

## 7.0 REGISTRY OF CYTOTOXICITY (RC) DATA (ZEBET)

### 7.1 The ZEBET Database

ZEBET was established in Germany in 1989 at the Federal Institute for Consumer Health Protection and Veterinary Medicine (BgVV; <http://www.bgvv.de>). The ZEBET database contains evaluated information from the field of biomedicine and related fields on alternative methods that address the 3Rs concept of research that involves animals: refinement of animal use in experimentation, reduction of animal use, and replacement of animals. The database information was obtained from approximately 800 different documents (e.g., books, journals, monographs, etc.). The RC is part of the database and provides *in vitro* IC50 values as well as acute oral toxicity data (LD50) for rats and mice for 347 chemicals. The LD50 values come from the RTECS database at NIOSH. The ZEBET database also includes data for the 50 chemicals from the MEIC database. The German Institute for Medical Documentation and Information (DIMDI) provides access to the ZEBET database (<http://www.dimdi.de>).

#### 7.1.1 Tables

Table 7.1: IC50 values in ascending order (all RC chemicals)

Table 7.2: Rat LD50 oral values in descending order (all RC chemicals)

Table 7.3: Alphabetical order (all RC chemicals)

Table 7.4: Rat LD50 oral values in descending order (MEIC chemicals)

The acute oral toxicity values are provided in mg/kg and mmol/l for rats and mice. Regression calculation values are in the last column of the data sheets. Rat LD50 values were used for the calculations if they were available; if not, then mouse LD50 values were used.

#### 7.1.2 Figures

Regression calculations between cytotoxicity and acute oral toxicity are illustrated in the figures following the data.

Figure 7.1: Regression between RC values (IC50x) and acute oral LD50 values (MEIC chemicals)

Figure 7.2: Regression between human cell lines (IC50m) and acute oral LD50 values (MEIC chemicals)

#### 7.1.3 German Organizational Names

**ZEBET:** Zentralstelle zur Erfassung und Bewertung von Ersatz- und Ergänzungsmethoden zum Tierversuch  
(*German Centre for the Documentation and Validation of Alternative Methods [at BgVV]*)

**DIMDI:** Deutsches Institut für Medizinische Dokumentation und Information  
(*The German Institute for Medical Documentation and Information*)

**BgVV:** Bundesinstitut für gesundheitlichen Verbraucherschutz und Veterinärmedizin  
(*Federal Institute for Health Protection of Consumers and Veterinary Medicine*)



**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC #   | Chemical                            | CAS #      | IC50x |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|----------|-------------------------------------|------------|-------|----------|----------|---------|------------|---------|--------|---|
|      |          |                                     |            | ug/ml | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 1    |          | Trenimon                            | 68-76-8    | 0.00  | 0.000033 | NA       | NA      | NA         | NA      | 231.28 |   |
| 2    |          | Actinomycin D                       | 50-76-0    | 0.01  | 0.000081 | 7.2      | 0.0057  | 12.6       | 0.01    | 1255.6 | 0.0057                                  |
| 3    |          | Aminopterin                         | 54-62-6    | 0.01  | 0.000012 | NA       | NA      | 3.0        | 0.0068  | 440.47 | 0.0068                                  |
| 4    |          | Vincristine sulfate                 | 2068-78-2  | 0.01  | 0.000015 | NA       | NA      | NA         | NA      | 923.14 |   |
| 5    | K-       | Strophantin                         |            | 0.03  | 0.000044 | NA       | NA      | NA         | NA      | 710.9  |   |
| 132  |          | Triphenyltin hydroxide              | 76-87-9    | 0.02  | 0.000049 | 44.0     | 0.12    | 245.9      | 0.67    | 367.03 | 0.12                                    |
| 6    |          | Colchicine                          | 64-86-8    | 0.02  | 0.000054 | NA       | NA      | 6.0        | 0.015   | 399.48 | 0.015                                   |
| 7    |          | Ouabain                             | 630-60-4   | 0.04  | 0.000072 | NA       | NA      | NA         | NA      | 584.73 |   |
| 133  |          | Cytochalasin D                      | 22144-77-0 | 0.05  | 0.000092 | NA       | NA      | 36.0       | 0.071   | 507.68 | 0.071                                   |
| 8    |          | Digitoxin                           | 71-63-6    | 0.08  | 0.00011  | 55.8     | 0.073   | NA         | NA      | 765.05 | 0.073                                   |
| 134  |          | Rotenone                            | 83-79-4    | 0.05  | 0.00013  | 130.2    | 0.33    | 351.1      | 0.89    | 394.45 | 0.33                                    |
| 9    |          | Amethopterin                        | 59-05-2    | 0.06  | 0.00014  | 136.4    | 0.3     | 145.4      | 0.32    | 454.5  | 0.3                                     |
| 10   |          | Emetine                             | 483-18-1   | 0.08  | 0.00016  | 67.3     | 0.14    | NA         | NA      | 480.71 | 0.14                                    |
| 135  | 2,3,7,8- | Tetrachloro-dibenzo-p-dioxin        | 1746-01-6  | 0.06  | 0.0002   | NA       | NA      | 0.1        | 0.00035 | 321.96 | 0.00035                                 |
| 11   |          | Doxorubicin * HCl                   | 25316-40-9 | 0.19  | 0.00033  | NA       | NA      | 696.0      | 1.2     | 580.03 | 1.2                                     |
| 12   |          | Puromycin                           | 53-79-2    | 0.16  | 0.00033  | NA       | NA      | 674.4      | 1.43    | 471.58 | 1.43                                    |
| 136  |          | Diethyldithiocarbamate sodium* 3H2O | 20624-25-3 | 0.09  | 0.00039  | 1500.7   | 6.66    | 1500.7     | 6.66    | 225.33 | 6.66                                    |
| 137  |          | Triethyltin chloride                | 994-31-0   | 0.11  | 0.00046  | 5.1      | 0.021   | NA         | NA      | 241.35 | 0.021                                   |
| 138  |          | Tributyltin chloride                | 1461-22-9  | 0.18  | 0.00054  | 120.4    | 0.37    | NA         | NA      | 325.53 | 0.37                                    |
| 139  |          | Retinol                             | 68-26-8    | 0.15  | 0.00054  | 1999.8   | 6.98    | 4011.0     | 14      | 286.5  | 6.98                                    |
| 140  | 6-       | Thioguanine                         | 154-42-7   | 0.10  | 0.00057  | NA       | NA      | 160.5      | 0.96    | 167.21 | 0.96                                    |
| 13   |          | Cycloheximide                       | 66-81-9    | 0.17  | 0.00059  | 2.0      | 0.0071  | 132.3      | 0.47    | 281.39 | 0.0071                                  |
| 141  |          | Cytosine arabinoside                | 147-94-4   | 0.17  | 0.00068  | NA       | NA      | 3137.9     | 12.9    | 243.25 | 12.9                                    |
| 142  |          | Methylmercury chloride              | 115-09-3   | 0.18  | 0.00071  | NA       | NA      | 57.7       | 0.23    | 251.08 | 0.23                                    |
| 143  |          | Triethylene melamine                | 51-18-3    | 0.16  | 0.00078  | 1.0      | 0.005   | 14.9       | 0.073   | 204.27 | 0.005                                   |
| 14   |          | Mitomycin C                         | 50-07-7    | 0.28  | 0.00084  | 14.0     | 0.042   | 17.1       | 0.051   | 334.37 | 0.042                                   |
| 144  |          | Sodium bichromate VI                | 10588-01-9 | 0.24  | 0.00093  | 49.8     | 0.19    | NA         | NA      | 261.98 | 0.19                                    |
| 15   | 8-       | Azaganine                           | 134-58-7   | 0.20  | 0.0013   | NA       | NA      | 1500.1     | 9.86    | 152.14 | 9.86                                    |
| 145  |          | Potassium chromate VI               | 7789-00-6  | 0.29  | 0.0015   | NA       | NA      | 180.6      | 0.93    | 194.2  | 0.93                                    |
| 16   |          | Azaserine                           | 115-02-6   | 0.35  | 0.002    | 169.7    | 0.98    | 150.6      | 0.87    | 173.15 | 0.98                                    |
| 146  |          | Potassium bichromate VI             |            | 0.59  | 0.002    | NA       | NA      | 191.2      | 0.65    | 294.2  | 0.65                                    |
| 147  |          | Mitoxantrone                        | 65271-80-9 | 1.07  | 0.0024   | 586.8    | 1.32    | NA         | NA      | 444.54 | 1.32                                    |
| 148  |          | Nitrogen mustard * HCl              | 55-86-7    | 0.50  | 0.0026   | 10.0     | 0.052   | 19.3       | 0.1     | 192.53 | 0.052                                   |
| 17   | 5-       | Fluorouracil                        | 51-21-8    | 0.34  | 0.0026   | 230.3    | 1.77    | 114.5      | 0.88    | 130.09 | 1.77                                    |
| 149  |          | Chromium VI trioxide                | 1333-82-0  | 0.27  | 0.0027   | 80.0     | 0.8     | 127.0      | 1.27    | 100    | 0.8                                     |
| 150  |          | Cis-platinum                        | 15663-27-1 | 0.84  | 0.0028   | 25.8     | 0.086   | 33.0       | 0.11    | 300.07 | 0.086                                   |
| 151  |          | Hexachlorocyclopentadiene           | 77-47-4    | 0.85  | 0.0031   | 111.8    | 0.41    | NA         | NA      | 272.75 | 0.41                                    |
| 152  | 8-       | Hydroxyquinoline                    | 148-24-3   | 0.48  | 0.0033   | 1200.6   | 8.27    | NA         | NA      | 145.17 | 8.27                                    |
| 18   |          | Captan                              | 133-06-2   | 1.17  | 0.0039   | 10009.6  | 33.3    | 7003.7     | 23.3    | 300.59 | 33.3                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |      | Chemical                             | CAS #      | IC50x |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|--------------------------------------|------------|-------|--------|----------|---------|------------|---------|--------|---|
|      |        |      |                                      |            | ug/ml | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 153  | 26     |      | Arsenic III trioxide                 | 1327-53-3  | 0.83  | 0.0042 | 19.8     | 0.1     | 45.5       | 0.23    | 197.84 | 0.1                                     |
| 154  |        |      | Maneb                                | 12427-38-2 | 1.12  | 0.0042 | 4500.6   | 16.9    | 3994.7     | 15      | 266.31 | 16.9                                    |
| 19   |        |      | Cytochalasin B                       | 14930-96-2 | 2.40  | 0.005  | NA       | NA      | NA         | NA      | 479.67 |   |
| 155  |        |      | Benzalkonium chloride                | 8001-54-5  | 1.90  | 0.0052 | 401.5    | 1.1     | 339.5      | 0.93    | 365    | 1.1                                     |
| 156  |        |      | Stearyltrimethylammoniumchloride     | 112-03-8   | 2.09  | 0.006  | NA       | NA      | 536.1      | 1.54    | 348.13 | 1.54                                    |
| 20   |        |      | Cadmium II chloride                  | 10108-64-2 | 1.17  | 0.0064 | 88.0     | 0.48    | 174.1      | 0.95    | 183.3  | 0.48                                    |
| 157  | 38     |      | Hexachlorophene                      | 70-30-4    | 3.21  | 0.0079 | 61.0     | 0.15    | 65.1       | 0.16    | 406.89 | 0.15                                    |
| 21   |        | 6-   | Mercaptopurine                       | 50-44-2    | 1.22  | 0.008  | NA       | NA      | 280.0      | 1.84    | 152.19 | 1.84                                    |
| 158  |        |      | Dichlorophene                        | 97-23-4    | 2.23  | 0.0083 | 2691.3   | 10      | 1001.2     | 3.72    | 269.13 | 10                                      |
| 22   | 6      |      | Digoxin                              | 20830-75-5 | 6.64  | 0.0085 | NA       | NA      | 18.0       | 0.023   | 781.05 | 0.023                                   |
| 159  |        |      | Hexadecyltrimethylammoniumbromide    | 57-09-0    | 3.24  | 0.0089 | 408.3    | 1.12    | NA         | NA      | 364.53 | 1.12                                    |
| 23   |        |      | Daraprim                             | 58-14-0    | 2.21  | 0.0089 | NA       | NA      | 126.9      | 0.51    | 248.74 | 0.51                                    |
| 24   |        |      | Ethylenediamine-tetraacetic acid     | 60-00-4    | 2.92  | 0.01   | NA       | NA      | NA         | NA      | 292.28 |   |
| 25   |        |      | Thio-TEPA                            | 52-24-4    | 2.08  | 0.011  | NA       | NA      | 37.8       | 0.2     | 189.24 | 0.2                                     |
| 160  |        | N-   | Methyl-N'-nitro-N-nitroso- guanidine | 70-25-7    | 1.77  | 0.012  | 89.7     | 0.61    | NA         | NA      | 147.12 | 0.61                                    |
| 26   |        |      | Kelthane                             | 115-32-2   | 4.45  | 0.012  | 574.2    | 1.55    | 418.6      | 1.13    | 370.48 | 1.55                                    |
| 161  |        |      | Silver I nitrate                     | 7761-88-8  | 2.21  | 0.013  | NA       | NA      | 49.3       | 0.29    | 169.88 | 0.29                                    |
| 27   |        |      | Chlorpromazine                       | 50-53-3    | 4.46  | 0.014  | 140.3    | 0.44    | 261.5      | 0.82    | 318.89 | 0.44                                    |
| 28   |        |      | Aldosterone                          | 52-39-1    | 5.05  | 0.014  | NA       | NA      | NA         | NA      | 360.44 |   |
| 29   | 28     |      | Mercury II chloride                  | 7487-94-7  | 4.07  | 0.015  | 1.0      | 0.0037  | 10.0       | 0.037   | 271.49 | 0.0037                                  |
| 162  |        |      | Chlorhexidine                        | 55-56-1    | 7.58  | 0.015  | 9200.5   | 18.2    | 9857.6     | 19.5    | 505.52 | 18.2                                    |
| 30   |        |      | Sodium arsenate, dibasic             | 7778-43-0  | 2.79  | 0.015  | NA       | NA      | NA         | NA      | 185.91 |   |
| 31   | 41     |      | Chloroquine diphosphate              | 50-63-5    | 8.77  | 0.017  | 969.9    | 1.88    | 500.4      | 0.97    | 515.92 | 1.88                                    |
| 164  |        |      | Oxatomide                            | 60607-34-3 | 8.11  | 0.019  | 1412.1   | 3.31    | 9598.7     | 22.5    | 426.61 | 3.31                                    |
| 163  |        |      | Cetyltrimethylammonium chloride      | 112-02-7   | 7.61  | 0.021  | 474.4    | 1.31    | NA         | NA      | 362.16 | 1.31                                    |
| 165  |        |      | Isoproterenol * HCl                  | 51-30-9    | 5.45  | 0.022  | 2219.8   | 8.96    | NA         | NA      | 247.75 | 8.96                                    |
| 32   |        |      | Hydrocortisone                       | 50-23-7    | 7.98  | 0.022  | NA       | NA      | NA         | NA      | 362.51 |   |
| 166  |        |      | Triisooctylamine                     | 2757-28-0  | 8.14  | 0.023  | 1620.2   | 4.58    | NA         | NA      | 353.76 | 4.58                                    |
| 167  |        | p,p' | DDD                                  | 72-54-8    | 7.68  | 0.024  | 112.0    | 0.35    | NA         | NA      | 320.04 | 0.35                                    |
| 33   |        | p-   | Chloromercuribenzoic acid            | 59-85-8    | 8.57  | 0.024  | NA       | NA      | 25.0       | 0.07    | 357.16 | 0.07                                    |
| 34   |        |      | Diethylstilbestrol                   | 56-53-1    | 6.71  | 0.025  | NA       | NA      | NA         | NA      | 268.38 |   |
| 168  |        |      | Dicoumarol                           | 66-76-2    | 9.08  | 0.027  | 709.6    | 2.11    | 232.1      | 0.69    | 336.31 | 2.11                                    |
| 169  |        |      | Epinephrine bitartrate               | 51-42-3    | 9.33  | 0.028  | NA       | NA      | 4.0        | 0.012   | 333.33 | 0.012                                   |
| 35   |        |      | Flufenamic acid                      | 530-78-9   | 8.16  | 0.029  | 272.8    | 0.97    | 714.4      | 2.54    | 281.25 | 0.97                                    |
| 170  | 29     |      | Thioridazine * HCl                   | 130-61-0   | 11.81 | 0.029  | NA       | NA      | 358.2      | 0.88    | 407.07 | 0.88                                    |
| 36   |        |      | Progesterone                         | 57-83-0    | 9.44  | 0.03   | NA       | NA      | NA         | NA      | 314.51 |   |
| 171  |        |      | Fumagillin                           | 297-95-0   | 14.22 | 0.031  | NA       | NA      | 1999.5     | 4.36    | 458.6  | 4.36                                    |
| 37   |        |      | Aflatoxin B1                         | 1162-65-8  | 10.62 | 0.034  | 5.0      | 0.016   | 9.1        | 0.029   | 312.29 | 0.016                                   |
| 172  |        |      | Nabam                                | 142-59-6   | 8.97  | 0.035  | 394.8    | 1.54    | 579.3      | 2.26    | 256.34 | 1.54                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |      | Chemical                          | CAS #      | IC50x |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|-----------------------------------|------------|-------|--------|----------|---------|------------|---------|--------|---|
|      |        |      |                                   |            | ug/ml | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 173  | 39     |      | Pentachlorophenol                 | 87-86-5    | 9.59  | 0.036  | 50.6     | 0.19    | NA         | NA      | 266.32 | 0.19                                    |
| 174  |        |      | Ambazone                          | 539-21-9   | 9.02  | 0.038  | 749.9    | 3.16    | 999.1      | 4.21    | 237.32 | 3.16                                    |
| 175  |        |      | Norepinephrine                    | 51-41-2    | 6.60  | 0.039  | NA       | NA      | 20.3       | 0.12    | 169.2  | 0.12                                    |
| 46   |        |      | Lead II chloride                  | 7758-95-4  | 11.96 | 0.043  | NA       | NA      | NA         | NA      | 278.09 |   |
| 176  |        |      | Papaverine                        | 58-74-2    | 15.27 | 0.045  | 325.8    | 0.96    | 230.8      | 0.68    | 339.42 | 0.96                                    |
| 177  |        |      | Busulphan                         | 55-98-1    | 11.33 | 0.046  | 1.9      | 0.0076  | 199.5      | 0.81    | 246.32 | 0.0076                                  |
| 178  |        |      | Salicylanilide                    | 87-17-2    | 9.81  | 0.046  | NA       | NA      | 2409.7     | 11.3    | 213.25 | 11.3                                    |
| 179  |        |      | Acrolein                          | 107-02-8   | 2.64  | 0.047  | 46.0     | 0.82    | 39.8       | 0.71    | 56.07  | 0.82                                    |
| 180  |        | p-   | Phenylenediamine                  | 106-50-3   | 5.41  | 0.05   | 80.0     | 0.74    | NA         | NA      | 108.16 | 0.74                                    |
| 38   |        |      | Imipramine * HCl                  | 113-52-0   | 17.11 | 0.054  | 304.2    | 0.96    | 374.0      | 1.18    | 316.91 | 0.96                                    |
| 181  | 30     |      | Thallium I sulfate                | 7446-18-6  | 27.26 | 0.054  | NA       | NA      | 28.8       | 0.057   | 504.8  | 0.057                                   |
| 39   |        | 2,4- | Dichlorophenol                    | 120-83-2   | 8.97  | 0.055  | 580.3    | 3.56    | 1600.7     | 9.82    | 163    | 3.56                                    |
| 182  |        |      | Triton X-100                      | 9002-93-1  | 35.59 | 0.055  | 1798.7   | 2.78    | NA         | NA      | 647    | 2.78                                    |
| 183  | 5      |      | Amitriptyline                     | 50-48-6    | 15.54 | 0.056  | 319.1    | 1.15    | 147.0      | 0.53    | 277.44 | 1.15                                    |
| 184  |        |      | Butylated hydroxytoluene          | 128-37-0   | 12.34 | 0.056  | 890.4    | 4.04    | 1040.2     | 4.72    | 220.39 | 4.04                                    |
| 185  |        |      | Heptachlor                        | 76-44-8    | 22.02 | 0.059  | 41.1     | 0.11    | 67.2       | 0.18    | 373.3  | 0.11                                    |
| 186  |        |      | Zineb                             | 12122-67-7 | 16.27 | 0.059  | 5211.3   | 18.9    | 7610.1     | 27.6    | 275.73 | 18.9                                    |
| 40   |        |      | Chlordan                          | 57-74-9    | 24.59 | 0.06   | 458.9    | 1.12    | NA         | NA      | 409.76 | 1.12                                    |
| 41   |        |      | Chloroquine sulfate               | 132-73-0   | 25.08 | 0.06   | 1086.8   | 2.6     | NA         | NA      | 418    | 2.6                                     |
| 42   |        | p-   | Aminophenol                       | 23-30-8    | 6.77  | 0.062  | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 187  |        | 4-   | Hexylresorcinol                   | 136-77-6   | 12.44 | 0.064  | 549.9    | 2.83    | NA         | NA      | 194.3  | 2.83                                    |
| 43   |        |      | Aldrin                            | 309-00-2   | 24.45 | 0.067  | 40.1     | 0.11    | 43.8       | 0.12    | 364.9  | 0.11                                    |
| 44   |        |      | Hydroxyzine * HCl                 | 1244-76-4  | 27.56 | 0.067  | 950.4    | 2.31    | NA         | NA      | 411.41 | 2.31                                    |
| 188  |        | t-   | Butyl hydroquinone                | 1948-33-0  | 11.47 | 0.069  | 799.6    | 4.81    | 1000.8     | 6.02    | 166.24 | 4.81                                    |
| 189  |        |      | Antimycin                         | 11118-72-2 | 17.52 | 0.07   | NA       | NA      | 112.6      | 0.45    | 250.27 | 0.45                                    |
| 45   |        |      | Quinine * HCl                     | 130-89-2   | 27.07 | 0.075  | 620.8    | 1.72    | 1158.6     | 3.21    | 360.92 | 1.72                                    |
| 190  |        |      | Chlorambucil                      | 305-03-3   | 23.12 | 0.076  | 76.1     | 0.25    | 100.4      | 0.33    | 304.24 | 0.25                                    |
| 191  |        |      | Dimenhydrinate                    | 523-87-5   | 35.72 | 0.076  | 1320.8   | 2.81    | 202.1      | 0.43    | 470.02 | 2.81                                    |
| 192  |        | 1,3- | Bis(2-chloroethyl)- 1-nitrosoarea | 154-93-8   | 16.70 | 0.078  | 19.9     | 0.093   | 19.1       | 0.089   | 214.07 | 0.093                                   |
| 193  |        | 5-   | Azacytidine                       | 320-67-2   | 19.29 | 0.079  | NA       | NA      | 571.5      | 2.34    | 244.24 | 2.34                                    |
| 47   |        |      | Naftipramide                      | 1505-95-9  | 25.07 | 0.084  | 1029.7   | 3.45    | 1086.4     | 3.64    | 298.47 | 3.45                                    |
| 48   |        |      | Mefenamic acid                    | 61-68-7    | 20.99 | 0.087  | 789.1    | 3.27    | 629.8      | 2.61    | 241.31 | 3.27                                    |
| 49   |        |      | Parathion                         | 56-38-2    | 27.09 | 0.093  | 2.0      | 0.0069  | 6.1        | 0.021   | 291.28 | 0.0069                                  |
| 194  |        | p-   | Toluyldiamine                     | 95-70-5    | 11.49 | 0.094  | 101.4    | 0.83    | NA         | NA      | 122.19 | 0.83                                    |
| 50   |        |      | Trypan blue                       | 72-57-1    | 91.66 | 0.095  | 6204.2   | 6.43    | NA         | NA      | 964.88 | 6.43                                    |
| 195  |        | p,p' | DDA                               | 83-05-6    | 27.83 | 0.099  | NA       | NA      | 590.4      | 2.1     | 281.14 | 2.1                                     |
| 196  | 40     |      | VerapamilHCl                      | 152-11-4   | 49.11 | 0.1    | 108.0    | 0.22    | 162.1      | 0.33    | 491.13 | 0.22                                    |
| 197  |        | p,p' | DDE                               | 72-55-9    | 31.80 | 0.1    | 880.9    | 2.77    | NA         | NA      | 318.02 | 2.77                                    |
| 51   |        |      | Disulfoton                        | 298-04-4   | 30.19 | 0.11   | 2.0      | 0.0073  | 5.5        | 0.02    | 274.42 | 0.0073                                  |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |         | Chemical                                  | CAS #      | IC50x  |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|---------|---|------------|--------|--------|----------|---------|------------|---------|--------|---|
|      |        |         |   |            | ug/ml  | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 198  |        |         | Ioxynil                                   | 1689-83-4  | 40.80  | 0.11   | 111.3    | 0.3     | NA         | NA      | 370.91 | 0.3                                     |
| 199  |        |         | Cupric chloride                           | 7447-39-4  | 14.79  | 0.11   | 139.8    | 1.04    | 189.6      | 1.41    | 134.44 | 1.04                                    |
| 200  |        |         | Dimethylaminoethyl methacrylate (polymer) | 2867-47-2  | 17.30  | 0.11   | 1745.4   | 11.1    | NA         | NA      | 157.24 | 11.1                                    |
| 52   |        |         | all-trans-Retinoic acid                   | 302-79-4   | 33.05  | 0.11   | 2001.2   | 6.66    | NA         | NA      | 300.48 | 6.66                                    |
| 53   | 43     |         | Quinidine sulfate                         | 50-54-4    | 50.70  | 0.12   | 456.3    | 1.08    | 595.8      | 1.41    | 422.54 | 1.08                                    |
| 202  |        |         | Formaldehyde                              | 50-00-0    | 3.60   | 0.12   | 798.8    | 26.6    | NA         | NA      | 30.03  | 26.6                                    |
| 54   | 23     |         | Propranolol * HCl                         | 318-98-9   | 35.50  | 0.12   | NA       | NA      | 470.4      | 1.59    | 295.84 | 1.59                                    |
| 201  |        | 13-cis- | Retinoic acid                             | 4759-48-2  | 36.06  | 0.12   | NA       | NA      | 3395.4     | 11.3    | 300.48 | 11.3                                    |
| 55   |        |         | Zinc II chloride                          | 7646-85-7  | 17.72  | 0.13   | 350.2    | 2.57    | 350.2      | 2.57    | 136.27 | 2.57                                    |
| 56   |        |         | Manganese IIchloride *4 H2O               | 13446-34-9 | 25.73  | 0.13   | 1484.4   | 7.5     | NA         | NA      | 197.92 | 7.5                                     |
| 57   |        | L-      | Dopa                                      | 59-92-7    | 25.64  | 0.13   | 1780.8   | 9.03    | 2366.5     | 12      | 197.21 | 9.03                                    |
| 204  |        |         | Azathioprine                              | 446-86-6   | 38.82  | 0.14   | 535.2    | 1.93    | 1389.2     | 5.01    | 277.29 | 1.93                                    |
| 58   |        |         | Dihydralazine sulfate                     | 7327-87-9  | 40.36  | 0.14   | 818.8    | 2.84    | 400.8      | 1.39    | 288.32 | 2.84                                    |
| 59   |        |         | Tetracycline * HCl                        | 64-75-5    | 67.33  | 0.14   | 6444.6   | 13.4    | NA         | NA      | 480.94 | 13.4                                    |
| 203  |        |         | Thallium I acetate                        | 563-68-8   | 36.88  | 0.14   | NA       | NA      | 34.2       | 0.13    | 263.42 | 0.13                                    |
| 205  |        |         | Versalide                                 | 88-29-9    | 38.77  | 0.15   | 315.3    | 1.22    | NA         | NA      | 258.44 | 1.22                                    |
| 60   |        |         | Indomethacin                              | 53-86-1    | 57.25  | 0.16   | 12.2     | 0.034   | 19.0       | 0.053   | 357.81 | 0.034                                   |
| 62   |        |         | Cobalt II chloride                        | 7646-79-9  | 20.77  | 0.16   | 80.5     | 0.62    | 80.5       | 0.62    | 129.83 | 0.62                                    |
| 61   |        | p,p'    | DDT                                       | 50-29-3    | 56.72  | 0.16   | 113.4    | 0.32    | 134.7      | 0.38    | 354.48 | 0.32                                    |
| 206  |        |         | Diquat dibromide                          | 85-00-7    | 55.05  | 0.16   | 230.5    | 0.67    | 234.0      | 0.68    | 344.08 | 0.67                                    |
| 63   | 4      |         | Diazepam                                  | 439-14-5   | 45.56  | 0.16   | 709.1    | 2.49    | 535.3      | 1.88    | 284.76 | 2.49                                    |
| 207  |        |         | Dieldrin                                  | 60-57-1    | 68.56  | 0.18   | 45.7     | 0.12    | 38.1       | 0.1     | 380.9  | 0.12                                    |
| 64   |        |         | Bendiocarb                                | 22781-23-3 | 40.19  | 0.18   | 178.6    | 0.8     | NA         | NA      | 223.25 | 0.8                                     |
| 208  |        |         | Undecylenic acid                          | 112-38-9   | 33.18  | 0.18   | 2506.6   | 13.6    | 8496.7     | 46.1    | 184.31 | 13.6                                    |
| 209  |        |         | Propylparaben                             | 94-13-3    | 32.44  | 0.18   | NA       | NA      | 6325.7     | 35.1    | 180.22 | 35.1                                    |
| 65   |        |         | Oxyphenbutazone                           | 129-20-4   | 61.64  | 0.19   | 999.2    | 3.08    | 480.1      | 1.48    | 324.41 | 3.08                                    |
| 66   |        |         | Cortisone                                 | 53-06-5    | 68.49  | 0.19   | NA       | NA      | NA         | NA      | 360.49 |   |
| 210  |        | p-      | Nitrophenol                               | 100-02-7   | 27.82  | 0.2    | 350.6    | 2.52    | 467.4      | 3.36    | 139.12 | 2.52                                    |
| 67   | 15     |         | Malathion                                 | 121-75-5   | 66.08  | 0.2    | 885.4    | 2.68    | 776.4      | 2.35    | 330.38 | 2.68                                    |
| 211  |        |         | Catechol                                  | 120-80-9   | 22.02  | 0.2    | 3887.2   | 35.3    | 259.9      | 2.36    | 110.12 | 35.3                                    |
| 68   |        | 2,4-    | Dinitrophenol                             | 51-28-5    | 38.67  | 0.21   | 29.5     | 0.16    | 44.2       | 0.24    | 184.12 | 0.16                                    |
| 69   |        |         | Secobarbital sodium                       | 309-43-3   | 54.66  | 0.21   | 124.9    | 0.48    | NA         | NA      | 260.3  | 0.48                                    |
| 212  |        | p-      | Cresol                                    | 106-44-5   | 23.79  | 0.22   | 206.6    | 1.91    | 343.9      | 3.18    | 108.15 | 1.91                                    |
| 70   | 49     |         | Atropine sulfate                          | 55-48-1    | 148.92 | 0.22   | 622.7    | 0.92    | 764.9      | 1.13    | 676.9  | 0.92                                    |
| 213  |        |         | Ammonium persulfate                       | 7727-54-0  | 52.49  | 0.23   | 819.3    | 3.59    | NA         | NA      | 228.22 | 3.59                                    |
| 214  |        |         | Thymol                                    | 89-83-8    | 34.56  | 0.23   | 979.6    | 6.52    | 1802.9     | 12      | 150.24 | 6.52                                    |
| 71   |        |         | Diphenhydramine * HCl                     | 147-24-0   | 70.04  | 0.24   | 855.1    | 2.93    | 113.8      | 0.39    | 291.85 | 2.93                                    |
| 72   |        |         | Butylated hydroxyanisole                  | 8003-24-5  | 43.26  | 0.24   | 2199.3   | 12.2    | 2001.0     | 11.1    | 180.27 | 12.2                                    |
| 215  |        |         | Chlorotetracycline                        | 57-62-5    | 114.94 | 0.24   | NA       | NA      | 2500.0     | 5.22    | 478.92 | 5.22                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |        | Chemical                       | CAS #      | IC50x  |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|--------------------------------|------------|--------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                                |            | ug/ml  | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 216  |        |        | Refortan                       |            | 78.28  | 0.25   | 3162.3   | 10.1    | NA         | NA      | 313.1  | 10.1                                    |
| 73   |        |        | Carbaryl                       | 63-25-2    | 52.32  | 0.26   | 249.5    | 1.24    | 438.7      | 2.18    | 201.24 | 1.24                                    |
| 74   |        |        | Nickel II chloride             | 7718-54-9  | 34.99  | 0.27   | 105.0    | 0.81    | NA         | NA      | 129.61 | 0.81                                    |
| 75   |        |        | Trichlorfon                    | 52-68-6    | 69.51  | 0.27   | 450.5    | 1.75    | 298.6      | 1.16    | 257.44 | 1.75                                    |
| 76   |        |        | Sodium dodecyl sulfate         | 151-21-3   | 78.15  | 0.27   | 1288.0   | 4.45    | NA         | NA      | 289.43 | 4.45                                    |
| 77   |        |        | Cinchophen                     | 132-60-5   | 67.31  | 0.27   | NA       | NA      | NA         | NA      | 249.28 |   |
| 217  |        |        | Amrinone                       | 60719-84-8 | 52.42  | 0.28   | 101.1    | 0.54    | 288.3      | 1.54    | 187.22 | 0.54                                    |
| 218  |        | o-     | Phenylenediamine               | 95-54-5    | 33.53  | 0.31   | 1069.7   | 9.89    | NA         | NA      | 108.16 | 9.89                                    |
| 78   |        | 6-     | Methylcoumarin                 | 92-48-8    | 49.66  | 0.31   | 1681.9   | 10.5    | NA         | NA      | 160.18 | 10.5                                    |
| 79   |        |        | Phenylbutazone                 | 50-33-9    | 98.69  | 0.32   | 376.3    | 1.22    | 441.0      | 1.43    | 308.41 | 1.22                                    |
| 80   |        | 2-     | Thiouracil                     | 141-90-2   | 41.01  | 0.32   | 999.6    | 7.8     | NA         | NA      | 128.16 | 7.8                                     |
| 219  |        |        | Hydralazine                    | 86-54-4    | 52.87  | 0.33   | 89.7     | 0.56    | 121.8      | 0.76    | 160.2  | 0.56                                    |
| 81   | 27     |        | Cupric sulfate * 5 H2O         | 7758-99-8  | 82.40  | 0.33   | 299.6    | 1.2     | NA         | NA      | 249.7  | 1.2                                     |
| 238  |        |        | Imidazolidinyl urea            | 39236-46-9 | 100.17 | 0.36   | 2598.9   | 9.34    | 3700.9     | 13.3    | 278.26 | 9.34                                    |
| 220  |        | m-     | Dinitrobenzene                 | 99-65-0    | 65.57  | 0.39   | 82.4     | 0.49    | NA         | NA      | 168.12 | 0.49                                    |
| 221  |        | 2-     | Nitro-p-phenylene-diamine      | 5307-14-2  | 59.73  | 0.39   | 3078.5   | 20.1    | NA         | NA      | 153.16 | 20.1                                    |
| 82   | 44     |        | Diphenylhydantoin              | 57-41-0    | 98.39  | 0.39   | NA       | NA      | 199.3      | 0.79    | 252.29 | 0.79                                    |
| 222  |        |        | Glibenclamide                  | 10238-21-8 | 197.62 | 0.4    | NA       | NA      | 3250.8     | 6.58    | 494.05 | 6.58                                    |
| 223  | 32     |        | Lindane                        | 58-89-9    | 119.24 | 0.41   | 75.6     | 0.26    | 87.2       | 0.3     | 290.82 | 0.26                                    |
| 224  |        | n-     | Butyl benzoate                 | 136-60-7   | 73.08  | 0.41   | 5133.6   | 28.8    | NA         | NA      | 178.25 | 28.8                                    |
| 225  |        |        | Ammonium sulfide               | 12135-76-1 | 21.47  | 0.42   | 168.2    | 3.29    | NA         | NA      | 51.12  | 3.29                                    |
| 226  |        |        | Dodecylbenzene sodiumsulfonate | 25155-30-0 | 146.38 | 0.42   | 1261.6   | 3.62    | 2000.5     | 5.74    | 348.52 | 3.62                                    |
| 227  | 46     |        | Sodium oxalate                 | 62-76-0    | 58.96  | 0.44   | 155.4    | 1.16    | NA         | NA      | 134    | 1.16                                    |
| 228  |        | 2,4,5- | Trichlorophen- oxyacetic acid  | 93-76-5    | 112.41 | 0.44   | 298.9    | 1.17    | 388.3      | 1.52    | 255.48 | 1.17                                    |
| 229  | 22     |        | Dextropropoxyphene * HCl       | 1639-60-7  | 184.23 | 0.49   | 82.7     | 0.22    | 82.7       | 0.22    | 375.98 | 0.22                                    |
| 230  | 42     |        | Orphenadrine * HCl             | 341-69-5   | 149.88 | 0.49   | 425.2    | 1.39    | 125.4      | 0.41    | 305.88 | 1.39                                    |
| 231  |        |        | Tween 80                       | 9005-65-6  | 641.90 | 0.49   | NA       | NA      | 25021.0    | 19.1    | 1310   | 19.1                                    |
| 232  |        | o-     | Cresol                         | 95-48-7    | 56.24  | 0.52   | 121.1    | 1.12    | 343.9      | 3.18    | 108.15 | 1.12                                    |
| 233  |        |        | Ibuprofen                      | 15687-27-1 | 107.28 | 0.52   | 1008.9   | 4.89    | 980.0      | 4.75    | 206.31 | 4.89                                    |
| 234  |        |        | Phenylthiourea                 | 103-85-5   | 82.20  | 0.54   | 3.0      | 0.02    | 10.0       | 0.066   | 152.23 | 0.02                                    |
| 235  | 25     |        | Paraquat                       | 4685-14-7  | 100.58 | 0.54   | 57.7     | 0.31    | 195.6      | 1.05    | 186.25 | 0.31                                    |
| 83   |        |        | Thiopental                     | 76-75-5    | 133.30 | 0.55   | NA       | NA      | 601.1      | 2.48    | 242.37 | 2.48                                    |
| 84   |        |        | Amobarbital                    | 57-43-2    | 126.73 | 0.56   | NA       | NA      | 344.0      | 1.52    | 226.31 | 1.52                                    |
| 236  |        |        | Hydrogen peroxide 90%          | 7722-84-1  | 19.05  | 0.56   | NA       | NA      | 2000.4     | 58.8    | 34.02  | 58.8                                    |
| 85   |        |        | Metamizol                      | 68-89-3    | 193.94 | 0.58   | 7189.2   | 21.5    | NA         | NA      | 334.38 | 21.5                                    |
| 237  |        |        | Beryllium II sulfate           | 13510-49-1 | 64.09  | 0.61   | 82.0     | 0.78    | 79.9       | 0.76    | 105.07 | 0.78                                    |
| 239  |        | m-     | Cresol                         | 108-39-4   | 71.38  | 0.66   | 242.3    | 2.24    | 828.4      | 7.66    | 108.15 | 2.24                                    |
| 240  |        |        | Pentoxifylline                 | 6493-05-6  | 183.71 | 0.66   | NA       | NA      | 1386.2     | 4.98    | 278.35 | 4.98                                    |
| 86   | 31     |        | Warfarin                       | 81-81-2    | 206.59 | 0.67   | 323.8    | 1.05    | 373.1      | 1.21    | 308.35 | 1.05                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |        | Chemical  | CAS #      | IC50x  |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|---|------------|--------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |   |            | ug/ml  | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 241  |        |        | Sodium azide  | 26628-22-8 | 46.16  | 0.71   | 44.9     | 0.69    | 27.3       | 0.42    | 65.02  | 0.69                                    |
| 87   |        |        | Pentobarbital sodium                                      | 57-33-0    | 176.29 | 0.71   | 201.1    | 0.81    | 280.6      | 1.13    | 248.29 | 0.81                                    |
| 242  |        | 1,2,4- | Trichlorobenzene  | 120-82-1   | 128.82 | 0.71   | 756.6    | 4.17    | 765.7      | 4.22    | 181.44 | 4.17                                    |
| 243  |        | p-     | Anisidine   | 104-94-9   | 89.91  | 0.73   | 1404.1   | 11.4    | NA         | NA      | 123.17 | 11.4                                    |
| 244  |        |        | Doxylamine succinate                                      | 562-10-7   | 291.38 | 0.75   | NA       | NA      | 470.1      | 1.21    | 388.51 | 1.21                                    |
| 88   |        |        | Dibutyl phthalate   | 84-74-2    | 211.57 | 0.76   | 11998.2  | 43.1    | NA         | NA      | 278.38 | 43.1                                    |
| 89   | 16     | 2,4-   | Dichlorophenoxy- acetic acid                              | 94-75-7    | 170.20 | 0.77   | 369.1    | 1.67    | 366.9      | 1.66    | 221.04 | 1.67                                    |
| 90   |        |        | Iproniazid  | 54-92-2    | 141.61 | 0.79   | 365.7    | 2.04    | 681.2      | 3.8     | 179.25 | 2.04                                    |
| 91   | 45     |        | Chloramphenicol   | 56-75-7    | 255.29 | 0.79   | 3393.1   | 10.5    | 2640.1     | 8.17    | 323.15 | 10.5                                    |
| 245  |        |        | Resorcinol  | 108-46-3   | 88.10  | 0.8    | 300.6    | 2.73    | NA         | NA      | 110.12 | 2.73                                    |
| 246  | 37     |        | Barium II nitrate   | 10022-31-8 | 211.70 | 0.81   | 355.4    | 1.36    | NA         | NA      | 261.36 | 1.36                                    |
| 247  |        | (+)    | Thalidomide   | 731-40-8   | 209.18 | 0.81   | NA       | NA      | 400.3      | 1.55    | 258.25 | 1.55                                    |
| 92   |        |        | Di(2-ethylhexyl)phthalate                                 | 117-81-7   | 328.12 | 0.84   | 31015.2  | 79.4    | 29999.6    | 76.8    | 390.62 | 79.4                                    |
| 93   |        |        | Sulfisoxazole   | 127-69-5   | 227.23 | 0.85   | NA       | NA      | 6790.2     | 25.4    | 267.33 | 25.4                                    |
| 248  |        | m-     | Aminophenol   | 591-27-5   | 93.86  | 0.86   | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 94   |        |        | Menthol   | 89-78-1    | 148.49 | 0.95   | 3172.9   | 20.3    | NA         | NA      | 156.3  | 20.3                                    |
| 249  |        | 3-     | Cyano-2-morpholino-5-(pyrid-4-yl)-pyridine (Chemical 122) |            | 255.66 | 0.96   | 346.2    | 1.3     | NA         | NA      | 266.31 | 1.3                                     |
| 250  |        |        | Valproate sodium  | 1069-66-5  | 166.22 | 1      | NA       | NA      | 1695.4     | 10.2    | 166.22 | 10.2                                    |
| 251  |        |        | Scopolamine * HBr   | 6533-68-2  | 415.05 | 1.08   | 1268.2   | 3.3     | 1879.3     | 4.89    | 384.31 | 3.3                                     |
| 95   |        |        | Salicylamide  | 65-45-2    | 148.12 | 1.08   | 1892.7   | 13.8    | 1398.9     | 10.2    | 137.15 | 13.8                                    |
| 252  | 19     |        | Potassium cyanide   | 151-50-8   | 72.93  | 1.12   | 9.8      | 0.15    | 8.5        | 0.13    | 65.12  | 0.15                                    |
| 96   |        |        | Cygon   | 60-51-5    | 284.29 | 1.24   | 151.3    | 0.66    | 59.6       | 0.26    | 229.27 | 0.66                                    |
| 97   |        |        | Phenacetin  | 62-44-2    | 227.63 | 1.27   | 1650.8   | 9.21    | 1220.6     | 6.81    | 179.24 | 9.21                                    |
| 253  |        |        | Isoxepac  | 55453-87-7 | 356.81 | 1.33   | 198.5    | 0.74    | NA         | NA      | 268.28 | 0.74                                    |
| 254  |        |        | Buflomedil  | 55837-25-7 | 415.03 | 1.35   | 365.8    | 1.19    | NA         | NA      | 307.43 | 1.19                                    |
| 98   |        |        | Methylparaben   | 99-76-3    | 216.07 | 1.42   | NA       | NA      | 1749.8     | 11.5    | 152.16 | 11.5                                    |
| 255  |        |        | Sodium monochloroacetate                                  | 3926-62-3  | 168.90 | 1.45   | 75.7     | 0.65    | NA         | NA      | 116.48 | 0.65                                    |
| 99   |        |        | Nalidixic acid  | 389-08-2   | 348.39 | 1.5    | 1349.4   | 5.81    | 571.4      | 2.46    | 232.26 | 5.81                                    |
| 256  |        |        | Tin II chloride   | 7772-99-8  | 286.28 | 1.51   | 699.6    | 3.69    | 1200.1     | 6.33    | 189.59 | 3.69                                    |
| 257  |        |        | Isononylaldehyde  | 5435-64-3  | 216.25 | 1.52   | 3243.8   | 22.8    | NA         | NA      | 142.27 | 22.8                                    |
| 100  |        | L-     | Ascorbic acid   | 50-81-7    | 267.73 | 1.52   | 11907.1  | 67.6    | 3364.3     | 19.1    | 176.14 | 67.6                                    |
| 101  |        |        | Glutethimide  | 77-21-4    | 338.97 | 1.56   | 599.7    | 2.76    | 360.7      | 1.66    | 217.29 | 2.76                                    |
| 102  |        |        | Acrylamide  | 79-06-1    | 114.45 | 1.61   | 169.9    | 2.39    | 169.9      | 2.39    | 71.09  | 2.39                                    |
| 258  |        |        | Diethyl sebacate  | 110-40-7   | 421.19 | 1.63   | 14470.4  | 56      | NA         | NA      | 258.4  | 56                                      |
| 259  |        |        | Methyl salicylate   | 119-36-8   | 258.67 | 1.7    | 887.1    | 5.83    | NA         | NA      | 152.16 | 5.83                                    |
| 260  |        |        | Coumarin  | 91-64-5    | 249.92 | 1.71   | 292.3    | 2       | 195.8      | 1.34    | 146.15 | 2                                       |
| 103  | 18     |        | Nicotine  | 54-11-5    | 290.45 | 1.79   | 50.3     | 0.31    | 24.3       | 0.15    | 162.26 | 0.31                                    |
| 104  |        |        | Tolbutamide   | 64-77-7    | 489.39 | 1.81   | NA       | NA      | 2601.1     | 9.62    | 270.38 | 9.62                                    |
| 105  | 21     |        | Theophylline  | 58-55-9    | 329.75 | 1.83   | NA       | NA      | 600.0      | 3.33    | 180.19 | 3.33                                    |



**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |      | Chemical                       | CAS #      | IC50x   |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|--------------------------------|------------|---------|--------|----------|---------|------------|---------|--------|---|
|      |        |      |                                |            | ug/ml   | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 106  | 14     |      | Sodium I fluoride              | 7681-49-4  | 77.68   | 1.85   | 180.1    | 4.29    | NA         | NA      | 41.99  | 4.29                                    |
| 261  | 3      |      | Ferrous sulfate                | 7720-78-7  | 281.03  | 1.85   | 319.0    | 2.1     | 978.3      | 6.44    | 151.91 | 2.1                                     |
| 262  | 47     |      | Amphetamine sulfate            | 60-13-9    | 726.02  | 1.97   | 55.3     | 0.15    | 24.0       | 0.065   | 368.54 | 0.15                                    |
| 107  | 2      |      | Acetylsalicylic acid           | 50-78-2    | 408.99  | 2.27   | 999.9    | 5.55    | 814.4      | 4.52    | 180.17 | 5.55                                    |
| 108  |        |      | Gibberellic acid               | 77-06-5    | 796.74  | 2.3    | 6304.7   | 18.2    | NA         | NA      | 346.41 | 18.2                                    |
| 109  |        |      | Frusemide                      | 54-31-9    | 770.67  | 2.33   | 2599.8   | 7.86    | 4597.6     | 13.9    | 330.76 | 7.86                                    |
| 110  |        |      | Acrylonitrile                  | 107-13-1   | 128.43  | 2.42   | 81.7     | 1.54    | 27.1       | 0.51    | 53.07  | 1.54                                    |
| 263  |        |      | Acetaldehyde                   | 75-07-0    | 107.95  | 2.45   | 1929.8   | 43.8    | NA         | NA      | 44.06  | 43.8                                    |
| 111  |        |      | Clofibrilic acid               | 882-09-7   | 560.26  | 2.61   | 1249.3   | 5.82    | 1169.9     | 5.45    | 214.66 | 5.82                                    |
| 112  | 48     |      | Caffeine                       | 58-08-2    | 512.74  | 2.64   | 192.3    | 0.99    | 619.6      | 3.19    | 194.22 | 0.99                                    |
| 264  |        |      | Chloral hydrate                | 302-17-0   | 438.31  | 2.65   | 479.7    | 2.9     | 1101.6     | 6.66    | 165.4  | 2.9                                     |
| 113  | 1      |      | Acetaminophen                  | 103-90-2   | 409.70  | 2.71   | 2403.8   | 15.9    | 338.6      | 2.24    | 151.18 | 15.9                                    |
| 265  |        |      | Streptomycin sulfate           | 298-39-5   | 3979.25 | 2.73   | NA       | NA      | 495.6      | 0.34    | 1457.6 | 0.34                                    |
| 114  |        |      | Natulan * HCl                  | 366-70-1   | 706.37  | 2.74   | 783.7    | 3.04    | NA         | NA      | 257.8  | 3.04                                    |
| 266  |        |      | Potassium hexacyanoferrate III | 13746-66-2 | 928.54  | 2.82   | NA       | NA      | 2970.0     | 9.02    | 329.27 | 9.02                                    |
| 267  |        | p-   | Hydroxybenzoic acid            | 99-96-7    | 403.34  | 2.92   | NA       | NA      | 2196.3     | 15.9    | 138.13 | 15.9                                    |
| 115  | 12     |      | Phenol                         | 108-95-2   | 283.30  | 3.01   | 414.1    | 4.4     | 300.2      | 3.19    | 94.12  | 4.4                                     |
| 268  |        | 1-   | Octanol                        | 111-87-5   | 398.60  | 3.06   | NA       | NA      | 1784.6     | 13.7    | 130.26 | 13.7                                    |
| 116  |        |      | Cyclophosphamide * H2O         | 6055-19-2  | 870.89  | 3.12   | 94.9     | 0.34    | 136.8      | 0.49    | 279.13 | 0.34                                    |
| 269  |        |      | Potassium I fluoride           | 7789-23-3  | 181.85  | 3.13   | 245.2    | 4.22    | NA         | NA      | 58.1   | 4.22                                    |
| 117  |        |      | Di(2-ethylhexyl)adipate        | 103-23-1   | 1167.52 | 3.15   | 9117.7   | 24.6    | NA         | NA      | 370.64 | 24.6                                    |
| 270  |        |      | Propionaldehyde                | 123-38-6   | 188.79  | 3.25   | 1411.6   | 24.3    | NA         | NA      | 58.09  | 24.3                                    |
| 271  |        |      | Styrene                        | 100-42-5   | 343.73  | 3.3    | 4999.7   | 48      | 315.6      | 3.03    | 104.16 | 48                                      |
| 272  |        |      | Salicylic acid                 | 69-72-7    | 466.88  | 3.38   | 890.9    | 6.45    | 479.3      | 3.47    | 138.13 | 6.45                                    |
| 273  |        |      | Bromobenzene                   | 108-86-1   | 543.29  | 3.46   | 2700.7   | 17.2    | NA         | NA      | 157.02 | 17.2                                    |
| 274  |        | L-   | Cysteine                       | 52-90-4    | 431.37  | 3.56   | NA       | NA      | 660.4      | 5.45    | 121.17 | 5.45                                    |
| 275  |        |      | Nitrilotriacetic acid          | 139-13-9   | 690.09  | 3.61   | 1470.0   | 7.69    | 3154.1     | 16.5    | 191.16 | 7.69                                    |
| 276  |        |      | Ambuphylline                   | 5634-34-4  | 988.51  | 3.67   | NA       | NA      | 600.7      | 2.23    | 269.35 | 2.23                                    |
| 118  | 24     |      | Phenobarbital                  | 50-06-6    | 884.91  | 3.81   | 162.6    | 0.7     | 167.2      | 0.72    | 232.26 | 0.7                                     |
| 277  |        |      | Potassium cyanate              | 590-28-3   | 335.84  | 4.14   | NA       | NA      | 843.6      | 10.4    | 81.12  | 10.4                                    |
| 278  |        |      | Phenylephrine * HCl            | 939-38-8   | 847.35  | 4.16   | 350.3    | 1.72    | 120.2      | 0.59    | 203.69 | 1.72                                    |
| 279  |        |      | Thioacetamide                  | 62-55-5    | 313.33  | 4.17   | 301.3    | 4.01    | NA         | NA      | 75.14  | 4.01                                    |
| 280  |        |      | Theophylline sodium acetate    | 8002-89-9  | 1098.74 | 4.19   | 582.2    | 2.22    | NA         | NA      | 262.23 | 2.22                                    |
| 281  |        | 1,2- | Dibromomethane                 | 106-93-4   | 730.17  | 4.2    | 107.8    | 0.62    | NA         | NA      | 173.85 | 0.62                                    |
| 119  |        |      | Sodium salicylate              | 54-21-7    | 693.28  | 4.33   | 1599.5   | 9.99    | 899.8      | 5.62    | 160.11 | 9.99                                    |
| 282  |        | (-)  | Phenylephrine                  | 59-42-7    | 744.17  | 4.45   | 349.5    | 2.09    | NA         | NA      | 167.23 | 2.09                                    |
| 283  |        |      | Milrinone                      | 78415-72-2 | 1007.61 | 4.77   | 90.8     | 0.43    | 137.3      | 0.65    | 211.24 | 0.43                                    |
| 120  |        | 5-   | Aminosalicic acid              | 89-57-6    | 776.47  | 5.07   | NA       | NA      | 7749.4     | 50.6    | 153.15 | 50.6                                    |
| 121  |        |      | Aminophenazone                 | 58-15-1    | 1246.87 | 5.39   | 999.3    | 4.32    | 358.6      | 1.55    | 231.33 | 4.32                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |        | Chemical                         | CAS #      | IC50x   |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|----------------------------------|------------|---------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                                  |            | ug/ml   | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 284  |        |        | Ammonium chloride                | 12125-02-9 | 295.32  | 5.52   | 1647.8   | 30.8    | NA         | NA      | 53.5   | 30.8                                    |
| 122  |        |        | Diethyl phthalate                | 84-66-2    | 1226.88 | 5.52   | 8601.5   | 38.7    | 6178.8     | 27.8    | 222.26 | 38.7                                    |
| 285  |        |        | Caffeine sodium benzoate         | 8000-95-1  | 1918.33 | 5.67   | 859.4    | 2.54    | 798.5      | 2.36    | 338.33 | 2.54                                    |
| 286  |        |        | Benzylpenicillin sodium          | 69-57-8    | 2042.17 | 5.73   | 6914.2   | 19.4    | NA         | NA      | 356.4  | 19.4                                    |
| 287  |        |        | Benzylalcohol                    | 100-51-6   | 628.35  | 5.81   | 1232.9   | 11.4    | 1579.0     | 14.6    | 108.15 | 11.4                                    |
| 288  |        | 1-     | Heptanol                         | 111-70-6   | 726.44  | 6.25   | 3254.4   | 28      | 1499.4     | 12.9    | 116.23 | 28                                      |
| 289  |        |        | Tetrachloroethene                | 127-18-4   | 1084.46 | 6.54   | 8854.8   | 53.4    | 8092.0     | 48.8    | 165.82 | 53.4                                    |
| 290  |        |        | Sodium sulfite                   | 7757-83-7  | 854.55  | 6.78   | NA       | NA      | 820.5      | 6.51    | 126.04 | 6.51                                    |
| 291  |        |        | Aniline                          | 62-53-3    | 642.67  | 6.9    | 439.6    | 4.72    | 439.6      | 4.72    | 93.14  | 4.72                                    |
| 292  |        |        | Allylalcohol                     | 107-18-6   | 403.14  | 6.94   | 63.9     | 1.1     | 95.8       | 1.65    | 58.09  | 1.1                                     |
| 293  |        |        | Diisopropylamine dichloroacetate | 660-27-5   | 1611.12 | 7      | NA       | NA      | 1700.9     | 7.39    | 230.16 | 7.39                                    |
| 123  | 35     |        | Isoniazid                        | 54-85-3    | 1027.33 | 7.49   | 650.1    | 4.74    | NA         | NA      | 137.16 | 4.74                                    |
| 294  |        |        | Trichloroacetic acid             | 76-03-9    | 1338.08 | 8.19   | 4999.4   | 30.6    | 5636.6     | 34.5    | 163.38 | 30.6                                    |
| 295  |        | 2,5-   | Hexanedione                      | 110-13-4   | 964.65  | 8.45   | 2705.6   | 23.7    | NA         | NA      | 114.16 | 23.7                                    |
| 124  |        |        | Acetazolamide                    | 59-66-5    | 1886.99 | 8.49   | NA       | NA      | 4289.6     | 19.3    | 222.26 | 19.3                                    |
| 125  | 34     |        | Carbon tetrachloride             | 56-23-5    | 1308.92 | 8.51   | 2799.3   | 18.2    | 12797.0    | 83.2    | 153.81 | 18.2                                    |
| 296  |        |        | Homatropine methylbromide        | 80-49-9    | 3332.97 | 9      | 1199.9   | 3.24    | 1399.8     | 3.78    | 370.33 | 3.24                                    |
| 297  | 11     | 1,1,1- | Trichloroethane                  | 71-55-6    | 1374.02 | 10.3   | 10298.5  | 77.2    | 11245.6    | 84.3    | 133.4  | 77.2                                    |
| 298  |        |        | Dichloroacetic acid              | 79-43-6    | 1482.81 | 11.5   | 2823.8   | 21.9    | 5518.6     | 42.8    | 128.94 | 21.9                                    |
| 299  |        |        | Imidazole                        | 288-32-4   | 783.04  | 11.5   | NA       | NA      | 1879.3     | 27.6    | 68.09  | 27.6                                    |
| 300  |        |        | Antipyrine                       | 60-80-0    | 2183.70 | 11.6   | 1799.7   | 9.56    | 1699.9     | 9.03    | 188.25 | 9.56                                    |
| 301  | 17     |        | Xylene                           | 1330-20-7  | 1274.16 | 12     | 4300.3   | 40.5    | NA         | NA      | 106.18 | 40.5                                    |
| 302  |        |        | Nitrobenzene                     | 98-95-3    | 1502.06 | 12.2   | 640.2    | 5.2     | NA         | NA      | 123.12 | 5.2                                     |
| 304  |        |        | Calcium II chloride              | 10043-52-4 | 1376.15 | 12.4   | 999.9    | 9.01    | NA         | NA      | 110.98 | 9.01                                    |
| 303  |        |        | Theophylline sodium              | 3485-82-3  | 2519.43 | 12.4   | NA       | NA      | 445.0      | 2.19    | 203.18 | 2.19                                    |
| 305  |        | n-     | Butanal                          | 123-72-8   | 923.14  | 12.8   | 2488.1   | 34.5    | NA         | NA      | 72.12  | 34.5                                    |
| 306  |        |        | Anisole                          | 100-66-3   | 1427.58 | 13.2   | 3698.7   | 34.2    | NA         | NA      | 108.15 | 34.2                                    |
| 307  |        | 2-     | Ethylbutanal                     | 97-96-1    | 1322.38 | 13.2   | 3977.1   | 39.7    | NA         | NA      | 100.18 | 39.7                                    |
| 308  | 33     |        | Chloroform                       | 67-66-3    | 1599.56 | 13.4   | 908.4    | 7.61    | 35.8       | 0.3     | 119.37 | 7.61                                    |
| 309  |        |        | Isobutanal                       | 78-84-2    | 973.62  | 13.5   | 2812.7   | 39      | NA         | NA      | 72.12  | 39                                      |
| 126  |        |        | Triethyl citrate                 | 77-93-0    | 4061.90 | 14.7   | 6990.9   | 25.3    | NA         | NA      | 276.32 | 25.3                                    |
| 310  |        |        | Tributylamine                    | 102-82-9   | 2855.16 | 15.4   | 539.5    | 2.91    | NA         | NA      | 185.4  | 2.91                                    |
| 311  |        | 1-     | Hexanol                          | 111-27-3   | 1573.88 | 15.4   | 719.5    | 7.04    | 1952.0     | 19.1    | 102.2  | 7.04                                    |
| 312  |        |        | Benzoic acid                     | 65-85-0    | 1917.44 | 15.7   | 2528.1   | 20.7    | 2369.3     | 19.4    | 122.13 | 20.7                                    |
| 313  |        |        | Xanthinol nicotinate             | 437-74-1   | 6865.26 | 15.8   | 14121.6  | 32.5    | 17336.9    | 39.9    | 434.51 | 32.5                                    |
| 314  |        |        | Saccharin                        | 81-07-2    | 3004.32 | 16.4   | NA       | NA      | 17000.0    | 92.8    | 183.19 | 92.8                                    |
| 315  |        |        | Isobenzoic furano dione          |            | 2518.04 | 17     | 4014.1   | 27.1    | 1999.6     | 13.5    | 148.12 | 27.1                                    |
| 316  |        |        | Toluene                          | 108-88-3   | 1575.77 | 17.1   | 5003.7   | 54.3    | NA         | NA      | 92.15  | 54.3                                    |
| 317  |        |        | Barbital sodium                  | 144-02-5   | 3835.32 | 18.6   | NA       | NA      | 800.1      | 3.88    | 206.2  | 3.88                                    |

**Section 7.2**  
**Table 7.1**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)**

| RC # | MEIC # |        | Chemical                        | CAS #      | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|---------------------------------|------------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                                 |            | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 318  |        |        | Trifluoroacetic acid            | 76-05-1    | 2337.62  | 20.5   | 199.6    | 1.75    | NA         | NA      | 114.03 | 1.75                                    |
| 127  |        |        | Dimethyl phthalate              | 131-11-3   | 4544.28  | 23.4   | 6894.1   | 35.5    | 7204.8     | 37.1    | 194.2  | 35.5                                    |
| 319  |        |        | Methylpentinol                  | 77-75-8    | 2336.21  | 23.8   | NA       | NA      | 525.2      | 5.35    | 98.16  | 5.35                                    |
| 320  |        | N,N-   | Dimethylacetamide               | 127-19-5   | 2108.79  | 24.2   | 5089.0   | 58.4    | 4618.4     | 53      | 87.14  | 58.4                                    |
| 321  |        |        | Acetic acid                     | 64-19-7    | 1459.46  | 24.3   | 3309.3   | 55.1    | 4961.0     | 82.6    | 60.06  | 55.1                                    |
| 322  |        | 1-     | Pentanol                        | 71-41-0    | 2195.43  | 24.9   | 3033.0   | 34.4    | 200.1      | 2.27    | 88.17  | 34.4                                    |
| 323  |        |        | Urethan                         | 51-79-6    | 2307.95  | 25.9   | NA       | NA      | 2504.0     | 28.1    | 89.11  | 28.1                                    |
| 324  |        | 2-     | Butoxyethanol                   | 111-76-2   | 3073.20  | 26     | 1477.5   | 12.5    | 1229.3     | 10.4    | 118.2  | 12.5                                    |
| 325  |        |        | Cyclohexanol                    | 108-93-0   | 2634.73  | 26.3   | 2063.7   | 20.6    | NA         | NA      | 100.18 | 20.6                                    |
| 326  |        |        | Halothane                       | 151-67-7   | 6138.83  | 31.1   | 5684.8   | 28.8    | NA         | NA      | 197.39 | 28.8                                    |
| 327  | 20     |        | Lithium I sulfate               | 10377-48-7 | 3704.98  | 33.7   | NA       | NA      | 1187.4     | 10.8    | 109.94 | 10.8                                    |
| 328  | 36     |        | Dichloromethane                 | 75-09-2    | 2964.06  | 34.9   | 1596.7   | 18.8    | NA         | NA      | 84.93  | 18.8                                    |
| 329  |        |        | Sodium cyclamate                | 139-05-9   | 7123.90  | 35.4   | 15254.0  | 75.8    | 17004.8    | 84.5    | 201.24 | 75.8                                    |
| 330  |        |        | Sulfuric acid                   | 7664-93-9  | 3530.88  | 36     | 2138.1   | 21.8    | NA         | NA      | 98.08  | 21.8                                    |
| 331  |        |        | Strontium II chloride           | 10476-85-4 | 5770.13  | 36.4   | 2251.0   | 14.2    | 3107.0     | 19.6    | 158.52 | 14.2                                    |
| 332  |        | 1,4-   | Dioxane                         | 123-91-1   | 3357.37  | 38.1   | 4203.3   | 47.7    | 5701.4     | 64.7    | 88.12  | 47.7                                    |
| 333  |        |        | Lithium I chloride              | 7447-41-8  | 1636.25  | 38.6   | 758.8    | 17.9    | 1165.7     | 27.5    | 42.39  | 17.9                                    |
| 334  |        |        | Isobutanol                      | 78-83-1    | 2973.01  | 40.1   | 2461.4   | 33.2    | NA         | NA      | 74.14  | 33.2                                    |
| 335  |        |        | Potassium hexacyano- ferrate II | 13943-58-3 | 15582.05 | 42.3   | 6409.6   | 17.4    | 5009.8     | 13.6    | 368.37 | 17.4                                    |
| 336  |        |        | Nicotinamide                    | 98-92-0    | 5423.02  | 44.4   | 3505.4   | 28.7    | NA         | NA      | 122.14 | 28.7                                    |
| 337  |        |        | Pyridine                        | 110-86-1   | 3710.26  | 46.9   | 893.9    | 11.3    | NA         | NA      | 79.11  | 11.3                                    |
| 338  |        | 1-     | Butanol                         | 71-36-3    | 3892.35  | 52.5   | 793.3    | 10.7    | NA         | NA      | 74.14  | 10.7                                    |
| 339  |        | 1-     | Nitropropane                    | 79-46-9    | 5159.47  | 57.9   | 455.4    | 5.11    | NA         | NA      | 89.11  | 5.11                                    |
| 340  |        |        | Diethylene glycol               | 111-46-6   | 6591.29  | 62.1   | 14753.5  | 139     | 23669.2    | 223     | 106.14 | 139                                     |
| 341  |        |        | Lactic acid                     | 598-82-3   | 5945.94  | 66     | 3729.7   | 41.4    | 4873.9     | 54.1    | 90.09  | 41.4                                    |
| 342  |        |        | Piperazine                      | 110-85-0   | 5789.95  | 67.2   | 1904.1   | 22.1    | 1438.9     | 16.7    | 86.16  | 22.1                                    |
| 343  |        |        | Magnesium II chloride * 6 H2O   | 7791-18-6  | 14314.43 | 70.4   | 8092.5   | 39.8    | NA         | NA      | 203.33 | 39.8                                    |
| 344  | 13     |        | Sodium chloride                 | 7647-14-5  | 4435.60  | 75.9   | 2998.0   | 51.3    | 3997.3     | 68.4    | 58.44  | 51.3                                    |
| 345  |        |        | Sodium I bromide                | 7647-15-6  | 8120.81  | 77.4   | 3504.3   | 33.4    | 6998.2     | 66.7    | 104.92 | 33.4                                    |
| 346  | 50     |        | Potassium I chloride            | 7447-40-7  | 6113.10  | 82     | 2601.8   | 34.9    | 1498.5     | 20.1    | 74.55  | 34.9                                    |
| 347  |        |        | Thiourea                        | 62-56-6    | 6547.18  | 86     | 124.9    | 1.64    | 8526.6     | 112     | 76.13  | 1.64                                    |
| 348  |        | 1-     | Propanol                        | 71-23-8    | 5800.62  | 96.5   | 5397.9   | 89.8    | NA         | NA      | 60.11  | 89.8                                    |
| 349  |        |        | Ethyl methyl ketone             | 78-93-3    | 7500.48  | 104    | 3396.9   | 47.1    | NA         | NA      | 72.12  | 47.1                                    |
| 350  |        |        | Tetrahydrofurfuryl alcohol      | 97-99-4    | 11338.65 | 111    | 2502.7   | 24.5    | 2298.4     | 22.5    | 102.15 | 24.5                                    |
| 351  |        |        | Dimethylformamide               | 68-12-2    | 8334.54  | 114    | 2800.1   | 38.3    | 3750.5     | 51.3    | 73.11  | 38.3                                    |
| 352  |        | 1,2,6- | Hexanetriol                     | 106-69-4   | 16506.60 | 123    | 15969.8  | 119     | NA         | NA      | 134.2  | 119                                     |
| 353  |        |        | Ethyl acetate                   | 141-78-6   | 11279.36 | 128    | 11015.0  | 125     | NA         | NA      | 88.12  | 125                                     |
| 128  | 10     | 2-     | Propanol                        | 67-63-0    | 10038.37 | 167    | 5842.7   | 97.2    | NA         | NA      | 60.11  | 97.2                                    |
| 354  |        | 1,3,5- | Trioxane                        | 110-88-3   | 19189.17 | 213    | 800.0    | 8.88    | NA         | NA      | 90.09  | 8.88                                    |

## Section 7.2

Table 7.1

Chemical Data from the Registry of Cytotoxicity Database (Sorted by IC50x mmol/l)

| RC # | MEIC # | Chemical           | CAS #    | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------------------|----------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |                    |          | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 355  |        | D-Glucose          | 50-99-7  | 40720.68 | 226    | 25765.7  | 143     | NA         | NA      | 180.18 | 143                                     |
| 356  |        | 2-Methoxyethanol   | 109-86-4 | 19103.61 | 251    | 2458.4   | 32.3    | NA         | NA      | 76.11  | 32.3                                    |
| 129  |        | Dimethyl sulfoxide | 75-18-3  | 19691.28 | 252    | 19691.3  | 252     | 16487.5    | 211     | 78.14  | 252                                     |
| 357  |        | Propylene glycol   | 57-55-6  | 26029.62 | 342    | 20016.9  | 263     | 23974.7    | 315     | 76.11  | 263                                     |
| 358  |        | Acetonitrile       | 75-05-8  | 15110.08 | 368    | 3798.1   | 92.5    | NA         | NA      | 41.06  | 92.5                                    |
| 130  | 9      | Ethanol            | 64-17-5  | 17464.32 | 379    | 14008.3  | 304     | 7787.5     | 169     | 46.08  | 304                                     |
| 359  |        | Acetone            | 67-64-1  | 25791.96 | 444    | 9759.1   | 168     | NA         | NA      | 58.09  | 168                                     |
| 360  | 7      | Ethylene glycol    | 107-21-1 | 34454.40 | 555    | 8567.0   | 138     | 7511.7     | 121     | 62.08  | 138                                     |
| 131  |        | Glycerol           | 56-81-5  | 57476.64 | 624    | 12619.1  | 137     | 25975.0    | 282     | 92.11  | 137                                     |
| 361  | 8      | Methanol           | 67-56-1  | 29806.50 | 930    | 13012.3  | 406     | NA         | NA      | 32.05  | 406                                     |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |      | Chemical                          | CAS #      | IC50x  |           | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|-----------------------------------|------------|--------|-----------|----------|---------|------------|---------|--------|---|
|      |        |      |                                   |            | ug/ml  | mmol/l    | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 29   | 28     |      | Mercury II chloride               | 7487-94-7  | 4.07   | 0.015     | 1.0      | 0.0037  | 10.0       | 0.037   | 271.49 | 0.0037                                  |
| 143  |        |      | Triethylene melamine              | 51-18-3    | 0.16   | 0.00078   | 1.0      | 0.005   | 14.9       | 0.073   | 204.27 | 0.005                                   |
| 177  |        |      | Busulphan                         | 55-98-1    | 11.33  | 0.046     | 1.9      | 0.0076  | 199.5      | 0.81    | 246.32 | 0.0076                                  |
| 13   |        |      | Cycloheximide                     | 66-81-9    | 0.17   | 0.00059   | 2.0      | 0.0071  | 132.3      | 0.47    | 281.39 | 0.0071                                  |
| 51   |        |      | Disulfoton                        | 298-04-4   | 30.19  | 0.11      | 2.0      | 0.0073  | 5.5        | 0.02    | 274.42 | 0.0073                                  |
| 49   |        |      | Parathion                         | 56-38-2    | 27.09  | 0.093     | 2.0      | 0.0069  | 6.1        | 0.021   | 291.28 | 0.0069                                  |
| 234  |        |      | Phenylthiourea                    | 103-85-5   | 82.20  | 0.54      | 3.0      | 0.02    | 10.0       | 0.066   | 152.23 | 0.02                                    |
| 37   |        |      | Aflatoxin B1                      | 1162-65-8  | 10.62  | 0.034     | 5.0      | 0.016   | 9.1        | 0.029   | 312.29 | 0.016                                   |
| 137  |        |      | Triethyltin chloride              | 994-31-0   | 0.11   | 0.00046   | 5.1      | 0.021   | NA         | NA      | 241.35 | 0.021                                   |
| 2    |        |      | Actinomycin D                     | 50-76-0    | 0.01   | 0.0000081 | 7.2      | 0.0057  | 12.6       | 0.01    | 1255.6 | 0.0057                                  |
| 252  | 19     |      | Potassium cyanide                 | 151-50-8   | 72.93  | 1.12      | 9.8      | 0.15    | 8.5        | 0.13    | 65.12  | 0.15                                    |
| 148  |        |      | Nitrogen mustard * HCl            | 55-86-7    | 0.50   | 0.0026    | 10.0     | 0.052   | 19.3       | 0.1     | 192.53 | 0.052                                   |
| 60   |        |      | Indomethacin                      | 53-86-1    | 57.25  | 0.16      | 12.2     | 0.034   | 19.0       | 0.053   | 357.81 | 0.034                                   |
| 14   |        |      | Mitomycin C                       | 50-07-7    | 0.28   | 0.00084   | 14.0     | 0.042   | 17.1       | 0.051   | 334.37 | 0.042                                   |
| 153  | 26     |      | Arsenic III trioxide              | 1327-53-3  | 0.83   | 0.0042    | 19.8     | 0.1     | 45.5       | 0.23    | 197.84 | 0.1                                     |
| 192  |        | 1,3- | Bis(2-chloroethyl)- 1-nitrosourea | 154-93-8   | 16.70  | 0.078     | 19.9     | 0.093   | 19.1       | 0.089   | 214.07 | 0.093                                   |
| 150  |        |      | Cis-platinum                      | 15663-27-1 | 0.84   | 0.0028    | 25.8     | 0.086   | 33.0       | 0.11    | 300.07 | 0.086                                   |
| 68   |        | 2,4- | Dinitrophenol                     | 51-28-5    | 38.67  | 0.21      | 29.5     | 0.16    | 44.2       | 0.24    | 184.12 | 0.16                                    |
| 43   |        |      | Aldrin                            | 309-00-2   | 24.45  | 0.067     | 40.1     | 0.11    | 43.8       | 0.12    | 364.9  | 0.11                                    |
| 185  |        |      | Heptachlor                        | 76-44-8    | 22.02  | 0.059     | 41.1     | 0.11    | 67.2       | 0.18    | 373.3  | 0.11                                    |
| 132  |        |      | Triphenyltin hydroxide            | 76-87-9    | 0.02   | 0.000049  | 44.0     | 0.12    | 245.9      | 0.67    | 367.03 | 0.12                                    |
| 241  |        |      | Sodium azide                      | 26628-22-8 | 46.16  | 0.71      | 44.9     | 0.69    | 27.3       | 0.42    | 65.02  | 0.69                                    |
| 207  |        |      | Dieldrin                          | 60-57-1    | 68.56  | 0.18      | 45.7     | 0.12    | 38.1       | 0.1     | 380.9  | 0.12                                    |
| 179  |        |      | Acrolein                          | 107-02-8   | 2.64   | 0.047     | 46.0     | 0.82    | 39.8       | 0.71    | 56.07  | 0.82                                    |
| 144  |        |      | Sodium bichromate VI              | 10588-01-9 | 0.24   | 0.00093   | 49.8     | 0.19    | NA         | NA      | 261.98 | 0.19                                    |
| 103  | 18     |      | Nicotine                          | 54-11-5    | 290.45 | 1.79      | 50.3     | 0.31    | 24.3       | 0.15    | 162.26 | 0.31                                    |
| 173  | 39     |      | Pentachlorophenol                 | 87-86-5    | 9.59   | 0.036     | 50.6     | 0.19    | NA         | NA      | 266.32 | 0.19                                    |
| 262  | 47     |      | Amphetamine sulfate               | 60-13-9    | 726.02 | 1.97      | 55.3     | 0.15    | 24.0       | 0.065   | 368.54 | 0.15                                    |
| 8    |        |      | Digitoxin                         | 71-63-6    | 0.08   | 0.00011   | 55.8     | 0.073   | NA         | NA      | 765.05 | 0.073                                   |
| 235  | 25     |      | Paraquat                          | 4685-14-7  | 100.58 | 0.54      | 57.7     | 0.31    | 195.6      | 1.05    | 186.25 | 0.31                                    |
| 157  | 38     |      | Hexachlorophene                   | 70-30-4    | 3.21   | 0.0079    | 61.0     | 0.15    | 65.1       | 0.16    | 406.89 | 0.15                                    |
| 292  |        |      | Allyl alcohol                     | 107-18-6   | 403.14 | 6.94      | 63.9     | 1.1     | 95.8       | 1.65    | 58.09  | 1.1                                     |
| 10   |        |      | Emetine                           | 483-18-1   | 0.08   | 0.00016   | 67.3     | 0.14    | NA         | NA      | 480.71 | 0.14                                    |
| 223  | 32     |      | Lindane                           | 58-89-9    | 119.24 | 0.41      | 75.6     | 0.26    | 87.2       | 0.3     | 290.82 | 0.26                                    |
| 255  |        |      | Sodium monochloroacetate          | 3926-62-3  | 168.90 | 1.45      | 75.7     | 0.65    | NA         | NA      | 116.48 | 0.65                                    |
| 190  |        |      | Chlorambucil                      | 305-03-3   | 23.12  | 0.076     | 76.1     | 0.25    | 100.4      | 0.33    | 304.24 | 0.25                                    |
| 149  |        |      | Chromium VI trioxide              | 1333-82-0  | 0.27   | 0.0027    | 80.0     | 0.8     | 127.0      | 1.27    | 100    | 0.8                                     |
| 180  |        | p-   | Phenylenediamine                  | 106-50-3   | 5.41   | 0.05      | 80.0     | 0.74    | NA         | NA      | 108.16 | 0.74                                    |
| 62   |        |      | Cobalt II chloride                | 7646-79-9  | 20.77  | 0.16      | 80.5     | 0.62    | 80.5       | 0.62    | 129.83 | 0.62                                    |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |      | Chemical                             | CAS #      | IC50x   |         | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|--------------------------------------|------------|---------|---------|----------|---------|------------|---------|--------|---|
|      |        |      |                                      |            | ug/ml   | mmol/l  | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 110  |        |      | Acrylonitrile                        | 107-13-1   | 128.43  | 2.42    | 81.7     | 1.54    | 27.1       | 0.51    | 53.07  | 1.54                                    |
| 237  |        |      | Beryllium II sulfate                 | 13510-49-1 | 64.09   | 0.61    | 82.0     | 0.78    | 79.9       | 0.76    | 105.07 | 0.78                                    |
| 220  |        | m-   | Dinitrobenzene                       | 99-65-0    | 65.57   | 0.39    | 82.4     | 0.49    | NA         | NA      | 168.12 | 0.49                                    |
| 229  | 22     |      | Dextropropoxyphene * HCl             | 1639-60-7  | 184.23  | 0.49    | 82.7     | 0.22    | 82.7       | 0.22    | 375.98 | 0.22                                    |
| 20   |        |      | Cadmium II chloride                  | 10108-64-2 | 1.17    | 0.0064  | 88.0     | 0.48    | 174.1      | 0.95    | 183.3  | 0.48                                    |
| 219  |        |      | Hydralazine                          | 86-54-4    | 52.87   | 0.33    | 89.7     | 0.56    | 121.8      | 0.76    | 160.2  | 0.56                                    |
| 160  |        | N-   | Methyl-N'-nitro-N-nitroso- guanidine | 70-25-7    | 1.77    | 0.012   | 89.7     | 0.61    | NA         | NA      | 147.12 | 0.61                                    |
| 283  |        |      | Milrinone                            | 78415-72-2 | 1007.61 | 4.77    | 90.8     | 0.43    | 137.3      | 0.65    | 211.24 | 0.43                                    |
| 116  |        |      | Cyclophosphamide * H2O               | 6055-19-2  | 870.89  | 3.12    | 94.9     | 0.34    | 136.8      | 0.49    | 279.13 | 0.34                                    |
| 217  |        |      | Amrinone                             | 60719-84-8 | 52.42   | 0.28    | 101.1    | 0.54    | 288.3      | 1.54    | 187.22 | 0.54                                    |
| 194  |        | p-   | Toluylendiamine                      | 95-70-5    | 11.49   | 0.094   | 101.4    | 0.83    | NA         | NA      | 122.19 | 0.83                                    |
| 74   |        |      | Nickel II chloride                   | 7718-54-9  | 34.99   | 0.27    | 105.0    | 0.81    | NA         | NA      | 129.61 | 0.81                                    |
| 281  |        | 1,2- | Dibromomethane                       | 106-93-4   | 730.17  | 4.2     | 107.8    | 0.62    | NA         | NA      | 173.85 | 0.62                                    |
| 196  | 40     |      | VerapamilHCl                         | 152-11-4   | 49.11   | 0.1     | 108.0    | 0.22    | 162.1      | 0.33    | 491.13 | 0.22                                    |
| 198  |        |      | Ioxynil                              | 1689-83-4  | 40.80   | 0.11    | 111.3    | 0.3     | NA         | NA      | 370.91 | 0.3                                     |
| 151  |        |      | Hexachlorocyclopentadiene            | 77-47-4    | 0.85    | 0.0031  | 111.8    | 0.41    | NA         | NA      | 272.75 | 0.41                                    |
| 167  |        | p,p' | DDD                                  | 72-54-8    | 7.68    | 0.024   | 112.0    | 0.35    | NA         | NA      | 320.04 | 0.35                                    |
| 61   |        | p,p' | DDT                                  | 50-29-3    | 56.72   | 0.16    | 113.4    | 0.32    | 134.7      | 0.38    | 354.48 | 0.32                                    |
| 138  |        |      | Tributyltin chloride                 | 1461-22-9  | 0.18    | 0.00054 | 120.4    | 0.37    | NA         | NA      | 325.53 | 0.37                                    |
| 232  |        | o-   | Cresol                               | 95-48-7    | 56.24   | 0.52    | 121.1    | 1.12    | 343.9      | 3.18    | 108.15 | 1.12                                    |
| 347  |        |      | Thiourea                             | 62-56-6    | 6547.18 | 86      | 124.9    | 1.64    | 8526.6     | 112     | 76.13  | 1.64                                    |
| 69   |        |      | Secobarbital sodium                  | 309-43-3   | 54.66   | 0.21    | 124.9    | 0.48    | NA         | NA      | 260.3  | 0.48                                    |
| 134  |        |      | Rotenone                             | 83-79-4    | 0.05    | 0.00013 | 130.2    | 0.33    | 351.1      | 0.89    | 394.45 | 0.33                                    |
| 9    |        |      | Amethopterin                         | 59-05-2    | 0.06    | 0.00014 | 136.4    | 0.3     | 145.4      | 0.32    | 454.5  | 0.3                                     |
| 199  |        |      | Cupric chloride                      | 7447-39-4  | 14.79   | 0.11    | 139.8    | 1.04    | 189.6      | 1.41    | 134.44 | 1.04                                    |
| 27   |        |      | Chlorpromazine                       | 50-53-3    | 4.46    | 0.014   | 140.3    | 0.44    | 261.5      | 0.82    | 318.89 | 0.44                                    |
| 96   |        |      | Cygon                                | 60-51-5    | 284.29  | 1.24    | 151.3    | 0.66    | 59.6       | 0.26    | 229.27 | 0.66                                    |
| 227  | 46     |      | Sodium oxalate                       | 62-76-0    | 58.96   | 0.44    | 155.4    | 1.16    | NA         | NA      | 134    | 1.16                                    |
| 118  | 24     |      | Phenobarbital                        | 50-06-6    | 884.91  | 3.81    | 162.6    | 0.7     | 167.2      | 0.72    | 232.26 | 0.7                                     |
| 225  |        |      | Ammonium sulfide                     | 12135-76-1 | 21.47   | 0.42    | 168.2    | 3.29    | NA         | NA      | 51.12  | 3.29                                    |
| 16   |        |      | Azaserine                            | 115-02-6   | 0.35    | 0.002   | 169.7    | 0.98    | 150.6      | 0.87    | 173.15 | 0.98                                    |
| 102  |        |      | Acrylamide                           | 79-06-1    | 114.45  | 1.61    | 169.9    | 2.39    | 169.9      | 2.39    | 71.09  | 2.39                                    |
| 64   |        |      | Bendiocarb                           | 22781-23-3 | 40.19   | 0.18    | 178.6    | 0.8     | NA         | NA      | 223.25 | 0.8                                     |
| 106  | 14     |      | Sodium I fluoride                    | 7681-49-4  | 77.68   | 1.85    | 180.1    | 4.29    | NA         | NA      | 41.99  | 4.29                                    |
| 112  | 48     |      | Caffeine                             | 58-08-2    | 512.74  | 2.64    | 192.3    | 0.99    | 619.6      | 3.19    | 194.22 | 0.99                                    |
| 253  |        |      | Isoxepac                             | 55453-87-7 | 356.81  | 1.33    | 198.5    | 0.74    | NA         | NA      | 268.28 | 0.74                                    |
| 318  |        |      | Trifluoroacetic acid                 | 76-05-1    | 2337.62 | 20.5    | 199.6    | 1.75    | NA         | NA      | 114.03 | 1.75                                    |
| 87   |        |      | Pentobarbital sodium                 | 57-33-0    | 176.29  | 0.71    | 201.1    | 0.81    | 280.6      | 1.13    | 248.29 | 0.81                                    |
| 212  |        | p-   | Cresol                               | 106-44-5   | 23.79   | 0.22    | 206.6    | 1.91    | 343.9      | 3.18    | 108.15 | 1.91                                    |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |        | Chemical  | CAS #      | IC50x   |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|---|------------|---------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |   |            | ug/ml   | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 17   |        | 5-     | Fluorouracil  | 51-21-8    | 0.34    | 0.0026 | 230.3    | 1.77    | 114.5      | 0.88    | 130.09 | 1.77                                    |
| 206  |        |        | Diquat dibromide  | 85-00-7    | 55.05   | 0.16   | 230.5    | 0.67    | 234.0      | 0.68    | 344.08 | 0.67                                    |
| 239  |        | m-     | Cresol  | 108-39-4   | 71.38   | 0.66   | 242.3    | 2.24    | 828.4      | 7.66    | 108.15 | 2.24                                    |
| 269  |        |        | Potassium I fluoride                                      | 7789-23-3  | 181.85  | 3.13   | 245.2    | 4.22    | NA         | NA      | 58.1   | 4.22                                    |
| 73   |        |        | Carbaryl  | 63-25-2    | 52.32   | 0.26   | 249.5    | 1.24    | 438.7      | 2.18    | 201.24 | 1.24                                    |
| 35   |        |        | Flufenamic acid   | 530-78-9   | 8.16    | 0.029  | 272.8    | 0.97    | 714.4      | 2.54    | 281.25 | 0.97                                    |
| 260  |        |        | Coumarin  | 91-64-5    | 249.92  | 1.71   | 292.3    | 2       | 195.8      | 1.34    | 146.15 | 2                                       |
| 228  |        | 2,4,5- | Trichlorophen- oxyacetic acid                             | 93-76-5    | 112.41  | 0.44   | 298.9    | 1.17    | 388.3      | 1.52    | 255.48 | 1.17                                    |
| 81   | 27     |        | Cupric sulfate * 5 H2O                                    | 7758-99-8  | 82.40   | 0.33   | 299.6    | 1.2     | NA         | NA      | 249.7  | 1.2                                     |
| 245  |        |        | Resorcinol  | 108-46-3   | 88.10   | 0.8    | 300.6    | 2.73    | NA         | NA      | 110.12 | 2.73                                    |
| 279  |        |        | Thioacetamide   | 62-55-5    | 313.33  | 4.17   | 301.3    | 4.01    | NA         | NA      | 75.14  | 4.01                                    |
| 38   |        |        | Imipramine * HCl  | 113-52-0   | 17.11   | 0.054  | 304.2    | 0.96    | 374.0      | 1.18    | 316.91 | 0.96                                    |
| 205  |        |        | Versalide   | 88-29-9    | 38.77   | 0.15   | 315.3    | 1.22    | NA         | NA      | 258.44 | 1.22                                    |
| 261  | 3      |        | Ferrous sulfate   | 7720-78-7  | 281.03  | 1.85   | 319.0    | 2.1     | 978.3      | 6.44    | 151.91 | 2.1                                     |
| 183  | 5      |        | Amitriptyline   | 50-48-6    | 15.54   | 0.056  | 319.1    | 1.15    | 147.0      | 0.53    | 277.44 | 1.15                                    |
| 86   | 31     |        | Warfarin  | 81-81-2    | 206.59  | 0.67   | 323.8    | 1.05    | 373.1      | 1.21    | 308.35 | 1.05                                    |
| 176  |        |        | Papaverine  | 58-74-2    | 15.27   | 0.045  | 325.8    | 0.96    | 230.8      | 0.68    | 339.42 | 0.96                                    |
| 249  |        | 3-     | Cyano-2-morpholino-5-(pyrid-4-yl)-pyridine (Chemical 122) |            | 255.66  | 0.96   | 346.2    | 1.3     | NA         | NA      | 266.31 | 1.3                                     |
| 282  |        | (-)    | Phenylephrine   | 59-42-7    | 744.17  | 4.45   | 349.5    | 2.09    | NA         | NA      | 167.23 | 2.09                                    |
| 55   |        |        | Zinc II chloride  | 7646-85-7  | 17.72   | 0.13   | 350.2    | 2.57    | 350.2      | 2.57    | 136.27 | 2.57                                    |
| 278  |        |        | Phenylephrine * HCl                                       | 939-38-8   | 847.35  | 4.16   | 350.3    | 1.72    | 120.2      | 0.59    | 203.69 | 1.72                                    |
| 210  |        | p-     | Nitrophenol   | 100-02-7   | 27.82   | 0.2    | 350.6    | 2.52    | 467.4      | 3.36    | 139.12 | 2.52                                    |
| 246  | 37     |        | Barium II nitrate   | 10022-31-8 | 211.70  | 0.81   | 355.4    | 1.36    | NA         | NA      | 261.36 | 1.36                                    |
| 90   |        |        | Iproniazid  | 54-92-2    | 141.61  | 0.79   | 365.7    | 2.04    | 681.2      | 3.8     | 179.25 | 2.04                                    |
| 254  |        |        | Buflomedil  | 55837-25-7 | 415.03  | 1.35   | 365.8    | 1.19    | NA         | NA      | 307.43 | 1.19                                    |
| 89   | 16     | 2,4-   | Dichlorophenoxy- acetic acid                              | 94-75-7    | 170.20  | 0.77   | 369.1    | 1.67    | 366.9      | 1.66    | 221.04 | 1.67                                    |
| 79   |        |        | Phenylbutazone  | 50-33-9    | 98.69   | 0.32   | 376.3    | 1.22    | 441.0      | 1.43    | 308.41 | 1.22                                    |
| 172  |        |        | Nabam   | 142-59-6   | 8.97    | 0.035  | 394.8    | 1.54    | 579.3      | 2.26    | 256.34 | 1.54                                    |
| 155  |        |        | Benzalkonium chloride                                     | 8001-54-5  | 1.90    | 0.0052 | 401.5    | 1.1     | 339.5      | 0.93    | 365    | 1.1                                     |
| 159  |        |        | Hexadecyltrimethylammoniumbromide                         | 57-09-0    | 3.24    | 0.0089 | 408.3    | 1.12    | NA         | NA      | 364.53 | 1.12                                    |
| 115  | 12     |        | Phenol  | 108-95-2   | 283.30  | 3.01   | 414.1    | 4.4     | 300.2      | 3.19    | 94.12  | 4.4                                     |
| 230  | 42     |        | Orphenadrine * HCl  | 341-69-5   | 149.88  | 0.49   | 425.2    | 1.39    | 125.4      | 0.41    | 305.88 | 1.39                                    |
| 291  |        |        | Aniline   | 62-53-3    | 642.67  | 6.9    | 439.6    | 4.72    | 439.6      | 4.72    | 93.14  | 4.72                                    |
| 75   |        |        | Trichlorfon   | 52-68-6    | 69.51   | 0.27   | 450.5    | 1.75    | 298.6      | 1.16    | 257.44 | 1.75                                    |
| 339  |        | 1-     | Nitropropane  | 79-46-9    | 5159.47 | 57.9   | 455.4    | 5.11    | NA         | NA      | 89.11  | 5.11                                    |
| 53   | 43     |        | Quindine sulfate  | 50-54-4    | 50.70   | 0.12   | 456.3    | 1.08    | 595.8      | 1.41    | 422.54 | 1.08                                    |
| 40   |        |        | Chlordan  | 57-74-9    | 24.59   | 0.06   | 458.9    | 1.12    | NA         | NA      | 409.76 | 1.12                                    |
| 163  |        |        | Cetyltrimethylammonium chloride                           | 112-02-7   | 7.61    | 0.021  | 474.4    | 1.31    | NA         | NA      | 362.16 | 1.31                                    |
| 264  |        |        | Chloral hydrate   | 302-17-0   | 438.31  | 2.65   | 479.7    | 2.9     | 1101.6     | 6.66    | 165.4  | 2.9                                     |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |        | Chemical                    | CAS #      | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|-----------------------------|------------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                             |            | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 204  |        |        | Azathioprine                | 446-86-6   | 38.82    | 0.14   | 535.2    | 1.93    | 1389.2     | 5.01    | 277.29 | 1.93                                    |
| 310  |        |        | Tributylamine               | 102-82-9   | 2855.16  | 15.4   | 539.5    | 2.91    | NA         | NA      | 185.4  | 2.91                                    |
| 187  |        | 4-     | Hexylresorcinol             | 136-77-6   | 12.44    | 0.064  | 549.9    | 2.83    | NA         | NA      | 194.3  | 2.83                                    |
| 26   |        |        | Kelthane                    | 115-32-2   | 4.45     | 0.012  | 574.2    | 1.55    | 418.6      | 1.13    | 370.48 | 1.55                                    |
| 39   |        | 2,4-   | Dichlorophenol              | 120-83-2   | 8.97     | 0.055  | 580.3    | 3.56    | 1600.7     | 9.82    | 163    | 3.56                                    |
| 280  |        |        | Theophylline sodium acetate | 8002-89-9  | 1098.74  | 4.19   | 582.2    | 2.22    | NA         | NA      | 262.23 | 2.22                                    |
| 147  |        |        | Mitoxantrone                | 65271-80-9 | 1.07     | 0.0024 | 586.8    | 1.32    | NA         | NA      | 444.54 | 1.32                                    |
| 101  |        |        | Glutethimide                | 77-21-4    | 338.97   | 1.56   | 599.7    | 2.76    | 360.7      | 1.66    | 217.29 | 2.76                                    |
| 45   |        |        | Quinine * HCl               | 130-89-2   | 27.07    | 0.075  | 620.8    | 1.72    | 1158.6     | 3.21    | 360.92 | 1.72                                    |
| 70   | 49     |        | Atropine sulfate            | 55-48-1    | 148.92   | 0.22   | 622.7    | 0.92    | 764.9      | 1.13    | 676.9  | 0.92                                    |
| 302  |        |        | Nitrobenzene                | 98-95-3    | 1502.06  | 12.2   | 640.2    | 5.2     | NA         | NA      | 123.12 | 5.2                                     |
| 123  | 35     |        | Isoniazid                   | 54-85-3    | 1027.33  | 7.49   | 650.1    | 4.74    | NA         | NA      | 137.16 | 4.74                                    |
| 256  |        |        | Tin II chloride             | 7772-99-8  | 286.28   | 1.51   | 699.6    | 3.69    | 1200.1     | 6.33    | 189.59 | 3.69                                    |
| 63   | 4      |        | Diazepam                    | 439-14-5   | 45.56    | 0.16   | 709.1    | 2.49    | 535.3      | 1.88    | 284.76 | 2.49                                    |
| 168  |        |        | Dicoumarol                  | 66-76-2    | 9.08     | 0.027  | 709.6    | 2.11    | 232.1      | 0.69    | 336.31 | 2.11                                    |
| 311  |        | 1-     | Hexanol                     | 111-27-3   | 1573.88  | 15.4   | 719.5    | 7.04    | 1952.0     | 19.1    | 102.2  | 7.04                                    |
| 174  |        |        | Ambazone                    | 539-21-9   | 9.02     | 0.038  | 749.9    | 3.16    | 999.1      | 4.21    | 237.32 | 3.16                                    |
| 242  |        | 1,2,4- | Trichlorobenzene            | 120-82-1   | 128.82   | 0.71   | 756.6    | 4.17    | 765.7      | 4.22    | 181.44 | 4.17                                    |
| 333  |        |        | Lithium I chloride          | 7447-41-8  | 1636.25  | 38.6   | 758.8    | 17.9    | 1165.7     | 27.5    | 42.39  | 17.9                                    |
| 114  |        |        | Natulan * HCl               | 366-70-1   | 706.37   | 2.74   | 783.7    | 3.04    | NA         | NA      | 257.8  | 3.04                                    |
| 48   |        |        | Mefenamic acid              | 61-68-7    | 20.99    | 0.087  | 789.1    | 3.27    | 629.8      | 2.61    | 241.31 | 3.27                                    |
| 338  |        | 1-     | Butanol                     | 71-36-3    | 3892.35  | 52.5   | 793.3    | 10.7    | NA         | NA      | 74.14  | 10.7                                    |
| 202  |        |        | Formaldehyde                | 50-00-0    | 3.60     | 0.12   | 798.8    | 26.6    | NA         | NA      | 30.03  | 26.6                                    |
| 188  |        | t-     | Butyl hydroquinone          | 1948-33-0  | 11.47    | 0.069  | 799.6    | 4.81    | 1000.8     | 6.02    | 166.24 | 4.81                                    |
| 354  |        | 1,3,5- | Trioxane                    | 110-88-3   | 19189.17 | 213    | 800.0    | 8.88    | NA         | NA      | 90.09  | 8.88                                    |
| 58   |        |        | Dihydralazine sulfate       | 7327-87-9  | 40.36    | 0.14   | 818.8    | 2.84    | 400.8      | 1.39    | 288.32 | 2.84                                    |
| 213  |        |        | Ammonium persulfate         | 7727-54-0  | 52.49    | 0.23   | 819.3    | 3.59    | NA         | NA      | 228.22 | 3.59                                    |
| 71   |        |        | Diphenhydramine * HCl       | 147-24-0   | 70.04    | 0.24   | 855.1    | 2.93    | 113.8      | 0.39    | 291.85 | 2.93                                    |
| 285  |        |        | Caffeine sodium benzoate    | 8000-95-1  | 1918.33  | 5.67   | 859.4    | 2.54    | 798.5      | 2.36    | 338.33 | 2.54                                    |
| 197  |        | p,p'   | DDE                         | 72-55-9    | 31.80    | 0.1    | 880.9    | 2.77    | NA         | NA      | 318.02 | 2.77                                    |
| 67   | 15     |        | Malathion                   | 121-75-5   | 66.08    | 0.2    | 885.4    | 2.68    | 776.4      | 2.35    | 330.38 | 2.68                                    |
| 259  |        |        | Methyl salicylate           | 119-36-8   | 258.67   | 1.7    | 887.1    | 5.83    | NA         | NA      | 152.16 | 5.83                                    |
| 184  |        |        | Butylated hydroxytoluene    | 128-37-0   | 12.34    | 0.056  | 890.4    | 4.04    | 1040.2     | 4.72    | 220.39 | 4.04                                    |
| 272  |        |        | Salicylic acid              | 69-72-7    | 466.88   | 3.38   | 890.9    | 6.45    | 479.3      | 3.47    | 138.13 | 6.45                                    |
| 337  |        |        | Pyridine                    | 110-86-1   | 3710.26  | 46.9   | 893.9    | 11.3    | NA         | NA      | 79.11  | 11.3                                    |
| 308  | 33     |        | Chloroform                  | 67-66-3    | 1599.56  | 13.4   | 908.4    | 7.61    | 35.8       | 0.3     | 119.37 | 7.61                                    |
| 44   |        |        | Hydroxyzine * HCl           | 1244-76-4  | 27.56    | 0.067  | 950.4    | 2.31    | NA         | NA      | 411.41 | 2.31                                    |
| 31   | 41     |        | Chloroquine diphosphate     | 50-63-5    | 8.77     | 0.017  | 969.9    | 1.88    | 500.4      | 0.97    | 515.92 | 1.88                                    |
| 214  |        |        | Thymol                      | 89-83-8    | 34.56    | 0.23   | 979.6    | 6.52    | 1802.9     | 12      | 150.24 | 6.52                                    |



**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |    | Chemical                                  | CAS #      | IC50x   |         | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----|---|------------|---------|---------|----------|---------|------------|---------|--------|---|
|      |        |    |   |            | ug/ml   | mmol/l  | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 65   |        |    | Oxyphenbutazone                           | 129-20-4   | 61.64   | 0.19    | 999.2    | 3.08    | 480.1      | 1.48    | 324.41 | 3.08                                    |
| 121  |        |    | Aminophenazone                            | 58-15-1    | 1246.87 | 5.39    | 999.3    | 4.32    | 358.6      | 1.55    | 231.33 | 4.32                                    |
| 80   |        | 2- | Thiouracil                                | 141-90-2   | 41.01   | 0.32    | 999.6    | 7.8     | NA         | NA      | 128.16 | 7.8                                     |
| 304  |        |    | Calcium II chloride                       | 10043-52-4 | 1376.15 | 12.4    | 999.9    | 9.01    | NA         | NA      | 110.98 | 9.01                                    |
| 107  | 2      |    | Acetylsalicylic acid                      | 50-78-2    | 408.99  | 2.27    | 999.9    | 5.55    | 814.4      | 4.52    | 180.17 | 5.55                                    |
| 233  |        |    | Ibuprofen                                 | 15687-27-1 | 107.28  | 0.52    | 1008.9   | 4.89    | 980.0      | 4.75    | 206.31 | 4.89                                    |
| 47   |        |    | Naftipramide                              | 1505-95-9  | 25.07   | 0.084   | 1029.7   | 3.45    | 1086.4     | 3.64    | 298.47 | 3.45                                    |
| 218  |        | o- | Phenylenediamine                          | 95-54-5    | 33.53   | 0.31    | 1069.7   | 9.89    | NA         | NA      | 108.16 | 9.89                                    |
| 41   |        |    | Chloroquine sulfate                       | 132-73-0   | 25.08   | 0.06    | 1086.8   | 2.6     | NA         | NA      | 418    | 2.6                                     |
| 296  |        |    | Homatropine methylbromide                 | 80-49-9    | 3332.97 | 9       | 1199.9   | 3.24    | 1399.8     | 3.78    | 370.33 | 3.24                                    |
| 152  |        | 8- | Hydroxyquinoline                          | 148-24-3   | 0.48    | 0.0033  | 1200.6   | 8.27    | NA         | NA      | 145.17 | 8.27                                    |
| 287  |        |    | Benzylalcohol                             | 100-51-6   | 628.35  | 5.81    | 1232.9   | 11.4    | 1579.0     | 14.6    | 108.15 | 11.4                                    |
| 111  |        |    | Clofibrilic acid                          | 882-09-7   | 560.26  | 2.61    | 1249.3   | 5.82    | 1169.9     | 5.45    | 214.66 | 5.82                                    |
| 226  |        |    | Dodecylbenzene sodiumsulfonate            | 25155-30-0 | 146.38  | 0.42    | 1261.6   | 3.62    | 2000.5     | 5.74    | 348.52 | 3.62                                    |
| 251  |        |    | Scopolamine * HBr                         | 6533-68-2  | 415.05  | 1.08    | 1268.2   | 3.3     | 1879.3     | 4.89    | 384.31 | 3.3                                     |
| 76   |        |    | Sodium dodecyl sulfate                    | 151-21-3   | 78.15   | 0.27    | 1288.0   | 4.45    | NA         | NA      | 289.43 | 4.45                                    |
| 191  |        |    | Dimenhydrinate                            | 523-87-5   | 35.72   | 0.076   | 1320.8   | 2.81    | 202.1      | 0.43    | 470.02 | 2.81                                    |
| 99   |        |    | Nalidixic acid                            | 389-08-2   | 348.39  | 1.5     | 1349.4   | 5.81    | 571.4      | 2.46    | 232.26 | 5.81                                    |
| 243  |        | p- | Anisidine                                 | 104-94-9   | 89.91   | 0.73    | 1404.1   | 11.4    | NA         | NA      | 123.17 | 11.4                                    |
| 270  |        |    | Propionaldehyde                           | 123-38-6   | 188.79  | 3.25    | 1411.6   | 24.3    | NA         | NA      | 58.09  | 24.3                                    |
| 164  |        |    | Oxatamide                                 | 60607-34-3 | 8.11    | 0.019   | 1412.1   | 3.31    | 9598.7     | 22.5    | 426.61 | 3.31                                    |
| 275  |        |    | Nitrilotriacetic acid                     | 139-13-9   | 690.09  | 3.61    | 1470.0   | 7.69    | 3154.1     | 16.5    | 191.16 | 7.69                                    |
| 324  |        | 2- | Butoxyethanol                             | 111-76-2   | 3073.20 | 26      | 1477.5   | 12.5    | 1229.3     | 10.4    | 118.2  | 12.5                                    |
| 56   |        |    | Manganese IIchloride *4 H2O               | 13446-34-9 | 25.73   | 0.13    | 1484.4   | 7.5     | NA         | NA      | 197.92 | 7.5                                     |
| 136  |        |    | Diethyldithiocarbamate sodium* 3H2O       | 20624-25-3 | 0.09    | 0.00039 | 1500.7   | 6.66    | 1500.7     | 6.66    | 225.33 | 6.66                                    |
| 328  | 36     |    | Dichloromethane                           | 75-09-2    | 2964.06 | 34.9    | 1596.7   | 18.8    | NA         | NA      | 84.93  | 18.8                                    |
| 119  |        |    | Sodium salicylate                         | 54-21-7    | 693.28  | 4.33    | 1599.5   | 9.99    | 899.8      | 5.62    | 160.11 | 9.99                                    |
| 166  |        |    | Triisooctylamine                          | 2757-28-0  | 8.14    | 0.023   | 1620.2   | 4.58    | NA         | NA      | 353.76 | 4.58                                    |
| 284  |        |    | Ammonium chloride                         | 12125-02-9 | 295.32  | 5.52    | 1647.8   | 30.8    | NA         | NA      | 53.5   | 30.8                                    |
| 97   |        |    | Phenacetin                                | 62-44-2    | 227.63  | 1.27    | 1650.8   | 9.21    | 1220.6     | 6.81    | 179.24 | 9.21                                    |
| 248  |        | m- | Aminophenol                               | 591-27-5   | 93.86   | 0.86    | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 42   |        | p- | Aminophenol                               | 23-30-8    | 6.77    | 0.062   | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 78   |        | 6- | Methylcoumarin                            | 92-48-8    | 49.66   | 0.31    | 1681.9   | 10.5    | NA         | NA      | 160.18 | 10.5                                    |
| 200  |        |    | Dimethylaminoethyl methacrylate (polymer) | 2867-47-2  | 17.30   | 0.11    | 1745.4   | 11.1    | NA         | NA      | 157.24 | 11.1                                    |
| 57   |        | L- | Dopa                                      | 59-92-7    | 25.64   | 0.13    | 1780.8   | 9.03    | 2366.5     | 12      | 197.21 | 9.03                                    |
| 182  |        |    | Triton X-100                              | 9002-93-1  | 35.59   | 0.055   | 1798.7   | 2.78    | NA         | NA      | 647    | 2.78                                    |
| 300  |        |    | Antipyrine                                | 60-80-0    | 2183.70 | 11.6    | 1799.7   | 9.56    | 1699.9     | 9.03    | 188.25 | 9.56                                    |
| 95   |        |    | Salicylamide                              | 65-45-2    | 148.12  | 1.08    | 1892.7   | 13.8    | 1398.9     | 10.2    | 137.15 | 13.8                                    |
| 342  |        |    | Piperazine                                | 110-85-0   | 5789.95 | 67.2    | 1904.1   | 22.1    | 1438.9     | 16.7    | 86.16  | 22.1                                    |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |      | Chemical                   | CAS #      | IC50x    |         | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|----------------------------|------------|----------|---------|----------|---------|------------|---------|--------|---|
|      |        |      |                            |            | ug/ml    | mmol/l  | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 263  |        |      | Acetaldehyde               | 75-07-0    | 107.95   | 2.45    | 1929.8   | 43.8    | NA         | NA      | 44.06  | 43.8                                    |
| 139  |        |      | Retinol                    | 68-26-8    | 0.15     | 0.00054 | 1999.8   | 6.98    | 4011.0     | 14      | 286.5  | 6.98                                    |
| 52   |        |      | all-trans-Retinoic acid    | 302-79-4   | 33.05    | 0.11    | 2001.2   | 6.66    | NA         | NA      | 300.48 | 6.66                                    |
| 325  |        |      | Cyclohexanol               | 108-93-0   | 2634.73  | 26.3    | 2063.7   | 20.6    | NA         | NA      | 100.18 | 20.6                                    |
| 330  |        |      | Sulfuric acid              | 7664-93-9  | 3530.88  | 36      | 2138.1   | 21.8    | NA         | NA      | 98.08  | 21.8                                    |
| 72   |        |      | Butylated hydroxyanisole   | 8003-24-5  | 43.26    | 0.24    | 2199.3   | 12.2    | 2001.0     | 11.1    | 180.27 | 12.2                                    |
| 165  |        |      | Isoproterenol * HCl        | 51-30-9    | 5.45     | 0.022   | 2219.8   | 8.96    | NA         | NA      | 247.75 | 8.96                                    |
| 331  |        |      | Strontium II chloride      | 10476-85-4 | 5770.13  | 36.4    | 2251.0   | 14.2    | 3107.0     | 19.6    | 158.52 | 14.2                                    |
| 113  | 1      |      | Acetaminophen              | 103-90-2   | 409.70   | 2.71    | 2403.8   | 15.9    | 338.6      | 2.24    | 151.18 | 15.9                                    |
| 356  |        | 2-   | Methoxyethanol             | 109-86-4   | 19103.61 | 251     | 2458.4   | 32.3    | NA         | NA      | 76.11  | 32.3                                    |
| 334  |        |      | Isobutanol                 | 78-83-1    | 2973.01  | 40.1    | 2461.4   | 33.2    | NA         | NA      | 74.14  | 33.2                                    |
| 305  |        | n-   | Butanal                    | 123-72-8   | 923.14   | 12.8    | 2488.1   | 34.5    | NA         | NA      | 72.12  | 34.5                                    |
| 350  |        |      | Tetrahydrofurfuryl alcohol | 97-99-4    | 11338.65 | 111     | 2502.7   | 24.5    | 2298.4     | 22.5    | 102.15 | 24.5                                    |
| 208  |        |      | Undecylenic acid           | 112-38-9   | 33.18    | 0.18    | 2506.6   | 13.6    | 8496.7     | 46.1    | 184.31 | 13.6                                    |
| 312  |        |      | Benzoic acid               | 65-85-0    | 1917.44  | 15.7    | 2528.1   | 20.7    | 2369.3     | 19.4    | 122.13 | 20.7                                    |
| 238  |        |      | Imidazolidinyl urea        | 39236-46-9 | 100.17   | 0.36    | 2598.9   | 9.34    | 3700.9     | 13.3    | 278.26 | 9.34                                    |
| 109  |        |      | Frusemide                  | 54-31-9    | 770.67   | 2.33    | 2599.8   | 7.86    | 4597.6     | 13.9    | 330.76 | 7.86                                    |
| 346  | 50     |      | Potassium I chloride       | 7447-40-7  | 6113.10  | 82      | 2601.8   | 34.9    | 1498.5     | 20.1    | 74.55  | 34.9                                    |
| 158  |        |      | Dichlorophene              | 97-23-4    | 2.23     | 0.0083  | 2691.3   | 10      | 1001.2     | 3.72    | 269.13 | 10                                      |
| 273  |        |      | Bromobenzene               | 108-86-1   | 543.29   | 3.46    | 2700.7   | 17.2    | NA         | NA      | 157.02 | 17.2                                    |
| 295  |        | 2,5- | Hexanedione                | 110-13-4   | 964.65   | 8.45    | 2705.6   | 23.7    | NA         | NA      | 114.16 | 23.7                                    |
| 125  | 34     |      | Carbon tetrachloride       | 56-23-5    | 1308.92  | 8.51    | 2799.3   | 18.2    | 12797.0    | 83.2    | 153.81 | 18.2                                    |
| 351  |        |      | Dimethylformamide          | 68-12-2    | 8334.54  | 114     | 2800.1   | 38.3    | 3750.5     | 51.3    | 73.11  | 38.3                                    |
| 309  |        |      | Isobutanol                 | 78-84-2    | 973.62   | 13.5    | 2812.7   | 39      | NA         | NA      | 72.12  | 39                                      |
| 298  |        |      | Dichloroacetic acid        | 79-43-6    | 1482.81  | 11.5    | 2823.8   | 21.9    | 5518.6     | 42.8    | 128.94 | 21.9                                    |
| 344  | 13     |      | Sodium chloride            | 7647-14-5  | 4435.60  | 75.9    | 2998.0   | 51.3    | 3997.3     | 68.4    | 58.44  | 51.3                                    |
| 322  |        | 1-   | Pentanol                   | 71-41-0    | 2195.43  | 24.9    | 3033.0   | 34.4    | 200.1      | 2.27    | 88.17  | 34.4                                    |
| 221  |        | 2-   | Nitro-p-phenylene-diamine  | 5307-14-2  | 59.73    | 0.39    | 3078.5   | 20.1    | NA         | NA      | 153.16 | 20.1                                    |
| 216  |        |      | Refortan                   |            | 78.28    | 0.25    | 3162.3   | 10.1    | NA         | NA      | 313.1  | 10.1                                    |
| 94   |        |      | Menthol                    | 89-78-1    | 148.49   | 0.95    | 3172.9   | 20.3    | NA         | NA      | 156.3  | 20.3                                    |
| 257  |        |      | Isononylaldehyde           | 5435-64-3  | 216.25   | 1.52    | 3243.8   | 22.8    | NA         | NA      | 142.27 | 22.8                                    |
| 288  |        | 1-   | Heptanol                   | 111-70-6   | 726.44   | 6.25    | 3254.4   | 28      | 1499.4     | 12.9    | 116.23 | 28                                      |
| 321  |        |      | Acetic acid                | 64-19-7    | 1459.46  | 24.3    | 3309.3   | 55.1    | 4961.0     | 82.6    | 60.06  | 55.1                                    |
| 91   | 45     |      | Chloramphenicol            | 56-75-7    | 255.29   | 0.79    | 3393.1   | 10.5    | 2640.1     | 8.17    | 323.15 | 10.5                                    |
| 349  |        |      | Ethyl methyl ketone        | 78-93-3    | 7500.48  | 104     | 3396.9   | 47.1    | NA         | NA      | 72.12  | 47.1                                    |
| 345  |        |      | Sodium I bromide           | 7647-15-6  | 8120.81  | 77.4    | 3504.3   | 33.4    | 6998.2     | 66.7    | 104.92 | 33.4                                    |
| 336  |        |      | Nicotinamide               | 98-92-0    | 5423.02  | 44.4    | 3505.4   | 28.7    | NA         | NA      | 122.14 | 28.7                                    |
| 306  |        |      | Anisole                    | 100-66-3   | 1427.58  | 13.2    | 3698.7   | 34.2    | NA         | NA      | 108.15 | 34.2                                    |
| 341  |        |      | Lactic acid                | 598-82-3   | 5945.94  | 66      | 3729.7   | 41.4    | 4873.9     | 54.1    | 90.09  | 41.4                                    |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |        | Chemical                        | CAS #      | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|---------------------------------|------------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                                 |            | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 358  |        |        | Acetonitrile                    | 75-05-8    | 15110.08 | 368    | 3798.1   | 92.5    | NA         | NA      | 41.06  | 92.5                                    |
| 211  |        |        | Catechol                        | 120-80-9   | 22.02    | 0.2    | 3887.2   | 35.3    | 259.9      | 2.36    | 110.12 | 35.3                                    |
| 307  |        | 2-     | Ethylbutanal                    | 97-96-1    | 1322.38  | 13.2   | 3977.1   | 39.7    | NA         | NA      | 100.18 | 39.7                                    |
| 315  |        |        | Isobenzoic furano dione         |            | 2518.04  | 17     | 4014.1   | 27.1    | 1999.6     | 13.5    | 148.12 | 27.1                                    |
| 332  |        | 1,4-   | Dioxane                         | 123-91-1   | 3357.37  | 38.1   | 4203.3   | 47.7    | 5701.4     | 64.7    | 88.12  | 47.7                                    |
| 301  | 17     |        | Xylene                          | 1330-20-7  | 1274.16  | 12     | 4300.3   | 40.5    | NA         | NA      | 106.18 | 40.5                                    |
| 154  |        |        | Maneb                           | 12427-38-2 | 1.12     | 0.0042 | 4500.6   | 16.9    | 3994.7     | 15      | 266.31 | 16.9                                    |
| 294  |        |        | Trichloroacetic acid            | 76-03-9    | 1338.08  | 8.19   | 4999.4   | 30.6    | 5636.6     | 34.5    | 163.38 | 30.6                                    |
| 271  |        |        | Styrene                         | 100-42-5   | 343.73   | 3.3    | 4999.7   | 48      | 315.6      | 3.03    | 104.16 | 48                                      |
| 316  |        |        | Toluene                         | 108-88-3   | 1575.77  | 17.1   | 5003.7   | 54.3    | NA         | NA      | 92.15  | 54.3                                    |
| 320  |        | N,N-   | Dimethylacetamide               | 127-19-5   | 2108.79  | 24.2   | 5089.0   | 58.4    | 4618.4     | 53      | 87.14  | 58.4                                    |
| 224  |        | n-     | Butyl benzoate                  | 136-60-7   | 73.08    | 0.41   | 5133.6   | 28.8    | NA         | NA      | 178.25 | 28.8                                    |
| 186  |        |        | Zineb                           | 12122-67-7 | 16.27    | 0.059  | 5211.3   | 18.9    | 7610.1     | 27.6    | 275.73 | 18.9                                    |
| 348  |        | 1-     | Propanol                        | 71-23-8    | 5800.62  | 96.5   | 5397.9   | 89.8    | NA         | NA      | 60.11  | 89.8                                    |
| 326  |        |        | Halothane                       | 151-67-7   | 6138.83  | 31.1   | 5684.8   | 28.8    | NA         | NA      | 197.39 | 28.8                                    |
| 128  | 10     | 2-     | Propanol                        | 67-63-0    | 10038.37 | 167    | 5842.7   | 97.2    | NA         | NA      | 60.11  | 97.2                                    |
| 50   |        |        | Trypan blue                     | 72-57-1    | 91.66    | 0.095  | 6204.2   | 6.43    | NA         | NA      | 964.88 | 6.43                                    |
| 108  |        |        | Gibberellic acid                | 77-06-5    | 796.74   | 2.3    | 6304.7   | 18.2    | NA         | NA      | 346.41 | 18.2                                    |
| 335  |        |        | Potassium hexacyano- ferrate II | 13943-58-3 | 15582.05 | 42.3   | 6409.6   | 17.4    | 5009.8     | 13.6    | 368.37 | 17.4                                    |
| 59   |        |        | Tetracycline * HCl              | 64-75-5    | 67.33    | 0.14   | 6444.6   | 13.4    | NA         | NA      | 480.94 | 13.4                                    |
| 127  |        |        | Dimethyl phthalate              | 131-11-3   | 4544.28  | 23.4   | 6894.1   | 35.5    | 7204.8     | 37.1    | 194.2  | 35.5                                    |
| 286  |        |        | Benzylpenicillin sodium         | 69-57-8    | 2042.17  | 5.73   | 6914.2   | 19.4    | NA         | NA      | 356.4  | 19.4                                    |
| 126  |        |        | Triethyl citrate                | 77-93-0    | 4061.90  | 14.7   | 6990.9   | 25.3    | NA         | NA      | 276.32 | 25.3                                    |
| 85   |        |        | Metamizol                       | 68-89-3    | 193.94   | 0.58   | 7189.2   | 21.5    | NA         | NA      | 334.38 | 21.5                                    |
| 343  |        |        | Magnesium II chloride * 6 H2O   | 7791-18-6  | 14314.43 | 70.4   | 8092.5   | 39.8    | NA         | NA      | 203.33 | 39.8                                    |
| 360  | 7      |        | Ethylene glycol                 | 107-21-1   | 34454.40 | 555    | 8567.0   | 138     | 7511.7     | 121     | 62.08  | 138                                     |
| 122  |        |        | Diethyl phthalate               | 84-66-2    | 1226.88  | 5.52   | 8601.5   | 38.7    | 6178.8     | 27.8    | 222.26 | 38.7                                    |
| 289  |        |        | Tetrachloroethene               | 127-18-4   | 1084.46  | 6.54   | 8854.8   | 53.4    | 8092.0     | 48.8    | 165.82 | 53.4                                    |
| 117  |        |        | Di(2-ethylhexyl)adipate         | 103-23-1   | 1167.52  | 3.15   | 9117.7   | 24.6    | NA         | NA      | 370.64 | 24.6                                    |
| 162  |        |        | Chlorhexidine                   | 55-56-1    | 7.58     | 0.015  | 9200.5   | 18.2    | 9857.6     | 19.5    | 505.52 | 18.2                                    |
| 359  |        |        | Acetone                         | 67-64-1    | 25791.96 | 444    | 9759.1   | 168     | NA         | NA      | 58.09  | 168                                     |
| 18   |        |        | Captan                          | 133-06-2   | 1.17     | 0.0039 | 10009.6  | 33.3    | 7003.7     | 23.3    | 300.59 | 33.3                                    |
| 297  | 11     | 1,1,1- | Trichloroethane                 | 71-55-6    | 1374.02  | 10.3   | 10298.5  | 77.2    | 11245.6    | 84.3    | 133.4  | 77.2                                    |
| 353  |        |        | Ethyl acetate                   | 141-78-6   | 11279.36 | 128    | 11015.0  | 125     | NA         | NA      | 88.12  | 125                                     |
| 100  |        | L-     | Ascorbic acid                   | 50-81-7    | 267.73   | 1.52   | 11907.1  | 67.6    | 3364.3     | 19.1    | 176.14 | 67.6                                    |
| 88   |        |        | Dibutyl phthalate               | 84-74-2    | 211.57   | 0.76   | 11998.2  | 43.1    | NA         | NA      | 278.38 | 43.1                                    |
| 131  |        |        | Glycerol                        | 56-81-5    | 57476.64 | 624    | 12619.1  | 137     | 25975.0    | 282     | 92.11  | 137                                     |
| 361  | 8      |        | Methanol                        | 67-56-1    | 29806.50 | 930    | 13012.3  | 406     | NA         | NA      | 32.05  | 406                                     |
| 130  | 9      |        | Ethanol                         | 64-17-5    | 17464.32 | 379    | 14008.3  | 304     | 7787.5     | 169     | 46.08  | 304                                     |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |        | Chemical                         | CAS #      | IC50x    |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|----------------------------------|------------|----------|----------|----------|---------|------------|---------|--------|---|
|      |        |        |                                  |            | ug/ml    | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 313  |        |        | Xanthinol nicotinate             | 437-74-1   | 6865.26  | 15.8     | 14121.6  | 32.5    | 17336.9    | 39.9    | 434.51 | 32.5                                    |
| 258  |        |        | Diethyl sebacate                 | 110-40-7   | 421.19   | 1.63     | 14470.4  | 56      | NA         | NA      | 258.4  | 56                                      |
| 340  |        |        | Diethylene glycol                | 111-46-6   | 6591.29  | 62.1     | 14753.5  | 139     | 23669.2    | 223     | 106.14 | 139                                     |
| 329  |        |        | Sodium cyclamate                 | 139-05-9   | 7123.90  | 35.4     | 15254.0  | 75.8    | 17004.8    | 84.5    | 201.24 | 75.8                                    |
| 352  |        | 1,2,6- | Hexanetriol                      | 106-69-4   | 16506.60 | 123      | 15969.8  | 119     | NA         | NA      | 134.2  | 119                                     |
| 129  |        |        | Dimethyl sulfoxide               | 75-18-3    | 19691.28 | 252      | 19691.3  | 252     | 16487.5    | 211     | 78.14  | 252                                     |
| 357  |        |        | Propylene glycol                 | 57-55-6    | 26029.62 | 342      | 20016.9  | 263     | 23974.7    | 315     | 76.11  | 263                                     |
| 355  |        |        | D-Glucose                        | 50-99-7    | 40720.68 | 226      | 25765.7  | 143     | NA         | NA      | 180.18 | 143                                     |
| 92   |        |        | Di(2-ethylhexyl)phthalate        | 117-81-7   | 328.12   | 0.84     | 31015.2  | 79.4    | 29999.6    | 76.8    | 390.62 | 79.4                                    |
| 124  |        |        | Acetazolamide                    | 59-66-5    | 1886.99  | 8.49     | NA       | NA      | 4289.6     | 19.3    | 222.26 | 19.3                                    |
| 28   |        |        | Aldosterone                      | 52-39-1    | 5.05     | 0.014    | NA       | NA      | NA         | NA      | 360.44 |   |
| 276  |        |        | Ambuphylline                     | 5634-34-4  | 988.51   | 3.67     | NA       | NA      | 600.7      | 2.23    | 269.35 | 2.23                                    |
| 3    |        |        | Aminopterin                      | 54-62-6    | 0.01     | 0.000012 | NA       | NA      | 3.0        | 0.0068  | 440.47 | 0.0068                                  |
| 120  |        | 5-     | Aminosalicylic acid              | 89-57-6    | 776.47   | 5.07     | NA       | NA      | 7749.4     | 50.6    | 153.15 | 50.6                                    |
| 84   |        |        | Amobarbital                      | 57-43-2    | 126.73   | 0.56     | NA       | NA      | 344.0      | 1.52    | 226.31 | 1.52                                    |
| 189  |        |        | Antimycin                        | 11118-72-2 | 17.52    | 0.07     | NA       | NA      | 112.6      | 0.45    | 250.27 | 0.45                                    |
| 193  |        | 5-     | Azacytidine                      | 320-67-2   | 19.29    | 0.079    | NA       | NA      | 571.5      | 2.34    | 244.24 | 2.34                                    |
| 15   |        | 8-     | Azaguanine                       | 134-58-7   | 0.20     | 0.0013   | NA       | NA      | 1500.1     | 9.86    | 152.14 | 9.86                                    |
| 317  |        |        | Barbital sodium                  | 144-02-5   | 3835.32  | 18.6     | NA       | NA      | 800.1      | 3.88    | 206.2  | 3.88                                    |
| 33   |        | p-     | Chloromercuribenzoic acid        | 59-85-8    | 8.57     | 0.024    | NA       | NA      | 25.0       | 0.07    | 357.16 | 0.07                                    |
| 215  |        |        | Chlorotetracycline               | 57-62-5    | 114.94   | 0.24     | NA       | NA      | 2500.0     | 5.22    | 478.92 | 5.22                                    |
| 77   |        |        | Cinchophen                       | 132-60-5   | 67.31    | 0.27     | NA       | NA      | NA         | NA      | 249.28 |   |
| 6    |        |        | Colchicine                       | 64-86-8    | 0.02     | 0.000054 | NA       | NA      | 6.0        | 0.015   | 399.48 | 0.015                                   |
| 66   |        |        | Cortisone                        | 53-06-5    | 68.49    | 0.19     | NA       | NA      | NA         | NA      | 360.49 |   |
| 274  |        | L-     | Cysteine                         | 52-90-4    | 431.37   | 3.56     | NA       | NA      | 660.4      | 5.45    | 121.17 | 5.45                                    |
| 19   |        |        | Cytochalasin B                   | 14930-96-2 | 2.40     | 0.005    | NA       | NA      | NA         | NA      | 479.67 |   |
| 133  |        |        | Cytochalasin D                   | 22144-77-0 | 0.05     | 0.000092 | NA       | NA      | 36.0       | 0.071   | 507.68 | 0.071                                   |
| 141  |        |        | Cytosine arabinoside             | 147-94-4   | 0.17     | 0.00068  | NA       | NA      | 3137.9     | 12.9    | 243.25 | 12.9                                    |
| 23   |        |        | Daraprim                         | 58-14-0    | 2.21     | 0.0089   | NA       | NA      | 126.9      | 0.51    | 248.74 | 0.51                                    |
| 195  |        | p,p'   | DDA                              | 83-05-6    | 27.83    | 0.099    | NA       | NA      | 590.4      | 2.1     | 281.14 | 2.1                                     |
| 34   |        |        | Diethylstilbestrol               | 56-53-1    | 6.71     | 0.025    | NA       | NA      | NA         | NA      | 268.38 |   |
| 22   | 6      |        | Digoxin                          | 20830-75-5 | 6.64     | 0.0085   | NA       | NA      | 18.0       | 0.023   | 781.05 | 0.023                                   |
| 293  |        |        | Diisopropylamine dichloroacetate | 660-27-5   | 1611.12  | 7        | NA       | NA      | 1700.9     | 7.39    | 230.16 | 7.39                                    |
| 82   | 44     |        | Diphenylhydantoin                | 57-41-0    | 98.39    | 0.39     | NA       | NA      | 199.3      | 0.79    | 252.29 | 0.79                                    |
| 11   |        |        | Doxorubicin * HCl                | 25316-40-9 | 0.19     | 0.00033  | NA       | NA      | 696.0      | 1.2     | 580.03 | 1.2                                     |
| 244  |        |        | Doxylamine succinate             | 562-10-7   | 291.38   | 0.75     | NA       | NA      | 470.1      | 1.21    | 388.51 | 1.21                                    |
| 169  |        |        | Epinephrine bitartrate           | 51-42-3    | 9.33     | 0.028    | NA       | NA      | 4.0        | 0.012   | 333.33 | 0.012                                   |
| 24   |        |        | Ethylenediamine-tetraacetic acid | 60-00-4    | 2.92     | 0.01     | NA       | NA      | NA         | NA      | 292.28 |   |
| 171  |        |        | Fumagillin                       | 297-95-0   | 14.22    | 0.031    | NA       | NA      | 1999.5     | 4.36    | 458.6  | 4.36                                    |

**Section 7.2**  
**Table 7.2**  
**Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |          | Chemical                         | CAS #      | IC50x   |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----------|----------------------------------|------------|---------|----------|----------|---------|------------|---------|--------|---|
|      |        |          |                                  |            | ug/ml   | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 222  |        |          | Glibenclamide                    | 10238-21-8 | 197.62  | 0.4      | NA       | NA      | 3250.8     | 6.58    | 494.05 | 6.58                                    |
| 32   |        |          | Hydrocortisone                   | 50-23-7    | 7.98    | 0.022    | NA       | NA      | NA         | NA      | 362.51 |   |
| 236  |        |          | Hydrogen peroxide 90%            | 7722-84-1  | 19.05   | 0.56     | NA       | NA      | 2000.4     | 58.8    | 34.02  | 58.8                                    |
| 267  |        | p-       | Hydroxybenzoic acid              | 99-96-7    | 403.34  | 2.92     | NA       | NA      | 2196.3     | 15.9    | 138.13 | 15.9                                    |
| 299  |        |          | Imidazole                        | 288-32-4   | 783.04  | 11.5     | NA       | NA      | 1879.3     | 27.6    | 68.09  | 27.6                                    |
| 46   |        |          | Lead II chloride                 | 7758-95-4  | 11.96   | 0.043    | NA       | NA      | NA         | NA      | 278.09 |   |
| 327  | 20     |          | Lithium I sulfate                | 10377-48-7 | 3704.98 | 33.7     | NA       | NA      | 1187.4     | 10.8    | 109.94 | 10.8                                    |
| 21   |        | 6-       | Mercaptopurine                   | 50-44-2    | 1.22    | 0.008    | NA       | NA      | 280.0      | 1.84    | 152.19 | 1.84                                    |
| 142  |        |          | Methylmercury chloride           | 115-09-3   | 0.18    | 0.00071  | NA       | NA      | 57.7       | 0.23    | 251.08 | 0.23                                    |
| 98   |        |          | Methylparaben                    | 99-76-3    | 216.07  | 1.42     | NA       | NA      | 1749.8     | 11.5    | 152.16 | 11.5                                    |
| 319  |        |          | Methylpentinol                   | 77-75-8    | 2336.21 | 23.8     | NA       | NA      | 525.2      | 5.35    | 98.16  | 5.35                                    |
| 175  |        |          | Norepinephrine                   | 51-41-2    | 6.60    | 0.039    | NA       | NA      | 20.3       | 0.12    | 169.2  | 0.12                                    |
| 268  |        | 1-       | Octanol                          | 111-87-5   | 398.60  | 3.06     | NA       | NA      | 1784.6     | 13.7    | 130.26 | 13.7                                    |
| 7    |        |          | Ouabain                          | 630-60-4   | 0.04    | 0.000072 | NA       | NA      | NA         | NA      | 584.73 |   |
| 240  |        |          | Pentoxifylline                   | 6493-05-6  | 183.71  | 0.66     | NA       | NA      | 1386.2     | 4.98    | 278.35 | 4.98                                    |
| 146  |        |          | Potassium bichromate VI          | 7778-50-9  | 0.59    | 0.002    | NA       | NA      | 191.2      | 0.65    | 294.2  | 0.65                                    |
| 145  |        |          | Potassium chromate VI            | 7789-00-6  | 0.29    | 0.0015   | NA       | NA      | 180.6      | 0.93    | 194.2  | 0.93                                    |
| 277  |        |          | Potassium cyanate                | 590-28-3   | 335.84  | 4.14     | NA       | NA      | 843.6      | 10.4    | 81.12  | 10.4                                    |
| 266  |        |          | Potassium hexacyanoferrate III   | 13746-66-2 | 928.54  | 2.82     | NA       | NA      | 2970.0     | 9.02    | 329.27 | 9.02                                    |
| 36   |        |          | Progesterone                     | 57-83-0    | 9.44    | 0.03     | NA       | NA      | NA         | NA      | 314.51 |   |
| 54   | 23     |          | Propranolol * HCl                | 318-98-9   | 35.50   | 0.12     | NA       | NA      | 470.4      | 1.59    | 295.84 | 1.59                                    |
| 209  |        |          | Propylparaben                    | 94-13-3    | 32.44   | 0.18     | NA       | NA      | 6325.7     | 35.1    | 180.22 | 35.1                                    |
| 12   |        |          | Puromycin                        | 53-79-2    | 0.16    | 0.00033  | NA       | NA      | 674.4      | 1.43    | 471.58 | 1.43                                    |
| 201  |        | 13-cis-  | Retinoic acid                    | 4759-48-2  | 36.06   | 0.12     | NA       | NA      | 3395.4     | 11.3    | 300.48 | 11.3                                    |
| 314  |        |          | Saccharin                        | 81-07-2    | 3004.32 | 16.4     | NA       | NA      | 17000.0    | 92.8    | 183.19 | 92.8                                    |
| 178  |        |          | Salicylanilide                   | 87-17-2    | 9.81    | 0.046    | NA       | NA      | 2409.7     | 11.3    | 213.25 | 11.3                                    |
| 161  |        |          | Silver I nitrate                 | 7761-88-8  | 2.21    | 0.013    | NA       | NA      | 49.3       | 0.29    | 169.88 | 0.29                                    |
| 30   |        |          | Sodium arsenate, dibasic         | 7778-43-0  | 2.79    | 0.015    | NA       | NA      | NA         | NA      | 185.91 |   |
| 290  |        |          | Sodium sulfite                   | 7757-83-7  | 854.55  | 6.78     | NA       | NA      | 820.5      | 6.51    | 126.04 | 6.51                                    |
| 156  |        |          | Stearyltrimethylammoniumchloride | 112-03-8   | 2.09    | 0.006    | NA       | NA      | 536.1      | 1.54    | 348.13 | 1.54                                    |
| 265  |        |          | Streptomycin sulfate             | 298-39-5   | 3979.25 | 2.73     | NA       | NA      | 495.6      | 0.34    | 1457.6 | 0.34                                    |
| 5    |        | K-       | Strophantin                      |            | 0.03    | 0.000044 | NA       | NA      | NA         | NA      | 710.9  |   |
| 93   |        |          | Sulfisoxazole                    | 127-69-5   | 227.23  | 0.85     | NA       | NA      | 6790.2     | 25.4    | 267.33 | 25.4                                    |
| 135  |        | 2,3,7,8- | Tetrachloro-dibenzo-p-dioxin     | 1746-01-6  | 0.06    | 0.0002   | NA       | NA      | 0.1        | 0.00035 | 321.96 | 0.00035                                 |
| 247  |        | (+)-     | Thalidomide                      | 731-40-8   | 209.18  | 0.81     | NA       | NA      | 400.3      | 1.55    | 258.25 | 1.55                                    |
| 203  |        |          | Thallium I acetate               | 563-68-8   | 36.88   | 0.14     | NA       | NA      | 34.2       | 0.13    | 263.42 | 0.13                                    |
| 181  | 30     |          | Thallium I sulfate               | 7446-18-6  | 27.26   | 0.054    | NA       | NA      | 28.8       | 0.057   | 504.8  | 0.057                                   |
| 105  | 21     |          | Theophylline                     | 58-55-9    | 329.75  | 1.83     | NA       | NA      | 600.0      | 3.33    | 180.19 | 3.33                                    |
| 303  |        |          | Theophylline sodium              | 3485-82-3  | 2519.43 | 12.4     | NA       | NA      | 445.0      | 2.19    | 203.18 | 2.19                                    |

## Section 7.2

Table 7.2

Chemical Data from the Registry of Cytotoxicity Database (Sorted by Rat LD50 Oral mg/kg)

| RC # | MEIC # | Chemical            | CAS #     | IC50x   |           | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|---------------------|-----------|---------|-----------|----------|---------|------------|---------|--------|---|
|      |        |                     |           | ug/ml   | mmol/l    | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 25   |        | Thio-TEPA           | 52-24-4   | 2.08    | 0.011     | NA       | NA      | 37.8       | 0.2     | 189.24 | 0.2                                     |
| 140  |        | 6-Thioguanine       | 154-42-7  | 0.10    | 0.00057   | NA       | NA      | 160.5      | 0.96    | 167.21 | 0.96                                    |
| 83   |        | Thiopental          | 76-75-5   | 133.30  | 0.55      | NA       | NA      | 601.1      | 2.48    | 242.37 | 2.48                                    |
| 170  | 29     | Thioridazine * HCl  | 130-61-0  | 11.81   | 0.029     | NA       | NA      | 358.2      | 0.88    | 407.07 | 0.88                                    |
| 104  |        | Tolbutamide         | 64-77-7   | 489.39  | 1.81      | NA       | NA      | 2601.1     | 9.62    | 270.38 | 9.62                                    |
| 1    |        | Trenimon            | 68-76-8   | 0.00    | 0.0000033 | NA       | NA      | NA         | NA      | 231.28 |   |
| 231  |        | Tween 80            | 9005-65-6 | 641.90  | 0.49      | NA       | NA      | 25021.0    | 19.1    | 1310   | 19.1                                    |
| 323  |        | Urethan             | 51-79-6   | 2307.95 | 25.9      | NA       | NA      | 2504.0     | 28.1    | 89.11  | 28.1                                    |
| 250  |        | Valproate sodium    | 1069-66-5 | 166.22  | 1         | NA       | NA      | 1695.4     | 10.2    | 166.22 | 10.2                                    |
| 4    |        | Vincristine sulfate | 2068-78-2 | 0.01    | 0.000015  | NA       | NA      | NA         | NA      | 923.14 |   |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |    | Chemical                | CAS #      | IC50x    |           | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----|-------------------------|------------|----------|-----------|----------|---------|------------|---------|--------|---|
|      |        |    |                         |            | ug/ml    | mmol/l    | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 263  |        |    | Acetaldehyde            | 75-07-0    | 107.95   | 2.45      | 1929.8   | 43.8    | NA         | NA      | 44.06  | 43.8                                    |
| 113  | 1      |    | Acetaminophen           | 103-90-2   | 409.70   | 2.71      | 2403.8   | 15.9    | 338.6      | 2.24    | 151.18 | 15.9                                    |
| 124  |        |    | Acetazolamide           | 59-66-5    | 1886.99  | 8.49      | NA       | NA      | 4289.6     | 19.3    | 222.26 | 19.3                                    |
| 321  |        |    | Acetic acid             | 64-19-7    | 1459.46  | 24.3      | 3309.3   | 55.1    | 4961.0     | 82.6    | 60.06  | 55.1                                    |
| 359  |        |    | Acetone                 | 67-64-1    | 25791.96 | 444       | 9759.1   | 168     | NA         | NA      | 58.09  | 168                                     |
| 358  |        |    | Acetonitrile            | 75-05-8    | 15110.08 | 368       | 3798.1   | 92.5    | NA         | NA      | 41.06  | 92.5                                    |
| 107  | 2      |    | Acetylsalicylic acid    | 50-78-2    | 408.99   | 2.27      | 999.9    | 5.55    | 814.4      | 4.52    | 180.17 | 5.55                                    |
| 179  |        |    | Acrolein                | 107-02-8   | 2.64     | 0.047     | 46.0     | 0.82    | 39.8       | 0.71    | 56.07  | 0.82                                    |
| 102  |        |    | Acrylamide              | 79-06-1    | 114.45   | 1.61      | 169.9    | 2.39    | 169.9      | 2.39    | 71.09  | 2.39                                    |
| 110  |        |    | Acrylonitrile           | 107-13-1   | 128.43   | 2.42      | 81.7     | 1.54    | 27.1       | 0.51    | 53.07  | 1.54                                    |
| 2    |        |    | Actinomycin D           | 50-76-0    | 0.01     | 0.0000081 | 7.2      | 0.0057  | 12.6       | 0.01    | 1255.6 | 0.0057                                  |
| 37   |        |    | Aflatoxin B1            | 1162-65-8  | 10.62    | 0.034     | 5.0      | 0.016   | 9.1        | 0.029   | 312.29 | 0.016                                   |
| 28   |        |    | Aldosterone             | 52-39-1    | 5.05     | 0.014     | NA       | NA      | NA         | NA      | 360.44 |   |
| 43   |        |    | Aldrin                  | 309-00-2   | 24.45    | 0.067     | 40.1     | 0.11    | 43.8       | 0.12    | 364.9  | 0.11                                    |
| 52   |        |    | all-trans-Retinoic acid | 302-79-4   | 33.05    | 0.11      | 2001.2   | 6.66    | NA         | NA      | 300.48 | 6.66                                    |
| 292  |        |    | Allyl alcohol           | 107-18-6   | 403.14   | 6.94      | 63.9     | 1.1     | 95.8       | 1.65    | 58.09  | 1.1                                     |
| 174  |        |    | Ambazone                | 539-21-9   | 9.02     | 0.038     | 749.9    | 3.16    | 999.1      | 4.21    | 237.32 | 3.16                                    |
| 276  |        |    | Ambuphylline            | 5634-34-4  | 988.51   | 3.67      | NA       | NA      | 600.7      | 2.23    | 269.35 | 2.23                                    |
| 9    |        |    | Amethopterin            | 59-05-2    | 0.06     | 0.00014   | 136.4    | 0.3     | 145.4      | 0.32    | 454.5  | 0.3                                     |
| 121  |        |    | Aminophenazone          | 58-15-1    | 1246.87  | 5.39      | 999.3    | 4.32    | 358.6      | 1.55    | 231.33 | 4.32                                    |
| 248  |        | m- | Aminophenol             | 591-27-5   | 93.86    | 0.86      | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 42   |        | p- | Aminophenol             | 23-30-8    | 6.77     | 0.062     | 1658.9   | 15.2    | NA         | NA      | 109.14 | 15.2                                    |
| 3    |        |    | Aminopterin             | 54-62-6    | 0.01     | 0.000012  | NA       | NA      | 3.0        | 0.0068  | 440.47 | 0.0068                                  |
| 120  |        | 5- | Aminosalicic acid       | 89-57-6    | 776.47   | 5.07      | NA       | NA      | 7749.4     | 50.6    | 153.15 | 50.6                                    |
| 183  | 5      |    | Amitriptyline           | 50-48-6    | 15.54    | 0.056     | 319.1    | 1.15    | 147.0      | 0.53    | 277.44 | 1.15                                    |
| 284  |        |    | Ammonium chloride       | 12125-02-9 | 295.32   | 5.52      | 1647.8   | 30.8    | NA         | NA      | 53.5   | 30.8                                    |
| 213  |        |    | Ammonium persulfate     | 7727-54-0  | 52.49    | 0.23      | 819.3    | 3.59    | NA         | NA      | 228.22 | 3.59                                    |
| 225  |        |    | Ammonium sulfide        | 12135-76-1 | 21.47    | 0.42      | 168.2    | 3.29    | NA         | NA      | 51.12  | 3.29                                    |
| 84   |        |    | Amobarbital             | 57-43-2    | 126.73   | 0.56      | NA       | NA      | 344.0      | 1.52    | 226.31 | 1.52                                    |
| 262  | 47     |    | Amphetamine sulfate     | 60-13-9    | 726.02   | 1.97      | 55.3     | 0.15    | 24.0       | 0.065   | 368.54 | 0.15                                    |
| 217  |        |    | Amrinone                | 60719-84-8 | 52.42    | 0.28      | 101.1    | 0.54    | 288.3      | 1.54    | 187.22 | 0.54                                    |
| 291  |        |    | Aniline                 | 62-53-3    | 642.67   | 6.9       | 439.6    | 4.72    | 439.6      | 4.72    | 93.14  | 4.72                                    |
| 243  |        | p- | Anisidine               | 104-94-9   | 89.91    | 0.73      | 1404.1   | 11.4    | NA         | NA      | 123.17 | 11.4                                    |
| 306  |        |    | Anisole                 | 100-66-3   | 1427.58  | 13.2      | 3698.7   | 34.2    | NA         | NA      | 108.15 | 34.2                                    |
| 189  |        |    | Antimycin               | 11118-72-2 | 17.52    | 0.07      | NA       | NA      | 112.6      | 0.45    | 250.27 | 0.45                                    |
| 300  |        |    | Antipyrine              | 60-80-0    | 2183.70  | 11.6      | 1799.7   | 9.56    | 1699.9     | 9.03    | 188.25 | 9.56                                    |
| 153  | 26     |    | Arsenic III trioxide    | 1327-53-3  | 0.83     | 0.0042    | 19.8     | 0.1     | 45.5       | 0.23    | 197.84 | 0.1                                     |
| 100  |        | L- | Ascorbic acid           | 50-81-7    | 267.73   | 1.52      | 11907.1  | 67.6    | 3364.3     | 19.1    | 176.14 | 67.6                                    |
| 70   | 49     |    | Atropine sulfate        | 55-48-1    | 148.92   | 0.22      | 622.7    | 0.92    | 764.9      | 1.13    | 676.9  | 0.92                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |      | Chemical                          | CAS #      | IC50x   |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|-----------------------------------|------------|---------|--------|----------|---------|------------|---------|--------|---|
|      |        |      |                                   |            | ug/ml   | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 193  |        | 5-   | Azacytidine                       | 320-67-2   | 19.29   | 0.079  | NA       | NA      | 571.5      | 2.34    | 244.24 | 2.34                                    |
| 15   |        | 8-   | Azaguanine                        | 134-58-7   | 0.20    | 0.0013 | NA       | NA      | 1500.1     | 9.86    | 152.14 | 9.86                                    |
| 16   |        |      | Azaserine                         | 115-02-6   | 0.35    | 0.002  | 169.7    | 0.98    | 150.6      | 0.87    | 173.15 | 0.98                                    |
| 204  |        |      | Azathioprine                      | 446-86-6   | 38.82   | 0.14   | 535.2    | 1.93    | 1389.2     | 5.01    | 277.29 | 1.93                                    |
| 317  |        |      | Barbital sodium                   | 144-02-5   | 3835.32 | 18.6   | NA       | NA      | 800.1      | 3.88    | 206.2  | 3.88                                    |
| 246  | 37     |      | Barium II nitrate                 | 10022-31-8 | 211.70  | 0.81   | 355.4    | 1.36    | NA         | NA      | 261.36 | 1.36                                    |
| 64   |        |      | Bendiocarb                        | 22781-23-3 | 40.19   | 0.18   | 178.6    | 0.8     | NA         | NA      | 223.25 | 0.8                                     |
| 155  |        |      | Benzalkonium chloride             | 8001-54-5  | 1.90    | 0.0052 | 401.5    | 1.1     | 339.5      | 0.93    | 365    | 1.1                                     |
| 312  |        |      | Benzoic acid                      | 65-85-0    | 1917.44 | 15.7   | 2528.1   | 20.7    | 2369.3     | 19.4    | 122.13 | 20.7                                    |
| 287  |        |      | Benzylalcohol                     | 100-51-6   | 628.35  | 5.81   | 1232.9   | 11.4    | 1579.0     | 14.6    | 108.15 | 11.4                                    |
| 286  |        |      | Benzylpenicillin sodium           | 69-57-8    | 2042.17 | 5.73   | 6914.2   | 19.4    | NA         | NA      | 356.4  | 19.4                                    |
| 237  |        |      | Beryllium II sulfate              | 13510-49-1 | 64.09   | 0.61   | 82.0     | 0.78    | 79.9       | 0.76    | 105.07 | 0.78                                    |
| 192  |        | 1,3- | Bis(2-chloroethyl)- 1-nitrosoarea | 154-93-8   | 16.70   | 0.078  | 19.9     | 0.093   | 19.1       | 0.089   | 214.07 | 0.093                                   |
| 273  |        |      | Bromobenzene                      | 108-86-1   | 543.29  | 3.46   | 2700.7   | 17.2    | NA         | NA      | 157.02 | 17.2                                    |
| 254  |        |      | Buflomedil                        | 55837-25-7 | 415.03  | 1.35   | 365.8    | 1.19    | NA         | NA      | 307.43 | 1.19                                    |
| 177  |        |      | Busulphan                         | 55-98-1    | 11.33   | 0.046  | 1.9      | 0.0076  | 199.5      | 0.81    | 246.32 | 0.0076                                  |
| 305  |        | n-   | Butanal                           | 123-72-8   | 923.14  | 12.8   | 2488.1   | 34.5    | NA         | NA      | 72.12  | 34.5                                    |
| 338  |        | 1-   | Butanol                           | 71-36-3    | 3892.35 | 52.5   | 793.3    | 10.7    | NA         | NA      | 74.14  | 10.7                                    |
| 324  |        | 2-   | Butoxyethanol                     | 111-76-2   | 3073.20 | 26     | 1477.5   | 12.5    | 1229.3     | 10.4    | 118.2  | 12.5                                    |
| 224  |        | n-   | Butyl benzoate                    | 136-60-7   | 73.08   | 0.41   | 5133.6   | 28.8    | NA         | NA      | 178.25 | 28.8                                    |
| 188  |        | t-   | Butyl hydroquinone                | 1948-33-0  | 11.47   | 0.069  | 799.6    | 4.81    | 1000.8     | 6.02    | 166.24 | 4.81                                    |
| 72   |        |      | Butylated hydroxyanisole          | 8003-24-5  | 43.26   | 0.24   | 2199.3   | 12.2    | 2001.0     | 11.1    | 180.27 | 12.2                                    |
| 184  |        |      | Butylated hydroxytoluene          | 128-37-0   | 12.34   | 0.056  | 890.4    | 4.04    | 1040.2     | 4.72    | 220.39 | 4.04                                    |
| 20   |        |      | Cadmium II chloride               | 10108-64-2 | 1.17    | 0.0064 | 88.0     | 0.48    | 174.1      | 0.95    | 183.3  | 0.48                                    |
| 112  | 48     |      | Caffeine                          | 58-08-2    | 512.74  | 2.64   | 192.3    | 0.99    | 619.6      | 3.19    | 194.22 | 0.99                                    |
| 285  |        |      | Caffeine sodium benzoate          | 8000-95-1  | 1918.33 | 5.67   | 859.4    | 2.54    | 798.5      | 2.36    | 338.33 | 2.54                                    |
| 304  |        |      | Calcium II chloride               | 10043-52-4 | 1376.15 | 12.4   | 999.9    | 9.01    | NA         | NA      | 110.98 | 9.01                                    |
| 18   |        |      | Captan                            | 133-06-2   | 1.17    | 0.0039 | 10009.6  | 33.3    | 7003.7     | 23.3    | 300.59 | 33.3                                    |
| 73   |        |      | Carbaryl                          | 63-25-2    | 52.32   | 0.26   | 249.5    | 1.24    | 438.7      | 2.18    | 201.24 | 1.24                                    |
| 125  | 34     |      | Carbon tetrachloride              | 56-23-5    | 1308.92 | 8.51   | 2799.3   | 18.2    | 12797.0    | 83.2    | 153.81 | 18.2                                    |
| 211  |        |      | Catechol                          | 120-80-9   | 22.02   | 0.2    | 3887.2   | 35.3    | 259.9      | 2.36    | 110.12 | 35.3                                    |
| 163  |        |      | Cetyltrimethylammonium chloride   | 112-02-7   | 7.61    | 0.021  | 474.4    | 1.31    | NA         | NA      | 362.16 | 1.31                                    |
| 264  |        |      | Chloral hydrate                   | 302-17-0   | 438.31  | 2.65   | 479.7    | 2.9     | 1101.6     | 6.66    | 165.4  | 2.9                                     |
| 190  |        |      | Chlorambucil                      | 305-03-3   | 23.12   | 0.076  | 76.1     | 0.25    | 100.4      | 0.33    | 304.24 | 0.25                                    |
| 91   | 45     |      | Chloramphenicol                   | 56-75-7    | 255.29  | 0.79   | 3393.1   | 10.5    | 2640.1     | 8.17    | 323.15 | 10.5                                    |
| 40   |        |      | Chlordan                          | 57-74-9    | 24.59   | 0.06   | 458.9    | 1.12    | NA         | NA      | 409.76 | 1.12                                    |
| 162  |        |      | Chlorhexidine                     | 55-56-1    | 7.58    | 0.015  | 9200.5   | 18.2    | 9857.6     | 19.5    | 505.52 | 18.2                                    |
| 308  | 33     |      | Chloroform                        | 67-66-3    | 1599.56 | 13.4   | 908.4    | 7.61    | 35.8       | 0.3     | 119.37 | 7.61                                    |
| 33   |        | p-   | Chloromercuribenzoic acid         | 59-85-8    | 8.57    | 0.024  | NA       | NA      | 25.0       | 0.07    | 357.16 | 0.07                                    |



**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |      | Chemical  | CAS #      | IC50x    |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|---|------------|----------|----------|----------|---------|------------|---------|--------|---|
|      |        |      |   |            | ug/ml    | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 31   | 41     |      | Chloroquine diphosphate                                     | 50-63-5    | 8.77     | 0.017    | 969.9    | 1.88    | 500.4      | 0.97    | 515.92 | 1.88                                    |
| 41   |        |      | Chloroquine sulfate   | 132-73-0   | 25.08    | 0.06     | 1086.8   | 2.6     | NA         | NA      | 418    | 2.6                                     |
| 215  |        |      | Chlorotetracycline  | 57-62-5    | 114.94   | 0.24     | NA       | NA      | 2500.0     | 5.22    | 478.92 | 5.22                                    |
| 27   |        |      | Chlorpromazine  | 50-53-3    | 4.46     | 0.014    | 140.3    | 0.44    | 261.5      | 0.82    | 318.89 | 0.44                                    |
| 149  |        |      | Chromium VI trioxide  | 1333-82-0  | 0.27     | 0.0027   | 80.0     | 0.8     | 127.0      | 1.27    | 100    | 0.8                                     |
| 77   |        |      | Cinchophen  | 132-60-5   | 67.31    | 0.27     | NA       | NA      | NA         | NA      | 249.28 |   |
| 150  |        |      | Cis-platinum  | 15663-27-1 | 0.84     | 0.0028   | 25.8     | 0.086   | 33.0       | 0.11    | 300.07 | 0.086                                   |
| 111  |        |      | Clofibrilic acid  | 882-09-7   | 560.26   | 2.61     | 1249.3   | 5.82    | 1169.9     | 5.45    | 214.66 | 5.82                                    |
| 62   |        |      | Cobalt II chloride  | 7646-79-9  | 20.77    | 0.16     | 80.5     | 0.62    | 80.5       | 0.62    | 129.83 | 0.62                                    |
| 6    |        |      | Colchicine  | 64-86-8    | 0.02     | 0.000054 | NA       | NA      | 6.0        | 0.015   | 399.48 | 0.015                                   |
| 66   |        |      | Cortisone   | 53-06-5    | 68.49    | 0.19     | NA       | NA      | NA         | NA      | 360.49 |   |
| 260  |        |      | Coumarin  | 91-64-5    | 249.92   | 1.71     | 292.3    | 2       | 195.8      | 1.34    | 146.15 | 2                                       |
| 239  |        | m-   | Cresol  | 108-39-4   | 71.38    | 0.66     | 242.3    | 2.24    | 828.4      | 7.66    | 108.15 | 2.24                                    |
| 232  |        | o-   | Cresol  | 95-48-7    | 56.24    | 0.52     | 121.1    | 1.12    | 343.9      | 3.18    | 108.15 | 1.12                                    |
| 212  |        | p-   | Cresol  | 106-44-5   | 23.79    | 0.22     | 206.6    | 1.91    | 343.9      | 3.18    | 108.15 | 1.91                                    |
| 199  |        |      | Cupric chloride   | 7447-39-4  | 14.79    | 0.11     | 139.8    | 1.04    | 189.6      | 1.41    | 134.44 | 1.04                                    |
| 81   | 27     |      | Cupric sulfate * 5 H2O                                      | 7758-99-8  | 82.40    | 0.33     | 299.6    | 1.2     | NA         | NA      | 249.7  | 1.2                                     |
| 249  |        | 3-   | Cyano-2-morpholino-5-(pyridin-4-yl)-pyridine (Chemical 122) |            | 255.66   | 0.96     | 346.2    | 1.3     | NA         | NA      | 266.31 | 1.3                                     |
| 325  |        |      | Cyclohexanol  | 108-93-0   | 2634.73  | 26.3     | 2063.7   | 20.6    | NA         | NA      | 100.18 | 20.6                                    |
| 13   |        |      | Cycloheximide   | 66-81-9    | 0.17     | 0.00059  | 2.0      | 0.0071  | 132.3      | 0.47    | 281.39 | 0.0071                                  |
| 116  |        |      | Cyclophosphamide * H2O                                      | 6055-19-2  | 870.89   | 3.12     | 94.9     | 0.34    | 136.8      | 0.49    | 279.13 | 0.34                                    |
| 96   |        |      | Cygon   | 60-51-5    | 284.29   | 1.24     | 151.3    | 0.66    | 59.6       | 0.26    | 229.27 | 0.66                                    |
| 274  |        | L-   | Cysteine  | 52-90-4    | 431.37   | 3.56     | NA       | NA      | 660.4      | 5.45    | 121.17 | 5.45                                    |
| 19   |        |      | Cytochalasin B  | 14930-96-2 | 2.40     | 0.005    | NA       | NA      | NA         | NA      | 479.67 |   |
| 133  |        |      | Cytochalasin D  | 22144-77-0 | 0.05     | 0.000092 | NA       | NA      | 36.0       | 0.071   | 507.68 | 0.071                                   |
| 141  |        |      | Cytosine arabinoside  | 147-94-4   | 0.17     | 0.00068  | NA       | NA      | 3137.9     | 12.9    | 243.25 | 12.9                                    |
| 355  |        |      | D-Glucose   | 50-99-7    | 40720.68 | 226      | 25765.7  | 143     | NA         | NA      | 180.18 | 143                                     |
| 23   |        |      | Daraprim  | 58-14-0    | 2.21     | 0.0089   | NA       | NA      | 126.9      | 0.51    | 248.74 | 0.51                                    |
| 195  |        | p,p' | DDA   | 83-05-6    | 27.83    | 0.099    | NA       | NA      | 590.4      | 2.1     | 281.14 | 2.1                                     |
| 167  |        | p,p' | DDD   | 72-54-8    | 7.68     | 0.024    | 112.0    | 0.35    | NA         | NA      | 320.04 | 0.35                                    |
| 197  |        | p,p' | DDE   | 72-55-9    | 31.80    | 0.1      | 880.9    | 2.77    | NA         | NA      | 318.02 | 2.77                                    |
| 61   |        | p,p' | DDT   | 50-29-3    | 56.72    | 0.16     | 113.4    | 0.32    | 134.7      | 0.38    | 354.48 | 0.32                                    |
| 229  | 22     |      | Dextropropoxyphene * HCl                                    | 1639-60-7  | 184.23   | 0.49     | 82.7     | 0.22    | 82.7       | 0.22    | 375.98 | 0.22                                    |
| 117  |        |      | Di(2-ethylhexyl)adipate                                     | 103-23-1   | 1167.52  | 3.15     | 9117.7   | 24.6    | NA         | NA      | 370.64 | 24.6                                    |
| 92   |        |      | Di(2-ethylhexyl)phthalate                                   | 117-81-7   | 328.12   | 0.84     | 31015.2  | 79.4    | 29999.6    | 76.8    | 390.62 | 79.4                                    |
| 63   | 4      |      | Diazepam  | 439-14-5   | 45.56    | 0.16     | 709.1    | 2.49    | 535.3      | 1.88    | 284.76 | 2.49                                    |
| 281  |        | 1,2- | Dibromomethane  | 106-93-4   | 730.17   | 4.2      | 107.8    | 0.62    | NA         | NA      | 173.85 | 0.62                                    |
| 88   |        |      | Dibutyl phthalate   | 84-74-2    | 211.57   | 0.76     | 11998.2  | 43.1    | NA         | NA      | 278.38 | 43.1                                    |
| 298  |        |      | Dichloroacetic acid   | 79-43-6    | 1482.81  | 11.5     | 2823.8   | 21.9    | 5518.6     | 42.8    | 128.94 | 21.9                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |      | Chemical                                  | CAS #      | IC50x    |         | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|---|------------|----------|---------|----------|---------|------------|---------|--------|---|
|      |        |      |   |            | ug/ml    | mmol/l  | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 328  | 36     |      | Dichloromethane                           | 75-09-2    | 2964.06  | 34.9    | 1596.7   | 18.8    | NA         | NA      | 84.93  | 18.8                                    |
| 158  |        |      | Dichlorophene                             | 97-23-4    | 2.23     | 0.0083  | 2691.3   | 10      | 1001.2     | 3.72    | 269.13 | 10                                      |
| 39   |        | 2,4- | Dichlorophenol                            | 120-83-2   | 8.97     | 0.055   | 580.3    | 3.56    | 1600.7     | 9.82    | 163    | 3.56                                    |
| 89   | 16     | 2,4- | Dichlorophenoxy- acetic acid              | 94-75-7    | 170.20   | 0.77    | 369.1    | 1.67    | 366.9      | 1.66    | 221.04 | 1.67                                    |
| 168  |        |      | Dicoumarol                                | 66-76-2    | 9.08     | 0.027   | 709.6    | 2.11    | 232.1      | 0.69    | 336.31 | 2.11                                    |
| 207  |        |      | Dieldrin                                  | 60-57-1    | 68.56    | 0.18    | 45.7     | 0.12    | 38.1       | 0.1     | 380.9  | 0.12                                    |
| 122  |        |      | Diethyl phthalate                         | 84-66-2    | 1226.88  | 5.52    | 8601.5   | 38.7    | 6178.8     | 27.8    | 222.26 | 38.7                                    |
| 258  |        |      | Diethyl sebacate                          | 110-40-7   | 421.19   | 1.63    | 14470.4  | 56      | NA         | NA      | 258.4  | 56                                      |
| 136  |        |      | Diethyldithiocarbamate sodium* 3H2O       | 20624-25-3 | 0.09     | 0.00039 | 1500.7   | 6.66    | 1500.7     | 6.66    | 225.33 | 6.66                                    |
| 340  |        |      | Diethylene glycol                         | 111-46-6   | 6591.29  | 62.1    | 14753.5  | 139     | 23669.2    | 223     | 106.14 | 139                                     |
| 34   |        |      | Diethylstilbestrol                        | 56-53-1    | 6.71     | 0.025   | NA       | NA      | NA         | NA      | 268.38 |   |
| 8    |        |      | Digitoxin                                 | 71-63-6    | 0.08     | 0.00011 | 55.8     | 0.073   | NA         | NA      | 765.05 | 0.073                                   |
| 22   | 6      |      | Digoxin                                   | 20830-75-5 | 6.64     | 0.0085  | NA       | NA      | 18.0       | 0.023   | 781.05 | 0.023                                   |
| 58   |        |      | Dihydralazine sulfate                     | 7327-87-9  | 40.36    | 0.14    | 818.8    | 2.84    | 400.8      | 1.39    | 288.32 | 2.84                                    |
| 293  |        |      | Diisopropylamine dichloroacetate          | 660-27-5   | 1611.12  | 7       | NA       | NA      | 1700.9     | 7.39    | 230.16 | 7.39                                    |
| 191  |        |      | Dimenhydrinate                            | 523-87-5   | 35.72    | 0.076   | 1320.8   | 2.81    | 202.1      | 0.43    | 470.02 | 2.81                                    |
| 127  |        |      | Dimethyl phthalate                        | 131-11-3   | 4544.28  | 23.4    | 6894.1   | 35.5    | 7204.8     | 37.1    | 194.2  | 35.5                                    |
| 129  |        |      | Dimethyl sulfoxide                        | 75-18-3    | 19691.28 | 252     | 19691.3  | 252     | 16487.5    | 211     | 78.14  | 252                                     |
| 320  |        | N,N- | Dimethylacetamide                         | 127-19-5   | 2108.79  | 24.2    | 5089.0   | 58.4    | 4618.4     | 53      | 87.14  | 58.4                                    |
| 200  |        |      | Dimethylaminoethyl methacrylate (polymer) | 2867-47-2  | 17.30    | 0.11    | 1745.4   | 11.1    | NA         | NA      | 157.24 | 11.1                                    |
| 351  |        |      | Dimethylformamide                         | 68-12-2    | 8334.54  | 114     | 2800.1   | 38.3    | 3750.5     | 51.3    | 73.11  | 38.3                                    |
| 220  |        | m-   | Dinitrobenzene                            | 99-65-0    | 65.57    | 0.39    | 82.4     | 0.49    | NA         | NA      | 168.12 | 0.49                                    |
| 68   |        | 2,4- | Dinitrophenol                             | 51-28-5    | 38.67    | 0.21    | 29.5     | 0.16    | 44.2       | 0.24    | 184.12 | 0.16                                    |
| 332  |        | 1,4- | Dioxane                                   | 123-91-1   | 3357.37  | 38.1    | 4203.3   | 47.7    | 5701.4     | 64.7    | 88.12  | 47.7                                    |
| 71   |        |      | Diphenhydramine * HCl                     | 147-24-0   | 70.04    | 0.24    | 855.1    | 2.93    | 113.8      | 0.39    | 291.85 | 2.93                                    |
| 82   | 44     |      | Diphenylhydantoin                         | 57-41-0    | 98.39    | 0.39    | NA       | NA      | 199.3      | 0.79    | 252.29 | 0.79                                    |
| 206  |        |      | Diquat dibromide                          | 85-00-7    | 55.05    | 0.16    | 230.5    | 0.67    | 234.0      | 0.68    | 344.08 | 0.67                                    |
| 51   |        |      | Disulfoton                                | 298-04-4   | 30.19    | 0.11    | 2.0      | 0.0073  | 5.5        | 0.02    | 274.42 | 0.0073                                  |
| 226  |        |      | Dodecylbenzene sodiumsulfonate            | 25155-30-0 | 146.38   | 0.42    | 1261.6   | 3.62    | 2000.5     | 5.74    | 348.52 | 3.62                                    |
| 57   |        | L-   | Dopa                                      | 59-92-7    | 25.64    | 0.13    | 1780.8   | 9.03    | 2366.5     | 12      | 197.21 | 9.03                                    |
| 11   |        |      | Doxorubicin * HCl                         | 25316-40-9 | 0.19     | 0.00033 | NA       | NA      | 696.0      | 1.2     | 580.03 | 1.2                                     |
| 244  |        |      | Doxylamine succinate                      | 562-10-7   | 291.38   | 0.75    | NA       | NA      | 470.1      | 1.21    | 388.51 | 1.21                                    |
| 10   |        |      | Emetine                                   | 483-18-1   | 0.08     | 0.00016 | 67.3     | 0.14    | NA         | NA      | 480.71 | 0.14                                    |
| 169  |        |      | Epinephrine bitartrate                    | 51-42-3    | 9.33     | 0.028   | NA       | NA      | 4.0        | 0.012   | 333.33 | 0.012                                   |
| 130  | 9      |      | Ethanol                                   | 64-17-5    | 17464.32 | 379     | 14008.3  | 304     | 7787.5     | 169     | 46.08  | 304                                     |
| 353  |        |      | Ethyl acetate                             | 141-78-6   | 11279.36 | 128     | 11015.0  | 125     | NA         | NA      | 88.12  | 125                                     |
| 349  |        |      | Ethyl methyl ketone                       | 78-93-3    | 7500.48  | 104     | 3396.9   | 47.1    | NA         | NA      | 72.12  | 47.1                                    |
| 307  |        | 2-   | Ethylbutanal                              | 97-96-1    | 1322.38  | 13.2    | 3977.1   | 39.7    | NA         | NA      | 100.18 | 39.7                                    |
| 360  | 7      |      | Ethylene glycol                           | 107-21-1   | 34454.40 | 555     | 8567.0   | 138     | 7511.7     | 121     | 62.08  | 138                                     |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |        | Chemical                          | CAS #      | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|-----------------------------------|------------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                                   |            | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 24   |        |        | Ethylenediamine-tetraacetic acid  | 60-00-4    | 2.92     | 0.01   | NA       | NA      | NA         | NA      | 292.28 |   |
| 261  | 3      |        | Ferrous sulfate                   | 7720-78-7  | 281.03   | 1.85   | 319.0    | 2.1     | 978.3      | 6.44    | 151.91 | 2.1                                     |
| 35   |        |        | Flufenamic acid                   | 530-78-9   | 8.16     | 0.029  | 272.8    | 0.97    | 714.4      | 2.54    | 281.25 | 0.97                                    |
| 17   |        | 5-     | Fluorouracil                      | 51-21-8    | 0.34     | 0.0026 | 230.3    | 1.77    | 114.5      | 0.88    | 130.09 | 1.77                                    |
| 202  |        |        | Formaldehyde                      | 50-00-0    | 3.60     | 0.12   | 798.8    | 26.6    | NA         | NA      | 30.03  | 26.6                                    |
| 109  |        |        | Frusemide                         | 54-31-9    | 770.67   | 2.33   | 2599.8   | 7.86    | 4597.6     | 13.9    | 330.76 | 7.86                                    |
| 171  |        |        | Fumagillin                        | 297-95-0   | 14.22    | 0.031  | NA       | NA      | 1999.5     | 4.36    | 458.6  | 4.36                                    |
| 108  |        |        | Gibberellic acid                  | 77-06-5    | 796.74   | 2.3    | 6304.7   | 18.2    | NA         | NA      | 346.41 | 18.2                                    |
| 222  |        |        | Glibenclamide                     | 10238-21-8 | 197.62   | 0.4    | NA       | NA      | 3250.8     | 6.58    | 494.05 | 6.58                                    |
| 101  |        |        | Glutethimide                      | 77-21-4    | 338.97   | 1.56   | 599.7    | 2.76    | 360.7      | 1.66    | 217.29 | 2.76                                    |
| 131  |        |        | Glycerol                          | 56-81-5    | 57476.64 | 624    | 12619.1  | 137     | 25975.0    | 282     | 92.11  | 137                                     |
| 326  |        |        | Halothane                         | 151-67-7   | 6138.83  | 31.1   | 5684.8   | 28.8    | NA         | NA      | 197.39 | 28.8                                    |
| 185  |        |        | Heptachlor                        | 76-44-8    | 22.02    | 0.059  | 41.1     | 0.11    | 67.2       | 0.18    | 373.3  | 0.11                                    |
| 288  |        | 1-     | Heptanol                          | 111-70-6   | 726.44   | 6.25   | 3254.4   | 28      | 1499.4     | 12.9    | 116.23 | 28                                      |
| 151  |        |        | Hexachlorocyclopentadiene         | 77-47-4    | 0.85     | 0.0031 | 111.8    | 0.41    | NA         | NA      | 272.75 | 0.41                                    |
| 157  | 38     |        | Hexachlorophene                   | 70-30-4    | 3.21     | 0.0079 | 61.0     | 0.15    | 65.1       | 0.16    | 406.89 | 0.15                                    |
| 159  |        |        | Hexadecyltrimethylammoniumbromide | 57-09-0    | 3.24     | 0.0089 | 408.3    | 1.12    | NA         | NA      | 364.53 | 1.12                                    |
| 295  |        | 2,5-   | Hexanedione                       | 110-13-4   | 964.65   | 8.45   | 2705.6   | 23.7    | NA         | NA      | 114.16 | 23.7                                    |
| 352  |        | 1,2,6- | Hexanetriol                       | 106-69-4   | 16506.60 | 123    | 15969.8  | 119     | NA         | NA      | 134.2  | 119                                     |
| 311  |        | 1-     | Hexanol                           | 111-27-3   | 1573.88  | 15.4   | 719.5    | 7.04    | 1952.0     | 19.1    | 102.2  | 7.04                                    |
| 187  |        | 4-     | Hexylresorcinol                   | 136-77-6   | 12.44    | 0.064  | 549.9    | 2.83    | NA         | NA      | 194.3  | 2.83                                    |
| 296  |        |        | Homatropine methylbromide         | 80-49-9    | 3332.97  | 9      | 1199.9   | 3.24    | 1399.8     | 3.78    | 370.33 | 3.24                                    |
| 219  |        |        | Hydralazine                       | 86-54-4    | 52.87    | 0.33   | 89.7     | 0.56    | 121.8      | 0.76    | 160.2  | 0.56                                    |
| 32   |        |        | Hydrocortisone                    | 50-23-7    | 7.98     | 0.022  | NA       | NA      | NA         | NA      | 362.51 |   |
| 236  |        |        | Hydrogen peroxide 90%             | 7722-84-1  | 19.05    | 0.56   | NA       | NA      | 2000.4     | 58.8    | 34.02  | 58.8                                    |
| 267  |        | p-     | Hydroxybenzoic acid               | 99-96-7    | 403.34   | 2.92   | NA       | NA      | 2196.3     | 15.9    | 138.13 | 15.9                                    |
| 152  |        | 8-     | Hydroxyquinoline                  | 148-24-3   | 0.48     | 0.0033 | 1200.6   | 8.27    | NA         | NA      | 145.17 | 8.27                                    |
| 44   |        |        | Hydroxyzine * HCl                 | 1244-76-4  | 27.56    | 0.067  | 950.4    | 2.31    | NA         | NA      | 411.41 | 2.31                                    |
| 233  |        |        | Ibuprofen                         | 15687-27-1 | 107.28   | 0.52   | 1008.9   | 4.89    | 980.0      | 4.75    | 206.31 | 4.89                                    |
| 299  |        |        | Imidazole                         | 288-32-4   | 783.04   | 11.5   | NA       | NA      | 1879.3     | 27.6    | 68.09  | 27.6                                    |
| 238  |        |        | Imidazolidinyl urea               | 39236-46-9 | 100.17   | 0.36   | 2598.9   | 9.34    | 3700.9     | 13.3    | 278.26 | 9.34                                    |
| 38   |        |        | Imipramine * HCl                  | 113-52-0   | 17.11    | 0.054  | 304.2    | 0.96    | 374.0      | 1.18    | 316.91 | 0.96                                    |
| 60   |        |        | Indomethacin                      | 53-86-1    | 57.25    | 0.16   | 12.2     | 0.034   | 19.0       | 0.053   | 357.81 | 0.034                                   |
| 198  |        |        | Ioxynil                           | 1689-83-4  | 40.80    | 0.11   | 111.3    | 0.3     | NA         | NA      | 370.91 | 0.3                                     |
| 90   |        |        | Iproniazid                        | 54-92-2    | 141.61   | 0.79   | 365.7    | 2.04    | 681.2      | 3.8     | 179.25 | 2.04                                    |
| 315  |        |        | Isobenzoic furano dione           |            | 2518.04  | 17     | 4014.1   | 27.1    | 1999.6     | 13.5    | 148.12 | 27.1                                    |
| 309  |        |        | Isobutanal                        | 78-84-2    | 973.62   | 13.5   | 2812.7   | 39      | NA         | NA      | 72.12  | 39                                      |
| 334  |        |        | Isobutanol                        | 78-83-1    | 2973.01  | 40.1   | 2461.4   | 33.2    | NA         | NA      | 74.14  | 33.2                                    |
| 123  | 35     |        | Isoniazid                         | 54-85-3    | 1027.33  | 7.49   | 650.1    | 4.74    | NA         | NA      | 137.16 | 4.74                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # | Chemical                               | CAS #      | IC50x    |         | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--|------------|----------|---------|----------|---------|------------|---------|--------|---|
|      |        |  |            | ug/ml    | mmol/l  | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 257  |        | Isononylaldehyde                       | 5435-64-3  | 216.25   | 1.52    | 3243.8   | 22.8    | NA         | NA      | 142.27 | 22.8                                    |
| 165  |        | Isoproterenol * HCl                    | 51-30-9    | 5.45     | 0.022   | 2219.8   | 8.96    | NA         | NA      | 247.75 | 8.96                                    |
| 253  |        | Isoxepac                               | 55453-87-7 | 356.81   | 1.33    | 198.5    | 0.74    | NA         | NA      | 268.28 | 0.74                                    |
| 26   |        | Kelthane                               | 115-32-2   | 4.45     | 0.012   | 574.2    | 1.55    | 418.6      | 1.13    | 370.48 | 1.55                                    |
| 341  |        | Lactic acid                            | 598-82-3   | 5945.94  | 66      | 3729.7   | 41.4    | 4873.9     | 54.1    | 90.09  | 41.4                                    |
| 46   |        | Lead II chloride                       | 7758-95-4  | 11.96    | 0.043   | NA       | NA      | NA         | NA      | 278.09 |   |
| 223  | 32     | Lindane                                | 58-89-9    | 119.24   | 0.41    | 75.6     | 0.26    | 87.2       | 0.3     | 290.82 | 0.26                                    |
| 333  |        | Lithium I chloride                     | 7447-41-8  | 1636.25  | 38.6    | 758.8    | 17.9    | 1165.7     | 27.5    | 42.39  | 17.9                                    |
| 327  | 20     | Lithium I sulfate                      | 10377-48-7 | 3704.98  | 33.7    | NA       | NA      | 1187.4     | 10.8    | 109.94 | 10.8                                    |
| 343  |        | Magnesium II chloride * 6 H2O          | 7791-18-6  | 14314.43 | 70.4    | 8092.5   | 39.8    | NA         | NA      | 203.33 | 39.8                                    |
| 67   | 15     | Malathion                              | 121-75-5   | 66.08    | 0.2     | 885.4    | 2.68    | 776.4      | 2.35    | 330.38 | 2.68                                    |
| 154  |        | Maneb                                  | 12427-38-2 | 1.12     | 0.0042  | 4500.6   | 16.9    | 3994.7     | 15      | 266.31 | 16.9                                    |
| 56   |        | Manganese IIchloride *4 H2O            | 13446-34-9 | 25.73    | 0.13    | 1484.4   | 7.5     | NA         | NA      | 197.92 | 7.5                                     |
| 48   |        | Mefenamic acid                         | 61-68-7    | 20.99    | 0.087   | 789.1    | 3.27    | 629.8      | 2.61    | 241.31 | 3.27                                    |
| 94   |        | Menthol                                | 89-78-1    | 148.49   | 0.95    | 3172.9   | 20.3    | NA         | NA      | 156.3  | 20.3                                    |
| 21   |        | 6-Mercaptopurine                       | 50-44-2    | 1.22     | 0.008   | NA       | NA      | 280.0      | 1.84    | 152.19 | 1.84                                    |
| 29   | 28     | Mercury II chloride                    | 7487-94-7  | 4.07     | 0.015   | 1.0      | 0.0037  | 10.0       | 0.037   | 271.49 | 0.0037                                  |
| 85   |        | Metamizol                              | 68-89-3    | 193.94   | 0.58    | 7189.2   | 21.5    | NA         | NA      | 334.38 | 21.5                                    |
| 361  | 8      | Methanol                               | 67-56-1    | 29806.50 | 930     | 13012.3  | 406     | NA         | NA      | 32.05  | 406                                     |
| 356  |        | 2-Methoxyethanol                       | 109-86-4   | 19103.61 | 251     | 2458.4   | 32.3    | NA         | NA      | 76.11  | 32.3                                    |
| 259  |        | Methyl salicylate                      | 119-36-8   | 258.67   | 1.7     | 887.1    | 5.83    | NA         | NA      | 152.16 | 5.83                                    |
| 160  |        | N-Methyl-N'-nitro-N-nitroso- guanidine | 70-25-7    | 1.77     | 0.012   | 89.7     | 0.61    | NA         | NA      | 147.12 | 0.61                                    |
| 78   |        | 6-Methylcoumarin                       | 92-48-8    | 49.66    | 0.31    | 1681.9   | 10.5    | NA         | NA      | 160.18 | 10.5                                    |
| 142  |        | Methylmercury chloride                 | 115-09-3   | 0.18     | 0.00071 | NA       | NA      | 57.7       | 0.23    | 251.08 | 0.23                                    |
| 98   |        | Methylparaben                          | 99-76-3    | 216.07   | 1.42    | NA       | NA      | 1749.8     | 11.5    | 152.16 | 11.5                                    |
| 319  |        | Methylpentinol                         | 77-75-8    | 2336.21  | 23.8    | NA       | NA      | 525.2      | 5.35    | 98.16  | 5.35                                    |
| 283  |        | Milrinone                              | 78415-72-2 | 1007.61  | 4.77    | 90.8     | 0.43    | 137.3      | 0.65    | 211.24 | 0.43                                    |
| 14   |        | Mitomycin C                            | 50-07-7    | 0.28     | 0.00084 | 14.0     | 0.042   | 17.1       | 0.051   | 334.37 | 0.042                                   |
| 147  |        | Mitoxantrone                           | 65271-80-9 | 1.07     | 0.0024  | 586.8    | 1.32    | NA         | NA      | 444.54 | 1.32                                    |
| 172  |        | Nabam                                  | 142-59-6   | 8.97     | 0.035   | 394.8    | 1.54    | 579.3      | 2.26    | 256.34 | 1.54                                    |
| 47   |        | Naftipramide                           | 1505-95-9  | 25.07    | 0.084   | 1029.7   | 3.45    | 1086.4     | 3.64    | 298.47 | 3.45                                    |
| 99   |        | Nalidixic acid                         | 389-08-2   | 348.39   | 1.5     | 1349.4   | 5.81    | 571.4      | 2.46    | 232.26 | 5.81                                    |
| 114  |        | Natulan * HCl                          | 366-70-1   | 706.37   | 2.74    | 783.7    | 3.04    | NA         | NA      | 257.8  | 3.04                                    |
| 74   |        | Nickel II chloride                     | 7718-54-9  | 34.99    | 0.27    | 105.0    | 0.81    | NA         | NA      | 129.61 | 0.81                                    |
| 336  |        | Nicotinamide                           | 98-92-0    | 5423.02  | 44.4    | 3505.4   | 28.7    | NA         | NA      | 122.14 | 28.7                                    |
| 103  | 18     | Nicotine                               | 54-11-5    | 290.45   | 1.79    | 50.3     | 0.31    | 24.3       | 0.15    | 162.26 | 0.31                                    |
| 275  |        | Nitriiotriacetic acid                  | 139-13-9   | 690.09   | 3.61    | 1470.0   | 7.69    | 3154.1     | 16.5    | 191.16 | 7.69                                    |
| 221  |        | 2-Nitro-p-phenylene-diamine            | 5307-14-2  | 59.73    | 0.39    | 3078.5   | 20.1    | NA         | NA      | 153.16 | 20.1                                    |
| 302  |        | Nitrobenzene                           | 98-95-3    | 1502.06  | 12.2    | 640.2    | 5.2     | NA         | NA      | 123.12 | 5.2                                     |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |      | Chemical                        | CAS #      | IC50x    |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|------|---------------------------------|------------|----------|----------|----------|---------|------------|---------|--------|---|
|      |        |      |                                 |            | ug/ml    | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 148  |        |      | Nitrogen mustard * HCl          | 55-86-7    | 0.50     | 0.0026   | 10.0     | 0.052   | 19.3       | 0.1     | 192.53 | 0.052                                   |
| 210  |        | p-   | Nitrophenol                     | 100-02-7   | 27.82    | 0.2      | 350.6    | 2.52    | 467.4      | 3.36    | 139.12 | 2.52                                    |
| 339  |        | 1-   | Nitropropane                    | 79-46-9    | 5159.47  | 57.9     | 455.4    | 5.11    | NA         | NA      | 89.11  | 5.11                                    |
| 175  |        |      | Norepinephrine                  | 51-41-2    | 6.60     | 0.039    | NA       | NA      | 20.3       | 0.12    | 169.2  | 0.12                                    |
| 268  |        | 1-   | Octanol                         | 111-87-5   | 398.60   | 3.06     | NA       | NA      | 1784.6     | 13.7    | 130.26 | 13.7                                    |
| 230  | 42     |      | Orphenadrine * HCl              | 341-69-5   | 149.88   | 0.49     | 425.2    | 1.39    | 125.4      | 0.41    | 305.88 | 1.39                                    |
| 7    |        |      | Ouabain                         | 630-60-4   | 0.04     | 0.000072 | NA       | NA      | NA         | NA      | 584.73 |   |
| 164  |        |      | Oxatomide                       | 60607-34-3 | 8.11     | 0.019    | 1412.1   | 3.31    | 9598.7     | 22.5    | 426.61 | 3.31                                    |
| 65   |        |      | Oxyphenbutazone                 | 129-20-4   | 61.64    | 0.19     | 999.2    | 3.08    | 480.1      | 1.48    | 324.41 | 3.08                                    |
| 176  |        |      | Papaverine                      | 58-74-2    | 15.27    | 0.045    | 325.8    | 0.96    | 230.8      | 0.68    | 339.42 | 0.96                                    |
| 235  | 25     |      | Paraquat                        | 4685-14-7  | 100.58   | 0.54     | 57.7     | 0.31    | 195.6      | 1.05    | 186.25 | 0.31                                    |
| 49   |        |      | Parathion                       | 56-38-2    | 27.09    | 0.093    | 2.0      | 0.0069  | 6.1        | 0.021   | 291.28 | 0.0069                                  |
| 173  | 39     |      | Pentachlorophenol               | 87-86-5    | 9.59     | 0.036    | 50.6     | 0.19    | NA         | NA      | 266.32 | 0.19                                    |
| 322  |        | 1-   | Pentanol                        | 71-41-0    | 2195.43  | 24.9     | 3033.0   | 34.4    | 200.1      | 2.27    | 88.17  | 34.4                                    |
| 87   |        |      | Pentobarbital sodium            | 57-33-0    | 176.29   | 0.71     | 201.1    | 0.81    | 280.6      | 1.13    | 248.29 | 0.81                                    |
| 240  |        |      | Pentoxifylline                  | 6493-05-6  | 183.71   | 0.66     | NA       | NA      | 1386.2     | 4.98    | 278.35 | 4.98                                    |
| 97   |        |      | Phenacetin                      | 62-44-2    | 227.63   | 1.27     | 1650.8   | 9.21    | 1220.6     | 6.81    | 179.24 | 9.21                                    |
| 118  | 24     |      | Phenobarbital                   | 50-06-6    | 884.91   | 3.81     | 162.6    | 0.7     | 167.2      | 0.72    | 232.26 | 0.7                                     |
| 115  | 12     |      | Phenol                          | 108-95-2   | 283.30   | 3.01     | 414.1    | 4.4     | 300.2      | 3.19    | 94.12  | 4.4                                     |
| 79   |        |      | Phenylbutazone                  | 50-33-9    | 98.69    | 0.32     | 376.3    | 1.22    | 441.0      | 1.43    | 308.41 | 1.22                                    |
| 218  |        | o-   | Phenylenediamine                | 95-54-5    | 33.53    | 0.31     | 1069.7   | 9.89    | NA         | NA      | 108.16 | 9.89                                    |
| 180  |        | p-   | Phenylenediamine                | 106-50-3   | 5.41     | 0.05     | 80.0     | 0.74    | NA         | NA      | 108.16 | 0.74                                    |
| 282  |        | (-)- | Phenylephrine                   | 59-42-7    | 744.17   | 4.45     | 349.5    | 2.09    | NA         | NA      | 167.23 | 2.09                                    |
| 278  |        |      | Phenylephrine * HCl             | 939-38-8   | 847.35   | 4.16     | 350.3    | 1.72    | 120.2      | 0.59    | 203.69 | 1.72                                    |
| 234  |        |      | Phenylthiourea                  | 103-85-5   | 82.20    | 0.54     | 3.0      | 0.02    | 10.0       | 0.066   | 152.23 | 0.02                                    |
| 342  |        |      | Piperazine                      | 110-85-0   | 5789.95  | 67.2     | 1904.1   | 22.1    | 1438.9     | 16.7    | 86.16  | 22.1                                    |
| 146  |        |      | Potassium bichromate VI         | 7778-50-9  | 0.59     | 0.002    | NA       | NA      | 191.2      | 0.65    | 294.2  | 0.65                                    |
| 145  |        |      | Potassium chromate VI           | 7789-00-6  | 0.29     | 0.0015   | NA       | NA      | 180.6      | 0.93    | 194.2  | 0.93                                    |
| 277  |        |      | Potassium cyanate               | 590-28-3   | 335.84   | 4.14     | NA       | NA      | 843.6      | 10.4    | 81.12  | 10.4                                    |
| 252  | 19     |      | Potassium cyanide               | 151-50-8   | 72.93    | 1.12     | 9.8      | 0.15    | 8.5        | 0.13    | 65.12  | 0.15                                    |
| 335  |        |      | Potassium hexacyano- ferrate II | 13943-58-3 | 15582.05 | 42.3     | 6409.6   | 17.4    | 5009.8     | 13.6    | 368.37 | 17.4                                    |
| 266  |        |      | Potassium hexacyanoferrate III  | 13746-66-2 | 928.54   | 2.82     | NA       | NA      | 2970.0     | 9.02    | 329.27 | 9.02                                    |
| 346  | 50     |      | Potassium I chloride            | 7447-40-7  | 6113.10  | 82       | 2601.8   | 34.9    | 1498.5     | 20.1    | 74.55  | 34.9                                    |
| 269  |        |      | Potassium I fluoride            | 7789-23-3  | 181.85   | 3.13     | 245.2    | 4.22    | NA         | NA      | 58.1   | 4.22                                    |
| 36   |        |      | Progesterone                    | 57-83-0    | 9.44     | 0.03     | NA       | NA      | NA         | NA      | 314.51 |   |
| 348  |        | 1-   | Propanol                        | 71-23-8    | 5800.62  | 96.5     | 5397.9   | 89.8    | NA         | NA      | 60.11  | 89.8                                    |
| 128  | 10     | 2-   | Propanol                        | 67-63-0    | 10038.37 | 167      | 5842.7   | 97.2    | NA         | NA      | 60.11  | 97.2                                    |
| 270  |        |      | Propionaldehyde                 | 123-38-6   | 188.79   | 3.25     | 1411.6   | 24.3    | NA         | NA      | 58.09  | 24.3                                    |
| 54   | 23     |      | Propranolol * HCl               | 318-98-9   | 35.50    | 0.12     | NA       | NA      | 470.4      | 1.59    | 295.84 | 1.59                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |          | Chemical                         | CAS #      | IC50x    |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----------|----------------------------------|------------|----------|----------|----------|---------|------------|---------|--------|---|
|      |        |          |                                  |            | ug/ml    | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 357  |        |          | Propylene glycol                 | 57-55-6    | 26029.62 | 342      | 20016.9  | 263     | 23974.7    | 315     | 76.11  | 263                                     |
| 209  |        |          | Propylparaben                    | 94-13-3    | 32.44    | 0.18     | NA       | NA      | 6325.7     | 35.1    | 180.22 | 35.1                                    |
| 12   |        |          | Puromycin                        | 53-79-2    | 0.16     | 0.00033  | NA       | NA      | 674.4      | 1.43    | 471.58 | 1.43                                    |
| 337  |        |          | Pyridine                         | 110-86-1   | 3710.26  | 46.9     | 893.9    | 11.3    | NA         | NA      | 79.11  | 11.3                                    |
| 53   | 43     |          | Quinidine sulfate                | 50-54-4    | 50.70    | 0.12     | 456.3    | 1.08    | 595.8      | 1.41    | 422.54 | 1.08                                    |
| 45   |        |          | Quinine * HCl                    | 130-89-2   | 27.07    | 0.075    | 620.8    | 1.72    | 1158.6     | 3.21    | 360.92 | 1.72                                    |
| 216  |        |          | Refortan                         |            | 78.28    | 0.25     | 3162.3   | 10.1    | NA         | NA      | 313.1  | 10.1                                    |
| 245  |        |          | Resorcinol                       | 108-46-3   | 88.10    | 0.8      | 300.6    | 2.73    | NA         | NA      | 110.12 | 2.73                                    |
| 201  |        | 13-cis-  | Retinoic acid                    | 4759-48-2  | 36.06    | 0.12     | NA       | NA      | 3395.4     | 11.3    | 300.48 | 11.3                                    |
| 139  |        |          | Retinol                          | 68-26-8    | 0.15     | 0.00054  | 1999.8   | 6.98    | 4011.0     | 14      | 286.5  | 6.98                                    |
| 134  |        |          | Rotenone                         | 83-79-4    | 0.05     | 0.00013  | 130.2    | 0.33    | 351.1      | 0.89    | 394.45 | 0.33                                    |
| 314  |        |          | Saccharin                        | 81-07-2    | 3004.32  | 16.4     | NA       | NA      | 17000.0    | 92.8    | 183.19 | 92.8                                    |
| 95   |        |          | Salicylamide                     | 65-45-2    | 148.12   | 1.08     | 1892.7   | 13.8    | 1398.9     | 10.2    | 137.15 | 13.8                                    |
| 178  |        |          | Salicylanilide                   | 87-17-2    | 9.81     | 0.046    | NA       | NA      | 2409.7     | 11.3    | 213.25 | 11.3                                    |
| 272  |        |          | Salicylic acid                   | 69-72-7    | 466.88   | 3.38     | 890.9    | 6.45    | 479.3      | 3.47    | 138.13 | 6.45                                    |
| 251  |        |          | Scopolamine * HBr                | 6533-68-2  | 415.05   | 1.08     | 1268.2   | 3.3     | 1879.3     | 4.89    | 384.31 | 3.3                                     |
| 69   |        |          | Secobarbital sodium              | 309-43-3   | 54.66    | 0.21     | 124.9    | 0.48    | NA         | NA      | 260.3  | 0.48                                    |
| 161  |        |          | Silver I nitrate                 | 7761-88-8  | 2.21     | 0.013    | NA       | NA      | 49.3       | 0.29    | 169.88 | 0.29                                    |
| 30   |        |          | Sodium arsenate, dibasic         | 7778-43-0  | 2.79     | 0.015    | NA       | NA      | NA         | NA      | 185.91 |   |
| 241  |        |          | Sodium azide                     | 26628-22-8 | 46.16    | 0.71     | 44.9     | 0.69    | 27.3       | 0.42    | 65.02  | 0.69                                    |
| 144  |        |          | Sodium bichromate VI             | 10588-01-9 | 0.24     | 0.00093  | 49.8     | 0.19    | NA         | NA      | 261.98 | 0.19                                    |
| 344  | 13     |          | Sodium chloride                  | 7647-14-5  | 4435.60  | 75.9     | 2998.0   | 51.3    | 3997.3     | 68.4    | 58.44  | 51.3                                    |
| 329  |        |          | Sodium cyclamate                 | 139-05-9   | 7123.90  | 35.4     | 15254.0  | 75.8    | 17004.8    | 84.5    | 201.24 | 75.8                                    |
| 76   |        |          | Sodium dodecyl sulfate           | 151-21-3   | 78.15    | 0.27     | 1288.0   | 4.45    | NA         | NA      | 289.43 | 4.45                                    |
| 345  |        |          | Sodium I bromide                 | 7647-15-6  | 8120.81  | 77.4     | 3504.3   | 33.4    | 6998.2     | 66.7    | 104.92 | 33.4                                    |
| 106  | 14     |          | Sodium I fluoride                | 7681-49-4  | 77.68    | 1.85     | 180.1    | 4.29    | NA         | NA      | 41.99  | 4.29                                    |
| 255  |        |          | Sodium monochloroacetate         | 3926-62-3  | 168.90   | 1.45     | 75.7     | 0.65    | NA         | NA      | 116.48 | 0.65                                    |
| 227  | 46     |          | Sodium oxalate                   | 62-76-0    | 58.96    | 0.44     | 155.4    | 1.16    | NA         | NA      | 134    | 1.16                                    |
| 119  |        |          | Sodium salicylate                | 54-21-7    | 693.28   | 4.33     | 1599.5   | 9.99    | 899.8      | 5.62    | 160.11 | 9.99                                    |
| 290  |        |          | Sodium sulfite                   | 7757-83-7  | 854.55   | 6.78     | NA       | NA      | 820.5      | 6.51    | 126.04 | 6.51                                    |
| 156  |        |          | Stearyltrimethylammoniumchloride | 112-03-8   | 2.09     | 0.006    | NA       | NA      | 536.1      | 1.54    | 348.13 | 1.54                                    |
| 265  |        |          | Streptomycin sulfate             | 298-39-5   | 3979.25  | 2.73     | NA       | NA      | 495.6      | 0.34    | 1457.6 | 0.34                                    |
| 331  |        |          | Strontium II chloride            | 10476-85-4 | 5770.13  | 36.4     | 2251.0   | 14.2    | 3107.0     | 19.6    | 158.52 | 14.2                                    |
| 5    |        | K-       | Strophantin                      |            | 0.03     | 0.000044 | NA       | NA      | NA         | NA      | 710.9  |   |
| 271  |        |          | Styrene                          | 100-42-5   | 343.73   | 3.3      | 4999.7   | 48      | 315.6      | 3.03    | 104.16 | 48                                      |
| 93   |        |          | Sulfisoxazole                    | 127-69-5   | 227.23   | 0.85     | NA       | NA      | 6790.2     | 25.4    | 267.33 | 25.4                                    |
| 330  |        |          | Sulfuric acid                    | 7664-93-9  | 3530.88  | 36       | 2138.1   | 21.8    | NA         | NA      | 98.08  | 21.8                                    |
| 135  |        | 2,3,7,8- | Tetrachloro-dibenzo-p-dioxin     | 1746-01-6  | 0.06     | 0.0002   | NA       | NA      | 0.1        | 0.00035 | 321.96 | 0.00035                                 |
| 289  |        |          | Tetrachloroethene                | 127-18-4   | 1084.46  | 6.54     | 8854.8   | 53.4    | 8092.0     | 48.8    | 165.82 | 53.4                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # |        | Chemical                      | CAS #     | IC50x    |           | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|-------------------------------|-----------|----------|-----------|----------|---------|------------|---------|--------|---|
|      |        |        |                               |           | ug/ml    | mmol/l    | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 59   |        |        | Tetracycline * HCl            | 64-75-5   | 67.33    | 0.14      | 6444.6   | 13.4    | NA         | NA      | 480.94 | 13.4                                    |
| 350  |        |        | Tetrahydrofurfuryl alcohol    | 97-99-4   | 11338.65 | 111       | 2502.7   | 24.5    | 2298.4     | 22.5    | 102.15 | 24.5                                    |
| 247  |        | (+)-   | Thalidomide                   | 731-40-8  | 209.18   | 0.81      | NA       | NA      | 400.3      | 1.55    | 258.25 | 1.55                                    |
| 203  |        |        | Thallium I acetate            | 563-68-8  | 36.88    | 0.14      | NA       | NA      | 34.2       | 0.13    | 263.42 | 0.13                                    |
| 181  | 30     |        | Thallium I sulfate            | 7446-18-6 | 27.26    | 0.054     | NA       | NA      | 28.8       | 0.057   | 504.8  | 0.057                                   |
| 105  | 21     |        | Theophylline                  | 58-55-9   | 329.75   | 1.83      | NA       | NA      | 600.0      | 3.33    | 180.19 | 3.33                                    |
| 303  |        |        | Theophylline sodium           | 3485-82-3 | 2519.43  | 12.4      | NA       | NA      | 445.0      | 2.19    | 203.18 | 2.19                                    |
| 280  |        |        | Theophylline sodium acetate   | 8002-89-9 | 1098.74  | 4.19      | 582.2    | 2.22    | NA         | NA      | 262.23 | 2.22                                    |
| 25   |        |        | Thio-TEPA                     | 52-24-4   | 2.08     | 0.011     | NA       | NA      | 37.8       | 0.2     | 189.24 | 0.2                                     |
| 279  |        |        | Thioacetamide                 | 62-55-5   | 313.33   | 4.17      | 301.3    | 4.01    | NA         | NA      | 75.14  | 4.01                                    |
| 140  |        | 6-     | Thioguanine                   | 154-42-7  | 0.10     | 0.00057   | NA       | NA      | 160.5      | 0.96    | 167.21 | 0.96                                    |
| 83   |        |        | Thiopental                    | 76-75-5   | 133.30   | 0.55      | NA       | NA      | 601.1      | 2.48    | 242.37 | 2.48                                    |
| 170  | 29     |        | Thioridazine * HCl            | 130-61-0  | 11.81    | 0.029     | NA       | NA      | 358.2      | 0.88    | 407.07 | 0.88                                    |
| 80   |        | 2-     | Thiouracil                    | 141-90-2  | 41.01    | 0.32      | 999.6    | 7.8     | NA         | NA      | 128.16 | 7.8                                     |
| 347  |        |        | Thiourea                      | 62-56-6   | 6547.18  | 86        | 124.9    | 1.64    | 8526.6     | 112     | 76.13  | 1.64                                    |
| 214  |        |        | Thymol                        | 89-83-8   | 34.56    | 0.23      | 979.6    | 6.52    | 1802.9     | 12      | 150.24 | 6.52                                    |
| 256  |        |        | Tin II chloride               | 7772-99-8 | 286.28   | 1.51      | 699.6    | 3.69    | 1200.1     | 6.33    | 189.59 | 3.69                                    |
| 104  |        |        | Tolbutamide                   | 64-77-7   | 489.39   | 1.81      | NA       | NA      | 2601.1     | 9.62    | 270.38 | 9.62                                    |
| 316  |        |        | Toluene                       | 108-88-3  | 1575.77  | 17.1      | 5003.7   | 54.3    | NA         | NA      | 92.15  | 54.3                                    |
| 194  |        | p-     | Toluyldiamine                 | 95-70-5   | 11.49    | 0.094     | 101.4    | 0.83    | NA         | NA      | 122.19 | 0.83                                    |
| 1    |        |        | Trenimon                      | 68-76-8   | 0.00     | 0.0000033 | NA       | NA      | NA         | NA      | 231.28 |   |
| 310  |        |        | Tributylamine                 | 102-82-9  | 2855.16  | 15.4      | 539.5    | 2.91    | NA         | NA      | 185.4  | 2.91                                    |
| 138  |        |        | Tributyltin chloride          | 1461-22-9 | 0.18     | 0.00054   | 120.4    | 0.37    | NA         | NA      | 325.53 | 0.37                                    |
| 75   |        |        | Trichlorfon                   | 52-68-6   | 69.51    | 0.27      | 450.5    | 1.75    | 298.6      | 1.16    | 257.44 | 1.75                                    |
| 294  |        |        | Trichloroacetic acid          | 76-03-9   | 1338.08  | 8.19      | 4999.4   | 30.6    | 5636.6     | 34.5    | 163.38 | 30.6                                    |
| 242  |        | 1,2,4- | Trichlorobenzene              | 120-82-1  | 128.82   | 0.71      | 756.6    | 4.17    | 765.7      | 4.22    | 181.44 | 4.17                                    |
| 297  | 11     | 1,1,1- | Trichloroethane               | 71-55-6   | 1374.02  | 10.3      | 10298.5  | 77.2    | 11245.6    | 84.3    | 133.4  | 77.2                                    |
| 228  |        | 2,4,5- | Trichlorophen- oxyacetic acid | 93-76-5   | 112.41   | 0.44      | 298.9    | 1.17    | 388.3      | 1.52    | 255.48 | 1.17                                    |
| 126  |        |        | Triethyl citrate              | 77-93-0   | 4061.90  | 14.7      | 6990.9   | 25.3    | NA         | NA      | 276.32 | 25.3                                    |
| 143  |        |        | Triethylene melamine          | 51-18-3   | 0.16     | 0.00078   | 1.0      | 0.005   | 14.9       | 0.073   | 204.27 | 0.005                                   |
| 137  |        |        | Triethyltin chloride          | 994-31-0  | 0.11     | 0.00046   | 5.1      | 0.021   | NA         | NA      | 241.35 | 0.021                                   |
| 318  |        |        | Trifluoroacetic acid          | 76-05-1   | 2337.62  | 20.5      | 199.6    | 1.75    | NA         | NA      | 114.03 | 1.75                                    |
| 166  |        |        | Triisooctylamine              | 2757-28-0 | 8.14     | 0.023     | 1620.2   | 4.58    | NA         | NA      | 353.76 | 4.58                                    |
| 354  |        | 1,3,5- | Trioxane                      | 110-88-3  | 19189.17 | 213       | 800.0    | 8.88    | NA         | NA      | 90.09  | 8.88                                    |
| 132  |        |        | Triphenyltin hydroxide        | 76-87-9   | 0.02     | 0.000049  | 44.0     | 0.12    | 245.9      | 0.67    | 367.03 | 0.12                                    |
| 182  |        |        | Triton X-100                  | 9002-93-1 | 35.59    | 0.055     | 1798.7   | 2.78    | NA         | NA      | 647    | 2.78                                    |
| 50   |        |        | Trypan blue                   | 72-57-1   | 91.66    | 0.095     | 6204.2   | 6.43    | NA         | NA      | 964.88 | 6.43                                    |
| 231  |        |        | Tween 80                      | 9005-65-6 | 641.90   | 0.49      | NA       | NA      | 25021.0    | 19.1    | 1310   | 19.1                                    |
| 208  |        |        | Undecylenic acid              | 112-38-9  | 33.18    | 0.18      | 2506.6   | 13.6    | 8496.7     | 46.1    | 184.31 | 13.6                                    |

**Section 7.2**  
**Table 7.3**  
**Chemical Data from the Registry of Cytotoxicity Data Bank (Alphabetical))**

| RC # | MEIC # | Chemical             | CAS #      | IC50x   |          | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----------------------|------------|---------|----------|----------|---------|------------|---------|--------|---|
|      |        |                      |            | ug/ml   | mmol/l   | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 323  |        | Urethan              | 51-79-6    | 2307.95 | 25.9     | NA       | NA      | 2504.0     | 28.1    | 89.11  | 28.1                                    |
| 250  |        | Valproate sodium     | 1069-66-5  | 166.22  | 1        | NA       | NA      | 1695.4     | 10.2    | 166.22 | 10.2                                    |
| 196  | 40     | VerapamilHCl         | 152-11-4   | 49.11   | 0.1      | 108.0    | 0.22    | 162.1      | 0.33    | 491.13 | 0.22                                    |
| 205  |        | Versalide            | 88-29-9    | 38.77   | 0.15     | 315.3    | 1.22    | NA         | NA      | 258.44 | 1.22                                    |
| 4    |        | Vincristine sulfate  | 2068-78-2  | 0.01    | 0.000015 | NA       | NA      | NA         | NA      | 923.14 |   |
| 86   | 31     | Warfarin             | 81-81-2    | 206.59  | 0.67     | 323.8    | 1.05    | 373.1      | 1.21    | 308.35 | 1.05                                    |
| 313  |        | Xanthinol nicotinate | 437-74-1   | 6865.26 | 15.8     | 14121.6  | 32.5    | 17336.9    | 39.9    | 434.51 | 32.5                                    |
| 301  | 17     | Xylene               | 1330-20-7  | 1274.16 | 12       | 4300.3   | 40.5    | NA         | NA      | 106.18 | 40.5                                    |
| 55   |        | Zinc II chloride     | 7646-85-7  | 17.72   | 0.13     | 350.2    | 2.57    | 350.2      | 2.57    | 136.27 | 2.57                                    |
| 186  |        | Zineb                | 12122-67-7 | 16.27   | 0.059    | 5211.3   | 18.9    | 7610.1     | 27.6    | 275.73 | 18.9                                    |



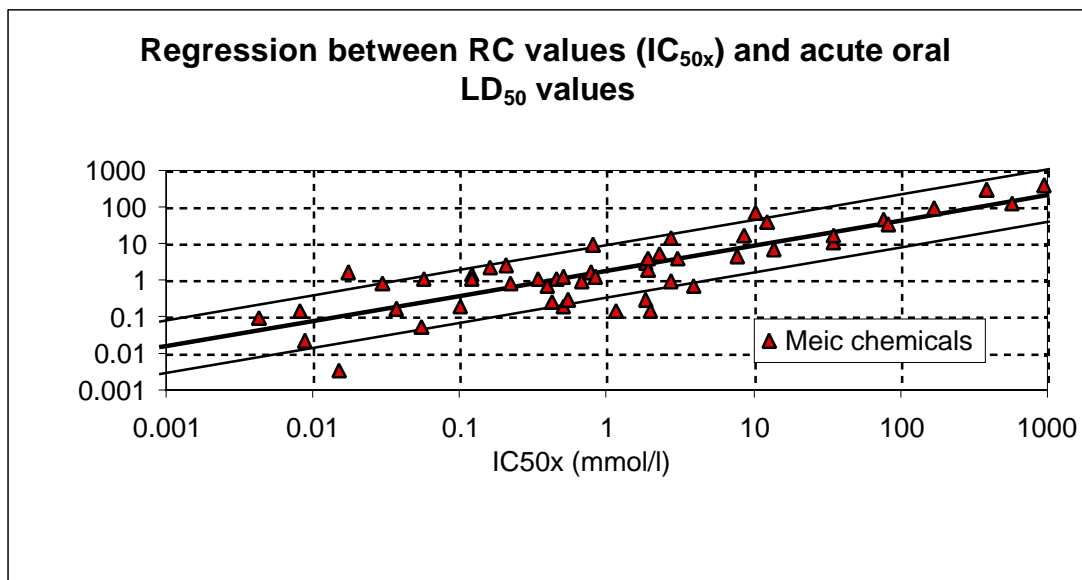
**Section 7.2**  
**Table 7.4**  
**Registry of Cytotoxicity Data - MEIC Chemicals (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # | Chemical                         | CAS #      | IC50x   |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|----------------------------------|------------|---------|--------|----------|---------|------------|---------|--------|---|
|      |        |                                  |            | ug/ml   | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 29   | 28     | Mercury II chloride              | 7487-94-7  | 4.07    | 0.015  | 1.0      | 0.0037  | 10.0       | 0.037   | 271.49 | 0.0037                                  |
| 252  | 19     | Potassium cyanide                | 151-50-8   | 72.93   | 1.12   | 9.8      | 0.15    | 8.5        | 0.13    | 65.12  | 0.15                                    |
| 153  | 26     | Arsenic III trioxide             | 1327-53-3  | 0.83    | 0.0042 | 19.8     | 0.1     | 45.5       | 0.23    | 197.84 | 0.1                                     |
| 103  | 18     | Nicotine                         | 54-11-5    | 290.45  | 1.79   | 50.3     | 0.31    | 24.3       | 0.15    | 162.26 | 0.31                                    |
| 173  | 39     | Pentachlorophenol                | 87-86-5    | 9.59    | 0.036  | 50.6     | 0.19    | NA         | NA      | 266.32 | 0.19                                    |
| 262  | 47     | Amphetamine sulfate              | 60-13-9    | 726.02  | 1.97   | 55.3     | 0.15    | 24.0       | 0.065   | 368.54 | 0.15                                    |
| 235  | 25     | Paraquat                         | 4685-14-7  | 100.58  | 0.54   | 57.7     | 0.31    | 195.6      | 1.05    | 186.25 | 0.31                                    |
| 157  | 38     | Hexachlorophene                  | 70-30-4    | 3.21    | 0.0079 | 61.0     | 0.15    | 65.1       | 0.16    | 406.89 | 0.15                                    |
| 223  | 32     | Lindane                          | 58-89-9    | 119.24  | 0.41   | 75.6     | 0.26    | 87.2       | 0.3     | 290.82 | 0.26                                    |
| 229  | 22     | Dextropropoxyphene * HCl         | 1639-60-7  | 184.23  | 0.49   | 82.7     | 0.22    | 82.7       | 0.22    | 375.98 | 0.22                                    |
| 196  | 40     | VerapamilHCl                     | 152-11-4   | 49.11   | 0.1    | 108.0    | 0.22    | 162.1      | 0.33    | 491.13 | 0.22                                    |
| 227  | 46     | Sodium oxalate                   | 62-76-0    | 58.96   | 0.44   | 155.4    | 1.16    | NA         | NA      | 134    | 1.16                                    |
| 118  | 24     | Phenobarbital                    | 50-06-6    | 884.91  | 3.81   | 162.6    | 0.7     | 167.2      | 0.72    | 232.26 | 0.7                                     |
| 106  | 14     | Sodium I fluoride                | 7681-49-4  | 77.68   | 1.85   | 180.1    | 4.29    | NA         | NA      | 41.99  | 4.29                                    |
| 112  | 48     | Caffeine                         | 58-08-2    | 512.74  | 2.64   | 192.3    | 0.99    | 619.6      | 3.19    | 194.22 | 0.99                                    |
| 81   | 27     | Cupric sulfate * 5 H2O           | 7758-99-8  | 82.40   | 0.33   | 299.6    | 1.2     | NA         | NA      | 249.7  | 1.2                                     |
| 261  | 3      | Ferrous sulfate                  | 7720-78-7  | 281.03  | 1.85   | 319.0    | 2.1     | 978.3      | 6.44    | 151.91 | 2.1                                     |
| 183  | 5      | Amitriptyline                    | 50-48-6    | 15.54   | 0.056  | 319.1    | 1.15    | 147.0      | 0.53    | 277.44 | 1.15                                    |
| 86   | 31     | Warfarin                         | 81-81-2    | 206.59  | 0.67   | 323.8    | 1.05    | 373.1      | 1.21    | 308.35 | 1.05                                    |
| 246  | 37     | Barium II nitrate                | 10022-31-8 | 211.70  | 0.81   | 355.4    | 1.36    | NA         | NA      | 261.36 | 1.36                                    |
| 89   | 16     | 2,4-Dichlorophenoxy- acetic acid | 94-75-7    | 170.20  | 0.77   | 369.1    | 1.67    | 366.9      | 1.66    | 221.04 | 1.67                                    |
| 115  | 12     | Phenol                           | 108-95-2   | 283.30  | 3.01   | 414.1    | 4.4     | 300.2      | 3.19    | 94.12  | 4.4                                     |
| 230  | 42     | Orphenadrine * HCl               | 341-69-5   | 149.88  | 0.49   | 425.2    | 1.39    | 125.4      | 0.41    | 305.88 | 1.39                                    |
| 53   | 43     | Quinidine sulfate                | 50-54-4    | 50.70   | 0.12   | 456.3    | 1.08    | 595.8      | 1.41    | 422.54 | 1.08                                    |
| 70   | 49     | Atropine sulfate                 | 55-48-1    | 148.92  | 0.22   | 622.7    | 0.92    | 764.9      | 1.13    | 676.9  | 0.92                                    |
| 123  | 35     | Isoniazid                        | 54-85-3    | 1027.33 | 7.49   | 650.1    | 4.74    | NA         | NA      | 137.16 | 4.74                                    |
| 63   | 4      | Diazepam                         | 439-14-5   | 45.56   | 0.16   | 709.1    | 2.49    | 535.3      | 1.88    | 284.76 | 2.49                                    |
| 67   | 15     | Malathion                        | 121-75-5   | 66.08   | 0.2    | 885.4    | 2.68    | 776.4      | 2.35    | 330.38 | 2.68                                    |
| 308  | 33     | Chloroform                       | 67-66-3    | 1599.56 | 13.4   | 908.4    | 7.61    | 35.8       | 0.3     | 119.37 | 7.61                                    |
| 31   | 41     | Chloroquine diphosphate          | 50-63-5    | 8.77    | 0.017  | 969.9    | 1.88    | 500.4      | 0.97    | 515.92 | 1.88                                    |
| 107  | 2      | Acetylsalicylic acid             | 50-78-2    | 408.99  | 2.27   | 999.9    | 5.55    | 814.4      | 4.52    | 180.17 | 5.55                                    |
| 328  | 36     | Dichloromethane                  | 75-09-2    | 2964.06 | 34.9   | 1596.7   | 18.8    | NA         | NA      | 84.93  | 18.8                                    |
| 113  | 1      | Acetaminophen                    | 103-90-2   | 409.70  | 2.71   | 2403.8   | 15.9    | 338.6      | 2.24    | 151.18 | 15.9                                    |
| 346  | 50     | Potassium I chloride             | 7447-40-7  | 6113.10 | 82     | 2601.8   | 34.9    | 1498.5     | 20.1    | 74.55  | 34.9                                    |
| 125  | 34     | Carbon tetrachloride             | 56-23-5    | 1308.92 | 8.51   | 2799.3   | 18.2    | 12797.0    | 83.2    | 153.81 | 18.2                                    |
| 344  | 13     | Sodium chloride                  | 7647-14-5  | 4435.60 | 75.9   | 2998.0   | 51.3    | 3997.3     | 68.4    | 58.44  | 51.3                                    |
| 91   | 45     | Chloramphenicol                  | 56-75-7    | 255.29  | 0.79   | 3393.1   | 10.5    | 2640.1     | 8.17    | 323.15 | 10.5                                    |

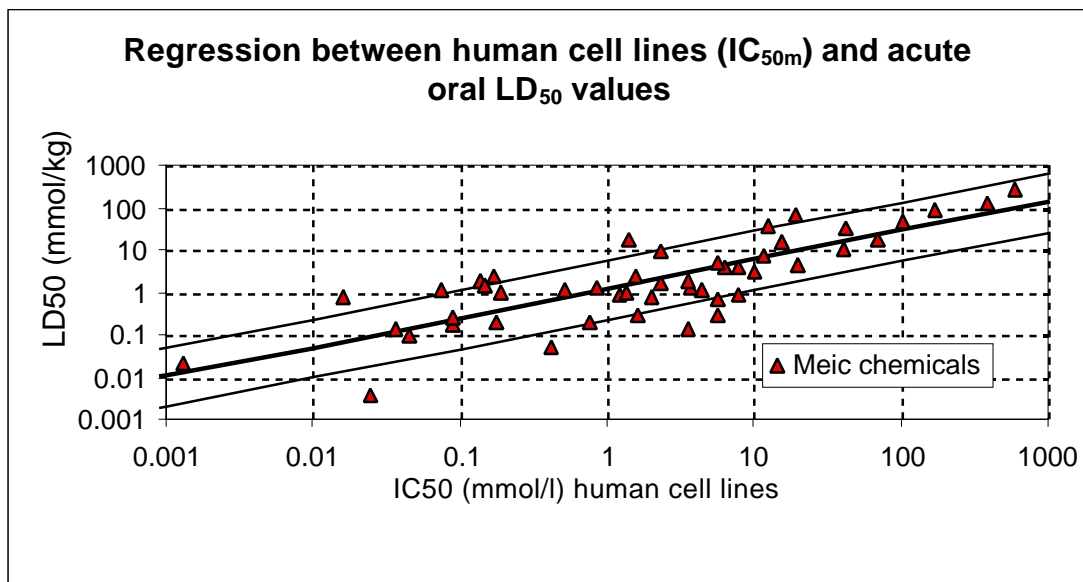
**Section 7.2**  
**Table 7.4**  
**Registry of Cytotoxicity Data - MEIC Chemicals (Sorted by Rat LD50 Oral mg/kg)**

| RC # | MEIC # |        | Chemical           | CAS #      | IC50x    |        | LD50 RAT |         | LD50 MOUSE |         | MW     | Rodent LD50 (mmol/kg)<br>for Regression |
|------|--------|--------|--------------------|------------|----------|--------|----------|---------|------------|---------|--------|---|
|      |        |        |                    |            | ug/ml    | mmol/l | mg/kg    | mmol/kg | mg/kg      | mmol/kg |        |   |
| 301  | 17     |        | Xylene             | 1330-20-7  | 1274.16  | 12     | 4300.3   | 40.5    | NA         | NA      | 106.18 | 40.5                                    |
| 128  | 10     | 2-     | Propanol           | 67-63-0    | 10038.37 | 167    | 5842.7   | 97.2    | NA         | NA      | 60.11  | 97.2                                    |
| 360  | 7      |        | Ethylene glycol    | 107-21-1   | 34454.40 | 555    | 8567.0   | 138     | 7511.7     | 121     | 62.08  | 138                                     |
| 297  | 11     | 1,1,1- | Trichloroethane    | 71-55-6    | 1374.02  | 10.3   | 10298.5  | 77.2    | 11245.6    | 84.3    | 133.4  | 77.2                                    |
| 361  | 8      |        | Methanol           | 67-56-1    | 29806.50 | 930    | 13012.3  | 406     | NA         | NA      | 32.05  | 406                                     |
| 130  | 9      |        | Ethanol            | 64-17-5    | 17464.32 | 379    | 14008.3  | 304     | 7787.5     | 169     | 46.08  | 304                                     |
| 22   | 6      |        | Digoxin            | 20830-75-5 | 6.64     | 0.0085 | NA       | NA      | 18.0       | 0.023   | 781.05 | 0.023                                   |
| 327  | 20     |        | Lithium I sulfate  | 10377-48-7 | 3704.98  | 33.7   | NA       | NA      | 1187.4     | 10.8    | 109.94 | 10.8                                    |
| 105  | 21     |        | Theophylline       | 58-55-9    | 329.75   | 1.83   | NA       | NA      | 600.0      | 3.33    | 180.19 | 3.33                                    |
| 54   | 23     |        | Propranolol * HCl  | 318-98-9   | 35.50    | 0.12   | NA       | NA      | 470.4      | 1.59    | 295.84 | 1.59                                    |
| 170  | 29     |        | Thioridazine * HCl | 130-61-0   | 11.81    | 0.029  | NA       | NA      | 358.2      | 0.88    | 407.07 | 0.88                                    |
| 181  | 30     |        | Thallium I sulfate | 7446-18-6  | 27.26    | 0.054  | NA       | NA      | 28.8       | 0.057   | 504.8  | 0.057                                   |
| 82   | 44     |        | Diphenylhydantoin  | 57-41-0    | 98.39    | 0.39   | NA       | NA      | 199.3      | 0.79    | 252.29 | 0.79                                    |

## Calculation of the Regression Between Cytotoxicity and Acute Oral Toxicity



**Figure 7.1** Regression between RC values ( $IC_{50x}$ ) and acute oral  $LD_{50}$  values (MEIC chemicals)



**Figure 7.2** Regression between human cell lines ( $IC_{50m}$ ) and acute oral  $LD_{50}$  values (MEIC chemicals)

