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Regulatory

Correlation of Structural Class with No-Observed-Effect Levels: A Proposal for Establishing a Threshold of Concern

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Summary—The relationship between chemical structure and toxicity was explored through the compilation of a large reference database consisting of over 600 chemical substances tested for a variety of endpoints resulting in over 2900 no-observed-effect levels (NOELs). Each substance in the database was classified into one of three structural classes using a decision tree approach. The resulting cumulative distributions of NOELs for each of the structural classes differed significantly from one another, supporting the contention that chemical structure defines toxicity. The database was used to derive a threshold of acceptable human exposure for each of the structural classes that could be applied in the absence of specific toxicity data on a substance within one of the three structural classes. The human exposure thresholds provide guidance on the degree of testing and evaluation required for substances that lack toxicity data. Copyright © 1996 Published by Elsevier Science Ltd

Introduction

Humans are exposed to thousands of chemicals over a lifetime (Fishbein, 1980; Flamm, 1981; Koren, 1991; NRC, 1994). These exposures are incurred from various sources ranging from the workplace to the low amounts of synthetic and naturally occurring substances present in the human environment and food supply. It is neither humanly possible nor necessary to test the toxicity of all these chemicals with the same degree of rigour.

A question that confronts regulatory agencies and international organizations is the extent of testing that is required to ensure, with reasonable certainty, that any given chemical to which humans are exposed can be used safely. Intuitively, toxicologists tend to be more concerned with substances having higher human exposures and reactive functional groups than with those substances not having these characteristics; however, there have been only limited attempts to integrate data on exposure and structure–activity relationships (SARs) into the risk assessment paradigm.

One of the first attempts to introduce a sense of priority into guidelines for testing chemicals based on these concepts was that of the US Food and Drug Administration (FDA). Using, in part, concepts proposed by Cramer *et al.* (1978) concerning presumed SARs, the FDA developed a procedure for ranking food and colour additives in terms of the extent of toxicity testing required. In the FDA 'Redbook' (FDA, 1982), which outlined requirements for testing of food and colour additives, knowledge of exposure was coupled with information on structure (and presumed SARs) to rank chemicals into various concern levels. Those substances of highest 'concern' were recommended for more extensive testing than those of lowest 'concern'. The concept that structure and exposure provide guidance on the degree of testing required has been embodied in toxicity testing guidelines emanating from other national and international organizations (FDA, 1993; Health and Welfare Canada, 1986; NRC, 1983 and 1994; OECD, 1993; WHO, 1967, 1978, 1987 and 1990). It is also in keeping with the long-standing principle that resources should be directed towards the testing and evaluation of those substances with the greatest potential to produce human risk and away from those with a low potential for risk.

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Abbreviations: ADI = acceptable daily intake; JECFA = Joint FAO/WHO Expert Committee on Food Additives; LOEL = lowest-observed-effect level; NOEL = no-observed-effect level; NTP = National Toxicology Program; SAR = structure–activity relationship.

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One of the practical problems in regulatory toxicology is defining when exposure to a substance of known structure is so low as to be of little or no toxicological significance, thus precluding the need for the usual degree of testing or evaluation. The concept that there is a level of exposure for all chemicals below which there is no significant risk is widely—and for non-carcinogenic endpoints, universally—accepted. It is also embodied in the practice of establishing acceptable daily intakes (ADIs) for chemicals and tolerable levels of adventitious substances in air, food and water. Establishment of ADIs is done with the virtual certainty that such exposures will produce no appreciable health risk (WHO, 1987). The FDA has recognized the *de minimus* concept and has established a threshold of regulation for indirect food additives (*Federal Register*, 1995).

The idea of establishing a generalized human exposure threshold for chemicals using historical data from well-conducted toxicity studies is not a new one, having been proposed initially by Frawley in 1967. Frawley (1967) suggested the concept of establishing a human exposure threshold for substances intended for use as food-packaging materials using data from multiple chronic rodent studies. He showed, on the basis of studies conducted on several well-tested substances (including food additives, industrial and consumer chemicals and pesticides), that a generic 'no-effect' level could be established that could preclude the need for toxicity studies and safety evaluation. He constructed a reference database of non-tumorigenic endpoints, using 220, 2-year rodents studies, and presented the no-observed-effect levels (NOELs) for all 220 compounds. Frawley (1967) reported that, if he excluded heavy metals and pesticides from the analysis, there was no compound in the remaining database (except for acrylamide) that showed evidence of chronic toxicity at dietary concentrations of less than 100 ppm. Application of a typical 100-fold safety factor to the 100 ppm generalized NOEL would mean that humans could safely consume any of the materials, provided that the dietary concentration did not exceed 1 ppm. Frawley (1967), noting that his database was incomplete, proposed adding an additional safety factor of 10 which would translate to a toxicologically inconsequential human exposure level of 0.1 ppm in the diet.

More recently, Rulis (1986) conducted an analysis of the FDA's Priority-Based Assessment of Food Additives (PAFA) database containing 159 compounds with subchronic or chronic toxicity data, LD_{50} values from 18,000 oral rodent studies contained in the Registry of Toxic Effects of Chemical Substances (RTECS), and TD_{50} values for 130 compounds found in the carcinogen potency database of Gold *et al.* (1984). Rulis (1986) came to the same conclusion as Frawley (1967): essentially, there is no risk of toxicity in rodents exposed to various chemical substances (except for some more potent substances, such as pesticides and related substances) at dietary exposures of less than 1 mg/kg body weight/day or, in human terms, approximately 1–10 μg/kg body weight/day, depending on the safety factor applied.

In addition to this work, Rulis (1986, 1989 and 1992) applied a probabilistic approach to the problem of threshold of regulation for food-contact materials. Rulis (1986) transformed the potencies (expressed as TD_{50} values) of 343 orally administered carcinogens, compiled by Gold *et al.* (1984), into a distribution of exposures calculated to present a constant assumed lifetime risk of one in 1,000,000. His analysis indicated that it was highly probable that dietary exposures to organic chemicals in the range of 50 ppt would not present a carcinogenic risk to humans, regardless of chemical structure, and therefore it was not necessary to obtain animal toxicity data to evaluate such exposures.

Munro (1990) re-analysed the data assessed by Rulis (1986) using the same methodology, and also applied this probabilistic approach to three alternate data sets consisting of (1) carcinogens from the updated database of Gold *et al.* (1989), (2) the National Toxicology Program (NTP) carcinogens as defined by Ashby and Tennant (1988) and Ashby *et al.* (1989) and (3) carcinogens carefully selected using conservative biological criteria. Overall, the results of the reanalysis indicated that there is a low probability that a dietary level of 1 ppb of a substance of unknown toxicity would present a greater than one in 1,000,000 risk of cancer.

As noted earlier, the FDA has recently established a "threshold of regulation" for indirect food additives of 0.5 ppb total diet (*Federal Register*, 1995). This is equivalent to a daily intake of 1.5 μg, assuming the consumption of 3000 g food and liquid. The FDA has stated that this threshold of regulation would be applied to indirect food additives that are not known to be carcinogens and that do not contain structural alerts indicative of carcinogenicity. Substances meeting the threshold of regulation criteria would not require toxicological testing.

The work conducted by the FDA (*Federal Register*, 1995), Frawley (1967), Rulis (1986, 1989 and 1992) and Munro (1990) is expanded on in this paper through the compilation of a large database consisting of over 600 reference substances from which distributions of NOELs were derived. The reference database presents the toxicity in terms of NOELs for a wide variety of organic chemicals of divergent structure, similar to the efforts of the previous workers but, in this case, grouped into three general classes based on chemical structure using the decision tree of Cramer *et al.* (1978). This database was used as a basis to derive a threshold of acceptable exposure for each of the structural classes that can be applied to substances lacking toxicity data. The structural classification was based on the

well-accepted tenet that inherent toxicity is dependent on chemical structure.

Methods

Overall, the reference database consists of 613 organic substances representing a range of industrial chemicals, pharmaceuticals, food substances and environmental, agricultural and consumer chemicals likely to be encountered in commerce. For many of the substances, more than one NOEL was identified from the literature, resulting from the fact that many substances in the reference database were tested in more than one species and sex and/or demonstrated a range of endpoints suitable for establishing a NOEL. This led, in some cases, to multiple NOELs for individual substances. In all, the reference database contains 2941 NOELs.

Compilation of the reference database

In compiling the reference database, emphasis was placed on retrieving data from certain databases known to contain well-validated toxicological endpoints for a series of well-defined chemical structures. Four data sources were chosen to represent a variety of chemical substances (e.g. pesticides, food additives, industrial chemicals, etc.). These included the National Toxicology Program (NTP) technical reports (post-1984), the toxicological monographs prepared by the Joint FAO/WHO Expert Committee on Food Additives (JECFA), the Integrated Risk Information System (IRIS) database, and the Developmental and Reproductive Toxicology (DART) database. No studies on organometallics, inorganic substances, chemical mixtures, or non-structurally defined substances (such as gums, resins, oils, etc.) were included in the reference database.

Only studies with oral exposure were entered into the database with the dosing method specified (i.e. gavage, diet, drinking water or capsule) for each study. The study types included those typically conducted in toxicology, such as subchronic, chronic, reproduction and teratology studies. Short-term and acute studies were not included, since these were considered not to be relevant to establishing chronic NOELs nor to be representative of other endpoints. Emphasis was placed on obtaining data from chronic studies. The database consisted mainly of studies in rodents and rabbits. Initially, studies conducted in other species, including humans, dogs and ferrets, also were included in the reference database; however, very few studies in these species were found that met the established criteria. An evaluation of randomly selected dog studies indicated that many had too few animals per group to derive a statistically valid NOEL. Moreover, for many dog studies, a common endpoint was reduced body weight and/or food consumption which was judged to be due, in many cases, either to palatability problems with the diet or to vomiting. In addition, most studies in dogs and other non-rodent species were simply too short in duration to be classified as chronic studies.

Although the intent was to develop a database consisting mainly of NOELs from chronic studies, in many cases, the lowest and thus most conservative NOEL for a substance came from a subchronic study. In order to group NOELs for substances with only subchronic studies with those with chronic studies to derive the cumulative distribution of NOELs, subchronic NOELs were divided by a factor of three to approximate the most likely NOEL that would be derived from a chronic study. This conversion factor is based on research defining the relationship between subchronic and chronic NOELs. Weil and McCollister (1963) compared 3-month NOELs with 2-year NOELs for 33 different substances (including pharmaceuticals, pesticides and food additives) fed to rats. They found that for most of the compounds (30), the ratio of the NOELs between subchronic and chronic studies was 5 or less and more than half of the compounds had a ratio equal to 2 or less. More recently, it has been determined through further analysis of more chemical substances that a more accurate adjustment factor for extrapolating NOELs derived from subchronic studies to chronic was between 2 and 3 (Beck *et al.*, 1993; Lewis *et al.*, 1990; McNamara, 1976; M. Dourson, personal communication). The data entered into the reference database included the name of the chemical, Chemical Abstracts Service Registry Numbers (CAS No.), structural classification as assessed using the decision tree of Cramer *et al.* (1978) (as discussed below), species, sex, route of administration, dose levels tested, study type, duration, endpoints reported, lowest-observed-effect level (LOEL), NOEL and references.

A further criterion for inclusion in the database was that a study had to have a demonstrated LOEL as well as a NOEL, thus ensuring that the study was rigorous enough to detect toxic effects. In some instances, however, NOELs were included for studies expected not to demonstrate a LOEL since these were substances, such as major food ingredients, that were without toxicity at the highest dose tested in well-conducted studies. In these cases, the NOEL was conservatively chosen as the highest dose tested. It should be noted that the inclusion of such substances in the database would not bias the database in favour of higher NOELs since the true NOEL for such substances probably would exceed the NOEL established from the available studies.

In an effort to be conservative in the construction of the reference database, NOELs selected by the author(s) of each study were used, even though in some cases authors tended to be highly conservative in the interpretation of their data. In some instances, it was found that the stated NOEL may have been based on a misjudgement of an adverse effect by the author (e.g. physiological *v.* toxicological effects) or

on artefactual effects (e.g. foetal toxicity as a result of maternal toxicity). An example of this is isopropyl alcohol, which has been reported to produce teratogenic effects at very low doses (0.018 mg/kg body weight) in one study; however, its structure, known metabolism and other toxicological data provide no evidence for concluding teratogenicity. Even though, scientifically, some of these author-derived NOELs were not thoroughly substantiated, they were included in the reference database, thereby increasing the degree of its conservative nature. NOELs selected by the US Environmental Protection Agency for the IRIS database were entered without further review.

For each of the 613 substances, the most conservative NOEL was selected, based on the most sensitive species, sex and endpoint.

Relating structure to toxicity

It is a well-known and basic precept of chemistry that properties of a substance, including its inherent toxicity, are determined by its chemical structure. Thus, in theory, the toxicity of a substance could be predicted completely from its structure. In practice, however, this is complicated by the complexities of biological systems. Although the structure and resulting chemical reactivity may be well known, it is far more difficult to predict how a molecule may react with biological molecules through active binding sites, direct chemical reactions, or interactions with enzymes that may convert the molecule into another structure. Additionally, it is necessary to know the quantitative aspects of the biological interactions—including the concentration of the chemical at the site of interaction, the biological molecule with which it is interacting, any catalysts or enzymes that may affect the interaction, and any other part of the chemical environment such as pH that may affect the interaction. Furthermore, it is necessary to know the kinetics of transport of the molecule to and from the reaction site, the kinetics of the interaction itself, and the kinetics of removal of the metabolites and transformed biochemicals. Taking all this together, a complicated picture emerges. Nevertheless, an empirical examination of large bodies of data on defined chemicals often results in the emergence of rational patterns of biological activity associated with particular chemical structures. Although these patterns may be difficult to condense into a set of rules clearly differentiating various chemical classes, the patterns can be characterized to categorize substances that fall into general classes. This exercise can be made more successful if the rules are developed with consideration of metabolic patterns and chemical reactivity and even intuitive considerations such as wide natural occurrence in the food supply.

Even the most conservative of toxicologists make generalized judgements resulting in structural groupings based on their experience (e.g. concerns regarding persistent, bioaccumulative chlorinated organic chemicals). On the other hand, some chemical structures are considered so innocuous as to allow JECFA to establish an ADI not specified, even in the absence of any classical toxicity studies—as was done for the fatty acid octanoic acid, based on its known natural occurrence in the body as well as in the food supply and its well-characterized metabolic fate (JECFA, 1986).

While the work of Frawley, Rulis and others clearly provides the framework for establishing thresholds for chemicals in general, it is recognized that correlation of structural class with potential toxicity is of fundamental importance in further extending the concept of toxicological threshold. Several methods have been proposed for using chemical structure to group substances according to their probable toxicity. For example, the efforts of Ashby and others to develop structural alerts for carcinogenicity and mutagenicity (Ashby, 1985 and 1994; Ashby and Paton, 1993; Ashby and Tennant, 1991; Tennant and Ashby, 1991) are well known but have a narrowly focused endpoint. Perhaps the best known attempt at a broader classification is the FDA's so-called Redbook structure category assignments (FDA, 1982), in which various substructures were assigned to one of three structural categories depending on presumed toxic potential. One of the most comprehensive efforts at correlation of structure with toxic potential is the decision tree approach of Cramer *et al.* (1978), in which a series of 33 questions—primarily about the structure but, in some cases, about other properties, such as propensity for hydrolysis and physiological occurrence—lead to one of three classes reflecting a presumption of low, moderate or serious toxicity.

All three of these methods have in common the fact that they deal only with defined organic chemicals and their salts and they are very conservative in their classification. For example, the mere occurrence of an aldehyde group in the Ashby classification is an alert for possible carcinogenicity or mutagenicity, even though it is known that aldehydes are rapidly detoxified *in vivo*. Similarly, both the Redbook and the decision tree classify all halogenated compounds in the most toxic category, although it is well known that some substances in this class have very low toxicity.

If these methods are truly discriminatory, it should be possible to use them to classify chemicals to produce separate groups of substances with clearly differing NOELs. Therefore, an effort was made to classify all substances in the reference database by chemical structure type using each of the three methods. The method of Ashby *et al.* (1989) quickly proved not to be very useful in this context because of its narrowly focused endpoints—carcinogenicity and mutagenicity—which are endpoints not included in this database. On the other hand, it was possible to classify all materials according to the FDA

Redbook. However, the over-conservative approach of this method became apparent when only one of the 613 substances in the reference database came out in the class of lowest presumed toxicity and 15 were in the intermediate class.

Classification by the decision tree method of Cramer *et al.* (1978) proved to be much more discriminatory, with 137 chemicals falling into the presumptively least toxic class (Class I), 28 into the intermediate class (Class II) and 448 into the presumptively most toxic class (Class III; see Table 1). The fact that there are far more substances in Class III than in Class I or II, reflects partially the conservative nature of this method, but also reflects the fact that the substances that toxicologists or regulators have chosen for the rather extensive testing required to meet the criteria necessary for inclusion in this database, were in many cases chosen at least in part on the basis of some suspicion arising from chemical structure.

The decision tree method was based on toxicological data then available and used a series of 33 questions, each leading either to another question or to classification into one of the three classes of presumptive toxicity. These questions were primarily based on chemical structure. Natural occurrence in bodily tissues or fluids, and natural occurrence in traditional foods, were also considered. The logic of the tree relies primarily on knowledge of common metabolic pathways. The three classes of substances are defined as follows:

Class I — Substances of simple chemical structure and efficient modes of metabolism that would suggest a low order of oral toxicity (e.g. L-glutamic acid, mannitol or propylene glycol).

Class II — Substances that are in a structural class in which there is less knowledge of the metabolism, pharmacology and toxicology, but for which there is no clear indication of toxicity (e.g. β-carotene, diallyl phthalate or maltol). Most substances in Class II belong to either of two categories; one includes substances with functional groups that are similar to, but somewhat more reactive than functional groups in Class I (e.g. allyl and alkyne); the other includes substances with more complex structures than substances in Class I, but that are common components of food.

Class III — Substances of a chemical structure that permit no strong initial presumption of safety, or that may even suggest significant toxicity (e.g. acetonitrile, 2,4-dinitrotoluene, chlorobenzene or *p*-aminophenol).

Table 1. Number of reference database substances in each Cramer *et al.* (1978) structural class

Structural class	No. of chemicals
I	137
II	28
III	448

Data analysis

On the basis of a graphical examination of the data, the logarithms of the 613 most conservative NOELs appeared to follow a normal distribution more closely than did the original NOELs. In order to examine the effect of structural class on toxicity, the distributions of the logarithms of NOELs were plotted separately for each Cramer *et al.* (1978) structural class. Because these distributions were only approximately normal, the distribution of NOELs for the entire reference database and the distributions of the NOELs for each structural class were treated both non-parametrically and parametrically. To evaluate differences among these distributions, pairwise comparisons among the empirical distributions of NOELs for each of the three classes of compounds were done using the Kolmogorov–Smirnov test (Press *et al.*, 1992).

Calculation of human exposure thresholds

A human exposure threshold was calculated from the respective distribution of NOELs for each of the structural classes. To accomplish this, the fifth percentile NOEL was calculated for each structural class and this in turn was converted through the application of a safety factor to a human exposure threshold. The fifth percentile NOEL was chosen because this value would provide 95% confidence that the NOEL of any other substance in the same structural class but of unknown toxicity would not have a NOEL less than that at the fifth percentile. In converting the fifth percentile NOELs to human exposure thresholds for the three structural classes, a 100-fold safety factor was used, since such a factor would inherently be applied in establishing safe intake levels for the substances comprising the database. The use of a 100-fold factor provides a substantive margin of safety, since the human exposure thresholds are based on a large database of approximately 613 compounds with good supporting toxicological data. Furthermore, fifth percentile NOELs were used to calculate the thresholds, providing a more conservative figure than the 50th percentile. Thus, it is believed that a 100-fold safety factor provides a reasonable margin of safety in translating the results of analysis of the reference database to humans.

Results

The cumulative distribution of the 613 most conservative NOELs derived from the reference

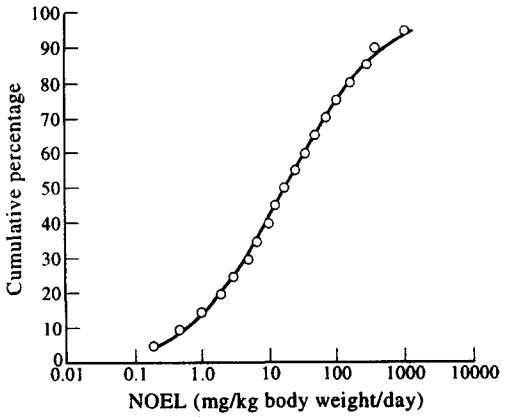

Fig. 1. Cumulative distribution of the most conservative NOELs for compounds in the reference database (□, percentiles; — fitted lognormal distribution).

database is shown in Fig. 1. The data points reflect the empirical distribution of NOELs. The fitted lognormal distribution used to describe the data set parametrically appeared to fit the data reasonably well. On the basis of the fitted lognormal distribution of NOELs it was found that 95% of the 613 compounds in the database had NOELs greater than 0.22 mg/kg body weight/day (i.e. the fifth percentile).

Figure 2 presents the cumulative distributions of NOELs of substances in the reference database separated into Cramer *et al.* (1978) structural classes I, II and III. As can be seen from Fig. 2, there is a clear effect of structure on toxicity, as indicated by the distinct separation of the cumulative distributions for each of the three structural classes. The three distributions were found to differ significantly (Class I *v.* Class II and Class I *v.* Class III, $P < 0.05$; Class II *v.* Class III, $P < 0.10$). The 50th percentiles of the distributions were 116, 26 and 9 mg/kg body weight/day, for structural classes I, II and III, respectively.

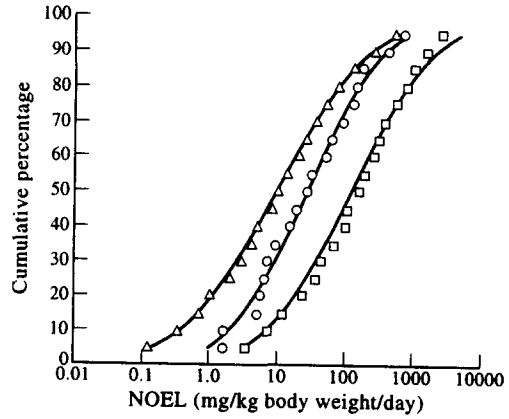

Fig. 2. Cumulative distribution of the most conservative NOELs for compounds in the reference database grouped into Cramer *et al.* (1978) structural classes I, II and III (□, class I percentiles; ○, class II percentiles; Δ, class III percentiles; — fitted lognormal distribution).

Using the lognormal distributions fit to the data for each structural class, estimates of the fifth percentiles of the distributions of NOELs were 3.0, 0.91 and 0.15 mg/kg body weight/day for classes I, II and III, respectively. Because the logarithms of the NOELs for these classes exhibited some evidence of non-normality, the fifth percentile was also estimated non-parametrically. The non-parametric estimates (3.3, 1.6 and 0.12 mg/kg body weight/day for classes I, II and III, respectively) were close to, or somewhat greater than, the parametric estimates. Consequently, the parametric estimates, which tended to be more conservative overall, were used to calculate the human exposure thresholds for each of the structural classes.

The calculated human exposure thresholds for each structural class are shown in Table 2. Clearly, other human exposure thresholds could be calculated, depending on the degree of conservatism deemed appropriate. It should be noted that within structural class III, for example, there are 24/448 substances with NOELs below the fifth percentile and the safety factors, relative to the human exposure threshold of 0.09 mg/day for this group of 24 substances, ranged from about three to 90. An alternative would be to use the first percentile to calculate the human exposure threshold (yielding a human exposure threshold of 0.02 mg/day for structural class III). Then only 8/448 substances would have NOELs below the first percentile and safety factors for these compounds would range from 15 to 90.

Discussion

Analysis of this large database provides evidence that there is a less than 5% probability that toxicological studies of any other substance not included in the database would result in a NOEL lower than the fifth percentile NOEL of 0.22 mg/kg body weight for the entire database. This is a useful concept in determining priorities for testing as well as for regulation. Moreover, it provides the basis for an argument that, with appropriate safety factors, a threshold can be established and, if human exposure to a substance is below that threshold, the substance can be judged, with reasonable confidence, to present a low probability of risk regardless of structure, even if there are no toxicological data available.

More importantly, this database demonstrates that if substances are grouped logically and with proper consideration of structure, metabolism, physiological occurrence, etc., a range of thresholds can be generated for certain structural classes. Although this is a concept that has long been used intuitively by toxicologists, this database provides the first firm support for that intuition and a method for determination of specific values for the various thresholds. With regard to the thousands of chemicals to which humans are exposed in a lifetime, the great majority of which have little or no

Table 2. Fifth percentile NOELs and human exposure thresholds for each Cramer (1978) structural class

Structural class	Fifth percentile NOEL (mg/kg body weight/day)	Human exposure threshold (mg/day)*
I	3.0	1.8
II	0.91	0.54
III	0.15	0.09

*The human exposure threshold was calculated by multiplying the fifth percentile NOEL by 60 (assuming an individual weighs 60 kg) and dividing by a safety factor of 100, as discussed in the text.

toxicological data, this database should give confidence that the majority of the substances to which we are exposed in trace amounts do not present a significant potential risk. It would, at the same time, allow the scientific community to focus its resources on those substances for which additional data are clearly necessary. Moreover, it provides a reasonable alternative to the need for extensive animal testing of substances with innocuous structures and trivial exposures.

The selection of the fifth percentile NOEL as opposed to the first percentile NOEL was considered to be reasonable for several reasons. First, the criteria used to select the NOELs were very strict and designed to err on the side of conservatism; thus, the NOELs in the database are considered to be conservative. In addition, the substances in the database were, for the most part, extensively tested for a variety of endpoints and thus the lowest NOEL for each substance in the reference database would be unlikely to be reduced through further testing. Secondly, in developing a threshold of regulation for carcinogenic substances, Rulis (1986) selected a threshold corresponding to the 15th percentile of the distribution of 10^{-6} risks for carcinogens in the Gold *et al.* (1984) database; in the present study the more conservative fifth percentile values were chosen. Thirdly, the 24/448 structural class III compounds that fell below the fifth percentile were pesticides, drugs or industrial chemicals; none was a food additive or commonly used food ingredient. Only 8/448 compounds in structural class III fell below the first percentile of the distribution of NOELs, corresponding to a safety margin of 15–90-fold of the human exposure threshold for that class. In comparison, the safety margin for those compounds below the fifth percentile ranged from 3 to 90. Therefore, use of the first percentile rather than the fifth percentile may reduce the number of compounds falling below the threshold; however, the margin of safety between the threshold and the NOEL is not substantially altered.

It is recognized that the human exposure thresholds for each of the structural classes derived from this study (see Table 2) are considerably higher than the intake of 1.5 μg/day calculated from the 0.5 ppb threshold of regulation indicated in the FDA ruling for food-packaging materials. The FDA has indicated, on the basis of an analysis of the distribution of one in 1,000,000 risks from the Gold database of carcinogens, that an exposure to an indirect food additive of unknown toxicity at a dietary level of 0.5 ppb or less would not present an unacceptable risk, even if it were later found to be a carcinogen (*Federal Register*, 1995). The human exposure thresholds presented here are intended to apply to chemically-defined substances for which there is no presumption of genotoxic carcinogenicity. Otherwise, the 1.5 μg/day threshold may be a more appropriate value.

In conclusion, the proposed approach takes advantage of knowledge of the relationship between structure and toxicity and incorporates this into the proposed threshold values. This study shows that structural class has an important bearing on toxicity. Such information should be incorporated in regulatory proposals which are aimed at establishing priorities for, and extent of, testing and evaluation of chemical substances.

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APPENDIX

Most Conservative NOELS for Substances in the Reference Database—Cramer *et al.*

Structural Class 1

	Chemical Name	CAS no.	Species Tested	Exposure Duration (days)	Study Type	Exposure Route	Endpoint Type	Doses Given By Author	LOEL (mg/kg/day)	Authors' NOEL (mg/kg/day)	Calculated NOEL (mg/kg/day)	Reference
1	Acetic acid	64-19-7	rat	105	sub	orl	nofx	0.01, 0.1, 0.25, 0.5% [c]	none	none	726*	Sollmann, 1921
2	Acetoin	513-86-0	rat	91	sub	orl	mult	0, 750, 3000, 12,000 ppm [a]	1286	330	330*	Gaunt *et al.*, 1972a
3	Acetone	67-64-1	rat	90	sub	gav	owt	0, 100, 500, 2500 mg/kg/day	500	100	100*	US EPA, 1986a
4	Adipic acid	124-04-9	rbt	13	terat	NG	nofx	0, 2.5, 12, 54, 250 mg/kg/day	none	none	250	Food and Drug Research Labs, 1974a
5	Allura Red AC	25956-17-6	rat	644	chr	fod	bdw	0, 0.37, 1.39, 5.19% in diet [c]	3739	none	1001	Olson and Voelker, 1970
6	Aminoundecanoic acid, 11-	2432-99-7	rat	91	sub	fod	bdw	0, 9000, 12,000, 15,000, 18,000, 21,000 ppm [c]	1800	none	1500*	NTP, 1982a
7	Ascorbic acid	50-81-7(a)	rat	10	terat	gav	msk	5.5–555 mg/kg	555	none	5.5	Food and Drug Research Labs, 1974b
8	Ascorbic acid, L-	50-81-7(b)	rat	721	chr	fod	bdw	0, 25,000, 50,000 ppm [a]	3051	none	1458	NTP, 1983a
9	Benzaldehyde	100-52-7	mus	91	sub	gav	kid	0, 75, 150, 300, 600, 1200 mg/kg/day	600	none	300*	Kluwe *et al.*, 1983
10	Benzoic acid	65-85-0	rat	NG	repro	fod	nofx	0, 0.5, 1% [c]	none	none	887	Kieckebusch and Lang, 1960
11	Benzyl acetate	140-11-4	rat	720	chr	fod	nofx	0, 3000, 6000, 12,000 ppm [a]	none	none	510	NTP, 1993a
12	Benzyl alcohol	100-51-6	mus	720	chr	gav	mult	0, 100, 200 mg/kg/day	200	none	100	NTP, 1989a
13	Bis(2-ethylhexyl)phthalate	117-81-7	mus	125	repro	fod	rep	0, 0.01, 0.1, 3.0% [c]	180	none	18*	Lamb, 1986
14	Brilliant Black PN	2519-30-4	rat	761	chr	fod	nofx	0.1% [a]	none	none	60	Hecht and Wingler, 1952; DFG, 1957
15	Butanediol, 1,3-	107-88-0	rat	730	chr	fod	nofx	0, 1, 3, 10% in diet [c]	none	6883	6883	Scala and Paynter, 1967
16	Butanol, 2-	78-92-2	rat	NG	repro	orl	mult	0, 0.3, 1.0, 3.0% [a]	5089	1644	1644	Cox *et al.*, 1975
17	Butanol, *n*-	71-36-3	rat	91	sub	gav	neu	0, 30, 125, 500 mg/kg/day	500	125	125*	US EPA, 1986b
18	Butyl benzyl phthalate	85-68-7	mus	91	sub	fod	bdw	0, 1600, 3100, 6300, 12,500, 25,000 ppm [c]	2438	none	1228*	NTP, 1982b
19	Butylated hydroxyanisole	25013-16-5	rat	90	sub	fod	git	0, 0.025, 0.125, 2% [c]	1843	none	115*	Altmann *et al.*, 1986
20	Butyrolactone, γ-	96-48-0	mus	90	sub	gav	mult	0, 65, 131, 262, 525, 1050 mg/kg/day	1050	none	525*	NTP, 1992a
21	Calcium cyclamate	139-06-0	rat	707	chr	fod	nofx	up to 10% [c]	none	none	7203	Friedman *et al.*, 1972
22	Calcium formate	544-17-2	rat	NG	repro	fod	nofx	0.2, 0.4% [c]	none	none	355	Malorny, 1969
23	Calcium stearoyl lactylate	5793-94-2	rat	98	sub	fod	mult	0, 0.5, 5, 12.5% [c]	11089	4435	4435*	Hodge, 1953
24	Carotenoic acid, beta-apo-8'-, methyl ester		rat	238	sub	gav	tes	0, 100, 500 mg/kg/day	500	none	100*	Anonymous, 1962; 1966
25	Cinnamaldehyde	104-55-2	rat	102	sub	fod	mult	0, 1000, 2500, 10,000 ppm in diet [a]	500	none	125*	Hagan *et al.*, 1967a
26	Citral	5392-40-5	rat	91	sub	fod	nofx	0, 0.1, 0.25, 1% [c]	none	none	887*	Hagan *et al.*, 1967b
27	Citranaxanthin	3604-90-8	rat	730	chr	fod	nofx	0, 86, 284, 860 ppm in diet [c]	none	none	59	Leuschner *et al.*, 1976
28	Cumene	98-82-8	rat	194	sub	gav	kid	0, 154, 462, 763 mg/kg/day	462	154	154*	Wolf *et al.*, 1956a
29	Di(2-ethylhexyl)adipate	103-23-1	rat	133	repro	fod	mult	0, 300, 1800, 12,000 ppm [a]	1080	170	170*	ICI Americas, Inc., 1988
30	Dibutyl phthalate	84-74-2	rat	365	sub	fod	ltl	0, 0.01, 0.05, 0.25, 1.25% [b,d]	600	125	125*	Smith, 1953
31	Diethyl phthalate	84-66-2	rat	730	chr	fod	bdw	0, 0.5, 2.5, 5.0% [c]	4435	none	2218	Food Research Labs, 1955
32	Diethylene glycol	111-46-6	mus	10	terat	gav	mult	0, 1250, 5000, 10,000 mg/kg/day	5000	none	1250	Bates *et al.*, 1991
33	Diethylene glycol monoethyl ether	111-90-0	rat	90	sub	fod	kid	0, 0.5, 5.0% [c]	2500	250	250*	Gaunt *et al.*, 1968
34	Dimethoxane	828-00-2	rat	455	chr	gav	git	0, 62.5, 125 mg/kg/day	125	none	62.5	NTP, 1989b
35	Dimethyl terephthalate	120-61-6	rat	60	repro	fod	rep	0, 250, 500, 1000 mg/kg/day	500	250	250*	Krasavage *et al.*, 1973
36	Dimethylcarbonate	616-38-6	rat	90	sub	orl	nofx	0, 0.1, 0.3, 1.0% [c]	none	none	1475*	Eiben *et al.*, 1982

[*Contd*]

37	Dimethyldicarbonate	4525-33-1	rat	100	repro	orl	nofx	0, 0, 4000 ppm [c]	none	none	590*	Eiben *et al.*, 1983
38	Dimethylphenol, 2,4-	105-67-9	mus	90	sub	gav	mult	5, 50, 250 mg/kg/day	250	50	50*	US EPA, 1989a
39	Dimethylphenol, 2,6-	576-26-1	rat	240	sub	NG	mult	0, 0.6, 6 mg/kg/day	6	0.6	0.6*	Veldre and Janes, 1979a
40	Dimethylphenol, 3,4-	95-65-8	rat	240	sub	NG	mult	1.4, 14 mg/kg/day	14	1.4	1.4*	Veldre and Janes, 1979b
41	Dioctyl sodium sulfosuccinate	577-11-7	rat	NG	repro	fod	bdw	0, 0.1, 0.5, 1% [c]	431	none	86	MacKenzie *et al.*, 1990
42	Disodium 5'-guanylate	5550-12-9	rat	7	terat	gav	nofx	0, 100 mg/kg/day	none	none	100	Kaziwara *et al.*, 1971
43	Disodium 5'-inosinate	4691-65-0	rat	NG	repro	fod	nofx	0, 0.5, 1, 2% [c]	none	none	1441	Palmer *et al.*, 1973
44	Dodecyl gallate	1166-52-5	rat	150	sub	fod	mult	10, 50, 250 mg/kg/day	50	10	10*	Mikhailova *et al.*, 1985
45	Ethanol	64-17-5	ham	NG	repro	orl	nofx	3.8 grams/day of 20% (v/v) solution [c]	none	none	5241	DiBattista, 1989
46	Ethyl acetate	141-78-6	rat	90	sub	gav	mult	0, 300, 900, 3600 mg/kg/day	3600	900	900*	US EPA, 1986c
47	Ethyl acrylate	140-88-5	rat	730	chr	orl	con	0, 6, 60, 2000 ppm [c]	248	none	8.4	Borzelleca *et al.*, 1964
48	Ethyl butyrate	105-54-4	rat	84	sub	fod	nofx	14.4 mg/kg/day	none	none	14.4*	Oser, 1967
49	Ethyl ether	60-29-7	rat	91	sub	gav	mult	0, 500, 2000, 3500 mg/kg/day	2000	500	500*	US EPA, 1986d
50	Ethyl formate	109-94-4	rat	119	sub	fod	nofx	0, 1000, 2500, 10,000 ppm [a]	none	none	500*	Hagan *et al.*, 1967a
51	Ethyl glycol monomethyl ether	109-86-4	rat	10	terat	gav	rep	0, 12.5, 25, 50, 100 mg/kg/day	25	none	12.5	Morrissey *et al.*, 1989
52	Ethyl heptanoate	106-30-9	rat	91	sub	fod	nofx	0, 0.1, 1% [c]	none	none	887*	Hagan *et al.*, 1967b
53	Ethyl nonanoate	123-29-5	rat	112	sub	fod	nofx	0, 1% [c]	none	none	887*	Hagan *et al.*, 1967b
54	Ethyl-1-hexanol, 2-	104-76-7	mus	90	sub	gav	owt	0, 25, 125, 250, 500 mg/kg/day	250	none	125*	BASF, 1992
55	Ethylbenzene	100-41-4	rat	182	sub	gav	mult	0, 13.6, 136, 408, 680 mg/kg/day	408	136	136*	Wolf *et al.*, 1956b
56	Ethylbutyric acid, 2-	88-09-5	rat	90	sub	fod	nofx	0, 0.62% [c]	none	534	534*	Amoore *et al.*, 1978
57	Ethylene glycol	107-21-1	rat	730	chr	fod	mult	0, 0.1, 0.2, 0.5, 1.0, 4.0% [b]	250	100	100	Blood, 1965
58	Ethylhexanoic acid, 2-	123-66-0	rat	10	terat	gav	ter	0, 100, 250, 500 mg/kg/day	250	none	100	Hendrickx *et al.*, 1993
59	Ethylphthalyl ethylglycolate	84-72-0	rat	730	chr	fod	mult	0, 0.05, 0.5, 5% [a]	2500	250	250	Hodge *et al.*, 1953
60	Eugenol	97-53-0	rat	84	sub	fod	nofx	79.3 mg/kg/day	none	none	79.3*	Oser, 1967
61	FD & C Blue No. 1	3844-45-9	rat	730	chr	fod	nofx	0, 0.5, 1, 2, 5% [c]	none	3502	3502	Hansen *et al.*, 1966a
62	FD & C Blue No. 2	860-22-0	mus	560	chr	fod	bld	0, 0.2, 0.4, 0.8, 1.6% in diet [d]	1100	550	550	Hooson *et al.*, 1974
63	Formaldehyde	50-00-0	rat	730	chr	orl	mult	0, 1, 15, 82 mg/kg/day	82	15	15	Til *et al.*, 1989
64	Fumaric acid	110-17-8	rat	730	chr	fod	mult	0, 0.5, 1.0, 1.5% [c]	1081	none	720	Fitzhugh and Nelson, 1947
65	Geranyl acetate	105-87-3	rat	119	sub	fod	nofx	0, 0.1, 0.25, 1% [c]	none	none	887*	Hagan *et al.*, 1967b
66	Glutamate, monosodium	142-47-2	rbt	15	terat	gav	nofx	0, 25 mg/kg/day	none	none	25	Yonetani, 1967
67	Glutamic acid hydrochloride	138-15-8	rbt	15	terat	gav	nofx	0, 25 mg/kg/day	none	none	25	Yonetani, 1967
68	Glutamic acid, L-	56-86-0	rat	730	chr	fod	nofx	0, 0.1, 0.4% [c]	none	none	288	Little, 1953
69	Glycerol	56-81-5	rat	730	chr	fod	owt	0, 5, 10, 20% [c]	6883	none	3442	Atlas Chemical Ind., 1969
70	Glyceryl tribenzoate	614-33-5	rat	90	sub	fod	con	0, 120, 604, 2571 mg/kg/day	2571	none	604*	Carson, 1972
71	Hexenal, 2- (trans)	505-57-7	rat	91	sub	fod	mult	0, 260, 640, 1600, 4000 ppm [a]	257	80	80*	Gaunt *et al.*, 1971a
72	Hexylresorcinol, 4-	136-77-6	mus	91	sub	gav	kid	0, 62.5, 125, 250, 500, 1000 mg/kg/day	125	none	62.5*	NTP, 1988a
73	Hydroquinone	123-31-9	rat	90	sub	gav	owt	0, 25, 50, 100, 200, 400 mg/kg/day	50	none	25*	NTP, 1989c
74	Hydroxybenzoic acid butyl ester, *p*-	94-26-8	rat	84	sub	fod	mult	0, 2, 8% [a]	5500	none	900*	Matthews *et al.*, 1956
75	Hydroxybenzoic acid ethyl ester, *p*-	120-47-8	rat	NG	chr	fod	nofx	0, 2% [c]	none	none	1441	Truhaut, 1962
76	Hydroxybenzoic acid methyl ester, *p*-	99-76-3	rat	540	chr	fod	bdw	150, 1500 mg/kg/day	1500	none	150	Sokol, 1952
77	Hydroxybenzoic acid propyl ester, *p*-	94-13-3	rat	540	chr	fod	bdw	150, 1500 mg/kg/day	1500	none	150	Sokol, 1952
78	Hydroxybenzyl acetone, *p*-	5471-51-2	rat	91	sub	fod	owt	0, 0.1, 0.2, 0.4, 1% [a]	240	100	100*	Gaunt *et al.*, 1970a
79	Inosine monophosphate	131-99-7	rat	NG	repro	fod	nofx	0, 0.5, 1, 2% [c]	none	none	1774	Palmer *et al.*, 1971
80	Ionone	8013-90-9	rat	90	sub	fod	mult	0, 10, 100 mg/kg/day	100	10	10*	Ford *et al.*, 1983a
81	Isoamyl butyrate	106-27-4	rat	112	sub	fod	nofx	0, 0.1, 0.25, 1% [c]	none	none	887*	Hagan *et al.*, 1967b
82	Isoamyl salicylate	87-20-7	rat	91	sub	fod	owt	0, 50 [a], 500, 5000 ppm [d]	47	4.7	4.7*	Drake *et al.*, 1975
83	Isobutyl alcohol	78-83-1	rat	91	sub	NG	mult	0, 100, 316, 1000 mg/kg/day	1000	316	316*	US EPA, 1986c
84	Isomaltitol	534-73-6	rat	90	sub	fod	git	0, 3.3, 10, 30% [c]	8871	none	2927*	Bomhard *et al.*, 1978
85	Isopropyl alcohol	67-63-0	rat	180	terat	NG	ter	0, 0.018, 0.18, 1.8, 18 mg/kg/day	0.18	0.018	0.018*	Antonova and Salmina, 1978
86	Isovaleric acid	503-74-2	rat	90	sub	fod	mult	0, 0.62, 1.25, 2.5, 5, 10% [c]	4307	2154	2154*	Amoore *et al.*, 1978

(Cont'd)

87	Lactitol	585-86-4	rat	NG	repro	fod	bdw	0, 2, 5, 10% [c]	3680	none	1472	Sinkeldam *et al.*, 1982
88	Limonene, *d*-	5989-27-5	mus	721	chr	gav	liv	0, 250, 500 mg/kg/day	500	none	250	NTP, 1990a
89	Lithocholic acid	434-13-9	rat	721	chr	gav	kid	0, 250, 500 mg/kg/day	500	none	250	NCI, 1978a
90	Malonaldehyde, sodium salt	24382-04-5	rat	91	sub	gav	kid	0, 30, 60, 125, 250, 500 mg/kg/day	60	none	30*	NTP, 1988b
91	Mannitol	69-65-8	rat	10	terat	NG	nofx	1600 mg/kg/day	none	none	1600	FDRL, 1972
92	Menthol	89-78-1	rat	721	chr	fod	bdw	0, 3750, 7500 ppm [c]	593	none	296	NCI, 1979a
93	Methanol	67-56-1	rat	90	sub	gav	mult	0, 100, 500, 2500 mg/kg/day	2500	500	500*	US EPA, 1986f
94	Methyl ethyl carbonate		rat	10	terat	orl	con	0, 0.01, 0.1, 1.0% [c]	1564	none	156	Machemer, 1976
95	Methyl methacrylate	79-41-4	rat	730	chr	orl	con	0, 6, 60, 2000 ppm [c]	248	none	8.4	Borzelleca *et al.*, 1964
96	Methyl salicylate	119-36-8	rat	730	chr	fod	msk	0, 0.1, 0.5, 1.0, 2.0% [c]	360	none	72	Webb and Hansen, 1963
97	Methyl-1-phenylpentan-2-ol, 4-	38502-29-3	rat	91	sub	fod	bld	0, 10, 40, 160 mg/kg/day	40	10	10*	Ford *et al.*, 1983b
98	Methylenebis, 2,2'-		rat	11	terat	gav	mult	187, 375, 750 mg/kg/day	375	none	187	Tanaka *et al.*, 1989
99	Methylphenol, 3-	108-39-4	rat	90	sub	gav	bdw	0, 50, 150, 450 mg/kg/day	150	50	50*	US EPA, 1986g
100	Methylphenylcarbinyl acetate	93-92-5	rat	91	sub	gav	owt	0, 15, 50, 150 mg/kg/day	150	15	50*	Gaunt *et al.*, 1974
101	Myrcene, β-	123-35-3	rat	NG	repro	gav	rep	250, 500, 1000, 1500 mg/kg/day	500	250	250	Delgado *et al.*, 1993
102	Nonalactone, γ-	104-61-0	rat	730	chr	fod	nofx	0, 0.1, 0.5% [c]	none	none	360	Baer and Griepentrog, 1967a
103	Octyl acetate	112-14-1	rat	10	terat	gav	mult	0, 100, 500, 1000 mg/kg/day	500	none	100	Daughtrey *et al.*, 1989
104	Octyl gallate	1034-01-1	rat	NG	repro	fod	rep	0, 1000, 5000 ppm in diet [c]	444	none	89	Hazelton Lab. Inc., 1970
105	Oleylamine	1838-19-3	rbt	13	terat	gav	mult	0, 3, 10, 30 mg/kg/day	10	none	3	Mercieca *et al.*, 1990
106	Oxalic acid	144-62-7	rat	730	chr	fod	nofx	0, 0.1, 0.5, 0.8, 1.2% [c]	none	none	840	Fitzhugh and Nelson, 1947
107	Phenol	108-95-2	rat	721	chr	orl	mult	0, 2500, 5000 ppm [a]	344	153	153	NCI, 1980
108	Phenoxyethanol	122-99-6	rat	91	sub	gav	kid	0, 80, 400, 2000 mg/kg/day	400	none	80*	Ben-Dyke *et al.*, 1977
109	Phenyl-1-propanol, 2-	698-87-3	rat	91	sub	fod	owt	0, 10, 40, 160 mg/kg/day	40	10	10*	Gaunt *et al.*, 1982
110	Phenylalanine	63-91-2	rat	NG	repro	orl	nofx	0, 0.45% [a]	none	none	835	Holder, 1989
111	Potassium sorbate	24634-61-5	rat	90	sub	fod	owt	0, 1, 2, 5, 10% [c]	4435	none	1774*	Mellon Institute, 1954
112	Propyl gallate	121-79-9	rat	730	chr	fod	mult	0, 0.001, 0.01, 0.12, 1.2, 2.3% [c]	864	none	86	Orten *et al.*, 1948
113	Propylene glycol	57-55-6	rat	105	sub	fod	nofx	0, 50,000 ppm [a]	none	2500	2500*	Gaunt *et al.*, 1972c
114	Resorcinol	108-46-3	rat	90	sub	gav	owt	0, 32, 65, 130, 260, 520 mg/kg/day	65	none	32*	NTP, 1992b
115	Retinol	68-26-2	mus	1	terat	gav	ter	10, 100 mg/kg/day	100	none	10	Eckhoff *et al.*, 1989
116	Riboflavin	83-88-5	rat	NG	repro	fod	nofx	4, 40 ppm [c]	none	none	4	Le Clerc, 1974
117	Sodium benzoate	532-32-1	rat	720	chr	fod	nofx	0, 1, 2% [a]	none	none	1000	Sodemoto and Enomoto, 1980
118	Sodium erythorbate	89-65-6	rat	728	chr	orl	bdw	0, 1.25, 2.5% [c, d]	1554	none	784	Abe *et al.*, 1984
119	Sodium lauryl glyccryl ether sulfonate		rat	735	repro	fod	nofx	0, 0.1, 0.5% [c]	none	none	360	Tusing *et al.*, 1962
120	Sodium lauryl trioxyethylene sulfate	13150-00-0	rat	35	repro	fod	nofx	0, 0.1, 0.5% [c]	none	none	360	Tusing *et al.*, 1962
121	Sodium stearoyl lactylate	25383-99-7	rat	02	sub	fod	mult	0, 0.5, 5, 12.5% [c]	11089	4435	4435*	Hodge, 1953
122	Sorbic acid	110-44-1	rat	511	chr	fod	nofx	0, 5% [c]	none	none	3602	Lang, 1962; Lang *et al.*, 1967
123	Stearyl tartrate		rat	NG	repro	fod	nofx	0, 1, 5% [c]	none	none	3600	Frazer *et al.*, 1954
124	Styrene	100-42-5	rat	730	chr	orl	bdw	0, 125, 250 ppm in drinking water [a]	21	none	12	Chemical Manufacturers Association, 1980
125	Sucrose monopalmitate	26446-38-8	rat	660	repro	fod	nofx	0, 1% [c]	none	none	720	Paynter, 1965
126	Sucrose monostearate	25168-73-4	rat	60	sub	NG	nofx	100, 200, 1000, 2000 mg/kg/day	none	none	2000*	Hara, 1959
127	Tartaric acid	133-37-9	rat	10	terat	NG	nofx	181 mg/kg/day	none	none	181	FDRL, 1973
128	Tertiary butyl hydroquinone	1948-33-0	rat	66	repro	fod	bdw	0, 0.015, 0.15, 0.5% in diet [c]	431	none	129*	Krasavage and Terhaar, 1970
129	Tocopherol, α-	59-02-9	rat	90	sub	fod	bld	35, 875, 1750, 3500, 35,000 mg/kg diet [c]	3105	none	310*	Dysmsza and Park, 1975
130	Tolualdehyde	1334-78-7	rat	91	sub	gav	owt	0, 50, 250, 500 mg/kg/day	500	250	250*	Brantom *et al.*, 1972
131	Toluene	108-88-3	rat	193	sub	gav	nofx	118, 354, 590 mg/kg/day	none	none	590*	Wolf *et al.*, 1956c
132	Triethylene glycol	112-27-6	mus	10	terat	gav	ter	0, 0.5, 5.0, 10.0 ml/kg/day	5	none	0.5	Neeper-Bradley *et al.*, 1994
133	Triethylene glycol monomethyl ether	112-35-6	rbt	13	terat	gav	ltl	0, 250, 500, 1000, 1500 mg/kg/day	1500	1000	1000	Krasavage *et al.*, 1992
134	Trimethylamine	75-50-3	rat	84	sub	fod	bdw	0, 0.08, 0.16, 0.31, 0.62% [c]	267	138	138*	Amoore *et al.*, 1978

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135	Undecalactone, γ-	104-67-6	rat	730	chr	fod	nofx	0, 0.1, 0.5% [c]	none	none	360	Baer and Griepentrog, 1967a
136	Vanillin	121-33-5	rat	730	chr	fod	nofx	0, 0.5, 1, 2% [c]	none	none	1441	Hagan *et al.*, 1967b
137	Xylitol	87-99-0	rat	330	repro	fod	nofx	100 mg/kg/day	none	none	100*	Mosinger, 1971

Structural Class 2

Chemical Name	CAS No.	Species Tested	Exposure Duration (days)	Study Type	Exposure Route	Endpoint Type	Doses Given By Author	LOEL (mg/kg/day)	Authors' NOEL (mg/kg/day)	Calculated NOEL (mg/kg/day)	Reference
1 Acrylic acid	79-10-7	rat	98	repro	orl	rep	0, 500, 2500, 5000 ppm [a]	240	53	53*	BASF, 1993
2 Allyl alcohol	107-18-6	rat	105	sub	orl	owt	0, 50, 100, 200, 800 mg/litre [d]	9.6	4.8	4.8*	Carpanini *et al.*, 1978
3 Allyl heptanoate	142-19-8	rat	90	sub	fod	bdw	0, 49.6, 157, 496 mg/kg/day	157	none	49.6*	Damske *et al.*, 1980
4 Allyl hexanoate	123-68-2	rat	365	sub	fod	nofx	2500 mg/kg [a]	none	none	125*	Hagan *et al.*, 1967c
5 Butylated hydroxytoluene	128-37-0	rat	90	repro	fod	rep	0, 25, 100, 500 mg/kg/day	100	none	25*	Olsen *et al.*, 1986
6 Caffeine	58-08-2	rat	21	terat	orl	ter	0.007, 0.018, 0.036, 0.07, 0.1, 0.15, 0.2% [a]	27.4	none	10.1	Collins *et al.*, 1983
7 Carotene, β-	7235-40-7	rat	770	repro	fod	nofx	0, 1000 ppm [c]	none	none	89	Bagdon *et al.*, 1960
8 Carvone	99-49-0	rat	365	sub	fod	nofx	2500 ppm [a]	none	none	125*	Hagan *et al.*, 1967c
9 Carvone, *d*-	2244-16-8	mus	730	chr	gav	nofx	0, 375, 750 mg/kg/day	none	750	750	NTP, 1990b
10 Diacetyl	431-03-8	rat	90	sub	gav	mult	0, 10, 30, 90, 540 mg/kg/day	540	90	90*	Colley *et al.*, 1969
11 Diallyl phthalate	131-17-9	mus	721	chr	gav	git	0, 150, 300 mg/kg/day	300	none	150	NTP, 1983b
12 Diketopiperazine	2990-68-9	mus	770	chr	fod	owt	0, 250, 500, 1000 mg/kg/day	1000	none	500	Anonymous, 1974
13 Ethyl maltol	4940-11-8	rat	90	repro	NG	nofx	0, 50, 100, 200 mg/kg/day	none	none	200*	Gralla *et al.*, 1969
14 Ethyl vanillin	121-32-4	rat	730	chr	fod	nofx	0, 0.5, 1, 2% [c]	none	none	1441	Hagan *et al.*, 1967b
15 Ethylhexyl phthalate, mono-2-		rat	10	terat	gav	bdw	0, 50, 100, 200 mg/kg/day	100	none	50	Ruddick *et al.*, 1981
16 Etretinate	54350-48-0	rat	1	terat	gav	ter	0, 1, 3, 6, 10, 15, 25 mg/kg/day	10	none	6	Agnish *et al.*, 1990
17 Fenthion	55-88-9	rat	91	sub	fod	bdw	0, 5, 20, 40, 80, 160, 320 ppm [c]	32	none	16*	NCI, 1978b
18 Furfural	98-01-1	rat	720	chr	gav	pul	0, 30, 60 mg/kg/day	60	none	30	NTP, 1990c
19 Isobornyl acetate	125-12-2	rat	91	sub	gav	kid	0, 15, 90, 270 mg/kg/day	90	15	15*	Gaunt *et al.*, 1971b
20 Isophorone	78-59-1	rat	91	sub	gav	nos	0, 62.5, 125, 250, 500, 1000 mg/kg/day	1000	none	500*	NTP, 1986a
21 Maltol	118-71-8	mus	180	sub	fod	ltl	0, 100, 200, 400 mg/kg in diet [c]	39	none	20*	Marshall and Bouchard, 1980
22 Methyl amyl ketone	110-43-0	rat	91	sub	gav	kid	0, 20, 100, 500 mg/kg/day	100	20	20*	Gaunt *et al.*, 1972b
23 Methyl anthranilate	134-20-3	rat	115	sub	fod	mult	0, 3000, 10,000 ppm in diet [a]	500	none	150*	Dow Chemical, 1967
24 Piperidine	110-89-4	rat	84	sub	fod	bdw	0, 0.08, 0.16, 0.31, 0.62% [c]	138	69	69*	Amoore *et al.* 1978
25 Piperonal	120-57-0	rat	730	chr	fod	nofx	0, 0.1, 0.5% [c]	none	none	360	Baer and Griepentrog, 1967b
26 Propargyl alcohol	107-19-7	rat	91	sub	NG	mult	0, 5, 15, 50 mg/kg/day	15	5	5*	US EPA, 1987
27 Pyridine	110-86-1	rat	90	sub	gav	owt	0, 0.25, 1, 10, 25, 50 mg/kg/day	10	1	1*	US EPA, 1986h
28 Thujone	546-80-5	rat	98	sub	gav	ltl	0, 5, 10, 20 mg/kg/day	10	5	5*	Margaria, 1963

Structural Class 3

Chemical Name	CAS No.	Species Tested	Exposure Duration (days)	Study Type	Exposure Route	Endpoint Type	Doses Given By Author	LOEL (mg/kg/day)	Authors' NOEL (mg/kg/day)	Calculated NOEL (mg/kg/day)	Reference
1 (1-naphthyl)ethylene-diamine dihydro chloride, *N*-	1465-25-4	rat	728	chr	fod	mult	0, 0.05, 0.10% [c]	79	none	39	NCI, 1979b
2 (2-chloroethyl)trimethyl-ammonium chloride	999-81-5	rat	756	chr	fod	bdw	0, 1500, 3000 ppm [c]	275	none	138	NCI, 1979c

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3	(chloroacetyl)-acetanilide, 4'-	140-49-8	rat	609	chr	fod	bdw	0, 1000, 2000 ppm [c]	1580	none	790	NCI, 1979d
4	1,1'-(2,2,2-trichloroethylidene) bis(4-chloro)-benzene	50-29-3	rat	546	chr	fod	mult	0, 210, 420 ppm	32	none	16	NCI, 1978c
5	11-oxo-11*H*-pyrido(2,1-*b*) quinazoline-2-carboxylic acid		rat	11	terat	gav	mult	20, 90, 400 mg/kg/day	400	none	90	Nishimura *et al.*, 1988
6	2(2,4,5-trichlorophenoxy) propionic acid	93-72-1	rat	730	chr	fod	mult	0[b], 10[c], 30[b], 100[c] ppm	8.7	2.6	2.6	Mullison, 1966
7	2-(2-methyl-4-chlorophenoxy) propionic acid	93-65-2	rat	90	sub	fod	owt	0, 50, 400, 3200 ppm [a]	20	2.5	2.5*	Verschuuren *et al.*, 1975
8	4-(2-methyl-4-chlorophenoxy) butyric acid	94-81-5	rat	91	sub	fod	mult	0, 4, 12, 40 mg/kg/day	40	12	12*	Rhodia Inc., 1970
9	C.I. Disperse Blue 1	2475-45-8	rat	91	sub	fod	mult	0, 1200, 2500, 5000, 10,000, 20,000 ppm [d]	129	none	62*	NTP, 1986c
10	C.I. Orange 3	6373-74-6	mus	91	sub	gav	kid	0, 250, 500, 1000, 2000 mg/kg/day	1000	none	500*	NTP, 1988e
11	C.I. Acid Red 14	3567-69-9	mus	91	sub	fod	bdw	0, 6000, 12,500, 25,000, 50,000, 100,000 ppm in diet [c]	2439	none	1171*	NTP, 1982e
12	C.I. Disperse Yellow	2832-40-8	rat	91	sub	fod	mult	0, 1250, 2500, 5000, 10,000, 20,000 ppm	500	none	250*	NTP, 1982f
13	C.I. Pigment Red 23	6471-49-4	rat	720	chr	fod	kid	0, 10,000, 25,000, 50,000 ppm [a]	2100	none	1100	NTP, 1992c
14	C.I. Solvent Yellow 14	842-07-9	rat	91	sub	fod	mult	0, 250, 500, 1000, 2000, 4000 ppm [c]	100	none	50*	NTP, 1982g
15	EDTA, disodium	139-33-3	rat	84	sub	fod	rep	0, 0.5, 1, 5% [c]	5000	none	1000*	Yang, 1964
16	HC Blue No. 1	2784-94-3	rat	91	sub	fod	bdw	0, 750, 1500, 3000, 6250, 12,500 ppm [c]	625	none	300*	NTP, 1985d
17	HC Blue No. 2	33229-34-4	rat	91	sub	fod	bdw	0, 3100, 6200, 12,500, 25,000, 50,000 ppm [c]	620	none	310*	NTP, 1985e
18	HC Yellow 4	59820-43-8	rat	720	chr	fod	nos	0, 2500, 5000 ppm [d]	229	none	115	NTP, 1992i
19	LY201116		rat	12	terat	gav	bdw	0, 10, 25, 50 mg/kg/day	25	10	10	Higdon *et al.*, date unknown
20	LY237733	121588-75-8	rat	12	terat	gav	mult	0, 3, 10, 30 mg/kg/day	30	10	10	Kelich *et al.*, 1991
21	Acenaphthene	83-32-9	mus	90	sub	gav	liv	0, 175, 350, 700 mg/kg/day	350	175	175*	US EPA, 1989b
22	Acephate	30560-19-1	rat	NG	repro	NG	mult	2.5, 25 mg/kg/day	25	2.5	2.5	Chevron, 1987
23	Acesulfame potassium	33665-90-6	rat	28	repro	fod	bdw	0, 0.3, 1.0, 3.0% [c]	887	none	266	Sinkeldam *et al.*, 1976
24	Acetaminophen	103-90-2	mus	720	chr	fod	cnd	0, 600, 3000, 6000 [a]	600	none	110	NTP, 1993b
25	Acetoacetamide	5977-14-0	rat	90	sub	fod	mult	0, 400, 2000, 10,000, 50,000 mg/kg diet [c]	887	177	177*	Mayer *et al.*, 1979
26	Acetoacetamide-*N*-sulfonic acid		rat	90	sub	fod	mult	0, 800, 20,000, 50,000 mg/kg diet [d]	4658	1863	1863*	Fuchs *et al.*, 1986
27	Acetochlor	34256-82-1	rat	730	chr	fod	liv	0, 40, 200, 1000 ppm [a]	50	none	10	Monsanto Co., 1986
28	Acetonitrile	75-05-8	rat	14	terat	gav	nos	0, 125, 190, 275 mg/kg/day	275	none	190	International Research and Development Corp., 1981
29	Acifluorin sodium	62476-59-9	rat	730	chr	fod	mult	25, 180 mg/kg/day	180	25	25	Rhone-Poulenc, 1983
30	Acrylamide	79-06-1	rat	90	sub	orl	neu	0, 0.05, 0.2, 1, 5, 20 mg/kg/day	1	0.2	0.2*	Burek *et al.*, 1980
31	Acrylonitrile	107-13-1	rat	10	terat	gav	mult	0, 10, 25, 65 mg/kg/day	65	none	25	Murray *et al.*, 1976; 1978
32	Alachlor	15972-60-8	rat	730	chr	fod	mult	0, 0.5, 2.5, 15 mg/kg/day	15	2.5	2.5	Monsanto Co., 1984a
33	Albendazole	54965-21-8	rat	60	sub	gav	nos	0, 1, 10, 30 mg/kg/day	10	1	1*	Boutemy, 1980
34	Albendazole sulfoxide		rat	8	terat	gav	rep	0, 5.3, 6, 6.62, 8.83, 10.6, 13.25 mg/kg/day	6.62	6	6	Martin, 1980
35	Aldicarb	116-06-3	rat	90	repro	fod	rep	0, 0.2, 0.3, 0.7 mg/kg/day	0.7	0.3	0.3*	Union Carbide, 1974
36	Aldicarb sulfone	1646-88-4	rat	90	sub	fod	mult	0, 0.2, 0.6, 2, 5, 16 mg/kg/day	2	none	0.6*	Union Carbide, 1968
37	Alinidine hydrobromide	33178-86-8	rat	NG	terat	NG	mult	0, 2, 6, 20 mg/kg/day	6	2	2	Matsuo *et al.*, 1989
38	Ally	74223-64-6	rat	NG	repro	NG	bdw	25, 250 mg/kg/day	250	25	25	du Pont, 1985a
39	Allyl isovalerate	2835-39-4	rat	91	sub	gav	mult	0, 15, 31, 62, 125, 250 mg/kg/day	125	none	62*	NTP, 1983c
40	Amaranth	915-67-3	rat	20	terat	gav	rep	0, 7.5, 15, 30, 100, 200 mg/kg/day	15	none	7.5	Collins *et al.*, 1972
41	Amdro	67485-29-4	rat	NG	repro	NG	bdw	2.5, 5 mg/kg/day	5	2.5	2.5	American Cyanamid, 1982
42	Ameltolide	787-93-9	rat	12	terat	gav	bdw	0, 10, 25, 50 mg/kg/day	25	10	10	Higdon *et al.*, 1991
43	Ametryn	834-12-8	rat	91	sub	gav	liv	0, 10, 100 mg/kg/day	100	10	10*	Ciba, 1961

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44	Amino-4-ethoxy-acetanilide, 3-	17026-81-2	rat	546	chr	fod	mult	0, 0.4, 1.5% [c]	1185	none	316	NCI, 1978d
45	Amino-4-nitrophenol, 2-	99-57-0	rat	91	sub	gav	mult	0, 62.5, 125, 250, 500, 1000 mg/kg/day	500	none	250*	NTP, 1988c
46	Amino-5-nitrophenol, 2-	121-88-0	rat	91	sub	gav	owt	0, 100, 200, 400, 800, 1600 mg/kg/day	200	none	100*	NTP, 1988d
47	Aminophenol, *p*-	123-30-8	rat	180	sub	fod	mult	0, 0.07, 0.2, 0.7% [c]	686	none	196*	Burnett *et al.*, 1989
48	Amitraz	33089-61-1	rbt	NG	repro	NG	ter	1, 5 mg/kg/day	5	1	1	Upjohn Co., 1973
49	Ammonium carmine		rat	21	terat	gav	rep	0, 200, 500, 1000 mg/kg/day	1000	none	500	Gaunt *et al.*, 1976
50	Amphetamine sulfate, *dl*-	60-13-9	rat	720	chr	fod	bdw	0, 20, 100 ppm [a]	5	none	1	NTP, 1991a
51	Ampicillin trihydrate	7177-48-2	mus	91	sub	gav	git	0, 250, 500, 1000, 2000, 3000 mg/kg/day	2000	none	1000*	NTP, 1987a
52	Anethole, *trans*-	104-46-1	rat	819	chr	fod	mult	0, 0.25, 0.5, 1% [c]	344	none	172	Truhaut *et al.*, 1988
53	Anilazine	101-05-3	rat	91	sub	fod	bdw	0, 250, 500, 1000, 2000, 4000, 8000, 16,000 ppm [c]	800	none	400*	NCI, 1978e
54	Anisidine hydrochloride, *p*-	20265-97-8	rat	721	chr	fod	bdw	0, 0.3, 0.6% [c]	474	none	237	NCI, 1978f
55	Anthranilic acid	118-92-3	rat	546	chr	fod	bdw	0, 15,000, 30,000 ppm [c]	2751	none	1376	NCI, 1978g
56	Apollo	74115-24-5	rat	NG	repro	NG	liv	2, 20 mg/kg/day	20	2	2	BCF Chemicals, 1984
57	Arochlor 1254	27323-18-8	rat	735	chr	fod	mult	0, 25, 50, 100 ppm [c]	4	none	2	NCI, 1978h
58	Aspartame	22389-47-0	rat	364	sub	fod	owt	0, 1, 2, 4 g/kg/day of diet [c]	147	none	74*	Ishii *et al.*, 1981
59	Assure	76578-14-8	rat	728	chr	fod	liv	0, 25, 100, 400 ppm [a]	3.7	0.9	0.9	du Pont, 1985b
60	Asulam	3337-71-1	rat	756	chr	fod	mult	36, 180 mg/kg/day	180	36	36	Rhone-Poulenc, 1981a
61	Atrazine	1912-24-9	rat	NG	repro	fod	mult	0, 10, 50, 500 ppm [a]	34.97	3.5	3.5	Ciba, 1987
62	Avermectin B1	65195-55-3	mus	NG	terat	NG	ter	0.03, 0.1 mg/kg/day	0.1	0.03	0.03	Merck & Co., 1985
63	Azaperone	1649-18-9	mus	10	terat	gav	mult	0, 2.5, 10, 40 mg/kg/day	10	2.5	2.5	Mosher *et al.*, 1973
64	Azinphos methyl	86-50-0	rat	730	chr	fod	bld	0, 2.5, 5, 20, 50 ppm in diet [c]	0.36	none	0.18	Huntingdon Research Centre, 1966
65	Azorubine	3567-69-0	rat	90	sub	fod	owt	0, 0.05, 0.1, 0.5, 1.0% [d]	500	250	250*	Gaunt *et al.*, 1967a
66	Azuletil sodium (KT1-32)	99287-30-6	rat	12	terat	gav	neu	0, 10, 77, 600 mg/kg/day	77	10	10	Tesh *et al.*, 1991
67	Baygon	114-26-1	rat	730	chr	fod	mult	10, 50 mg/kg/day	50	10	10	Mobay Chemical, 1984a
68	Bayleton	43121-43-3	rat	730	chr	fod	mult	0, 50, 500, 5000 ppm [b]	25	2.5	2.5	Mobay Chemical, 1978
69	Baythroid	68359-37-5	rat	NG	repro	NG	rep	2.5, 7.5 mg/kg/day	7.5	2.5	2.5	Mobay Chemical, 1983
70	Benomyl	17804-35-2	rat	NG	repro	fod	rep	0, 100, 500, 2500 ppm [a]	25	5	5	du Pont, 1968
71	Bentazon	25057-89-0	rat	90	sub	fod	tes	3.5, 10 mg/kg/day	10	3.5	3.5*	BASF, 1970
72	Benzofuran	271-89-6	rat	90	sub	gav	nos	0, 31.25, 62.5, 125, 250, 500 mg/kg/day	62.5	none	31.25*	NTP, 1989d
73	Benzoin	119-53-9	rat	90	sub	fod	kid	0, 30, 60, 125, 250, 500 ppm [c]	25	none	12.5*	NTP, 1980a
74	Benzyl Violet 4B	1684-09-3	rat	730	chr	fod	git	0.1, 0.5, 1% in diet [c]	720	none	360	FDA, 1964
75	Benzyl-*p*-chlorophenol, *o*-	120-32-1	rat	91	sub	gav	kid	0, 30, 60, 120, 240, 480 mg/kg/day	240	none	120*	NTP, 1994
76	Betaxolol	63659-18-7	rbt	13	terat	gav	rep	0, 1, 4, 12, 36 mg/kg/day	36	12	12	Tesh *et al.*, 1990
77	Bidrin	141-66-2	rat	NG	repro	fod	rep	0, 2, 5, 15, 50 ppm [b]	0.25	0.1	0.1	Shell Chemical Co., 1965
78	Biphenthrin	82657-04-3	rat	NG	terat	NG	mult	1, 2 mg/kg/day	2	1	1	FMC Corp., 1984
79	Biphenyl, 1,1-	92-52-4	rat	700	chr	fod	mult	0, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, 1.0% [a]	250	50	50	Ambrose *et al.*, 1960
80	Biphenylamine hydrochloride, 2-	2185-92-4	mus	91	sub	fod	spl	0, 300, 1000, 3000, 10,000, 30,000 ppm [c]	180	none	54*	NTP, 1982c
81	Bis(2-chloro-1-methyl-ethyl)ether, Technical Grade	108-60-1	rat	91	sub	gav	bdw	0, 10, 25, 50, 100, 250 mg/kg/day	250	none	100*	NCI, 1979e
82	Bis(2-chloroisopropyl)ether	39638-32-9	mus	728	chr	fod	bld	0, 80 [d], 400 [a], 2000 [d], 10,000 [d] ppm	198	36	36	Mitsumori *et al.*, 1979
83	Bisphenol A	80-05-7	rat	91	sub	fod	bdw	0, 250, 500, 1000, 2000, 4000 ppm [c]	113	none	56*	NTP, 1982d
84	Bromoacetic acid, 2-	79-08-3	rat	10	terat	gav	ter	0, 25, 50, 100 mg/kg/day	100	none	50	Randall *et al.*, 1991
85	Bromodichloromethane	75-27-4	rat	540	chr	cap	bdw	0, 0.014, 0.055, 0.22% [a]	130	none	24	Tobe *et al.*, 1982
86	Bromomethane	74-83-9	rat	91	sub	gav	mult	0, 0.4, 2, 10, 50 mg/kg/day	10	2	2*	Danse *et al.*, 1984
87	Bromoxynil	1689-84-5	rat	10	terat	gav	mult	1.7, 5, 15 mg/kg/day	15	none	5	Rogers *et al.*, 1990
88	Bromoxynil octanoate	1689-99-2	rat	NG	terat	NG	mult	15, 35 mg/kg/day	35	15	15	Union Carbide, 1981
89	Brown FK	6300-61-4	mus	560	chr	fod	nos	0, 0.0125, 0.0375, 0.075, 0.125, 0.625% in diet [c]	64	none	21	Wilson *et al.*, 1970
90	Butyl chloride, *n*-	109-69-3	rat	91	sub	gav	mult	0, 30, 60, 120, 250, 500 mg/kg/day	250	none	120*	NTP, 1986b

91	Butylate	2008-41-5	rat	NG	repro	NG	con	10, 50 mg/kg/day	50	10	10	Stauffer Chemical Co., 1986
92	Calcium cyanamide	156-62-7	mus	700	chr	fod	ltl	0, 500, 2000 ppm [c]	344	none	86	NCI, 1979f
93	Canthaxanthin	514-78-3	rat	91	sub	fod	owt	0, 125, 250, 500, 1000, 2000 mg/kg/day	1000	none	500*	Steiger and Buser, 1982
94	Caprolactam	105-60-2	rat	90	sub	fod	bld	50, 250 mg/kg/day	250	50	50*	Powers *et al.*, 1984
95	Captafol	2425-06-1	rat	730	chr	NG	mult	2.8, 12 mg/kg/day	12	2.8	2.8	Chevron, 1985a
96	Captan	133-06-2	rbt	NG	terat	NG	bdw	25, 60 mg/kg/day	60	25	25	Chevron, 1981
97	Carazolol	57775-29-8	rat	90	sub	fod	bdw	0, 40, 120, 400 mg/kg food [a]	30.4	none	9.5*	Rebel *et al.*, 1976
98	Carbaryl	63-25-2	rat	730	chr	fod	mult	0, 50, 100, 200, 400 ppm [a]	15.6	9.6	9.6	Carpenter *et al.*, 1961
99	Carbendazim	10605-21-7	rat	8	terat	gav	mult	0, 25, 50, 100, 200, 400, 1000 mg/kg/day	1000	none	400	Cummings and Harris, 1990
100	Carbofuran	1563-66-2	rat	NG	terat	NG	rep	1, 3 mg/kg/day	3	1	1	FMC Corp., 1981
101	Carbon tetrachloride	56-23-5	rat	84	sub	gav	liv	1, 10, 33 mg/kg/day, 5 days/wk [a]	7.1	0.71	0.71*	Bruckner *et al.*, 1986
102	Carbosulfan	55285-14-8	rat	NG	repro	NG	rep	1, 12.5 mg/kg/day	12.5	1	1	FMC Corp., 1982
103	Carboxin	5234-68-4	rat	730	chr	fod	mult	0, 100, 200, 600 ppm [b]	30	10	10	Uniroyal Chemical, 1969
104	Carmoisine	3567-64-9	rat	90	sub	fod	owt	0, 0.05, 0.1, 0.5, 1% in diet [c]	887	none	444*	Gaunt *et al.*, 1967b
105	Chloramben	133-90-4	rat	NG	terat	NG	msk	25, 75 mg/kg/day	75	25	25	Union Carbide, 1976
106	Chlordane	57-74-9	rat	910	chr	fod	liv	0, 1, 5, 25 ppm in diet [a]	0.273	0.055	0.055	Velsicol Chemical, 1983
107	Chlorendic acid	115-28-6	rat	91	sub	fod	bdw	0, 620, 1250, 2500, 5000, 10,000 ppm in diet [c]	141	none	70*	NTP, 1987b
108	Chlorimuron-ethyl	90982-32-4	rbt	NG	terat	NG	ter	13, 48 mg/kg/day	48	13	13	du Pont, 1985c
109	Chloro-*p*-toluidine, 3-	95-74-9	mus	546	chr	fod	bdw	0, 300, 600 ppm [c]	104	none	52	NCI, 1978i
110	Chloroacetic acid	79-11-8	rat	730	chr	gav	ltl	0, 15, 30 mg/kg/day	30	none	15	NTP, 1992d
111	Chloroaniline hydrochloride, *p*-	20265-96-7	rat	750	chr	gav	mult	0, 2, 6, 18 mg/kg/day	6	none	2	NTP, 1989e
112	Chlorobenzene	108-90-7	rat	90	sub	fod	owt	50, 100 mg/kg/day	100	50	50*	Monsanto Co., 1967; Knapp *et al.*, 1971
113	Chlorobenzilate	510-15-6	rat	NG	repro	fod	tes	0, 25, 50 ppm in diet [c]	4.4	none	2.2	Woodward, 1965
114	Chlorodibromomethane	124-48-1	rat	91	sub	gav	mult	0, 15, 30, 60, 125, 250 mg/kg/day	250	none	125*	NTP, 1985a
115	Chloroform	67-66-3	rat	90	sub	NG	mult	15, 30, 410 mg/kg/day	410	30	30*	Anonymous, date unknown {a}
116	Chlorofructose, 6-		rat	70	repro	gav	rep	0, 3, 9 mg/kg/day	9	none	3*	Tesh *et al.*, 1984
117	Chloronaphthalene, β-	91-58-7	mus	91	sub	gav	mult	0, 100, 250, 600 mg/kg/day	600	250	250*	US EPA, 1989c
118	Chlorophenol, 2-	95-57-8	rat	NG	repro	orl	mult	0, 5, 50, 500 ppm [b]	50	5	5	Exon and Koller, 1986
119	Chloropropylate	5836-10-2	rat	730	chr	fod	mult	0, 40, 125 ppm in diet [c]	9	none	2.9	Woodard, 1966
120	Chlorothalonil	1897-45-6	rbt	NG	terat	NG	rep	5, 50 mg/kg/day	50	5	5	Diamond Shamrock, 1975
121	Chlorotoluene, *o*-	95-49-8	rat	104	sub	gav	mult	0, 20, 80, 320 mg/kg/day	80	20	20*	Gibson *et al.*, 1974
122	Chlorpheniramine maleate	113-92-8	rat	91	sub	gav	mult	0, 3.75, 7.5, 15, 30, 60 mg/kg/day	60	none	30*	NTP, 1986d
123	Chlorpromazine	50-53-3	rat	10	terat	gav	rep	0, 1, 3, 9 mg/kg/day	3	none	1	Robertson *et al.*, 1980
124	Chlorsulfuron	64902-72-3	rat	730	chr	fod	bdw	0, 100, 500, 2500 ppm [b]	25	5	5	du Pont, 1980
125	Chocolate Brown HT	4553-89-3	rat	730	chr	fod	ltl	0, 500, 2000, 10,000 ppm in diet	736	none	147	Carpanini *et al.*, 1975
126	Cimetidine	51481-61-9	rat	NG	repro	orl	mult	0, 0.15, 0.75, 4 mg/ml [a]	400	none	130	Shapiro *et al.*, 1988
127	Clonitralid	1420-04-8	mus	546	chr	fod	bdw	0, 274, 549 ppm [c]	94	none	47	NCI, 1978j
128	Closantel	57808-65-8	rat	NG	repro	gav	tes	0, 2.5, 10, 40 mg/kg/day	10	2.5	2.5	Dirx and Marsboom, 1984
129	Codeine	76-57-3	mus	10	terat	gav	rep	0, 37.5, 75, 150 mg/kg BID	300	150	150	Williams *et al.*, 1991
130	Coumaphos	56-72-4	rat	730	chr	fod	mult	0, 5, 10, 25, 100 ppm in diet [c]	0.8	0.4	0.4	Doull *et al.*, 1960
131	Coumarin	91-64-5	mus	90	sub	gav	bdw	0, 19, 38, 75, 150, 300 mg/kg/day	300	none	150*	NTP, 1993c
132	Crufomate	299-86-5	rat	600	chr	fod	bld	0, 20, 40, 60, 80 ppm in diet [c]	4	none	3	McCollister *et al.*, 1968
133	Curcumin	458-37-7	mus	90	sub	fod	bld	0, 0.1, 0.5, 1.0, 2.5, 5.0% [d]	928	none	186*	Lilja *et al.*, 1983
134	Cyclodextrin, β-	7585-39-9	rat	183	sub	gav	bdw	0, 100, 400, 1600 mg/kg/day	1600	400	400*	Makita *et al.*, 1975
135	Cyclohexylamine	108-91-8	rat	NG	repro	fod	bdw	0, 15, 50, 100, 150 mg/kg/day	50	none	15	Oser *et al.*, 1976
136	Cyclophosphamide	50-18-0	rat	28	repro	gav	rep	3.4, 5.1 mg/kg/day	5.1	none	3.4	Hales *et al.*, 1992
137	Cyhalothrin	68085-85-8	rat	NG	repro	fod	bdw	0, 10, 30, 100 ppm [b]	1.5	0.5	0.5	Imperial Chemicals Industries, 1984
138	Cypermethrin	52315-07-8	rat	NG	repro	NG	bdw	0.5, 5 mg/kg/day	5	0.5	0.5	ICI Americas, Inc., 1979

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139	Cyromazine	66215-27-8	rat	730	chr	fod	bdw	1.5, 15 mg/kg/day	15	1.5	1.5	Ciba, 1981a
140	Dacthal	1861-32-1	rat	730	chr	fod	owt	0, 100, 1000, 10,000 ppm [b]	500	50	50	Diamond Shamrock, 1964
141	Dalapony sodium salt	75-99-0	rat	730	chr	fod	owt	0, 5, 15, 50 mg/kg/day [b]	28.17	8.45	8.45	Paynter *et al.*, 1960
142	Daminozide	1596-84-5	rat	NG	repro	NG	ter	390, 1800 mg/kg/day	1800	390	390	Uniroyal Chemical, 1978
143	Decabromodiphenyl oxide	1163-19-5	mus	721	chr	fod	git	0, 25,000, 50,000 ppm [a]	7780	none	3760	NTP, 1986e
144	Deoxyquinine		rbt	13	terat	gav	mult	0, 20, 40, 80 mg/kg/day	80	none	40	Edwards *et al.*, 1982
145	Diamino-2,2′-stilbenedisulfonic acid, 4,4′-, disodium salt	7336-20-1	rat	90	sub	fod	mult	0, 6250, 12,500, 25,000, 50,000, 100,000 ppm [d]	2356	none	1207*	NTP, 1992e
146	Diaminophenol dihydrochloride, 2,4-	137-09-7	rat	720	chr	gav	mult	0, 12.5, 25 mg/kg/day	25	none	12.5	NTP, 1992f
147	Diazinon	333-41-5	mus	91	sub	fod	bdw	0, 50, 100, 200, 400, 800, 1600, 3200 ppm [c]	144	none	72*	NCI, 1979g
148	Dibenzo-*p*-dioxin	262-12-4	mus	630	chr	fod	mult	0, 5000, 10,000 ppm [c]	1728	none	864	NCI, 1978k
149	Dibromobenzene, 1,4-	106-37-6	rat	90	sub	NG	mult	0, 5, 10, 20 mg/kg/day	20	10	10*	Carlson and Tardiff, 1977
150	Dicamba	1918-00-9	rbt	NG	repro	fod	rep	0, 1, 3, 10 mg/kg/day	10	3	3	Velsicol Chemical, 1978
151	Dichloro-2-propanol, 1,3-	96-23-1	rat	90	sub	gav	owt	0, 0.1, 1, 10, 100 mg/kg/day	10	1	1*	Jersey *et al.*, 1991
152	Dichloro-*p*-phenylenediamine, 2,6-	609-20-1	rat	91	sub	fod	bdw	0, 1000, 2000, 4000, 6000, 8000 ppm	200	none	100*	NTP, 1982h
153	Dichlorobenzene, 1,2-	95-50-1	rat	91	sub	gav	mult	0, 30, 60, 125, 250, 500 mg/kg/day	125	none	60*	NTP, 1985b
154	Dichlorobenzene, 1,4-	106-46-7	rat	91	sub	gav	kid	0, 37.5, 75, 150, 300, 600 mg/kg/day	600	none	300*	NTP, 1987c
155	Dichlorobenzilic acid	23851-46-9	rat	99	sub	fod	owt	0, 20, 100, 500, 2500 ppm in diet [c]	221.8	none	44.4*	Domenjoz, 1965
156	Dichlorodifluoromethane	75-71-8	rat	730	chr	fod	bdw	0, 300, 3000 ppm [b]	150	15	15	Sherman, 1974
157	Dichloroethane, 1,1-	75-34-3	mus	546	chr	gav	ltl	0, 1442, 2885 mg/kg/day	2885	none	1442	NCI, 1978l
158	Dichloroethane, 1,2-	107-06-2	rat	90	sub	orl	owt	0, 500, 1000, 2000, 4000, 8000 ppm [d]	59	none	34*	Morgan *et al.*, 1990
159	Dichloroethylene, 1,1-	75-35-4	mus	91	sub	gav	bdw	0, 5, 15, 40, 100, 250 mg/kg/day	40	none	15*	NTP, 1982i
160	Dichloroethylene, *trans*-1,2-	156-60-5	mus	90	sub	orl	liv	0, 0.1, 1.0, or 2.0 mg/ml [a]	175	17	17*	Barnes *et al.*, 1985
161	Dichloromethane	75-09-2	rat	720	chr	orl	liv	0, 5, 50, 125, 250 mg/kg/day	50	5	5	National Coffee Assoc., 1982
162	Dichlorophenol, 2,4-	120-83-2	rat	NG	repro	orl	mult	0, 3, 30, 300 ppm [a]	3	0.3	0.3	Exon and Koller, 1985
163	Dichlorophenoxyacetic acid, 2,4-	94-75-7	rat	91	sub	fod	bld	0, 1, 5, 15, 45 mg/kg/day	5	1	1*	Dow Chemical, 1983
164	Dichloropropanol, 2,3-	616-23-9	rat	92	sub	gav	mult	0, 10, 35, 100 mg/kg/day	35	10	10*	US EPA, 1989d
165	Dichloropropene, 1,3-	542-75-6	rat	90	sub	fod	owt	0, 1, 3, 10, 30 mg/kg/day	10	3	3*	Dow Chemical, 1973
166	Dichlorvos	62-73-7	rat	730	chr	fod	mult	0, 0.047, 0.46, 4.67, 46.7, 234 ppm in diet [a]	2.3	0.23	0.23	Shell Chemical Co., 1967
167	Dicofol	115-32-2	rat	730	chr	fod	mult	0, 20, 100, 250, 500, 1000 ppm in diet [c]	20	none	8	Larson, 1957
168	Dieldrin	60-57-1	rat	730	chr	fod	liv	0, 0.1, 1.0, 10.0 ppm [a]	0.05	0.005	0.005	Walker *et al.*, 1969
169	Diethyldithiocarbamate	148-18-5	rat	90	sub	NG	bdw	0, 30, 100, 300 mg/kg/day	100	30	30*	Sunderman *et al.*, 1967
170	Diethylthiourea, *N,N′*-	105-55-5	mus	721	chr	fod	bdw	0, 250, 500 ppm [c]	86	none	43	NCI, 1979h
171	Difenzoquat	43222-48-6	rat	730	chr	fod	bdw	0, 100, 500, 2500 ppm [b]	125	25	25	Amercian Cyanamid, 1975
172	Diflubenzuron	35367-38-5	rat	730	chr	fod	bld	2, 8 mg/kg/day	8	2	2	Thompson-Hayward Chemical Corp., 1973
173	Dihydroavermectin-B1a, 22,23-	71827-03-7	mus	10	terat	gav	neu	0, 0.2, 0.4, 0.8, 1.6 mg/kg/day	0.4	none	0.2	Merck & Co., 1979
174	Dihydroavermectin-B1b, 22,23-		mus	10	terat	gav	nos	0, 0.4, 0.8, 1.6 mg/kg/day	0.8	none	0.4	Merck & Co., 1979
175	Dihydrocoumarin, 3,4-	119-84-6	rat	90	sub	gav	mult	0, 75, 150, 300, 600, 1200 mg/kg/day	300	none	150*	NTP, 1993h
176	Diiodomethyl *p*-tolyl sulfone	20018-09-1	rat	10	terat	fod	mult	0, 0.125, 0.25, 0.5, 1.0% [c]	251	none	126	Ema *et al.*, 1992
177	Dimethipin	55290-64-7	rat	742	chr	fod	liv	0, 40, 200, 1000 ppm [a]	10	2	2	Uniroyal Chemical, 1981
178	Dimethoate	60-51-5	rat	730	chr	fod	neu	0, 1, 5, 25, 100 ppm [a]	0.25	0.05	0.05	American Cyanamid, 1986a
179	Dimethoxyaniline hydrochloride, 2,4-	54150-69-5	rat	728	chr	fod	bdw	0, 1500, 3000 ppm [c]	276	none	138	NCI, 1979i
180	Dimethoxybenzidine-4,4′-diisocyanate, 3,3′-	91-93-0	mus	546	chr	fod	bdw	0, 22000, 44000 ppm [c]	7550	none	3775	NCI, 1978m
181	Dimethyl hydrogen phosphite	868-85-9	rat	728	chr	gav	mult	0, 50, 100 mg/kg/day	100	none	50	NTP, 1985c
182	Dimethyl methylphosphonate	756-79-6	rat	91	sub	gav	mult	0, 250, 500, 1000, 2000, 4000 mg/kg/day	2000	none	1000*	NTP, 1987h

183	Dimethyl morpholinophosphoramidate	597-25-1	rat	91	sub	gav	owt	0, 200, 400, 800, 1200, 1600 mg/kg/day	400	none	200*	NTP, 1986f
184	Dimethylaniline, *N,N'*-	121-69-7	mus	90	sub	gav	spl	0, 31, 62, 125, 250, 500 mg/kg/day	62	none	31*	NTP, 1989f
185	Dinitrobenzene, *m*-	99-65-0	rat	112	sub	orl	owt	0, 3, 8, 20 ppm [b]	1.1	0.4	0.4*	Cody *et al.*, 1981
186	Dinitrotoluene, 2,4-	121-14-2	rat	720	chr	fod	mult	0, 0.6, 4, 34 mg/kg/day	34	4	4	Lee *et al.*, 1985
187	Dinocap	39300-45-3	ham	8	terat	gav	nos	0, 50, 100, 200 mg/kg/day	100	none	50	Rogers *et al.*, 1989
188	Dinoseb	88-85-7	rbt	NG	terat	NG	ter	3, 10 mg/kg/day	10	3	3	American Hoechst Corp., 1986
189	Diphenamid	957-51-7	rat	730	chr	fod	owt	10, 30 mg/kg/day	30	10	10	Upjohn Co., 1966
190	Diphenhydramine hydrochloride	147-24-0	rat	90	sub	fod	liv	0, 156, 313, 625, 1250, 2500 ppm [c]	31	none	16*	NTP, 1989g
191	Diphenylamine	122-39-4	rat	730	chr	fod	kid	3.1, 31 mg/kg/day	31	3.1	3.1	Chemley Products, 1967
192	Diphenylhydantoin, 5,5'-	57-41-0	rat	10	terat	gav	bdw	0, 150, 375, 750, 1125, 1500 mg/kg/day	375	none	150	Rowland *et al.*, 1990
193	Diphenylhydantoin, 5,5-	57-41-0	rat	90	sub	fod	bdw	0, 300, 600, 1200, 2400, 4800 ppm [a]	122.2	none	60.7*	NTP, 1993d
194	Diquat	85-00-7	rat	730	chr	fod	eye	0, 5 [d], 15 [a], 75 [a], 375 [d] ppm in diet	0.58	0.19	0.19	Chevron, 1985b
195	Disulfoton	298-04-4	rat	730	chr	fod	mult	0.05, 0.1 mg/kg/day	0.1	0.05	0.05	Mobay Chemical, 1975
196	Dithiobiurea, 2,5-	142-46-1	rat	546	chr	fod	ltl	0, 0.6, 1.2% [c]	947	none	473	NCI, 1979s
197	Diuron	330-54-1	rat	730	chr	fod	bld	1, 6 mg/kg/day	6	1	1	du Pont, 1964
198	Dodecylguanidine acetate, *n*-	2439-10-3	rat	730	chr	fod	bdw	7, 10, 29, 45 mg/kg/day	29–45	7–10	7	Amercian Cyanamid, 1959
199	Endothall	145-73-3	mus	NG	terat	NG	ltl	5, 20 mg/kg/day	20	5	5	Penwalt Corp, 1981
200	Ephedrine sulfate	134-72-5	rat	91	sub	fod	bdw	0, 125, 250, 500, 1000, 2000 ppm [c]	50	none	25*	NTP, 1986g
201	Epichlorohydrin	106-89-8	rat	NG	repro	gav	rep	0, 2, 10 mg/kg/day	10	2	2	Van Esch, 1981
202	Erythromycin stearate	643-22-1	rat	91	sub	fod	liv	0, 5000, 10,000 ppm [a]	370	none	180*	NTP, 1988f
203	Erythrosine	16423-68-0	rat	NG	repro	fod	bdw	0, 0.25, 1.0, 4.0% [c]	799	none	200	Albridge *et al.*, 1981
204	Ethalfuralin	55283-68-6	rbt	13	terat	gav	mult	0, 25, 75, 150, 300 mg/kg/day	150	75	75	Byrd *et al.*, 1990
205	Ethephon	16672-87-0	rat	728	chr	fod	bld	15, 150 mg/kg/day	150	15	15	Union Carbide, 1978
206	Ethion	563-12-2	rat	NG	repro	NG	bld	0.2, 1.025 mg/kg/day	1.025	0.2	0.2	FMC Corp., 1985
207	Ethyl dipropylthiocarbamate, *s*-	759-94-4	rat	NG	repro	fod	bdw	0, 50, 200, 800 ppm [b]	10	3	3	PPG Industries, 1986
208	Ethyl *p*-nitrophenyl phenylphosphorothioate	2104-64-5	rat	90	sub	fod	bld	0.25, 1.25 mg/kg/day	1.25	0.25	0.25*	Moribani, Nissan, du Pont, Velsicol, 1986
209	Ethylene chlorohydrin	107-07-3	rat	84	sub	gav	owt	0, 30, 45, 67.5 mg/kg/day	67.5	45	45*	Oser *et al.*, 1975
210	Ethylene thiourea	96-45-7	mus	90	sub	fod	end	0, 1 [d], 10 [a], 100 [d], 1000 [d] ppm	17	1.7	1.7*	Rohm and Haas Co., 1985a
211	Ethylmethylphenylglycidate	77-83-8	rat	730	chr	fod	nos	0, 0.02, 0.1, 0.5% [d]	175	35	35	Dunnington *et al.*, 1981
212	Express	101200-48-0	rat	NG	repro	NG	bdw	1, 13 mg/kg/day	13	1	1	du Pont, 1986a
213	Fast Green FCF	2353-45-9	mus	730	chr	fod	ltl	0, 1, 2% in diet	3432	none	1716	Hansen *et al.*, 1966b
214	Febantel	58306-30-2	rat	150	sub	fod	mult	0, 20, 100, 500 ppm in diet [a]	10	2	2*	Eiben, 1985
215	Fenamiphos	22224-92-6	rbt	730	terat	fod	bdw	0.1, 0.3 mg/kg/day	0.3	0.1	0.1	Mobay Chemical, 1982
216	Fenbendazole	43210-67-9	rat	875	chr	fod	mult	0, 5, 15, 45, 135 mg/kg/day	15	5	5	Goldenthal, 1981; Brown, 1982; Sauer, 1986
217	Fenchlorphos	299-84-3	rat	105	sub	fod	mult	0, 0.5, 1.5, 5, 15, 50 mg/kg/day	50	none	15*	McCollister *et al.*, 1959
218	Fluometuron	2164-17-2	rat	90	sub	fod	mult	8, 75 mg/kg/day	75	8	8*	Ciba, 1965
219	Fluoranthene	206-44-0	mus	91	sub	gav	mult	0, 125, 250, 500 mg/kg/day	250	125	125*	US EPA, 1988a
220	Fluorene	86-73-7	mus	91	sub	gav	mult	0, 125, 250, 500 mg/kg/day	250	125	125*	US EPA, 1989e
221	Fluridone	59756-60-4	rat	730	chr	fod	mult	0, 200, 650, 2000 ppm [a]	25	8	8	Elanco Products, 1980a
222	Flurprimidol	56425-91-3	rat	NG	repro	fod	mult	0, 25, 100, 1000 ppm [b]	7	2	2	Eli Lilly & Co., 1986
223	Flutolanil	66332-96-5	rbt	NG	terat	NG	rep	40, 200 mg/kg/day	200	40	40	Nor-Am Chemical Co., 1987
224	Fluvalinate	69409-94-5	rat	730	chr	gav	mult	0, 0.25, 0.5, 1, 2.5 mg/kg/day	2.5	1	1	Zoecon, 1984

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225	Folpet	133-07-3	rbt	NG	terat	NG	rep	10, 40 mg/kg/day	40	10	10	Chevron, 1965
226	Fonofos	944-22-9	rat	730	chr	fod	bld	0, 5, 1.58 mg/kg/day	1.58	0.5	0.5	Stauffer Chemical Co., 1968
227	Fosetyl-al	39148-24-8	rat	NG	repro	NG	rep	300, 600 mg/kg/day	600	300	300	Rhone-Poulenc, 1981b
228	Glufosinate-ammonium	77182-82-2	rat	91	sub	fod	owt	0, 8, 64, 500, 4000 ppm [b]	3.2	0.4	0.4*	Hoescht, 1982
229	Glyphosate	1071-83-6	rat	NG	repro	fod	rep	0, 3, 10, 30 mg/kg/day	30	10	10	Monsanto Co., 1981
230	Haloxyfop-methyl	69806-40-2	rats	NG	repro	fod	owt	0, 0.005, 0.05, 1 mg/kg/day	0.05	0.005	0.005	Dow Chemical, 1985
231	Harmony	79277-27-3	rat	730	chr	fod	mult	0, 25, 500, 2500 ppm [b]	25	1	1	du Pont, 1986b
232	Heptachlor	76-44-8	rat	NG	repro	fod	rep	0.25, 0.35 mg/kg/day	0.35	0.25	0.25	Velsicol Chemical, 1955
233	Heptachlor epoxide	1024-57-3	rat	NG	repro	NG	rep	0.25, 0.5 mg/kg/day	0.5	0.25	0.25	Velsicol Chemical, 1959
234	Hexabromobenzene	87-82-1	rat	84	sub	fod	bld	0, 10, 20, 40, 80, 160 ppm in diet [b]	2	1	1*	Mendoza *et al.*, 1977
235	Hexachlorobenzene	118-74-1	rat	NG	repro	fod	liv	0, 0.32, 1.6, 8.0, 40 ppm [b]	0.3	0.08	0.08	Arnold *et al.*, 1985
236	Hexachlorobutadiene	87-68-3	rat	91	sub	gav	kid	0, 0.4, 1, 2.5, 6.3, 15.6 mg/kg/day	2.5	1	1*	Harleman and Scinen, 1979
237	Hexachlorocyclohexane, γ-	58-89-9	rat	730	chr	fod	mult	5, 10, 50, 100, 400, 800 or 1600 ppm [d]	5	2.5	2.5	Fitzhugh, 1950
238	Hexachlorocyclopentadiene	77-47-4	rat	91	sub	gav	git	0, 10, 19, 38, 75, 150 mg/kg/day	19	10	10*	Abdo *et al.*, 1984
239	Hexachloroethane	67-72-1	rat	112	sub	fod	kid	0, 1, 15, 62 mg/kg/day	15	1	1*	Gorzinski *et al.*, 1985
240	Hexachlorophene	70-30-4	rat	NG	repro	NG	rep	1, 3 mg/kg/day	3	1	1	Kalo Laboratories, 1979
241	Hexahydro-1,3,5-trinitro-1,3,5-triazine	121-82-4	rat	720	chr	fod	mult	0, 0.3, 1.5, 8, 40 mg/kg/day	1.5	0.3	0.3	US DOD, 1983
242	Hexamethylenetetramine	100-97-0	mus	420	chr	orl	bdw	0, 0.5, 1, 5% [c]	2359	1180	1180	Della Porta *et al.*, 1968
243	Hexazinone	51235-04-2	rat	730	chr	fod	bdw	0, 200, 1000, 2500 ppm [b]	50	10	10	du Pont, 1977
244	Hydralazine	86-54-4	rat	12	terat	gav	nofx	0, 15, 30 mg/kg/day	none	none	30	Pryde *et al.*, 1993
245	Hydrazobenzene	122-66-7	mus	546	chr	fod	mult	0, 0.008%, 0.04% [c]	69	none	14	NCI, 1978n
246	Hydrochlorothiazide	58-93-5	mus	90	sub	fod	kid	0, 3125, 6250, 12,500, 25,000, 50,000 ppm [c]	1219	none	609*	NTP, 1989h
247	Hydroxypropyl methanethiol-sulfonate, 2-		rbt	13	terat	gav	mult	0, 0.75, 4, 7.5 mg/kg/day	4	none	0.75	Adam *et al.*, 1990
248	Hydroxyquinoline, 8-	148-24-3	rat	721	chr	fod	bdw	0, 1500, 3000 ppm [a]	143	none	73	NTP, 1985f
249	Imazalil	35554-44-0	rat	730	chr	fod	owt	10, 40 mg/kg/day	40	10	10	Janssen R & D, Inc., 1967
250	Imazaquin	81335-37-7	mus	540	chr	NG	bdw	150, 600 mg/kg/day	600	150	150	American Cyanamid, 1985
251	Iodinated glycerol	5634-39-9	mus	91	sub	gav	kid	0, 31, 62, 125, 250, 500 mg/kg/day	250	none	125*	NTP, 1990d
252	Ipazilide	115436-73-2	rbt	13	terat	gav	nofx	0, 12.5, 25, 50 mg/kg/day	none	50	50	Brown *et al.*, 1991
253	Iprodione	36734-19-7	rat	NG	repro	NG	owt	25, 100 mg/kg/day	100	25	25	Rhone-Poulenc, 1976
254	Ipronidazole	14885-29-1	rat	80	repro	fod	bdw	0, 20, 200, 2000 ppm [a]	100	10	10*	Dale, 1976
255	Isopropalin	33820-53-0	rat	90	sub	fod	mult	0, 250, 750, 2250 ppm [d]	70.5	23.5	23.5*	Elanco Products, 1969
256	Isoxaben	82558-50-7	rat	730	chr	fod	mult	0, 125, 1250, 12,500 ppm [a]	50.7	5	5	Elanco Products, 1985
257	Jervine	469-59-0	mus	1	terat	gav	nofx	70, 150, 300 mg/kg/day	none	none	300	Omnell *et al.*, 1990
258	Lactofen	77501-63-4	rat	NG	repro	NG	mult	2.5, 25 mg/kg/day	25	2.5	2.5	PPG Industries, 1983
259	Lansoprazole	103577-45-3	rbt	NG	terat	gav	mult	3, 10, 30 mg/kg/day	30	none	10	Schardein *et al.*, 1990
260	Levamisole	5036-02-2	rat	91	sub	fod	mult	0, 100, 400, 1600 ppm [a]	40	none	10*	Marsboom *et al.*, 1969
261	Linamarin	554-35-8	ham	1	terat	NG	mult	0, 70, 100, 120, 140 mg/kg/day	120	none	100	Frakes *et al.*, 1985
262	Linuron	330-55-2	rat	NG	repro	NG	mult	1.25, 6.25 mg/kg/day	6.25	1.25	1.25	du Pont, 1984
263	Londax	83055-99-6	rat	730	chr	fod	mult	30, 309 mg/kg/day	309	30	30	du Pont, 1986c
264	Malaoxon	1634-78-2	rat	91	sub	fod	ltl	0, 125, 250, 500, 1000, 2000, 4000, 8000 ppm [c]	400	none	200*	NCI, 1979j
265	Malathion	121-75-5	rat	730	chr	fod	mult	5, 50 mg/kg/day	50	5	5	American Cyanamid, 1980
266	Maleic anhydride	108-31-6	rat	90	sub	fod	kid	0, 20, 40, 100, 250, 600 mg/kg/day	100	40	40*	US EPA, 1975

267	Maleic hydrazine	123-33-1	rbt	NG	terat	NG	ter	100, 300 mg/kg/day	300	100	100	Uniroyal Chemical, 1983
268	Manidipine hydrochloride	126229-12-7	rbt	13	terat	gav	mult	0, 10, 30, 100 mg/kg/day	100	30	30	Morseth and Ihara, 1989
269	Melamine	108-78-1	rat	91	sub	fod	kid	0, 750, 1500, 3000, 6000, 12,000 ppm [c]	339	none	170*	NTP, 1983d
270	Mepiquat chloride	24307-26-4	rat	730	chr	fod	bdw	50, 150 mg/kg/day	150	50	50	BASF, 1979
271	Mercaptobenzothiazole, 2-	149-30-4	mus	91	sub	gav	nos	0, 94, 188, 375, 750, 1500 mg/kg/day	375	none	188*	NTP, 1988g
272	Merphos	150-50-5	rat	112	sub	fod	bld	0.1, 0.25 mg/kg/day	0.25	0.1	0.1*	Virginia Carolina Chemical Corp., 1958
273	Merphos oxide	78-48-8	rat	730	chr	fod	neu	0.25, 1.25 mg/kg/day	1.25	0.25	0.25	Mobay Chemical, 1969
274	Meso-2,3-dimercaptosuccinic acid	304-55-2	mus	35	repro	gav	mult	0, 200, 400, 800 mg/kg/day	800	400	400	Domingo *et al.*, 1990
275	Metalaxyl	57837-19-1	rat	730	chr	fod	liv	0, 250, 1250 ppm [a]	62.5	12.5	12.5	Ciba, 1980a
276	Methamidophos	10265-92-6	rat	NG	terat	fod	mult	1, 3 mg/kg/day	3	1	1	Mobay Chemical, 1984b
277	Methidathion	950-37-8	rat	730	chr	fod	mult	0.2, 2 mg/kg/day	2	0.2	0.2	Ciba, 1986
278	Methomyl	16752-77-5	rat	730	chr	fod	mult	5, 10 mg/kg/day	10	5	5	du Pont, 1981a
279	Methoxychlor	72-43-5	rbt	13	terat	fod	mult	0, 5, 36, 251 mg/kg/day	36	5	5	Kincaid Enterprises, Inc., 1986
280	Methoxypsoralen, 8-	298-81-7	rat	90	sub	gav	owt	0, 25, 50, 100, 200, 400 mg/kg/day	50	none	25*	NTP, 1989i
281	Methyl carbamate	598-55-0	rat	90	sub	gav	liv	0, 50, 100, 200, 400, 800 mg/kg/day	200	none	100*	Quest *et al.*, 1987
282	Methyl ethyl ketoxime	96-29-7	rbt	13	terat	gav	mult	0, 8, 14, 24, 40 mg/kg/day	24	none	14	Mercieca *et al.*, 1991
283	Methyl parathion	298-00-0	rat	730	chr	fod	owt	0, 0.5, 5, 50 ppm in diet [b]	0.25	0.025	0.025	Monsanto Co., 1984b
284	Methyl-4-chlorophenoxyacetic acid, 2-	94-74-6	rat	364	repro	NG	rep	7.5, 22.5 mg/kg/day	22.5	7.5	7.5*	Industry Task Force on MCPA, 1986
285	Methyl-*N*-methylanthranilate	85-91-6	rat	90	sub	fod	owt	0, 300, 1200, 3600 ppm in diet [a]	60	none	15*	Gaunt *et al.*, 1970b
286	Methyldopa sesquihydrate, α-	41372-80-1	rat	91	sub	fod	mult	0, 3100, 6300, 12,500, 25,000, 50,000 ppm [c]	712	none	350*	NTP, 1989j
287	Methylolacrylamide, *N*-	924-42-5	rat	90	sub	gav	neu	0, 12.5, 25, 50, 100, 200 mg/kg/day	25	none	12.5*	NTP, 1989k
288	Metolachlor	51218-45-2	rat	157	repro	fod	mult	0, 30, 300, 1000 ppm [a]	50	15	15*	Ciba, 1981b
289	Metribuzin	21087-64-9	rat	730	chr	fod	mult	5, 15 mg/kg/day	15	5	5	Mobay Chemical, 1974
290	Mexacarbate	315-18-4	mus	546	chr	fod	ova	0, 68, 135 ppm [c]	23	none	12	NCI, 1978o
291	Miporamicin	73684-69-2	rat	NG	terat	NG	con	40, 200, 1000 mg/kg/day	200	40	40	Furuhashi *et al.*, 1989
292	Mirex	2385-85-5	mus	540	chr	fod	liv	0, 1, 5, 15, 30 ppm [b]	0.86	0.17	0.17	Fulfs *et al.*, 1977
293	Molinate	2212-67-1	rat	NG	repro	gav	rep	0, 0.2, 4, 12, 30, 60 mg/kg/day	4	0.2	0.2	Stauffer Chemical Co., 1981
294	Monodiethanolamine salt of riboflavin-5′-phosphate		rat	203	sub	fod	bld	1, 4, 10, 40 mg daily [a]	50	none	20*	Randall, 1950
295	Monuron	150-68-5	rat	91	sub	fod	bdw	0, 750, 1500, 3000, 6000, 12,000 ppm [c]	150	none	75*	NTP, 1988h
296	Naled	300-76-5	rat	730	chr	gav	nos	0, 0.2, 2, 10 mg/kg/day	2	0.2	0.2	Chevron, 1984a
297	Nalidixic acid	389-08-2	rat	90	sub	fod	owt	0, 1000, 2000, 4000, 8000, 16,000 ppm [c]	200	none	100*	NTP, 1989l
298	Naphthoxy acetic acid, 2-	120-23-0	rat	NG	terat	NG	bdw	0, 62.5, 125, 250 mg/kg/day	250	125	125	Henwood and Osimitz, date unknown
299	Napropamide	15299-99-7	rat	NG	repro	fod	bdw	0, 10, 30, 100 mg/kg/day	100	30	30	Stauffer Chemical Co., 1978
300	Natamycin	7681-93-8	rat	730	chr	fod	bdw	0, 125, 250, 500, 1000 ppm [c]	72	none	36	Levinskas *et al.*, 1966
301	Nitro-*o*-toluidine, 5-	99-55-8	rat	546	chr	fod	bdw	0, 0.005, 0.01% ppm [c]	8	none	4	NCI, 1978p
302	Nitro-*p*-phenylenediamine, 2-	5307-14-2	rat	546	chr	fod	bdw	0, 550, 1100 ppm [c]	87	none	43	NCI, 1978q
303	Nitroaniline, *p*-	100-01-6	mus	90	sub	gav	liv	0, 1, 3, 10, 30, 100 mg/kg/day	10	none	3*	NTP, 1993e
304	Nitroanthranilic acid, 4-	619-17-0	rat	546	chr	fod	mult	0, 0.46, 1.50% [c]	1185	none	363	NCI, 1978r
305	Nitrofurantoin	67-20-9	rat	91	sub	fod	tes	0, 600, 1300, 2500, 5000, 10,000 ppm [c]	250	none	130*	NTP, 1989q
306	Nitrofurazone	59-87-0	mus	721	chr	fod	mult	0, 150, 310 ppm [a]	33	none	16	NTP, 1988i
307	Nitroguanidine	556-88-7	rat	90	sub	fod	bdw	0, 100, 316, 1000 mg/kg/day	1000	316	316*	Morgan *et al.*, 1988
308	Nitronaphthalene, 1-	86-57-7	rat	546	chr	fod	bdw	0, 0.06, 0.18% [c]	165	none	55	NCI, 1978s

[*Contd*]

309	Nitrosodiphenylamine, *N*-	86-30-6	rat	77	sub	fod	bdw	0, 1000, 2000, 3000, 4000, 6000, 8000, 10,000 ppm [c]	300	400	400*	NCI, 1979k
310	Norflurazon	27314-13-2	rbt	NG	terat	NG	rep	10, 30 mg/kg/day	30	10	10	Sandoz, Inc., 1983
311	Ochratoxin A	303-47-9	mus	1	terat	gav	ter	0, 1, 2, 4 mg/kg/day	2	none	1	Arora and Frolen, 1981
312	Octabromodiphenyl ether	32536-52-0	rat	90	sub	gav	liv	0, 0.62, 1.25, 2.51, 5.01, 10.02, 20.04 mg/kg/day	5	2.51	2.51*	Carlson, 1980a
313	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	2691-41-0	rat	91	sub	fod	liv	0, 50, 150, 450, 1350, 4000 mg/kg/day	150	50	50*	US DOD, 1985
314	Olaquindox	23696-28-8	rat	91	sub	gav	owt	0, 1, 5, 20 mg/kg/day	5	1	1*	Hoffmann, 1972; Urwin and Spicer, 1971
315	Orange RN	1934-20-9	rat	730	chr	fod	owt	0, 0.05, 0.25% in diet [c]	180	none	36	Dacre, 1969
316	Oryzalin	19044-88-3	rat	NG	repro	NG	rep	12.5, 37.5 mg/kg/day	37.5	12.5	12.5	Elanco Products, 1980b
317	Oxadiazon	19666-30-9	rat	730	chr	fod	mult	0, 10, 100, 1000, 3000 ppm [b]	5	0.5	0.5	Rhone-Poulenc, 1981c
318	Oxamyl	23135-22-0	rat	730	chr	fod	bdw	0, 50, 100, 150 ppm [b]	5	2.5	2.5	du Pont, 1972
319	Oxfendazole	53716-50-0	rat	90	sub	fod	bld	0, 50, 100, 200, 600, 2000 ppm [a]	7.7	none	3.8*	Killeen and Rapp, 1974
320	Oxyfluorfen	42874-03-3	mus	600	chr	fod	liv	0, 2, 20, 200 ppm [b]	3	0.3	0.3	Rohm and Haas Co., 1977
321	Oxytetracycline	79-57-2	mus	10	terat	gav	owt	0, 1325, 1670, 2100 mg/kg/day	2100	1670	1670	Morrissey *et al.*, 1986
322	Oxytetracycline hydrochloride	2058-46-0	mus	91	sub	fod	bdw	0, 3100, 6300, 12,500, 25,000, 50,000 ppm [d]	7950	none	3450*	NTP, 1987d
323	Oxythioquinox	2439-01-2	rat	112	sub	fod	bdw	0, 10, 25, 50 ppm in diet [c]	4.4	none	2.2*	Doull *et al.*, 1963
324	Paclobutrazol	76738-62-0	rat	90	sub	fod	mult	0, 50, 250, 1250 ppm [b]	62.5	12.5	12.5*	ICI Americas, Inc., 1983
325	Paraquat	1910-42-5	rat	NG	terat	NG	mult	1, 5 mg/kg/day	5	1	1	Chevron, 1977
326	Parathion	56-38-2	rat	560	chr	fod	mult	0, 23, 45 ppm [c]	3.5	none	1.8	NCI, 1979l
327	Patulin	149-29-1	rat	730	repro	gav	bdw	0, 0.1, 0.5, 1.5 mg/kg bw x 3/week	0.2	none	0.04	Becci *et al.*, 1981
328	Pendimethalin	40487-42-1	rat	90	sub	fod	mult	25, 250 mg/kg/day	250	25	25*	American Cyanamid, 1974
329	Penicillin VK	132-98-9	rat	91	sub	gav	git	0, 180, 370, 750, 1500, 3000 mg/kg/day	750	none	370*	NTP, 1988j
330	Pentabromodiphenyl ether	32534-81-9	rat	90	sub	gav	liv	0, 0.44, 0.88, 1.77, 3.53, 7.06, 14.12 mg/kg/day	3.3	1.77	1.77*	Carlson, 1980b
331	Pentachloroethane	76-01-7	rat	91	sub	gav	bdw	0, 5, 10, 50, 125, 250 mg/kg/day	250	none	125*	NTP, 1983e
332	Pentachloronitrobenzene	82-68-8	mus	91	sub	fod	owt	0, 1250, 2500, 5000, 10,000, 20,000 ppm [c]	450	none	225*	NTP, 1987e
333	Pentachlorophenol	87-86-5	rat	730	chr	fod	mult	0, 3, 10, 30 mg/kg/day	10	3	3	Schwetz *et al.*, 1978
334	Pentaerythritol tetranitrate	78-11-5	rat	98	sub	fod	owt	0, 3100, 6200, 12,500, 25,000, 50,000 ppm [c]	1411	none	700*	NTP, 1989m
335	Permethrin	52645-53-1	mus	730	chr	fod	owt	3, 375 mg/kg/day	375	3	3	FMC Corp., 1979
336	Phenformin	114-86-3	rat	546	chr	fod	bdw	0, 400, 800 ppm [c]	73	none	37	NCI, 1977a
337	Phenyl-2-naphthylamine, *n*-	135-88-6	rat	91	sub	fod	owt	0, 2500, 5000, 10,000, 20,000, 40,000 ppm [c]	565	none	282*	NTP, 1988k
338	Phenyl-3-methyl-5-pyrazolone, 1-	89-25-8	mus	714	chr	fod	bdw	0, 7500, 15,000 ppm [c]	2595	none	1297	NCI, 1978t
339	Phenylbutazone	50-33-9	rat	90	sub	gav	kid	0, 25, 50, 100, 200, 300 mg/kg/day	50	none	25*	NTP, 1990e
340	Phenylenediamine, *m*-	108-45-2	rat	90	sub	orl	mult	0, 2, 6, 18 mg/kg/day	18	6	6*	Hofer *et al.*, 1982
341	Phenylephrine hydrochloride	61-76-7	rat	84	sub	fod	bdw	0, 1250, 2500, 5000, 10,000, 20,000 ppm [c]	282	none	141*	NTP, 1987f
342	Phosmet	732-11-6	rat	730	chr	fod	mult	0, 20, 40, 400 ppm [b]	20	2	2	Stauffer Chemical Co., 1967
343	Phosphamidon	13171-21-6	rat	560	chr	fod	mult	0, 80, 160 ppm [c]	12.3	none	6.2	NCI, 1979m
344	Photodieldrin	13366-73-9	rat	560	chr	fod	neu	0, 5, 10 ppm [c]	0.7	none	0.35	NCI, 1977b
345	Phthalamide	88-96-0	mus	742	chr	fod	mult	0, 6200, 12,500, 25,000 ppm [c]	2163	none	1073	NCI, 1979n
346	Phthalic anhydride	85-44-9	rat	735	chr	fod	bdw	0, 7500, 15,000 ppm [c]	1185	none	592	NCI, 1979o
347	Picloram	1918-02-1	rat	730	chr	fod	liv	20, 60 mg/kg/day	60	20	20	Dow Chemical, 1986
348	Pilsicainide hydrochloride	88069-67-4	rbt	13	terat	gav	nofx	0, 5, 10, 20 mg/kg/day	none	20	20	Yamamori *et al.*, 1991
349	Pirimiphos-methyl	29232-93-7	rat	730	chr	fod	bld	0.5, 2.5 mg/kg/day	2.5	0.5	0.5	ICI Americas, Inc., 1973
350	Ponceau 4R	2611-82-7	mus	574	chr	fod	kid	0, 0.01, 0.05, 0.25, 1.25% [c]	432	86	86	Mason *et al.*, 1974

351	Pravadoline	92623-83-1	rat	71	repro	NG	rep	0, 32, 100, 300 mg/kg/day	300	none	100*	Dennis *et al.*, 1990
352	Probenecid	57-66-9	mus	90	sub	gav	mult	0, 100, 200, 400, 800, 1600 mg/kg/day	200	none	100*	NTP, 1991b
353	Prochloraz	67747-09-5	rat	NG	terat	NG	bdw	5, 22 mg/kg/day	22	5	5	Nor-Am Chemical Co., 1980
354	Proflavine monohydrochloride hemihydrate	952-23-8	rat	763	chr	fod	liv	0, 300, 600 ppm [c]	47	none	24	NCI, 1977c
355	Promethazine hydrochloride	58-33-3	mus	90	sub	gav	owt	0, 5, 15, 45, 135, 405 mg/kg/day	15	none	5*	NTP, 1993f
356	Prometon	1610-18-0	rbt	NG	terat	NG	bdw	3.5, 24.5 mg/kg/day	24.5	3.5	3.5	Ciba, 1982a
357	Prometryn	7287-19-6	rbt	NG	terat	fod	mult	0, 15, 150, 1500 ppm [b]	72	12	12	Ciba, 1985
358	Pronamide	23950-58-5	rat	90	sub	fod	owt	2.5, 7.5 mg/kg/day	7.5	2.5	2.5*	Rohm and Haas Co., 1970
359	Propachlor	1918-16-7	rat	90	sub	fod	mult	0, 1.3, 13.3, 133.3 mg/kg/day	133.3	13.3	13.3*	Monsanto Co., 1964
360	Propanil	709-98-8	rat	730	chr	fod	owt	0, 100, 400, 1600 ppm [b]	20	5	5	Rohm and Haas Co., 1964
361	Propargite	2312-35-8	rbt	13	terat	gav	bdw	0, 2, 6, 10, 18 mg/kg/day	6	2	2	Uniroyal Chemical, 1966
362	Propazine	139-40-2	rat	NG	repro	NG	rep	5, 50 mg/kg/day	50	5	5	Ciba, 1979
363	Propham	122-42-9	rat	90	sub	fod	owt	0, 250, 1000, 2000 ppm [b]	100	50	50*	PPG Industries, 1979
364	Propiconazole	60207-90-1	rat	730	chr	NG	git	5, 25 mg/kg/day	25	5	5	Ciba, 1982b
365	Propiverine hydrochloride (P-4)	54556-98-8	rat	91	sub	NG	nos	0, 2, 10, 50 mg/kg/day	10	2	2*	Saito *et al.*, 1989
366	Propylene dichloride	78-87-5	rat	10	terat	gav	mult	0, 10, 30, 125 mg/kg/day	125	none	30	Hanley *et al.*, 1990
367	Pursuit	81335-77-5	rbt	NG	terat	fod	nos	300, 1000 mg/kg/day	1000	300	300	American Cyanamid, 1986b
368	Pydrin	51630-58-1	rat	91	sub	fod	neu	0, 50, 150, 300, 500 ppm [b]	7.5	2.5	2.5*	Shell Chemical Co., 1984
369	Pyrazinamide	98-96-4	rat	546	chr	fod	bdw	0, 5000, 10,000 ppm [c]	789	none	385	NCI, 1977d
370	Pyrene	129-00-0	mus	91	sub	gav	owt	0, 75, 125, 250 mg/kg/day	125	75	75*	US EPA, 1989f
371	Quercetin	117-39-5	rat	730	chr	fod	bdw	0, 1000, 10,000, 40,000 ppm [d]	2034	none	400	NTP, 1992j
372	Quinalphos	13593-03-8	mus	540	chr	fod	bld	0.03, 0.15 mg/kg/day	0.15	0.03	0.03	Sandoz Inc., 1980
373	Quinine hydrochloride	130-89-2	rat	91	sub	fod	mult	0, 1, 10, 40, 100, 200 mg/kg/day	100	40	40*	Colley *et al.*, 1989
374	Red 2G	3734-67-6	rat	730	chr	fod	spl	0.004, 0.016, 0.064, 0.16% [c]	46	none	12	Unilever, 1974
375	Reserpine	50-55-5	mus	91	sub	fod	bdw	0, 0.4, 0.8, 1.5, 3.0, 6.0 ppm [c]	1.2	none	0.58*	NTP, 1982j
376	Resmethrin	10453-86-8	rat	NG	terat	NG	ter	40, 80 mg/kg/day	80	40	40	Penwick Corp., 1979
377	Rhodamine 6G	989-38-8	rat	720	chr	fod	end	0, 120, 200 ppm [a]	12	none	5	NTP, 1989n
378	Ronidazole	7681-76-7	rbt	9	terat	gav	bdw	0, 3, 10, 30 mg/kg/day	30	none	10	Zwickey *et al.*, 1975
379	Rotenone	83-79-4	rat	NG	repro	fod	rep	0, 8, 37.5, 75 ppm [b]	1.88	0.38	0.38	US Fish and Wildlife Service, 1983
380	Saccharin	81-07-2	rat	730	chr	fod	mult	0, 0.005, 0.05, 0.5, 5% [c]	3602	none	360	Lessel, 1967
381	Savey	78587-05-0	rat	730	chr	fod	owt	23, 160 mg/kg/day	160	23	23	du Pont, 1985d
382	Sethoxydim	74051-80-2	rat	NG	repro	NG	rep	18, 162 mg/kg/day	162	18	18	BASF, 1980
383	Simazine	122-34-9	rat	730	chr	fod	mult	0, 10, 100, 1000 ppm [a]	5	0.52	0.52	Ciba, 1988a
384	Sodium cyclamate	139-05-9	rat	720	chr	fod	bdw	0, 0.01, 0.1, 0.5, 1, 5% [c]	3602	none	720	Fitzhugh *et al.*, 1951
385	Sodium fluoroacetate	62-74-8	rat	91	sub	gav	mult	0, 0,05, 0.2, 0.5 mg/kg/day	0.2	0.05	0.05*	US EPA, 1988b
386	Sodium naphthionate		rat	20	terat	gav	rep	0, 15, 30, 100, 200 mg/kg/day	100	none	30	Collins *et al.*, 1973
387	Sorbitan monolaurate	1338-39-2	rat	730	chr	fod	bdw	0, 5, 10% in diet [c]	6883	none	3442	Anonymous, date unknown{b}
388	Sorbitan monostearate	1338-41-6	rat	730	chr	fod	mult	2, 5, 10, 25% in diet [c]	7203	none	3602	Fitzhugh *et al.*, 1959
389	Succinic anhydride	108-30-5	mus	90	sub	gav	mult	0, 37, 75, 150, 300, 600 mg/kg/day	150	none	75*	NTP, 1990f
390	Sucrose acetate isobutyrate	126-13-6	rat	1	repro	gav	rep	0, 20, 200, 2000 mg/kg/day	2000	none	200	Krasavage, 1973
391	Sulfadimidine	57-68-1	rat	730	chr	fod	end	0, 10, 40, 600, 1200, 2400 ppm in diet [c]	33	none	2.2	Fullerton *et al.*, 1987

{*Contd*}

392	Sulfisoxazole	127-69-5	rat	91	sub	gav	kid	0, 100, 215, 464, 1000, 2160 mg/kg/day	1000	none	464*	NCI, 1979p
393	Sulfolene, 3-	77-79-2	mus	546	chr	gav	ltl	0, 311, 622 mg/kg/day	622	none	311	NCI, 1978u
394	Sunset Yellow FCF	2783-94-0	rat	84	sub	fod	bdw	0, 6000, 12,500, 25,000, 50,000, 100,000 ppm [c]	1412	none	678*	NTP, 1981
395	Suplatast tosilate	94055-76-2	rat	NG	repro	NG	mult	0, 200, 600, 1800 mg/kg/day	1800	600	600	Aso *et al.*, 1992
396	Systhane	88671-89-0	rat	NG	repro	NG	mult	2.32, 4.28 mg/kg/day	4.28	2.32	2.32	Rohm and Haas Co., 1985b
397	Tebuthiuron	34014-18-1	rat	NG	repro	fod	bdw	0, 100, 200, 400 ppm [a]	14	7	7	Elanco Products, 1981
398	Terbacil	5902-51-2	mus	730	chr	fod	mult	7.5, 187.5 mg/kg/day	187.5	7.5	7.5	du Pont, 1981b
399	Terbutryn	886-50-0	rat	730	chr	fod	bld	0, 2, 300, 3000 ppm [b]	15	0.1	0.1	Ciba, 1980b
400	Tert-butyl-2-chlorophenol, 4-		rat	730	chr	fod	mult	0, 100, 300, 1000, 3000 ppm in diet [c]	216	none	72	McCollister, 1964
401	Tetrachlorobenzene, 1,2,4,5-	95-94-3	rat	91	sub	fod	kid	0, 0.5, 5.0, 50, 500 ppm [a]	3.4	0.34	0.34*	Chu *et al.*, 1984
402	Tetrachloroethane, 1,1,1,2-	630-20-6	rat	91	sub	gav	neu	0, 5, 10, 50, 100, 500 mg/kg/day	500	none	100*	NTP, 1983f
403	Tetrachloroethane, 1,1,2,2-	79-34-5	rat	546	chr	gav	ltl	0, 62, 108 mg/kg/day	108	none	62	NCI, 1978v
404	Tetrachloroethylene	127-18-4	rat	NG	sub	orl	bdw	14, 400, 1400 mg/kg/day	1400	14	14*	Hayes *et al.*, 1986
405	Tetrachlorophenol, 2,3,4,6-	58-90-2	rat	90	sub	gav	mult	0, 25, 100, 200 mg/kg/day	100	25	25*	US EPA, 1986i
406	Tetrachloropyridine, 2,3,5,6-	2402-79-1	rat	NG	repro	gav	kid	0, 5, 25, 150 mg/kg/day	150	25	25	Zielke *et al.*, 1993
407	Tetrachlorvinphos	961-11-5	rat	730	chr	fod	mult	6, 100 mg/kg/day	100	6	6	Shell Chemical Co., 1966
408	Tetracycline hydrochloride	64-75-5	rat	91	sub	fod	bld	0, 3100, 6300, 12,500, 25,000, 50,000 ppm [c]	630	none	310*	NTP, 1989o
409	Tetraethyldithiopyrophosphate	3689-24-5	rat	90	sub	fod	bld	0, 5, 10, 20, 50 ppm [b]	1	0.5	0.5*	Kimmerle *et al.*, 1974
410	Tetraethylthiourea disulfide	97-77-8	mus	756	chr	fod	mult	0, 100, 500 ppm [c]	86	none	17	NCI, 1979q
411	Tetrahydrocannabinol, δ-9-	1972-08-3	rat	21	terat	fod	nofx	0, 15, 50 mg/kg/day	none	none	50	Hutchings *et al.*, 1989
412	Tetrakis(hydroxymethyl)phosphonium chloride (THPC)	124-64-1	rat	91	sub	gav	liv	0, 3.75, 7.5, 15, 30, 60 mg/kg/day	7.5	none	3.75*	NTP, 1987g
413	Tetrakis(hydroxymethyl)phosphonium sulphate (THPS)	55566-30-8	rat	91	sub	gav	bdw	0, 5, 10, 20, 40, 60 mg/kg/day	10	none	5*	NTP, 1987g
414	Thiabendazole	148-79-8	rat	12	terat	gav	bdw	10, 40, 80 mg/kg/day	40	10	10	Lankas and Wise, 1993
415	Thiobencarb	28249-77-6	rat	730	chr	fod	mult	0, 20, 100, 500 ppm [b]	5	1	1	Chevron, 1984b
416	Thiophanate-methyl	23564-05-8	rat	730	chr	fod	mult	10, 40, 160, 640 ppm [b]	32	8	8	Pennwalt Corporation, 1972
417	Thiram	137-26-8	rat	730	chr	fod	neu	0, 100, 300, 1000, 2500 ppm [b]	15	5	5	du Pont, 1954
418	Tocopheryl acetate, *dl*-α-	52225-20-4	rat	730	chr	fod	bld	0, 500, 1000, 2000 mg/kg/day	2000	none	1000	Wheldon *et al.*, 1983
419	Toluenediamine hydrochloride, 2,6-	15481-70-6	mus	91	sub	fod	bdw	0, 100, 300, 1000, 3000, 10,000 ppm [c]	52	none	16*	NTP, 1980b
420	Toluenediamine sulfate, 2,5-	6369-59-1	rat	546	chr	fod	bdw	0, 0.06, 0.2% [c]	184	none	55	NCI, 1978w
421	Tralomethrin	66841-25-6	rat	730	chr	gav	bdw	0, 0.75, 3, 12 mg/kg/day	3	0.75	0.75	Roussel UCLAF, 1984
422	Trenbolone acetate	10161-34-8	rat	NG	repro	fod	rep	0, 0.1, 0.3, 0.5, 3, 18 ppm in diet [c]	0.266	none	0.044	James *et al.*, 1986
423	Trenbolone hydroxide, 17-α-		rat	161	sub	gav	bld	0, 0.01, 0.04, 0.36, 3.6 mg/kg/day	0.36	0.04	0.04*	Dean, 1988; Hooks *et al.*, 1988
424	Triallate	2303-17-5	mus	730	chr	fod	spl	3, 9 mg/kg/day	9	3	3	Monsanto Co., 1983
425	Triamterene	396-01-0	rat	90	sub	fod	mult	0, 150, 300, 600, 1200, 2400 ppm [a]	70	none	40*	NTP, 1993g
426	Tribromomethane	75-25-2	mus	91	sub	gav	liv	0, 25, 50, 100, 200, 400 mg/kg/day	200	none	100*	NTP, 1989p
427	Trichloroacetonitrile	545-06-2	rat	13	terat	gav	ter	0, 1, 7.5, 15, 35, 55 mg/kg/day	7.5	1	1	Smith *et al.*, 1988
428	Trichlorobenzene, 1,2,4-	120-82-1	rat	NG	repro	orl	owt	0, 25, 100, 400 ppm [b,d]	53.6	14.8	14.8	Robinson *et al.*, 1981
429	Trichloroethane, 1,1 2-	79-00-5	mus	90	sub	orl	mult	0, 20, 200 or 2000 mg/litre [a]	46	none	4*	White *et al.*, 1985; Sanders *et al.*, 1985
430	Trichloroethane, 1,1,1-	71-55-6	mus	NG	repro	orl	nofx	0, 100, 300, 1000 mg/kg/day	none	none	1000	Lane *et al.*, 1982
431	Trichloroethylene	79-01-6(a)	mus	91	sub	gav	mult	0, 375, 750, 1500, 3000, 6000 mg/kg/day	750	none	375*	NTP, 1990g
432	Trichloroethylene, 1,1,2-	79-01-6(b)	mus	120	sub	orl	owt	0, 0.1, 1.0, 2.5, 5.0 mg/ml [a]	216.7	none	18.4*	Tucker *et al.*, 1982
433	Trichlorogalactosucrose	56038-13-2	rat	NG	repro	fod	owt	0, 3000, 10,000, 30,000 ppm [c]	980	none	294	Tesh and Willoughby, 1986

434	Trichlorophenol, 2,4,5-	95-95-4	rat	98	sub	fod	mult	100-10000 ppm [b]	300	100	100*	McCollister *et al.*, 1961
435	Trichlorophenoxyacetic acid, 2,4,5-	93-76-5	rat	730	chr	fod	kid	0, 3, 10, 30 mg/kg/day	10	3	3	Kociba *et al.*, 1979
436	Tridiphane	58138-08-2	rat	NG	repro	fod	rep	0.33, 1.67 mg/kg/day	1.67	0.33	0.33	Dow Chemical, 1984
437	Triethylene tetramine dihydrochloride	38260-01-4	mus	NG	terat	orl	liv	0, 3000, 6000, 12,000 ppm [c]	1585	none	793	Tanaka *et al.*, 1991
438	Trifluralin	1582-09-8	rat	730	chr	fod	bdw	10, 40 mg/kg/day	40	10	10	Hoescht, 1986
439	Trimethylaniline, 2,4,5-	137-17-7	rat	707	chr	fod	spl	0, 200, 800 ppm [c]	63	none	16	NCI, 1979r
440	Trinitrotoluene, 2,4,6-	118-96-7	mus	730	chr	fod	mult	0, 1.5, 10, 70 mg/kg/day	70	none	10	US DOD, 1984
441	Tris-(2-chloroethyl) phosphate	115-96-8	rat	112	sub	gav	owt	0, 22, 44, 88, 175, 350 mg/kg/day	44	none	22*	NTP, 1991c
442	Trisulfuron	82097-50-5	mus	730	chr	fod	liv	0, 10, 1000, 5000, 10,000 ppm [a]	129	1	1	Ciba, 1988b
443	Tylosin	1401-69-0	rat	365	sub	fod	nofx	0, 0.1, 0.5, 0.1% [a]	500	500	50*	Broddle *et al.*, 1978
444	Vinclozolin	50471-44-8	rat	721	chr	fod	mult	24.3, 72.9 mg/kg/day	72.9	24.3	24.3	BASF, 1977
445	Vinyl chloride	75-01-4	rat	91	sub	gav	bld	0, 30, 100, 300 mg/kg/day	100	none	30*	Feron *et al.*, 1975
446	Zatosetron maleate	123482-23-5	rat	12	terat	gav	mult	0, 10, 25, 70 mg/kg/day	25	10	10	Byrd *et al.*, 1991
447	Zearalenone	17924-92-4	rat	91	sub	fod	bdw	0, 30, 100, 300, 1000, 3000 ppm	10	none	3*	NTP, 1982k
448	Zeranol	55331-29-8	rat	730	chr	fod	ova	0, 0.25, 2.5, 25 ppm in diet [c]	0.2	none	0.02	Everett *et al.*, 1987

bdw = body weight changes; bld = blood effects; cap = capsule; chr = chronic (over 365 days); con = food consumption; cvs = cardiovascular effects; drm = dermal; end = endocrine; eye = ocular; fod = diet; gav = gavage; git = gastrointestinal; ham = hamster; imt = immunotoxicity; kid = renal effects; liv = hepatic effects; ltl = lethal; msk = musculo-skeletal, mult = multiple effects; mus = mouse; neu = neurological; NG = not given; nofx = no effects; nos = non-specific effects; orl = drinking water; ova = ovarian; owt = organ weight changes; pul = pulmonary effects; rbt = rabbit; rep = reproductive, effects; repro = reproduction study; exposure duration not specified; resp = respiratory tract; spl = spleen; sub = subchronic (60 to 365 days); ter = teratogenic; terat = teratology study; exposure duration not, specified; tes = testicular; [a] = author provided converted dose; [b] = JECFA provided converted doses; [c] = conversions were calculated by using standard values; [d] = doses were calculated from data provided, by the author; none = no toxicity reported at any dose; NOEL = highest dose tested; * = NOEL divided by a factor of 3 (see text for explanation)

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