No 75-56-9 QSA11.Simple aldehyde No 75-56-9 QSA12.Quinones No 75-56-9 QSA13.Hydrazine No 75-56-9 QSA14.Aliphatic azo and azoxy No 75-56-9 QSA15.Isocyanate and isothiocyanate groups No 75-56-9 QSA16.Alkyl carbamate and thiocarbamate No 75-56-9 QSA18.Polycyclic Aromatic Hydrocarbons No 75-56-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 75-56-9 QSA21.Alkyl and aryl N-nitroso groups No 75-56-9 QSA22.Azide and triazene groups No 75-56-9 QSA23.Aliphatic N-nitro No 75-56-9 QSA24.α,β unsaturated alkoxy No 75-56-9 QSA25.Aromatic nitroso group No 75-56-9 QSA26.Aromatic ring N-oxide No 75-56-9 QSA27.Nitro aromatic No 75-56-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 75-56-9 QSA28bis.Aromatic mono- and dialkylamine No 75-56-9 QSA28ter.Aromatic N-acyl amine No 75-56-9 QSA29.Aromatic diazo No 75-56-9 QSA30.Coumarins and Furocoumarins No 75-56-9 QSA32.1,3-dialkoxy-benzene No 75-56-9 QSA33.1-phenoxy-benzene No 75-56-9 QSA34.H-acceptor-path3-H-acceptor No 75-56-9 QSA35.Oxolane No 75-56-9

Table 18 Continued

		QSA36.Carbodiimides No 75-56-9 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
1,2-Polybutadiene	0	
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	1	QSA1.Acyl halides No 26115-70-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 26115-70-8 QSA3.N-methylol derivatives No 26115-70-8 QSA4.Monohaloalkene No 26115-70-8 QSA5.S or N mustard No 26115-70-8 QSA6.Propiolactones and propiosultones No 26115-70-8 QSA7.Epoxides and aziridines No 26115-70-8 QSA8.Aliphatic halogens No 26115-70-8 QSA9.Alkyl nitrite No 26115-70-8 QSA10.α,β unsaturated carbonyls No 26115-70-8 QSA11.Simple aldehyde No 26115-70-8 QSA12.Quinones No 26115-70-8 QSA13.Hydrazine No 26115-70-8 QSA14.Aliphatic azo and azoxy No 26115-70-8 QSA15.Isocyanate and isothiocyanate groups No 26115-70-8 QSA16.Alkyl carbamate and thiocarbamate No 26115-70-8 QSA18.Polycyclic Aromatic Hydrocarbons No 26115-70-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 26115-70-8 QSA21.Alkyl and aryl N-nitroso groups No 26115-70-8 QSA22.Azide and triazene groups No 26115-70-8 QSA23.Aliphatic N-nitro No 26115-70-8 QSA24.α,β unsaturated alkoxy No 26115-70-8 QSA25.Aromatic nitroso group No 26115-70-8 QSA26.Aromatic ring N-oxide No 26115-70-8 QSA27.Nitro aromatic No 26115-70-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 26115-70-8 QSA28bis.Aromatic mono- and dialkylamine No 26115-70-8 QSA28ter.Aromatic N-acyl amine No 26115-70-8 QSA29.Aromatic diazo No 26115-70-8 QSA30.Coumarins and Furocoumarins No 26115-70-8 QSA32.1,3-dialkoxy-benzene No 26115-70-8 QSA33.1-phenoxy-benzene No 26115-70-8 QSA34.H-acceptor-path3-H-acceptor Yes 26115-70-8 QSA35.Oxolane No 26115-70-8 QSA36.Carbodiimides No 26115-70-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	1	QSA1.Acyl halides No 3006-93-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 3006-93-7 QSA3.N-methylol derivatives No 3006-93-7 QSA4.Monohaloalkene No 3006-93-7 QSA5.S or N mustard No 3006-93-7 QSA6.Propiolactones and propiosultones No 3006-93-7 QSA7.Epoxides and aziridines No 3006-93-7 QSA8.Aliphatic halogens No 3006-93-7 QSA9.Alkyl nitrite No 3006-93-7 QSA10.α,β

Table 18 Continued

		unsaturated carbonyls Yes 3006-93-7 QSA11.Simple aldehyde No 3006-93-7 QSA12.Quinones No 3006-93-7 QSA13.Hydrazine No 3006-93-7 QSA14.Aliphatic azo and azoxy No 3006-93-7 QSA15.Isocyanate and isothiocyanate groups No 3006-93-7 QSA16.Alkyl carbamate and thiocarbamate No 3006-93-7 QSA18.Polycyclic Aromatic Hydrocarbons No 3006-93-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 3006-93-7 QSA21.Alkyl and aryl N-nitroso groups No 3006-93-7 QSA22.Azide and triazene groups No 3006-93-7 QSA23.Aliphatic N-nitro No 3006-93-7 QSA24.α,β unsaturated alkoxy No 3006-93-7 QSA25.Aromatic nitroso group No 3006-93-7 QSA26.Aromatic ring N-oxide No 3006-93-7 QSA27.Nitro aromatic No 3006-93-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 3006-93-7 QSA28bis.Aromatic mono- and dialkylamine No 3006-93-7 QSA28ter.Aromatic N-acyl amine No 3006-93-7 QSA29.Aromatic diazo No 3006-93-7 QSA30.Coumarins and Furocoumarins No 3006-93-7 QSA32.1,3-dialkoxy-benzene No 3006-93-7 QSA33.1-phenoxy-benzene No 3006-93-7 QSA34.H-acceptor-path3-H-acceptor Yes 3006-93-7 QSA35.Oxolane No 3006-93-7 QSA36.Carbodiimides No 3006-93-7 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
2,2 dimethyl-pentane	0	
2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	0	
2-deoxyadenosine	1	QSA1.Acyl halides No 958-09-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 958-09-8 QSA3.N-methylol derivatives No 958-09-8 QSA4.Monohaloalkene No 958-09-8 QSA5.S or N mustard No 958-09-8 QSA6.Propiolactones and propiosultones No 958-09-8 QSA7.Epoxides and aziridines No 958-09-8 QSA8.Aliphatic halogens No 958-09-8 QSA9.Alkyl nitrite No 958-09-8 QSA10.α,β unsaturated carbonyls No 958-09-8 QSA11.Simple aldehyde No 958-09-8 QSA12.Quinones No 958-09-8 QSA13.Hydrazine No 958-09-8 QSA14.Aliphatic azo and azoxy No 958-09-8 QSA15.Isocyanate and isothiocyanate groups No 958-09-8 QSA16.Alkyl carbamate and thiocarbamate No 958-09-8 QSA18.Polycyclic Aromatic Hydrocarbons No 958-09-8 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 958-09-8 QSA21.Alkyl and aryl N-nitroso groups No 958-09-8 QSA22.Azide and triazene groups No 958-09-8 QSA23.Aliphatic N-nitro No 958-09-8 QSA24.α,β unsaturated alkoxy No 958-09-8 QSA25.Aromatic nitroso group No 958-09-8 QSA26.Aromatic ring N-oxide No 958-09-8 QSA27.Nitro aromatic No 958-09-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 958-09-8 QSA28bis.Aromatic mono- and dialkylamine No 958-09-8 QSA28ter.Aromatic N-acyl amine No 958-09-8 QSA29.Aromatic diazo No 958-09-8 QSA30.Coumarins and Furocoumarins No 958-09-8 QSA32.1,3-dialkoxy-benzene No 958-09-8 QSA33.1-phenoxy-benzene No 958-09-8 QSA34.H-acceptor-path3-H-acceptor Yes 958-09-8 QSA35.Oxolane Yes 958-09-8 QSA36.Carbodiimides No 958-09-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
2'-deoxycytidine	1	QSA1.Acyl halides No 951-77-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 951-77-9 QSA3.N-methylol derivatives No 951-77-9 QSA4.Monohaloalkene No 951-77-9 QSA5.S or N mustard No 951-77-9 QSA6.Propiolactones and propiosultones No 951-77-9 QSA7.Epoxides and aziridines No 951-77-9 QSA8.Aliphatic halogens No 951-77-9 QSA9.Alkyl nitrite No 951-77-9 QSA10.α,β unsaturated carbonyls No 951-77-9 QSA11.Simple aldehyde No 951-77-9 QSA12.Quinones No 951-77-9 QSA13.Hydrazine No 951-77-9 QSA14.Aliphatic azo and azoxy No 951-77-9 QSA15.Isocyanate and isothiocyanate groups No 951-77-9 QSA16.Alkyl carbamate and thiocarbamate No 951-77-9 QSA18.Polycyclic Aromatic Hydrocarbons No 951-77-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 951-77-9 QSA21.Alkyl and aryl N-nitroso groups No 951-77-9 QSA22.Azide and triazene groups No 951-77-9 QSA23.Aliphatic N-nitro No 951-77-9 QSA24.α,β unsaturated alkoxy No 951-77-9 QSA25.Aromatic nitroso group No 951-77-9 QSA26.Aromatic ring N-oxide No 951-77-9 QSA27.Nitro aromatic No 951-77-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 951-77-9 QSA28bis.Aromatic mono- and dialkylamine No 951-77-9 QSA28ter.Aromatic N-acyl amine No 951-77-9 QSA29.Aromatic diazo No 951-77-9 QSA30.Coumarins and Furocoumarins No 951-77-9 QSA32.1,3-dialkoxy-benzene No 951-77-9 QSA33.1-phenoxy-benzene No 951-77-9 QSA34.H-acceptor-path3-H-acceptor Yes 951-77-9 QSA35.Oxolane Yes 951-77-9 QSA36.Carbodiimides No 951-77-9 QAny alert?.At least one

Table 18 Continued

		alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
2'-deoxyguanosine	1	QSA1.Acyl halides No 961-07-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 961-07-9 QSA3.N-methylol derivatives No 961-07-9 QSA4.Monohaloalkene No 961-07-9 QSA5.S or N mustard No 961-07-9 QSA6.Propiolactones and propiosultones No 961-07-9 QSA7.Epoxides and aziridines No 961-07-9 QSA8.Aliphatic halogens No 961-07-9 QSA9.Alkyl nitrite No 961-07-9 QSA10.α,β unsaturated carbonyls No 961-07-9 QSA11.Simple aldehyde No 961-07-9 QSA12.Quinones No 961-07-9 QSA13.Hydrazine No 961-07-9 QSA14.Aliphatic azo and azoxy No 961-07-9 QSA15.Isocyanate and isothiocyanate groups No 961-07-9 QSA16.Alkyl carbamate and thiocarbamate No 961-07-9 QSA18.Polycyclic Aromatic Hydrocarbons No 961-07-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 961-07-9 QSA21.Alkyl and aryl N-nitroso groups No 961-07-9 QSA22.Azide and triazene groups No 961-07-9 QSA23.Aliphatic N-nitro No 961-07-9 QSA24.α,β unsaturated alkoxy No 961-07-9 QSA25.Aromatic nitroso group No 961-07-9 QSA26.Aromatic ring N-oxide No 961-07-9 QSA27.Nitro aromatic No 961-07-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 961-07-9 QSA28bis.Aromatic mono- and dialkylamine No 961-07-9 QSA28ter.Aromatic N-acyl amine No 961-07-9 QSA29.Aromatic diazo No 961-07-9 QSA30.Coumarins and Furocoumarins No 961-07-9 QSA32.1,3-dialkoxy-benzene No 961-07-9 QSA33.1-phenoxy-benzene No 961-07-9 QSA34.H-acceptor-path3-H-acceptor Yes 961-07-9 QSA35.Oxolane Yes 961-07-9 QSA36.Carbodiimides No 961-07-9 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
2-phenoxyethanol	1	QSA1.Acyl halides No 122-99-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 122-99-6 QSA3.N-methylol derivatives No 122-99-6 QSA4.Monohaloalkene No 122-99-6 QSA5.S or N mustard No 122-99-6 QSA6.Propiolactones and propiosultones No 122-99-6 QSA7.Epoxides and aziridines No 122-99-6 QSA8.Aliphatic halogens No 122-99-6 QSA9.Alkyl nitrite No 122-99-6 QSA10.α,β unsaturated carbonyls No 122-99-6 QSA11.Simple aldehyde No 122-99-6 QSA12.Quinones No 122-99-6 QSA13.Hydrazine No 122-99-6 QSA14.Aliphatic azo and azoxy No 122-99-6 QSA15.Isocyanate and isothiocyanate groups No 122-99-6 QSA16.Alkyl carbamate and thiocarbamate No 122-99-6 QSA18.Polycyclic Aromatic

Table 18 Continued

		Hydrocarbons No 122-99-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 122-99-6 QSA21.Alkyl and aryl N-nitroso groups No 122-99-6 QSA22.Azide and triazene groups No 122-99-6 QSA23.Aliphatic N-nitro No 122-99-6 QSA24.α,β unsaturated alkoxy No 122-99-6 QSA25.Aromatic nitroso group No 122-99-6 QSA26.Aromatic ring N-oxide No 122-99-6 QSA27.Nitro aromatic No 122-99-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 122-99-6 QSA28bis.Aromatic mono- and dialkylamine No 122-99-6 QSA28ter.Aromatic N-acyl amine No 122-99-6 QSA29.Aromatic diazo No 122-99-6 QSA30.Coumarins and Furocoumarins No 122-99-6 QSA32.1,3-dialkoxy-benzene No 122-99-6 QSA33.1-phenoxy-benzene No 122-99-6 QSA34.H-acceptor-path3-H-acceptor Yes 122-99-6 QSA35.Oxolane No 122-99-6 QSA36.Carbodiimides No 122-99-6 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
3-methylpentane	0	
5-methyldeoxycytidine	1	QSA1.Acyl halides No 838-07-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 838-07-3 QSA3.N-methylol derivatives No 838-07-3 QSA4.Monohaloalkene No 838-07-3 QSA5.S or N mustard No 838-07-3 QSA6.Propiolactones and propiosultones No 838-07-3 QSA7.Epoxides and aziridines No 838-07-3 QSA8.Aliphatic halogens No 838-07-3 QSA9.Alkyl nitrite No 838-07-3 QSA10.α,β unsaturated carbonyls No 838-07-3 QSA11.Simple aldehyde No 838-07-3 QSA12.Quinones No 838-07-3 QSA13.Hydrazine No 838-07-3 QSA14.Aliphatic azo and azoxy No 838-07-3 QSA15.Isocyanate and isothiocyanate groups No 838-07-3 QSA16.Alkyl carbamate and thiocarbamate No 838-07-3 QSA18.Polycyclic Aromatic Hydrocarbons No 838-07-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 838-07-3 QSA21.Alkyl and aryl N-nitroso groups No 838-07-3 QSA22.Azide and triazene groups No 838-07-3 QSA23.Aliphatic N-nitro No 838-07-3 QSA24.α,β unsaturated alkoxy No 838-07-3 QSA25.Aromatic nitroso group No 838-07-3 QSA26.Aromatic ring N-oxide No 838-07-3 QSA27.Nitro aromatic No 838-07-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 838-07-3 QSA28bis.Aromatic mono- and dialkylamine No 838-07-3 QSA28ter.Aromatic N-acyl amine No 838-07-3 QSA29.Aromatic diazo No 838-07-3 QSA30.Coumarins and Furocoumarins No 838-07-3 QSA32.1,3-dialkoxy-benzene No 838-07-3 QSA33.1-

Table 18 Continued

		phenoxy-benzene No 838-07-3 QSA34.H-acceptor-path3-H-acceptor Yes 838-07-3 QSA35.Oxolane Yes 838-07-3 QSA36.Carbodiimides No 838-07-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
6,15-dihydroanthrazine-5,9,14,18-tetrone	1	QSA1.Acyl halides No 81-77-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 81-77-6 QSA3.N-methylol derivatives No 81-77-6 QSA4.Monohaloalkene No 81-77-6 QSA5.S or N mustard No 81-77-6 QSA6.Propiolactones and propiosultones No 81-77-6 QSA7.Epoxides and aziridines No 81-77-6 QSA8.Aliphatic halogens No 81-77-6 QSA9.Alkyl nitrite No 81-77-6 QSA10.α,β unsaturated carbonyls No 81-77-6 QSA11.Simple aldehyde No 81-77-6 QSA12.Quinones Yes 81-77-6 QSA13.Hydrazine No 81-77-6 QSA14.Aliphatic azo and azoxy No 81-77-6 QSA15.Isocyanate and isothiocyanate groups No 81-77-6 QSA16.Alkyl carbamate and thiocarbamate No 81-77-6 QSA18.Polycyclic Aromatic Hydrocarbons Yes 81-77-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 81-77-6 QSA21.Alkyl and aryl N-nitroso groups No 81-77-6 QSA22.Azide and triazene groups No 81-77-6 QSA23.Aliphatic N-nitro No 81-77-6 QSA24.α,β unsaturated alkoxy No 81-77-6 QSA25.Aromatic nitroso group No 81-77-6 QSA26.Aromatic ring N-oxide No 81-77-6 QSA27.Nitro aromatic No 81-77-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 81-77-6 QSA28bis.Aromatic mono- and dialkylamine No 81-77-6 QSA28ter.Aromatic N-acyl amine No 81-77-6 QSA29.Aromatic diazo No 81-77-6 QSA30.Coumarins and Furocoumarins No 81-77-6 QSA32.1,3-dialkoxy-benzene No 81-77-6 QSA33.1-phenoxy-benzene No 81-77-6 QSA34.H-acceptor-path3-H-acceptor Yes 81-77-6 QSA35.Oxolane No 81-77-6 QSA36.Carbodiimides No 81-77-6 QAny alert?.At least one alert fired? Yes
acrylonitrile	0	
adenosine	1	QSA1.Acyl halides No 58-61-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 58-61-7 QSA3.N-methylol derivatives No 58-61-7 QSA4.Monohaloalkene No 58-61-7 QSA5.S or N mustard No 58-61-7 QSA6.Propiolactones and propiosultones No 58-61-7 QSA7.Epoxides and aziridines No 58-61-7 QSA8.Aliphatic halogens No 58-61-7 QSA9.Alkyl nitrite No 58-61-7 QSA10.α,β unsaturated carbonyls No 58-61-7 QSA11.Simple aldehyde No 58-61-7 QSA12.Quinones No 58-61-7 QSA13.Hydrazine No 58-61-7 QSA14.Aliphatic azo and

Table 18 Continued

		azoxy No 58-61-7 QSA15.Isocyanate and isothiocyanate groups No 58-61-7 QSA16.Alkyl carbamate and thiocarbamate No 58-61-7 QSA18.Polycyclic Aromatic Hydrocarbons No 58-61-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 58-61-7 QSA21.Alkyl and aryl N-nitroso groups No 58-61-7 QSA22.Azide and triazene groups No 58-61-7 QSA23.Aliphatic N-nitro No 58-61-7 QSA24.α,β unsaturated alkoxy No 58-61-7 QSA25.Aromatic nitroso group No 58-61-7 QSA26.Aromatic ring N-oxide No 58-61-7 QSA27.Nitro aromatic No 58-61-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 58-61-7 QSA28bis.Aromatic mono- and dialkylamine No 58-61-7 QSA28ter.Aromatic N-acyl amine No 58-61-7 QSA29.Aromatic diazo No 58-61-7 QSA30.Coumarins and Furocoumarins No 58-61-7 QSA32.1,3-dialkoxy-benzene No 58-61-7 QSA33.1-phenoxy-benzene No 58-61-7 QSA34.H-acceptor-path3-H-acceptor Yes 58-61-7 QSA35.Oxolane Yes 58-61-7 QSA36.Carbodiimides No 58-61-7 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
aluminum (used toxicity measures for aluminum chloride)	0	
aluminum hydroxide	0	
aluminum phosphate	1	QSA1.Acyl halides No 7784-30-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7784-30-7 QSA3.N-methylol derivatives No 7784-30-7 QSA4.Monohaloalkene No 7784-30-7 QSA5.S or N mustard No 7784-30-7 QSA6.Propiolactones and propiosultones No 7784-30-7 QSA7.Epoxides and aziridines No 7784-30-7 QSA8.Aliphatic halogens No 7784-30-7 QSA9.Alkyl nitrite No 7784-30-7 QSA10.α,β unsaturated carbonyls No 7784-30-7 QSA11.Simple aldehyde No 7784-30-7 QSA12.Quinones No 7784-30-7 QSA13.Hydrazine No 7784-30-7 QSA14.Aliphatic azo and azoxy No 7784-30-7 QSA15.Isocyanate and isothiocyanate groups No 7784-30-7 QSA16.Alkyl carbamate and thiocarbamate No 7784-30-7 QSA18.Polycyclic Aromatic Hydrocarbons No 7784-30-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7784-30-7 QSA21.Alkyl and aryl N-nitroso groups No 7784-30-7 QSA22.Azide and triazene groups No 7784-30-7 QSA23.Aliphatic N-nitro No 7784-30-7

Table 18 Continued

		QSA24.α,β unsaturated alkoxy No 7784-30-7 QSA25.Aromatic nitroso group No 7784-30-7 QSA26.Aromatic ring N-oxide No 7784-30-7 QSA27.Nitro aromatic No 7784-30-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7784-30-7 QSA28bis.Aromatic mono- and dialkylamine No 7784-30-7 QSA28ter.Aromatic N-acyl amine No 7784-30-7 QSA29.Aromatic diazo No 7784-30-7 QSA30.Coumarins and Furocoumarins No 7784-30-7 QSA32.1,3-dialkoxy-benzene No 7784-30-7 QSA33.1-phenoxy-benzene No 7784-30-7 QSA34.H-acceptor-path3-H-acceptor Yes 7784-30-7 QSA35.Oxolane No 7784-30-7 QSA36.Carbodiimides No 7784-30-7 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
aluminum silicate	0	
aluminum sulfate	1	QSA1.Acyl halides No 10043-01-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 10043-01-3 QSA3.N-methylol derivatives No 10043-01-3 QSA4.Monohaloalkene No 10043-01-3 QSA5.S or N mustard No 10043-01-3 QSA6.Propiolactones and propiosultones No 10043-01-3 QSA7.Epoxides and aziridines No 10043-01-3 QSA8.Aliphatic halogens No 10043-01-3 QSA9.Alkyl nitrite No 10043-01-3 QSA10.α,β unsaturated carbonyls No 10043-01-3 QSA11.Simple aldehyde No 10043-01-3 QSA12.Quinones No 10043-01-3 QSA13.Hydrazine No 10043-01-3 QSA14.Aliphatic azo and azoxy No 10043-01-3 QSA15.Isocyanate and isothiocyanate groups No 10043-01-3 QSA16.Alkyl carbamate and thiocarbamate No 10043-01-3 QSA18.Polycyclic Aromatic Hydrocarbons No 10043-01-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 10043-01-3 QSA21.Alkyl and aryl N-nitroso groups No 10043-01-3 QSA22.Azide and triazene groups No 10043-01-3 QSA23.Aliphatic N-nitro No 10043-01-3 QSA24.α,β unsaturated alkoxy No 10043-01-3 QSA25.Aromatic nitroso group No 10043-01-3 QSA26.Aromatic ring N-oxide No 10043-01-3 QSA27.Nitro aromatic No 10043-01-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 10043-01-3 QSA28bis.Aromatic mono- and dialkylamine No 10043-01-3 QSA28ter.Aromatic N-acyl amine No 10043-01-3 QSA29.Aromatic diazo No 10043-01-3 QSA30.Coumarins and Furocoumarins No 10043-01-3 QSA32.1,3-dialkoxy-benzene No 10043-01-3 QSA33.1-phenoxy-benzene No 10043-01-3 QSA34.H-acceptor-path3-H-acceptor Yes 10043-

Table 18 Continued

		01-3 QSA35.Oxolane No 10043-01-3 QSA36.Carbodiimides No 10043-01-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
ammonium sulfate	1	QSA1.Acyl halides No 7783-20-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7783-20-2 QSA3.N-methylol derivatives No 7783-20-2 QSA4.Monohaloalkene No 7783-20-2 QSA5.S or N mustard No 7783-20-2 QSA6.Propiolactones and propiosultones No 7783-20-2 QSA7.Epoxides and aziridines No 7783-20-2 QSA8.Aliphatic halogens No 7783-20-2 QSA9.Alkyl nitrite No 7783-20-2 QSA10.α,β unsaturated carbonyls No 7783-20-2 QSA11.Simple aldehyde No 7783-20-2 QSA12.Quinones No 7783-20-2 QSA13.Hydrazine No 7783-20-2 QSA14.Aliphatic azo and azoxy No 7783-20-2 QSA15.Isocyanate and isothiocyanate groups No 7783-20-2 QSA16.Alkyl carbamate and thiocarbamate No 7783-20-2 QSA18.Polycyclic Aromatic Hydrocarbons No 7783-20-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7783-20-2 QSA21.Alkyl and aryl N-nitroso groups No 7783-20-2 QSA22.Azide and triazene groups No 7783-20-2 QSA23.Aliphatic N-nitro No 7783-20-2 QSA24.α,β unsaturated alkoxy No 7783-20-2 QSA25.Aromatic nitroso group No 7783-20-2 QSA26.Aromatic ring N-oxide No 7783-20-2 QSA27.Nitro aromatic No 7783-20-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7783-20-2 QSA28bis.Aromatic mono- and dialkylamine No 7783-20-2 QSA28ter.Aromatic N-acyl amine No 7783-20-2 QSA29.Aromatic diazo No 7783-20-2 QSA30.Coumarins and Furocoumarins No 7783-20-2 QSA32.1,3-dialkoxy-benzene No 7783-20-2 QSA33.1-phenoxy-benzene No 7783-20-2 QSA34.H-acceptor-path3-H-acceptor Yes 7783-20-2 QSA35.Oxolane No 7783-20-2 QSA36.Carbodiimides No 7783-20-2 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
amphotericin B	1	QSA1.Acyl halides No 1397-89-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1397-89-3 QSA3.N-methylol derivatives No 1397-89-3 QSA4.Monohaloalkene No 1397-89-3 QSA5.S or N mustard No 1397-89-3 QSA6.Propiolactones and propiosultones No 1397-89-3 QSA7.Epoxides and aziridines No 1397-89-3 QSA8.Aliphatic halogens No 1397-89-3 QSA9.Alkyl nitrite No 1397-89-3 QSA10.α,β unsaturated carbonyls No 1397-89-3 QSA11.Simple

Table 18 Continued

		aldehyde No 1397-89-3 QSA12.Quinones No 1397-89-3 QSA13.Hydrazine No 1397-89-3 QSA14.Aliphatic azo and azoxy No 1397-89-3 QSA15.Isocyanate and isothiocyanate groups No 1397-89-3 QSA16.Alkyl carbamate and thiocarbamate No 1397-89-3 QSA18.Polycyclic Aromatic Hydrocarbons No 1397-89-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1397-89-3 QSA21.Alkyl and aryl N-nitroso groups No 1397-89-3 QSA22.Azide and triazene groups No 1397-89-3 QSA23.Aliphatic N-nitro No 1397-89-3 QSA24.α,β unsaturated alkoxy No 1397-89-3 QSA25.Aromatic nitroso group No 1397-89-3 QSA26.Aromatic ring N-oxide No 1397-89-3 QSA27.Nitro aromatic No 1397-89-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1397-89-3 QSA28bis.Aromatic mono- and dialkylamine No 1397-89-3 QSA28ter.Aromatic N-acyl amine No 1397-89-3 QSA29.Aromatic diazo No 1397-89-3 QSA30.Coumarins and Furocoumarins No 1397-89-3 QSA32.1,3-dialkoxy-benzene No 1397-89-3 QSA33.1-phenoxy-benzene No 1397-89-3 QSA34.H-acceptor-path3-H-acceptor Yes 1397-89-3 QSA35.Oxolane No 1397-89-3 QSA36.Carbodiimides No 1397-89-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
arsenic	0	
benzethonium chloride	1	QSA1.Acyl halides No 121-54-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 121-54-0 QSA3.N-methylol derivatives No 121-54-0 QSA4.Monohaloalkene No 121-54-0 QSA5.S or N mustard No 121-54-0 QSA6.Propiolactones and propiosultones No 121-54-0 QSA7.Epoxides and aziridines No 121-54-0 QSA8.Aliphatic halogens No 121-54-0 QSA9.Alkyl nitrite No 121-54-0 QSA10.α,β unsaturated carbonyls No 121-54-0 QSA11.Simple aldehyde No 121-54-0 QSA12.Quinones No 121-54-0 QSA13.Hydrazine No 121-54-0 QSA14.Aliphatic azo and azoxy No 121-54-0 QSA15.Isocyanate and isothiocyanate groups No 121-54-0 QSA16.Alkyl carbamate and thiocarbamate No 121-54-0 QSA18.Polycyclic Aromatic Hydrocarbons No 121-54-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 121-54-0 QSA21.Alkyl and aryl N-nitroso groups No 121-54-0 QSA22.Azide and triazene groups No 121-54-0 QSA23.Aliphatic N-nitro No 121-54-0 QSA24.α,β unsaturated alkoxy No 121-54-0 QSA25.Aromatic nitroso group No 121-54-0 QSA26.Aromatic ring N-oxide No 121-54-0 QSA27.Nitro aromatic No 121-54-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived

Table 18 Continued

		esters (with restrictions) No 121-54-0 QSA28bis.Aromatic mono- and dialkylamine No 121-54-0 QSA28ter.Aromatic N-acyl amine No 121-54-0 QSA29.Aromatic diazo No 121-54-0 QSA30.Coumarins and Furocoumarins No 121-54-0 QSA32.1,3-dialkoxy-benzene No 121-54-0 QSA33.1-phenoxy-benzene No 121-54-0 QSA34.H-acceptor-path3-H-acceptor Yes 121-54-0 QSA35.Oxolane No 121-54-0 QSA36.Carbodiimides No 121-54-0 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
benzoic acid	1	QSA1.Acyl halides No 65-85-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 65-85-0 QSA3.N-methylol derivatives No 65-85-0 QSA4.Monohaloalkene No 65-85-0 QSA5.S or N mustard No 65-85-0 QSA6.Propiolactones and propiosultones No 65-85-0 QSA7.Epoxides and aziridines No 65-85-0 QSA8.Aliphatic halogens No 65-85-0 QSA9.Alkyl nitrite No 65-85-0 QSA10.α,β unsaturated carbonyls No 65-85-0 QSA11.Simple aldehyde No 65-85-0 QSA12.Quinones No 65-85-0 QSA13.Hydrazine No 65-85-0 QSA14.Aliphatic azo and azoxy No 65-85-0 QSA15.Isocyanate and isothiocyanate groups No 65-85-0 QSA16.Alkyl carbamate and thiocarbamate No 65-85-0 QSA18.Polycyclic Aromatic Hydrocarbons No 65-85-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 65-85-0 QSA21.Alkyl and aryl N-nitroso groups No 65-85-0 QSA22.Azide and triazene groups No 65-85-0 QSA23.Aliphatic N-nitro No 65-85-0 QSA24.α,β unsaturated alkoxy No 65-85-0 QSA25.Aromatic nitroso group No 65-85-0 QSA26.Aromatic ring N-oxide No 65-85-0 QSA27.Nitro aromatic No 65-85-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 65-85-0 QSA28bis.Aromatic mono- and dialkylamine No 65-85-0 QSA28ter.Aromatic N-acyl amine No 65-85-0 QSA29.Aromatic diazo No 65-85-0 QSA30.Coumarins and Furocoumarins No 65-85-0 QSA32.1,3-dialkoxy-benzene No 65-85-0 QSA33.1-phenoxy-benzene No 65-85-0 QSA34.H-acceptor-path3-H-acceptor Yes 65-85-0 QSA35.Oxolane No 65-85-0 QSA36.Carbodiimides No 65-85-0 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
beta-propriolactone	1	QSA1.Acyl halides No 57-57-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-57-8 QSA3.N-methylol derivatives No 57-57-8 QSA4.Monohaloalkene No 57-57-8 QSA5.S or N mustard No 57-57-8 QSA6.Propiolactones and propiosultones Yes 57-57-8

Table 18 Continued

		QSA7.Epoxides and aziridines No 57-57-8 QSA8.Aliphatic halogens No 57-57-8 QSA9.Alkyl nitrite No 57-57-8 QSA10.α,β unsaturated carbonyls No 57-57-8 QSA11.Simple aldehyde No 57-57-8 QSA12.Quinones No 57-57-8 QSA13.Hydrazine No 57-57-8 QSA14.Aliphatic azo and azoxy No 57-57-8 QSA15.Isocyanate and isothiocyanate groups No 57-57-8 QSA16.Alkyl carbamate and thiocarbamate No 57-57-8 QSA18.Polycyclic Aromatic Hydrocarbons No 57-57-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 57-57-8 QSA21.Alkyl and aryl N-nitroso groups No 57-57-8 QSA22.Azide and triazene groups No 57-57-8 QSA23.Aliphatic N-nitro No 57-57-8 QSA24.α,β unsaturated alkoxy No 57-57-8 QSA25.Aromatic nitroso group No 57-57-8 QSA26.Aromatic ring N-oxide No 57-57-8 QSA27.Nitro aromatic No 57-57-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 57-57-8 QSA28bis.Aromatic mono- and dialkylamine No 57-57-8 QSA28ter.Aromatic N-acyl amine No 57-57-8 QSA29.Aromatic diazo No 57-57-8 QSA30.Coumarins and Furocoumarins No 57-57-8 QSA32.1,3-dialkoxy-benzene No 57-57-8 QSA33.1-phenoxy-benzene No 57-57-8 QSA34.H-acceptor-path3-H-acceptor Yes 57-57-8 QSA35.Oxolane No 57-57-8 QSA36.Carbodiimides No 57-57-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
biotin	1	QSA1.Acyl halides No 58-85-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 58-85-5 QSA3.N-methylol derivatives No 58-85-5 QSA4.Monohaloalkene No 58-85-5 QSA5.S or N mustard No 58-85-5 QSA6.Propiolactones and propiosultones No 58-85-5 QSA7.Epoxides and aziridines No 58-85-5 QSA8.Aliphatic halogens No 58-85-5 QSA9.Alkyl nitrite No 58-85-5 QSA10.α,β unsaturated carbonyls No 58-85-5 QSA11.Simple aldehyde No 58-85-5 QSA12.Quinones No 58-85-5 QSA13.Hydrazine No 58-85-5 QSA14.Aliphatic azo and azoxy No 58-85-5 QSA15.Isocyanate and isothiocyanate groups No 58-85-5 QSA16.Alkyl carbamate and thiocarbamate No 58-85-5 QSA18.Polycyclic Aromatic Hydrocarbons No 58-85-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 58-85-5 QSA21.Alkyl and aryl N-nitroso groups No 58-85-5 QSA22.Azide and triazene groups No 58-85-5 QSA23.Aliphatic N-nitro No 58-85-5 QSA24.α,β unsaturated alkoxy No 58-85-5 QSA25.Aromatic nitroso group No 58-85-5 QSA26.Aromatic ring N-oxide No 58-85-5 QSA27.Nitro aromatic No 58-85-5 QSA28.Primary

Table 18 Continued

		aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 58-85-5 QSA28bis.Aromatic mono- and dialkylamine No 58-85-5 QSA28ter.Aromatic N-acyl amine No 58-85-5 QSA29.Aromatic diazo No 58-85-5 QSA30.Coumarins and Furocoumarins No 58-85-5 QSA32.1,3-dialkoxy-benzene No 58-85-5 QSA33.1-phenoxy-benzene No 58-85-5 QSA34.H-acceptor-path3-H-acceptor Yes 58-85-5 QSA35.Oxolane No 58-85-5 QSA36.Carbodiimides No 58-85-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
boron	0	
bromine	0	
butylated hydroxytoluene (BHT)	0	
calcium carbonate	1	QSA1.Acyl halides No 471-34-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 471-34-1 QSA3.N-methylol derivatives No 471-34-1 QSA4.Monohaloalkene No 471-34-1 QSA5.S or N mustard No 471-34-1 QSA6.Propiolactones and propiosultones No 471-34-1 QSA7.Epoxides and aziridines No 471-34-1 QSA8.Aliphatic halogens No 471-34-1 QSA9.Alkyl nitrite No 471-34-1 QSA10.α,β unsaturated carbonyls No 471-34-1 QSA11.Simple aldehyde No 471-34-1 QSA12.Quinones No 471-34-1 QSA13.Hydrazine No 471-34-1 QSA14.Aliphatic azo and azoxy No 471-34-1 QSA15.Isocyanate and isothiocyanate groups No 471-34-1 QSA16.Alkyl carbamate and thiocarbamate No 471-34-1 QSA18.Polycyclic Aromatic Hydrocarbons No 471-34-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 471-34-1 QSA21.Alkyl and aryl N-nitroso groups No 471-34-1 QSA22.Azide and triazene groups No 471-34-1 QSA23.Aliphatic N-nitro No 471-34-1 QSA24.α,β unsaturated alkoxy No 471-34-1 QSA25.Aromatic nitroso group No 471-34-1 QSA26.Aromatic ring N-oxide No 471-34-1 QSA27.Nitro aromatic No 471-34-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 471-34-1 QSA28bis.Aromatic mono- and dialkylamine No 471-34-1 QSA28ter.Aromatic N-acyl amine No 471-34-1 QSA29.Aromatic diazo No 471-34-1 QSA30.Coumarins and Furocoumarins No 471-34-1 QSA32.1,3-dialkoxy-benzene No 471-34-1 QSA33.1-phenoxy-benzene No 471-34-1 QSA34.H-acceptor-path3-H-acceptor Yes 471-34-1 QSA35.Oxolane No 471-34-1 QSA36.Carbodiimides No 471-34-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the

Table 18 Continued

		micronucleus assay (Class I)
calcium chloride	0	
calcium chloride dihydrate	0	
calcium pantothenate (vitamin B5)	1	QSA1.Acyl halides No 137-08-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 137-08-6 QSA3.N-methylol derivatives No 137-08-6 QSA4.Monohaloalkene No 137-08-6 QSA5.S or N mustard No 137-08-6 QSA6.Propiolactones and propiosultones No 137-08-6 QSA7.Epoxides and aziridines No 137-08-6 QSA8.Aliphatic halogens No 137-08-6 QSA9.Alkyl nitrite No 137-08-6 QSA10.α,β unsaturated carbonyls No 137-08-6 QSA11.Simple aldehyde No 137-08-6 QSA12.Quinones No 137-08-6 QSA13.Hydrazine No 137-08-6 QSA14.Aliphatic azo and azoxy No 137-08-6 QSA15.Isocyanate and isothiocyanate groups No 137-08-6 QSA16.Alkyl carbamate and thiocarbamate No 137-08-6 QSA18.Polycyclic Aromatic Hydrocarbons No 137-08-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 137-08-6 QSA21.Alkyl and aryl N-nitroso groups No 137-08-6 QSA22.Azide and triazene groups No 137-08-6 QSA23.Aliphatic N-nitro No 137-08-6 QSA24.α,β unsaturated alkoxy No 137-08-6 QSA25.Aromatic nitroso group No 137-08-6 QSA26.Aromatic ring N-oxide No 137-08-6 QSA27.Nitro aromatic No 137-08-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 137-08-6 QSA28bis.Aromatic mono- and dialkylamine No 137-08-6 QSA28ter.Aromatic N-acyl amine No 137-08-6 QSA29.Aromatic diazo No 137-08-6 QSA30.Coumarins and Furocoumarins No 137-08-6 QSA32.1,3-dialkoxy-benzene No 137-08-6 QSA33.1-phenoxy-benzene No 137-08-6 QSA34.H-acceptor-path3-H-acceptor Yes 137-08-6 QSA35.Oxolane No 137-08-6 QSA36.Carbodiimides No 137-08-6 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I) 137-08-6
carbon	0	
cesium hydroxide	0	
cetrimonium bromide (CTAB)	0	
chlortetracycline	1	QSA1.Acyl halides No 57-62-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-62-5 QSA3.N-methylol derivatives No 57-62-5 QSA4.Monohaloalkene No

Table 18 Continued

		57-62-5 QSA5.S or N mustard No 57-62-5 QSA6.Propiolactones and propiosultones No 57-62-5 QSA7.Epoxides and aziridines No 57-62-5 QSA8.Aliphatic halogens No 57-62-5 QSA9.Alkyl nitrite No 57-62-5 QSA10.α,β unsaturated carbonyls Yes 57-62-5 QSA11.Simple aldehyde No 57-62-5 QSA12.Quinones No 57-62-5 QSA13.Hydrazine No 57-62-5 QSA14.Aliphatic azo and azoxy No 57-62-5 QSA15.Isocyanate and isothiocyanate groups No 57-62-5 QSA16.Alkyl carbamate and thiocarbamate No 57-62-5 QSA18.Polycyclic Aromatic Hydrocarbons No 57-62-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 57-62-5 QSA21.Alkyl and aryl N-nitroso groups No 57-62-5 QSA22.Azide and triazene groups No 57-62-5 QSA23.Aliphatic N-nitro No 57-62-5 QSA24.α,β unsaturated alkoxy No 57-62-5 QSA25.Aromatic nitroso group No 57-62-5 QSA26.Aromatic ring N-oxide No 57-62-5 QSA27.Nitro aromatic No 57-62-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 57-62-5 QSA28bis.Aromatic mono- and dialkylamine No 57-62-5 QSA28ter.Aromatic N-acyl amine No 57-62-5 QSA29.Aromatic diazo No 57-62-5 QSA30.Coumarins and Furocoumarins No 57-62-5 QSA32.1,3-dialkoxy-benzene No 57-62-5 QSA33.1-phenoxy-benzene No 57-62-5 QSA34.H-acceptor-path3-H-acceptor Yes 57-62-5 QSA35.Oxolane No 57-62-5 QSA36.Carbodiimides No 57-62-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
cholesterol	0	
choline chloride	1	QSA1.Acyl halides No 67-48-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 67-48-1 QSA3.N-methylol derivatives No 67-48-1 QSA4.Monohaloalkene No 67-48-1 QSA5.S or N mustard No 67-48-1 QSA6.Propiolactones and propiosultones No 67-48-1 QSA7.Epoxides and aziridines No 67-48-1 QSA8.Aliphatic halogens No 67-48-1 QSA9.Alkyl nitrite No 67-48-1 QSA10.α,β unsaturated carbonyls No 67-48-1 QSA11.Simple aldehyde No 67-48-1 QSA12.Quinones No 67-48-1 QSA13.Hydrazine No 67-48-1 QSA14.Aliphatic azo and azoxy No 67-48-1 QSA15.Isocyanate and isothiocyanate groups No 67-48-1 QSA16.Alkyl carbamate and thiocarbamate No 67-48-1 QSA18.Polycyclic Aromatic Hydrocarbons No 67-48-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 67-48-1 QSA21.Alkyl and aryl N-nitroso groups No 67-48-1 QSA22.Azide and triazene groups No 67-48-1 QSA23.Aliphatic N-nitro No 67-48-1

Table 18 Continued

		QSA24.α,β unsaturated alkoxy No 67-48-1 QSA25.Aromatic nitroso group No 67-48-1 QSA26.Aromatic ring N-oxide No 67-48-1 QSA27.Nitro aromatic No 67-48-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 67-48-1 QSA28bis.Aromatic mono- and dialkylamine No 67-48-1 QSA28ter.Aromatic N-acyl amine No 67-48-1 QSA29.Aromatic diazo No 67-48-1 QSA30.Coumarins and Furocoumarins No 67-48-1 QSA32.1,3-dialkoxy-benzene No 67-48-1 QSA33.1-phenoxy-benzene No 67-48-1 QSA34.H-acceptor-path3-H-acceptor Yes 67-48-1 QSA35.Oxolane No 67-48-1 QSA36.Carbodiimides No 67-48-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
citric acid	1	QSA1.Acyl halides No 77-92-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 77-92-9 QSA3.N-methylol derivatives No 77-92-9 QSA4.Monohaloalkene No 77-92-9 QSA5.S or N mustard No 77-92-9 QSA6.Propiolactones and propiosultones No 77-92-9 QSA7.Epoxides and aziridines No 77-92-9 QSA8.Aliphatic halogens No 77-92-9 QSA9.Alkyl nitrite No 77-92-9 QSA10.α,β unsaturated carbonyls No 77-92-9 QSA11.Simple aldehyde No 77-92-9 QSA12.Quinones No 77-92-9 QSA13.Hydrazine No 77-92-9 QSA14.Aliphatic azo and azoxy No 77-92-9 QSA15.Isocyanate and isothiocyanate groups No 77-92-9 QSA16.Alkyl carbamate and thiocarbamate No 77-92-9 QSA18.Polycyclic Aromatic Hydrocarbons No 77-92-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 77-92-9 QSA21.Alkyl and aryl N-nitroso groups No 77-92-9 QSA22.Azide and triazene groups No 77-92-9 QSA23.Aliphatic N-nitro No 77-92-9 QSA24.α,β unsaturated alkoxy No 77-92-9 QSA25.Aromatic nitroso group No 77-92-9 QSA26.Aromatic ring N-oxide No 77-92-9 QSA27.Nitro aromatic No 77-92-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 77-92-9 QSA28bis.Aromatic mono- and dialkylamine No 77-92-9 QSA28ter.Aromatic N-acyl amine No 77-92-9 QSA29.Aromatic diazo No 77-92-9 QSA30.Coumarins and Furocoumarins No 77-92-9 QSA32.1,3-dialkoxy-benzene No 77-92-9 QSA33.1-phenoxy-benzene No 77-92-9 QSA34.H-acceptor-path3-H-acceptor Yes 77-92-9 QSA35.Oxolane No 77-92-9 QSA36.Carbodiimides No 77-92-9 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
co-carboxylase	1	QSA1.Acyl halides No 154-87-0 QSA2.Alkyl (C5) or benzyl

Table 18 Continued

		ester of sulphonic or phosphonic acid No 154-87-0 QSA3.N-methylol derivatives No 154-87-0 QSA4.Monohaloalkene No 154-87-0 QSA5.S or N mustard No 154-87-0 QSA6.Propiolactones and propiosultones No 154-87-0 QSA7.Epoxides and aziridines No 154-87-0 QSA8.Aliphatic halogens No 154-87-0 QSA9.Alkyl nitrite No 154-87-0 QSA10.α,β unsaturated carbonyls No 154-87-0 QSA11.Simple aldehyde No 154-87-0 QSA12.Quinones No 154-87-0 QSA13.Hydrazine No 154-87-0 QSA14.Aliphatic azo and azoxy No 154-87-0 QSA15.Isocyanate and isothiocyanate groups No 154-87-0 QSA16.Alkyl carbamate and thiocarbamate No 154-87-0 QSA18.Polycyclic Aromatic Hydrocarbons No 154-87-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 154-87-0 QSA21.Alkyl and aryl N-nitroso groups No 154-87-0 QSA22.Azide and triazene groups No 154-87-0 QSA23.Aliphatic N-nitro No 154-87-0 QSA24.α,β unsaturated alkoxy No 154-87-0 QSA25.Aromatic nitroso group No 154-87-0 QSA26.Aromatic ring N-oxide No 154-87-0 QSA27.Nitro aromatic No 154-87-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 154-87-0 QSA28bis.Aromatic mono- and dialkylamine No 154-87-0 QSA28ter.Aromatic N-acyl amine No 154-87-0 QSA29.Aromatic diazo No 154-87-0 QSA30.Coumarins and Furocoumarins No 154-87-0 QSA32.1,3-dialkoxy-benzene No 154-87-0 QSA33.1-phenoxy-benzene No 154-87-0 QSA34.H-acceptor-path3-H-acceptor Yes 154-87-0 QSA35.Oxolane No 154-87-0 QSA36.Carbodiimides No 154-87-0 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
cyclohexane	0	
DDT (dichlorodiphenyltrichloroethane)	0	
deoxycholic acid	1	QSA1.Acyl halides No 83-44-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 83-44-3 QSA3.N-methylol derivatives No 83-44-3 QSA4.Monohaloalkene No 83-44-3 QSA5.S or N mustard No 83-44-3 QSA6.Propiolactones and propiosultones No 83-44-3 QSA7.Epoxides and aziridines No 83-44-3 QSA8.Aliphatic halogens No 83-44-3 QSA9.Alkyl nitrite No 83-44-3 QSA10.α,β unsaturated carbonyls No 83-44-3 QSA11.Simple aldehyde No 83-44-3 QSA12.Quinones No 83-44-3 QSA13.Hydrazine No 83-44-3 QSA14.Aliphatic azo and azoxy No 83-44-3 QSA15.Isocyanate and isothiocyanate

Table 18 Continued

		groups No 83-44-3 QSA16.Alkyl carbamate and thiocarbamate No 83-44-3 QSA18.Polycyclic Aromatic Hydrocarbons No 83-44-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 83-44-3 QSA21.Alkyl and aryl N-nitroso groups No 83-44-3 QSA22.Azide and triazene groups No 83-44-3 QSA23.Aliphatic N-nitro No 83-44-3 QSA24.α,β unsaturated alkoxy No 83-44-3 QSA25.Aromatic nitroso group No 83-44-3 QSA26.Aromatic ring N-oxide No 83-44-3 QSA27.Nitro aromatic No 83-44-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 83-44-3 QSA28bis.Aromatic mono- and dialkylamine No 83-44-3 QSA28ter.Aromatic N-acyl amine No 83-44-3 QSA29.Aromatic diazo No 83-44-3 QSA30.Coumarins and Furocoumarins No 83-44-3 QSA32.1,3-dialkoxy-benzene No 83-44-3 QSA33.1-phenoxy-benzene No 83-44-3 QSA34.H-acceptor-path3-H-acceptor Yes 83-44-3 QSA35.Oxolane No 83-44-3 QSA36.Carbodiimides No 83-44-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
dextran	1	QSA1.Acyl halides No 9004-54-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9004-54-0 QSA3.N-methylol derivatives No 9004-54-0 QSA4.Monohaloalkene No 9004-54-0 QSA5.S or N mustard No 9004-54-0 QSA6.Propiolactones and propiosultones No 9004-54-0 QSA7.Epoxides and aziridines No 9004-54-0 QSA8.Aliphatic halogens No 9004-54-0 QSA9.Alkyl nitrite No 9004-54-0 QSA10.α,β unsaturated carbonyls No 9004-54-0 QSA11.Simple aldehyde Yes 9004-54-0 QSA12.Quinones No 9004-54-0 QSA13.Hydrazine No 9004-54-0 QSA14.Aliphatic azo and azoxy No 9004-54-0 QSA15.Isocyanate and isothiocyanate groups No 9004-54-0 QSA16.Alkyl carbamate and thiocarbamate No 9004-54-0 QSA18.Polycyclic Aromatic Hydrocarbons No 9004-54-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9004-54-0 QSA21.Alkyl and aryl N-nitroso groups No 9004-54-0 QSA22.Azide and triazene groups No 9004-54-0 QSA23.Aliphatic N-nitro No 9004-54-0 QSA24.α,β unsaturated alkoxy No 9004-54-0 QSA25.Aromatic nitroso group No 9004-54-0 QSA26.Aromatic ring N-oxide No 9004-54-0 QSA27.Nitro aromatic No 9004-54-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9004-54-0 QSA28bis.Aromatic mono- and dialkylamine No 9004-54-0 QSA28ter.Aromatic N-acyl amine No 9004-54-0 QSA29.Aromatic diazo No 9004-54-0 QSA30.Coumarins and

Table 18 Continued

		Furocoumarins No 9004-54-0 QSA32.1,3-dialkoxy-benzene No 9004-54-0 QSA33.1-phenoxy-benzene No 9004-54-0 QSA34.H-acceptor-path3-H-acceptor Yes 9004-54-0 QSA35.Oxolane No 9004-54-0 QSA36.Carbodiimides No 9004-54-0 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
D-galactose	1	QSA1.Acyl halides No 59-23-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-23-4 QSA3.N-methylol derivatives No 59-23-4 QSA4.Monohaloalkene No 59-23-4 QSA5.S or N mustard No 59-23-4 QSA6.Propiolactones and propiosultones No 59-23-4 QSA7.Epoxides and aziridines No 59-23-4 QSA8.Aliphatic halogens No 59-23-4 QSA9.Alkyl nitrite No 59-23-4 QSA10.α,β unsaturated carbonyls No 59-23-4 QSA11.Simple aldehyde No 59-23-4 QSA12.Quinones No 59-23-4 QSA13.Hydrazine No 59-23-4 QSA14.Aliphatic azo and azoxy No 59-23-4 QSA15.Isocyanate and isothiocyanate groups No 59-23-4 QSA16.Alkyl carbamate and thiocarbamate No 59-23-4 QSA18.Polycyclic Aromatic Hydrocarbons No 59-23-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 59-23-4 QSA21.Alkyl and aryl N-nitroso groups No 59-23-4 QSA22.Azide and triazene groups No 59-23-4 QSA23.Aliphatic N-nitro No 59-23-4 QSA24.α,β unsaturated alkoxy No 59-23-4 QSA25.Aromatic nitroso group No 59-23-4 QSA26.Aromatic ring N-oxide No 59-23-4 QSA27.Nitro aromatic No 59-23-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 59-23-4 QSA28bis.Aromatic mono- and dialkylamine No 59-23-4 QSA28ter.Aromatic N-acyl amine No 59-23-4 QSA29.Aromatic diazo No 59-23-4 QSA30.Coumarins and Furocoumarins No 59-23-4 QSA32.1,3-dialkoxy-benzene No 59-23-4 QSA33.1-phenoxy-benzene No 59-23-4 QSA34.H-acceptor-path3-H-acceptor Yes 59-23-4 QSA35.Oxolane No 59-23-4 QSA36.Carbodiimides No 59-23-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
diadenine sulfate	1	QSA1.Acyl halides No 321-30-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 321-30-2 QSA3.N-methylol derivatives No 321-30-2 QSA4.Monohaloalkene No 321-30-2 QSA5.S or N mustard No 321-30-2 QSA6.Propiolactones and propiosultones No 321-30-2 QSA7.Epoxides and aziridines No 321-30-2 QSA8.Aliphatic halogens No 321-30-2 QSA9.Alkyl nitrite No 321-30-2 QSA10.α,β unsaturated carbonyls No 321-30-2

Table 18 Continued

		QSA11.Simple aldehyde No 321-30-2 QSA12.Quinones No 321-30-2 QSA13.Hydrazine No 321-30-2 QSA14.Aliphatic azo and azoxy No 321-30-2 QSA15.Isocyanate and isothiocyanate groups No 321-30-2 QSA16.Alkyl carbamate and thiocarbamate No 321-30-2 QSA18.Polycyclic Aromatic Hydrocarbons No 321-30-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 321-30-2 QSA21.Alkyl and aryl N-nitroso groups No 321-30-2 QSA22.Azide and triazene groups No 321-30-2 QSA23.Aliphatic N-nitro No 321-30-2 QSA24.α,β unsaturated alkoxy No 321-30-2 QSA25.Aromatic nitroso group No 321-30-2 QSA26.Aromatic ring N-oxide No 321-30-2 QSA27.Nitro aromatic No 321-30-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 321-30-2 QSA28bis.Aromatic mono- and dialkylamine No 321-30-2 QSA28ter.Aromatic N-acyl amine No 321-30-2 QSA29.Aromatic diazo No 321-30-2 QSA30.Coumarins and Furocoumarins No 321-30-2 QSA32.1,3-dialkoxy-benzene No 321-30-2 QSA33.1-phenoxy-benzene No 321-30-2 QSA34.H-acceptor-path3-H-acceptor Yes 321-30-2 QSA35.Oxolane No 321-30-2 QSA36.Carbodiimides No 321-30-2 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
disodium phosphate	1	QSA1.Acyl halides No 7558-79-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7558-79-4 QSA3.N-methylol derivatives No 7558-79-4 QSA4.Monohaloalkene No 7558-79-4 QSA5.S or N mustard No 7558-79-4 QSA6.Propiolactones and propiosultones No 7558-79-4 QSA7.Epoxides and aziridines No 7558-79-4 QSA8.Aliphatic halogens No 7558-79-4 QSA9.Alkyl nitrite No 7558-79-4 QSA10.α,β unsaturated carbonyls No 7558-79-4 QSA11.Simple aldehyde No 7558-79-4 QSA12.Quinones No 7558-79-4 QSA13.Hydrazine No 7558-79-4 QSA14.Aliphatic azo and azoxy No 7558-79-4 QSA15.Isocyanate and isothiocyanate groups No 7558-79-4 QSA16.Alkyl carbamate and thiocarbamate No 7558-79-4 QSA18.Polycyclic Aromatic Hydrocarbons No 7558-79-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7558-79-4 QSA21.Alkyl and aryl N-nitroso groups No 7558-79-4 QSA22.Azide and triazene groups No 7558-79-4 QSA23.Aliphatic N-nitro No 7558-79-4 QSA24.α,β unsaturated alkoxy No 7558-79-4 QSA25.Aromatic nitroso group No 7558-79-4 QSA26.Aromatic ring N-oxide No 7558-79-4 QSA27.Nitro aromatic No 7558-79-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No

Table 18 Continued

		7558-79-4 QSA28bis.Aromatic mono- and dialkylamine No 7558-79-4 QSA28ter.Aromatic N-acyl amine No 7558-79-4 QSA29.Aromatic diazo No 7558-79-4 QSA30.Coumarins and Furocoumarins No 7558-79-4 QSA32.1,3-dialkoxy-benzene No 7558-79-4 QSA33.1-phenoxy-benzene No 7558-79-4 QSA34.H-acceptor-path3-H-acceptor Yes 7558-79-4 QSA35.Oxolane No 7558-79-4 QSA36.Carbodiimides No 7558-79-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
disodium phosphate dodecahydrate	1	QSA1.Acyl halides No 10039-32-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 10039-32-4 QSA3.N-methylol derivatives No 10039-32-4 QSA4.Monohaloalkene No 10039-32-4 QSA5.S or N mustard No 10039-32-4 QSA6.Propiolactones and propiosultones No 10039-32-4 QSA7.Epoxides and aziridines No 10039-32-4 QSA8.Aliphatic halogens No 10039-32-4 QSA9.Alkyl nitrite No 10039-32-4 QSA10.α,β unsaturated carbonyls No 10039-32-4 QSA11.Simple aldehyde No 10039-32-4 QSA12.Quinones No 10039-32-4 QSA13.Hydrazine No 10039-32-4 QSA14.Aliphatic azo and azoxy No 10039-32-4 QSA15.Isocyanate and isothiocyanate groups No 10039-32-4 QSA16.Alkyl carbamate and thiocarbamate No 10039-32-4 QSA18.Polycyclic Aromatic Hydrocarbons No 10039-32-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 10039-32-4 QSA21.Alkyl and aryl N-nitroso groups No 10039-32-4 QSA22.Azide and triazene groups No 10039-32-4 QSA23.Aliphatic N-nitro No 10039-32-4 QSA24.α,β unsaturated alkoxy No 10039-32-4 QSA25.Aromatic nitroso group No 10039-32-4 QSA26.Aromatic ring N-oxide No 10039-32-4 QSA27.Nitro aromatic No 10039-32-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 10039-32-4 QSA28bis.Aromatic mono- and dialkylamine No 10039-32-4 QSA28ter.Aromatic N-acyl amine No 10039-32-4 QSA29.Aromatic diazo No 10039-32-4 QSA30.Coumarins and Furocoumarins No 10039-32-4 QSA32.1,3-dialkoxy-benzene No 10039-32-4 QSA33.1-phenoxy-benzene No 10039-32-4 QSA34.H-acceptor-path3-H-acceptor Yes 10039-32-4 QSA35.Oxolane No 10039-32-4 QSA36.Carbodiimides No 10039-32-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
DL-aspartic acid	1	QSA1.Acyl halides No 617-45-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 617-45-8 QSA3.N-methylol derivatives No 617-45-8 QSA4.Monohaloalkene No

Table 18 Continued

		617-45-8 QSA5.S or N mustard No 617-45-8 QSA6.Propiolactones and propiosultones No 617-45-8 QSA7.Epoxides and aziridines No 617-45-8 QSA8.Aliphatic halogens No 617-45-8 QSA9.Alkyl nitrite No 617-45-8 QSA10.α,β unsaturated carbonyls No 617-45-8 QSA11.Simple aldehyde No 617-45-8 QSA12.Quinones No 617-45-8 QSA13.Hydrazine No 617-45-8 QSA14.Aliphatic azo and azoxy No 617-45-8 QSA15.Isocyanate and isothiocyanate groups No 617-45-8 QSA16.Alkyl carbamate and thiocarbamate No 617-45-8 QSA18.Polycyclic Aromatic Hydrocarbons No 617-45-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 617-45-8 QSA21.Alkyl and aryl N-nitroso groups No 617-45-8 QSA22.Azide and triazene groups No 617-45-8 QSA23.Aliphatic N-nitro No 617-45-8 QSA24.α,β unsaturated alkoxy No 617-45-8 QSA25.Aromatic nitroso group No 617-45-8 QSA26.Aromatic ring N-oxide No 617-45-8 QSA27.Nitro aromatic No 617-45-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 617-45-8 QSA28bis.Aromatic mono- and dialkylamine No 617-45-8 QSA28ter.Aromatic N-acyl amine No 617-45-8 QSA29.Aromatic diazo No 617-45-8 QSA30.Coumarins and Furocoumarins No 617-45-8 QSA32.1,3-dialkoxy-benzene No 617-45-8 QSA33.1-phenoxy-benzene No 617-45-8 QSA34.H-acceptor-path3-H-acceptor Yes 617-45-8 QSA35.Oxolane No 617-45-8 QSA36.Carbodiimides No 617-45-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
DL-glutamic acid	1	QSA1.Acyl halides No 617-65-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 617-65-2 QSA3.N-methylol derivatives No 617-65-2 QSA4.Monohaloalkene No 617-65-2 QSA5.S or N mustard No 617-65-2 QSA6.Propiolactones and propiosultones No 617-65-2 QSA7.Epoxides and aziridines No 617-65-2 QSA8.Aliphatic halogens No 617-65-2 QSA9.Alkyl nitrite No 617-65-2 QSA10.α,β unsaturated carbonyls No 617-65-2 QSA11.Simple aldehyde No 617-65-2 QSA12.Quinones No 617-65-2 QSA13.Hydrazine No 617-65-2 QSA14.Aliphatic azo and azoxy No 617-65-2 QSA15.Isocyanate and isothiocyanate groups No 617-65-2 QSA16.Alkyl carbamate and thiocarbamate No 617-65-2 QSA18.Polycyclic Aromatic Hydrocarbons No 617-65-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 617-65-2 QSA21.Alkyl and aryl N-nitroso groups No 617-65-2 QSA22.Azide and triazene groups No 617-65-2 QSA23.Aliphatic N-nitro No 617-65-2 QSA24.α,β unsaturated alkoxy No 617-65-2 QSA25.Aromatic

Table 18 Continued

		nitroso group No 617-65-2 QSA26.Aromatic ring N-oxide No 617-65-2 QSA27.Nitro aromatic No 617-65-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 617-65-2 QSA28bis.Aromatic mono- and dialkylamine No 617-65-2 QSA28ter.Aromatic N-acyl amine No 617-65-2 QSA29.Aromatic diazo No 617-65-2 QSA30.Coumarins and Furocoumarins No 617-65-2 QSA32.1,3-dialkoxy-benzene No 617-65-2 QSA33.1-phenoxy-benzene No 617-65-2 QSA34.H-acceptor-path3-H-acceptor Yes 617-65-2 QSA35.Oxolane No 617-65-2 QSA36.Carbodiimides No 617-65-2 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
D-ribose	1	QSA1.Acyl halides No 50-69-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-69-1 QSA3.N-methylol derivatives No 50-69-1 QSA4.Monohaloalkene No 50-69-1 QSA5.S or N mustard No 50-69-1 QSA6.Propiolactones and propiosultones No 50-69-1 QSA7.Epoxides and aziridines No 50-69-1 QSA8.Aliphatic halogens No 50-69-1 QSA9.Alkyl nitrite No 50-69-1 QSA10.α,β unsaturated carbonyls No 50-69-1 QSA11.Simple aldehyde No 50-69-1 QSA12.Quinones No 50-69-1 QSA13.Hydrazine No 50-69-1 QSA14.Aliphatic azo and azoxy No 50-69-1 QSA15.Isocyanate and isothiocyanate groups No 50-69-1 QSA16.Alkyl carbamate and thiocarbamate No 50-69-1 QSA18.Polycyclic Aromatic Hydrocarbons No 50-69-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-69-1 QSA21.Alkyl and aryl N-nitroso groups No 50-69-1 QSA22.Azide and triazene groups No 50-69-1 QSA23.Aliphatic N-nitro No 50-69-1 QSA24.α,β unsaturated alkoxy No 50-69-1 QSA25.Aromatic nitroso group No 50-69-1 QSA26.Aromatic ring N-oxide No 50-69-1 QSA27.Nitro aromatic No 50-69-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-69-1 QSA28bis.Aromatic mono- and dialkylamine No 50-69-1 QSA28ter.Aromatic N-acyl amine No 50-69-1 QSA29.Aromatic diazo No 50-69-1 QSA30.Coumarins and Furocoumarins No 50-69-1 QSA32.1,3-dialkoxy-benzene No 50-69-1 QSA33.1-phenoxy-benzene No 50-69-1 QSA34.H-acceptor-path3-H-acceptor Yes 50-69-1 QSA35.Oxolane Yes 50-69-1 QSA36.Carbodiimides No 50-69-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
d-sorbitol	1	QSA1.Acyl halides No 50-70-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-70-4 QSA3.N-

Table 18 Continued

		methylol derivatives No 50-70-4 QSA4.Monohaloalkene No 50-70-4 QSA5.S or N mustard No 50-70-4 QSA6.Propiolactones and propiosultones No 50-70-4 QSA7.Epoxides and aziridines No 50-70-4 QSA8.Aliphatic halogens No 50-70-4 QSA9.Alkyl nitrite No 50-70-4 QSA10.α,β unsaturated carbonyls No 50-70-4 QSA11.Simple aldehyde No 50-70-4 QSA12.Quinones No 50-70-4 QSA13.Hydrazine No 50-70-4 QSA14.Aliphatic azo and azoxy No 50-70-4 QSA15.Isocyanate and isothiocyanate groups No 50-70-4 QSA16.Alkyl carbamate and thiocarbamate No 50-70-4 QSA18.Polycyclic Aromatic Hydrocarbons No 50-70-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-70-4 QSA21.Alkyl and aryl N-nitroso groups No 50-70-4 QSA22.Azide and triazene groups No 50-70-4 QSA23.Aliphatic N-nitro No 50-70-4 QSA24.α,β unsaturated alkoxy No 50-70-4 QSA25.Aromatic nitroso group No 50-70-4 QSA26.Aromatic ring N-oxide No 50-70-4 QSA27.Nitro aromatic No 50-70-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-70-4 QSA28bis.Aromatic mono- and dialkylamine No 50-70-4 QSA28ter.Aromatic N-acyl amine No 50-70-4 QSA29.Aromatic diazo No 50-70-4 QSA30.Coumarins and Furocoumarins No 50-70-4 QSA32.1,3-dialkoxy-benzene No 50-70-4 QSA33.1-phenoxy-benzene No 50-70-4 QSA34.H-acceptor-path3-H-acceptor Yes 50-70-4 QSA35.Oxolane No 50-70-4 QSA36.Carbodiimides No 50-70-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
edetate disodium (EDTA)	1	QSA1.Acyl halides No 6381-92-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 6381-92-6 QSA3.N-methylol derivatives No 6381-92-6 QSA4.Monohaloalkene No 6381-92-6 QSA5.S or N mustard No 6381-92-6 QSA6.Propiolactones and propiosultones No 6381-92-6 QSA7.Epoxides and aziridines No 6381-92-6 QSA8.Aliphatic halogens No 6381-92-6 QSA9.Alkyl nitrite No 6381-92-6 QSA10.α,β unsaturated carbonyls No 6381-92-6 QSA11.Simple aldehyde No 6381-92-6 QSA12.Quinones No 6381-92-6 QSA13.Hydrazine No 6381-92-6 QSA14.Aliphatic azo and azoxy No 6381-92-6 QSA15.Isocyanate and isothiocyanate groups No 6381-92-6 QSA16.Alkyl carbamate and thiocarbamate No 6381-92-6 QSA18.Polycyclic Aromatic Hydrocarbons No 6381-92-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 6381-92-6 QSA21.Alkyl and aryl N-nitroso groups No 6381-92-6 QSA22.Azide and triazene

Table 18 Continued

		groups No 6381-92-6 QSA23.Aliphatic N-nitro No 6381-92-6 QSA24.α,β unsaturated alkoxy No 6381-92-6 QSA25.Aromatic nitroso group No 6381-92-6 QSA26.Aromatic ring N-oxide No 6381-92-6 QSA27.Nitro aromatic No 6381-92-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 6381-92-6 QSA28bis.Aromatic mono- and dialkylamine No 6381-92-6 QSA28ter.Aromatic N-acyl amine No 6381-92-6 QSA29.Aromatic diazo No 6381-92-6 QSA30.Coumarins and Furocoumarins No 6381-92-6 QSA32.1,3-dialkoxy-benzene No 6381-92-6 QSA33.1-phenoxy-benzene No 6381-92-6 QSA34.H-acceptor-path3-H-acceptor Yes 6381-92-6 QSA35.Oxolane No 6381-92-6 QSA36.Carbodiimides No 6381-92-6 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
ergocalciferol (vitamin D2)	0	
ethanolamine	1	QSA1.Acyl halides No 141-43-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 141-43-5 QSA3.N-methylol derivatives No 141-43-5 QSA4.Monohaloalkene No 141-43-5 QSA5.S or N mustard No 141-43-5 QSA6.Propiolactones and propiosultones No 141-43-5 QSA7.Epoxides and aziridines No 141-43-5 QSA8.Aliphatic halogens No 141-43-5 QSA9.Alkyl nitrite No 141-43-5 QSA10.α,β unsaturated carbonyls No 141-43-5 QSA11.Simple aldehyde No 141-43-5 QSA12.Quinones No 141-43-5 QSA13.Hydrazine No 141-43-5 QSA14.Aliphatic azo and azoxy No 141-43-5 QSA15.Isocyanate and isothiocyanate groups No 141-43-5 QSA16.Alkyl carbamate and thiocarbamate No 141-43-5 QSA18.Polycyclic Aromatic Hydrocarbons No 141-43-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 141-43-5 QSA21.Alkyl and aryl N-nitroso groups No 141-43-5 QSA22.Azide and triazene groups No 141-43-5 QSA23.Aliphatic N-nitro No 141-43-5 QSA24.α,β unsaturated alkoxy No 141-43-5 QSA25.Aromatic nitroso group No 141-43-5 QSA26.Aromatic ring N-oxide No 141-43-5 QSA27.Nitro aromatic No 141-43-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 141-43-5 QSA28bis.Aromatic mono- and dialkylamine No 141-43-5 QSA28ter.Aromatic N-acyl amine No 141-43-5 QSA29.Aromatic diazo No 141-43-5 QSA30.Coumarins and Furocoumarins No 141-43-5 QSA32.1,3-dialkoxy-benzene No 141-43-5 QSA33.1-phenoxy-benzene No 141-43-5 QSA34.H-acceptor-path3-H-acceptor Yes 141-43-5 QSA35.Oxolane No 141-43-5

Table 18 Continued

		QSA36.Carbodiimides No 141-43-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
ethyl acrylate	1	QSA1.Acyl halides No 9003-32-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9003-32-1 QSA3.N-methylol derivatives No 9003-32-1 QSA4.Monohaloalkene No 9003-32-1 QSA5.S or N mustard No 9003-32-1 QSA6.Propiolactones and propiosultones No 9003-32-1 QSA7.Epoxides and aziridines No 9003-32-1 QSA8.Aliphatic halogens No 9003-32-1 QSA9.Alkyl nitrite No 9003-32-1 QSA10.α,β unsaturated carbonyls No 9003-32-1 QSA11.Simple aldehyde No 9003-32-1 QSA12.Quinones No 9003-32-1 QSA13.Hydrazine No 9003-32-1 QSA14.Aliphatic azo and azoxy No 9003-32-1 QSA15.Isocyanate and isothiocyanate groups No 9003-32-1 QSA16.Alkyl carbamate and thiocarbamate No 9003-32-1 QSA18.Polycyclic Aromatic Hydrocarbons No 9003-32-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9003-32-1 QSA21.Alkyl and aryl N-nitroso groups No 9003-32-1 QSA22.Azide and triazene groups No 9003-32-1 QSA23.Aliphatic N-nitro No 9003-32-1 QSA24.α,β unsaturated alkoxy No 9003-32-1 QSA25.Aromatic nitroso group No 9003-32-1 QSA26.Aromatic ring N-oxide No 9003-32-1 QSA27.Nitro aromatic No 9003-32-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9003-32-1 QSA28bis.Aromatic mono- and dialkylamine No 9003-32-1 QSA28ter.Aromatic N-acyl amine No 9003-32-1 QSA29.Aromatic diazo No 9003-32-1 QSA30.Coumarins and Furocoumarins No 9003-32-1 QSA32.1,3-dialkoxy-benzene No 9003-32-1 QSA33.1-phenoxy-benzene No 9003-32-1 QSA34.H-acceptor-path3-H-acceptor Yes 9003-32-1 QSA35.Oxolane No 9003-32-1 QSA36.Carbodiimides No 9003-32-1 QAny alert?.At least one alert fired? Yes
ethylene oxide	1	QSA1.Acyl halides No 75-21-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 75-21-8 QSA3.N-methylol derivatives No 75-21-8 QSA4.Monohaloalkene No 75-21-8 QSA5.S or N mustard No 75-21-8 QSA6.Propiolactones and propiosultones No 75-21-8 QSA7.Epoxides and aziridines Yes 75-21-8 QSA8.Aliphatic halogens No 75-21-8 QSA9.Alkyl nitrite No 75-21-8 QSA10.α,β unsaturated carbonyls No 75-21-8 QSA11.Simple aldehyde No 75-21-8 QSA12.Quinones No 75-21-8 QSA13.Hydrazine No 75-21-8 QSA14.Aliphatic azo and azoxy No 75-21-8 QSA15.Isocyanate and isothiocyanate groups No 75-21-8 QSA16.Alkyl carbamate and

Table 18 Continued

		thiocarbamate No 75-21-8 QSA18.Polycyclic Aromatic Hydrocarbons No 75-21-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 75-21-8 QSA21.Alkyl and aryl N-nitroso groups No 75-21-8 QSA22.Azide and triazene groups No 75-21-8 QSA23.Aliphatic N-nitro No 75-21-8 QSA24.α,β unsaturated alkoxy No 75-21-8 QSA25.Aromatic nitroso group No 75-21-8 QSA26.Aromatic ring N-oxide No 75-21-8 QSA27.Nitro aromatic No 75-21-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 75-21-8 QSA28bis.Aromatic mono- and dialkylamine No 75-21-8 QSA28ter.Aromatic N-acyl amine No 75-21-8 QSA29.Aromatic diazo No 75-21-8 QSA30.Coumarins and Furocoumarins No 75-21-8 QSA32.1,3-dialkoxy-benzene No 75-21-8 QSA33.1-phenoxy-benzene No 75-21-8 QSA34.H-acceptor-path3-H-acceptor No 75-21-8 QSA35.Oxolane No 75-21-8 QSA36.Carbodiimides No 75-21-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
ethylene; (5E)-5-ethylidenebicyclo[2.2.1]hept-2-ene; prop-1-ene	0	
ferric (III) nitrate	1	QSA1.Acyl halides No 10421-48-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 10421-48-4 QSA3.N-methylol derivatives No 10421-48-4 QSA4.Monohaloalkene No 10421-48-4 QSA5.S or N mustard No 10421-48-4 QSA6.Propiolactones and propiosultones No 10421-48-4 QSA7.Epoxides and aziridines No 10421-48-4 QSA8.Aliphatic halogens No 10421-48-4 QSA9.Alkyl nitrite No 10421-48-4 QSA10.α,β unsaturated carbonyls No 10421-48-4 QSA11.Simple aldehyde No 10421-48-4 QSA12.Quinones No 10421-48-4 QSA13.Hydrazine No 10421-48-4 QSA14.Aliphatic azo and azoxy No 10421-48-4 QSA15.Isocyanate and isothiocyanate groups No 10421-48-4 QSA16.Alkyl carbamate and thiocarbamate No 10421-48-4 QSA18.Polycyclic Aromatic Hydrocarbons No 10421-48-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 10421-48-4 QSA21.Alkyl and aryl N-nitroso groups No 10421-48-4 QSA22.Azide and triazene groups No 10421-48-4 QSA23.Aliphatic N-nitro No 10421-48-4 QSA24.α,β unsaturated alkoxy No 10421-48-4 QSA25.Aromatic nitroso group No 10421-48-4 QSA26.Aromatic ring N-oxide No 10421-48-4 QSA27.Nitro

Table 18 Continued

		aromatic No 10421-48-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 10421-48-4 QSA28bis.Aromatic mono- and dialkylamine No 10421-48-4 QSA28ter.Aromatic N-acyl amine No 10421-48-4 QSA29.Aromatic diazo No 10421-48-4 QSA30.Coumarins and Furocoumarins No 10421-48-4 QSA32.1,3-dialkoxy-benzene No 10421-48-4 QSA33.1-phenoxy-benzene No 10421-48-4 QSA34.H-acceptor-path3-H-acceptor Yes 10421-48-4 QSA35.Oxolane No 10421-48-4 QSA36.Carbodiimides No 10421-48-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
ferrous succinate (butanedioic acid)	1	QSA1.Acyl halides No 10030-90-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 10030-90-7 QSA3.N-methylol derivatives No 10030-90-7 QSA4.Monohaloalkene No 10030-90-7 QSA5.S or N mustard No 10030-90-7 QSA6.Propiolactones and propiosultones No 10030-90-7 QSA7.Epoxides and aziridines No 10030-90-7 QSA8.Aliphatic halogens No 10030-90-7 QSA9.Alkyl nitrite No 10030-90-7 QSA10.α,β unsaturated carbonyls No 10030-90-7 QSA11.Simple aldehyde No 10030-90-7 QSA12.Quinones No 10030-90-7 QSA13.Hydrazine No 10030-90-7 QSA14.Aliphatic azo and azoxy No 10030-90-7 QSA15.Isocyanate and isothiocyanate groups No 10030-90-7 QSA16.Alkyl carbamate and thiocarbamate No 10030-90-7 QSA18.Polycyclic Aromatic Hydrocarbons No 10030-90-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 10030-90-7 QSA21.Alkyl and aryl N-nitroso groups No 10030-90-7 QSA22.Azide and triazene groups No 10030-90-7 QSA23.Aliphatic N-nitro No 10030-90-7 QSA24.α,β unsaturated alkoxy No 10030-90-7 QSA25.Aromatic nitroso group No 10030-90-7 QSA26.Aromatic ring N-oxide No 10030-90-7 QSA27.Nitro aromatic No 10030-90-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 10030-90-7 QSA28bis.Aromatic mono- and dialkylamine No 10030-90-7 QSA28ter.Aromatic N-acyl amine No 10030-90-7 QSA29.Aromatic diazo No 10030-90-7 QSA30.Coumarins and Furocoumarins No 10030-90-7 QSA32.1,3-dialkoxy-benzene No 10030-90-7 QSA33.1-phenoxy-benzene No 10030-90-7 QSA34.H-acceptor-path3-H-acceptor Yes 10030-90-7 QSA35.Oxolane No 10030-90-7 QSA36.Carbodiimides No 10030-90-7 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)

Table 18 Continued

flavin adenine dinucleotide (FAD)	1	QSA1.Acyl halides No 146-14-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 146-14-5 QSA3.N-methylol derivatives No 146-14-5 QSA4.Monohaloalkene No 146-14-5 QSA5.S or N mustard No 146-14-5 QSA6.Propiolactones and propiosultones No 146-14-5 QSA7.Epoxides and aziridines No 146-14-5 QSA8.Aliphatic halogens No 146-14-5 QSA9.Alkyl nitrite No 146-14-5 QSA10.α,β unsaturated carbonyls No 146-14-5 QSA11.Simple aldehyde No 146-14-5 QSA12.Quinones No 146-14-5 QSA13.Hydrazine No 146-14-5 QSA14.Aliphatic azo and azoxy No 146-14-5 QSA15.Isocyanate and isothiocyanate groups No 146-14-5 QSA16.Alkyl carbamate and thiocarbamate No 146-14-5 QSA18.Polycyclic Aromatic Hydrocarbons No 146-14-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 146-14-5 QSA21.Alkyl and aryl N-nitroso groups No 146-14-5 QSA22.Azide and triazene groups No 146-14-5 QSA23.Aliphatic N-nitro No 146-14-5 QSA24.α,β unsaturated alkoxy No 146-14-5 QSA25.Aromatic nitroso group No 146-14-5 QSA26.Aromatic ring N-oxide No 146-14-5 QSA27.Nitro aromatic No 146-14-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 146-14-5 QSA28bis.Aromatic mono- and dialkylamine No 146-14-5 QSA28ter.Aromatic N-acyl amine No 146-14-5 QSA29.Aromatic diazo No 146-14-5 QSA30.Coumarins and Furocoumarins No 146-14-5 QSA32.1,3-dialkoxy-benzene No 146-14-5 QSA33.1-phenoxy-benzene No 146-14-5 QSA34.H-acceptor-path3-H-acceptor Yes 146-14-5 QSA35.Oxolane Yes 146-14-5 QSA36.Carbodiimides No 146-14-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
folic acid	1	QSA1.Acyl halides No 59-30-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-30-3 QSA3.N-methylol derivatives No 59-30-3 QSA4.Monohaloalkene No 59-30-3 QSA5.S or N mustard No 59-30-3 QSA6.Propiolactones and propiosultones No 59-30-3 QSA7.Epoxides and aziridines No 59-30-3 QSA8.Aliphatic halogens No 59-30-3 QSA9.Alkyl nitrite No 59-30-3 QSA10.α,β unsaturated carbonyls No 59-30-3 QSA11.Simple aldehyde No 59-30-3 QSA12.Quinones No 59-30-3 QSA13.Hydrazine No 59-30-3 QSA14.Aliphatic azo and azoxy No 59-30-3 QSA15.Isocyanate and isothiocyanate groups No 59-30-3 QSA16.Alkyl carbamate and thiocarbamate No 59-30-3 QSA18.Polycyclic Aromatic Hydrocarbons No 59-30-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 59-30-3 QSA21.Alkyl and aryl N-

Table 18 Continued

		nitroso groups No 59-30-3 QSA22.Azide and triazene groups No 59-30-3 QSA23.Aliphatic N-nitro No 59-30-3 QSA24.α,β unsaturated alkoxy No 59-30-3 QSA25.Aromatic nitroso group No 59-30-3 QSA26.Aromatic ring N-oxide No 59-30-3 QSA27.Nitro aromatic No 59-30-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 59-30-3 QSA28bis.Aromatic mono- and dialkylamine No 59-30-3 QSA28ter.Aromatic N-acyl amine No 59-30-3 QSA29.Aromatic diazo No 59-30-3 QSA30.Coumarins and Furocoumarins No 59-30-3 QSA32.1,3-dialkoxy-benzene No 59-30-3 QSA33.1-phenoxy-benzene No 59-30-3 QSA34.H-acceptor-path3-H-acceptor Yes 59-30-3 QSA35.Oxolane No 59-30-3 QSA36.Carbodiimides No 59-30-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
formaldehyde	0	
gentamicin	1	QSA1.Acyl halides No 1403-66-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1403-66-3 QSA3.N-methylol derivatives No 1403-66-3 QSA4.Monohaloalkene No 1403-66-3 QSA5.S or N mustard No 1403-66-3 QSA6.Propiolactones and propiosultones No 1403-66-3 QSA7.Epoxides and aziridines No 1403-66-3 QSA8.Aliphatic halogens No 1403-66-3 QSA9.Alkyl nitrite No 1403-66-3 QSA10.α,β unsaturated carbonyls No 1403-66-3 QSA11.Simple aldehyde No 1403-66-3 QSA12.Quinones No 1403-66-3 QSA13.Hydrazine No 1403-66-3 QSA14.Aliphatic azo and azoxy No 1403-66-3 QSA15.Isocyanate and isothiocyanate groups No 1403-66-3 QSA16.Alkyl carbamate and thiocarbamate No 1403-66-3 QSA18.Polycyclic Aromatic Hydrocarbons No 1403-66-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1403-66-3 QSA21.Alkyl and aryl N-nitroso groups No 1403-66-3 QSA22.Azide and triazene groups No 1403-66-3 QSA23.Aliphatic N-nitro No 1403-66-3 QSA24.α,β unsaturated alkoxy No 1403-66-3 QSA25.Aromatic nitroso group No 1403-66-3 QSA26.Aromatic ring N-oxide No 1403-66-3 QSA27.Nitro aromatic No 1403-66-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1403-66-3 QSA28bis.Aromatic mono- and dialkylamine No 1403-66-3 QSA28ter.Aromatic N-acyl amine No 1403-66-3 QSA29.Aromatic diazo No 1403-66-3 QSA30.Coumarins and Furocoumarins No 1403-66-3 QSA32.1,3-dialkoxy-benzene No 1403-66-3 QSA33.1-phenoxy-benzene No 1403-66-3 QSA34.H-acceptor-path3-H-acceptor Yes 1403-66-3

Table 18 Continued

		QSA35.Oxolane No 1403-66-3 QSA36.Carbodiimides No 1403-66-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
glutaral	1	QSA1.Acyl halides No 111-30-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 111-30-8 QSA3.N-methylol derivatives No 111-30-8 QSA4.Monohaloalkene No 111-30-8 QSA5.S or N mustard No 111-30-8 QSA6.Propiolactones and propiosultones No 111-30-8 QSA7.Epoxides and aziridines No 111-30-8 QSA8.Aliphatic halogens No 111-30-8 QSA9.Alkyl nitrite No 111-30-8 QSA10.α,β unsaturated carbonyls No 111-30-8 QSA11.Simple aldehyde Yes 111-30-8 QSA12.Quinones No 111-30-8 QSA13.Hydrazine No 111-30-8 QSA14.Aliphatic azo and azoxy No 111-30-8 QSA15.Isocyanate and isothiocyanate groups No 111-30-8 QSA16.Alkyl carbamate and thiocarbamate No 111-30-8 QSA18.Polycyclic Aromatic Hydrocarbons No 111-30-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 111-30-8 QSA21.Alkyl and aryl N-nitroso groups No 111-30-8 QSA22.Azide and triazene groups No 111-30-8 QSA23.Aliphatic N-nitro No 111-30-8 QSA24.α,β unsaturated alkoxy No 111-30-8 QSA25.Aromatic nitroso group No 111-30-8 QSA26.Aromatic ring N-oxide No 111-30-8 QSA27.Nitro aromatic No 111-30-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 111-30-8 QSA28bis.Aromatic mono- and dialkylamine No 111-30-8 QSA28ter.Aromatic N-acyl amine No 111-30-8 QSA29.Aromatic diazo No 111-30-8 QSA30.Coumarins and Furocoumarins No 111-30-8 QSA32.1,3-dialkoxy-benzene No 111-30-8 QSA33.1-phenoxy-benzene No 111-30-8 QSA34.H-acceptor-path3-H-acceptor No 111-30-8 QSA35.Oxolane No 111-30-8 QSA36.Carbodiimides No 111-30-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
glutathione	1	QSA1.Acyl halides No 70-18-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 70-18-8 QSA3.N-methylol derivatives No 70-18-8 QSA4.Monohaloalkene No 70-18-8 QSA5.S or N mustard No 70-18-8 QSA6.Propiolactones and propiosultones No 70-18-8 QSA7.Epoxides and aziridines No 70-18-8 QSA8.Aliphatic halogens No 70-18-8 QSA9.Alkyl nitrite No 70-18-8 QSA10.α,β unsaturated carbonyls No 70-18-8 QSA11.Simple aldehyde No 70-18-8 QSA12.Quinones No 70-18-8 QSA13.Hydrazine No 70-18-8 QSA14.Aliphatic azo and azoxy No 70-18-8 QSA15.Isocyanate and isothiocyanate

Table 18 Continued

		groups No 70-18-8 QSA16.Alkyl carbamate and thiocarbamate No 70-18-8 QSA18.Polycyclic Aromatic Hydrocarbons No 70-18-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 70-18-8 QSA21.Alkyl and aryl N-nitroso groups No 70-18-8 QSA22.Azide and triazene groups No 70-18-8 QSA23.Aliphatic N-nitro No 70-18-8 QSA24.α,β unsaturated alkoxy No 70-18-8 QSA25.Aromatic nitroso group No 70-18-8 QSA26.Aromatic ring N-oxide No 70-18-8 QSA27.Nitro aromatic No 70-18-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 70-18-8 QSA28bis.Aromatic mono- and dialkylamine No 70-18-8 QSA28ter.Aromatic N-acyl amine No 70-18-8 QSA29.Aromatic diazo No 70-18-8 QSA30.Coumarins and Furocoumarins No 70-18-8 QSA32.1,3-dialkoxy-benzene No 70-18-8 QSA33.1-phenoxy-benzene No 70-18-8 QSA34.H-acceptor-path3-H-acceptor Yes 70-18-8 QSA35.Oxolane No 70-18-8 QSA36.Carbodiimides No 70-18-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
glycerin	1	QSA1.Acyl halides No 56-81-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-81-5 QSA3.N-methylol derivatives No 56-81-5 QSA4.Monohaloalkene No 56-81-5 QSA5.S or N mustard No 56-81-5 QSA6.Propiolactones and propiosultones No 56-81-5 QSA7.Epoxides and aziridines No 56-81-5 QSA8.Aliphatic halogens No 56-81-5 QSA9.Alkyl nitrite No 56-81-5 QSA10.α,β unsaturated carbonyls No 56-81-5 QSA11.Simple aldehyde No 56-81-5 QSA12.Quinones No 56-81-5 QSA13.Hydrazine No 56-81-5 QSA14.Aliphatic azo and azoxy No 56-81-5 QSA15.Isocyanate and isothiocyanate groups No 56-81-5 QSA16.Alkyl carbamate and thiocarbamate No 56-81-5 QSA18.Polycyclic Aromatic Hydrocarbons No 56-81-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-81-5 QSA21.Alkyl and aryl N-nitroso groups No 56-81-5 QSA22.Azide and triazene groups No 56-81-5 QSA23.Aliphatic N-nitro No 56-81-5 QSA24.α,β unsaturated alkoxy No 56-81-5 QSA25.Aromatic nitroso group No 56-81-5 QSA26.Aromatic ring N-oxide No 56-81-5 QSA27.Nitro aromatic No 56-81-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-81-5 QSA28bis.Aromatic mono- and dialkylamine No 56-81-5 QSA28ter.Aromatic N-acyl amine No 56-81-5 QSA29.Aromatic diazo No 56-81-5 QSA30.Coumarins and Furocoumarins No 56-81-5 QSA32.1,3-dialkoxy-benzene No 56-81-5 QSA33.1-phenoxy-

Table 18 Continued

		benzene No 56-81-5 QSA34.H-acceptor-path3-H-acceptor Yes 56-81-5 QSA35.Oxolane No 56-81-5 QSA36.Carbodiimides No 56-81-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
glycine	1	QSA1.Acyl halides No 56-40-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-40-6 QSA3.N-methylol derivatives No 56-40-6 QSA4.Monohaloalkene No 56-40-6 QSA5.S or N mustard No 56-40-6 QSA6.Propiolactones and propiosultones No 56-40-6 QSA7.Epoxides and aziridines No 56-40-6 QSA8.Aliphatic halogens No 56-40-6 QSA9.Alkyl nitrite No 56-40-6 QSA10.α,β unsaturated carbonyls No 56-40-6 QSA11.Simple aldehyde No 56-40-6 QSA12.Quinones No 56-40-6 QSA13.Hydrazine No 56-40-6 QSA14.Aliphatic azo and azoxy No 56-40-6 QSA15.Isocyanate and isothiocyanate groups No 56-40-6 QSA16.Alkyl carbamate and thiocarbamate No 56-40-6 QSA18.Polycyclic Aromatic Hydrocarbons No 56-40-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-40-6 QSA21.Alkyl and aryl N-nitroso groups No 56-40-6 QSA22.Azide and triazene groups No 56-40-6 QSA23.Aliphatic N-nitro No 56-40-6 QSA24.α,β unsaturated alkoxy No 56-40-6 QSA25.Aromatic nitroso group No 56-40-6 QSA26.Aromatic ring N-oxide No 56-40-6 QSA27.Nitro aromatic No 56-40-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-40-6 QSA28bis.Aromatic mono- and dialkylamine No 56-40-6 QSA28ter.Aromatic N-acyl amine No 56-40-6 QSA29.Aromatic diazo No 56-40-6 QSA30.Coumarins and Furocoumarins No 56-40-6 QSA32.1,3-dialkoxy-benzene No 56-40-6 QSA33.1-phenoxy-benzene No 56-40-6 QSA34.H-acceptor-path3-H-acceptor Yes 56-40-6 QSA35.Oxolane No 56-40-6 QSA36.Carbodiimides No 56-40-6 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I) 56-40-6
guanine hydrochloride	1	QSA1.Acyl halides No 33735-91-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 33735-91-0 QSA3.N-methylol derivatives No 33735-91-0 QSA4.Monohaloalkene No 33735-91-0 QSA5.S or N mustard No 33735-91-0 QSA6.Propiolactones and propiosultones No 33735-91-0 QSA7.Epoxides and aziridines No 33735-91-0 QSA8.Aliphatic halogens No 33735-91-0 QSA9.Alkyl nitrite No 33735-91-0 QSA10.α,β unsaturated carbonyls No 33735-91-0 QSA11.Simple aldehyde No 33735-91-0 QSA12.Quinones No 33735-91-0

Table 18 Continued

		QSA13.Hydrazine No 33735-91-0 QSA14.Aliphatic azo and azoxy No 33735-91-0 QSA15.Isocyanate and isothiocyanate groups No 33735-91-0 QSA16.Alkyl carbamate and thiocarbamate No 33735-91-0 QSA18.Polycyclic Aromatic Hydrocarbons No 33735-91-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 33735-91-0 QSA21.Alkyl and aryl N-nitroso groups No 33735-91-0 QSA22.Azide and triazene groups No 33735-91-0 QSA23.Aliphatic N-nitro No 33735-91-0 QSA24.α,β unsaturated alkoxy No 33735-91-0 QSA25.Aromatic nitroso group No 33735-91-0 QSA26.Aromatic ring N-oxide No 33735-91-0 QSA27.Nitro aromatic No 33735-91-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 33735-91-0 QSA28bis.Aromatic mono- and dialkylamine No 33735-91-0 QSA28ter.Aromatic N-acyl amine No 33735-91-0 QSA29.Aromatic diazo No 33735-91-0 QSA30.Coumarins and Furocoumarins No 33735-91-0 QSA32.1,3-dialkoxy-benzene No 33735-91-0 QSA33.1-phenoxy-benzene No 33735-91-0 QSA34.H-acceptor-path3-H-acceptor Yes 33735-91-0 QSA35.Oxolane No 33735-91-0 QSA36.Carbodiimides No 33735-91-0 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
hemin chloride	1	QSA1.Acyl halides No 16009-13-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 16009-13-5 QSA3.N-methylol derivatives No 16009-13-5 QSA4.Monohaloalkene No 16009-13-5 QSA5.S or N mustard No 16009-13-5 QSA6.Propiolactones and propiosultones No 16009-13-5 QSA7.Epoxides and aziridines No 16009-13-5 QSA8.Aliphatic halogens No 16009-13-5 QSA9.Alkyl nitrite No 16009-13-5 QSA10.α,β unsaturated carbonyls No 16009-13-5 QSA11.Simple aldehyde No 16009-13-5 QSA12.Quinones No 16009-13-5 QSA13.Hydrazine No 16009-13-5 QSA14.Aliphatic azo and azoxy No 16009-13-5 QSA15.Isocyanate and isothiocyanate groups No 16009-13-5 QSA16.Alkyl carbamate and thiocarbamate No 16009-13-5 QSA18.Polycyclic Aromatic Hydrocarbons No 16009-13-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 16009-13-5 QSA21.Alkyl and aryl N-nitroso groups No 16009-13-5 QSA22.Azide and triazene groups No 16009-13-5 QSA23.Aliphatic N-nitro No 16009-13-5 QSA24.α,β unsaturated alkoxy No 16009-13-5 QSA25.Aromatic nitroso group No 16009-13-5 QSA26.Aromatic ring N-oxide No 16009-13-5 QSA27.Nitro aromatic No 16009-13-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No

Table 18 Continued

		16009-13-5 QSA28bis.Aromatic mono- and dialkylamine No 16009-13-5 QSA28ter.Aromatic N-acyl amine No 16009-13-5 QSA29.Aromatic diazo No 16009-13-5 QSA30.Coumarins and Furocoumarins No 16009-13-5 QSA32.1,3-dialkoxy-benzene No 16009-13-5 QSA33.1-phenoxy-benzene No 16009-13-5 QSA34.H-acceptor-path3-H-acceptor Yes 16009-13-5 QSA35.Oxolane No 16009-13-5 QSA36.Carbodiimides No 16009-13-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	1	QSA1.Acyl halides No 7365-45-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7365-45-9 QSA3.N-methylol derivatives No 7365-45-9 QSA4.Monohaloalkene No 7365-45-9 QSA5.S or N mustard No 7365-45-9 QSA6.Propiolactones and propiosultones No 7365-45-9 QSA7.Epoxides and aziridines No 7365-45-9 QSA8.Aliphatic halogens No 7365-45-9 QSA9.Alkyl nitrite No 7365-45-9 QSA10.α,β unsaturated carbonyls No 7365-45-9 QSA11.Simple aldehyde No 7365-45-9 QSA12.Quinones No 7365-45-9 QSA13.Hydrazine No 7365-45-9 QSA14.Aliphatic azo and azoxy No 7365-45-9 QSA15.Isocyanate and isothiocyanate groups No 7365-45-9 QSA16.Alkyl carbamate and thiocarbamate No 7365-45-9 QSA18.Polycyclic Aromatic Hydrocarbons No 7365-45-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7365-45-9 QSA21.Alkyl and aryl N-nitroso groups No 7365-45-9 QSA22.Azide and triazene groups No 7365-45-9 QSA23.Aliphatic N-nitro No 7365-45-9 QSA24.α,β unsaturated alkoxy No 7365-45-9 QSA25.Aromatic nitroso group No 7365-45-9 QSA26.Aromatic ring N-oxide No 7365-45-9 QSA27.Nitro aromatic No 7365-45-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7365-45-9 QSA28bis.Aromatic mono- and dialkylamine No 7365-45-9 QSA28ter.Aromatic N-acyl amine No 7365-45-9 QSA29.Aromatic diazo No 7365-45-9 QSA30.Coumarins and Furocoumarins No 7365-45-9 QSA32.1,3-dialkoxy-benzene No 7365-45-9 QSA33.1-phenoxy-benzene No 7365-45-9 QSA34.H-acceptor-path3-H-acceptor Yes 7365-45-9 QSA35.Oxolane No 7365-45-9 QSA36.Carbodiimides No 7365-45-9 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
heptakis(2,6-O-dimethyl)beta-	1	QSA1.Acyl halides No QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No QSA3.N-methylol derivatives No QSA4.Monohaloalkene No QSA5.S or N

Table 18 Continued

cyclodextrin		mustard No QSA6.Propiolactones and propiosultones No QSA7.Epoxides and aziridines No QSA8.Aliphatic halogens No QSA9.Alkyl nitrite No QSA10.α,β unsaturated carbonyls No QSA11.Simple aldehyde No QSA12.Quinones No QSA13.Hydrazine No QSA14.Aliphatic azo and azoxy No QSA15.Isocyanate and isothiocyanate groups No QSA16.Alkyl carbamate and thiocarbamate No QSA18.Polycyclic Aromatic Hydrocarbons No QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No QSA21.Alkyl and aryl N-nitroso groups No QSA22.Azide and triazene groups No QSA23.Aliphatic N-nitro No QSA24.α,β unsaturated alkoxy No QSA25.Aromatic nitroso group No QSA26.Aromatic ring N-oxide No QSA27.Nitro aromatic No QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No QSA28bis.Aromatic mono- and dialkylamine No QSA28ter.Aromatic N-acyl amine No QSA29.Aromatic diazo No QSA30.Coumarins and Furocoumarins No QSA32.1,3-dialkoxy-benzene No QSA33.1-phenoxy-benzene No QSA35.Oxolane No QSA36.Carbodiimides No QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
hexachlorobenzene	0	
hexamethyldisiloxane	0	
hydrocortisone	1	QSA1.Acyl halides No 50-23-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-23-7 QSA3.N-methylol derivatives No 50-23-7 QSA4.Monohaloalkene No 50-23-7 QSA5.S or N mustard No 50-23-7 QSA6.Propiolactones and propiosultones No 50-23-7 QSA7.Epoxides and aziridines No 50-23-7 QSA8.Aliphatic halogens No 50-23-7 QSA9.Alkyl nitrite No 50-23-7 QSA10.α,β unsaturated carbonyls Yes 50-23-7 QSA11.Simple aldehyde No 50-23-7 QSA12.Quinones No 50-23-7 QSA13.Hydrazine No 50-23-7 QSA14.Aliphatic azo and azoxy No 50-23-7 QSA15.Isocyanate and isothiocyanate groups No 50-23-7 QSA16.Alkyl carbamate and thiocarbamate No 50-23-7 QSA18.Polycyclic Aromatic Hydrocarbons No 50-23-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-23-7 QSA21.Alkyl and aryl N-nitroso groups No 50-23-7 QSA22.Azide and triazene groups No 50-23-7 QSA23.Aliphatic N-nitro No 50-23-7 QSA24.α,β unsaturated alkoxy No 50-23-7 QSA25.Aromatic

Table 18 Continued

		nitroso group No 50-23-7 QSA26.Aromatic ring N-oxide No 50-23-7 QSA27.Nitro aromatic No 50-23-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-23-7 QSA28bis.Aromatic mono- and dialkylamine No 50-23-7 QSA28ter.Aromatic N-acyl amine No 50-23-7 QSA29.Aromatic diazo No 50-23-7 QSA30.Coumarins and Furocoumarins No 50-23-7 QSA32.1,3-dialkoxy-benzene No 50-23-7 QSA33.1-phenoxy-benzene No 50-23-7 QSA34.H-acceptor-path3-H-acceptor Yes 50-23-7 QSA35.Oxolane No 50-23-7 QSA36.Carbodiimides No 50-23-7 QAny alert?.At least one alert fired? Yes Class
hydroxy L proline	1	QSA1.Acyl halides No 51-35-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 51-35-4 QSA3.N-methylol derivatives No 51-35-4 QSA4.Monohaloalkene No 51-35-4 QSA5.S or N mustard No 51-35-4 QSA6.Propiolactones and propiosultones No 51-35-4 QSA7.Epoxides and aziridines No 51-35-4 QSA8.Aliphatic halogens No 51-35-4 QSA9.Alkyl nitrite No 51-35-4 QSA10.α,β unsaturated carbonyls No 51-35-4 QSA11.Simple aldehyde No 51-35-4 QSA12.Quinones No 51-35-4 QSA13.Hydrazine No 51-35-4 QSA14.Aliphatic azo and azoxy No 51-35-4 QSA15.Isocyanate and isothiocyanate groups No 51-35-4 QSA16.Alkyl carbamate and thiocarbamate No 51-35-4 QSA18.Polycyclic Aromatic Hydrocarbons No 51-35-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 51-35-4 QSA21.Alkyl and aryl N-nitroso groups No 51-35-4 QSA22.Azide and triazene groups No 51-35-4 QSA23.Aliphatic N-nitro No 51-35-4 QSA24.α,β unsaturated alkoxy No 51-35-4 QSA25.Aromatic nitroso group No 51-35-4 QSA26.Aromatic ring N-oxide No 51-35-4 QSA27.Nitro aromatic No 51-35-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 51-35-4 QSA28bis.Aromatic mono- and dialkylamine No 51-35-4 QSA28ter.Aromatic N-acyl amine No 51-35-4 QSA29.Aromatic diazo No 51-35-4 QSA30.Coumarins and Furocoumarins No 51-35-4 QSA32.1,3-dialkoxy-benzene No 51-35-4 QSA33.1-phenoxy-benzene No 51-35-4 QSA34.H-acceptor-path3-H-acceptor Yes 51-35-4 QSA35.Oxolane No 51-35-4 QSA36.Carbodiimides No 51-35-4 QAny alert?.At least one alert fired? Yes
hydroxylysine	1	QSA1.Acyl halides No hydroxylysine QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No hydroxylysine QSA3.N-methylol derivatives No hydroxylysine QSA4.Monohaloalkene No hydroxylysine QSA5.S or N

Table 18 Continued

		mustard No hydroxylysine QSA6.Propiolactones and propiosultones No hydroxylysine QSA7.Epoxides and aziridines No hydroxylysine QSA8.Aliphatic halogens No hydroxylysine QSA9.Alkyl nitrite No hydroxylysine QSA10.α,β unsaturated carbonyls No hydroxylysine QSA11.Simple aldehyde No hydroxylysine QSA12.Quinones No hydroxylysine QSA13.Hydrazine No hydroxylysine QSA14.Aliphatic azo and azoxy No hydroxylysine QSA15.Isocyanate and isothiocyanate groups No hydroxylysine QSA16.Alkyl carbamate and thiocarbamate No hydroxylysine QSA18.Polycyclic Aromatic Hydrocarbons No hydroxylysine QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No hydroxylysine QSA21.Alkyl and aryl N-nitroso groups No hydroxylysine QSA22.Azide and triazene groups No hydroxylysine QSA23.Aliphatic N-nitro No hydroxylysine QSA24.α,β unsaturated alkoxy No hydroxylysine QSA25.Aromatic nitroso group No hydroxylysine QSA26.Aromatic ring N-oxide No hydroxylysine QSA27.Nitro aromatic No hydroxylysine QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No hydroxylysine QSA28bis.Aromatic mono- and dialkylamine No hydroxylysine QSA28ter.Aromatic N-acyl amine No hydroxylysine QSA29.Aromatic diazo No hydroxylysine QSA30.Coumarins and Furocoumarins No hydroxylysine QSA32.1,3-dialkoxy-benzene No hydroxylysine QSA33.1-phenoxy-benzene No hydroxylysine QSA34.H-acceptor-path3-H-acceptor Yes hydroxylysine QSA35.Oxolane No hydroxylysine QSA36.Carbodiimides No hydroxylysine QAny alert?.At least one alert fired? Yes
hypoxanthine	1	QSA1.Acyl halides No 68-94-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 68-94-0 QSA3.N-methylol derivatives No 68-94-0 QSA4.Monohaloalkene No 68-94-0 QSA5.S or N mustard No 68-94-0 QSA6.Propiolactones and propiosultones No 68-94-0 QSA7.Epoxides and aziridines No 68-94-0 QSA8.Aliphatic halogens No 68-94-0 QSA9.Alkyl nitrite No 68-94-0 QSA10.α,β unsaturated carbonyls No 68-94-0 QSA11.Simple aldehyde No 68-94-0 QSA12.Quinones No 68-94-0 QSA13.Hydrazine No 68-94-0 QSA14.Aliphatic azo and azoxy No 68-94-0 QSA15.Isocyanate and isothiocyanate groups No 68-94-0 QSA16.Alkyl carbamate and thiocarbamate No 68-94-0 QSA18.Polycyclic Aromatic Hydrocarbons No 68-94-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 68-94-0 QSA21.Alkyl and aryl N-nitroso groups No 68-94-0 QSA22.Azide and triazene

Table 18 Continued

		groups No 68-94-0 QSA23.Aliphatic N-nitro No 68-94-0 QSA24.α,β unsaturated alkoxy No 68-94-0 QSA25.Aromatic nitroso group No 68-94-0 QSA26.Aromatic ring N-oxide No 68-94-0 QSA27.Nitro aromatic No 68-94-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 68-94-0 QSA28bis.Aromatic mono- and dialkylamine No 68-94-0 QSA28ter.Aromatic N-acyl amine No 68-94-0 QSA29.Aromatic diazo No 68-94-0 QSA30.Coumarins and Furocoumarins No 68-94-0 QSA32.1,3-dialkoxy-benzene No 68-94-0 QSA33.1-phenoxy-benzene No 68-94-0 QSA34.H-acceptor-path3-H-acceptor Yes 68-94-0 QSA35.Oxolane No 68-94-0 QSA36.Carbodiimides No 68-94-0 QAny alert?.At least one alert fired? Yes
i-Inositol	1	QSA1.Acyl halides No 87-89-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 87-89-8 QSA3.N-methylol derivatives No 87-89-8 QSA4.Monohaloalkene No 87-89-8 QSA5.S or N mustard No 87-89-8 QSA6.Propiolactones and propiosultones No 87-89-8 QSA7.Epoxides and aziridines No 87-89-8 QSA8.Aliphatic halogens No 87-89-8 QSA9.Alkyl nitrite No 87-89-8 QSA10.α,β unsaturated carbonyls No 87-89-8 QSA11.Simple aldehyde No 87-89-8 QSA12.Quinones No 87-89-8 QSA13.Hydrazine No 87-89-8 QSA14.Aliphatic azo and azoxy No 87-89-8 QSA15.Isocyanate and isothiocyanate groups No 87-89-8 QSA16.Alkyl carbamate and thiocarbamate No 87-89-8 QSA18.Polycyclic Aromatic Hydrocarbons No 87-89-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 87-89-8 QSA21.Alkyl and aryl N-nitroso groups No 87-89-8 QSA22.Azide and triazene groups No 87-89-8 QSA23.Aliphatic N-nitro No 87-89-8 QSA24.α,β unsaturated alkoxy No 87-89-8 QSA25.Aromatic nitroso group No 87-89-8 QSA26.Aromatic ring N-oxide No 87-89-8 QSA27.Nitro aromatic No 87-89-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 87-89-8 QSA28bis.Aromatic mono- and dialkylamine No 87-89-8 QSA28ter.Aromatic N-acyl amine No 87-89-8 QSA29.Aromatic diazo No 87-89-8 QSA30.Coumarins and Furocoumarins No 87-89-8 QSA32.1,3-dialkoxy-benzene No 87-89-8 QSA33.1-phenoxy-benzene No 87-89-8 QSA34.H-acceptor-path3-H-acceptor Yes 87-89-8 QSA35.Oxolane No 87-89-8 QSA36.Carbodiimides No 87-89-8 QAny alert?.At least one alert fired? Yes
indigo	1	QSA1.Acyl halides No 482-89-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 482-89-3 QSA3.N-

Table 18 Continued

		methylol derivatives No 482-89-3 QSA4.Monohaloalkene No 482-89-3 QSA5.S or N mustard No 482-89-3 QSA6.Propiolactones and propiosultones No 482-89-3 QSA7.Epoxides and aziridines No 482-89-3 QSA8.Aliphatic halogens No 482-89-3 QSA9.Alkyl nitrite No 482-89-3 QSA10.α,β unsaturated carbonyls Yes 482-89-3 QSA11.Simple aldehyde No 482-89-3 QSA12.Quinones No 482-89-3 QSA13.Hydrazine No 482-89-3 QSA14.Aliphatic azo and azoxy No 482-89-3 QSA15.Isocyanate and isothiocyanate groups No 482-89-3 QSA16.Alkyl carbamate and thiocarbamate No 482-89-3 QSA18.Polycyclic Aromatic Hydrocarbons No 482-89-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 482-89-3 QSA21.Alkyl and aryl N-nitroso groups No 482-89-3 QSA22.Azide and triazene groups No 482-89-3 QSA23.Aliphatic N-nitro No 482-89-3 QSA24.α,β unsaturated alkoxy No 482-89-3 QSA25.Aromatic nitroso group No 482-89-3 QSA26.Aromatic ring N-oxide No 482-89-3 QSA27.Nitro aromatic No 482-89-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 482-89-3 QSA28bis.Aromatic mono- and dialkylamine No 482-89-3 QSA28ter.Aromatic N-acyl amine No 482-89-3 QSA29.Aromatic diazo No 482-89-3 QSA30.Coumarins and Furocoumarins No 482-89-3 QSA32.1,3-dialkoxy-benzene No 482-89-3 QSA33.1-phenoxy-benzene No 482-89-3 QSA34.H-acceptor-path3-H-acceptor Yes 482-89-3 QSA35.Oxolane No 482-89-3 QSA36.Carbodiimides No 482-89-3 QAny alert?.At least one alert fired? Yes
insulin	1	QSA1.Acyl halides No 11061-68-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 11061-68-0 QSA3.N-methylol derivatives No 11061-68-0 QSA4.Monohaloalkene No 11061-68-0 QSA5.S or N mustard No 11061-68-0 QSA6.Propiolactones and propiosultones No 11061-68-0 QSA7.Epoxides and aziridines No 11061-68-0 QSA8.Aliphatic halogens No 11061-68-0 QSA9.Alkyl nitrite No 11061-68-0 QSA10.α,β unsaturated carbonyls No 11061-68-0 QSA11.Simple aldehyde No 11061-68-0 QSA12.Quinones No 11061-68-0 QSA13.Hydrazine No 11061-68-0 QSA14.Aliphatic azo and azoxy No 11061-68-0 QSA15.Isocyanate and isothiocyanate groups No 11061-68-0 QSA16.Alkyl carbamate and thiocarbamate No 11061-68-0 QSA18.Polycyclic Aromatic Hydrocarbons No 11061-68-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 11061-68-0 QSA21.Alkyl and aryl N-nitroso groups No 11061-68-0 QSA22.Azide and triazene groups No 11061-68-0 QSA23.Aliphatic N-nitro No 11061-

Table 18 Continued

		68-0 QSA24.α,β unsaturated alkoxy No 11061-68-0 QSA25.Aromatic nitroso group No 11061-68-0 QSA26.Aromatic ring N-oxide No 11061-68-0 QSA27.Nitro aromatic No 11061-68-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 11061-68-0 QSA28bis.Aromatic mono- and dialkylamine No 11061-68-0 QSA28ter.Aromatic N-acyl amine No 11061-68-0 QSA29.Aromatic diazo No 11061-68-0 QSA30.Coumarins and Furocoumarins No 11061-68-0 QSA32.1,3-dialkoxy-benzene No 11061-68-0 QSA33.1-phenoxy-benzene No 11061-68-0 QSA34.H-acceptor-path3-H-acceptor Yes 11061-68-0 QSA35.Oxolane No 11061-68-0 QSA36.Carbodiimides No 11061-68-0 QAny alert?.At least one alert fired? Yes
iron	0	
iron (II) sulfate heptahydrate	1	QSA1.Acyl halides No 7782-63-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7782-63-0 QSA3.N-methylol derivatives No 7782-63-0 QSA4.Monohaloalkene No 7782-63-0 QSA5.S or N mustard No 7782-63-0 QSA6.Propiolactones and propiosultones No 7782-63-0 QSA7.Epoxides and aziridines No 7782-63-0 QSA8.Aliphatic halogens No 7782-63-0 QSA9.Alkyl nitrite No 7782-63-0 QSA10.α,β unsaturated carbonyls No 7782-63-0 QSA11.Simple aldehyde No 7782-63-0 QSA12.Quinones No 7782-63-0 QSA13.Hydrazine No 7782-63-0 QSA14.Aliphatic azo and azoxy No 7782-63-0 QSA15.Isocyanate and isothiocyanate groups No 7782-63-0 QSA16.Alkyl carbamate and thiocarbamate No 7782-63-0 QSA18.Polycyclic Aromatic Hydrocarbons No 7782-63-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7782-63-0 QSA21.Alkyl and aryl N-nitroso groups No 7782-63-0 QSA22.Azide and triazene groups No 7782-63-0 QSA23.Aliphatic N-nitro No 7782-63-0 QSA24.α,β unsaturated alkoxy No 7782-63-0 QSA25.Aromatic nitroso group No 7782-63-0 QSA26.Aromatic ring N-oxide No 7782-63-0 QSA27.Nitro aromatic No 7782-63-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7782-63-0 QSA28bis.Aromatic mono- and dialkylamine No 7782-63-0 QSA28ter.Aromatic N-acyl amine No 7782-63-0 QSA29.Aromatic diazo No 7782-63-0 QSA30.Coumarins and Furocoumarins No 7782-63-0 QSA32.1,3-dialkoxy-benzene No 7782-63-0 QSA33.1-phenoxy-benzene No 7782-63-0 QSA34.H-acceptor-path3-H-acceptor Yes 7782-63-0 QSA35.Oxolane No 7782-63-0 QSA36.Carbodiimides No 7782-63-0 QAny alert?.At least one alert fired? Yes Class At

Table 18 Continued

		least one positive structural alerts for the micronucleus assay (Class I)
iron ammonium citrate (FERRIC AMMONIUM CITRATE)	1	QSA1.Acyl halides No 1185-57-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1185-57-5 QSA3.N-methylol derivatives No 1185-57-5 QSA4.Monohaloalkene No 1185-57-5 QSA5.S or N mustard No 1185-57-5 QSA6.Propiolactones and propiosultones No 1185-57-5 QSA7.Epoxides and aziridines No 1185-57-5 QSA8.Aliphatic halogens No 1185-57-5 QSA9.Alkyl nitrite No 1185-57-5 QSA10.α,β unsaturated carbonyls No 1185-57-5 QSA11.Simple aldehyde No 1185-57-5 QSA12.Quinones No 1185-57-5 QSA13.Hydrazine No 1185-57-5 QSA14.Aliphatic azo and azoxy No 1185-57-5 QSA15.Isocyanate and isothiocyanate groups No 1185-57-5 QSA16.Alkyl carbamate and thiocarbamate No 1185-57-5 QSA18.Polycyclic Aromatic Hydrocarbons No 1185-57-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1185-57-5 QSA21.Alkyl and aryl N-nitroso groups No 1185-57-5 QSA22.Azide and triazene groups No 1185-57-5 QSA23.Aliphatic N-nitro No 1185-57-5 QSA24.α,β unsaturated alkoxy No 1185-57-5 QSA25.Aromatic nitroso group No 1185-57-5 QSA26.Aromatic ring N-oxide No 1185-57-5 QSA27.Nitro aromatic No 1185-57-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1185-57-5 QSA28bis.Aromatic mono- and dialkylamine No 1185-57-5 QSA28ter.Aromatic N-acyl amine No 1185-57-5 QSA29.Aromatic diazo No 1185-57-5 QSA30.Coumarins and Furocoumarins No 1185-57-5 QSA32.1,3-dialkoxy-benzene No 1185-57-5 QSA33.1-phenoxy-benzene No 1185-57-5 QSA34.H-acceptor-path3-H-acceptor Yes 1185-57-5 QSA35.Oxolane No 1185-57-5 QSA36.Carbodiimides No 1185-57-5 QAny alert?.At least one alert fired? Yes
iron III nitrate	1	QSA1.Acyl halides No 7782-61-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7782-61-8 QSA3.N-methylol derivatives No 7782-61-8 QSA4.Monohaloalkene No 7782-61-8 QSA5.S or N mustard No 7782-61-8 QSA6.Propiolactones and propiosultones No 7782-61-8 QSA7.Epoxides and aziridines No 7782-61-8 QSA8.Aliphatic halogens No 7782-61-8 QSA9.Alkyl nitrite No 7782-61-8 QSA10.α,β unsaturated carbonyls No 7782-61-8 QSA11.Simple aldehyde No 7782-61-8 QSA12.Quinones No 7782-61-8 QSA13.Hydrazine No 7782-61-8 QSA14.Aliphatic azo and azoxy No 7782-61-8 QSA15.Isocyanate and isothiocyanate groups No 7782-61-8 QSA16.Alkyl carbamate and

Table 18 Continued

		thiocarbamate No 7782-61-8 QSA18.Polycyclic Aromatic Hydrocarbons No 7782-61-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7782-61-8 QSA21.Alkyl and aryl N-nitroso groups No 7782-61-8 QSA22.Azide and triazene groups No 7782-61-8 QSA23.Aliphatic N-nitro No 7782-61-8 QSA24.α,β unsaturated alkoxy No 7782-61-8 QSA25.Aromatic nitroso group No 7782-61-8 QSA26.Aromatic ring N-oxide No 7782-61-8 QSA27.Nitro aromatic No 7782-61-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7782-61-8 QSA28bis.Aromatic mono- and dialkylamine No 7782-61-8 QSA28ter.Aromatic N-acyl amine No 7782-61-8 QSA29.Aromatic diazo No 7782-61-8 QSA30.Coumarins and Furocoumarins No 7782-61-8 QSA32.1,3-dialkoxy-benzene No 7782-61-8 QSA33.1-phenoxy-benzene No 7782-61-8 QSA34.H-acceptor-path3-H-acceptor Yes 7782-61-8 QSA35.Oxolane No 7782-61-8 QSA36.Carbodiimides No 7782-61-8 QAny alert?.At least one alert fired? Yes
kanamycin	1	QSA1.Acyl halides No 59-01-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-01-8 QSA3.N-methylol derivatives No 59-01-8 QSA4.Monohaloalkene No 59-01-8 QSA5.S or N mustard No 59-01-8 QSA6.Propiolactones and propiosultones No 59-01-8 QSA7.Epoxides and aziridines No 59-01-8 QSA8.Aliphatic halogens No 59-01-8 QSA9.Alkyl nitrite No 59-01-8 QSA10.α,β unsaturated carbonyls No 59-01-8 QSA11.Simple aldehyde No 59-01-8 QSA12.Quinones No 59-01-8 QSA13.Hydrazine No 59-01-8 QSA14.Aliphatic azo and azoxy No 59-01-8 QSA15.Isocyanate and isothiocyanate groups No 59-01-8 QSA16.Alkyl carbamate and thiocarbamate No 59-01-8 QSA18.Polycyclic Aromatic Hydrocarbons No 59-01-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 59-01-8 QSA21.Alkyl and aryl N-nitroso groups No 59-01-8 QSA22.Azide and triazene groups No 59-01-8 QSA23.Aliphatic N-nitro No 59-01-8 QSA24.α,β unsaturated alkoxy No 59-01-8 QSA25.Aromatic nitroso group No 59-01-8 QSA26.Aromatic ring N-oxide No 59-01-8 QSA27.Nitro aromatic No 59-01-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 59-01-8 QSA28bis.Aromatic mono- and dialkylamine No 59-01-8 QSA28ter.Aromatic N-acyl amine No 59-01-8 QSA29.Aromatic diazo No 59-01-8 QSA30.Coumarins and Furocoumarins No 59-01-8 QSA32.1,3-dialkoxy-benzene No 59-01-8 QSA33.1-phenoxy-benzene No 59-01-8 QSA34.H-acceptor-path3-H-acceptor Yes 59-01-8 QSA35.Oxolane No 59-01-8

Table 18 Continued

		QSA36.Carbodiimides No 59-01-8 QAny alert?.At least one alert fired? Yes
lactose	1	QSA1.Acyl halides No 63-42-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 63-42-3 QSA3.N-methylol derivatives No 63-42-3 QSA4.Monohaloalkene No 63-42-3 QSA5.S or N mustard No 63-42-3 QSA6.Propiolactones and propiosultones No 63-42-3 QSA7.Epoxides and aziridines No 63-42-3 QSA8.Aliphatic halogens No 63-42-3 QSA9.Alkyl nitrite No 63-42-3 QSA10.α,β unsaturated carbonyls No 63-42-3 QSA11.Simple aldehyde No 63-42-3 QSA12.Quinones No 63-42-3 QSA13.Hydrazine No 63-42-3 QSA14.Aliphatic azo and azoxy No 63-42-3 QSA15.Isocyanate and isothiocyanate groups No 63-42-3 QSA16.Alkyl carbamate and thiocarbamate No 63-42-3 QSA18.Polycyclic Aromatic Hydrocarbons No 63-42-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 63-42-3 QSA21.Alkyl and aryl N-nitroso groups No 63-42-3 QSA22.Azide and triazene groups No 63-42-3 QSA23.Aliphatic N-nitro No 63-42-3 QSA24.α,β unsaturated alkoxy No 63-42-3 QSA25.Aromatic nitroso group No 63-42-3 QSA26.Aromatic ring N-oxide No 63-42-3 QSA27.Nitro aromatic No 63-42-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 63-42-3 QSA28bis.Aromatic mono- and dialkylamine No 63-42-3 QSA28ter.Aromatic N-acyl amine No 63-42-3 QSA29.Aromatic diazo No 63-42-3 QSA30.Coumarins and Furocoumarins No 63-42-3 QSA32.1,3-dialkoxy-benzene No 63-42-3 QSA33.1-phenoxy-benzene No 63-42-3 QSA34.H-acceptor-path3-H-acceptor Yes 63-42-3 QSA35.Oxolane No 63-42-3 QSA36.Carbodiimides No 63-42-3 QAny alert?.At least one alert fired? Yes
L-alanine	1	QSA1.Acyl halides No 56-41-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-41-7 QSA3.N-methylol derivatives No 56-41-7 QSA4.Monohaloalkene No 56-41-7 QSA5.S or N mustard No 56-41-7 QSA6.Propiolactones and propiosultones No 56-41-7 QSA7.Epoxides and aziridines No 56-41-7 QSA8.Aliphatic halogens No 56-41-7 QSA9.Alkyl nitrite No 56-41-7 QSA10.α,β unsaturated carbonyls No 56-41-7 QSA11.Simple aldehyde No 56-41-7 QSA12.Quinones No 56-41-7 QSA13.Hydrazine No 56-41-7 QSA14.Aliphatic azo and azoxy No 56-41-7 QSA15.Isocyanate and isothiocyanate groups No 56-41-7 QSA16.Alkyl carbamate and thiocarbamate No 56-41-7 QSA18.Polycyclic Aromatic Hydrocarbons No 56-41-7 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 56-41-7 QSA21.Alkyl and aryl N-nitroso groups No 56-41-7 QSA22.Azide and triazene groups No 56-41-7 QSA23.Aliphatic N-nitro No 56-41-7 QSA24.α,β unsaturated alkoxy No 56-41-7 QSA25.Aromatic nitroso group No 56-41-7 QSA26.Aromatic ring N-oxide No 56-41-7 QSA27.Nitro aromatic No 56-41-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-41-7 QSA28bis.Aromatic mono- and dialkylamine No 56-41-7 QSA28ter.Aromatic N-acyl amine No 56-41-7 QSA29.Aromatic diazo No 56-41-7 QSA30.Coumarins and Furocoumarins No 56-41-7 QSA32.1,3-dialkoxy-benzene No 56-41-7 QSA33.1-phenoxy-benzene No 56-41-7 QSA34.H-acceptor-path3-H-acceptor Yes 56-41-7 QSA35.Oxolane No 56-41-7 QSA36.Carbodiimides No 56-41-7 QAny alert?.At least one alert fired? Yes
L-arginine	1	QSA1.Acyl halides No 74-79-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 74-79-3 QSA3.N-methylol derivatives No 74-79-3 QSA4.Monohaloalkene No 74-79-3 QSA5.S or N mustard No 74-79-3 QSA6.Propiolactones and propiosultones No 74-79-3 QSA7.Epoxides and aziridines No 74-79-3 QSA8.Aliphatic halogens No 74-79-3 QSA9.Alkyl nitrite No 74-79-3 QSA10.α,β unsaturated carbonyls No 74-79-3 QSA11.Simple aldehyde No 74-79-3 QSA12.Quinones No 74-79-3 QSA13.Hydrazine No 74-79-3 QSA14.Aliphatic azo and azoxy No 74-79-3 QSA15.Isocyanate and isothiocyanate groups No 74-79-3 QSA16.Alkyl carbamate and thiocarbamate No 74-79-3 QSA18.Polycyclic Aromatic Hydrocarbons No 74-79-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 74-79-3 QSA21.Alkyl and aryl N-nitroso groups No 74-79-3 QSA22.Azide and triazene groups No 74-79-3 QSA23.Aliphatic N-nitro No 74-79-3 QSA24.α,β unsaturated alkoxy No 74-79-3 QSA25.Aromatic nitroso group No 74-79-3 QSA26.Aromatic ring N-oxide No 74-79-3 QSA27.Nitro aromatic No 74-79-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 74-79-3 QSA28bis.Aromatic mono- and dialkylamine No 74-79-3 QSA28ter.Aromatic N-acyl amine No 74-79-3 QSA29.Aromatic diazo No 74-79-3 QSA30.Coumarins and Furocoumarins No 74-79-3 QSA32.1,3-dialkoxy-benzene No 74-79-3 QSA33.1-phenoxy-benzene No 74-79-3 QSA34.H-acceptor-path3-H-acceptor Yes 74-79-3 QSA35.Oxolane No 74-79-3 QSA36.Carbodiimides No 74-79-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the

Table 18 Continued

		micronucleus assay (Class I)
L-ascorbic acid	1	QSA1.Acyl halides No 50-81-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-81-7 QSA3.N-methylol derivatives No 50-81-7 QSA4.Monohaloalkene No 50-81-7 QSA5.S or N mustard No 50-81-7 QSA6.Propiolactones and propiosultones No 50-81-7 QSA7.Epoxides and aziridines No 50-81-7 QSA8.Aliphatic halogens No 50-81-7 QSA9.Alkyl nitrite No 50-81-7 QSA10.α,β unsaturated carbonyls No 50-81-7 QSA11.Simple aldehyde No 50-81-7 QSA12.Quinones No 50-81-7 QSA13.Hydrazine No 50-81-7 QSA14.Aliphatic azo and azoxy No 50-81-7 QSA15.Isocyanate and isothiocyanate groups No 50-81-7 QSA16.Alkyl carbamate and thiocarbamate No 50-81-7 QSA18.Polycyclic Aromatic Hydrocarbons No 50-81-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-81-7 QSA21.Alkyl and aryl N-nitroso groups No 50-81-7 QSA22.Azide and triazene groups No 50-81-7 QSA23.Aliphatic N-nitro No 50-81-7 QSA24.α,β unsaturated alkoxy No 50-81-7 QSA25.Aromatic nitroso group No 50-81-7 QSA26.Aromatic ring N-oxide No 50-81-7 QSA27.Nitro aromatic No 50-81-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-81-7 QSA28bis.Aromatic mono- and dialkylamine No 50-81-7 QSA28ter.Aromatic N-acyl amine No 50-81-7 QSA29.Aromatic diazo No 50-81-7 QSA30.Coumarins and Furocoumarins No 50-81-7 QSA32.1,3-dialkoxy-benzene No 50-81-7 QSA33.1-phenoxy-benzene No 50-81-7 QSA34.H-acceptor-path3-H-acceptor Yes 50-81-7 QSA35.Oxolane No 50-81-7 QSA36.Carbodiimides No 50-81-7 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-asparagine	1	QSA1.Acyl halides No 70-47-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 70-47-3 QSA3.N-methylol derivatives No 70-47-3 QSA4.Monohaloalkene No 70-47-3 QSA5.S or N mustard No 70-47-3 QSA6.Propiolactones and propiosultones No 70-47-3 QSA7.Epoxides and aziridines No 70-47-3 QSA8.Aliphatic halogens No 70-47-3 QSA9.Alkyl nitrite No 70-47-3 QSA10.α,β unsaturated carbonyls No 70-47-3 QSA11.Simple aldehyde No 70-47-3 QSA12.Quinones No 70-47-3 QSA13.Hydrazine No 70-47-3 QSA14.Aliphatic azo and azoxy No 70-47-3 QSA15.Isocyanate and isothiocyanate groups No 70-47-3 QSA16.Alkyl carbamate and thiocarbamate No 70-47-3 QSA18.Polycyclic Aromatic Hydrocarbons No 70-47-3 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 70-47-3 QSA21.Alkyl and aryl N-nitroso groups No 70-47-3 QSA22.Azide and triazene groups No 70-47-3 QSA23.Aliphatic N-nitro No 70-47-3 QSA24.α,β unsaturated alkoxy No 70-47-3 QSA25.Aromatic nitroso group No 70-47-3 QSA26.Aromatic ring N-oxide No 70-47-3 QSA27.Nitro aromatic No 70-47-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 70-47-3 QSA28bis.Aromatic mono- and dialkylamine No 70-47-3 QSA28ter.Aromatic N-acyl amine No 70-47-3 QSA29.Aromatic diazo No 70-47-3 QSA30.Coumarins and Furocoumarins No 70-47-3 QSA32.1,3-dialkoxy-benzene No 70-47-3 QSA33.1-phenoxy-benzene No 70-47-3 QSA34.H-acceptor-path3-H-acceptor Yes 70-47-3 QSA35.Oxolane No 70-47-3 QSA36.Carbodiimides No 70-47-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-cysteine	1	QSA1.Acyl halides No 52-90-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 52-90-4 QSA3.N-methylol derivatives No 52-90-4 QSA4.Monohaloalkene No 52-90-4 QSA5.S or N mustard No 52-90-4 QSA6.Propiolactones and propiosultones No 52-90-4 QSA7.Epoxides and aziridines No 52-90-4 QSA8.Aliphatic halogens No 52-90-4 QSA9.Alkyl nitrite No 52-90-4 QSA10.α,β unsaturated carbonyls No 52-90-4 QSA11.Simple aldehyde No 52-90-4 QSA12.Quinones No 52-90-4 QSA13.Hydrazine No 52-90-4 QSA14.Aliphatic azo and azoxy No 52-90-4 QSA15.Isocyanate and isothiocyanate groups No 52-90-4 QSA16.Alkyl carbamate and thiocarbamate No 52-90-4 QSA18.Polycyclic Aromatic Hydrocarbons No 52-90-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 52-90-4 QSA21.Alkyl and aryl N-nitroso groups No 52-90-4 QSA22.Azide and triazene groups No 52-90-4 QSA23.Aliphatic N-nitro No 52-90-4 QSA24.α,β unsaturated alkoxy No 52-90-4 QSA25.Aromatic nitroso group No 52-90-4 QSA26.Aromatic ring N-oxide No 52-90-4 QSA27.Nitro aromatic No 52-90-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 52-90-4 QSA28bis.Aromatic mono- and dialkylamine No 52-90-4 QSA28ter.Aromatic N-acyl amine No 52-90-4 QSA29.Aromatic diazo No 52-90-4 QSA30.Coumarins and Furocoumarins No 52-90-4 QSA32.1,3-dialkoxy-benzene No 52-90-4 QSA33.1-phenoxy-benzene No 52-90-4 QSA34.H-acceptor-path3-H-acceptor Yes 52-90-4 QSA35.Oxolane No 52-90-4 QSA36.Carbodiimides No 52-90-4 QAny alert?.At least one

Table 18 Continued

		alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-cystine	1	QSA1.Acyl halides No 56-89-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-89-3 QSA3.N-methylol derivatives No 56-89-3 QSA4.Monohaloalkene No 56-89-3 QSA5.S or N mustard No 56-89-3 QSA6.Propiolactones and propiosultones No 56-89-3 QSA7.Epoxides and aziridines No 56-89-3 QSA8.Aliphatic halogens No 56-89-3 QSA9.Alkyl nitrite No 56-89-3 QSA10.α,β unsaturated carbonyls No 56-89-3 QSA11.Simple aldehyde No 56-89-3 QSA12.Quinones No 56-89-3 QSA13.Hydrazine No 56-89-3 QSA14.Aliphatic azo and azoxy No 56-89-3 QSA15.Isocyanate and isothiocyanate groups No 56-89-3 QSA16.Alkyl carbamate and thiocarbamate No 56-89-3 QSA18.Polycyclic Aromatic Hydrocarbons No 56-89-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-89-3 QSA21.Alkyl and aryl N-nitroso groups No 56-89-3 QSA22.Azide and triazene groups No 56-89-3 QSA23.Aliphatic N-nitro No 56-89-3 QSA24.α,β unsaturated alkoxy No 56-89-3 QSA25.Aromatic nitroso group No 56-89-3 QSA26.Aromatic ring N-oxide No 56-89-3 QSA27.Nitro aromatic No 56-89-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-89-3 QSA28bis.Aromatic mono- and dialkylamine No 56-89-3 QSA28ter.Aromatic N-acyl amine No 56-89-3 QSA29.Aromatic diazo No 56-89-3 QSA30.Coumarins and Furocoumarins No 56-89-3 QSA32.1,3-dialkoxy-benzene No 56-89-3 QSA33.1-phenoxy-benzene No 56-89-3 QSA34.H-acceptor-path3-H-acceptor Yes 56-89-3 QSA35.Oxolane No 56-89-3 QSA36.Carbodiimides No 56-89-3 QAny alert?.At least one alert fired? Yes
L-glutamic acid	1	QSA1.Acyl halides No 56-86-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-86-0 QSA3.N-methylol derivatives No 56-86-0 QSA4.Monohaloalkene No 56-86-0 QSA5.S or N mustard No 56-86-0 QSA6.Propiolactones and propiosultones No 56-86-0 QSA7.Epoxides and aziridines No 56-86-0 QSA8.Aliphatic halogens No 56-86-0 QSA9.Alkyl nitrite No 56-86-0 QSA10.α,β unsaturated carbonyls No 56-86-0 QSA11.Simple aldehyde No 56-86-0 QSA12.Quinones No 56-86-0 QSA13.Hydrazine No 56-86-0 QSA14.Aliphatic azo and azoxy No 56-86-0 QSA15.Isocyanate and isothiocyanate groups No 56-86-0 QSA16.Alkyl carbamate and thiocarbamate No 56-86-0 QSA18.Polycyclic Aromatic Hydrocarbons No 56-86-0 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 56-86-0 QSA21.Alkyl and aryl N-nitroso groups No 56-86-0 QSA22.Azide and triazene groups No 56-86-0 QSA23.Aliphatic N-nitro No 56-86-0 QSA24.α,β unsaturated alkoxy No 56-86-0 QSA25.Aromatic nitroso group No 56-86-0 QSA26.Aromatic ring N-oxide No 56-86-0 QSA27.Nitro aromatic No 56-86-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-86-0 QSA28bis.Aromatic mono- and dialkylamine No 56-86-0 QSA28ter.Aromatic N-acyl amine No 56-86-0 QSA29.Aromatic diazo No 56-86-0 QSA30.Coumarins and Furocoumarins No 56-86-0 QSA32.1,3-dialkoxy-benzene No 56-86-0 QSA33.1-phenoxy-benzene No 56-86-0 QSA34.H-acceptor-path3-H-acceptor Yes 56-86-0 QSA35.Oxolane No 56-86-0 QSA36.Carbodiimides No 56-86-0 QAny alert?.At least one alert fired? Yes
L-glutamine	1	QSA1.Acyl halides No 56-86-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-86-0 QSA3.N-methylol derivatives No 56-86-0 QSA4.Monohaloalkene No 56-86-0 QSA5.S or N mustard No 56-86-0 QSA6.Propiolactones and propiosultones No 56-86-0 QSA7.Epoxides and aziridines No 56-86-0 QSA8.Aliphatic halogens No 56-86-0 QSA9.Alkyl nitrite No 56-86-0 QSA10.α,β unsaturated carbonyls No 56-86-0 QSA11.Simple aldehyde No 56-86-0 QSA12.Quinones No 56-86-0 QSA13.Hydrazine No 56-86-0 QSA14.Aliphatic azo and azoxy No 56-86-0 QSA15.Isocyanate and isothiocyanate groups No 56-86-0 QSA16.Alkyl carbamate and thiocarbamate No 56-86-0 QSA18.Polycyclic Aromatic Hydrocarbons No 56-86-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-86-0 QSA21.Alkyl and aryl N-nitroso groups No 56-86-0 QSA22.Azide and triazene groups No 56-86-0 QSA23.Aliphatic N-nitro No 56-86-0 QSA24.α,β unsaturated alkoxy No 56-86-0 QSA25.Aromatic nitroso group No 56-86-0 QSA26.Aromatic ring N-oxide No 56-86-0 QSA27.Nitro aromatic No 56-86-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-86-0 QSA28bis.Aromatic mono- and dialkylamine No 56-86-0 QSA28ter.Aromatic N-acyl amine No 56-86-0 QSA29.Aromatic diazo No 56-86-0 QSA30.Coumarins and Furocoumarins No 56-86-0 QSA32.1,3-dialkoxy-benzene No 56-86-0 QSA33.1-phenoxy-benzene No 56-86-0 QSA34.H-acceptor-path3-H-acceptor Yes 56-86-0 QSA35.Oxolane No 56-86-0 QSA36.Carbodiimides No 56-86-0 QAny alert?.At least one alert fired? Yes

Table 18 Continued

L-histidine	1	QSA1.Acyl halides No 71-00-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 71-00-1 QSA3.N-methylol derivatives No 71-00-1 QSA4.Monohaloalkene No 71-00-1 QSA5.S or N mustard No 71-00-1 QSA6.Propiolactones and propiosultones No 71-00-1 QSA7.Epoxides and aziridines No 71-00-1 QSA8.Aliphatic halogens No 71-00-1 QSA9.Alkyl nitrite No 71-00-1 QSA10.α,β unsaturated carbonyls No 71-00-1 QSA11.Simple aldehyde No 71-00-1 QSA12.Quinones No 71-00-1 QSA13.Hydrazine No 71-00-1 QSA14.Aliphatic azo and azoxy No 71-00-1 QSA15.Isocyanate and isothiocyanate groups No 71-00-1 QSA16.Alkyl carbamate and thiocarbamate No 71-00-1 QSA18.Polycyclic Aromatic Hydrocarbons No 71-00-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 71-00-1 QSA21.Alkyl and aryl N-nitroso groups No 71-00-1 QSA22.Azide and triazene groups No 71-00-1 QSA23.Aliphatic N-nitro No 71-00-1 QSA24.α,β unsaturated alkoxy No 71-00-1 QSA25.Aromatic nitroso group No 71-00-1 QSA26.Aromatic ring N-oxide No 71-00-1 QSA27.Nitro aromatic No 71-00-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 71-00-1 QSA28bis.Aromatic mono- and dialkylamine No 71-00-1 QSA28ter.Aromatic N-acyl amine No 71-00-1 QSA29.Aromatic diazo No 71-00-1 QSA30.Coumarins and Furocoumarins No 71-00-1 QSA32.1,3-dialkoxy-benzene No 71-00-1 QSA33.1-phenoxy-benzene No 71-00-1 QSA34.H-acceptor-path3-H-acceptor Yes 71-00-1 QSA35.Oxolane No 71-00-1 QSA36.Carbodiimides No 71-00-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-isoleucine	1	QSA1.Acyl halides No 73-32-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 73-32-5 QSA3.N-methylol derivatives No 73-32-5 QSA4.Monohaloalkene No 73-32-5 QSA5.S or N mustard No 73-32-5 QSA6.Propiolactones and propiosultones No 73-32-5 QSA7.Epoxides and aziridines No 73-32-5 QSA8.Aliphatic halogens No 73-32-5 QSA9.Alkyl nitrite No 73-32-5 QSA10.α,β unsaturated carbonyls No 73-32-5 QSA11.Simple aldehyde No 73-32-5 QSA12.Quinones No 73-32-5 QSA13.Hydrazine No 73-32-5 QSA14.Aliphatic azo and azoxy No 73-32-5 QSA15.Isocyanate and isothiocyanate groups No 73-32-5 QSA16.Alkyl carbamate and thiocarbamate No 73-32-5 QSA18.Polycyclic Aromatic Hydrocarbons No 73-32-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 73-32-5 QSA21.Alkyl and aryl N-

Table 18 Continued

		nitroso groups No 73-32-5 QSA22.Azide and triazene groups No 73-32-5 QSA23.Aliphatic N-nitro No 73-32-5 QSA24.α,β unsaturated alkoxy No 73-32-5 QSA25.Aromatic nitroso group No 73-32-5 QSA26.Aromatic ring N-oxide No 73-32-5 QSA27.Nitro aromatic No 73-32-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 73-32-5 QSA28bis.Aromatic mono- and dialkylamine No 73-32-5 QSA28ter.Aromatic N-acyl amine No 73-32-5 QSA29.Aromatic diazo No 73-32-5 QSA30.Coumarins and Furocoumarins No 73-32-5 QSA32.1,3-dialkoxy-benzene No 73-32-5 QSA33.1-phenoxy-benzene No 73-32-5 QSA34.H-acceptor-path3-H-acceptor Yes 73-32-5 QSA35.Oxolane No 73-32-5 QSA36.Carbodiimides No 73-32-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-leucine	1	QSA1.Acyl halides No 73-32-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 73-32-5 QSA3.N-methylol derivatives No 73-32-5 QSA4.Monohaloalkene No 73-32-5 QSA5.S or N mustard No 73-32-5 QSA6.Propiolactones and propiosultones No 73-32-5 QSA7.Epoxides and aziridines No 73-32-5 QSA8.Aliphatic halogens No 73-32-5 QSA9.Alkyl nitrite No 73-32-5 QSA10.α,β unsaturated carbonyls No 73-32-5 QSA11.Simple aldehyde No 73-32-5 QSA12.Quinones No 73-32-5 QSA13.Hydrazine No 73-32-5 QSA14.Aliphatic azo and azoxy No 73-32-5 QSA15.Isocyanate and isothiocyanate groups No 73-32-5 QSA16.Alkyl carbamate and thiocarbamate No 73-32-5 QSA18.Polycyclic Aromatic Hydrocarbons No 73-32-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 73-32-5 QSA21.Alkyl and aryl N-nitroso groups No 73-32-5 QSA22.Azide and triazene groups No 73-32-5 QSA23.Aliphatic N-nitro No 73-32-5 QSA24.α,β unsaturated alkoxy No 73-32-5 QSA25.Aromatic nitroso group No 73-32-5 QSA26.Aromatic ring N-oxide No 73-32-5 QSA27.Nitro aromatic No 73-32-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 73-32-5 QSA28bis.Aromatic mono- and dialkylamine No 73-32-5 QSA28ter.Aromatic N-acyl amine No 73-32-5 QSA29.Aromatic diazo No 73-32-5 QSA30.Coumarins and Furocoumarins No 73-32-5 QSA32.1,3-dialkoxy-benzene No 73-32-5 QSA33.1-phenoxy-benzene No 73-32-5 QSA34.H-acceptor-path3-H-acceptor Yes 73-32-5 QSA35.Oxolane No 73-32-5 QSA36.Carbodiimides No 73-32-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the

Table 18 Continued

		micronucleus assay (Class I)
L-lysine	1	QSA1.Acyl halides No 56-87-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-87-1 QSA3.N-methylol derivatives No 56-87-1 QSA4.Monohaloalkene No 56-87-1 QSA5.S or N mustard No 56-87-1 QSA6.Propiolactones and propiosultones No 56-87-1 QSA7.Epoxides and aziridines No 56-87-1 QSA8.Aliphatic halogens No 56-87-1 QSA9.Alkyl nitrite No 56-87-1 QSA10.α,β unsaturated carbonyls No 56-87-1 QSA11.Simple aldehyde No 56-87-1 QSA12.Quinones No 56-87-1 QSA13.Hydrazine No 56-87-1 QSA14.Aliphatic azo and azoxy No 56-87-1 QSA15.Isocyanate and isothiocyanate groups No 56-87-1 QSA16.Alkyl carbamate and thiocarbamate No 56-87-1 QSA18.Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA21.Alkyl and aryl N-nitroso groups No 56-87-1 QSA22.Azide and triazene groups No 56-87-1 QSA23.Aliphatic N-nitro No 56-87-1 QSA24.α,β unsaturated alkoxy No 56-87-1 QSA25.Aromatic nitroso group No 56-87-1 QSA26.Aromatic ring N-oxide No 56-87-1 QSA27.Nitro aromatic No 56-87-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-87-1 QSA28bis.Aromatic mono- and dialkylamine No 56-87-1 QSA28ter.Aromatic N-acyl amine No 56-87-1 QSA29.Aromatic diazo No 56-87-1 QSA30.Coumarins and Furocoumarins No 56-87-1 QSA32.1,3-dialkoxy-benzene No 56-87-1 QSA33.1-phenoxy-benzene No 56-87-1 QSA34.H-acceptor-path3-H-acceptor Yes 56-87-1 QSA35.Oxolane No 56-87-1 QSA36.Carbodiimides No 56-87-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-methionine	1	QSA1.Acyl halides No 56-87-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-87-1 QSA3.N-methylol derivatives No 56-87-1 QSA4.Monohaloalkene No 56-87-1 QSA5.S or N mustard No 56-87-1 QSA6.Propiolactones and propiosultones No 56-87-1 QSA7.Epoxides and aziridines No 56-87-1 QSA8.Aliphatic halogens No 56-87-1 QSA9.Alkyl nitrite No 56-87-1 QSA10.α,β unsaturated carbonyls No 56-87-1 QSA11.Simple aldehyde No 56-87-1 QSA12.Quinones No 56-87-1 QSA13.Hydrazine No 56-87-1 QSA14.Aliphatic azo and azoxy No 56-87-1 QSA15.Isocyanate and isothiocyanate groups No 56-87-1 QSA16.Alkyl carbamate and thiocarbamate No 56-87-1 QSA18.Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 56-87-1 QSA21.Alkyl and aryl N-nitroso groups No 56-87-1 QSA22.Azide and triazene groups No 56-87-1 QSA23.Aliphatic N-nitro No 56-87-1 QSA24.α,β unsaturated alkoxy No 56-87-1 QSA25.Aromatic nitroso group No 56-87-1 QSA26.Aromatic ring N-oxide No 56-87-1 QSA27.Nitro aromatic No 56-87-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-87-1 QSA28bis.Aromatic mono- and dialkylamine No 56-87-1 QSA28ter.Aromatic N-acyl amine No 56-87-1 QSA29.Aromatic diazo No 56-87-1 QSA30.Coumarins and Furocoumarins No 56-87-1 QSA32.1,3-dialkoxy-benzene No 56-87-1 QSA33.1-phenoxy-benzene No 56-87-1 QSA34.H-acceptor-path3-H-acceptor Yes 56-87-1 QSA35.Oxolane No 56-87-1 QSA36.Carbodiimides No 56-87-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-phenylalanine	1	QSA1.Acyl halides No 56-87-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-87-1 QSA3.N-methylol derivatives No 56-87-1 QSA4.Monohaloalkene No 56-87-1 QSA5.S or N mustard No 56-87-1 QSA6.Propiolactones and propiosultones No 56-87-1 QSA7.Epoxides and aziridines No 56-87-1 QSA8.Aliphatic halogens No 56-87-1 QSA9.Alkyl nitrite No 56-87-1 QSA10.α,β unsaturated carbonyls No 56-87-1 QSA11.Simple aldehyde No 56-87-1 QSA12.Quinones No 56-87-1 QSA13.Hydrazine No 56-87-1 QSA14.Aliphatic azo and azoxy No 56-87-1 QSA15.Isocyanate and isothiocyanate groups No 56-87-1 QSA16.Alkyl carbamate and thiocarbamate No 56-87-1 QSA18.Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA21.Alkyl and aryl N-nitroso groups No 56-87-1 QSA22.Azide and triazene groups No 56-87-1 QSA23.Aliphatic N-nitro No 56-87-1 QSA24.α,β unsaturated alkoxy No 56-87-1 QSA25.Aromatic nitroso group No 56-87-1 QSA26.Aromatic ring N-oxide No 56-87-1 QSA27.Nitro aromatic No 56-87-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-87-1 QSA28bis.Aromatic mono- and dialkylamine No 56-87-1 QSA28ter.Aromatic N-acyl amine No 56-87-1 QSA29.Aromatic diazo No 56-87-1 QSA30.Coumarins and Furocoumarins No 56-87-1 QSA32.1,3-dialkoxy-benzene No 56-87-1 QSA33.1-phenoxy-benzene No 56-87-1 QSA34.H-acceptor-path3-H-acceptor Yes 56-87-1 QSA35.Oxolane No 56-87-1 QSA36.Carbodiimides No 56-87-1 QAny alert?.At least one

Table 18 Continued

		alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-proline	1	QSA1.Acyl halides No 56-87-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-87-1 QSA3.N-methylol derivatives No 56-87-1 QSA4.Monohaloalkene No 56-87-1 QSA5.S or N mustard No 56-87-1 QSA6.Propiolactones and propiosultones No 56-87-1 QSA7.Epoxides and aziridines No 56-87-1 QSA8.Aliphatic halogens No 56-87-1 QSA9.Alkyl nitrite No 56-87-1 QSA10.α,β unsaturated carbonyls No 56-87-1 QSA11.Simple aldehyde No 56-87-1 QSA12.Quinones No 56-87-1 QSA13.Hydrazine No 56-87-1 QSA14.Aliphatic azo and azoxy No 56-87-1 QSA15.Isocyanate and isothiocyanate groups No 56-87-1 QSA16.Alkyl carbamate and thiocarbamate No 56-87-1 QSA18.Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA21.Alkyl and aryl N-nitroso groups No 56-87-1 QSA22.Azide and triazene groups No 56-87-1 QSA23.Aliphatic N-nitro No 56-87-1 QSA24.α,β unsaturated alkoxy No 56-87-1 QSA25.Aromatic nitroso group No 56-87-1 QSA26.Aromatic ring N-oxide No 56-87-1 QSA27.Nitro aromatic No 56-87-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-87-1 QSA28bis.Aromatic mono- and dialkylamine No 56-87-1 QSA28ter.Aromatic N-acyl amine No 56-87-1 QSA29.Aromatic diazo No 56-87-1 QSA30.Coumarins and Furocoumarins No 56-87-1 QSA32.1,3-dialkoxy-benzene No 56-87-1 QSA33.1-phenoxy-benzene No 56-87-1 QSA34.H-acceptor-path3-H-acceptor Yes 56-87-1 QSA35.Oxolane No 56-87-1 QSA36.Carbodiimides No 56-87-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-serine	1	QSA1.Acyl halides No 56-87-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 56-87-1 QSA3.N-methylol derivatives No 56-87-1 QSA4.Monohaloalkene No 56-87-1 QSA5.S or N mustard No 56-87-1 QSA6.Propiolactones and propiosultones No 56-87-1 QSA7.Epoxides and aziridines No 56-87-1 QSA8.Aliphatic halogens No 56-87-1 QSA9.Alkyl nitrite No 56-87-1 QSA10.α,β unsaturated carbonyls No 56-87-1 QSA11.Simple aldehyde No 56-87-1 QSA12.Quinones No 56-87-1 QSA13.Hydrazine No 56-87-1 QSA14.Aliphatic azo and azoxy No 56-87-1 QSA15.Isocyanate and isothiocyanate groups No 56-87-1 QSA16.Alkyl carbamate and thiocarbamate No 56-87-1 QSA18.Polycyclic Aromatic

Table 18 Continued

		Hydrocarbons No 56-87-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 56-87-1 QSA21.Alkyl and aryl N-nitroso groups No 56-87-1 QSA22.Azide and triazene groups No 56-87-1 QSA23.Aliphatic N-nitro No 56-87-1 QSA24.α,β unsaturated alkoxy No 56-87-1 QSA25.Aromatic nitroso group No 56-87-1 QSA26.Aromatic ring N-oxide No 56-87-1 QSA27.Nitro aromatic No 56-87-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 56-87-1 QSA28bis.Aromatic mono- and dialkylamine No 56-87-1 QSA28ter.Aromatic N-acyl amine No 56-87-1 QSA29.Aromatic diazo No 56-87-1 QSA30.Coumarins and Furocoumarins No 56-87-1 QSA32.1,3-dialkoxy-benzene No 56-87-1 QSA33.1-phenoxy-benzene No 56-87-1 QSA34.H-acceptor-path3-H-acceptor Yes 56-87-1 QSA35.Oxolane No 56-87-1 QSA36.Carbodiimides No 56-87-1 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-threonine	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5

Table 18 Continued

		QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-tryptophan	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-tyrosine	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and

Table 18 Continued

		thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
L-valine	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-

Table 18 Continued

		acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
magnesium	0	
magnesium chloride	0	
magnesium silicate (talc)	0	
magnesium stearate	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
magnesium sulfate	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic

Table 18 Continued

		halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
mannitol	1	QSA1.Acyl halides No 72-19-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 72-19-5 QSA3.N-methylol derivatives No 72-19-5 QSA4.Monohaloalkene No 72-19-5 QSA5.S or N mustard No 72-19-5 QSA6.Propiolactones and propiosultones No 72-19-5 QSA7.Epoxides and aziridines No 72-19-5 QSA8.Aliphatic halogens No 72-19-5 QSA9.Alkyl nitrite No 72-19-5 QSA10.α,β unsaturated carbonyls No 72-19-5 QSA11.Simple aldehyde No 72-19-5 QSA12.Quinones No 72-19-5 QSA13.Hydrazine No 72-19-5 QSA14.Aliphatic azo and azoxy No 72-19-5 QSA15.Isocyanate and isothiocyanate groups No 72-19-5 QSA16.Alkyl carbamate and thiocarbamate No 72-19-5 QSA18.Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 72-19-5 QSA21.Alkyl and aryl N-nitroso groups No 72-19-5 QSA22.Azide and triazene groups No 72-19-5 QSA23.Aliphatic N-nitro No 72-19-5 QSA24.α,β unsaturated alkoxy No 72-19-5 QSA25.Aromatic nitroso group No 72-19-5 QSA26.Aromatic ring N-oxide No 72-19-5 QSA27.Nitro aromatic No 72-19-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with

Table 18 Continued

		restrictions) No 72-19-5 QSA28bis.Aromatic mono- and dialkylamine No 72-19-5 QSA28ter.Aromatic N-acyl amine No 72-19-5 QSA29.Aromatic diazo No 72-19-5 QSA30.Coumarins and Furocoumarins No 72-19-5 QSA32.1,3-dialkoxy-benzene No 72-19-5 QSA33.1-phenoxy-benzene No 72-19-5 QSA34.H-acceptor-path3-H-acceptor Yes 72-19-5 QSA35.Oxolane No 72-19-5 QSA36.Carbodiimides No 72-19-5 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
menadione	1	QSA1.Acyl halides No 58-27-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 58-27-5 QSA3.N-methylol derivatives No 58-27-5 QSA4.Monohaloalkene No 58-27-5 QSA5.S or N mustard No 58-27-5 QSA6.Propiolactones and propiosultones No 58-27-5 QSA7.Epoxides and aziridines No 58-27-5 QSA8.Aliphatic halogens No 58-27-5 QSA9.Alkyl nitrite No 58-27-5 QSA10.α,β unsaturated carbonyls No 58-27-5 QSA11.Simple aldehyde No 58-27-5 QSA12.Quinones Yes 58-27-5 QSA13.Hydrazine No 58-27-5 QSA14.Aliphatic azo and azoxy No 58-27-5 QSA15.Isocyanate and isothiocyanate groups No 58-27-5 QSA16.Alkyl carbamate and thiocarbamate No 58-27-5 QSA18.Polycyclic Aromatic Hydrocarbons No 58-27-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 58-27-5 QSA21.Alkyl and aryl N-nitroso groups No 58-27-5 QSA22.Azide and triazene groups No 58-27-5 QSA23.Aliphatic N-nitro No 58-27-5 QSA24.α,β unsaturated alkoxy No 58-27-5 QSA25.Aromatic nitroso group No 58-27-5 QSA26.Aromatic ring N-oxide No 58-27-5 QSA27.Nitro aromatic No 58-27-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 58-27-5 QSA28bis.Aromatic mono- and dialkylamine No 58-27-5 QSA28ter.Aromatic N-acyl amine No 58-27-5 QSA29.Aromatic diazo No 58-27-5 QSA30.Coumarins and Furocoumarins No 58-27-5 QSA32.1,3-dialkoxy-benzene No 58-27-5 QSA33.1-phenoxy-benzene No 58-27-5 QSA34.H-acceptor-path3-H-acceptor Yes 58-27-5 QSA35.Oxolane No 58-27-5 QSA36.Carbodiimides No 58-27-5 QAny alert?.At least one alert fired? Yes
mercury	0	
methylcyclopentane	0	
methyltrimethoxysilane	0	
monobasic	1	QSA1.Acyl halides No 7778-77-0 QSA2.Alkyl (C5) or benzyl

Table 18 Continued

potassium phosphate		ester of sulphonic or phosphonic acid No 7778-77-0 QSA3.N-methylol derivatives No 7778-77-0 QSA4.Monohaloalkene No 7778-77-0 QSA5.S or N mustard No 7778-77-0 QSA6.Propiolactones and propiosultones No 7778-77-0 QSA7.Epoxides and aziridines No 7778-77-0 QSA8.Aliphatic halogens No 7778-77-0 QSA9.Alkyl nitrite No 7778-77-0 QSA10.α,β unsaturated carbonyls No 7778-77-0 QSA11.Simple aldehyde No 7778-77-0 QSA12.Quinones No 7778-77-0 QSA13.Hydrazine No 7778-77-0 QSA14.Aliphatic azo and azoxy No 7778-77-0 QSA15.Isocyanate and isothiocyanate groups No 7778-77-0 QSA16.Alkyl carbamate and thiocarbamate No 7778-77-0 QSA18.Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA21.Alkyl and aryl N-nitroso groups No 7778-77-0 QSA22.Azide and triazene groups No 7778-77-0 QSA23.Aliphatic N-nitro No 7778-77-0 QSA24.α,β unsaturated alkoxy No 7778-77-0 QSA25.Aromatic nitroso group No 7778-77-0 QSA26.Aromatic ring N-oxide No 7778-77-0 QSA27.Nitro aromatic No 7778-77-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7778-77-0 QSA28bis.Aromatic mono- and dialkylamine No 7778-77-0 QSA28ter.Aromatic N-acyl amine No 7778-77-0 QSA29.Aromatic diazo No 7778-77-0 QSA30.Coumarins and Furocoumarins No 7778-77-0 QSA32.1,3-dialkoxy-benzene No 7778-77-0 QSA33.1-phenoxy-benzene No 7778-77-0 QSA34.H-acceptor-path3-H-acceptor Yes 7778-77-0 QSA35.Oxolane No 7778-77-0 QSA36.Carbodiimides No 7778-77-0 QAny alert?.At least one alert fired? Ye
monobasic sodium phosphate	1	QSA1.Acyl halides No 7778-77-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7778-77-0 QSA3.N-methylol derivatives No 7778-77-0 QSA4.Monohaloalkene No 7778-77-0 QSA5.S or N mustard No 7778-77-0 QSA6.Propiolactones and propiosultones No 7778-77-0 QSA7.Epoxides and aziridines No 7778-77-0 QSA8.Aliphatic halogens No 7778-77-0 QSA9.Alkyl nitrite No 7778-77-0 QSA10.α,β unsaturated carbonyls No 7778-77-0 QSA11.Simple aldehyde No 7778-77-0 QSA12.Quinones No 7778-77-0 QSA13.Hydrazine No 7778-77-0 QSA14.Aliphatic azo and azoxy No 7778-77-0 QSA15.Isocyanate and isothiocyanate groups No 7778-77-0 QSA16.Alkyl carbamate and thiocarbamate No 7778-77-0 QSA18.Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA21.Alkyl and aryl

Table 18 Continued

		N-nitroso groups No 7778-77-0 QSA22.Azide and triazene groups No 7778-77-0 QSA23.Aliphatic N-nitro No 7778-77-0 QSA24.α,β unsaturated alkoxy No 7778-77-0 QSA25.Aromatic nitroso group No 7778-77-0 QSA26.Aromatic ring N-oxide No 7778-77-0 QSA27.Nitro aromatic No 7778-77-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7778-77-0 QSA28bis.Aromatic mono- and dialkylamine No 7778-77-0 QSA28ter.Aromatic N-acyl amine No 7778-77-0 QSA29.Aromatic diazo No 7778-77-0 QSA30.Coumarins and Furocoumarins No 7778-77-0 QSA32.1,3-dialkoxy-benzene No 7778-77-0 QSA33.1-phenoxy-benzene No 7778-77-0 QSA34.H-acceptor-path3-H-acceptor Yes 7778-77-0 QSA35.Oxolane No 7778-77-0 QSA36.Carbodiimides No 7778-77-0 QAny alert?.At least one alert fired? Ye
monosodium L glutamate	1	QSA1.Acyl halides No 7778-77-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7778-77-0 QSA3.N-methylol derivatives No 7778-77-0 QSA4.Monohaloalkene No 7778-77-0 QSA5.S or N mustard No 7778-77-0 QSA6.Propiolactones and propiosultones No 7778-77-0 QSA7.Epoxides and aziridines No 7778-77-0 QSA8.Aliphatic halogens No 7778-77-0 QSA9.Alkyl nitrite No 7778-77-0 QSA10.α,β unsaturated carbonyls No 7778-77-0 QSA11.Simple aldehyde No 7778-77-0 QSA12.Quinones No 7778-77-0 QSA13.Hydrazine No 7778-77-0 QSA14.Aliphatic azo and azoxy No 7778-77-0 QSA15.Isocyanate and isothiocyanate groups No 7778-77-0 QSA16.Alkyl carbamate and thiocarbamate No 7778-77-0 QSA18.Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 7778-77-0 QSA21.Alkyl and aryl N-nitroso groups No 7778-77-0 QSA22.Azide and triazene groups No 7778-77-0 QSA23.Aliphatic N-nitro No 7778-77-0 QSA24.α,β unsaturated alkoxy No 7778-77-0 QSA25.Aromatic nitroso group No 7778-77-0 QSA26.Aromatic ring N-oxide No 7778-77-0 QSA27.Nitro aromatic No 7778-77-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 7778-77-0 QSA28bis.Aromatic mono- and dialkylamine No 7778-77-0 QSA28ter.Aromatic N-acyl amine No 7778-77-0 QSA29.Aromatic diazo No 7778-77-0 QSA30.Coumarins and Furocoumarins No 7778-77-0 QSA32.1,3-dialkoxy-benzene No 7778-77-0 QSA33.1-phenoxy-benzene No 7778-77-0 QSA34.H-acceptor-path3-H-acceptor Yes 7778-77-0 QSA35.Oxolane No 7778-77-0 QSA36.Carbodiimides No 7778-77-0 QAny alert?.At least one alert fired? Ye

Table 18 Continued

m-xylene	0	
nadide (NAD)	1	QSA1.Acyl halides No 53-84-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 53-84-9 QSA3.N-methylol derivatives No 53-84-9 QSA4.Monohaloalkene No 53-84-9 QSA5.S or N mustard No 53-84-9 QSA6.Propiolactones and propiosultones No 53-84-9 QSA7.Epoxides and aziridines No 53-84-9 QSA8.Aliphatic halogens No 53-84-9 QSA9.Alkyl nitrite No 53-84-9 QSA10.α,β unsaturated carbonyls No 53-84-9 QSA11.Simple aldehyde No 53-84-9 QSA12.Quinones No 53-84-9 QSA13.Hydrazine No 53-84-9 QSA14.Aliphatic azo and azoxy No 53-84-9 QSA15.Isocyanate and isothiocyanate groups No 53-84-9 QSA16.Alkyl carbamate and thiocarbamate No 53-84-9 QSA18.Polycyclic Aromatic Hydrocarbons No 53-84-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 53-84-9 QSA21.Alkyl and aryl N-nitroso groups No 53-84-9 QSA22.Azide and triazene groups No 53-84-9 QSA23.Aliphatic N-nitro No 53-84-9 QSA24.α,β unsaturated alkoxy No 53-84-9 QSA25.Aromatic nitroso group No 53-84-9 QSA26.Aromatic ring N-oxide No 53-84-9 QSA27.Nitro aromatic No 53-84-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 53-84-9 QSA28bis.Aromatic mono- and dialkylamine No 53-84-9 QSA28ter.Aromatic N-acyl amine No 53-84-9 QSA29.Aromatic diazo No 53-84-9 QSA30.Coumarins and Furocoumarins No 53-84-9 QSA32.1,3-dialkoxy-benzene No 53-84-9 QSA33.1-phenoxy-benzene No 53-84-9 QSA34.H-acceptor-path3-H-acceptor Yes 53-84-9 QSA35.Oxolane Yes 53-84-9 QSA36.Carbodiimides No 53-84-9 QAny alert?.At least one alert fired? Yes
n-dodecane	0	
neomycin	1	QSA1.Acyl halides No 1404-04-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1404-04-2 QSA3.N-methylol derivatives No 1404-04-2 QSA4.Monohaloalkene No 1404-04-2 QSA5.S or N mustard No 1404-04-2 QSA6.Propiolactones and propiosultones No 1404-04-2 QSA7.Epoxides and aziridines No 1404-04-2 QSA8.Aliphatic halogens No 1404-04-2 QSA9.Alkyl nitrite No 1404-04-2 QSA10.α,β unsaturated carbonyls No 1404-04-2 QSA11.Simple aldehyde No 1404-04-2 QSA12.Quinones No 1404-04-2 QSA13.Hydrazine No 1404-04-2 QSA14.Aliphatic azo and azoxy No 1404-04-2 QSA15.Isocyanate and isothiocyanate groups No 1404-04-2 QSA16.Alkyl carbamate and thiocarbamate No 1404-04-2 QSA18.Polycyclic Aromatic

Table 18 Continued

		Hydrocarbons No 1404-04-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1404-04-2 QSA21.Alkyl and aryl N-nitroso groups No 1404-04-2 QSA22.Azide and triazene groups No 1404-04-2 QSA23.Aliphatic N-nitro No 1404-04-2 QSA24.α,β unsaturated alkoxy No 1404-04-2 QSA25.Aromatic nitroso group No 1404-04-2 QSA26.Aromatic ring N-oxide No 1404-04-2 QSA27.Nitro aromatic No 1404-04-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1404-04-2 QSA28bis.Aromatic mono- and dialkylamine No 1404-04-2 QSA28ter.Aromatic N-acyl amine No 1404-04-2 QSA29.Aromatic diazo No 1404-04-2 QSA30.Coumarins and Furocoumarins No 1404-04-2 QSA32.1,3-dialkoxy-benzene No 1404-04-2 QSA33.1-phenoxy-benzene No 1404-04-2 QSA34.H-acceptor-path3-H-acceptor Yes 1404-04-2 QSA35.Oxolane No 1404-04-2 QSA36.Carbodiimides No 1404-04-2 QAny alert?.At least one alert fired? Yes
n-hexadecane	0	
n-hexane	0	
nicotinamide	1	QSA1.Acyl halides No 98-92-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 98-92-0 QSA3.N-methylol derivatives No 98-92-0 QSA4.Monohaloalkene No 98-92-0 QSA5.S or N mustard No 98-92-0 QSA6.Propiolactones and propiosultones No 98-92-0 QSA7.Epoxides and aziridines No 98-92-0 QSA8.Aliphatic halogens No 98-92-0 QSA9.Alkyl nitrite No 98-92-0 QSA10.α,β unsaturated carbonyls No 98-92-0 QSA11.Simple aldehyde No 98-92-0 QSA12.Quinones No 98-92-0 QSA13.Hydrazine No 98-92-0 QSA14.Aliphatic azo and azoxy No 98-92-0 QSA15.Isocyanate and isothiocyanate groups No 98-92-0 QSA16.Alkyl carbamate and thiocarbamate No 98-92-0 QSA18.Polycyclic Aromatic Hydrocarbons No 98-92-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 98-92-0 QSA21.Alkyl and aryl N-nitroso groups No 98-92-0 QSA22.Azide and triazene groups No 98-92-0 QSA23.Aliphatic N-nitro No 98-92-0 QSA24.α,β unsaturated alkoxy No 98-92-0 QSA25.Aromatic nitroso group No 98-92-0 QSA26.Aromatic ring N-oxide No 98-92-0 QSA27.Nitro aromatic No 98-92-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 98-92-0 QSA28bis.Aromatic mono- and dialkylamine No 98-92-0 QSA28ter.Aromatic N-acyl amine No 98-92-0 QSA29.Aromatic diazo No 98-92-0 QSA30.Coumarins and Furocoumarins No 98-92-0 QSA32.1,3-dialkoxy-benzene No 98-92-0 QSA33.1-phenoxy-benzene No 98-92-0 QSA34.H-acceptor-path3-H-

Table 18 Continued

		acceptor Yes 98-92-0 QSA35.Oxolane No 98-92-0 QSA36.Carbodiimides No 98-92-0 QAny alert?.At least one alert fired? Yes
nicotinic acid	1	QSA1.Acyl halides No 59-67-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-67-6 QSA3.N-methylol derivatives No 59-67-6 QSA4.Monohaloalkene No 59-67-6 QSA5.S or N mustard No 59-67-6 QSA6.Propiolactones and propiosultones No 59-67-6 QSA7.Epoxides and aziridines No 59-67-6 QSA8.Aliphatic halogens No 59-67-6 QSA9.Alkyl nitrite No 59-67-6 QSA10.α,β unsaturated carbonyls No 59-67-6 QSA11.Simple aldehyde No 59-67-6 QSA12.Quinones No 59-67-6 QSA13.Hydrazine No 59-67-6 QSA14.Aliphatic azo and azoxy No 59-67-6 QSA15.Isocyanate and isothiocyanate groups No 59-67-6 QSA16.Alkyl carbamate and thiocarbamate No 59-67-6 QSA18.Polycyclic Aromatic Hydrocarbons No 59-67-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 59-67-6 QSA21.Alkyl and aryl N-nitroso groups No 59-67-6 QSA22.Azide and triazene groups No 59-67-6 QSA23.Aliphatic N-nitro No 59-67-6 QSA24.α,β unsaturated alkoxy No 59-67-6 QSA25.Aromatic nitroso group No 59-67-6 QSA26.Aromatic ring N-oxide No 59-67-6 QSA27.Nitro aromatic No 59-67-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 59-67-6 QSA28bis.Aromatic mono- and dialkylamine No 59-67-6 QSA28ter.Aromatic N-acyl amine No 59-67-6 QSA29.Aromatic diazo No 59-67-6 QSA30.Coumarins and Furocoumarins No 59-67-6 QSA32.1,3-dialkoxy-benzene No 59-67-6 QSA33.1-phenoxy-benzene No 59-67-6 QSA34.H-acceptor-path3-H-acceptor Yes 59-67-6 QSA35.Oxolane No 59-67-6 QSA36.Carbodiimides No 59-67-6 QAny alert?.At least one alert fired? Yes
n-octadecane	0	
n-tetradecane	0	
octoxynol 9	1	QSA1.Acyl halides No 9002-93-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9002-93-1 QSA3.N-methylol derivatives No 9002-93-1 QSA4.Monohaloalkene No 9002-93-1 QSA5.S or N mustard No 9002-93-1 QSA6.Propiolactones and propiosultones No 9002-93-1 QSA7.Epoxides and aziridines No 9002-93-1 QSA8.Aliphatic halogens No 9002-93-1 QSA9.Alkyl nitrite No 9002-93-1 QSA10.α,β unsaturated carbonyls No 9002-93-1 QSA11.Simple aldehyde No 9002-93-1 QSA12.Quinones No 9002-93-1 QSA13.Hydrazine No 9002-93-1 QSA14.Aliphatic azo and

Table 18 Continued

		azoxy No 9002-93-1 QSA15.Isocyanate and isothiocyanate groups No 9002-93-1 QSA16.Alkyl carbamate and thiocarbamate No 9002-93-1 QSA18.Polycyclic Aromatic Hydrocarbons No 9002-93-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9002-93-1 QSA21.Alkyl and aryl N-nitroso groups No 9002-93-1 QSA22.Azide and triazene groups No 9002-93-1 QSA23.Aliphatic N-nitro No 9002-93-1 QSA24.α,β unsaturated alkoxy No 9002-93-1 QSA25.Aromatic nitroso group No 9002-93-1 QSA26.Aromatic ring N-oxide No 9002-93-1 QSA27.Nitro aromatic No 9002-93-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9002-93-1 QSA28bis.Aromatic mono- and dialkylamine No 9002-93-1 QSA28ter.Aromatic N-acyl amine No 9002-93-1 QSA29.Aromatic diazo No 9002-93-1 QSA30.Coumarins and Furocoumarins No 9002-93-1 QSA32.1,3-dialkoxy-benzene No 9002-93-1 QSA33.1-phenoxy-benzene No 9002-93-1 QSA34.H-acceptor-path3-H-acceptor Yes 9002-93-1 QSA35.Oxolane No 9002-93-1 QSA36.Carbodiimides No 9002-93-1 QAny alert?.At least one alert fired? Yes
palmitic acid	1	QSA1.Acyl halides No 57-10-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-10-3 QSA3.N-methylol derivatives No 57-10-3 QSA4.Monohaloalkene No 57-10-3 QSA5.S or N mustard No 57-10-3 QSA6.Propiolactones and propiosultones No 57-10-3 QSA7.Epoxides and aziridines No 57-10-3 QSA8.Aliphatic halogens No 57-10-3 QSA9.Alkyl nitrite No 57-10-3 QSA10.α,β unsaturated carbonyls No 57-10-3 QSA11.Simple aldehyde No 57-10-3 QSA12.Quinones No 57-10-3 QSA13.Hydrazine No 57-10-3 QSA14.Aliphatic azo and azoxy No 57-10-3 QSA15.Isocyanate and isothiocyanate groups No 57-10-3 QSA16.Alkyl carbamate and thiocarbamate No 57-10-3 QSA18.Polycyclic Aromatic Hydrocarbons No 57-10-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 57-10-3 QSA21.Alkyl and aryl N-nitroso groups No 57-10-3 QSA22.Azide and triazene groups No 57-10-3 QSA23.Aliphatic N-nitro No 57-10-3 QSA24.α,β unsaturated alkoxy No 57-10-3 QSA25.Aromatic nitroso group No 57-10-3 QSA26.Aromatic ring N-oxide No 57-10-3 QSA27.Nitro aromatic No 57-10-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 57-10-3 QSA28bis.Aromatic mono- and dialkylamine No 57-10-3 QSA28ter.Aromatic N-acyl amine No 57-10-3 QSA29.Aromatic diazo No 57-10-3 QSA30.Coumarins and Furocoumarins No 57-10-3 QSA32.1,3-dialkoxy-benzene No 57-10-3 QSA33.1-phenoxy-

Table 18 Continued

		benzene No 57-10-3 QSA34.H-acceptor-path3-H-acceptor Yes 57-10-3 QSA35.Oxolane No 57-10-3 QSA36.Carbodiimides No 57-10-3 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
p-aminobenzoic acid (4-AMINOBENZOIC ACID)	1	QSA1.Acyl halides No 150-13-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 150-13-0 QSA3.N-methylol derivatives No 150-13-0 QSA4.Monohaloalkene No 150-13-0 QSA5.S or N mustard No 150-13-0 QSA6.Propiolactones and propiosultones No 150-13-0 QSA7.Epoxides and aziridines No 150-13-0 QSA8.Aliphatic halogens No 150-13-0 QSA9.Alkyl nitrite No 150-13-0 QSA10.α,β unsaturated carbonyls No 150-13-0 QSA11.Simple aldehyde No 150-13-0 QSA12.Quinones No 150-13-0 QSA13.Hydrazine No 150-13-0 QSA14.Aliphatic azo and azoxy No 150-13-0 QSA15.Isocyanate and isothiocyanate groups No 150-13-0 QSA16.Alkyl carbamate and thiocarbamate No 150-13-0 QSA18.Polycyclic Aromatic Hydrocarbons No 150-13-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 150-13-0 QSA21.Alkyl and aryl N-nitroso groups No 150-13-0 QSA22.Azide and triazene groups No 150-13-0 QSA23.Aliphatic N-nitro No 150-13-0 QSA24.α,β unsaturated alkoxy No 150-13-0 QSA25.Aromatic nitroso group No 150-13-0 QSA26.Aromatic ring N-oxide No 150-13-0 QSA27.Nitro aromatic No 150-13-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 150-13-0 QSA28bis.Aromatic mono- and dialkylamine No 150-13-0 QSA28ter.Aromatic N-acyl amine No 150-13-0 QSA29.Aromatic diazo No 150-13-0 QSA30.Coumarins and Furocoumarins No 150-13-0 QSA32.1,3-dialkoxy-benzene No 150-13-0 QSA33.1-phenoxy-benzene No 150-13-0 QSA34.H-acceptor-path3-H-acceptor Yes 150-13-0 QSA35.Oxolane No 150-13-0 QSA36.Carbodiimides No 150-13-0 QAny alert?.At least one alert fired? Yes
PCB 1221	0	
PCB 1242	0	
PCB 1248	0	
PCB 1254	0	
PCB 1260	0	
p-cymene	0	
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylide	1	QSA1.Acyl halides No 25155-25-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 25155-25-3 QSA3.N-methylol derivatives No 25155-25-3 QSA4.Monohaloalkene No 25155-25-3 QSA5.S or N mustard No 25155-25-3 QSA6.Propiolactones and

Table 18 Continued

ne)]bis[(1,1-dimethylethyl)		propiosultones No 25155-25-3 QSA7.Epoxides and aziridines No 25155-25-3 QSA8.Aliphatic halogens No 25155-25-3 QSA9.Alkyl nitrite No 25155-25-3 QSA10.α,β unsaturated carbonyls No 25155-25-3 QSA11.Simple aldehyde No 25155-25-3 QSA12.Quinones No 25155-25-3 QSA13.Hydrazine No 25155-25-3 QSA14.Aliphatic azo and azoxy No 25155-25-3 QSA15.Isocyanate and isothiocyanate groups No 25155-25-3 QSA16.Alkyl carbamate and thiocarbamate No 25155-25-3 QSA18.Polycyclic Aromatic Hydrocarbons No 25155-25-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 25155-25-3 QSA21.Alkyl and aryl N-nitroso groups No 25155-25-3 QSA22.Azide and triazene groups No 25155-25-3 QSA23.Aliphatic N-nitro No 25155-25-3 QSA24.α,β unsaturated alkoxy No 25155-25-3 QSA25.Aromatic nitroso group No 25155-25-3 QSA26.Aromatic ring N-oxide No 25155-25-3 QSA27.Nitro aromatic No 25155-25-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 25155-25-3 QSA28bis.Aromatic mono- and dialkylamine No 25155-25-3 QSA28ter.Aromatic N-acyl amine No 25155-25-3 QSA29.Aromatic diazo No 25155-25-3 QSA30.Coumarins and Furocoumarins No 25155-25-3 QSA32.1,3-dialkoxy-benzene No 25155-25-3 QSA33.1-phenoxy-benzene No 25155-25-3 QSA34.H-acceptor-path3-H-acceptor Yes 25155-25-3 QSA35.Oxolane No 25155-25-3 QSA36.Carbodiimides No 25155-25-3 QAny alert?.At least one alert fired? Yes
phenol	0	
phenol red (phenolsulfonphthalein)	1	QSA1.Acyl halides No 143-74-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 143-74-8 QSA3.N-methylol derivatives No 143-74-8 QSA4.Monohaloalkene No 143-74-8 QSA5.S or N mustard No 143-74-8 QSA6.Propiolactones and propiosultones No 143-74-8 QSA7.Epoxides and aziridines No 143-74-8 QSA8.Aliphatic halogens No 143-74-8 QSA9.Alkyl nitrite No 143-74-8 QSA10.α,β unsaturated carbonyls No 143-74-8 QSA11.Simple aldehyde No 143-74-8 QSA12.Quinones No 143-74-8 QSA13.Hydrazine No 143-74-8 QSA14.Aliphatic azo and azoxy No 143-74-8 QSA15.Isocyanate and isothiocyanate groups No 143-74-8 QSA16.Alkyl carbamate and thiocarbamate No 143-74-8 QSA18.Polycyclic Aromatic Hydrocarbons No 143-74-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 143-74-8 QSA21.Alkyl and aryl N-nitroso groups No 143-74-8 QSA22.Azide and triazene groups No 143-74-8 QSA23.Aliphatic N-nitro No 143-74-8 QSA24.α,β unsaturated alkoxy No 143-74-8 QSA25.Aromatic

Table 18 Continued

		nitroso group No 143-74-8 QSA26.Aromatic ring N-oxide No 143-74-8 QSA27.Nitro aromatic No 143-74-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 143-74-8 QSA28bis.Aromatic mono- and dialkylamine No 143-74-8 QSA28ter.Aromatic N-acyl amine No 143-74-8 QSA29.Aromatic diazo No 143-74-8 QSA30.Coumarins and Furocoumarins No 143-74-8 QSA32.1,3-dialkoxy-benzene No 143-74-8 QSA33.1-phenoxy-benzene No 143-74-8 QSA34.H-acceptor-path3-H-acceptor Yes 143-74-8 QSA35.Oxolane No 143-74-8 QSA36.Carbodiimides No 143-74-8 QAny alert?.At least one alert fired? Yes
poly(tetrafluoroethylene) (PTFE) (teflon)	0	
polydimethylsiloxanes	0	
polyethylene glycol nonylphenyl ether	1	QSA1.Acyl halides No 9016-45-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9016-45-9 QSA3.N-methylol derivatives No 9016-45-9 QSA4.Monohaloalkene No 9016-45-9 QSA5.S or N mustard No 9016-45-9 QSA6.Propiolactones and propiosultones No 9016-45-9 QSA7.Epoxides and aziridines No 9016-45-9 QSA8.Aliphatic halogens No 9016-45-9 QSA9.Alkyl nitrite No 9016-45-9 QSA10.α,β unsaturated carbonyls No 9016-45-9 QSA11.Simple aldehyde No 9016-45-9 QSA12.Quinones No 9016-45-9 QSA13.Hydrazine No 9016-45-9 QSA14.Aliphatic azo and azoxy No 9016-45-9 QSA15.Isocyanate and isothiocyanate groups No 9016-45-9 QSA16.Alkyl carbamate and thiocarbamate No 9016-45-9 QSA18.Polycyclic Aromatic Hydrocarbons No 9016-45-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9016-45-9 QSA21.Alkyl and aryl N-nitroso groups No 9016-45-9 QSA22.Azide and triazene groups No 9016-45-9 QSA23.Aliphatic N-nitro No 9016-45-9 QSA24.α,β unsaturated alkoxy No 9016-45-9 QSA25.Aromatic nitroso group No 9016-45-9 QSA26.Aromatic ring N-oxide No 9016-45-9 QSA27.Nitro aromatic No 9016-45-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9016-45-9 QSA28bis.Aromatic mono- and dialkylamine No 9016-45-9 QSA28ter.Aromatic N-acyl amine No 9016-45-9 QSA29.Aromatic diazo No 9016-45-9 QSA30.Coumarins and Furocoumarins No 9016-45-9 QSA32.1,3-dialkoxy-benzene No 9016-45-9 QSA33.1-phenoxy-benzene No 9016-

Table 18 Continued

		45-9 QSA34.H-acceptor-path3-H-acceptor Yes 9016-45-9 QSA35.Oxolane No 9016-45-9 QSA36.Carbodiimides No 9016-45-9 QAny alert?.At least one alert fired? Yes
polymyxin B	1	QSA1.Acyl halides No 1404-26-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1404-26-8 QSA3.N-methylol derivatives No 1404-26-8 QSA4.Monohaloalkene No 1404-26-8 QSA5.S or N mustard No 1404-26-8 QSA6.Propiolactones and propiosultones No 1404-26-8 QSA7.Epoxides and aziridines No 1404-26-8 QSA8.Aliphatic halogens No 1404-26-8 QSA9.Alkyl nitrite No 1404-26-8 QSA10.α,β unsaturated carbonyls No 1404-26-8 QSA11.Simple aldehyde No 1404-26-8 QSA12.Quinones No 1404-26-8 QSA13.Hydrazine No 1404-26-8 QSA14.Aliphatic azo and azoxy No 1404-26-8 QSA15.Isocyanate and isothiocyanate groups No 1404-26-8 QSA16.Alkyl carbamate and thiocarbamate No 1404-26-8 QSA18.Polycyclic Aromatic Hydrocarbons No 1404-26-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1404-26-8 QSA21.Alkyl and aryl N-nitroso groups No 1404-26-8 QSA22.Azide and triazene groups No 1404-26-8 QSA23.Aliphatic N-nitro No 1404-26-8 QSA24.α,β unsaturated alkoxy No 1404-26-8 QSA25.Aromatic nitroso group No 1404-26-8 QSA26.Aromatic ring N-oxide No 1404-26-8 QSA27.Nitro aromatic No 1404-26-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1404-26-8 QSA28bis.Aromatic mono- and dialkylamine No 1404-26-8 QSA28ter.Aromatic N-acyl amine No 1404-26-8 QSA29.Aromatic diazo No 1404-26-8 QSA30.Coumarins and Furocoumarins No 1404-26-8 QSA32.1,3-dialkoxy-benzene No 1404-26-8 QSA33.1-phenoxy-benzene No 1404-26-8 QSA34.H-acceptor-path3-H-acceptor Yes 1404-26-8 QSA35.Oxolane No 1404-26-8 QSA36.Carbodiimides No 1404-26-8 QAny alert?.At least one alert fired? Yes
polypropylene	0	
polysorbate 20	1	QSA1.Acyl halides No 9005-64-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9005-64-5 QSA3.N-methylol derivatives No 9005-64-5 QSA4.Monohaloalkene No 9005-64-5 QSA5.S or N mustard No 9005-64-5 QSA6.Propiolactones and propiosultones No 9005-64-5 QSA7.Epoxides and aziridines No 9005-64-5 QSA8.Aliphatic halogens No 9005-64-5 QSA9.Alkyl nitrite No 9005-64-5 QSA10.α,β unsaturated carbonyls No 9005-64-5 QSA11.Simple aldehyde No 9005-64-5 QSA12.Quinones No 9005-64-5 QSA13.Hydrazine No 9005-64-5 QSA14.Aliphatic azo and

Table 18 Continued

		azoxy No 9005-64-5 QSA15.Isocyanate and isothiocyanate groups No 9005-64-5 QSA16.Alkyl carbamate and thiocarbamate No 9005-64-5 QSA18.Polycyclic Aromatic Hydrocarbons No 9005-64-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9005-64-5 QSA21.Alkyl and aryl N-nitroso groups No 9005-64-5 QSA22.Azide and triazene groups No 9005-64-5 QSA23.Aliphatic N-nitro No 9005-64-5 QSA24.α,β unsaturated alkoxy No 9005-64-5 QSA25.Aromatic nitroso group No 9005-64-5 QSA26.Aromatic ring N-oxide No 9005-64-5 QSA27.Nitro aromatic No 9005-64-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9005-64-5 QSA28bis.Aromatic mono- and dialkylamine No 9005-64-5 QSA28ter.Aromatic N-acyl amine No 9005-64-5 QSA29.Aromatic diazo No 9005-64-5 QSA30.Coumarins and Furocoumarins No 9005-64-5 QSA32.1,3-dialkoxy-benzene No 9005-64-5 QSA33.1-phenoxy-benzene No 9005-64-5 QSA34.H-acceptor-path3-H-acceptor Yes 9005-64-5 QSA35.Oxolane Yes 9005-64-5 QSA36.Carbodiimides No 9005-64-5 QAny alert?.At least one alert fired? Yes
polysorbate 80 (tween 80)	1	QSA1.Acyl halides No 9005-65-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9005-65-6 QSA3.N-methylol derivatives No 9005-65-6 QSA4.Monohaloalkene No 9005-65-6 QSA5.S or N mustard No 9005-65-6 QSA6.Propiolactones and propiosultones No 9005-65-6 QSA7.Epoxides and aziridines No 9005-65-6 QSA8.Aliphatic halogens No 9005-65-6 QSA9.Alkyl nitrite No 9005-65-6 QSA10.α,β unsaturated carbonyls No 9005-65-6 QSA11.Simple aldehyde No 9005-65-6 QSA12.Quinones No 9005-65-6 QSA13.Hydrazine No 9005-65-6 QSA14.Aliphatic azo and azoxy No 9005-65-6 QSA15.Isocyanate and isothiocyanate groups No 9005-65-6 QSA16.Alkyl carbamate and thiocarbamate No 9005-65-6 QSA18.Polycyclic Aromatic Hydrocarbons No 9005-65-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9005-65-6 QSA21.Alkyl and aryl N-nitroso groups No 9005-65-6 QSA22.Azide and triazene groups No 9005-65-6 QSA23.Aliphatic N-nitro No 9005-65-6 QSA24.α,β unsaturated alkoxy No 9005-65-6 QSA25.Aromatic nitroso group No 9005-65-6 QSA26.Aromatic ring N-oxide No 9005-65-6 QSA27.Nitro aromatic No 9005-65-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9005-65-6 QSA28bis.Aromatic mono- and dialkylamine No 9005-65-6 QSA28ter.Aromatic N-acyl amine No 9005-65-6 QSA29.Aromatic diazo No 9005-65-6 QSA30.Coumarins and

Table 18 Continued

		Furocoumarins No 9005-65-6 QSA32.1,3-dialkoxy-benzene No 9005-65-6 QSA33.1-phenoxy-benzene No 9005-65-6 QSA34.H-acceptor-path3-H-acceptor Yes 9005-65-6 QSA35.Oxolane Yes 9005-65-6 QSA36.Carbodiimides No 9005-65-6 QAny alert?.At least one alert fired? Yes
polystyrene	0	
polyvinyl alcohol	0	
potassium	0	
potassium chloride	0	
potassium glutamate	1	QSA1.Acyl halides No 19473-49-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 19473-49-5 QSA3.N-methylol derivatives No 19473-49-5 QSA4.Monohaloalkene No 19473-49-5 QSA5.S or N mustard No 19473-49-5 QSA6.Propiolactones and propiosultones No 19473-49-5 QSA7.Epoxides and aziridines No 19473-49-5 QSA8.Aliphatic halogens No 19473-49-5 QSA9.Alkyl nitrite No 19473-49-5 QSA10.α,β unsaturated carbonyls No 19473-49-5 QSA11.Simple aldehyde No 19473-49-5 QSA12.Quinones No 19473-49-5 QSA13.Hydrazine No 19473-49-5 QSA14.Aliphatic azo and azoxy No 19473-49-5 QSA15.Isocyanate and isothiocyanate groups No 19473-49-5 QSA16.Alkyl carbamate and thiocarbamate No 19473-49-5 QSA18.Polycyclic Aromatic Hydrocarbons No 19473-49-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 19473-49-5 QSA21.Alkyl and aryl N-nitroso groups No 19473-49-5 QSA22.Azide and triazene groups No 19473-49-5 QSA23.Aliphatic N-nitro No 19473-49-5 QSA24.α,β unsaturated alkoxy No 19473-49-5 QSA25.Aromatic nitroso group No 19473-49-5 QSA26.Aromatic ring N-oxide No 19473-49-5 QSA27.Nitro aromatic No 19473-49-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 19473-49-5 QSA28bis.Aromatic mono- and dialkylamine No 19473-49-5 QSA28ter.Aromatic N-acyl amine No 19473-49-5 QSA29.Aromatic diazo No 19473-49-5 QSA30.Coumarins and Furocoumarins No 19473-49-5 QSA32.1,3-dialkoxy-benzene No 19473-49-5 QSA33.1-phenoxy-benzene No 19473-49-5 QSA34.H-acceptor-path3-H-acceptor Yes 19473-49-5 QSA35.Oxolane No 19473-49-5 QSA36.Carbodiimides No 19473-49-5 QAny alert?.At least one alert fired? Yes
p-xylene	0	
pyridoxal	1	QSA1.Acyl halides No 66-72-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 66-72-8 QSA3.N-

Table 18 Continued

		methylol derivatives No 66-72-8 QSA4.Monohaloalkene No 66-72-8 QSA5.S or N mustard No 66-72-8 QSA6.Propiolactones and propiosultones No 66-72-8 QSA7.Epoxides and aziridines No 66-72-8 QSA8.Aliphatic halogens No 66-72-8 QSA9.Alkyl nitrite No 66-72-8 QSA10.α,β unsaturated carbonyls No 66-72-8 QSA11.Simple aldehyde Yes 66-72-8 QSA12.Quinones No 66-72-8 QSA13.Hydrazine No 66-72-8 QSA14.Aliphatic azo and azoxy No 66-72-8 QSA15.Isocyanate and isothiocyanate groups No 66-72-8 QSA16.Alkyl carbamate and thiocarbamate No 66-72-8 QSA18.Polycyclic Aromatic Hydrocarbons No 66-72-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 66-72-8 QSA21.Alkyl and aryl N-nitroso groups No 66-72-8 QSA22.Azide and triazene groups No 66-72-8 QSA23.Aliphatic N-nitro No 66-72-8 QSA24.α,β unsaturated alkoxy No 66-72-8 QSA25.Aromatic nitroso group No 66-72-8 QSA26.Aromatic ring N-oxide No 66-72-8 QSA27.Nitro aromatic No 66-72-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 66-72-8 QSA28bis.Aromatic mono- and dialkylamine No 66-72-8 QSA28ter.Aromatic N-acyl amine No 66-72-8 QSA29.Aromatic diazo No 66-72-8 QSA30.Coumarins and Furocoumarins No 66-72-8 QSA32.1,3-dialkoxy-benzene No 66-72-8 QSA33.1-phenoxy-benzene No 66-72-8 QSA34.H-acceptor-path3-H-acceptor Yes 66-72-8 QSA35.Oxolane No 66-72-8 QSA36.Carbodiimides No 66-72-8 QAny alert?.At least one alert fired? Yes
pyridoxine	1	QSA1.Acyl halides No 65-23-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 65-23-6 QSA3.N-methylol derivatives No 65-23-6 QSA4.Monohaloalkene No 65-23-6 QSA5.S or N mustard No 65-23-6 QSA6.Propiolactones and propiosultones No 65-23-6 QSA7.Epoxides and aziridines No 65-23-6 QSA8.Aliphatic halogens No 65-23-6 QSA9.Alkyl nitrite No 65-23-6 QSA10.α,β unsaturated carbonyls No 65-23-6 QSA11.Simple aldehyde No 65-23-6 QSA12.Quinones No 65-23-6 QSA13.Hydrazine No 65-23-6 QSA14.Aliphatic azo and azoxy No 65-23-6 QSA15.Isocyanate and isothiocyanate groups No 65-23-6 QSA16.Alkyl carbamate and thiocarbamate No 65-23-6 QSA18.Polycyclic Aromatic Hydrocarbons No 65-23-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 65-23-6 QSA21.Alkyl and aryl N-nitroso groups No 65-23-6 QSA22.Azide and triazene groups No 65-23-6 QSA23.Aliphatic N-nitro No 65-23-6 QSA24.α,β unsaturated alkoxy No 65-23-6 QSA25.Aromatic

Table 18 Continued

		nitroso group No 65-23-6 QSA26.Aromatic ring N-oxide No 65-23-6 QSA27.Nitro aromatic No 65-23-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 65-23-6 QSA28bis.Aromatic mono- and dialkylamine No 65-23-6 QSA28ter.Aromatic N-acyl amine No 65-23-6 QSA29.Aromatic diazo No 65-23-6 QSA30.Coumarins and Furocoumarins No 65-23-6 QSA32.1,3-dialkoxy-benzene No 65-23-6 QSA33.1-phenoxy-benzene No 65-23-6 QSA34.H-acceptor-path3-H-acceptor Yes 65-23-6 QSA35.Oxolane No 65-23-6 QSA36.Carbodiimides No 65-23-6 QAny alert?.At least one alert fired? Yes
retinyl acetate	1	QSA1.Acyl halides No 127-47-9 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 127-47-9 QSA3.N-methylol derivatives No 127-47-9 QSA4.Monohaloalkene No 127-47-9 QSA5.S or N mustard No 127-47-9 QSA6.Propiolactones and propiosultones No 127-47-9 QSA7.Epoxides and aziridines No 127-47-9 QSA8.Aliphatic halogens No 127-47-9 QSA9.Alkyl nitrite No 127-47-9 QSA10.α,β unsaturated carbonyls No 127-47-9 QSA11.Simple aldehyde No 127-47-9 QSA12.Quinones No 127-47-9 QSA13.Hydrazine No 127-47-9 QSA14.Aliphatic azo and azoxy No 127-47-9 QSA15.Isocyanate and isothiocyanate groups No 127-47-9 QSA16.Alkyl carbamate and thiocarbamate No 127-47-9 QSA18.Polycyclic Aromatic Hydrocarbons No 127-47-9 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 127-47-9 QSA21.Alkyl and aryl N-nitroso groups No 127-47-9 QSA22.Azide and triazene groups No 127-47-9 QSA23.Aliphatic N-nitro No 127-47-9 QSA24.α,β unsaturated alkoxy No 127-47-9 QSA25.Aromatic nitroso group No 127-47-9 QSA26.Aromatic ring N-oxide No 127-47-9 QSA27.Nitro aromatic No 127-47-9 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 127-47-9 QSA28bis.Aromatic mono- and dialkylamine No 127-47-9 QSA28ter.Aromatic N-acyl amine No 127-47-9 QSA29.Aromatic diazo No 127-47-9 QSA30.Coumarins and Furocoumarins No 127-47-9 QSA32.1,3-dialkoxy-benzene No 127-47-9 QSA33.1-phenoxy-benzene No 127-47-9 QSA34.H-acceptor-path3-H-acceptor Yes 127-47-9 QSA35.Oxolane No 127-47-9 QSA36.Carbodiimides No 127-47-9 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
riboflavin	1	QSA1.Acyl halides No 83-88-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 83-88-5 QSA3.N-methylol derivatives No 83-88-5 QSA4.Monohaloalkene No

Table 18 Continued

		83-88-5 QSA5.S or N mustard No 83-88-5 QSA6.Propiolactones and propiosultones No 83-88-5 QSA7.Epoxides and aziridines No 83-88-5 QSA8.Aliphatic halogens No 83-88-5 QSA9.Alkyl nitrite No 83-88-5 QSA10.α,β unsaturated carbonyls No 83-88-5 QSA11.Simple aldehyde No 83-88-5 QSA12.Quinones No 83-88-5 QSA13.Hydrazine No 83-88-5 QSA14.Aliphatic azo and azoxy No 83-88-5 QSA15.Isocyanate and isothiocyanate groups No 83-88-5 QSA16.Alkyl carbamate and thiocarbamate No 83-88-5 QSA18.Polycyclic Aromatic Hydrocarbons No 83-88-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 83-88-5 QSA21.Alkyl and aryl N-nitroso groups No 83-88-5 QSA22.Azide and triazene groups No 83-88-5 QSA23.Aliphatic N-nitro No 83-88-5 QSA24.α,β unsaturated alkoxy No 83-88-5 QSA25.Aromatic nitroso group No 83-88-5 QSA26.Aromatic ring N-oxide No 83-88-5 QSA27.Nitro aromatic No 83-88-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 83-88-5 QSA28bis.Aromatic mono- and dialkylamine No 83-88-5 QSA28ter.Aromatic N-acyl amine No 83-88-5 QSA29.Aromatic diazo No 83-88-5 QSA30.Coumarins and Furocoumarins No 83-88-5 QSA32.1,3-dialkoxy-benzene No 83-88-5 QSA33.1-phenoxy-benzene No 83-88-5 QSA34.H-acceptor-path3-H-acceptor Yes 83-88-5 QSA35.Oxolane No 83-88-5 QSA36.Carbodiimides No 83-88-5 QAny alert?.At least one alert fired? Yes
silicon	0	
silicon dioxide	0	
sodium	0	
sodium acetate	1	QSA1.Acyl halides No 127-09-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 127-09-3 QSA3.N-methylol derivatives No 127-09-3 QSA4.Monohaloalkene No 127-09-3 QSA5.S or N mustard No 127-09-3 QSA6.Propiolactones and propiosultones No 127-09-3 QSA7.Epoxides and aziridines No 127-09-3 QSA8.Aliphatic halogens No 127-09-3 QSA9.Alkyl nitrite No 127-09-3 QSA10.α,β unsaturated carbonyls No 127-09-3 QSA11.Simple aldehyde No 127-09-3 QSA12.Quinones No 127-09-3 QSA13.Hydrazine No 127-09-3 QSA14.Aliphatic azo and azoxy No 127-09-3 QSA15.Isocyanate and isothiocyanate groups No 127-09-3 QSA16.Alkyl carbamate and thiocarbamate No 127-09-3 QSA18.Polycyclic Aromatic Hydrocarbons No 127-09-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 127-09-3 QSA21.Alkyl and aryl N-nitroso groups No 127-09-3 QSA22.Azide and triazene

Table 18 Continued

		groups No 127-09-3 QSA23.Aliphatic N-nitro No 127-09-3 QSA24.α,β unsaturated alkoxy No 127-09-3 QSA25.Aromatic nitroso group No 127-09-3 QSA26.Aromatic ring N-oxide No 127-09-3 QSA27.Nitro aromatic No 127-09-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 127-09-3 QSA28bis.Aromatic mono- and dialkylamine No 127-09-3 QSA28ter.Aromatic N-acyl amine No 127-09-3 QSA29.Aromatic diazo No 127-09-3 QSA30.Coumarins and Furocoumarins No 127-09-3 QSA32.1,3-dialkoxy-benzene No 127-09-3 QSA33.1-phenoxy-benzene No 127-09-3 QSA34.H-acceptor-path3-H-acceptor Yes 127-09-3 QSA35.Oxolane No 127-09-3 QSA36.Carbodiimides No 127-09-3 QAny alert?.At least one alert fired? Yes
sodium bicarbonate	1	QSA1.Acyl halides No 144-55-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 144-55-8 QSA3.N-methylol derivatives No 144-55-8 QSA4.Monohaloalkene No 144-55-8 QSA5.S or N mustard No 144-55-8 QSA6.Propiolactones and propiosultones No 144-55-8 QSA7.Epoxides and aziridines No 144-55-8 QSA8.Aliphatic halogens No 144-55-8 QSA9.Alkyl nitrite No 144-55-8 QSA10.α,β unsaturated carbonyls No 144-55-8 QSA11.Simple aldehyde No 144-55-8 QSA12.Quinones No 144-55-8 QSA13.Hydrazine No 144-55-8 QSA14.Aliphatic azo and azoxy No 144-55-8 QSA15.Isocyanate and isothiocyanate groups No 144-55-8 QSA16.Alkyl carbamate and thiocarbamate No 144-55-8 QSA18.Polycyclic Aromatic Hydrocarbons No 144-55-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 144-55-8 QSA21.Alkyl and aryl N-nitroso groups No 144-55-8 QSA22.Azide and triazene groups No 144-55-8 QSA23.Aliphatic N-nitro No 144-55-8 QSA24.α,β unsaturated alkoxy No 144-55-8 QSA25.Aromatic nitroso group No 144-55-8 QSA26.Aromatic ring N-oxide No 144-55-8 QSA27.Nitro aromatic No 144-55-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 144-55-8 QSA28bis.Aromatic mono- and dialkylamine No 144-55-8 QSA28ter.Aromatic N-acyl amine No 144-55-8 QSA29.Aromatic diazo No 144-55-8 QSA30.Coumarins and Furocoumarins No 144-55-8 QSA32.1,3-dialkoxy-benzene No 144-55-8 QSA33.1-phenoxy-benzene No 144-55-8 QSA34.H-acceptor-path3-H-acceptor Yes 144-55-8 QSA35.Oxolane No 144-55-8 QSA36.Carbodiimides No 144-55-8 QAny alert?.At least one alert fired? Yes
sodium borate	0	
sodium	0	

Table 18 Continued

chloride		
sodium citrate	1	QSA1.Acyl halides No 68-04-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 68-04-2 QSA3.N-methylol derivatives No 68-04-2 QSA4.Monohaloalkene No 68-04-2 QSA5.S or N mustard No 68-04-2 QSA6.Propiolactones and propiosultones No 68-04-2 QSA7.Epoxides and aziridines No 68-04-2 QSA8.Aliphatic halogens No 68-04-2 QSA9.Alkyl nitrite No 68-04-2 QSA10.α,β unsaturated carbonyls No 68-04-2 QSA11.Simple aldehyde No 68-04-2 QSA12.Quinones No 68-04-2 QSA13.Hydrazine No 68-04-2 QSA14.Aliphatic azo and azoxy No 68-04-2 QSA15.Isocyanate and isothiocyanate groups No 68-04-2 QSA16.Alkyl carbamate and thiocarbamate No 68-04-2 QSA18.Polycyclic Aromatic Hydrocarbons No 68-04-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 68-04-2 QSA21.Alkyl and aryl N-nitroso groups No 68-04-2 QSA22.Azide and triazene groups No 68-04-2 QSA23.Aliphatic N-nitro No 68-04-2 QSA24.α,β unsaturated alkoxy No 68-04-2 QSA25.Aromatic nitroso group No 68-04-2 QSA26.Aromatic ring N-oxide No 68-04-2 QSA27.Nitro aromatic No 68-04-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 68-04-2 QSA28bis.Aromatic mono- and dialkylamine No 68-04-2 QSA28ter.Aromatic N-acyl amine No 68-04-2 QSA29.Aromatic diazo No 68-04-2 QSA30.Coumarins and Furocoumarins No 68-04-2 QSA32.1,3-dialkoxy-benzene No 68-04-2 QSA33.1-phenoxy-benzene No 68-04-2 QSA34.H-acceptor-path3-H-acceptor Yes 68-04-2 QSA35.Oxolane No 68-04-2 QSA36.Carbodiimides No 68-04-2 QAny alert?.At least one alert fired? Yes
sodium dihydrogen phosphate dihydrate	1	QSA1.Acyl halides No 13472-35-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 13472-35-0 QSA3.N-methylol derivatives No 13472-35-0 QSA4.Monohaloalkene No 13472-35-0 QSA5.S or N mustard No 13472-35-0 QSA6.Propiolactones and propiosultones No 13472-35-0 QSA7.Epoxides and aziridines No 13472-35-0 QSA8.Aliphatic halogens No 13472-35-0 QSA9.Alkyl nitrite No 13472-35-0 QSA10.α,β unsaturated carbonyls No 13472-35-0 QSA11.Simple aldehyde No 13472-35-0 QSA12.Quinones No 13472-35-0 QSA13.Hydrazine No 13472-35-0 QSA14.Aliphatic azo and azoxy No 13472-35-0 QSA15.Isocyanate and isothiocyanate groups No 13472-35-0 QSA16.Alkyl carbamate and thiocarbamate No 13472-35-0 QSA18.Polycyclic Aromatic Hydrocarbons No 13472-35-0 QSA19.Heterocyclic Polycyclic

Table 18 Continued

		Aromatic Hydrocarbons No 13472-35-0 QSA21.Alkyl and aryl N-nitroso groups No 13472-35-0 QSA22.Azide and triazene groups No 13472-35-0 QSA23.Aliphatic N-nitro No 13472-35-0 QSA24.α,β unsaturated alkoxy No 13472-35-0 QSA25.Aromatic nitroso group No 13472-35-0 QSA26.Aromatic ring N-oxide No 13472-35-0 QSA27.Nitro aromatic No 13472-35-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 13472-35-0 QSA28bis.Aromatic mono- and dialkylamine No 13472-35-0 QSA28ter.Aromatic N-acyl amine No 13472-35-0 QSA29.Aromatic diazo No 13472-35-0 QSA30.Coumarins and Furocoumarins No 13472-35-0 QSA32.1,3-dialkoxy-benzene No 13472-35-0 QSA33.1-phenoxy-benzene No 13472-35-0 QSA34.H-acceptor-path3-H-acceptor Yes 13472-35-0 QSA35.Oxolane No 13472-35-0 QSA36.Carbodiimides No 13472-35-0 QAny alert?.At least one alert fired? Yes
sodium glucuronate	1	QSA1.Acyl halides No 14984-34-0 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 14984-34-0 QSA3.N-methylol derivatives No 14984-34-0 QSA4.Monohaloalkene No 14984-34-0 QSA5.S or N mustard No 14984-34-0 QSA6.Propiolactones and propiosultones No 14984-34-0 QSA7.Epoxides and aziridines No 14984-34-0 QSA8.Aliphatic halogens No 14984-34-0 QSA9.Alkyl nitrite No 14984-34-0 QSA10.α,β unsaturated carbonyls No 14984-34-0 QSA11.Simple aldehyde Yes 14984-34-0 QSA12.Quinones No 14984-34-0 QSA13.Hydrazine No 14984-34-0 QSA14.Aliphatic azo and azoxy No 14984-34-0 QSA15.Isocyanate and isothiocyanate groups No 14984-34-0 QSA16.Alkyl carbamate and thiocarbamate No 14984-34-0 QSA18.Polycyclic Aromatic Hydrocarbons No 14984-34-0 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 14984-34-0 QSA21.Alkyl and aryl N-nitroso groups No 14984-34-0 QSA22.Azide and triazene groups No 14984-34-0 QSA23.Aliphatic N-nitro No 14984-34-0 QSA24.α,β unsaturated alkoxy No 14984-34-0 QSA25.Aromatic nitroso group No 14984-34-0 QSA26.Aromatic ring N-oxide No 14984-34-0 QSA27.Nitro aromatic No 14984-34-0 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 14984-34-0 QSA28bis.Aromatic mono- and dialkylamine No 14984-34-0 QSA28ter.Aromatic N-acyl amine No 14984-34-0 QSA29.Aromatic diazo No 14984-34-0 QSA30.Coumarins and Furocoumarins No 14984-34-0 QSA32.1,3-dialkoxy-benzene No 14984-34-0 QSA33.1-phenoxy-benzene No 14984-34-0 QSA34.H-acceptor-path3-H-acceptor Yes 14984-

Table 18 Continued

		34-0 QSA35.Oxolane No 14984-34-0 QSA36.Carbodiimides No 14984-34-0 QAny alert?.At least one alert fired? Yes
sodium hydroxide	0	
sodium metabisulphite	0	
Sodium phosphate dibasic heptahydrate	0	
sodium pyruvate	1	QSA1.Acyl halides No 113-24-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 113-24-6 QSA3.N-methylol derivatives No 113-24-6 QSA4.Monohaloalkene No 113-24-6 QSA5.S or N mustard No 113-24-6 QSA6.Propiolactones and propiosultones No 113-24-6 QSA7.Epoxides and aziridines No 113-24-6 QSA8.Aliphatic halogens No 113-24-6 QSA9.Alkyl nitrite No 113-24-6 QSA10.α,β unsaturated carbonyls No 113-24-6 QSA11.Simple aldehyde No 113-24-6 QSA12.Quinones No 113-24-6 QSA13.Hydrazine No 113-24-6 QSA14.Aliphatic azo and azoxy No 113-24-6 QSA15.Isocyanate and isothiocyanate groups No 113-24-6 QSA16.Alkyl carbamate and thiocarbamate No 113-24-6 QSA18.Polycyclic Aromatic Hydrocarbons No 113-24-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 113-24-6 QSA21.Alkyl and aryl N-nitroso groups No 113-24-6 QSA22.Azide and triazene groups No 113-24-6 QSA23.Aliphatic N-nitro No 113-24-6 QSA24.α,β unsaturated alkoxy No 113-24-6 QSA25.Aromatic nitroso group No 113-24-6 QSA26.Aromatic ring N-oxide No 113-24-6 QSA27.Nitro aromatic No 113-24-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 113-24-6 QSA28bis.Aromatic mono- and dialkylamine No 113-24-6 QSA28ter.Aromatic N-acyl amine No 113-24-6 QSA29.Aromatic diazo No 113-24-6 QSA30.Coumarins and Furocoumarins No 113-24-6 QSA32.1,3-dialkoxy-benzene No 113-24-6 QSA33.1-phenoxy-benzene No 113-24-6 QSA34.H-acceptor-path3-H-acceptor Yes 113-24-6 QSA35.Oxolane No 113-24-6 QSA36.Carbodiimides No 113-24-6 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I) 113-24-6
sorbitan monoleate	1	QSA1.Acyl halides No 1338-43-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 1338-43-8 QSA3.N-methylol derivatives No 1338-43-8 QSA4.Monohaloalkene No 1338-43-8 QSA5.S or N

Table 18 Continued

		mustard No 1338-43-8 QSA6.Propiolactones and propiosultones No 1338-43-8 QSA7.Epoxides and aziridines No 1338-43-8 QSA8.Aliphatic halogens No 1338-43-8 QSA9.Alkyl nitrite No 1338-43-8 QSA10.α,β unsaturated carbonyls No 1338-43-8 QSA11.Simple aldehyde No 1338-43-8 QSA12.Quinones No 1338-43-8 QSA13.Hydrazine No 1338-43-8 QSA14.Aliphatic azo and azoxy No 1338-43-8 QSA15.Isocyanate and isothiocyanate groups No 1338-43-8 QSA16.Alkyl carbamate and thiocarbamate No 1338-43-8 QSA18.Polycyclic Aromatic Hydrocarbons No 1338-43-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 1338-43-8 QSA21.Alkyl and aryl N-nitroso groups No 1338-43-8 QSA22.Azide and triazene groups No 1338-43-8 QSA23.Aliphatic N-nitro No 1338-43-8 QSA24.α,β unsaturated alkoxy No 1338-43-8 QSA25.Aromatic nitroso group No 1338-43-8 QSA26.Aromatic ring N-oxide No 1338-43-8 QSA27.Nitro aromatic No 1338-43-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 1338-43-8 QSA28bis.Aromatic mono- and dialkylamine No 1338-43-8 QSA28ter.Aromatic N-acyl amine No 1338-43-8 QSA29.Aromatic diazo No 1338-43-8 QSA30.Coumarins and Furocoumarins No 1338-43-8 QSA32.1,3-dialkoxy-benzene No 1338-43-8 QSA33.1-phenoxy-benzene No 1338-43-8 QSA34.H-acceptor-path3-H-acceptor Yes 1338-43-8 QSA35.Oxolane Yes 1338-43-8 QSA36.Carbodiimides No 1338-43-8 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
sorbitol	1	QSA1.Acyl halides No 50-70-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-70-4 QSA3.N-methylol derivatives No 50-70-4 QSA4.Monohaloalkene No 50-70-4 QSA5.S or N mustard No 50-70-4 QSA6.Propiolactones and propiosultones No 50-70-4 QSA7.Epoxides and aziridines No 50-70-4 QSA8.Aliphatic halogens No 50-70-4 QSA9.Alkyl nitrite No 50-70-4 QSA10.α,β unsaturated carbonyls No 50-70-4 QSA11.Simple aldehyde No 50-70-4 QSA12.Quinones No 50-70-4 QSA13.Hydrazine No 50-70-4 QSA14.Aliphatic azo and azoxy No 50-70-4 QSA15.Isocyanate and isothiocyanate groups No 50-70-4 QSA16.Alkyl carbamate and thiocarbamate No 50-70-4 QSA18.Polycyclic Aromatic Hydrocarbons No 50-70-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-70-4 QSA21.Alkyl and aryl N-nitroso groups No 50-70-4 QSA22.Azide and triazene groups No 50-70-4 QSA23.Aliphatic N-nitro No 50-70-4

Table 18 Continued

		QSA24.α,β unsaturated alkoxy No 50-70-4 QSA25.Aromatic nitroso group No 50-70-4 QSA26.Aromatic ring N-oxide No 50-70-4 QSA27.Nitro aromatic No 50-70-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-70-4 QSA28bis.Aromatic mono- and dialkylamine No 50-70-4 QSA28ter.Aromatic N-acyl amine No 50-70-4 QSA29.Aromatic diazo No 50-70-4 QSA30.Coumarins and Furocoumarins No 50-70-4 QSA32.1,3-dialkoxy-benzene No 50-70-4 QSA33.1-phenoxy-benzene No 50-70-4 QSA34.H-acceptor-path3-H-acceptor Yes 50-70-4 QSA35.Oxolane No 50-70-4 QSA36.Carbodiimides No 50-70-4 QAny alert?.At least one alert fired? Yes Class At least one positive structural alerts for the micronucleus assay (Class I)
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	0	
stearic acid	0	
streptomycin	1	QSA1.Acyl halides No 57-92-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-92-1 QSA3.N-methylol derivatives No 57-92-1 QSA4.Monohaloalkene No 57-92-1 QSA5.S or N mustard No 57-92-1 QSA6.Propiolactones and propiosultones No 57-92-1 QSA7.Epoxides and aziridines No 57-92-1 QSA8.Aliphatic halogens No 57-92-1 QSA9.Alkyl nitrite No 57-92-1 QSA10.α,β unsaturated carbonyls No 57-92-1 QSA11.Simple aldehyde Yes 57-92-1 QSA12.Quinones No 57-92-1 QSA13.Hydrazine No 57-92-1 QSA14.Aliphatic azo and azoxy No 57-92-1 QSA15.Isocyanate and isothiocyanate groups No 57-92-1 QSA16.Alkyl carbamate and thiocarbamate No 57-92-1 QSA18.Polycyclic Aromatic Hydrocarbons No 57-92-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 57-92-1 QSA21.Alkyl and aryl N-nitroso groups No 57-92-1 QSA22.Azide and triazene groups No 57-92-1 QSA23.Aliphatic N-nitro No 57-92-1 QSA24.α,β unsaturated alkoxy No 57-92-1 QSA25.Aromatic nitroso group No 57-92-1 QSA26.Aromatic ring N-oxide No 57-92-1 QSA27.Nitro aromatic No 57-92-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 57-92-1 QSA28bis.Aromatic mono- and dialkylamine No 57-92-1 QSA28ter.Aromatic N-acyl amine No 57-92-1 QSA29.Aromatic diazo No 57-92-1

Table 18 Continued

		QSA30.Coumarins and Furocoumarins No 57-92-1 QSA32.1,3-dialkoxy-benzene No 57-92-1 QSA33.1-phenoxy-benzene No 57-92-1 QSA34.H-acceptor-path3-H-acceptor Yes 57-92-1 QSA35.Oxolane Yes 57-92-1 QSA36.Carbodiimides No 57-92-1 QAny alert?.At least one alert fired? Yes
sucrose	1	QSA1.Acyl halides No 57-50-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-50-1 QSA3.N-methylol derivatives No 57-50-1 QSA4.Monohaloalkene No 57-50-1 QSA5.S or N mustard No 57-50-1 QSA6.Propiolactones and propiosultones No 57-50-1 QSA7.Epoxides and aziridines No 57-50-1 QSA8.Aliphatic halogens No 57-50-1 QSA9.Alkyl nitrite No 57-50-1 QSA10.α,β unsaturated carbonyls No 57-50-1 QSA11.Simple aldehyde No 57-50-1 QSA12.Quinones No 57-50-1 QSA13.Hydrazine No 57-50-1 QSA14.Aliphatic azo and azoxy No 57-50-1 QSA15.Isocyanate and isothiocyanate groups No 57-50-1 QSA16.Alkyl carbamate and thiocarbamate No 57-50-1 QSA18.Polycyclic Aromatic Hydrocarbons No 57-50-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 57-50-1 QSA21.Alkyl and aryl N-nitroso groups No 57-50-1 QSA22.Azide and triazene groups No 57-50-1 QSA23.Aliphatic N-nitro No 57-50-1 QSA24.α,β unsaturated alkoxy No 57-50-1 QSA25.Aromatic nitroso group No 57-50-1 QSA26.Aromatic ring N-oxide No 57-50-1 QSA27.Nitro aromatic No 57-50-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 57-50-1 QSA28bis.Aromatic mono- and dialkylamine No 57-50-1 QSA28ter.Aromatic N-acyl amine No 57-50-1 QSA29.Aromatic diazo No 57-50-1 QSA30.Coumarins and Furocoumarins No 57-50-1 QSA32.1,3-dialkoxy-benzene No 57-50-1 QSA33.1-phenoxy-benzene No 57-50-1 QSA34.H-acceptor-path3-H-acceptor Yes 57-50-1 QSA35.Oxolane Yes 57-50-1 QSA36.Carbodiimides No 57-50-1 QAny alert?.At least one alert fired? Yes
sulfur	0	
thiamine	1	QSA1.Acyl halides No 59-43-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-43-8 QSA3.N-methylol derivatives No 59-43-8 QSA4.Monohaloalkene No 59-43-8 QSA5.S or N mustard No 59-43-8 QSA6.Propiolactones and propiosultones No 59-43-8 QSA7.Epoxides and aziridines No 59-43-8 QSA8.Aliphatic halogens No 59-43-8 QSA9.Alkyl nitrite No 59-43-8 QSA10.α,β unsaturated carbonyls No 59-43-8 QSA11.Simple aldehyde No 59-43-8 QSA12.Quinones No 59-43-8

Table 18 Continued

		QSA13.Hydrazine No 59-43-8 QSA14.Aliphatic azo and azoxy No 59-43-8 QSA15.Isocyanate and isothiocyanate groups No 59-43-8 QSA16.Alkyl carbamate and thiocarbamate No 59-43-8 QSA18.Polycyclic Aromatic Hydrocarbons No 59-43-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 59-43-8 QSA21.Alkyl and aryl N-nitroso groups No 59-43-8 QSA22.Azide and triazene groups No 59-43-8 QSA23.Aliphatic N-nitro No 59-43-8 QSA24.α,β unsaturated alkoxy No 59-43-8 QSA25.Aromatic nitroso group No 59-43-8 QSA26.Aromatic ring N-oxide No 59-43-8 QSA27.Nitro aromatic No 59-43-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 59-43-8 QSA28bis.Aromatic mono- and dialkylamine No 59-43-8 QSA28ter.Aromatic N-acyl amine No 59-43-8 QSA29.Aromatic diazo No 59-43-8 QSA30.Coumarins and Furocoumarins No 59-43-8 QSA32.1,3-dialkoxy-benzene No 59-43-8 QSA33.1-phenoxy-benzene No 59-43-8 QSA34.H-acceptor-path3-H-acceptor No 59-43-8 QSA35.Oxolane No 59-43-8 QSA36.Carbodiimides No 59-43-8 QAny alert?.At least one alert fired? Yes
thimerosal	0	
thymidine	1	QSA1.Acyl halides No 50-89-5 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-89-5 QSA3.N-methylol derivatives No 50-89-5 QSA4.Monohaloalkene No 50-89-5 QSA5.S or N mustard No 50-89-5 QSA6.Propiolactones and propiosultones No 50-89-5 QSA7.Epoxides and aziridines No 50-89-5 QSA8.Aliphatic halogens No 50-89-5 QSA9.Alkyl nitrite No 50-89-5 QSA10.α,β unsaturated carbonyls Yes 50-89-5 QSA11.Simple aldehyde No 50-89-5 QSA12.Quinones No 50-89-5 QSA13.Hydrazine No 50-89-5 QSA14.Aliphatic azo and azoxy No 50-89-5 QSA15.Isocyanate and isothiocyanate groups No 50-89-5 QSA16.Alkyl carbamate and thiocarbamate No 50-89-5 QSA18.Polycyclic Aromatic Hydrocarbons No 50-89-5 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 50-89-5 QSA21.Alkyl and aryl N-nitroso groups No 50-89-5 QSA22.Azide and triazene groups No 50-89-5 QSA23.Aliphatic N-nitro No 50-89-5 QSA24.α,β unsaturated alkoxy No 50-89-5 QSA25.Aromatic nitroso group No 50-89-5 QSA26.Aromatic ring N-oxide No 50-89-5 QSA27.Nitro aromatic No 50-89-5 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 50-89-5 QSA28bis.Aromatic mono- and dialkylamine No 50-89-5 QSA28ter.Aromatic N-acyl amine No 50-89-5 QSA29.Aromatic diazo No 50-89-5

Table 18 Continued

		QSA30.Coumarins and Furocoumarins No 50-89-5 QSA32.1,3-dialkoxy-benzene No 50-89-5 QSA33.1-phenoxy-benzene No 50-89-5 QSA34.H-acceptor-path3-H-acceptor Yes 50-89-5 QSA35.Oxolane Yes 50-89-5 QSA36.Carbodiimides No 50-89-5 QAny alert?.At least one alert fired? Yes
thymine	1	QSA1.Acyl halides No 65-71-4 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 65-71-4 QSA3.N-methylol derivatives No 65-71-4 QSA4.Monohaloalkene No 65-71-4 QSA5.S or N mustard No 65-71-4 QSA6.Propiolactones and propiosultones No 65-71-4 QSA7.Epoxides and aziridines No 65-71-4 QSA8.Aliphatic halogens No 65-71-4 QSA9.Alkyl nitrite No 65-71-4 QSA10.α,β unsaturated carbonyls Yes 65-71-4 QSA11.Simple aldehyde No 65-71-4 QSA12.Quinones No 65-71-4 QSA13.Hydrazine No 65-71-4 QSA14.Aliphatic azo and azoxy No 65-71-4 QSA15.Isocyanate and isothiocyanate groups No 65-71-4 QSA16.Alkyl carbamate and thiocarbamate No 65-71-4 QSA18.Polycyclic Aromatic Hydrocarbons No 65-71-4 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 65-71-4 QSA21.Alkyl and aryl N-nitroso groups No 65-71-4 QSA22.Azide and triazene groups No 65-71-4 QSA23.Aliphatic N-nitro No 65-71-4 QSA24.α,β unsaturated alkoxy No 65-71-4 QSA25.Aromatic nitroso group No 65-71-4 QSA26.Aromatic ring N-oxide No 65-71-4 QSA27.Nitro aromatic No 65-71-4 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 65-71-4 QSA28bis.Aromatic mono- and dialkylamine No 65-71-4 QSA28ter.Aromatic N-acyl amine No 65-71-4 QSA29.Aromatic diazo No 65-71-4 QSA30.Coumarins and Furocoumarins No 65-71-4 QSA32.1,3-dialkoxy-benzene No 65-71-4 QSA33.1-phenoxy-benzene No 65-71-4 QSA34.H-acceptor-path3-H-acceptor Yes 65-71-4 QSA35.Oxolane No 65-71-4 QSA36.Carbodiimides No 65-71-4 QAny alert?.At least one alert fired? Yes
titanium dioxide	0	
triphosphopyridine nucleotide (NADP)	1	QSA1.Acyl halides No 53-59-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 53-59-8 QSA3.N-methylol derivatives No 53-59-8 QSA4.Monohaloalkene No 53-59-8 QSA5.S or N mustard No 53-59-8 QSA6.Propiolactones and propiosultones No 53-59-8 QSA7.Epoxides and aziridines No 53-59-8 QSA8.Aliphatic halogens No 53-59-8 QSA9.Alkyl nitrite No 53-59-8 QSA10.α,β unsaturated carbonyls No 53-59-8 QSA11.Simple

Table 18 Continued

		aldehyde No 53-59-8 QSA12.Quinones No 53-59-8 QSA13.Hydrazine No 53-59-8 QSA14.Aliphatic azo and azoxy No 53-59-8 QSA15.Isocyanate and isothiocyanate groups No 53-59-8 QSA16.Alkyl carbamate and thiocarbamate No 53-59-8 QSA18.Polycyclic Aromatic Hydrocarbons No 53-59-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 53-59-8 QSA21.Alkyl and aryl N-nitroso groups No 53-59-8 QSA22.Azide and triazene groups No 53-59-8 QSA23.Aliphatic N-nitro No 53-59-8 QSA24.α,β unsaturated alkoxy No 53-59-8 QSA25.Aromatic nitroso group No 53-59-8 QSA26.Aromatic ring N-oxide No 53-59-8 QSA27.Nitro aromatic No 53-59-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) Yes 53-59-8 QSA28bis.Aromatic mono- and dialkylamine No 53-59-8 QSA28ter.Aromatic N-acyl amine No 53-59-8 QSA29.Aromatic diazo No 53-59-8 QSA30.Coumarins and Furocoumarins No 53-59-8 QSA32.1,3-dialkoxy-benzene No 53-59-8 QSA33.1-phenoxy-benzene No 53-59-8 QSA34.H-acceptor-path3-H-acceptor Yes 53-59-8 QSA35.Oxolane Yes 53-59-8 QSA36.Carbodiimides No 53-59-8 QAny alert?.At least one alert fired? Yes
tromethamine	1	QSA1.Acyl halides No 77-86-1 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 77-86-1 QSA3.N-methylol derivatives No 77-86-1 QSA4.Monohaloalkene No 77-86-1 QSA5.S or N mustard No 77-86-1 QSA6.Propiolactones and propiosultones No 77-86-1 QSA7.Epoxides and aziridines No 77-86-1 QSA8.Aliphatic halogens No 77-86-1 QSA9.Alkyl nitrite No 77-86-1 QSA10.α,β unsaturated carbonyls No 77-86-1 QSA11.Simple aldehyde No 77-86-1 QSA12.Quinones No 77-86-1 QSA13.Hydrazine No 77-86-1 QSA14.Aliphatic azo and azoxy No 77-86-1 QSA15.Isocyanate and isothiocyanate groups No 77-86-1 QSA16.Alkyl carbamate and thiocarbamate No 77-86-1 QSA18.Polycyclic Aromatic Hydrocarbons No 77-86-1 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 77-86-1 QSA21.Alkyl and aryl N-nitroso groups No 77-86-1 QSA22.Azide and triazene groups No 77-86-1 QSA23.Aliphatic N-nitro No 77-86-1 QSA24.α,β unsaturated alkoxy No 77-86-1 QSA25.Aromatic nitroso group No 77-86-1 QSA26.Aromatic ring N-oxide No 77-86-1 QSA27.Nitro aromatic No 77-86-1 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 77-86-1 QSA28bis.Aromatic mono- and dialkylamine No 77-86-1 QSA28ter.Aromatic N-acyl amine No 77-86-1 QSA29.Aromatic diazo No 77-86-1

Table 18 Continued

		QSA30.Coumarins and Furocoumarins No 77-86-1 QSA32.1,3-dialkoxy-benzene No 77-86-1 QSA33.1-phenoxy-benzene No 77-86-1 QSA34.H-acceptor-path3-H-acceptor Yes 77-86-1 QSA35.Oxolane No 77-86-1 QSA36.Carbodiimides No 77-86-1 QAny alert?.At least one alert fired? Yes
uracil	1	QSA1.Acyl halides No 66-22-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 66-22-8 QSA3.N-methylol derivatives No 66-22-8 QSA4.Monohaloalkene No 66-22-8 QSA5.S or N mustard No 66-22-8 QSA6.Propiolactones and propiosultones No 66-22-8 QSA7.Epoxides and aziridines No 66-22-8 QSA8.Aliphatic halogens No 66-22-8 QSA9.Alkyl nitrite No 66-22-8 QSA10.α,β unsaturated carbonyls Yes 66-22-8 QSA11.Simple aldehyde No 66-22-8 QSA12.Quinones No 66-22-8 QSA13.Hydrazine No 66-22-8 QSA14.Aliphatic azo and azoxy No 66-22-8 QSA15.Isocyanate and isothiocyanate groups No 66-22-8 QSA16.Alkyl carbamate and thiocarbamate No 66-22-8 QSA18.Polycyclic Aromatic Hydrocarbons No 66-22-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 66-22-8 QSA21.Alkyl and aryl N-nitroso groups No 66-22-8 QSA22.Azide and triazene groups No 66-22-8 QSA23.Aliphatic N-nitro No 66-22-8 QSA24.α,β unsaturated alkoxy No 66-22-8 QSA25.Aromatic nitroso group No 66-22-8 QSA26.Aromatic ring N-oxide No 66-22-8 QSA27.Nitro aromatic No 66-22-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 66-22-8 QSA28bis.Aromatic mono- and dialkylamine No 66-22-8 QSA28ter.Aromatic N-acyl amine No 66-22-8 QSA29.Aromatic diazo No 66-22-8 QSA30.Coumarins and Furocoumarins No 66-22-8 QSA32.1,3-dialkoxy-benzene No 66-22-8 QSA33.1-phenoxy-benzene No 66-22-8 QSA34.H-acceptor-path3-H-acceptor Yes 66-22-8 QSA35.Oxolane No 66-22-8 QSA36.Carbodiimides No 66-22-8 QAny alert?.At least one alert fired? Yes
urea	0	
uridine 5'-triphosphate	1	QSA1.Acyl halides No 63-39-8 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 63-39-8 QSA3.N-methylol derivatives No 63-39-8 QSA4.Monohaloalkene No 63-39-8 QSA5.S or N mustard No 63-39-8 QSA6.Propiolactones and propiosultones No 63-39-8 QSA7.Epoxides and aziridines No 63-39-8 QSA8.Aliphatic halogens No 63-39-8 QSA9.Alkyl nitrite No 63-39-8 QSA10.α,β unsaturated carbonyls Yes 63-39-8 QSA11.Simple aldehyde No 63-39-8 QSA12.Quinones No 63-39-8

Table 18 Continued

		QSA13.Hydrazine No 63-39-8 QSA14.Aliphatic azo and azoxy No 63-39-8 QSA15.Isocyanate and isothiocyanate groups No 63-39-8 QSA16.Alkyl carbamate and thiocarbamate No 63-39-8 QSA18.Polycyclic Aromatic Hydrocarbons No 63-39-8 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 63-39-8 QSA21.Alkyl and aryl N-nitroso groups No 63-39-8 QSA22.Azide and triazene groups No 63-39-8 QSA23.Aliphatic N-nitro No 63-39-8 QSA24.α,β unsaturated alkoxy No 63-39-8 QSA25.Aromatic nitroso group No 63-39-8 QSA26.Aromatic ring N-oxide No 63-39-8 QSA27.Nitro aromatic No 63-39-8 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 63-39-8 QSA28bis.Aromatic mono- and dialkylamine No 63-39-8 QSA28ter.Aromatic N-acyl amine No 63-39-8 QSA29.Aromatic diazo No 63-39-8 QSA30.Coumarins and Furocoumarins No 63-39-8 QSA32.1,3-dialkoxy-benzene No 63-39-8 QSA33.1-phenoxy-benzene No 63-39-8 QSA34.H-acceptor-path3-H-acceptor Yes 63-39-8 QSA35.Oxolane Yes 63-39-8 QSA36.Carbodiimides No 63-39-8 QAny alert?.At least one alert fired? Yes
vinyl acetate-chloroethene	1	QSA1.Acyl halides No 9003-20-7 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9003-20-7 QSA3.N-methylol derivatives No 9003-20-7 QSA4.Monohaloalkene No 9003-20-7 QSA5.S or N mustard No 9003-20-7 QSA6.Propiolactones and propiosultones No 9003-20-7 QSA7.Epoxides and aziridines No 9003-20-7 QSA8.Aliphatic halogens No 9003-20-7 QSA9.Alkyl nitrite No 9003-20-7 QSA10.α,β unsaturated carbonyls No 9003-20-7 QSA11.Simple aldehyde No 9003-20-7 QSA12.Quinones No 9003-20-7 QSA13.Hydrazine No 9003-20-7 QSA14.Aliphatic azo and azoxy No 9003-20-7 QSA15.Isocyanate and isothiocyanate groups No 9003-20-7 QSA16.Alkyl carbamate and thiocarbamate No 9003-20-7 QSA18.Polycyclic Aromatic Hydrocarbons No 9003-20-7 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 9003-20-7 QSA21.Alkyl and aryl N-nitroso groups No 9003-20-7 QSA22.Azide and triazene groups No 9003-20-7 QSA23.Aliphatic N-nitro No 9003-20-7 QSA24.α,β unsaturated alkoxy No 9003-20-7 QSA25.Aromatic nitroso group No 9003-20-7 QSA26.Aromatic ring N-oxide No 9003-20-7 QSA27.Nitro aromatic No 9003-20-7 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 9003-20-7 QSA28bis.Aromatic mono- and dialkylamine No 9003-20-7 QSA28ter.Aromatic N-acyl amine No 9003-20-7

Table 18 Continued

		QSA29.Aromatic diazo No 9003-20-7 QSA30.Coumarins and Furocoumarins No 9003-20-7 QSA32.1,3-dialkoxy-benzene No 9003-20-7 QSA33.1-phenoxy-benzene No 9003-20-7 QSA34.H-acceptor-path3-H-acceptor Yes 9003-20-7 QSA35.Oxolane No 9003-20-7 QSA36.Carbodiimides No 9003-20-7 QAny alert?.At least one alert fired? Ye
vitamin E succinate	1	QSA1.Acyl halides No 4345-03-3 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 4345-03-3 QSA3.N-methylol derivatives No 4345-03-3 QSA4.Monohaloalkene No 4345-03-3 QSA5.S or N mustard No 4345-03-3 QSA6.Propiolactones and propiosultones No 4345-03-3 QSA7.Epoxides and aziridines No 4345-03-3 QSA8.Aliphatic halogens No 4345-03-3 QSA9.Alkyl nitrite No 4345-03-3 QSA10.α,β unsaturated carbonyls No 4345-03-3 QSA11.Simple aldehyde No 4345-03-3 QSA12.Quinones No 4345-03-3 QSA13.Hydrazine No 4345-03-3 QSA14.Aliphatic azo and azoxy No 4345-03-3 QSA15.Isocyanate and isothiocyanate groups No 4345-03-3 QSA16.Alkyl carbamate and thiocarbamate No 4345-03-3 QSA18.Polycyclic Aromatic Hydrocarbons No 4345-03-3 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 4345-03-3 QSA21.Alkyl and aryl N-nitroso groups No 4345-03-3 QSA22.Azide and triazene groups No 4345-03-3 QSA23.Aliphatic N-nitro No 4345-03-3 QSA24.α,β unsaturated alkoxy No 4345-03-3 QSA25.Aromatic nitroso group No 4345-03-3 QSA26.Aromatic ring N-oxide No 4345-03-3 QSA27.Nitro aromatic No 4345-03-3 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 4345-03-3 QSA28bis.Aromatic mono- and dialkylamine No 4345-03-3 QSA28ter.Aromatic N-acyl amine No 4345-03-3 QSA29.Aromatic diazo No 4345-03-3 QSA30.Coumarins and Furocoumarins No 4345-03-3 QSA32.1,3-dialkoxy-benzene No 4345-03-3 QSA33.1-phenoxy-benzene No 4345-03-3 QSA34.H-acceptor-path3-H-acceptor Yes 4345-03-3 QSA35.Oxolane No 4345-03-3 QSA36.Carbodiimides No 4345-03-3 QAny alert?.At least one alert fired? Ye
xanthan gum	1	QSA1.Acyl halides No 11138-66-2 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 11138-66-2 QSA3.N-methylol derivatives No 11138-66-2 QSA4.Monohaloalkene No 11138-66-2 QSA5.S or N mustard No 11138-66-2 QSA6.Propiolactones and propiosultones No 11138-66-2 QSA7.Epoxides and aziridines No 11138-66-2 QSA8.Aliphatic halogens No 11138-66-2 QSA9.Alkyl nitrite No 11138-66-2 QSA10.α,β unsaturated carbonyls No 11138-66-2 QSA11.Simple

Table 18 Continued

		aldehyde No 11138-66-2 QSA12.Quinones No 11138-66-2 QSA13.Hydrazine No 11138-66-2 QSA14.Aliphatic azo and azoxy No 11138-66-2 QSA15.Isocyanate and isothiocyanate groups No 11138-66-2 QSA16.Alkyl carbamate and thiocarbamate No 11138-66-2 QSA18.Polycyclic Aromatic Hydrocarbons No 11138-66-2 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 11138-66-2 QSA21.Alkyl and aryl N-nitroso groups No 11138-66-2 QSA22.Azide and triazene groups No 11138-66-2 QSA23.Aliphatic N-nitro No 11138-66-2 QSA24.α,β unsaturated alkoxy No 11138-66-2 QSA25.Aromatic nitroso group No 11138-66-2 QSA26.Aromatic ring N-oxide No 11138-66-2 QSA27.Nitro aromatic No 11138-66-2 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 11138-66-2 QSA28bis.Aromatic mono- and dialkylamine No 11138-66-2 QSA28ter.Aromatic N-acyl amine No 11138-66-2 QSA29.Aromatic diazo No 11138-66-2 QSA30.Coumarins and Furocoumarins No 11138-66-2 QSA32.1,3-dialkoxy-benzene No 11138-66-2 QSA33.1-phenoxy-benzene Yes 11138-66-2 QSA34.H-acceptor-path3-H-acceptor No 11138-66-2 QSA35.Oxolane No 11138-66-2 QSA36.Carbodiimides No 11138-66-2 QAny alert?.At least one alert fired? Ye
xanthine	1	QSA1.Acyl halides No 69-89-6 QSA2.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 69-89-6 QSA3.N-methylol derivatives No 69-89-6 QSA4.Monohaloalkene No 69-89-6 QSA5.S or N mustard No 69-89-6 QSA6.Propiolactones and propiosultones No 69-89-6 QSA7.Epoxides and aziridines No 69-89-6 QSA8.Aliphatic halogens No 69-89-6 QSA9.Alkyl nitrite No 69-89-6 QSA10.α,β unsaturated carbonyls No 69-89-6 QSA11.Simple aldehyde No 69-89-6 QSA12.Quinones No 69-89-6 QSA13.Hydrazine No 69-89-6 QSA14.Aliphatic azo and azoxy No 69-89-6 QSA15.Isocyanate and isothiocyanate groups No 69-89-6 QSA16.Alkyl carbamate and thiocarbamate No 69-89-6 QSA18.Polycyclic Aromatic Hydrocarbons No 69-89-6 QSA19.Heterocyclic Polycyclic Aromatic Hydrocarbons No 69-89-6 QSA21.Alkyl and aryl N-nitroso groups No 69-89-6 QSA22.Azide and triazene groups No 69-89-6 QSA23.Aliphatic N-nitro No 69-89-6 QSA24.α,β unsaturated alkoxy No 69-89-6 QSA25.Aromatic nitroso group No 69-89-6 QSA26.Aromatic ring N-oxide No 69-89-6 QSA27.Nitro aromatic No 69-89-6 QSA28.Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) No 69-89-6 QSA28bis.Aromatic mono- and dialkylamine No 69-89-6 QSA28ter.Aromatic N-acyl

Table 18 Continued

		amine No 69-89-6 QSA29.Aromatic diazo No 69-89-6 QSA30.Coumarins and Furocoumarins No 69-89-6 QSA32.1,3-dialkoxy-benzene No 69-89-6 QSA33.1-phenoxy-benzene No 69-89-6 QSA34.H-acceptor-path3-H-acceptor Yes 69-89-6 QSA35.Oxolane No 69-89-6 QSA36.Carbodiimides No 69-89-6 QAny alert?.At least one alert fired? Yes
zinc	0	
zinc oxide	0	

Table 19. Classification of the Test Set by the Benigni-Bossa Algorithm

Chemical	Non-Genotoxic Carcinogen Class	Genotoxic Carcinogen Class	Verbose Explanation
1,2 polybutadiene	0	0	
1,2 propylene oxide	0	1	QSA1_gen.Acyl halides No 75-56-9 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 75-56-9 QSA3_gen.N-methylol derivatives No 75-56-9 QSA4_gen.Monohaloalkene No 75-56-9 QSA5_gen.S or N mustard No 75-56-9 QSA6_gen.P
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	0	0	
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	1	1	QSA1_gen.Acyl halides No 3006-93-7 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 3006-93-7 QSA3_gen.N-methylol derivatives No 3006-93-7 QSA4_gen.Monohaloalkene No 3006-93-7 QSA5_gen.S or N mustard No 3006-93-7
2,2 dimethyl-pentane	0	0	

Table 19 Continued

2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	0	0	
2-deoxyadenosine	0	1	QSA1_gen.Acyl halides No 958-09-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 958-09-8 QSA3_gen.N-methylol derivatives No 958-09-8 QSA4_gen.Monohaloalkene No 958-09-8 QSA5_gen.S or N mustard No 958-09-8 QSA6_
2'-deoxycytidine	0	0	
2'-deoxyguanosine	0	0	
2-phenoxyethanol	0	0	
3-methylpentane	0	0	
5-methyldeoxycytidine	0	0	
6,15-dihydroanthrazine-5,9,14,18-tetrone.	0	1	QSA1_gen.Acyl halides No 81-77-6 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 81-77-6 QSA3_gen.N-methylol derivatives No 81-77-6 QSA4_gen.Monohaloalkene No 81-77-6 QSA5_gen.S or N mustard No 81-77-6 QSA6_gen.P
acrylonitrile	0	0	
adenosine	0	1	QSA1_gen.Acyl halides No 58-61-7 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 58-61-7 QSA3_gen.N-methylol derivatives No 58-61-7 QSA4_gen.Monohaloalkene No 58-61-7 QSA5_gen.S or N mustard No 58-61-7 QSA6_gen.P
aluminum (used values for aluminum	0	0	

Table 19 Continued

chloride)			
aluminum hydroxide	0	0	
aluminum phosphate	0	0	
aluminum silicate	0	0	
aluminum sulfate	0	0	
ammonium sulfate	0	0	
amphotericin B	0	0	
arsenic	1	0	QSA1_gen.Acyl halides No 7440-38-2 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7440-38-2 QSA3_gen.N-methylol derivatives No 7440-38-2 QSA4_gen.Monohaloalkene No 7440-38-2 QSA5_gen.S or N mustard No 7440-38-2
benzethonium chloride	0	0	
benzoic acid	0	0	
beta-propriolactone	0	1	QSA1_gen.Acyl halides No 57-57-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-57-8 QSA3_gen.N-methylol derivatives No 57-57-8 QSA4_gen.Monohaloalkene No 57-57-8 QSA5_gen.S or N mustard No 57-57-8 QSA6_gen.P
biotin	0	0	
boron	0	0	
bromine	0	0	
butylated hydroxytoluene (BHT)	0	0	
calcium carbonate	0	0	
calcium chloride	0	0	
calcium chloride dihydrate	0	0	
calcium pantothenate (vitamin B5)	1	0	QSA1_gen.Acyl halides No 137-08-6 QSA2_gen.Alkyl (C5) or benzyl ester of

Table 19 Continued

			sulphonic or phosphonic acid No 137-08-6 QSA3_gen.N-methylol derivatives No 137-08-6 QSA4_gen.Monohaloalkene No 137-08-6 QSA5_gen.S or N mustard No 137-08-6 QSA6_
carbon	0	0	
cesium hydroxide	0	0	
cetrimonium bromide (CTAB)	0	0	
chlortetracycline	0	1	QSA1_gen.Acyl halides No 57-62-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-62-5 QSA3_gen.N-methylol derivatives No 57-62-5 QSA4_gen.Monohaloalkene No 57-62-5 QSA5_gen.S or N mustard No 57-62-5 QSA6_gen.P
cholesterol	0	0	
choline chloride	0	0	
citric acid	1	0	QSA1_gen.Acyl halides No 77-92-9 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 77-92-9 QSA3_gen.N-methylol derivatives No 77-92-9 QSA4_gen.Monohaloalkene No 77-92-9 QSA5_gen.S or N mustard No 77-92-9 QSA6_gen.P
co-carboxylase	0	0	
coenzyme A	1	1	QSA1_gen.Acyl halides No coenzyme A QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No coenzyme A QSA3_gen.N-methylol derivatives No coenzyme A QSA4_gen.Monohaloalkene

Table 19 Continued

			No coenzyme A QSA5_gen.S or N mustard No coenzyme
cyclohexane	0	0	
DDT (dichlorodiphenyltrichloroethane)	1	0	QSA1_gen.Acyl halides No 50-29-3 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-29-3 QSA3_gen.N-methylol derivatives No 50-29-3 QSA4_gen.Monohaloalkene No 50-29-3 QSA5_gen.S or N mustard No 50-29-3 QSA6_gen.P
deoxycholic acid	0	0	
dextran	0	1	QSA1_gen.Acyl halides No 9004-54-0 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 9004-54-0 QSA3_gen.N-methylol derivatives No 9004-54-0 QSA4_gen.Monohaloalkene No 9004-54-0 QSA5_gen.S or N mustard No 9004-54-0
D-galactose	0	0	
diadenine sulfate	1	1	QSA1_gen.Acyl halides No 321-30-2 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 321-30-2 QSA3_gen.N-methylol derivatives No 321-30-2 QSA4_gen.Monohaloalkene No 321-30-2 QSA5_gen.S or N mustard No 321-30-2 QSA6_
disodium phosphate	0	0	
disodium phosphate dodecahydrate	0	0	
DL-aspartic acid	0	0	
DL-glutamic acid	0	0	
D-ribose	0	0	
d-sorbitol	0	0	

Table 19 Continued

edetate disodium (EDTA)	0	0	
ergocalciferol (vitamin D2)	0	0	
ethanolamine	0	0	
ethyl acrylate		0	
ethylene oxide	0	1	QSA1_gen.Acyl halides No 75-21-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 75-21-8 QSA3_gen.N-methylol derivatives No 75-21-8 QSA4_gen.Monohaloalkene No 75-21-8 QSA5_gen.S or N mustard No 75-21-8 QSA6_gen.P
ethylene; (5E)-5-ethylidenebicyclo[2.2.1]hept-2-ene; prop-1-ene	0	0	
ferric (III) nitrate	0	0	
ferrous succinate (butanedioic acid)	0	0	
flavin adenine dinucleotide (FAD)	0	1	QSA1_gen.Acyl halides No 146-14-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 146-14-5 QSA3_gen.N-methylol derivatives No 146-14-5 QSA4_gen.Monohaloalkene No 146-14-5 QSA5_gen.S or N mustard No 146-14-5 QSA6_
folic acid	0	0	
formaldehyde	0	0	
gentamicin	0	0	
glutaral	0	1	QSA1_gen.Acyl halides No 111-30-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 111-30-8 QSA3_gen.N-methylol derivatives No 111-30-8

Table 19 Continued

			QSA4_gen.Monohaloalkene No 111-30-8 QSA5_gen.S or N mustard No 111-30-8 QSA6_
glutathione	0	0	
glycerin	0	0	
glycine	0	0	
guanine hydrochloride	1	0	QSA1_gen.Acyl halides No 33735-91-0 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 33735-91-0 QSA3_gen.N-methylol derivatives No 33735-91-0 QSA4_gen.Monohaloalkene No 33735-91-0 QSA5_gen.S or N mustard No 33735-91
hemin chloride	0	1	QSA1_gen.Acyl halides No 16009-13-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 16009-13-5 QSA3_gen.N-methylol derivatives No 16009-13-5 QSA4_gen.Monohaloalkene No 16009-13-5 QSA5_gen.S or N mustard No 16009-13
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	0	0	
0	0		
hexachlorobenzene	0	0	
hexamethyldisiloxane	0	0	QSA1_gen.Acyl halides No 63148-62-9 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 63148-62-9 QSA3_gen.N-methylol derivatives No 63148-62-9 QSA4_gen.Monohaloalkene No 63148-62-9 QSA5_gen.S or N mustard No 63148-62

Table 19 Continued

hydrocortisone	0	1	QSA1_gen.Acyl halides No 50-23-7 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-23-7 QSA3_gen.N-methylol derivatives No 50-23-7 QSA4_gen.Monohaloalkene No 50-23-7 QSA5_gen.S or N mustard No 50-23-7 QSA6_gen.P
hydroxy L proline	0	0	
hydroxylysine	0	0	
hypoxanthine	1	0	QSA1_gen.Acyl halides No 68-94-0 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 68-94-0 QSA3_gen.N-methylol derivatives No 68-94-0 QSA4_gen.Monohaloalkene No 68-94-0 QSA5_gen.S or N mustard No 68-94-0 QSA6_gen.P
i-Inositol	0	0	
indigo	0	1	QSA1_gen.Acyl halides No 482-89-3 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 482-89-3 QSA3_gen.N-methylol derivatives No 482-89-3 QSA4_gen.Monohaloalkene No 482-89-3 QSA5_gen.S or N mustard No 482-89-3 QSA6_
iron	0	0	
iron (II) sulfate heptahydrate	0	0	
iron ammonium citrate (FERRIC AMMONIUM CITRATE)	0	0	
iron III nitrate	0	0	
kanamycin	0	0	
lactose	0	0	

Table 19 Continued

L-alanine	0	0	
L-arginine	0	0	
L-ascorbic acid	0	0	
L-asparagine	0	0	
L-cysteine	0	0	
L-cystine	0	0	
L-glutamic acid	0	0	
L-glutamine	0	0	
L-histidine	1	0	QSA1_gen.Acyl halides No 71-00-1 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 71-00-1 QSA3_gen.N-methylol derivatives No 71-00-1 QSA4_gen.Monohaloalkene No 71-00-1 QSA5_gen.S or N mustard No 71-00-1 QSA6_gen.P
L-isoleucine	0	0	
L-leucine	0	0	
L-lysine	0	0	
L-methionine	0	0	
L-phenylalanine	0	0	
L-proline	0	0	
L-serine	0	0	
L-threonine	0	0	
L-tryptophan	0	0	
L-tyrosine	0	0	
L-valine	0	0	
magnesium	0	0	
magnesium chloride	0	0	
magnesium silicate (talc)	0	0	
magnesium stearate	0	0	
magnesium sulfate	0	0	
menadione	0	1	QSA1_gen.Acyl halides No 58-27-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 58-27-5 QSA3_gen.N-methylol derivatives No 58-27-5 QSA4_gen.Monohaloalkene No 58-27-5 QSA5_gen.S or

Table 19 Continued

			N mustard No 58-27-5 QSA6_gen.P
mercury	1	0	QSA1_gen.Acyl halides No 7439-97-6 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 7439-97-6 QSA3_gen.N-methylol derivatives No 7439-97-6 QSA4_gen.Monohaloalkene No 7439-97-6 QSA5_gen.S or N mustard No 7439-97-6
methylcyclopentane	0	0	
methyltrimethoxysilane	0	0	
monobasic potassium phosphate	0	0	
monobasic sodium phosphate	0	0	
monosodium L glutamate	0	0	
m-xylene	0	0	
nadide (NAD)	0	1	QSA1_gen.Acyl halides No 53-84-9 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 53-84-9 QSA3_gen.N-methylol derivatives No 53-84-9 QSA4_gen.Monohaloalkene No 53-84-9 QSA5_gen.S or N mustard No 53-84-9 QSA6_gen.P
n-dodecane	0	0	
neomycin	0	0	
n-hexadecane	0	0	
n-hexane	0	0	
nicotinamide	0	0	
nicotinic acid	0	0	
n-octadecane	0	0	
n-tetradecane	0	0	
octoxynol 9	0	0	
palmitic acid	0	0	
p-aminobenzoic acid	0	1	QSA1_gen.Acyl halides No

Table 19 Continued

(4-AMINOBENZOIC ACID)			150-13-0 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 150-13-0 QSA3_gen.N-methylol derivatives No 150-13-0 QSA4_gen.Monohaloalkene No 150-13-0 QSA5_gen.S or N mustard No 150-13-0 QSA6_
PCB 1221	0	0	
PCB 1242	0	0	
PCB 1248	0	0	
PCB 1254	0	0	
PCB 1260	1	0	QSA1_gen.Acyl halides No 11096-82-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 11096-82-5 QSA3_gen.N-methylol derivatives No 11096-82-5 QSA4_gen.Monohaloalkene No 11096-82-5 QSA5_gen.S or N mustard No 11096-82
p-cymene	0	0	
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	0	0	
phenol	0	0	
phenol red (phenolsulfonphthalein)	0	0	
polyethylene glycol nonylphenyl ether	0	0	
polymyxin B	0	0	
polypropylene	0	0	
polysorbate 20	0	0	
polysorbate 80 (tween 80)	0	0	
polystyrene	0	0	
polyvinyl alcohol	0	0	
potassium	0	0	

Table 19 Continued

potassium chloride	0	0	
potassium glutamate	0	0	
p-xylene	0	0	
pyridoxal	0	1	QSA1_gen.Acyl halides No 66-72-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 66-72-8 QSA3_gen.N-methylol derivatives No 66-72-8 QSA4_gen.Monohaloalkene No 66-72-8 QSA5_gen.S or N mustard No 66-72-8 QSA6_gen.P
pyridoxine	0	0	
retinyl acetate	0	0	QSA1_gen.Acyl halides No 127-47-9 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 127-47-9 QSA3_gen.N-methylol derivatives No 127-47-9 QSA4_gen.Monohaloalkene No 127-47-9 QSA5_gen.S or N mustard No 127-47-9 QSA6_
riboflavin	0	0	
silicon	0	0	
silicon dioxide	0	0	
sodium	0	0	
sodium acetate	0	0	
sodium bicarbonate	0	0	
sodium borate	0	0	
sodium chloride	0	0	
sodium citrate	0	0	
sodium dihydrogen phosphate dihydrate	0	0	
sodium glucuronate	0	1	QSA1_gen.Acyl halides No 14984-34-0 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 14984-34-0 QSA3_gen.N-methylol derivatives No 14984-34-0 QSA4_gen.Monohaloalkene

Table 19 Continued

			No 14984-34-0 QSA5_gen.S or N mustard No 14984-34
sodium hydroxide	0	0	
sodium metabisulphite	0	0	
sodium phosphate	0	0	
sodium phosphate dibasic heptahydrate	0	0	
sodium pyruvate	0	0	
sodium taurodeoxycholate	0	0	
sorbitan monoleate	0	0	
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	0	0	
stearic acid	0	0	
streptomycin	0	1	QSA1_gen.Acyl halides No 57-92-1 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-92-1 QSA3_gen.N-methylol derivatives No 57-92-1 QSA4_gen.Monohaloalkene No 57-92-1 QSA5_gen.S or N mustard No 57-92-1 QSA6_gen.P
sucrose	0	0	
sulfur	0	0	
tetrafluoroethylene	0	0	
thiamine	0	1	QSA1_gen.Acyl halides No 59-43-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 59-43-8 QSA3_gen.N-methylol derivatives No 59-43-8 QSA4_gen.Monohaloalkene No 59-43-8 QSA5_gen.S or N mustard No 59-43-8 QSA6_gen.P
thimerosal	1	0	QSA1_gen.Acyl halides No 54-64-8 QSA2_gen.Alkyl

Table 19 Continued

			(C5) or benzyl ester of sulphonic or phosphonic acid No 54-64-8 QSA3_gen.N-methylol derivatives No 54-64-8 QSA4_gen.Monohaloalkene No 54-64-8 QSA5_gen.S or N mustard No 54-64-8 QSA6_gen.P
thymidine	0	1	QSA1_gen.Acyl halides No 50-89-5 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 50-89-5 QSA3_gen.N-methylol derivatives No 50-89-5 QSA4_gen.Monohaloalkene No 50-89-5 QSA5_gen.S or N mustard No 50-89-5 QSA6_gen.P
thymine	0	1	QSA1_gen.Acyl halides No 65-71-4 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 65-71-4 QSA3_gen.N-methylol derivatives No 65-71-4 QSA4_gen.Monohaloalkene No 65-71-4 QSA5_gen.S or N mustard No 65-71-4 QSA6_gen.P
titanium	0	0	
titanium dioxide	0	0	
triphosphopyridine nucleotide (NADP)	0	1	QSA1_gen.Acyl halides No 53-59-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 53-59-8 QSA3_gen.N-methylol derivatives No 53-59-8 QSA4_gen.Monohaloalkene No 53-59-8 QSA5_gen.S or N mustard No 53-59-8 QSA6_gen.P
tromethamine	0	0	
uracil	0	1	QSA1_gen.Acyl halides No

Table 19 Continued

			66-22-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 66-22-8 QSA3_gen.N-methylol derivatives No 66-22-8 QSA4_gen.Monohaloalkene No 66-22-8 QSA5_gen.S or N mustard No 66-22-8 QSA6_gen.P
urea	0	0	QSA1_gen.Acyl halides No 57-13-6 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 57-13-6 QSA3_gen.N-methylol derivatives No 57-13-6 QSA4_gen.Monohaloalkene No 57-13-6 QSA5_gen.S or N mustard No 57-13-6 QSA6_gen.P
uridine 5'-triphosphate	0	1	QSA1_gen.Acyl halides No 63-39-8 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 63-39-8 QSA3_gen.N-methylol derivatives No 63-39-8 QSA4_gen.Monohaloalkene No 63-39-8 QSA5_gen.S or N mustard No 63-39-8 QSA6_gen.P
vitamin E succinate	0	0	
xanthine	1	0	QSA1_gen.Acyl halides No 69-89-6 QSA2_gen.Alkyl (C5) or benzyl ester of sulphonic or phosphonic acid No 69-89-6 QSA3_gen.N-methylol derivatives No 69-89-6 QSA4_gen.Monohaloalkene No 69-89-6 QSA5_gen.S or N mustard No 69-89-6 QSA6_gen.P
zinc	0	0	
zinc oxide	0	0	

Table 20. Classification of Test Set Sorted by Cramer Extended Algorithm

Chemical	Cramer Class	Verbose Explanation
1,2 polybutadiene	1	Q1.Normal constituent of the body No, Q2 Contains functional groups associated with enhanced toxicity No, Q3.Contains elements other than C,H,O,N,divalent S No, Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
2,2 dimethyl-pentane	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No, Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents Yes Q18.One of the list (see explanation) No Class Low (Class I)
2-deoxyadenosine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
2'-deoxycytidine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
2'-deoxyguanosine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
3-methylpentane	1	Q1.Normal constituent of the body No Q2.Contains functional

Table 20 Continued

		groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
adenosine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
benzoic acid	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes Q27.Rings with substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents No Q18.One of the list (see explanation) No Class Low (Class I)
beta-propriolactone	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester Yes Q9.Lactone, fused to another ring, or 5- or 6-membered a,b-unsaturated lactone? No Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
biotin	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)

Table 20 Continued

carbon	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
cholesterol	1	Q1.Normal constituent of the body Yes Class Low (Class I) 57-88-5
citric acid	1	Q1.Normal constituent of the body Yes Class Low (Class I)
cyclohexane	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents Yes Q18.One of the list (see explanation) No Class Low (Class I)
D-galactose	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
DL-aspartic acid	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
DL-glutamic acid	1	Q1.Normal constituent of the body Yes Class Low (Class I)
D-ribose	1	Q1.Normal constituent of the body No 50-69-1 Q2.Contains functional groups associated with enhanced toxicity No 50-69-1 Q3.Contains elements other than C,H,O,N,divalent S No 50-69-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
d-sorbitol	1	Q1.Normal constituent of the body Yes Class Low (Class I)
ethanolamine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
ethyl acrylate	1	Q1.Normal constituent of the body No 9003-32-1 Q2.Contains functional groups associated with enhanced toxicity No 9003-32-1 Q3.Contains elements other than

Table 20 Continued

		C,H,O,N,divalent S No 9003-32-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 9003-32-1 Q6.Benzene derivative with certain substituents No 9003-32-1 Q7.Heterocyclic No 9003-32-1 Q16.Common terpene No 9003-32-1 Q17.Readily hydrolysed to a common terpene No 9003-32-1 Q19.Open chain Yes 9003-32-1 Q20.Aliphatic with some functional groups (see explanation) Yes 9003-32-1 Q21.3 or more different functional groups No 9003-32-1 Q18.One of the list (see explanation) No Class Low (Class I)
formaldehyde	1	Q1.Normal constituent of the body Yes Class Low (Class I)
glutaral	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
glutathione	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
glycerin	1	Q1.Normal constituent of the body Yes Class Low (Class I)
glycine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. No Q12.Heteroaromatic No Q22.Common component of food No Q33.Has sufficient number of sulphonate or

Table 20 Continued

		sulphamate groups Yes Class Low (Class I)
heptakis(2,6-O-dimethyl)beta-cyclodextrin	1	Q3.Contains elements other than C,H,O,N,divalent S Yes 137-08-6
hydroxy L proline	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. No Q12.Heteroaromatic No Q22.Common component of food Yes Class Intermediate (Class II)
hypoxanthine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
i-Inositol	1	Q1.Normal constituent of the body Yes Class Low (Class I)
L-alanine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
L-arginine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
L-ascorbic acid	1	Q1.Normal constituent of the body Yes Class Low (Class I)
L-asparagine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily

Table 20 Continued

		hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food Yes Class Intermediate (Class II)
L-cysteine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups Yes Class High (Class III)
L-glutamic acid	1	Q1.Normal constituent of the body Yes Class Low (Class I)
L-glutamine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food Yes Class Intermediate (Class II)
L-histidine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
L-isoleucine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)

Table 20 Continued

L-leucine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
L-lysine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food Yes Class Intermediate (Class II)
L-methionine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups Yes Class High (Class III)
L-phenylalanine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes 63-91-2 Q27.Rings with substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents Yes Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. No Q22.Common component of food Yes Class Intermediate (Class II)

Table 20 Continued

L-proline	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. No Q12.Heteroaromatic No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
L-serine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups Yes Class High (Class III)
L-threonine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
L-tryptophan	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
L-tyrosine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes Q27.Rings with substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents Yes Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No Q32.Contains only the functional groups listed in Q30 or Q31 and those listed

Table 20 Continued

		below. No Q22.Common component of food Yes Class Intermediate (Class II)
L-valine	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
menadione	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes Q27.Rings with substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents No Q18.One of the list (see explanation) No Class Low (Class I)
methylcyclopentane	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents Yes Q18.One of the list (see explanation) No Class Low (Class I)
m-xylene	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No 108-38-3 Q7.Heterocyclic No 108-38-3 Q16.Common terpene No 108-38-3 Q17.Readily hydrolysed to a common terpene No 108-38-3 Q19.Open chain No 108-38-3 Q23.Aromatic Yes 108-38-3 Q27.Rings with substituents Yes 108-38-3 Q28.More than one aromatic ring No 108-38-3 Q30.Aromatic Ring with

Table 20 Continued

		complex substituents No 108-38-3 Q18.One of the list (see explanation) No Class Low (Class I)
n-dodecane	1	Q1.Normal constituent of the body No 112-40-3 Q2.Contains functional groups associated with enhanced toxicity No 112-40-3 Q3.Contains elements other than C,H,O,N,divalent S No 112-40-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
n-hexadecane	1	Q1.Normal constituent of the body No 544-76-3 Q2.Contains functional groups associated with enhanced toxicity No 544-76-3 Q3.Contains elements other than C,H,O,N,divalent S No 544-76-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
n-hexane	1	Q1.Normal constituent of the body No 110-54-3 Q2.Contains functional groups associated with enhanced toxicity No 110-54-3 Q3.Contains elements other than C,H,O,N,divalent S No 110-54-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
nicotinamide	1	Q1.Normal constituent of the body Yes Class Low (Class I)
n-octadecane	1	Q1.Normal constituent of the body No 593-45-3 Q2.Contains functional groups associated with enhanced toxicity No 593-45-3 Q3.Contains elements other than C,H,O,N,divalent S No 593-45-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
n-tetradecane	1	Q1.Normal constituent of the body No 629-59-4 Q2.Contains functional groups associated with enhanced toxicity No 629-59-4 Q3.Contains elements other than C,H,O,N,divalent S No 629-59-4 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
palmitic acid	1	Q1.Normal constituent of the body Yes Class Low (Class I)
p-cymene	1	Q1.Normal constituent of the body No 99-87-6 Q2.Contains functional groups associated with enhanced toxicity No 99-87-6 Q3.Contains elements other than C,H,O,N,divalent S No 99-87-6 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 99-87-6 Q6.Benzene derivative with certain substituents No 99-87-6 Q7.Heterocyclic No 99-87-6 Q16.Common terpene No 99-87-6 Q17.Readily hydrolysed to a common terpene No 99-87-6 Q19.Open chain No 99-87-6 Q23.Aromatic Yes 99-87-6 Q27.Rings with substituents Yes 99-87-6 Q28.More than one aromatic ring No 99-87-6 Q30.Aromatic Ring with complex substituents No 99-87-6 Q18.One of the list (see

Table 20 Continued

		explanation) No Class Low (Class I) 99-87-6
phenol	1	Q1.Normal constituent of the body No 108-95-2 Q2.Contains functional groups associated with enhanced toxicity No 108-95-2 Q3.Contains elements other than C,H,O,N,divalent S No 108-95-2 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 108-95-2 Q6.Benzene derivative with certain substituents No 108-95-2 Q7.Heterocyclic No 108-95-2 Q16.Common terpene No 108-95-2 Q17.Readily hydrolysed to a common terpene No 108-95-2 Q19.Open chain No 108-95-2 Q23.Aromatic Yes 108-95-2 Q27.Rings with substituents Yes 108-95-2 Q28.More than one aromatic ring No 108-95-2 Q30.Aromatic Ring with complex substituents No 108-95-2 Q18.One of the list (see explanation) No Class Low (Class I)
phenol red (phenolsulfonphthalein)	1	Q1.Normal constituent of the body No 143-74-8 Q2.Contains functional groups associated with enhanced toxicity No 143-74-8 Q3.Contains elements other than C,H,O,N,divalent S Yes 143-74-8 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes 143-74-8 Q7.Heterocyclic Yes 143-74-8 Q8.Lactone or cyclic diester No 143-74-8 Q10.3-membered heterocycle No 143-74-8 Q11.Has a heterocyclic ring with complex substituents. Yes 143-74-8 Q33.Has sufficient number of sulphonate or sulphamate groups Yes Class Low (Class I)
polystyrene	1	Q1.Normal constituent of the body No 9003-53-6 Q2.Contains functional groups associated with enhanced toxicity No 9003-53-6 Q3.Contains elements other than C,H,O,N,divalent S No 9003-53-6 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 9003-53-6 Q6.Benzene derivative with certain substituents No 9003-53-6 Q7.Heterocyclic No 9003-53-6 Q16.Common terpene No 9003-53-6 Q17.Readily hydrolysed to a common terpene No 9003-53-6 Q19.Open chain No 9003-53-6 Q23.Aromatic Yes 9003-53-6 Q27.Rings with substituents Yes 9003-53-6 Q28.More than one aromatic ring No 9003-53-6 Q30.Aromatic Ring with complex substituents No 9003-53-6 Q18.One of the list (see explanation) No Class Low (Class I)
polyvinyl alcohol	1	Q1.Normal constituent of the body No 9002-89-5 Q2.Contains functional groups associated with enhanced toxicity No 9002-89-5 Q3.Contains elements other than C,H,O,N,divalent S No 9002-89-5 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 9002-89-5 Q6.Benzene derivative with certain substituents No

Table 20 Continued

		9002-89-5 Q7.Heterocyclic No 9002-89-5 Q16.Common terpene No 9002-89-5 Q17.Readily hydrolysed to a common terpene No 9002-89-5 Q19.Open chain Yes 9002-89-5 Q20.Aliphatic with some functional groups (see explanation) Yes 9002-89-5 Q21.3 or more different functional groups No 9002-89-5 Q18.One of the list (see explanation) No Class Low (Class I)
p-xylene	1	Q1.Normal constituent of the body No 106-42-3 Q2.Contains functional groups associated with enhanced toxicity No 106-42-3 Q3.Contains elements other than C,H,O,N,divalent S No 106-42-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 106-42-3 Q6.Benzene derivative with certain substituents No 106-42-3 Q7.Heterocyclic No 106-42-3 Q16.Common terpene No 106-42-3 Q17.Readily hydrolysed to a common terpene No 106-42-3 Q19.Open chain No 106-42-3 Q23.Aromatic Yes 106-42-3 Q27.Rings with substituents Yes 106-42-3 Q28.More than one aromatic ring No 106-42-3 Q30.Aromatic Ring with complex substituents No 106-42-3 Q18.One of the list (see explanation) No Class Low (Class I)
pyridoxal	1	Q1.Normal constituent of the body Yes Class Low (Class I)
pyridoxine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
retinyl acetate	1	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents Yes Q18.One of the list (see explanation) No Class Low (Class I)
riboflavin	1	Q1.Normal constituent of the body No 83-88-5 Q2.Contains functional groups associated with enhanced toxicity No 83-88-5 Q3.Contains elements other than C,H,O,N,divalent S No 83-88-5 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 83-88-5 Q6.Benzene derivative with certain substituents No 83-88-5 Q7.Heterocyclic Yes 83-88-5 Q8.Lactone or cyclic diester No 83-88-5 Q10.3-membered heterocycle No 83-88-5 Q11.Has a heterocyclic ring with complex substituents. Yes 83-88-5 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
sorbitan monoleate	1	Q1.Normal constituent of the body No 1338-43-8 Q2.Contains functional groups associated with enhanced

Table 20 Continued

		toxicity No 1338-43-8 Q3.Contains elements other than C,H,O,N,divalent S No 1338-43-8 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 1338-43-8 Q6.Benzene derivative with certain substituents No 1338-43-8 Q7.Heterocyclic Yes 1338-43-8 Q8.Lactone or cyclic diester No 1338-43-8 Q10.3-membered heterocycle No 1338-43-8 Q11.Has a heterocyclic ring with complex substituents. No 1338-43-8 Q12.Heteroaromatic No 1338-43-8 Q22.Common component of food No 1338-43-8 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	1	Q1.Normal constituent of the body No 111-02-4 Q2.Contains functional groups associated with enhanced toxicity No 111-02-4 Q3.Contains elements other than C,H,O,N,divalent S No 111-02-4 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
stearic acid	1	Q1.Normal constituent of the body No 57-11-4 Q2.Contains functional groups associated with enhanced toxicity No 57-11-4 Q3.Contains elements other than C,H,O,N,divalent S No 57-11-4 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 57-11-4 Q6.Benzene derivative with certain substituents No 57-11-4 Q7.Heterocyclic No 57-11-4 Q16.Common terpene No 57-11-4 Q17.Readily hydrolysed to a common terpene No 57-11-4 Q19.Open chain Yes 57-11-4 Q20.Aliphatic with some functional groups (see explanation) Yes 57-11-4 Q21.3 or more different functional groups No 57-11-4 Q18.One of the list (see explanation) No Class Low (Class I)
sucrose	1	Q1.Normal constituent of the body No 57-50-1 Q2.Contains functional groups associated with enhanced toxicity No 57-50-1 Q3.Contains elements other than C,H,O,N,divalent S No 57-50-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 57-50-1 Q6.Benzene derivative with certain substituents No 57-50-1 Q7.Heterocyclic Yes 57-50-1 Q8.Lactone or cyclic diester No 57-50-1 Q10.3-membered heterocycle No 57-50-1 Q11.Has a heterocyclic ring with complex substituents. Yes 57-50-1 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
thymidine	1	Q1.Normal constituent of the body No 50-89-5 Q2.Contains functional groups associated with enhanced toxicity No 50-89-5 Q3.Contains elements other than C,H,O,N,divalent S No 50-89-5 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 50-89-5 Q6.Benzene derivative

Table 20 Continued

		with certain substituents No 50-89-5 Q7.Heterocyclic Yes 50-89-5 Q8.Lactone or cyclic diester No 50-89-5 Q10.3-membered heterocycle No 50-89-5 Q11.Has a heterocyclic ring with complex substituents. Yes 50-89-5 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
thymine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
tromethamine	1	Q1.Normal constituent of the body No 77-86-1 Q2.Contains functional groups associated with enhanced toxicity No 77-86-1 Q3.Contains elements other than C,H,O,N,divalent S No 77-86-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 77-86-1 Q6.Benzene derivative with certain substituents No 77-86-1 Q7.Heterocyclic No 77-86-1 Q16.Common terpene No 77-86-1 Q17.Readily hydrolysed to a common terpene No 77-86-1 Q19.Open chain Yes 77-86-1 Q20.Aliphatic with some functional groups (see explanation) Yes 77-86-1 Q21.3 or more different functional groups No 77-86-1 Q18.One of the list (see explanation) No Class Low (Class I)
uracil	1	Q1.Normal constituent of the body Yes Class Low (Class I)
urea	1	Q1.Normal constituent of the body Yes Class Low (Class I)
uridine 5'-triphosphate	1	Q1.Normal constituent of the body Yes Class Low (Class I)
xanthine	1	Q1.Normal constituent of the body Yes Class Low (Class I)
2-phenoxyethanol	2 *	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5 Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes Q27.Rings with substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents Yes Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. Yes Class Intermediate (Class II) 122-99-6
butylated hydroxytoluene (BHT)	2	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic Yes Q27.Rings with

Table 20 Continued

		substituents Yes Q28.More than one aromatic ring No Q30.Aromatic Ring with complex substituents No Q18.One of the list (see explanation) Yes Class Intermediate (Class II)
L-cystine	2	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S N Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food Yes Class Intermediate (Class II)
nicotinic acid	2	Q1.Normal constituent of the body No 59-67-6 Q2.Contains functional groups associated with enhanced toxicity No 59-67-6 Q3.Contains elements other than C,H,O,N,divalent S No 59-67-6 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 59-67-6 Q6.Benzene derivative with certain substituents No 59-67-6 Q7.Heterocyclic Yes 59-67-6 Q8.Lactone or cyclic diester No 59-67-6 Q10.3-membered heterocycle No 59-67-6 Q11.Has a heterocyclic ring with complex substituents. No 59-67-6 Q12.Heteroaromatic Yes 59-67-6 Q13.Does the ring bear any substituents? Yes 59-67-6 Q14.More than one aromatic ring No 59-67-6 Q22.Common component of food Yes Class Intermediate (Class II)
octoxynol 9	2	Q1.Normal constituent of the body No 9002-93-1 Q2.Contains functional groups associated with enhanced toxicity No 9002-93-1 Q3.Contains elements other than C,H,O,N,divalent S No 9002-93-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 9002-93-1 Q6.Benzene derivative with certain substituents No 9002-93-1 Q7.Heterocyclic No 9002-93-1 Q16.Common terpene No 9002-93-1 Q17.Readily hydrolysed to a common terpene No 9002-93-1 Q19.Open chain No 9002-93-1 Q23.Aromatic Yes 9002-93-1 Q27.Rings with substituents Yes 9002-93-1 Q28.More than one aromatic ring No 9002-93-1 Q30.Aromatic Ring with complex substituents Yes 9002-93-1 Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No 9002-93-1 Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. Yes Class Intermediate (Class II)
polyethylene glycol nonylphenyl ether	2	Q1.Normal constituent of the body No 9016-45-9 Q2.Contains functional groups associated with enhanced toxicity No 9016-45-9 Q3.Contains elements other than C,H,O,N,divalent S No 9016-45-9 Q5.Simply branched

Table 20 Continued

		aliphatic hydrocarbon or a common carbohydrate No 9016-45-9 Q6.Benzene derivative with certain substituents No 9016-45-9 Q7.Heterocyclic No 9016-45-9 Q16.Common terpene No 9016-45-9 Q17.Readily hydrolysed to a common terpene No 9016-45-9 Q19.Open chain No 9016-45-9 Q23.Aromatic Yes 9016-45-9 Q27.Rings with substituents Yes 9016-45-9 Q28.More than one aromatic ring No 9016-45-9 Q30.Aromatic Ring with complex substituents Yes 9016-45-9 Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No 9016-45-9 Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. Yes Class Intermediate (Class II)
1,2 propylene oxide	3	Q1.Normal constituent of the body No 75-56-9 Q2.Contains functional groups associated with enhanced toxicity No 75-56-9 Q3.Contains elements other than C,H,O,N,divalent S No 75-56-9 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 75-56-9 Q6.Benzene derivative with certain substituents No 75-56-9 Q7.Heterocyclic Yes 75-56-9 Q8.Lactone or cyclic diester No 75-56-9 Q10.3-membered heterocycle Yes Class High (Class III)
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
5-methyldeoxycytidine	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)

Table 20 Continued

6,15-dihydroanthrazine-5,9,14,18-tetrone	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. No Q12.Heteroaromatic No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
acrylonitrile	3	Q1.Normal constituent of the body No C=CC#N Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III) C=CC#N
aluminum (used toxicity values for aluminum chloride)	3	Q1.Normal constituent of the body No 7429-90-5 Q2.Contains functional groups associated with enhanced toxicity No 7429-90-5 Q3.Contains elements other than C,H,O,N,divalent S Yes 7429-90-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III) 7429-90-5
aluminum hydroxide	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
aluminum phosphate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
aluminum silicate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
aluminum sulfate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
ammonium sulfate	3	Q1.Normal constituent of the body No Q2.Contains functional

Table 20 Continued

		groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
amphotericin B	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester Yes Q9.Lactone, fused to another ring, or 5- or 6-membered a,b-unsaturated lactone? Yes Class High (Class III)
arsenic	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
benzethonium chloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
boron	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
bromine	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
calcium carbonate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes Q7.Heterocyclic No Acid [H]OC(=O)[O-] Q16.Common terpene No Acid [H]OC(=O)[O-] Q17.Readily hydrolysed to a common terpene No Acid [H]OC(=O)[O-] Q19.Open chain Yes Acid [H]OC(=O)[O-] Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)

Table 20 Continued

calcium chloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
calcium chloride dihydrate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
calcium pantothenate (vitamin B5)	3	Q1.Normal constituent of the body No 137-08-6
cesium hydroxide	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
cetrimonium bromide (CTAB)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes
chlortetracycline	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
choline chloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
co-carboxylase	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
DDT (dichlorodiphenyltrichloroethane)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
deoxycholic acid	3	Q1.Normal constituent of the body No 83-44-3 Q2.Contains functional groups associated with enhanced toxicity No 83-44-3 Q3.Contains elements other than C,H,O,N,divalent S No 83-44-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 83-44-3 Q6.Benzene derivative

Table 20 Continued

		with certain substituents No 83-44-3 Q7.Heterocyclic No 83-44-3 Q16.Common terpene No 83-44-3 Q17.Readily hydrolysed to a common terpene No 83-44-3 Q19.Open chain No 83-44-3 Q23.Aromatic No 83-44-3 Q24.Monocarbocyclic with simple substituents No 83-44-3 Q25.Cyclopropane, etc. (see explanation) No 83-44-3 Q26.Monocycloalkanone or a bicyclocompound No 83-44-3 Q22.Common component of food No 83-44-3 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
dextran	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. No Q12.Heteroaromatic No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
diadenine sulfate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
disodium phosphate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
disodium phosphate dodecahydrate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
edetate disodium (EDTA)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No

Table 20 Continued

		Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food N Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
ergocalciferol (vitamin D2)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents No Q25.Cyclopropane, etc. (see explanation) No Q26.Monocycloalkanone or a bicyclocompound No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
ethylene oxide	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle Yes Class High (Class III)
ethylene-ethylidenenorbomene-propylene terpolymer	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents No Q25.Cyclopropane, etc. (see explanation) No Q26.Monocycloalkanone or a bicyclocompound No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
ferric (III) nitrate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
ferrous succinate (butanedioic acid)	3	Q1.Normal constituent of the body No 10030-90-7 Q2.Contains functional groups associated with enhanced toxicity No 10030-90-7 Q3.Contains elements other than C,H,O,N,divalent S Yes 10030-90-7 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate,

Table 20 Continued

		sulphonate, sulphate, hydrochloride ... No Class High (Class III)
flavin adenine dinucleotide (FAD)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
folic acid	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
gentamicin	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
guanine hydrochloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
hemin chloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
hexachlorobenzene	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)

Table 20 Continued

hexamethyldisiloxane	3	Q1.Normal constituent of the body No 9006-65-9 Q2.Contains functional groups associated with enhanced toxicity No 9006-65-9 Q3.Contains elements other than C,H,O,N,divalent S Yes 9006-65-9 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
hydrocortisone	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain No Q23.Aromatic No Q24.Monocarbocyclic with simple substituents No Q25.Cyclopropane, etc. (see explanation) No Q26.Monocycloalkanone or a bicyclocompound No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
hydroxylysine	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) No Q22.Common component of food No Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
indigo	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
insulin	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic

Table 20 Continued

		hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
iron	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
iron (II) sulfate heptahydrate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
iron ammonium citrate (FERRIC AMMONIUM CITRATE)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
iron III nitrate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
kanamycin	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No Q6.Benzene derivative with certain substituents No Q7.Heterocyclic Yes Q8.Lactone or cyclic diester No Q10.3-membered heterocycle No Q11.Has a heterocyclic ring with complex substituents. Yes Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
lactose	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S No Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate Yes Class Low (Class I)
magnesium	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs

Table 20 Continued

		only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
magnesium chloride	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
magnesium silicate (talc)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
magnesium stearate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I) Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
magnesium sulfate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
mercury	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
methyltrimethoxysilane	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements

Table 20 Continued

		not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
monobasic potassium phosphate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
monobasic sodium phosphate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
monosodium L glutamate	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
nadide (NAD)	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
neomycin	3	Q1.Normal constituent of the body No 1404-04-2 Q2.Contains functional groups associated with enhanced toxicity No 1404-04-2 Q3.Contains elements other than C,H,O,N,divalent S No 1404-04-2 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 1404-04-2 Q6.Benzene derivative with certain substituents No 1404-04-2 Q7.Heterocyclic Yes 1404-04-2 Q8.Lactone or cyclic diester No 1404-04-2 Q10.3-membered heterocycle No 1404-04-2 Q11.Has a heterocyclic ring with complex substituents. Yes 1404-04-2 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
p-aminobenzoic acid (4-AMINOBENZOIC ACID)	3	Q1.Normal constituent of the body No 150-13-0 Q2.Contains functional groups associated with enhanced toxicity No 150-13-0 Q3.Contains elements other than C,H,O,N,divalent S No 150-13-0 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 150-13-0 Q6.Benzene derivative with certain substituents No 150-13-0 Q7.Heterocyclic No 150-13-0 Q16.Common terpene No 150-13-0 Q17.Readily hydrolysed to a common terpene No 150-13-0 Q19.Open chain No 150-13-0 Q23.Aromatic Yes 150-13-0 Q27.Rings with

Table 20 Continued

		substituents Yes 150-13-0 Q28.More than one aromatic ring No 150-13-0 Q30.Aromatic Ring with complex substituents Yes 150-13-0 Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No 150-13-0 Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. No 150-13-0 Q22.Common component of food No 150-13-0 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
PCB 1221	3	Q1.Normal constituent of the body No 11104-28-2 Q2.Contains functional groups associated with enhanced toxicity No 11104-28-2 Q3.Contains elements other than C,H,O,N,divalent S Yes 11104-28-2 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
PCB 1242	3	Q1.Normal constituent of the body No 53469-21-9 Q2.Contains functional groups associated with enhanced toxicity No 53469-21-9 Q3.Contains elements other than C,H,O,N,divalent S Yes 53469-21-9 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
PCB 1248	3	Q1.Normal constituent of the body No 12672-29-6 Q2.Contains functional groups associated with enhanced toxicity No 12672-29-6 Q3.Contains elements other than C,H,O,N,divalent S Yes 12672-29-6 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
PCB 1254	3	Q1.Normal constituent of the body No 11097-69-1 Q2.Contains functional groups associated with enhanced toxicity No 11097-69-1 Q3.Contains elements other than C,H,O,N,divalent S Yes 11097-69-1 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
PCB 1260	3	Q1.Normal constituent of the body No 11096-82-5 Q2.Contains functional groups associated with enhanced toxicity No 11096-82-5 Q3.Contains elements other than C,H,O,N,divalent S Yes 11096-82-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
peroxide, [1,3(or 1,4)-phenylenebis(1-	3	Q1.Normal constituent of the body No 25155-25-3 Q2.Contains functional groups associated with enhanced toxicity No 25155-25-3 Q3.Contains elements other than

Table 20 Continued

methylethylidene)] bis[(1,1-dimethylethyl)		C,H,O,N,divalent S No 25155-25-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 25155-25-3 Q6.Benzene derivative with certain substituents No 25155-25-3 Q7.Heterocyclic No 25155-25-3 Q16.Common terpene No 25155-25-3 Q17.Readily hydrolysed to a common terpene No 25155-25-3 Q19.Open chain No 25155-25-3 Q23.Aromatic Yes 25155-25-3 Q27.Rings with substituents Yes 25155-25-3 Q28.More than one aromatic ring No 25155-25-3 Q30.Aromatic Ring with complex substituents Yes 25155-25-3 Q31.Is the substance an acyclic acetal or ester of substances defined in Q30? No 25155-25-3 Q32.Contains only the functional groups listed in Q30 or Q31 and those listed below. No 25155-25-3 Q22.Common component of food No 25155-25-3 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III) 25155-25-3
polymyxin B	3	Q1.Normal constituent of the body No 1404-26-8 Q2.Contains functional groups associated with enhanced toxicity No 1404-26-8 Q3.Contains elements other than C,H,O,N,divalent S Yes 1404-26-8 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
polypropylene	3	Q1.Normal constituent of the body No 9003-07-0 Q2.Contains functional groups associated with enhanced toxicity No 9003-07-0 Q3.Contains elements other than C,H,O,N,divalent S Yes 9003-07-0 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
polysorbate 20	3	Q1.Normal constituent of the body No 9005-64-5 Q2.Contains functional groups associated with enhanced toxicity No 9005-64-5 Q3.Contains elements other than C,H,O,N,divalent S No 9005-64-5 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 9005-64-5 Q6.Benzene derivative with certain substituents No 9005-64-5 Q7.Heterocyclic Yes 9005-64-5 Q8.Lactone or cyclic diester No 9005-64-5 Q10.3-membered heterocycle No 9005-64-5 Q11.Has a heterocyclic ring with complex substituents. Yes 9005-64-5 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
polysorbate 80 (tween 80)	3	Q1.Normal constituent of the body No 9005-65-6 Q2.Contains functional groups associated with enhanced toxicity No 9005-65-6 Q3.Contains elements other than C,H,O,N,divalent S No 9005-65-6 Q5.Simply branched

Table 20 Continued

		aliphatic hydrocarbon or a common carbohydrate No 9005-65-6 Q6.Benzene derivative with certain substituents No 9005-65-6 Q7.Heterocyclic Yes 9005-65-6 Q8.Lactone or cyclic diester No 9005-65-6 Q10.3-membered heterocycle No 9005-65-6 Q11.Has a heterocyclic ring with complex substituents. Yes 9005-65-6 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
potassium	3	Q1.Normal constituent of the body No 7440-09-7 Q2.Contains functional groups associated with enhanced toxicity No 7440-09-7 Q3.Contains elements other than C,H,O,N,divalent S Yes 7440-09-7 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
potassium chloride	3	Q1.Normal constituent of the body No 7447-40-7 Q2.Contains functional groups associated with enhanced toxicity No 7447-40-7 Q3.Contains elements other than C,H,O,N,divalent S Yes 7447-40-7 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
potassium glutamate	3	Q1.Normal constituent of the body No 19473-49-5 Q2.Contains functional groups associated with enhanced toxicity No 19473-49-5 Q3.Contains elements other than C,H,O,N,divalent S Yes 19473-49-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes 19473-49-5 Q7.Heterocyclic No Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q16.Common terpene No Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q17.Readily hydrolysed to a common terpene No Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q19.Open chain Yes Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q20.Aliphatic with some functional groups (see explanation) Yes Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q21.3 or more different functional groups No Acid [H]OC(=O)C([H])([H])C([H])([H])C([H])(C(=O)O[H])N([H])[H] Q18.One of the list (see explanation) No Class Low (Class I)
silicon	3	Q1.Normal constituent of the body No 7440-21-3 Q2.Contains functional groups associated with enhanced toxicity No 7440-21-3 Q3.Contains elements other than

Table 20 Continued

		C,H,O,N,divalent S Yes 7440-21-3 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
silicon dioxide	3	Q1.Normal constituent of the body No 7631-86-9 Q2.Contains functional groups associated with enhanced toxicity No 7631-86-9 Q3.Contains elements other than C,H,O,N,divalent S Yes 7631-86-9 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium	3	Q1.Normal constituent of the body No 7440-23-5 Q2.Contains functional groups associated with enhanced toxicity No 7440-23-5 Q3.Contains elements other than C,H,O,N,divalent S Yes 7440-23-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium acetate	3	Q1.Normal constituent of the body No 127-09-3 Q2.Contains functional groups associated with enhanced toxicity No 127-09-3 Q3.Contains elements other than C,H,O,N,divalent S Yes 127-09-3 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes 127-09-3 Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
sodium bicarbonate	3	Q1.Normal constituent of the body No 144-55-8 Q2.Contains functional groups associated with enhanced toxicity No 144-55-8 Q3.Contains elements other than C,H,O,N,divalent S Yes 144-55-8 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III) 144-55-8
sodium borate	3	Q1.Normal constituent of the body No 1303-96-4 Q2.Contains functional groups associated with enhanced toxicity No 1303-96-4 Q3.Contains elements other than C,H,O,N,divalent S Yes 1303-96-4 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium chloride	3	Q1.Normal constituent of the body No 7647-14-5 Q2.Contains functional groups associated with enhanced

Table 20 Continued

		toxicity No 7647-14-5 Q3.Contains elements other than C,H,O,N,divalent S Yes 7647-14-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium citrate	3	Q1.Normal constituent of the body No 68-04-2 Q2.Contains functional groups associated with enhanced toxicity No 68-04-2 Q3.Contains elements other than C,H,O,N,divalent S Yes 68-04-2 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III) 68-04-2
sodium dihydrogen phosphate dihydrate	3	Q1.Normal constituent of the body No 13472-35-0 Q2.Contains functional groups associated with enhanced toxicity No 13472-35-0 Q3.Contains elements other than C,H,O,N,divalent S Yes 13472-35-0 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium glucuronate	3	Q1.Normal constituent of the body No 14984-34-0 Q2.Contains functional groups associated with enhanced toxicity No 14984-34-0 Q3.Contains elements other than C,H,O,N,divalent S Yes 14984-34-0 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes 14984-34-0 Q7.Heterocyclic No Q16.Common terpene No Acid Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups Yes Class High (Class III)
sodium hydroxide	3	Q1.Normal constituent of the body No 1310-73-2 Q2.Contains functional groups associated with enhanced toxicity No 1310-73-2 Q3.Contains elements other than C,H,O,N,divalent S Yes 1310-73-2 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium metabisulphite	3	Q1.Normal constituent of the body No 7681-57-4 Q2.Contains functional groups associated with enhanced toxicity No 7681-57-4 Q3.Contains elements other than C,H,O,N,divalent S Yes 7681-57-4 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium phosphate	3	Q1.Normal constituent of the body No 7632-05-5 Q2.Contains functional groups associated with enhanced toxicity No 7632-05-5 Q3.Contains elements other than

Table 20 Continued

		C,H,O,N,divalent S Yes 7632-05-5 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium phosphate dibasic heptahydrate	3	Q1.Normal constituent of the body No 7782-85-6 Q2.Contains functional groups associated with enhanced toxicity No 7782-85-6 Q3.Contains elements other than C,H,O,N,divalent S Yes 7782-85-6 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
sodium pyruvate	3	Q1.Normal constituent of the body No 113-24-6 Q2.Contains functional groups associated with enhanced toxicity No 113-24-6 Q3.Contains elements other than C,H,O,N,divalent S Yes 113-24-6 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... Yes 113-24-6 Q7.Heterocyclic No Q16.Common terpene No Q17.Readily hydrolysed to a common terpene No Q19.Open chain Yes Q20.Aliphatic with some functional groups (see explanation) Yes Q21.3 or more different functional groups No Q18.One of the list (see explanation) No Class Low (Class I)
streptomycin	3	Q1.Normal constituent of the body No 57-92-1 Q2.Contains functional groups associated with enhanced toxicity No 57-92-1 Q3.Contains elements other than C,H,O,N,divalent S No 57-92-1 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 57-92-1 Q6.Benzene derivative with certain substituents No 57-92-1 Q7.Heterocyclic Yes 57-92-1 Q8.Lactone or cyclic diester No 57-92-1 Q10.3-membered heterocycle No 57-92-1 Q11.Has a heterocyclic ring with complex substituents. Yes 57-92-1 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High (Class III)
sulfur	3	Q1.Normal constituent of the body No 7704-34-9 Q2.Contains functional groups associated with enhanced toxicity No 7704-34-9 Q3.Contains elements other than C,H,O,N,divalent S No 7704-34-9 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 7704-34-9 Q6.Benzene derivative with certain substituents No 7704-34-9 Q7.Heterocyclic No 7704-34-9 Q16.Common terpene No 7704-34-9 Q17.Readily hydrolysed to a common terpene No 7704-34-9 Q19.Open chain Yes 7704-34-9 Q20.Aliphatic with some functional groups (see explanation) No 7704-34-9 Q22.Common component of food No 7704-34-9 Q33.Has sufficient number of

Table 20 Continued

		sulphonate or sulphamate groups No Class High (Class III)
tetrafluoroethylene	3	Q1.Normal constituent of the body No 9002-84-0 Q2.Contains functional groups associated with enhanced toxicity No 9002-84-0 Q3.Contains elements other than C,H,O,N,divalent S Yes 9002-84-0 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
thiamine	3	Q1.Normal constituent of the body No 59-43-8 Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
thimerosal	3	Q1.Normal constituent of the body No 54-64-8 Q2.Contains functional groups associated with enhanced toxicity No 54-64-8 Q3.Contains elements other than C,H,O,N,divalent S Yes 54-64-8 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
titanium dioxide	3	Q1.Normal constituent of the body No 13463-67-7 Q2.Contains functional groups associated with enhanced toxicity No 13463-67-7 Q3.Contains elements other than C,H,O,N,divalent S Yes 13463-67-7 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
triphosphopyridine nucleotide (NADP)	3	Q1.Normal constituent of the body No 53-59-8 Q2.Contains functional groups associated with enhanced toxicity Yes Class High (Class III)
vinyl acetate-chloroethene	3	Q1.Normal constituent of the body No Q2.Contains functional groups associated with enhanced toxicity No Q3.Contains elements other than C,H,O,N,divalent S Yes Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
vitamin E succinate	3	Q1.Normal constituent of the body No 4345-03-3 Q2.Contains functional groups associated with enhanced toxicity No 4345-03-3 Q3.Contains elements other than C,H,O,N,divalent S No 4345-03-3 Q5.Simply branched aliphatic hydrocarbon or a common carbohydrate No 4345-03-3 Q6.Benzene derivative with certain substituents No 4345-03-3 Q7.Heterocyclic Yes 4345-03-3 Q8.Lactone or cyclic diester No 4345-03-3 Q10.3-membered heterocycle No 4345-03-3 Q11.Has a heterocyclic ring with complex substituents. No 4345-03-3 Q12.Heteroaromatic No 4345-03-3 Q22.Common component of food No 4345-03-3 Q33.Has sufficient number of sulphonate or sulphamate groups No Class High

Table 20 Continued

		(Class III)
zinc	3	Q1.Normal constituent of the body No 7440-66-6 Q2.Contains functional groups associated with enhanced toxicity No 7440-66-6 Q3.Contains elements other than C,H,O,N,divalent S Yes 7440-66-6 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)
zinc oxide	3	Q1.Normal constituent of the body No 1314-13-2 Q2.Contains functional groups associated with enhanced toxicity No 1314-13-2 Q3.Contains elements other than C,H,O,N,divalent S Yes 1314-13-2 Q4.Elements not listed in Q3 occurs only as a Na,K,Ca,Mg,N salt, sulphamate, sulphonate, sulphate, hydrochloride ... No Class High (Class III)

* All class II compounds reassigned to class III

Table 21. Internal Validation Data for the Benigni- Bossa Algorithm

Chemical	CPDB	CCRIS (M)	CCRIS (C)	GT	IARC	EPA	BB	FP	FN	TP	TN
1,2 propylene oxide	1			1	2B	B2	1			1	
2-deoxyadenosine			1	0			1			1	
2'-deoxycytidine			0				0				1
2-phenoxyethanol			0				0				1
acrylonitrile					2B	B1	0		1		
adenosine			0				1	1			
ammonium sulfate				0			0				1
amphotericin B			0	1			0		1		
benzethonium chloride		0	0				0				1
beta-propriolactone	1	1	1	1	2B		1			1	

Table 21 Continued

biotin			0				0				1
bromine				1			0		1		
calcium carbonate			0				0				1
calcium chloride	0		0				0				1
calcium pantothenate (vitamin B5)			0				1	1			
carbon			0				0				1
choline chloride	0		0	1			0		1		
citric acid	0		0				1	1			
cyclohexane				0			0				1
DDT (dichlorodiphenyl trichloroethane)					2B	B2	1			1	
deoxycholic acid			1				0		1		
dextran	0	0	0				1	1			
disodium phosphate			0				0				1
d-sorbitol			1	0			0		1		
ergocalciferol (vitamin D2)	0						0				1
ethanolamine			1				0		1		
ethyl acrylate	1	1	1	1	2B		0		1		
ethylene oxide	1	1	1	1	1		1			1	
folic acid			0				0				1
gentamicin				0			0				1
glutaral	0	1	1	1			1			1	
glutathione			1	1			0		1		
glycerin			0	0			0				1
glycine	1	0	0				0		1		
hemin chloride			0				1	1			
hexachlorobenzene	1	1	1	1	2B	B2	0		1		
hexamethyldisiloxane			0				0				1
hydrocortisone			1				1			1	
hypoxanthine				0			1	1			
indigo			1	0			1			1	
kanamycin				0			0				1
lactose		1					0		1		
L-alanine			0				0				1
L-ascorbic acid	0	0	1	1			0				1
L-asparagine			1				0		1		
L-cysteine				1			0		1		

Table 21 Continued

L-glutamic acid	0		0				0				1
L-glutamine			0				0				1
L-lysine				0			0				1
L-methionine	0			0			0				1
L-phenylalanine			0				0				1
L-proline				0			0				1
L-serine			0				0				1
L-threonine			1				0		1		
L-tryptophan	0	0	0				0				1
L-tyrosine			0				0				1
L-valine			0				0				1
magnesium chloride				0			0				1
magnesium silicate (talc)		1	0		2B		0		1		
magnesium sulfate			0				0				1
menadione			1				1			1	
methylcyclopentane			0				0				1
monosodium L glutamate			0	0			0				1
m-xylene			0				0				1
neomycin				1			0		1		
n-hexane	1		0				0		1		
nicotinamide	0		0	1			0		1		
nicotinic acid	0		0				0				1
octoxynol 9			0				0				1
palmitic acid			0				0				1
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)			0				0				1
polysorbate 80 (tween 80)	0	0					0				1
potassium chloride	0	0	1				0		1		
potassium glutamate			0	0			0				1
p-xylene			0				0				1
retinyl acetate	1	1	1	1			0		1		
riboflavin			1				0		1		
silicon		1					0		1		

Table 21 Continued

sodium acetate				0			0				1
sodium bicarbonate	0		0				0				1
sodium borate			0				0				1
sodium chloride	0		1	0			0		1		
sodium hydroxide				0			0				1
sodium metabisulphite		0	0	0			0				1
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)			0				0				1
stearic acid			0	0			0				1
streptomycin			1	1			1			1	
sucrose	0		1				0		1		
thymidine			1	1			1			1	
thymine		1	0				1			1	
uracil	1	1					1			1	
urea	0		1	1			0		1		
vinyl acetate-chloroethene					2B		1			1	
vitamin E succinate			0				0				1
xanthine			0				1	1	0	0	0
Totals								7	26	14	48
Chemical	CPDB	CCRIS (M)	CCRIS (C)	GT	IARC	EPA	CRAM	FP	FN	TP	TN
1,2 propylene oxide	1			1	2B	B2	1			1	
2-deoxyadenosine			1	0			0		1		
2'-deoxycytidine			0				0				1
2-phenoxyethanol			0				1	1			
acrylonitrile					2B	B1	1			1	
adenosine			0				0				1
aluminum (used toxicity values for aluminum chloride)			1	1			1			1	
aluminum sulfate			1	0			1			1	
ammonium sulfate				0			1	1			
amphotericin B			0	1			1			1	
arsenic			1	1	1	A	1			1	

Table 21 Continued

benzethonium chloride		0	0				1	1			
beta-propriolactone	1	1	1	1	2B		0		1		
biotin			0				0				1
bromine				1			1			1	
calcium carbonate			0				1	1			
calcium chloride	0		0				1	1			
calcium pantothenate (vitamin B5)			0				1	1			
carbon			0				0				1
choline chloride	0		0	1			1			1	
citric acid	0		0				0				1
cyclohexane				0			0				1
DDT (dichlorodiphenyl trichloroethane)					2B	B2	1			1	
deoxycholic acid			1				1			1	
dextran	0	0	0				1	1			
disodium phosphate			0				1	1			
ethanolamine			1				0		1		
ethyl acrylate	1	1	1	1	2B		0		1		
ethylene oxide	1	1	1	1	1		1			1	
folic acid			0				1	1			
formaldehyde	1	1	1	1	1	B1	0		1		
gentamicin				0			1	1			
glutaral	0	1	1	1			0		1		
glutathione			1	1			0		1		
glycerin			0	0			0				1
glycine	1	0	0				0		1		
hemin chloride			0				1	1			
hexachlorobenzene	1	1	1	1	2B	B2	1			1	
hexamethyldisiloxane			0				1	1			
hydrocortisone			1				1			1	
hypoxanthine				0			0				1
indigo			1	0			1			1	
iron			0				1	1			
iron (II) sulfate heptahydrate			1	0			1			1	
kanamycin				0			1	1			
lactose		1					0		1		

Table 21 Continued

L-alanine			0				0				1
L-asparagine			1				0		1		
L-cysteine				1			0		1		
L-glutamic acid	0		0				0				1
L-glutamine			0				0				1
L-lysine				0			0				1
L-methionine	0			0			0				1
L-phenylalanine			0				0				1
L-proline				0			0				1
L-serine			0				0				1
L-threonine			1				0		1		
L-tryptophan	0	0	0				0				1
L-tyrosine			0				0				1
L-valine			0				0				1
magnesium chloride				0			1	1			
magnesium silicate (talc)		1	0		2B		1			1	
magnesium sulfate			0				1	1			
menadione			1				0		1		
methylcyclopentane			0				0				1
monosodium L glutamate			0	0			1	1			
m-xylene			0				0				1
neomycin				1			1			1	
n-hexane	1		0				0		1		
nicotinamide	0		0	1			0		1		
nicotinic acid	0		0				1	1			
octoxynol 9			0				1	1			
palmitic acid			0				0				1
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)			0				1	1			
PCB 1242		1	0	0	1	B2	1			1	
PCB 1254	1	1	0	0	1	B2	1			1	
PCB 1260	1	1			1	B2	1	0	0	1	0
polysorbate 80 (tween 80)	0	0					1	1			
potassium chloride	0	0	1				1			1	

Table 21 Continued

potassium glutamate			0	0			1	1			
p-xylene			0				0				1
silicon		1					1			1	
sodium acetate				0			1	1			
sodium bicarbonate	0		0				1	1			
sodium borate			0				1	1			
sodium chloride	0		1	0			1			1	
sodium hydroxide				0			1	1			
sodium metabisulphite		0	0	0			1	1			
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)			0				0				1
stearic acid			0	0			0				1
streptomycin			1	1			1			1	
sucrose	0		1				0		1		
thimerosal			1	1			1			1	
thymidine			1	1			0		1		
thymine		1	0				0		1		
titanium dioxide	0	1		0	2B		1			1	
uracil	1	1					0		1		
urea	0		1	1			0		1		
vinyl acetate-chloroethene					2B		1			1	
xanthine			0				0				1
zinc			0				1	1			
zinc oxide			1				1			1	
Totals								28	20	28	26

Table 22. Internal Validation Data for the Extended Cramer Method

Chemical	**CPDB**	**CCRIS (M)**	**CCRIS (C)**	**GT**	**IARC**	**EPA**	**CRAM**	**FP**	**FN**	**TP**	**TN**
1,2 propylene oxide	1			1	2B	B2	1			1	
2-deoxyadenosine			1	0			0		1		
2'-deoxycytidine			0				0				1
2-phenoxyethanol			0				1	1			
acrylonitrile					2B	B1	1			1	

Table 22 Continued

adenosine			0				0				1
aluminum (used toxicity values for aluminum chloride)			1	1			1			1	
aluminum sulfate			1	0			1			1	
ammonium sulfate				0			1	1			
amphotericin B			0	1			1			1	
arsenic			1	1	1	A	1			1	
benzethonium chloride		0	0				1	1			
beta-propriolactone	1	1	1	1	2B		0		1		
biotin			0				0				1
bromine				1			1			1	
calcium carbonate			0				1	1			
calcium chloride	0		0				1	1			
calcium pantothenate (vitamin B5)			0				1	1			
carbon			0				0				1
choline chloride	0		0	1			1			1	
citric acid	0		0				0				1
cyclohexane				0			0				1
DDT (dichlorodiphenyl trichloroethane)					2B	B2	1			1	
deoxycholic acid			1				1			1	
dextran	0	0	0				1	1			
disodium phosphate			0				1	1			
ethanolamine			1				0		1		
ethyl acrylate	1	1	1	1	2B		0		1		
ethylene oxide	1	1	1	1	1		1			1	
folic acid			0				1	1			
formaldehyde	1	1	1	1	1	B1	0		1		
gentamicin				0			1	1			
glutaral	0	1	1	1			0		1		
glutathione			1	1			0		1		
glycerin			0	0			0				1
glycine	1	0	0				0		1		

Table 22 Continued

hemin chloride			0				1	1			
hexachlorobenzene	1	1	1	1	2B	B2	1			1	
hexamethyldisiloxane			0				1	1			
hydrocortisone			1				1			1	
hypoxanthine				0			0				1
indigo			1	0			1			1	
iron			0				1	1			
iron (II) sulfate heptahydrate			1	0			1			1	
kanamycin				0			1	1			
lactose		1					0		1		
L-alanine			0				0				1
L-asparagine			1				0		1		
L-cysteine				1			0		1		
L-glutamic acid	0		0				0				1
L-glutamine			0				0				1
L-lysine				0			0				1
L-methionine	0			0			0				1
L-phenylalanine			0				0				1
L-proline				0			0				1
L-serine			0				0				1
L-threonine			1				0		1		
L-tryptophan	0	0	0				0				1
L-tyrosine			0				0				1
L-valine			0				0				1
magnesium chloride				0			1	1			
magnesium silicate (talc)		1	0		2B		1			1	
magnesium sulfate			0				1	1			
menadione			1				0		1		
methylcyclopentane			0				0				1
monosodium L glutamate			0	0			1	1			
m-xylene			0				0				1
neomycin				1			1			1	
n-hexane	1		0				0		1		
nicotinamide	0		0	1			0		1		
nicotinic acid	0		0				1	1			
octoxynol 9			0				1	1			
palmitic acid			0				0				1

Table 22 Continued

peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)			0				1	1			
PCB 1242		1	0	0	1	B2	1			1	
PCB 1254	1	1	0	0	1	B2	1			1	
PCB 1260	1	1			1	B2	1	0	0	1	0
polysorbate 80 (tween 80)	0	0					1	1			
potassium chloride	0	0	1				1			1	
potassium glutamate			0	0			1	1			
p-xylene			0				0				1
silicon		1					1			1	
sodium acetate				0			1	1			
sodium bicarbonate	0		0				1	1			
sodium borate			0				1	1			
sodium chloride	0		1	0			1			1	
sodium hydroxide				0			1	1			
sodium metabisulphite		0	0	0			1	1			
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)			0				0				1
stearic acid			0	0			0				1
streptomycin			1	1			1			1	
sucrose	0		1				0		1		
thimerosal			1	1			1			1	
thymidine			1	1			0		1		
thymine		1	0				0		1		
titanium dioxide	0	1		0	2B		1			1	
uracil	1	1					0		1		
urea	0		1	1			0		1		
vinyl acetate-chloroethene					2B		1			1	
xanthine			0				0				1
zinc			0				1	1			
zinc oxide			1				1			1	
Totals								28	20	28	26

Table 23. Structural Alerts in the Benigni-Bossa Rule Base

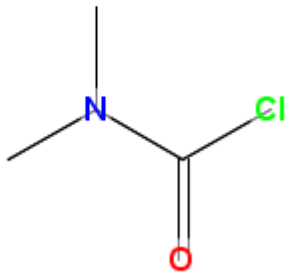
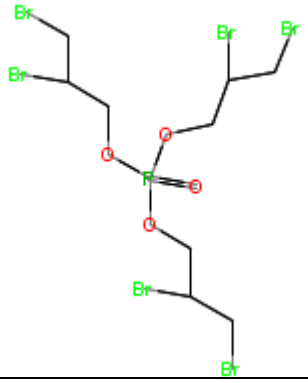
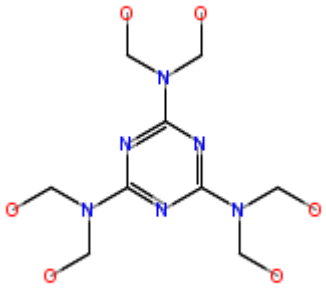
Structural Alert	Explanation And Example
Acyl halides	Acyl halide: RC(=O) [Br, Cl, F, I], where R is not OH or SH. Example: Dimethylcarbamoyl Chloride (79-44-7) 
Alkyl or benzyl ester of sulphonic or phosphonic acid	R= Alkyl with C<5 (also substituted with halogens), or benzyl R1= any atom/group except OH, SH, O-, S- Example: Tris(2,3-dibromopropyl) phosphate (126-72-7) 
N-methylol derivatives	R= Any atom/ group Example: Hexa(hydroxymethyl)melamine (531-18-0) 
Monohaloalkene	R1, R2 (or R3) = H or Alkyl R3 (or R2) = any atom/group except halogens Example: Dimethylvinyl Chloride (513-37-1)

Table 23 Continued

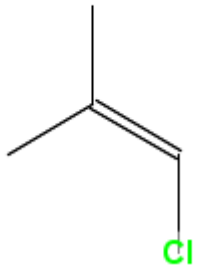
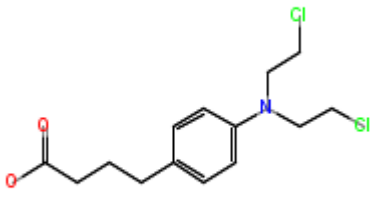
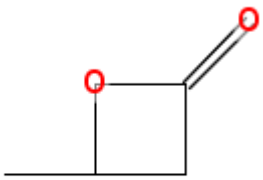
	
S or N mustard	R = any atom/group Example: Chloroambucil (305-03-3) 
Propiolactones or propiosultones	Example: Beta-butyrolactone (3068-88-0) 
Epoxides and aziridines	R = any atom/group Example: Thiotepa (52-24-4)

Table 23 Continued

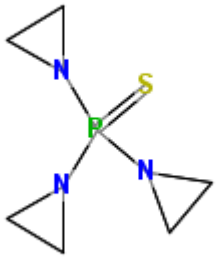
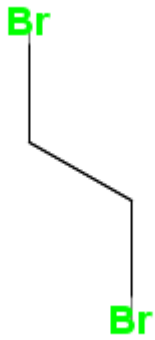
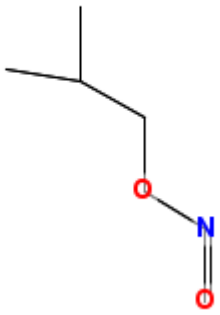
	
Aliphatic halogens	R = any atom/group Example: 1,2-dibromoethane (106-93-4) 
Alkyl nitrite	R= any alkyl group Example: Isobutyl nitrite (542-56-3) 
α, β unsaturated carbonyls	R1 and R2 = any atom/group, except alkyl chains with C>5 or aromatic rings. R= any atom/group, except OH, O- Example: 2,4-Hexadienal (142-83-6)

Table 23 Continued

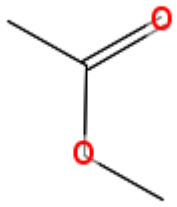
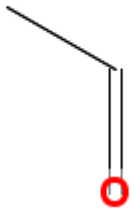
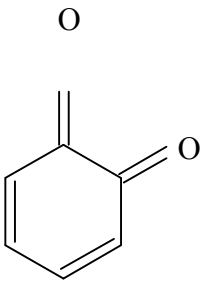
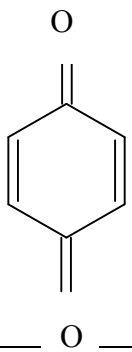
	
Simple aldehyde	R= aliphatic or aromatic carbon a,b unsaturated aldehydes are excluded Example: Acetaldehyde (75-07-0) 
Quinones	Any substance with the displayed substructures  

Table 23 Continued

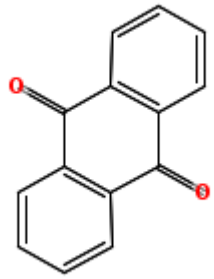
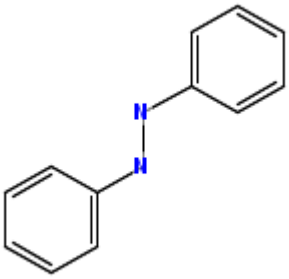
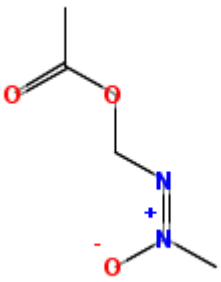
	Example: 9,10-Anthraquinone (84-65-1) 
Hydrazine	R= any atom/group Example: Hydrazobenzene (122-66-7) 
Aliphatic azo and azoxy	R1= Aliphatic carbon or hydrogen R2, R3 = Any atom/group R4 = Aliphatic carbon Example: Methylazoxymethanol Acetate (592-62-1) 
Isocyanate and isothiocyanate groups	R= any atom/group Example: Toluene Diisocyanate (26471-62-5)

Table 23 Continued

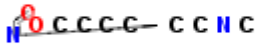
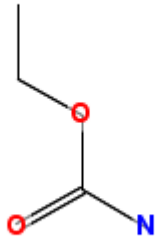
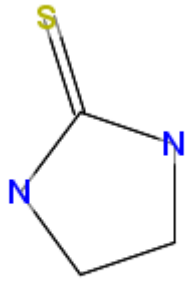
	
Alkyl carbamate and thiocarbamate	R = Aliphatic carbon or hydrogen R1 = Aliphatic carbon Example: Urethane (51-79-6) 
Thiocarbonyl (nongenotoxic)	R, R1, R2 = Any atom/group R3 = Any atom/group except OH, SH, O-, S-; Thiocarbamates are excluded. Example: Ethylenethiourea (96-45-7) 
Polycyclic Aromatic Hydrocarbons	Three or more fused rings, not heteroaromatic Example: Benzo(a)pyrene (50-32-8)

Table 23 Continued

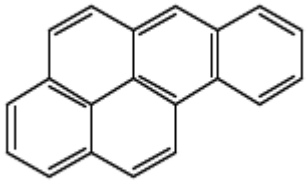
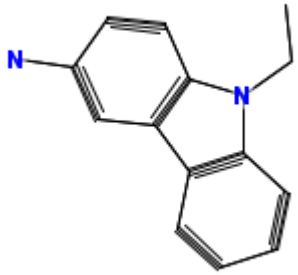
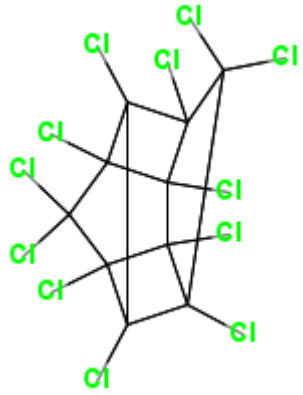
	
Heterocyclic Polycyclic Aromatic Hydrocarbons	Three or more fused rings, heteroaromatic Example: 3-Amino-9-Ethylcarbazole (132-32-1) 
(Poly) Halogenated Cycloalkanes (nongenotoxic)	Any cycloalkane skeleton with three or more halogens directly bound to the same ring Example: Mirex (2385-85-5) 
Alkyl and aryl N-nitroso groups	R1= Aliphatic or aromatic carbon, R2= Any atom/group Example: 1-(2-Hydroxyethyl)-1-Nitrosourea (13743-07-2)

Table 23 Continued

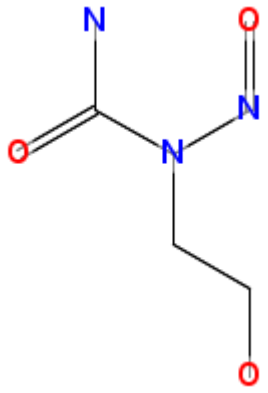
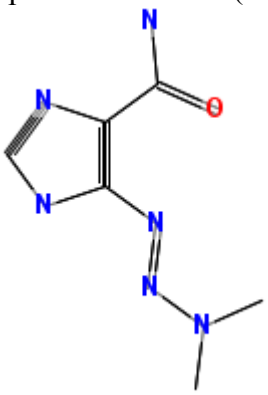
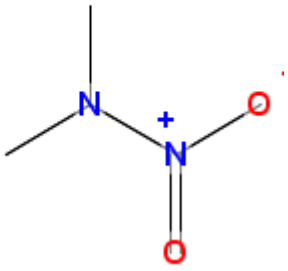
	
Azide and triazene groups	R= Any atom/group Example: Dacarbazine (4342-03-4) 
Aliphatic N-nitro group	R = Aliphatic Carbon or hydrogen Example: Dimethylnitramine (4164-28-7) 
α, β unsaturated aliphatic alkoxy group	R1= Any aliphatic Carbon R2 = Aliphatic or aromatic carbon Example: 1'-Acetoxysafrole (108-05-4)

Table 23 Continued

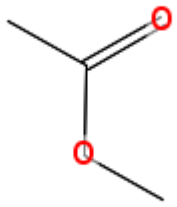
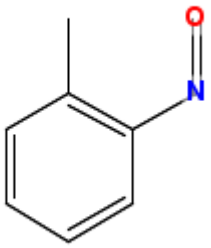
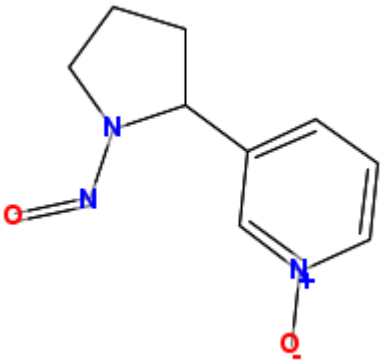
	
Aromatic nitroso group	Ar = Any aromatic/heteroaromatic ring Example: o-Nitrosotoluene (611-23-4) 
Aromatic ring N-oxide	Any aromatic or heteroaromatic ring Example: N'-nitrosonornicotine-1-N-oxide (78246-24-9) 
Nitro-aromatic	Ar = Any aromatic/heteroaromatic ring Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. Chemicals with a sulfonic acid group (-SO3H) on the same ring of the nitro group are excluded . Example: 2-Nitrotoluene (88-72-2)

Table 23 Continued

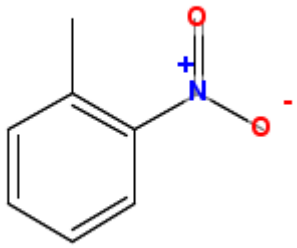
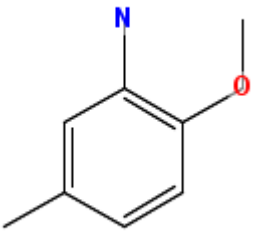
	
Primary aromatic amine, hydroxyl amine and its derived esters	Ar = Any aromatic/heteroaromatic ring R= Any atom/group Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. Chemicals with a sulfonic acid group (-SO3H) on the same ring of the amino group are excluded . Example: para-Cresidine (120-71-8) 
Aromatic mono- and dialkylamine	Ar = Any aromatic/heteroaromatic ring R1 = Hydrogen, methyl, ethyl R2 = Methyl, ethyl Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. Chemicals with a sulfonic acid group (-SO3H) on the same ring of the amino group are excluded . Example: Auramine (492-80-8)

Table 23 Continued

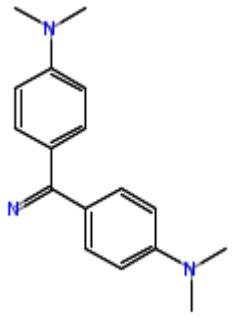
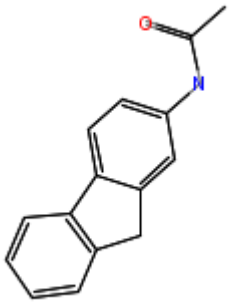
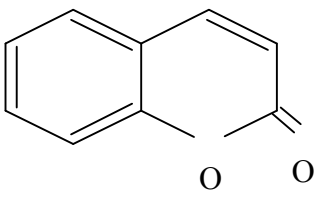
	
Aromatic N-acyl amine	Ar = Any aromatic/heteroaromatic ring R = Hydrogen, methyl Chemicals with ortho-disubstitution, or with an ortho carboxylic acid substituent are excluded. Chemicals with a sulfonic acid group (-SO3H) on the same ring of the amino group are excluded . Example: 2-Acetylaminofluorene (53-96-3)
Aromatic diazo	Ar = Any aromatic/heteroaromatic ring Chemicals with a sulfonic acid group (-SO3H) on both rings linked to the diazo group are excluded. Example: Salicylazosulfapyridine (599-79-1) 
Coumarins and Furocoumarins	Any substance with the displayed substructure  Example: Aflatoxin B1 (1162-65-8)

Table 23 Continued

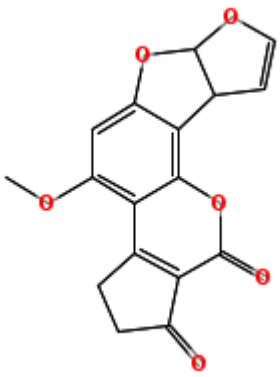
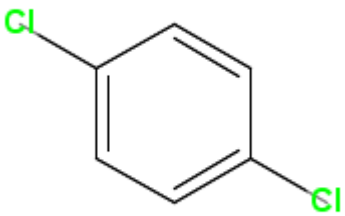
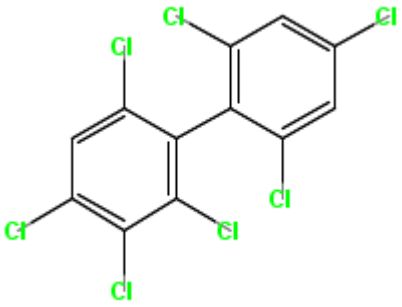
	
Halogenated benzene (nongenotoxic)	Chemicals with two halogens in ortho or meta are excluded. Chemicals with three or more hydroxyl groups are excluded. Example: 1,4-Dichlorobenzene (106-46-7) 
Halogenated PAH (nongenotoxic)	Ar = naphthalene, biphenyl, diphenyl Example: Aroclor 1260 (11096-82-5) 
Halogenated dibenzodioxins	X= F, Cl, Br, I Only chemicals with at least one halogen in one of the four lateral positions are considered. Example: 2,3,7,8-Tetrachlorodibenzo-p-dioxin (1746-01-6)

Table 23 Continued

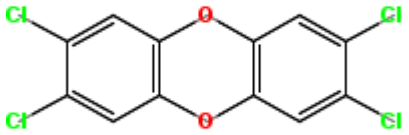
	

Table 24. Final Test Set of Chemicals with Benigni-Bossa Alerts

Chemical	CASRN	Structural Alerts
1,2 polybutadiene	9003-17-2	None
1,2 propylene oxide	75-56-9	Epoxides and aziridines
1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tris(3-(trimethoxysilyl)propyl)-	26115-70-8	None
1H-Pyrrole-2,5-dione, 1,1'-(1,3-phenylene)bis-	3006-93-7	α,β unsaturated carbonyls (geno), dicarboximide (nongeno)
2,2 dimethyl-pentane	590-35-2	None
2,6-di-tert-butyl-4-methylene-2,5-cyclohexadiene	2607-52-5	None
2-deoxyadenosine	958-09-8	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
2-deoxycytidine	951-77-9	None
2-deoxyguanosine	961-07-9	None
2-phenoxyethanol	122-99-6	None
3-methylpentane	96-14-0	None
5-methyldeoxycytidine	838-07-3	None
6,15-dihydroanthrazine-5,9,14,18-tetrone	81-77-6	Quinones, Polycyclic Aromatic Hydrocarbons
acetic acid	64-19-7	None
acrylonitrile	107-13-1	None
adenosine	58-61-7	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
ammonium sulfate	7783-20-2	None
amphotericin B	1397-89-3	None
benzethonium chloride	121-54-0	None
benzoic acid	65-85-0	None
beta-propriolactone	57-57-8	Propiolactones and propiosultones
biotin	58-85-5	None

Table 24 Continued

boron	7440-42-8	None
bromine	7726-95-6	None
butylated hydroxytoluene (BHT)	128-37-0	None
calcium carbonate	471-34-1	None
calcium chloride	10043-52-4	None
calcium chloride dihydrate	10035-04-8	None
calcium pantothenate (vitamin B5)	137-08-6	substituted n-alkylcarboxylic acids
carbon	7440-44-0	None
cesium hydroxide	21351-79-1	None
cetrimonium bromide (CTAB)	57-09-0	None
chlortetracycline	57-62-5	Alkenylbenzenes, α,β unsaturated carbonyls
cholesterol	57-88-5	None
choline chloride	67-48-1	None
citric acid	77-92-9	substituted n-alkylcarboxylic acids
co-carboxylase	154-87-0	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
cyclohexane	110-82-7	None
DDT (dichlorodiphenyltrichloroethane)	50-29-3	Halogenated PAH (naphthalenes, biphenyls, diphenyls) (Nongenotoxic carcinogens), alkyl halides
deoxycholic acid	83-44-3	None
dextran	9004-54-0	Simple aldehyde
D-galactose	59-23-4	None
diadenine sulfate	321-30-2	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions) (geno), imidazole and benzimidazole (nongeno)
disodium phosphate	7558-79-4	None
disodium phosphate dodecahydrate	10039-32-4	None
DL-aspartic acid	617-45-8	None
DL-glutamic acid	617-65-2	None
D-ribose	50-69-1	None
D-sorbitol	50-70-4	None
edetate disodium (EDTA)	6381-92-6	None
ergocalciferol (vitamin D2)	50-14-6	None
ethanolamine	141-43-5	None
ethyl acrylate	140-88-5	None
ethylene oxide	75-21-8	Epoxides and aziridines
ethylene-ethylidenenorbomene-propylene terpolymer	25038-36-2	None
ferrous succinate (butanedioic	10030-90-7	None

Table 24 Continued

acid)		
flavin adenine dinucleotide (FAD)	146-14-5	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
folic acid	59-30-3	None
gentamicin	1403-66-3	None
glutaral	111-30-8	Simple aldehyde
glutathione	70-18-8	None
glycerin	56-81-5	None
glycine	56-40-6	None
guanine hydrochloride	33735-91-0	imidazole and benzimidazole
hemin chloride	16009-13-5	Heterocyclic Polycyclic Aromatic Hydrocarbons
HEPES (4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid)	7365-45-9	None
heptakis(2,6-O-dimethyl)beta-cyclodextrin	51166-71-3	None
hexachlorobenzene	118-74-1	None
hexamethyldisiloxane	9006-65-9	None
hydrocortisone	50-23-7	α,β unsaturated carbonyls
hydroxy L proline	51-35-4	None
hydroxylysine	28902-93-4	None
hypoxanthine	68-94-0	imidazole and benzimidazole
i-Inositol	87-89-8	None
indigo	482-89-3	α,β unsaturated carbonyls
insulin	11061-68-0	imidazole and benzimidazole
kanamycin	59-01-8	None
lactose	63-42-3	None
L-alanine	56-41-7	None
L-arginine	74-79-3	None
L-ascorbic acid	50-81-7	None
L-asparagine	70-47-3	None
L-cysteine	52-90-4	None
L-cystine	56-89-3	None
L-glutamic acid	56-86-0	None
L-glutamine	56-85-9	None
L-histidine	71-00-1	imidazole and benzimidazole
L-isoleucine	73-32-5	None
L-leucine	61-90-5	None
L-lysine	56-87-1	None
L-methionine	63-68-3	None
L-phenylalanine	63-91-2	None

Table 24 Continued

L-proline	147-85-3	None
L-serine	56-45-1	None
L-threonine	72-19-5	None
L-tryptophan	73-22-3	None
L-tyrosine	60-18-4	None
L-valine	72-18-4	None
magnesium	7439-95-4	None
magnesium chloride	7786-30-3	None
magnesium silicate (talc)	14807-96-6	None
magnesium stearate	557-04-0	None
magnesium sulfate	7487-88-9	None
menadione	58-27-5	Quinones
methylcyclopentane	96-37-7	None
methyltrimethoxysilane	1185-55-3	None
monobasic potassium phosphate	7778-77-0	None
monobasic sodium phosphate	7558-80-7	None
monosodium L glutamate	142-47-2	None
m-xylene	108-38-3	None
nadide (NAD)	53-84-9	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
n-dodecane	112-40-3	None
neomycin	1404-04-2	None
n-hexadecane	544-76-3	None
n-hexane	110-54-3	None
nicotinamide	98-92-0	None
nicotinic acid	59-67-6	None
n-octadecane	593-45-3	None
n-tetradecane	629-59-4	None
octoxynol 9	9002-93-1	None
palmitic acid	57-10-3	None
p-aminobenzoic acid (4-AMINOBENZOIC ACID)	150-13-0	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions), Aromatic amine without sulfonic group on the same ring
p-cymene	99-87-6	None
peroxide, [1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[(1,1-dimethylethyl)	25155-25-3	None
phenol	108-95-2	None
phenol red (phenolsulfonphthalein)	143-74-8	None
polyethylene glycol nonylphenyl	9016-45-9	None

Table 24 Continued

ether		
polymyxin B	1404-26-8	None
polypropylene	9003-07-0	None
polysorbate 20	9005-64-5	None
polysorbate 80 (tween 80)	9005-65-6	None
polystyrene	9003-53-6	None
polyvinyl alcohol	9002-89-5	None
potassium	(7440-09-7)	None
potassium chloride	7447-40-7	None
potassium glutamate	19473-49-5	None
p-xylene	106-42-3	None
pyridoxal	66-72-8	Simple aldehyde
pyridoxine	65-23-6	None
retinyl acetate	127-47-9	None
riboflavin	83-88-5	None
silicon	7440-21-3	None
silicon dioxide	7631-86-9	None
sodium	7440-23-5	None
sodium acetate	127-09-3	None
sodium bicarbonate	144-55-8	None
sodium borate	1303-96-4	None
sodium chloride	7647-14-5	None
sodium citrate	68-04-2	None
sodium dihydrogen phosphate dihydrate	13472-35-0	None
sodium glucuronate	14984-34-0	Simple aldehyde
sodium hydroxide	1310-73-2	None
sodium metabisulphite	7681-57-4	None
sodium phosphate	7632 05 5	None
sodium phosphate dibasic heptahydrate	7782-85-6	None
sodium pyruvate	113-24-6	None
sorbitan monoleate	1338-43-8	None
squalene (2,6,10,15,19,23-hexamethyl-2,6,10,14,18,22-tetracosahexaene)	111-02-4	None
stearic acid	57-11-4	None
streptomycin	57-92-1	Simple aldehyde
sucrose	57-50-1	None
sulfur	7704-34-9	None
tetrafluoroethylene	9002-84-0	None
thiamine	59-43-8	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)

Table 24 Continued

thymidine	50-89-5	α,β unsaturated carbonyls
thymine	65-71-4	α,β unsaturated carbonyls
triphosphopyridine nucleotide (NADP)	53-59-8	Primary aromatic amine, hydroxyl amine and its derived esters (with restrictions)
tromethamine	77-86-1	None
uracil	66-22-8	α,β unsaturated carbonyls
urea	57-13-6	None
uridine 5'- triphosphate	63-39-8	α,β unsaturated carbonyls
vinyl acetate-chloroethene		Monohaloalkene, α,β unsaturated alkoxy
vitamin E succinate	(4345-03-3)	None
xanthine	69-89-6	imidazole and benzimidazole

Table 25. List of Benigni-Bossa Structural Alerts with External Validation Results (Benigni, Bossa, et. Al, 2008)**.**

Structural Alert	**No. of Chemicals Fired**	**No. of Carcinogens**	**True Positives Rate**
Acyl halides	1	1	100%
Alkyl or benzyl ester of sulphonic or phosphonic acid	12	10	83.33%
N-methylol derivatives	2	2	100%
Monohaloalkene	6	6	100%
S or N mustard	10	10	100%
Propiolactones or propiosultones	4	4	100%
Epoxides and aziridines	22	18	81.82%
Aliphatic halogens	66	49	74.24%
Alkyl nitrite	1	1	100%
a, b unsaturated carbonyls	38	29	76.32%
Simple aldehyde	8	7	87.5%
Quinones	12	10	83.33%
Hydrazine	53	51	96.23%
Aliphatic azo and azoxy	7	7	100%
Isocyanate and isothiocyanate groups	3	3	100%
Alkyl carbamate and thiocarbamate	6	6	100%
Thiocarbonyl (nongenotoxic)	19	13	68.42%
Polycyclic Aromatic Hydrocarbons	12	9	75%

Table 25 Continued

Heterocyclic Polycyclic Aromatic Hydrocarbons	12	11	91.67%
(Poly) Halogenated Cycloalkanes (nongenotoxic)	17	14	82.35%
Alkyl and aryl N-nitroso groups	79	78	98.73%
Azide and triazene groups	5	3	60%
Aliphatic N-nitro group	4	4	100%
A, b unsaturated aliphatic alkoxy group	2	2	100%
Aromatic nitroso group	3	3	100%
Aromatic ring N-oxide	3	2	66.67%
Nitro-aromatic	74	56	75.68%
Primary aromatic amine, hydroxyl amine and its derived esters	93	78	83.87%
Aromatic mono- and dialkylamine	11	9	81.82%
Aromatic N-acyl amine	16	12	75%
Aromatic diazo	20	16	80%
Coumarins and Furocoumarins	6	5	83.33%
Halogenated benzene (nongenotoxic)	11	4	36.36%
Halogenated PAH (nongenotoxic)	9	8	88.89%
Halogenated dibenzodioxins	4	2	50%