**On the Prediction of Cytotoxicity of Diverse Chemicals for Topminnow (*Poeciliopsis lucida*) Hepatoma Cell Line, PLHC-1**

**Supplementary Material**

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Table S1. Type and meaning of the descriptors appeared in the generated QSTR models.

|  |  |  |
| --- | --- | --- |
| Descriptor | Meaning of descriptor | Type |
| NaasC | Number of atoms of type aasC Atom-type | E-state indices |
| CATS2D\_01\_AN | CATS2D Acceptor-Negative at lag 01 | CATS 2D |
| CATS2D\_01\_DN | CATS2D Donor-Negative at lag 01 | CATS 2D |
| Mor28e | signal 28 / weighted by Sanderson electronegativity | 3D-MoRSE descriptors |
| DLS\_04 | modified drug-like score from Chen et al. (7 rules) | Drug-like indices |

Table S2. External set chemicals, predicted pEC50, NR[PLHC-1] (mM), descriptor and hat values and experimental pLC50 values for the NR data set.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* | |
| 5-fluorocytosine | 2022-85-7 | -1.215 | 0.164 | 0 | 0 | 0.4 | - | |
| 5-fluorouracil | 51-21-8 | -1.215 | 0.164 | 0 | 0 | 0.4 | - | |
| Acebutolol | 37517-30-9 | 1.212 | 0.101 | 3 | 0 | 1 | - | |
| Acetaminophen | 103-90-2 | -0.013 | 0.053 | 2 | 0 | 0.6 | - | |
| Acridine | 260-94-6 | -1.007 | 0.146 | 0 | 0 | 0.5 | - | |
| Acrivastine | 87848-99-5 | 0.007 | 0.084 | 4 | 1 | 0.8 | - | |
| Acyclovir | 59277-89-3 | 0.819 | 0.110 | 2 | 0 | 1 | - | |
| Alprenolol | 13655-52-2 | 0.819 | 0.110 | 2 | 0 | 1 | - | |
| Amitriptyline | 50-48-6 | 0.980 | 0.044 | 4 | 0 | 0.7 | - | |
| Amobarbital | 57-43-2 | 0.034 | 0.179 | 0 | 0 | 1 | - | |
| Ampicillin | 69-53-4 | -0.755 | 0.136 | 1 | 1 | 1 | - | |
| Antipyrine | 60-80-0 | -0.406 | 0.086 | 1 | 0 | 0.6 | - | |
| Atovaquone | 95233-18-4 | 1.188 | 0.057 | 4 | 0 | 0.8 | - | |
| Bumetanide | 28395-03-1 | 0.400 | 0.110 | 5 | 1 | 0.8 | - | |
| Bupropion | 34841-39-9 | 0.819 | 0.110 | 2 | 0 | 1 | - | |
| Caffeine | 58-08-2 | 0.403 | 0.065 | 2 | 0 | 0.8 | - | |
| Camptothecin | 7689-03-4 | 0.403 | 0.065 | 2 | 0 | 0.8 | - | |
| Capecitabine | 154361-50-9 | 0.034 | 0.179 | 0 | 0 | 1 | - | |
| Carvedilol | 72956-09-3 | 0.796 | 0.053 | 3 | 0 | 0.8 | - | |
| Cefurexime axetil | 64544-07-6 | 0.010 | 0.094 | 1 | 0 | 0.8 | - | |
| Cefuroxime | 55268-75-2 | -1.587 | 0.108 | 1 | 1 | 0.6 | - | |
| Cephalexin | 15686-71-2 | -0.755 | 0.136 | 1 | 1 | 1 | - | |
| Chloramphenicol | 56-75-7 | 0.819 | 0.110 | 2 | 0 | 1 | - | |
| Chlorotetracycline | 57-62-5 | 1.396 | 0.079 | 4 | 0 | 0.9 | - |
| Chlorpromazine | 50-53-3 | 1.581 | 0.079 | 5 | 0 | 0.8 | - |
| Chlorpropamide | 94-20-2 | 0.403 | 0.065 | 2 | 0 | 0.8 | - | |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Cimetidine | 51481-61-9 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Ciprofloxacin | 85721-33-1 | 0.423 | 0.125 | 4 | 1 | 1 | - |
| Clonazepam | 1622-61-3 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| Clonidine | 4205-90-7 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Cytarabine | 147-94-4 | -0.175 | 0.156 | 0 | 0 | 0.9 | - |
| Deoxytetracycline | 564-25-0 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Desipramine | 50-47-5 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Doxycycline | 564-25-0 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Estradiol | 50-28-2 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Ethinylestradiol | 57-63-6 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Famciclovir | 104227-87-4 | 0.426 | 0.136 | 1 | 0 | 1 | - |
| Famotidine | 76824-35-6 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| Finasteride | 98319-26-7 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Fleroxacin | 79660-72-3 | 0.816 | 0.154 | 5 | 1 | 1 | - |
| Florfenicol | 73231-34-2 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Flunitrazepam | 1622-62-4 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| Flutamide | 13311-84-7 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Furaltadone | 139-91-3 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Fusidic acid | 6990-06-3 | -1.356 | 0.156 | 0 | 1 | 0.9 | - |
| Gemcitabine | 95058-81-4 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Glibenclamid | 10238-21-8 | 1.997 | 0.134 | 5 | 0 | 1 | - |
| Hydrochlorothiazide | 58-93-5 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| Hydrocortisone | 50-23-7 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Imipramine | 50-49-7 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Indomethacin | 53-86-1 | -0.016 | 0.099 | 5 | 1 | 0.6 | - |
| Isoniazid | 54-85-3 | -0.406 | 0.086 | 1 | 0 | 0.6 | - |
| Isotretinoin | 4759-48-2 | -1.148 | 0.174 | 0 | 1 | 1 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Itraconazole | 84625-61-6 | 1.743 | 0.142 | 7 | 0 | 0.5 | - |
| Ketoconazole | 65277-42-1 | 1.789 | 0.102 | 5 | 0 | 0.9 | - |
| Ketoprofen | 22071-15-4 | -0.802 | 0.070 | 3 | 1 | 0.6 | - |
| Labetalol | 36894-69-6 | 1.604 | 0.109 | 4 | 0 | 1 | - |
| Lamotrigine | 84057-84-1 | 1.142 | 0.100 | 6 | 0 | 0.4 | - |
| Lansoprazole | 103577-45-3 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Levofloxacin | 100986-85-4 | 0.816 | 0.154 | 5 | 1 | 1 | - |
| Lidocaine | 137-58-6 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Lomefloxacin | 98079-51-7 | 0.816 | 0.154 | 5 | 1 | 1 | - |
| L-tryptophan | 73-22-3 | -1.795 | 0.122 | 1 | 1 | 0.5 | - |
| Metaxalone | 1665-48-1 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Metformin | 657-24-9 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Methylprednisolone | 83-43-2 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Metipranolol | 22664-55-7 | 1.997 | 0.134 | 5 | 0 | 1 | - |
| Metoprolol | 37350-58-6 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Metronidazole | 443-48-1 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Midazolam | 59467-70-8 | 1.951 | 0.143 | 7 | 0 | 0.6 | - |
| Nadolol | 42200-33-9 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Naproxen | 22204-53-1 | -0.779 | 0.081 | 2 | 1 | 0.8 | - |
| Nicotine | 22083-74-5 | 0.010 | 0.094 | 1 | 0 | 0.8 | - |
| Nisoldipine | 63675-72-9 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Nitrofurazone | 59-87-0 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| Norfloxacin | 70458-96-7 | 0.423 | 0.125 | 4 | 1 | 1 | - |
| Novobiocin | 303-81-1 | 2.159 | 0.154 | 7 | 0 | 0.7 | - |
| Ofloxacin | 82419-36-1 | 0.816 | 0.154 | 5 | 1 | 1 | - |
| Oxprenolol | 6452-71-7 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Oxyphenbutazone | 129-20-4 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Oxytetracycline | 79-57-2 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| Paracetamol | 103-90-2 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Paroxetine | 61869-08-7 | 1.581 | 0.079 | 5 | 0 | 0.8 | - |
| Pentobarbital | 76-74-4 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Phenobarbital | 50-06-6 | 0.010 | 0.094 | 1 | 0 | 0.8 | - |
| Phenoxymethylpenicillinic Acid | 87-08-1 | -0.755 | 0.136 | 1 | 1 | 1 | - |
| Phenylbutazone | 50-33-9 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Phenytoin | 57-41-0 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Pindolol | 13523-86-9 | 0.426 | 0.136 | 1 | 0 | 1 | - |
| Piperazine | 110-85-0 | -0.383 | 0.141 | 0 | 0 | 0.8 | - |
| Prazosin | 19216-56-9 | 1.581 | 0.079 | 5 | 0 | 0.8 | - |
| Prednisolone | 50-24-8 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Procaine | 59-46-1 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Progesterone | 57-83-0 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Promazine | 58-40-2 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Propylthiouracil | 51-52-5 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Quinidine | 56-54-2 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Quinine | 130-95-0 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Ranitidine | 66357-35-5 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Risperidone | 106266-06-2 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Sotalol | 3930-20-9 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Sulfaguanidine | 57-67-0 | -0.221 | 0.060 | 2 | 0 | 0.5 | - |
| Sulfaphenazole | 526-08-9 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| Sulfasalazine | 599-79-1 | -0.040 | 0.158 | 6 | 1 | 0.4 | - |
| Sumatriptan | 103628-46-2 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Terazosin | 63590-64-7 | 1.604 | 0.109 | 4 | 0 | 1 | - |
| Terbinafine | 91161-71-6 | -0.198 | 0.086 | 1 | 0 | 0.7 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Testosterone | 58-22-0 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Theophylline | 58-55-9 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Timolol | 26839-75-8 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Tolazamide | 1156-19-0 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Tolbutamide | 64-77-7 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Trenbolone acetate | 10161-34-9 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Triamterene | 396-01-0 | 0.541 | 0.087 | 5 | 0 | 0.3 | - |
| Triflupromazine | 146-54-3 | 1.581 | 0.079 | 5 | 0 | 0.8 | - |
| Warfarin | 81-81-2 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2,6-Dichlorobenzonitrile | 1194-65-6 | -0.244 | 0.078 | 3 | 0 | 0.3 | - |
| Acetochlor | 34256-82-1 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Acroleine | 107-02-8 | -1.215 | 0.164 | 0 | 0 | 0.4 | - |
| Ametryn | 834-12-8 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Anilofos | 64249-01-0 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Azocyclotin | 41083-11-8 | -0.175 | 0.156 | 0 | 0 | 0.9 | - |
| Benalaxyl | 71626-11-4 | 1.604 | 0.109 | 4 | 0 | 1 | - |
| Benomyl | 17804-35-2 | 0.010 | 0.094 | 1 | 0 | 0.8 | - |
| Bensulfuron-methyl | 83055-99-6 | 1.373 | 0.063 | 5 | 0 | 0.7 | - |
| Beta-cyfluthrin | 68359-37-5 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Bromoxynil | 1689-84-5 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| Chloridazon | 1698-60-8 | -0.822 | 0.111 | 1 | 0 | 0.4 | - |
| Chlorimuron-ethyl | 90982-32-4 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| Chlorothalonil | 1897-45-6 | 1.142 | 0.100 | 6 | 0 | 0.4 | - |
| Chlorotoluron | 15545-48-9 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Chlorsulfuron | 64902-72-3 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| Cyanazine | 21725-46-2 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Cyhexatin | 13121-70-5 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Decanoic acid | 334-48-5 | -1.564 | 0.147 | 0 | 1 | 0.8 | - |
| Diclofop methyl | 51338-27-3 | 1.165 | 0.057 | 5 | 0 | 0.6 | - |
| Diclofop P | 40843-25-2 | -0.016 | 0.099 | 5 | 1 | 0.6 | - |
| Dimethachlon | 24096-53-5 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| Endosulfan | 115-29-7 | -0.799 | 0.136 | 0 | 0 | 0.6 | - |
| Ethalfluraline | 55283-68-6 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Ethametsulfuron | 111353-84-5 | -0.640 | 0.145 | 5 | 1 | 0.3 | - |
| Ethoxyquin | 91-53-2 | 1.212 | 0.101 | 3 | 0 | 1 | 1.51 |
| Fenamiphos | 22224-92-6 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Fenhexamid | 126833-17-8 | 1.604 | 0.109 | 4 | 0 | 1 | - |
| Fenoxaprop | 95617-09-7 | -0.825 | 0.102 | 4 | 1 | 0.4 | - |
| Fenpropidin | 67306-00-7 | 0.611 | 0.084 | 2 | 0 | 0.9 | - |
| Fentin hydroxide | 76-87-9 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| Fluazifop P | 83066-88-0 | -0.825 | 0.102 | 4 | 1 | 0.4 | - |
| Flumetsulam | 98967-40-9 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| Fluroxypyr | 69377-81-7 | -0.432 | 0.122 | 5 | 1 | 0.4 | - |
| Iprodione | 36734-19-7 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Cybutryne | 28159-98-0 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Isoproturon | 34123-59-6 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Lindane | 58-89-9 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| Mefenacet | 73250-68-7 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Metalaxyl | 57837-19-1 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Methabenzthiazuron | 18691-97-9 | -0.406 | 0.086 | 1 | 0 | 0.6 | - |
| Metolachlor | 51218-45-2 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Metribuzin | 21087-64-9 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Metsulfuron-methyl | 74223-64-6 | 0.541 | 0.087 | 5 | 0 | 0.3 | - |
| Molinate | 2212-67-1 | 0.034 | 0.179 | 0 | 0 | 1 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Nicosulfuron | 111991-09-4 | 1.373 | 0.063 | 5 | 0 | 0.7 | - |
| Oxadiargyl | 39807-15-3 | 1.188 | 0.057 | 4 | 0 | 0.8 | - |
| Oxadiazon | 19666-30-9 | 1.604 | 0.109 | 4 | 0 | 1 | - |
| Oxadixyl | 77732-09-3 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Pendimethalin | 40487-42-1 | 1.997 | 0.134 | 5 | 0 | 1 | - |
| Phenmedipham | 13684-63-4 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| Pretilachlor | 51218-49-6 | 1.212 | 0.101 | 3 | 0 | 1 | 2.11 |
| Prometryn | 7287-19-6 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Quinclorac | 84087-01-4 | -1.218 | 0.099 | 3 | 1 | 0.4 | - |
| Quizalofop P | 94051-08-8 | -0.825 | 0.102 | 4 | 1 | 0.4 | - |
| Tebuthiuron | 34014-18-1 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Terbumeton | 33693-04-8 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Terbuthylazine | 5915-41-3 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Terbutryn | 886-50-0 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| Thiobencarb | 28249-77-6 | 0.819 | 0.110 | 2 | 0 | 1 | 2.30 |
| Thiophanate methyl | 23564-05-8 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| Tribenuron | 106040-48-6 | -0.640 | 0.145 | 5 | 1 | 0.3 | - |
| 1,1,2,2-Tetrachloroethane | 79-34-5 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| 1,1,2-Trichloroethane | 79-00-5 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| 1,1-Dichloroethane | 75-34-3 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 1,1-Dichloroethylene | 75-35-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.33 |
| 1,2,3-Trichloropropane | 96-18-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 1,2-Dibromo-3-chloropropane | 96-12-8 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.78 |
| 1,2-Dichloroethane | 107-06-2 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 1,2-Dichloropropane | 78-87-5 | -1.007 | 0.146 | 0 | 0 | 0.5 | -0.15 |
| 1,3-Dibromopropane | 109-64-8 | -1.007 | 0.146 | 0 | 0 | 0.5 | **1.41** |
| 1,3-Dichloropropane | 142-28-9 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 1,3-Dichloropropene | 542-75-6 | -0.591 | 0.134 | 0 | 0 | 0.7 | **1.87** |
| 1-Chlorobutane | 109-69-3 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 3,4-Dichlorobut-1-ene | 760-23-6 | -0.175 | 0.156 | 0 | 0 | 0.9 | 0.67 |
| Acetic acid, bromo-, 2-butene-1,4-diyl ester | 20679-58-7 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Bromodichloromethane | 75-27-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.77 |
| Carbon tetrachloride | 56-23-5 | -1.423 | 0.191 | 0 | 0 | 0.3 | **1.31** |
| Cyclohexane | 110-82-7 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Dibromochloromethane | 124-48-1 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.42 |
| Ethyl bromide | 74-96-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Ethylcyclohexane | 1678-91-7 | -1.007 | 0.146 | 0 | 0 | 0.5 | **2.18** |
| Methylcyclohexane | 108-87-2 | -1.007 | 0.146 | 0 | 0 | 0.5 | **1.67** |
| Pentachloroethane | 76-01-7 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Tetrachloroethene | 127-18-4 | -1.423 | 0.191 | 0 | 0 | 0.3 | **1.07** |
| Trichloroethylene | 79-01-6 | -1.423 | 0.191 | 0 | 0 | 0.3 | 0.54 |
| 1-(N-phenylamino)-naphthalene | 90-30-2 | -0.221 | 0.060 | 2 | 0 | 0.5 | **2.50** |
| 1,2-Dimethylnaphthalene | 573-98-8 | 0.195 | 0.055 | 2 | 0 | 0.7 | 1.83 |
| 1,3-Dimethylnapthalene | 575-41-7 | 0.195 | 0.055 | 2 | 0 | 0.7 | 1.94 |
| 1,5-Napthalenediamine | 2243-62-1 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.97 |
| 1,8-Naphthylenediamine | 479-27-6 | -0.013 | 0.053 | 2 | 0 | 0.6 | 1.45 |
| 1-Methylnaphthalene | 90-12-0 | -0.614 | 0.095 | 1 | 0 | 0.5 | **1.40** |
| 2,7-Dimethylnaphthalene | 582-16-1 | 0.195 | 0.055 | 2 | 0 | 0.7 | 1.94 |
| 2-Methylnaphthalene | 91-57-6 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.87 |
| 3-Hydroxy-2-naphthoic acid | 92-70-6 | -1.611 | 0.113 | 2 | 1 | 0.4 | - |
| Isopropylnaphthalene | 29253-36-9 | -0.198 | 0.086 | 1 | 0 | 0.7 | **2.36** |
| N-phenyl-2-naphthylamine | 135-88-6 | -0.221 | 0.060 | 2 | 0 | 0.5 | - |
| ß-Naphthol | 135-19-3 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.56 |
| ß-Naphthylamine | 91-59-8 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.56 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (*h*\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Tetralin | 119-64-2 | 0.195 | 0.055 | 2 | 0 | 0.7 | 1.34 |
| 1,2,3-Trichlorobenzene | 87-61-6 | -0.244 | 0.078 | 3 | 0 | 0.3 | 1.75 |
| 1,2-Dichlorobenzene | 95-50-1 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.59 |
| 1,3-Dichlorobenzene | 541-73-1 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.41 |
| 1,4-Benzenediamine, N,N'-bis(1-methylpropyl)- | 101-96-2 | 0.819 | 0.110 | 2 | 0 | 1 | **2.78** |
| 1,4-Dichlorobenzene | 106-46-7 | -0.221 | 0.060 | 2 | 0 | 0.5 | **1.82** |
| 2,4,6-Trichlorophenylhydrazine | 5329-12-4 | 0.772 | 0.039 | 4 | 0 | 0.6 | 2.33 |
| 2,4,6-Trinitrotoluene | 118-96-7 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 2,4-Diamino-6-nitrotoluene | 6629-29-4 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| 2,4-Diaminotoluene | 95-80-7 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2,4-Dichlorotoluene | 95-73-8 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| 2,4-dinitrotoluene | 121-14-2 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| 2,5-Diaminotoluene | 95-70-5 | 0.380 | 0.038 | 3 | 0 | 0.6 | **2.81** |
| 2,5-Dichlorotoluene | 19398-61-9 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.60 |
| 2,6-Diamino-4-nitrotoluene | 59229-75-3 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| 2,6-Diaminotoluene | 823-40-5 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2,6-dichlorotoluene | 118-69-4 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.85 |
| 2,6-Dinitrotoluene | 606-20-2 | -0.036 | 0.056 | 3 | 0 | 0.4 | **0.73** |
| 2-Amino-4,6-dinitrotoluene | 35572-78-2 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 2-Amino-4-nitrotoluene | 99-55-8 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2-Amino-6-nitrotoluene | 603-83-8 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2-Chlorohydroquinonedimethylether | 2100-42-7 | 0.796 | 0.053 | 3 | 0 | 0.8 | 0.79 |
| 2-Chlorotoluene | 95-49-8 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.22 |
| 2-methyl-4-chlorophenoxyacetic acid | 94-74-6 | -0.386 | 0.074 | 3 | 1 | 0.8 | - |
| 2-Phenylpropene | 98-83-9 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.21 |
| 3,4-Dichlorotoluene | 95-75-0 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.57 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 3,5-Bis(trifluoromethyl)benzylamine | 85068-29-7 | 0.588 | 0.041 | 3 | 0 | 0.7 | 1.34 |
| 3-Chlorotoluene | 108-41-8 | -0.221 | 0.060 | 2 | 0 | 0.5 | - |
| 4,6-Dichlororesorcinol | 137-19-9 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 4-Allyl-1,2-dimethoxybenzene | 93-15-2 | 1.212 | 0.101 | 3 | 0 | 1 | 1.10 |
| 4-Chlororesorcinol | 95-88-5 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 4-Chlorotoluene | 106-43-4 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.32 |
| 4-Nitrotoluene-2-sulphonic acid | 121-03-9 | -1.218 | 0.099 | 3 | 1 | 0.4 | - |
| 4-tert-Butyltoluene | 98-51-1 | 0.611 | 0.084 | 2 | 0 | 0.9 | 1.94 |
| 4-Toluenesulfonyl chloride | 98-59-9 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.39 |
| Atenolol | 29122-68-7 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Benzalacetone | 122-57-6 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.41 |
| Benzotrifluoride ((Trifluoromethyl)Benzene) | 98-08-8 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.01 |
| Benzyl alcohol | 100-51-6 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Benzyl cyanide | 140-29-4 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Benzylamine | 100-46-9 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Bromobenzene | 108-86-1 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.56 |
| Butylbenzene | 104-51-8 | -0.198 | 0.086 | 1 | 0 | 0.7 | 1.61 |
| Catechol | 120-80-9 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Chlorobenzene | 108-90-7 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.23 |
| Cyclohexylbenzene | 827-52-1 | -0.198 | 0.086 | 1 | 0 | 0.7 | **2.13** |
| Diisopropylbenzene | 25321-09-9 | 0.611 | 0.084 | 2 | 0 | 0.9 | 2.30 |
| Dimethyl phthalate | 131-11-3 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Diuron | 330-54-1 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Divinylbenzene | 1321-74-0 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.49 |
| Ethylbenzene | 100-41-4 | -0.198 | 0.086 | 1 | 0 | 0.7 | - |
| Fenobucarb | 3766-81-2 | 0.819 | 0.110 | 2 | 0 | 1 | 1.33 |
| Isopropylbenzene | 98-82-8 | -0.198 | 0.086 | 1 | 0 | 0.7 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Metaxylene hexafluoride | 402-31-3 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.47 |
| m-Phenylenebis(methylamine) | 1477-55-0 | 0.403 | 0.065 | 2 | 0 | 0.8 | **0.19** |
| m-Phenylenediamine | 108-45-2 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| n-Propylbenzene | 103-65-1 | -0.198 | 0.086 | 1 | 0 | 0.7 | - |
| o-Phenylenediamine | 95-54-5 | -0.013 | 0.053 | 2 | 0 | 0.6 | 1.37 |
| o-Toluenesulfonamide | 88-19-7 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Oxyfluorfen | 42874-03-3 | 1.142 | 0.100 | 6 | 0 | 0.4 | - |
| p-Cymene | 99-87-6 | 0.195 | 0.055 | 2 | 0 | 0.7 | 1.83 |
| p-Phenylenediamine | 106-50-3 | -0.013 | 0.053 | 2 | 0 | 0.6 | **3.21** |
| Propoxur | 114-26-1 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Resorcinol | 108-46-3 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Sulphanilamide | 63-74-1 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| Thiamphenicol | 15318-45-3 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Toluene | 108-88-3 | -0.614 | 0.095 | 1 | 0 | 0.5 | 0.57 |
| Trans-cinnamic acid | 140-10-3 | -1.587 | 0.108 | 1 | 1 | 0.6 | - |
| 2-(1,1-Dimethyl)-4,6-dimethylphenol | 1879-09-0 | 1.396 | 0.079 | 4 | 0 | 0.9 | 1.85 |
| 2,3,4,5-tetrachlorophenol | 4901-51-3 | 0.541 | 0.087 | 5 | 0 | 0.3 | - |
| 2,3,5,6-tetrachlorophenol | 935-95-5 | 0.541 | 0.087 | 5 | 0 | 0.3 | - |
| 2,3,5-trichlorophenol | 933-78-8 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 2,3,5-trimethylphenol | 697-82-5 | 0.980 | 0.044 | 4 | 0 | 0.7 | - |
| 2,3,6-trichlorophenol | 933-75-5 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 2,3,6-trimethylphenol | 2416-94-6 | 0.980 | 0.044 | 4 | 0 | 0.7 | - |
| 2,3-dimethylphenol | 526-75-0 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 2,4,6-Tribromophenol | 118-79-6 | 0.148 | 0.074 | 4 | 0 | 0.3 | 2.34 |
| 2,4,6-trimethylphenol | 527-60-6 | 0.980 | 0.044 | 4 | 0 | 0.7 | - |
| 2,4-Dibromophenol | 615-58-7 | -0.244 | 0.078 | 3 | 0 | 0.3 | 1.84 |
| 2,4-di-tert-butylphenol | 96-76-4 | 1.004 | 0.073 | 3 | 0 | 0.9 | 2.48 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 2,5-dimethylphenol | 95-87-4 | 0.588 | 0.041 | 3 | 0 | 0.7 | 1.33 |
| 2,6-dimethylphenol | 576-26-1 | 0.588 | 0.041 | 3 | 0 | 0.7 | 0.91 |
| 2,6-Di-sec-butylphenol | 5510-99-6 | 1.004 | 0.073 | 3 | 0 | 0.9 | **3.14** |
| 2-Allylphenol | 1745-81-9 | -0.221 | 0.060 | 2 | 0 | 0.5 | - |
| 2-ethylphenol | 90-00-6 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| 2-methoxyphenol | 90-05-1 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| 2-n-propylphenol | 644-35-9 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| 2-tert-butyl phenol | 88-18-6 | 0.611 | 0.084 | 2 | 0 | 0.9 | 1.61 |
| 2-tert-Butyl-p-cresol | 2409-55-4 | 1.004 | 0.073 | 3 | 0 | 0.9 | 1.94 |
| 3,4,5-trichloroguaiacol | 57057-83-7 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 3,4,5-trichlorophenol | 609-19-8 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 3,4-dimethylphenol | 95-65-8 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 3-ethylphenol | 620-17-7 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| 3-Trifluoromethyl-4-nitrophenol | 88-30-2 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| 4-(1-Methylethenyl)phenol | 4286-23-1 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.16 |
| 4-(2,4-dichlorophenoxy)-phenol | 40843-73-0 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 4,5,6-trichloroguaiacol | 2668-24-8 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 4,5-Dichloroguaiacol | 2460-49-3 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| 4-Chloro-2-methylphenol | 1570-64-5 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| 4-Chloro-2-nitrophenol | 89-64-5 | -0.036 | 0.056 | 3 | 0 | 0.4 | 1.20 |
| 4-ethylphenol | 123-07-9 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| 4-n-Nonylphenol | 104-40-5 | 0.403 | 0.065 | 2 | 0 | 0.8 | - |
| 4-n-octylphenol | 1806-26-4 | 0.611 | 0.084 | 2 | 0 | 0.9 | **3.37** |
| 4-Pentylphenol | 14938-35-3 | 0.611 | 0.084 | 2 | 0 | 0.9 | 2.07 |
| 6-tert-Butyl-m-cresol | 88-60-8 | 1.004 | 0.073 | 3 | 0 | 0.9 | 1.78 |
| 6-Tert-butyl-o-cresol | 2219-82-1 | 1.004 | 0.073 | 3 | 0 | 0.9 | 1.58 |
| Butylated hydroxyanisole | 25013-16-5 | 1.212 | 0.101 | 3 | 0 | 1 | 1.49 |

Table S2. Continued

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | | pLC50 (mM)\* |
| Methyl p-hydroxybenzoate | 99-76-3 | -0.013 | 0.053 | 2 | 0 | 0.6 | | 0.40 |
| o-sec-Butylphenol | 89-72-5 | 0.611 | 0.084 | 2 | 0 | 0.9 | | 1.40 |
| p-sec-Butylphenol | 99-71-8 | 0.611 | 0.084 | 2 | 0 | 0.9 | | 1.76 |
| p-tert-butylphenol | 98-54-4 | 0.611 | 0.084 | 2 | 0 | 0.9 | | - |
| Tetrachloroguaiacol | 2539-17-5 | 1.142 | 0.100 | 6 | 0 | 0.4 | | - |
| Thymol | 89-83-8 | 1.004 | 0.073 | 3 | 0 | 0.9 | | 1.50 |
| Trichlorosyringol | 2539-26-6 | 2.390 | 0.175 | 6 | 0 | 1 | | - |
| 1-Nitropyrene | 5522-43-0 | -0.822 | 0.111 | 1 | 0 | 0.4 | | - |
| 2-acetamidophenoxazin-3-one | 1916-55-8 | -0.429 | 0.075 | 2 | 0 | 0.4 | | - |
| 2-amino-7-methoxyphenoxazin-3-one |  | -0.036 | 0.056 | 3 | 0 | 0.4 |
| 2-aminophenoxazin-3-one | 1916-59-2 | -0.429 | 0.075 | 2 | 0 | 0.4 | | - |
| 9-Vinylcarbazole | 1484-13-5 | -1.007 | 0.146 | 0 | 0 | 0.5 | | - |
| Acenaphthene | 83-32-9 | 0.195 | 0.055 | 2 | 0 | 0.7 | | - |
| Dibenzo[b,f]cyclohepten-1-one | 2222-33-5 | 0.564 | 0.042 | 4 | 0 | 0.5 | | - |
| Dibenzothiophene | 132-65-0 | -1.007 | 0.146 | 0 | 0 | 0.5 | | **2.12** |
| Fluorene | 86-73-7 | 0.564 | 0.042 | 4 | 0 | 0.5 | |  |
| Phenanthrene | 85-01-8 | -1.007 | 0.146 | 0 | 0 | 0.5 | | **2.10** |
| Phenothiazine | 92-84-2 | 0.564 | 0.042 | 4 | 0 | 0.5 | | 2.41 |
| 1-Decanol | 112-30-1 | -1.423 | 0.191 | 0 | 0 | 0.3 | | **1.75** |
| 1-Nonanol | 143-08-8 | -1.423 | 0.191 | 0 | 0 | 0.3 | | **1.65** |
| 2-(2-Butoxyethoxy)ethanol | 112-34-5 | -0.799 | 0.136 | 0 | 0 | 0.6 | | - |
| 2-Butoxyethanol | 111-76-2 | -0.799 | 0.136 | 0 | 0 | 0.6 | | - |
| 2-Isoproxyethanol | 109-59-1 | -0.799 | 0.136 | 0 | 0 | 0.6 | | - |
| 3-Pentanol | 71-41-0 | -1.423 | 0.191 | 0 | 0 | 0.3 | | - |
| Cyclohexanol | 108-93-0 | -1.007 | 0.146 | 0 | 0 | 0.5 | | - |
| Hexanol | 111-27-3 | -1.423 | 0.191 | 0 | 0 | 0.3 | | - |
| Isodecyl alcohol | 25339-17-7 | -1.423 | 0.191 | 0 | 0 | 0.3 | | **1.43** |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 1,6-Hexanediamine | 124-09-4 | -0.799 | 0.136 | 0 | 0 | 0.6 | 0.21 |
| 2-(Dibutylamino)ethanol | 102-81-8 | -1.215 | 0.164 | 0 | 0 | 0.4 | 0.78 |
| 2,2'-Dimethyl-4,4'-methylenebis(cyclohexylamine) | 6864-37-5 | -0.799 | 0.136 | 0 | 0 | 0.6 | 1.04 |
| 2-Amino-2-ethylpropanediol | 115-70-8 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Cyclohexylamine | 108-91-8 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.48 |
| Dibutylamine | 111-92-2 | -1.423 | 0.191 | 0 | 0 | 0.3 | - |
| Diethanolamine | 111-42-2 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| Diethylamine | 109-89-7 | -1.215 | 0.164 | 0 | 0 | 0.4 | 0.43 |
| Diethylnitrosamine | 55-18-5 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Diisopropylamine | 108-18-9 | -1.423 | 0.191 | 0 | 0 | 0.3 | - |
| Dimethylamine | 124-40-3 | -0.799 | 0.136 | 0 | 0 | 0.6 | - |
| N,N,N',N'-Tetramethylhexamethylenediamine | 111-18-2 | -1.215 | 0.164 | 0 | 0 | 0.4 | - |
| Piperidine | 110-89-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| t-Butylamine | 75-64-9 | -1.215 | 0.164 | 0 | 0 | 0.4 | - |
| Triethylamine | 121-44-8 | -1.423 | 0.191 | 0 | 0 | 0.3 | 0.63 |
| 2-(Dimethylamino)ethyl methacrylate | 2867-47-2 | 0.034 | 0.179 | 0 | 0 | 1 | 0.92 |
| 2-Ethylhexyl methacrylate | 688-84-6 | 0.034 | 0.179 | 0 | 0 | 1 | 1.85 |
| 2-hydroxyethyl acrylate | 818-61-1 | 0.034 | 0.179 | 0 | 0 | 1 | 1.25 |
| 2-hydroxyethyl methacrylate | 868-77-9 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Ethyl trichloroacetate | 515-84-4 | 0.034 | 0.179 | 0 | 0 | 1 | 0.64 |
| Ethylacrylate | 140-88-5 | 0.034 | 0.179 | 0 | 0 | 1 | 1.92 |
| Isobutyl acetate | 110-19-0 | 0.034 | 0.179 | 0 | 0 | 1 | 0.83 |
| Methyl acrylate | 96-33-3 | 0.034 | 0.179 | 0 | 0 | 1 | 1.79 |
| Methyl methacrylate | 80-62-6 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| n-Butyl acrylate | 141-32-2 | 0.034 | 0.179 | 0 | 0 | 1 | 1.73 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| n-butyl methacrylate | 97-88-1 | 0.034 | 0.179 | 0 | 0 | 1 | 1.40 |
| Testosterone propionate | 57-85-2 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Tetracaine | 94-24-6 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Vinyl acetate | 108-05-4 | 0.034 | 0.179 | 0 | 0 | 1 | 1.55 |
| 2,3,4-trichloroaniline | 634-67-3 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 2,3-dichloroaniline | 608-27-5 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| 2,3-Dimethylaniline | 87-59-2 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 2,4,5-Trichloroaniline | 636-30-6 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 2,4,6-trichloroaniline | 634-93-5 | 0.148 | 0.074 | 4 | 0 | 0.3 | 1.57 |
| 2,4,6-Trimethylaniline | 88-05-1 | 0.980 | 0.044 | 4 | 0 | 0.7 | **0.39** |
| 2,4-Dichloroaniline | 554-00-7 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.30 |
| 2,4-dimethylaniline | 95-68-1 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 2,5-dichloroaniline | 95-82-9 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.87 |
| 2,5-dimethylaniline | 95-78-3 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 2,6-dichloroaniline | 608-31-1 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| 2,6-diethylaniline | 579-66-8 | 1.004 | 0.073 | 3 | 0 | 0.9 | - |
| 2,6-dimethylaniline | 87-62-7 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |
| 2-Chloro-5-methylaniline | 95-81-8 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.11 |
| 2-Chloroaniline | 95-51-2 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.24 |
| 2-ethylaniline | 578-54-1 | 0.195 | 0.055 | 2 | 0 | 0.7 | - |
| 2-Methyl-4-nitroaniline | 99-52-5 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 2-Methylaniline | 95-53-4 | -0.221 | 0.060 | 2 | 0 | 0.5 | -0.15 |
| 2-Nitroaniline | 88-74-4 | -0.429 | 0.075 | 2 | 0 | 0.4 | 0.52 |
| 2-Nitro-p-anisidine | 96-96-8 | 0.380 | 0.038 | 3 | 0 | 0.6 | 0.61 |
| 3,4,5-Trichloroaniline | 634-91-3 | 0.148 | 0.074 | 4 | 0 | 0.3 | - |
| 3,4-Dichloroaniline | 95-76-1 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.17 |
| 3,4-Dimethylaniline | 95-64-7 | 0.588 | 0.041 | 3 | 0 | 0.7 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | | NaasC | CATS2D\_01\_DN | | DLS\_04 | | | pLC50 (mM)\* |
| 3,5-dichloroaniline | 626-43-7 | 0.172 | 0.043 | | 3 | 0 | | 0.5 | | | - |
| 3,5-dimethylaniline | 108-69-0 | 0.588 | 0.041 | | 3 | 0 | | 0.7 | | | 0.55 |
| 3-chloroaniline | 108-42-9 | -0.221 | 0.060 | | 2 | 0 | | 0.5 | | | 1.16 |
| 3-ethylaniline | 587-02-0 | 0.195 | 0.055 | | 2 | 0 | | 0.7 | | | - |
| 3-methylaniline | 108-44-1 | -0.221 | 0.060 | | 2 | 0 | | 0.5 | | | - |
| 3-Nitroaniline | 99-09-2 | -0.429 | 0.075 | | 2 | 0 | | 0.4 | | | 0.19 |
| 4-Chloro-2-nitroaniline | 89-63-4 | -0.036 | 0.056 | | 3 | 0 | | 0.4 | | | 1.01 |
| 4-chloroaniline | 106-47-8 | -0.221 | 0.060 | | 2 | 0 | | 0.5 | | | 1.34 |
| 4-ethylaniline | 589-16-2 | 0.195 | 0.055 | | 2 | 0 | | 0.7 | | | - |
| 4-Fluoroaniline | 371-40-4 | -0.221 | 0.060 | | 2 | 0 | | 0.5 | | | - |
| 4-Isopropylaniline | 99-88-7 | 0.195 | 0.055 | | 2 | 0 | | 0.7 | | | 0.47 |
| 4-Methylaniline | 106-49-0 | -0.221 | 0.060 | | 2 | 0 | | 0.5 | | | -0.05 |
| 4-Nitroaniline | 100-01-6 | -0.429 | 0.075 | | 2 | 0 | | 0.4 | | | 0.21 |
| Aniline, p-(phenylazo)-(p-Aminoazobenzene) | 60-09-3 | 0.380 | 0.038 | | 3 | 0 | | 0.6 | | | 2.75 |
| Chlorfluoroaniline | 21397-08-0 | 0.172 | 0.043 | | 3 | 0 | | 0.5 | | | - |
| Dithiodianiline | 722-27-0 | 0.772 | 0.039 | | 4 | 0 | | 0.6 | | | - |
| N,N-Diethylaniline | 91-66-7 | 0.218 | 0.111 | | 1 | 0 | | 0.9 | | | 0.76 |
| N,N'-dimethylaniline |  | -0.198 | 0.086 | 1 | | | 0 | | 0.7 |
| N,N-Dimethylaniline | 121-69-7 | -0.198 | 0.086 | | 1 | 0 | | 0.7 | | | - |
| N-Ethylaniline | 103-69-5 | -0.198 | 0.086 | | 1 | 0 | | 0.7 | | | 0.22 |
| p-Anisidine | 104-94-9 | -0.013 | 0.053 | | 2 | 0 | | 0.6 | | | - |
| 2-ethyl-Butanoic acid | 88-09-5 | -1.148 | 0.174 | | 0 | 1 | | 1 | | | 0.14 |
| 2-Methylbutanoic acid | 600-07-7 | -1.148 | 0.174 | | 0 | 1 | | 1 | | | - |
| 3-Methylbutanoic acid | 503-74-2 | -1.148 | 0.174 | | 0 | 1 | | 1 | | | - |
| Acrylic acid | 79-10-7 | -2.188 | 0.168 | | 0 | 1 | | 0.5 | | | 0.07 |
| A-fluoro-b-alanine | 3821-81-6 | -1.148 | 0.174 | | 0 | 1 | | 1 | | | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Chloroacetic acid | 79-11-8 | -1.148 | 0.174 | 0 | 1 | 1 | 0.12 |
| Dansylglycine | 1091-85-6 | -1.195 | 0.080 | 2 | 1 | 0.6 | - |
| Flumequine | 42835-25-6 | 0.007 | 0.084 | 4 | 1 | 0.8 | - |
| Gentisic acid | 490-79-9 | -1.218 | 0.099 | 3 | 1 | 0.4 | - |
| Heptanoic acid | 111-14-8 | -1.148 | 0.174 | 0 | 1 | 1 | 0.24 |
| Isocyanuric acid | 108-80-5 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| Malonic acid diethylester | 105-53-3 | 0.034 | 0.179 | 0 | 0 | 1 | 0.61 |
| Methacrylic acid | 79-41-4 | -1.148 | 0.174 | 0 | 1 | 1 | - |
| Octanoic acid | 124-07-2 | -1.564 | 0.147 | 0 | 1 | 0.8 | 0.45 |
| Orthoformic acid trimethylester | 149-73-5 | -0.383 | 0.141 | 0 | 0 | 0.8 | - |
| Oxolinic acid | 14698-29-4 | -0.409 | 0.076 | 4 | 1 | 0.6 | - |
| Perfluorooctanoic acid | 335-67-1 | -1.564 | 0.147 | 0 | 1 | 0.8 | - |
| Pivalic acid | 75-98-9 | -1.148 | 0.174 | 0 | 1 | 1 | - |
| Pyridaphenthion | 119-12-0 | 0.426 | 0.136 | 1 | 0 | 1 | - |
| Sorbic acid | 110-44-1 | -1.564 | 0.147 | 0 | 1 | 0.8 | 0.17 |
| 2-Methylvaleraldehyde | 123-15-9 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| Capronaldehyde | 66-25-1 | -0.591 | 0.134 | 0 | 0 | 0.7 | - |
| Crotonaldehyde | 4170-30-3 | -0.799 | 0.136 | 0 | 0 | 0.6 | **2.99** |
| Dodecanal | 112-54-9 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Glutaraldehyde | 111-30-8 | 0.034 | 0.179 | 0 | 0 | 1 | 1.06 |
| Propionaldehyde | 123-38-6 | -0.383 | 0.141 | 0 | 0 | 0.8 | - |
| 1,2,4-trichloro-5-nitrobenzene | 89-69-0 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 2-Chloro-1-fluoro-4-nitrobenzene | 350-30-1 | -0.036 | 0.056 | 3 | 0 | 0.4 | 1.94 |
| 2-Chloronitrobenzene | 88-73-3 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 2-Nitroanisole | 91-23-6 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.51 |
| 2-Nitrotoluene | 88-72-2 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| 3,4-Dichloronitrobenzene | 99-54-7 | -0.036 | 0.056 | 3 | 0 | 0.4 | 1.61 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 3-Chloronitrobenzene | 121-73-3 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 3-Nitroanisole | 555-03-3 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.41 |
| 4-Amino-2,6-dinitrotoluene | 19406-51-0 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 4-Amino-2-nitrotoluene | 119-32-4 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 4-Chloro-3-methylnitrobenzene | 13290-74-9 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| 4-Chloronitrobenzene | 100-00-5 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 4-Methylnitrobenzene | 99-99-0 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.57 |
| alpha-Chloro-4-nitrotoluene | 100-14-1 | -0.429 | 0.075 | 2 | 0 | 0.4 | **2.45** |
| Nitrobenzene | 98-95-3 | -0.822 | 0.111 | 1 | 0 | 0.4 | - |
| 1,3-Diphenylguanidine | 102-06-7 | -0.013 | 0.053 | 2 | 0 | 0.6 | 1.09 |
| 2,2-Bis[4-(2-hydroxyethoxy)phenyl]propane | 901-44-0 | 1.604 | 0.109 | 4 | 0 | 1 | 1.18 |
| 2,3,4,4'-Tetrahydroxybenzophenon | 31127-54-5 | 1.142 | 0.100 | 6 | 0 | 0.4 | 0.84 |
| 2,4-Diamino-6-phenyl-s-triazine | 91-76-9 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| 2-Hydroxy-4-methoxybenzophenone | 131-57-7 | 0.772 | 0.039 | 4 | 0 | 0.6 | 1.78 |
| 3,4,4'-Trichlorodiphenylurea | 101-20-2 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 4,4'-Diaminodiphenyl ether | 101-80-4 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| 4,4'-Dihydroxydiphenylmethane | 620-92-8 | 0.772 | 0.039 | 4 | 0 | 0.6 | 1.19 |
| 4,4'-Methylenedianiline | 101-77-9 | 0.772 | 0.039 | 4 | 0 | 0.6 | 0.98 |
| Benzenamine,2,5-diethoxy-4-(4-morpholinyl)- | 51963-82-7 | 1.604 | 0.109 | 4 | 0 | 1 | 1.08 |
| Benzophenone | 119-61-9 | -0.221 | 0.060 | 2 | 0 | 0.5 | - |
| Bis(4-hydroxyphenyl)sulfone | 80-09-1 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| Bisphenol A | 80-05-7 | 1.188 | 0.057 | 4 | 0 | 0.8 | 1.46 |
| Dibenzyl ether | 103-50-4 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.46 |
| Dibromocresyl glycidyl ether | 30171-80-3 | 0.819 | 0.110 | 2 | 0 | 1 | 2.39 |
| Diphenyl ether | 101-84-8 | -0.221 | 0.060 | 2 | 0 | 0.5 | **1.98** |
| Diphenylamine | 122-39-4 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.41 |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Di-p-tolylamine | 620-93-9 | 0.564 | 0.042 | 4 | 0 | 0.5 | 2.66 |
| Hydrazobenzene | 122-66-7 | -0.013 | 0.053 | 2 | 0 | 0.6 | **3.63** |
| N,N'-Bis(2-methylphenyl)guanidine | 97-39-2 | 0.772 | 0.039 | 4 | 0 | 0.6 | 1.10 |
| Procymidone | 32809-16-8 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Pyrimethamine | 58-14-0 | 1.558 | 0.092 | 6 | 0 | 0.6 | - |
| Styrene-7,8-oxide | 96-09-3 | -0.198 | 0.086 | 1 | 0 | 0.7 | 1.14 |
| Sulfadiazine | 68-35-9 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| Sulfadimethoxine | 122-11-2 | 1.165 | 0.057 | 5 | 0 | 0.6 | - |
| Sulfamethazine\_\_Sulfadimidine | 57-68-1 | 1.165 | 0.057 | 5 | 0 | 0.6 | - |
| Sulfamethoxazole | 723-46-6 | 0.772 | 0.039 | 4 | 0 | 0.6 | - |
| Tetrabromobisphenol A | 79-94-7 | 2.343 | 0.212 | 8 | 0 | 0.6 | 1.77 |
| 1,1'-oxybis-butane | 142-96-1 | -1.423 | 0.191 | 0 | 0 | 0.3 | - |
| 1,2,3-trihydroxybenzene | 87-66-1 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 1,5-Cyclooctadiene | 111-78-4 | -0.175 | 0.156 | 0 | 0 | 0.9 | 0.92 |
| 1-Benzo[b]thien-2-ylethan-1-one | 22720-75-8 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.25 |
| 1-Chloro-2,4-dinitrobenzene | 97-00-7 | -0.036 | 0.056 | 3 | 0 | 0.4 | **3.10** |
| 1-Cyclohexene-1-carbonitrile | 1855-63-6 | -0.591 | 0.134 | 0 | 0 | 0.7 | 0.42 |
| 1-Mercaptooctane [n-Octylmercaptan] | 111-88-6 | -1.423 | 0.191 | 0 | 0 | 0.3 | **2.65** |
| 1-Methoxy-2-propanol | 107-98-2 | -0.799 | 0.136 | 0 | 0 | 0.6 | - |
| 2-(1'-Cyclohexenyl)cyclohexanone | 1502-22-3 | -0.175 | 0.156 | 0 | 0 | 0.9 | 0.79 |
| 2,2,5,5,-Tetramethylhydrofuran | 15045-43-9 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 2,2,6,6-Tetramethylpiperidin-4-ol | 2403-88-5 | -0.799 | 0.136 | 0 | 0 | 0.6 | - |
| 2,2'-Dithiobisbenzothiazole | 120-78-5 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 2,3,3,3,2',3',3',3'-Octachlorodipropyl ether | 127-90-2 | -1.007 | 0.146 | 0 | 0 | 0.5 | **2.81** |
| 2,3-Dichloro-1,4-napthoquinone | 117-80-6 | -0.429 | 0.075 | 2 | 0 | 0.4 | **3.86** |
| 2,4,6-Trimethylbenzaldehyde | 487-68-3 | 0.980 | 0.044 | 4 | 0 | 0.7 | 1.09 |
| 2-acetoxy-1,4-naphthoquinone | 1785-65-5 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 2-aminophenol | 95-55-6 | -0.013 | 0.053 | 2 | 0 | 0.6 | **2.21** |
| 2-Aminopyridine | 504-29-0 | -0.406 | 0.086 | 1 | 0 | 0.6 | 0.93 |
| 2-Butanone oxime | 96-29-7 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| 2-Butenedinitrile, (E)- | 764-42-1 | -1.215 | 0.164 | 0 | 0 | 0.4 | 2.34 |
| 2-Chlorobenzyl chloride | 611-19-8 | -0.221 | 0.060 | 2 | 0 | 0.5 | **2.78** |
| 2-Decanone | 693-54-9 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 2-hydroxy-1,4-naphthoquinone | 83-72-7 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 2-Mercaptobenzothiazole | 149-30-4 | -0.637 | 0.099 | 2 | 0 | 0.3 | - |
| 2-Mercaptoethanol | 60-24-2 | -0.175 | 0.156 | 0 | 0 | 0.9 | 0.43 |
| 2-methyl-1,4-naphthoquinone | 58-27-5 | -0.013 | 0.053 | 2 | 0 | 0.6 | - |
| 2-Methyl-4(5)-nitroimidazole | 696-23-1 | -0.429 | 0.075 | 2 | 0 | 0.4 | - |
| 2-methylthio-4-tert-butylamino-6-amino-s-triazine | 30125-65-6 | 1.212 | 0.101 | 3 | 0 | 1 | - |
| 2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- | 470-82-6 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 2-Phenylindole | 948-65-2 | -0.221 | 0.060 | 2 | 0 | 0.5 | **2.85** |
| 2-Phenylphenol | 90-43-7 | 0.172 | 0.043 | 3 | 0 | 0.5 | - |
| 2-Propenenitrile, 2-chloro- | 920-37-6 | -1.423 | 0.191 | 0 | 0 | 0.3 | **3.02** |
| 2-Propenenitrile | 107-13-1 | -1.215 | 0.164 | 0 | 0 | 0.4 | 1.02 |
| 2-Undecanone | 112-12-9 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| 2-Vinylpyridine | 100-69-6 | -0.614 | 0.095 | 1 | 0 | 0.5 | 1.21 |
| 3-(Methylthio)propionaldehyde | 3268-49-3 | -0.175 | 0.156 | 0 | 0 | 0.9 | 1.17 |
| 3,3'-Dichlorobenzidine | 91-94-1 | 1.558 | 0.092 | 6 | 0 | 0.6 | **2.70** |
| 3,4,5-Trichlorocatechol | 56961-20-7 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 3,4,6-Trichlorocatechol | 32139-72-3 | 0.749 | 0.069 | 5 | 0 | 0.4 | - |
| 3,4-Dichlorocatechol | 3978-67-4 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 3,5,5-Trimethyl-2-cyclohexen-1-one | 78-59-1 | -0.175 | 0.156 | 0 | 0 | 0.9 | - |
| 3,5-Dichlorocatechol | 13673-92-2 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| 3,5-Di-tert-butylsalicylic acid | 19715-19-6 | 0.423 | 0.125 | 4 | 1 | 1 | 1.97 |
| 3a,4,7,7a-Tetrahydro-1H-indene | 3048-65-5 | -0.591 | 0.134 | 0 | 0 | 0.7 | 1.44 |
| 3-Amino-1,2,4-triazole | 61-82-5 | -0.406 | 0.086 | 1 | 0 | 0.6 | - |
| 3-amino-2-Butenenitrile | 1118-61-2 | -0.383 | 0.141 | 0 | 0 | 0.8 | 0.68 |
| 3-Amino-4-chlorobenzoic acid | 2840-28-0 | -1.218 | 0.099 | 3 | 1 | 0.4 | - |
| 3-Aminophenol | 591-27-5 | -0.013 | 0.053 | 2 | 0 | 0.6 | -0.04 |
| 3-Aminopyridine | 462-08-8 | -0.406 | 0.086 | 1 | 0 | 0.6 | 1.04 |
| 4,4,4-Trifluorocrotonitrile | 406-86-0 | -1.007 | 0.146 | 0 | 0 | 0.5 | **2.78** |
| 4,4'-Dihydroxy-biphenyl | 92-88-6 | 0.772 | 0.039 | 4 | 0 | 0.6 | 1.16 |
| 4,5-Dichlorocatechol | 3428-24-8 | 0.356 | 0.054 | 4 | 0 | 0.4 | - |
| 4,6-Dinitro-o-cresol | 534-52-1 | 0.356 | 0.054 | 4 | 0 | 0.4 | 2.26 |
| 4-Amino-2-nitrophenol | 119-34-6 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| 4-Aminophenol | 123-30-8 | -0.013 | 0.053 | 2 | 0 | 0.6 | 2.07 |
| 4-Aminopyridine | 504-24-5 | -0.406 | 0.086 | 1 | 0 | 0.6 | 1.44 |
| 4-Chlorocatechol | 2138-22-9 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| 4-ethyl-1,1'-Biphenyl | 5707-44-8 | 0.172 | 0.043 | 3 | 0 | 0.5 | 2.48 |
| 4-Hydroxybenzoic acid | 99-96-7 | -1.611 | 0.113 | 2 | 1 | 0.4 | 0.17 |
| 4-Methylbenzoic acid | 99-94-5 | -1.195 | 0.080 | 2 | 1 | 0.6 | 0.33 |
| 4-Vinylpyridine | 100-43-6 | -0.614 | 0.095 | 1 | 0 | 0.5 | **2.02** |
| 5-Ethylidene-8,9,10-trinorborn-2-ene | 16219-75-3 | -0.591 | 0.134 | 0 | 0 | 0.7 | 1.23 |
| 6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline | 91-53-2 | 1.212 | 0.101 | 3 | 0 | 1 | 1.51 |
| 6-Methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one | 2439-01-2 | -0.036 | 0.056 | 3 | 0 | 0.4 | - |
| 8-Hydroxyquinoline | 148-24-3 | -0.406 | 0.086 | 1 | 0 | 0.6 | 1.76 |
| Acetophenone | 98-86-2 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Acetylsalicylic acid | 50-78-2 | -1.195 | 0.080 | 2 | 1 | 0.6 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| alpha,alpha-Dichlorotoluene | 98-87-3 | -0.614 | 0.095 | 1 | 0 | 0.5 | 0.85 |
| Anisol | 100-66-3 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Atrazine-deisopropyl | 1007-28-9 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Benazolin ethyl | 25059-80-7 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Benzaldehyde | 100-52-7 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Benzenethiol | 108-98-5 | -0.614 | 0.095 | 1 | 0 | 0.5 | **4.09** |
| Benzoyl-chloride | 98-88-4 | -0.614 | 0.095 | 1 | 0 | 0.5 | - |
| Benzyl-chloroformiate | 501-53-1 | -0.406 | 0.086 | 1 | 0 | 0.6 | - |
| Betariboacetate | 13035-61-5 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Biphenyl | 92-52-4 | -0.221 | 0.060 | 2 | 0 | 0.5 | 1.60 |
| Bis(2-chloroethyl) ether | 111-44-4 | -1.007 | 0.146 | 0 | 0 | 0.5 | - |
| Bismerthiazol | 79319-85-0 | -0.799 | 0.136 | 0 | 0 | 0.6 | - |
| Buparvaquone | 88426-33-9 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| But-3-en-3-olide | 674-82-8 | 0.034 | 0.179 | 0 | 0 | 1 | 0.98 |
| Butachlor | 23184-66-9 | 1.212 | 0.101 | 3 | 0 | 1 | **3.05** |
| Butylbenzyl phthalate | 85-68-7 | 0.796 | 0.053 | 3 | 0 | 0.8 | - |
| Captopril | 62571-86-2 | -1.148 | 0.174 | 0 | 1 | 1 | - |
| Chlorohydroquinone | 615-67-8 | 0.380 | 0.038 | 3 | 0 | 0.6 | - |
| Cinmethylin | 87818-31-3 | 0.819 | 0.110 | 2 | 0 | 1 | - |
| Cotinine | 486-56-6 | 0.010 | 0.094 | 1 | 0 | 0.8 | - |
| Cyclohexanone oxime | 100-64-1 | 0.034 | 0.179 | 0 | 0 | 1 | - |
| Cyclohexanone | 108-94-1 | -0.175 | 0.156 | 0 | 0 | 0.9 | - |
| Cyclosulfamuron | 136849-15-5 | 1.789 | 0.102 | 5 | 0 | 0.9 | - |
| Diallyl phthalate | 131-17-9 | -0.013 | 0.053 | 2 | 0 | 0.6 | **2.75** |
| Diethyl disulfide | 110-81-6 | -1.007 | 0.146 | 0 | 0 | 0.5 | 1.01 |
| Diethyl malonate | 105-53-3 | 0.034 | 0.179 | 0 | 0 | 1 | 0.61 |
| Diethyl phthalate | 84-66-2 | 0.819 | 0.110 | 2 | 0 | 1 | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | | NaasC | CATS2D\_01\_DN | | DLS\_04 | | | pLC50 (mM)\* |
| Diisobutyl phthalate | 84-69-5 | 0.819 | 0.110 | | 2 | 0 | | 1 | | | 1.92 |
| Dimethyl disulphide | 624-92-0 | -0.175 | 0.156 | | 0 | 0 | | 0.9 | | | **1.93** |
| Dimethylformamide | 68-12-2 | -0.175 | 0.156 | | 0 | 0 | | 0.9 | | | - |
| Dimethylnitrosamine | 62-75-9 | -0.175 | 0.156 | | 0 | 0 | | 0.9 | | | - |
| Dinitramine | 29091-05-2 | 1.188 | 0.057 | | 4 | 0 | | 0.8 | | |  |
| Diphenylpropanediol |  | 0.403 | 0.065 | 2 | | | 0 | | 0.8 |
| Droperidol | 548-73-2 | 1.188 | 0.057 | | 4 | 0 | | 0.8 | | | - |
| Enrofloxacin | 93106-60-6 | 0.423 | 0.125 | | 4 | 1 | | 1 | | | - |
| Ethanethiol | 75-08-1 | -0.799 | 0.136 | | 0 | 0 | | 0.6 | | | 1.45 |
| Flumazenil | 78755-81-4 | 1.581 | 0.079 | | 5 | 0 | | 0.8 | | | - |
| Glycidyl methacrylate | 106-91-2 | 0.034 | 0.179 | | 0 | 0 | | 1 | | | 1.71 |
| Haloxyfop R | 72619-32-0 | 1.581 | 0.079 | | 5 | 0 | | 0.8 | | | - |
| Hexamethylene diacrylate | 13048-33-4 | 0.034 | 0.179 | | 0 | 0 | | 1 | | | **2.77** |
| Hydrogenatedbisphenol A | 80-04-6 | -0.799 | 0.136 | | 0 | 0 | | 0.6 | | | 1.10 |
| Hydroquinone | 123-31-9 | -0.013 | 0.053 | | 2 | 0 | | 0.6 | | | - |
| Isoprene | 78-79-5 | -1.215 | 0.164 | | 0 | 0 | | 0.4 | | | 0.66 |
| Maleic anhydride | 108-31-6 | -1.215 | 0.164 | | 0 | 0 | | 0.4 | | | - |
| Medazepam | 2898-12-6 | 1.188 | 0.057 | | 4 | 0 | | 0.8 | | | - |
| Methacrylonitrile | 126-98-7 | -0.799 | 0.136 | | 0 | 0 | | 0.6 | | | - |
| Methyl isothiocyanate | 556-61-6 | -0.799 | 0.136 | | 0 | 0 | | 0.6 | | | **2.78** |
| Methylhydrazine | 60-34-4 | -0.799 | 0.136 | | 0 | 0 | | 0.6 | | | **2.08** |
| m-Toluic acid | 99-04-7 | -1.195 | 0.080 | | 2 | 1 | | 0.6 | | | 0.22 |
| N-(tert-Butyl)-2-benzothiazolylsulfenamide | 95-31-8 | 0.010 | 0.094 | | 1 | 0 | | 0.8 | | | **2.23** |
| N,N-Dimethylhydrazine | 57-14-7 | -0.591 | 0.134 | | 0 | 0 | | 0.7 | | | - |
| N-Cyclohexyl-2-benzothiazolylsulfenamide | 95-33-0 | 0.010 | 0.094 | | 1 | 0 | | 0.8 | | | **2.10** |
| Nitroglycerin | 55-63-0 | -0.591 | 0.134 | | 0 | 0 | | 0.7 | | | - |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| N-Methyl-N,N-bis(2-dimethylaminoethyl)amine | 3030-47-5 | -0.799 | 0.136 | 0 | 0 | 0.6 |  |
| o-Acetoacetotoluidide | 93-68-5 | 0.403 | 0.065 | 2 | 0 | 0.8 |  |
| o-Chlorobenzonitrile | 873-32-5 | -0.637 | 0.099 | 2 | 0 | 0.3 | 0.57 |
| Octanedinitrile | 629-40-3 | -0.383 | 0.141 | 0 | 0 | 0.8 | -0.61 |
| Olaquindox | 23696-28-8 | 0.403 | 0.065 | 2 | 0 | 0.8 |  |
| Ondansetron | 99614-02-5 | 0.796 | 0.053 | 3 | 0 | 0.8 |  |
| o-Tolidine | 119-93-7 | 1.558 | 0.092 | 6 | 0 | 0.6 | 1.21 |
| Pentane-1-thiol | 110-66-7 | -1.423 | 0.191 | 0 | 0 | 0.3 | **1.90** |
| Perfluorooctane sulfonic acid | 1763-23-1 | -1.772 | 0.145 | 0 | 1 | 0.7 |  |
| Phenol,4,4',4''-ethylidynetris- | 27955-94-8 | 1.558 | 0.092 | 6 | 0 | 0.6 |  |
| Phthalic anhydride | 85-44-9 | -0.429 | 0.075 | 2 | 0 | 0.4 |  |
| Phthalonitrile | 91-15-6 | -0.429 | 0.075 | 2 | 0 | 0.4 | 0.75 |
| Pivaloyl chloride | 3282-30-2 | -0.175 | 0.156 | 0 | 0 | 0.9 |  |
| p-Methoxybenzaldehyde | 123-11-5 | -0.013 | 0.053 | 2 | 0 | 0.6 | 0.53 |
| p-Phenylphenol | 92-69-3 | 0.172 | 0.043 | 3 | 0 | 0.5 | 1.70 |
| Propyl gallate | 121-79-9 | 1.604 | 0.109 | 4 | 0 | 1 |  |
| Propyzamide | 23950-58-5 | 0.796 | 0.053 | 3 | 0 | 0.8 |  |
| Pyrazosulfuron ethyl | 93697-74-6 | 1.789 | 0.102 | 5 | 0 | 0.9 |  |
| Quinoline | 91-22-5 | 0.195 | 0.055 | 2 | 0 | 0.7 | 0.30 |
| Secobarbital | 76-73-3 | 0.034 | 0.179 | 0 | 0 | 1 |  |
| Simazine | 122-34-9 | 1.212 | 0.101 | 3 | 0 | 1 |  |
| Sulfaquinoxaline | 59-40-5 | -0.036 | 0.056 | 3 | 0 | 0.4 |  |
| tert-Butyl 2-ethylperoxyhexanoate | 3006-82-4 | -0.383 | 0.141 | 0 | 0 | 0.8 | 1.67 |
| tert-Butylhydroperoxide | 75-91-2 | -0.799 | 0.136 | 0 | 0 | 0.6 | -0.02 |
| Tetrachlorocatechol | 1198-55-6 | 1.142 | 0.100 | 6 | 0 | 0.4 |  |
| Tetrachlorohydroquinone | 87-87-6 | 1.142 | 0.100 | 6 | 0 | 0.4 |  |

Table S2. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| NAME | CAS | Pred.  pEC50, NR[PLHC-1] | HAT i/i (h\*=0.308) | NaasC | CATS2D\_01\_DN | DLS\_04 | pLC50 (mM)\* |
| Tetrachlorophthalic anhydride | 117-08-8 | 1.142 | 0.100 | 6 | 0 | 0.4 |  |
| Tetrahydromethylphthalic anhydride | 11070-44-3 | -0.383 | 0.141 | 0 | 0 | 0.8 |  |
| Thiopental | 76-75-5 | 0.034 | 0.179 | 0 | 0 | 1 |  |
| Thiophene | 110-02-1 | -1.007 | 0.146 | 0 | 0 | 0.5 | 0.43 |
| Thiosemicarbazide | 79-19-6 | -0.591 | 0.134 | 0 | 0 | 0.7 | 0.64 |
| Thiourea dioxide | 4189-44-0 | -1.007 | 0.146 | 0 | 0 | 0.5 |  |
| Thiourea | 62-56-6 | -0.799 | 0.136 | 0 | 0 | 0.6 |  |
| Triclosan | 3380-34-5 | 1.142 | 0.100 | 6 | 0 | 0.4 | 2.64 |
| Trifluralin | 1582-09-8 | 1.604 | 0.109 | 4 | 0 | 1 |  |
| Trimethylquinone | 935-92-2 | -0.383 | 0.141 | 0 | 0 | 0.8 |  |
| Triphenyl phosphate | 115-86-6 | 0.380 | 0.038 | 3 | 0 | 0.6 | 2.40 |
| Tris-(2,3-dibromopropyl) phosphate | 126-72-7 | -0.175 | 0.156 | 0 | 0 | 0.9 | **2.56** |
| Tris(2-chloroethyl) phosphate | 115-96-8 | 0.034 | 0.179 | 0 | 0 | 1 |  |

\*pLC50 (mM) values were obtained from the literature [31]. Bold values indicate pLC50 data with very weak relationship with the pEC50, NR[PLHC-1] prediction.

Table S3. External set chemicals, predicted pEC50, MTT[PLHC-1] (mM), descriptor and hat values and experimental pLC50 values for the MTT data set.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | | pLC50 (mM)\*\* |
| 5-fluorocytosine | 2022-85-7 | -1.118 | 0.205 | 0.247 | 0 | 0 | - | |
| 5-fluorouracil | 51-21-8 | -1.031 | 0.189 | 0.183 | 0 | 0 | - | |
| Acebutolol | 37517-30-9 | 0.844 | 0.072 | -0.526 | 3 | 0 | - | |
| Acetaminophen | 103-90-2 | -0.015 | 0.058 | -0.119 | 2 | 0 | - | |
| Acridine | 260-94-6 | -0.324 | 0.137 | -0.333 | 0 | 0 | - | |
| Acrivastine | 87848-99-5 | 0.217 | 0.101 | -0.475 | 4 | 1 | - | |
| Acyclovir | 59277-89-3 | -0.205 | 0.070 | 0.020 | 2 | 0 | - | |
| Alprenolol | 13655-52-2 | 0.448 | 0.070 | -0.457 | 2 | 0 | - | |
| Amitriptyline | 50-48-6 | 0.890 | 0.058 | -0.340 | 4 | 0 | - | |
| Amobarbital | 57-43-2 | 0.153 | 0.178 | -0.681 | 0 | 0 | - | |
| Ampicillin | 69-53-4 | -1.152 | 0.121 | -0.135 | 1 | 1 | - | |
| Antipyrine | 60-80-0 | -0.071 | 0.087 | -0.298 | 1 | 0 | - | |
| Atovaquone | 95233-18-4 | 0.494 | 0.054 | -0.051 | 4 | 0 | - | |
| Bumetanide | 28395-03-1 | -0.264 | 0.097 | 0.096 | 5 | 1 | - | |
| Bupropion | 34841-39-9 | 0.814 | 0.120 | -0.724 | 2 | 0 | - | |
| Caffeine | 58-08-2 | -0.029 | 0.059 | -0.109 | 2 | 0 | - | |
| Camptothecin | 7689-03-4 | 0.319 | 0.061 | -0.363 | 2 | 0 | - | |
| Capecitabine | 154361-50-9 | 0.068 | 0.166 | -0.619 | 0 | 0 | - | |
| Carvedilol | 72956-09-3 | 0.664 | 0.054 | -0.395 | 3 | 0 | - | |
| Cefurexime axetil | 64544-07-6 | 0.433 | 0.131 | -0.666 | 1 | 0 | - | |
| Cefuroxime | 55268-75-2 | -1.518 | 0.147 | 0.132 | 1 | 1 | - | |
| Cephalexin | 15686-71-2 | -1.319 | 0.128 | -0.013 | 1 | 1 | - | |
| Chloramphenicol | 56-75-7 | -0.223 | 0.072 | 0.033 | 2 | 0 | - | |
| Chlorotetracycline | 57-62-5 | 0.574 | 0.051 | -0.109 | 4 | 0 | - | |
| Chlorpromazine | 50-53-3 | 1.376 | 0.104 | -0.475 | 5 | 0 | - | |
| Chlorpropamide | 94-20-2 | -0.201 | 0.070 | 0.017 | 2 | 0 | - | |
| Cimetidine | 51481-61-9 | 0.358 | 0.063 | -0.391 | 2 | 0 | - | |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Clonazepam | 1622-61-3 | 0.428 | 0.107 | 0.217 | 5 | 0 | - |
| Clonidine | 4205-90-7 | 0.129 | 0.053 | -0.004 | 3 | 0 | - |
| Cromolyn | 16110-51-3 | -0.583 | 0.313 | -0.078 | 6 | 2 | - |
| Cytarabine | 147-94-4 | -0.650 | 0.144 | -0.095 | 0 | 0 | - |
| Deoxytetracycline | 564-25-0 | 0.077 | 0.057 | 0.034 | 3 | 0 | - |
| Desipramine | 50-47-5 | 0.756 | 0.052 | -0.242 | 4 | 0 | - |
| Doxycycline | 564-25-0 | 0.751 | 0.062 | -0.458 | 3 | 0 | - |
| Estradiol | 50-28-2 | 0.489 | 0.045 | -0.267 | 3 | 0 | - |
| Ethinylestradiol | 57-63-6 | 0.547 | 0.047 | -0.309 | 3 | 0 | - |
| Famciclovir | 104227-87-4 | 0.117 | 0.096 | -0.435 | 1 | 0 | - |
| Famotidine | 76824-35-6 | -0.215 | 0.071 | 0.027 | 2 | 0 | - |
| Fleroxacin | 79660-72-3 | 0.200 | 0.095 | -0.243 | 5 | 1 | - |
| Florfenicol | 73231-34-2 | -0.015 | 0.058 | -0.119 | 2 | 0 | - |
| Flunitrazepam | 1622-62-4 | 0.323 | 0.123 | 0.294 | 5 | 0 | - |
| Flutamide | 13311-84-7 | 0.347 | 0.044 | -0.163 | 3 | 0 | - |
| Furaltadone | 139-91-3 | 0.065 | 0.056 | -0.177 | 2 | 0 | - |
| Gemcitabine | 95058-81-4 | -0.851 | 0.163 | 0.052 | 0 | 0 | - |
| Glibenclamid | 10238-21-8 | 1.823 | 0.187 | -0.801 | 5 | 0 | - |
| Hydrochlorothiazide | 58-93-5 | -0.217 | 0.152 | 0.468 | 4 | 0 | - |
| Hydrocortisone | 50-23-7 | -0.610 | 0.142 | -0.124 | 0 | 0 | - |
| Imipramine | 50-49-7 | 0.890 | 0.058 | -0.340 | 4 | 0 | - |
| Indomethacin | 53-86-1 | -0.044 | 0.089 | -0.065 | 5 | 1 | - |
| Isoniazid | 54-85-3 | -0.253 | 0.088 | -0.165 | 1 | 0 | - |
| Isotretinoin | 4759-48-2 | -0.560 | 0.254 | -0.787 | 0 | 1 | - |
| Ketoconazole | 65277-42-1 | 1.275 | 0.093 | -0.401 | 5 | 0 | - |
| Ketoprofen | 22071-15-4 | -0.662 | 0.069 | -0.053 | 3 | 1 | - |
| Labetalol | 36894-69-6 | 0.719 | 0.051 | -0.215 | 4 | 0 | - |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Lamotrigine | 84057-84-1 | 0.799 | 0.139 | 0.166 | 6 | 0 | - |
| Lansoprazole | 103577-45-3 | 0.661 | 0.050 | -0.173 | 4 | 0 | - |
| Levofloxacin | 100986-85-4 | 0.250 | 0.098 | -0.279 | 5 | 1 | - |
| Lidocaine | 137-58-6 | 0.956 | 0.087 | -0.608 | 3 | 0 | - |
| Lomefloxacin | 98079-51-7 | 0.250 | 0.098 | -0.279 | 5 | 1 | - |
| L-tryptophan | 73-22-3 | -1.440 | 0.138 | 0.075 | 1 | 1 | - |
| Metaxalone | 1665-48-1 | 0.430 | 0.044 | -0.224 | 3 | 0 | - |
| Metformin | 657-24-9 | -0.981 | 0.181 | 0.147 | 0 | 0 | - |
| Methotrexate | 59-05-2 | -0.295 | 0.333 | -0.508 | 5 | 2 | - |
| Methylprednisolone | 83-43-2 | 0.313 | 0.206 | -0.798 | 0 | 0 | - |
| Metipranolol | 22664-55-7 | 1.343 | 0.100 | -0.451 | 5 | 0 | - |
| Metoprolol | 37350-58-6 | 0.267 | 0.059 | -0.325 | 2 | 0 | - |
| Metronidazole | 443-48-1 | 0.137 | 0.056 | -0.230 | 2 | 0 | - |
| Midazolam | 59467-70-8 | 1.358 | 0.183 | -0.022 | 7 | 0 | - |
| Nadolol | 42200-33-9 | 0.789 | 0.066 | -0.486 | 3 | 0 | - |
| Naproxen | 22204-53-1 | -0.591 | 0.090 | -0.325 | 2 | 1 | - |
| Nicotine | 22083-74-5 | 0.109 | 0.095 | -0.429 | 1 | 0 | - |
| Nisoldipine | 63675-72-9 | 0.524 | 0.078 | -0.512 | 2 | 0 | - |
| Nitrofurazone | 59-87-0 | -0.241 | 0.074 | 0.046 | 2 | 0 | - |
| Norfloxacin | 70458-96-7 | 0.003 | 0.079 | -0.319 | 4 | 1 | - |
| Ofloxacin | 82419-36-1 | 0.241 | 0.097 | -0.273 | 5 | 1 | - |
| Oxprenolol | 6452-71-7 | 0.419 | 0.068 | -0.436 | 2 | 0 | - |
| Oxyphenbutazone | 129-20-4 | 0.481 | 0.045 | -0.261 | 3 | 0 | - |
| Oxytetracycline | 79-57-2 | 0.440 | 0.044 | -0.231 | 3 | 0 | - |
| Paracetamol | 103-90-2 | -0.016 | 0.059 | -0.118 | 2 | 0 | - |
| Paroxetine | 61869-08-7 | 1.394 | 0.106 | -0.488 | 5 | 0 | - |
| Pentobarbital | 76-74-4 | -0.065 | 0.152 | -0.522 | 0 | 0 | - |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Phenobarbital | 50-06-6 | -0.252 | 0.088 | -0.166 | 1 | 0 | - |
| Phenoxymethylpenicillinic Acid | 87-08-1 | -1.038 | 0.120 | -0.218 | 1 | 1 | - |
| Phenylbutazone | 50-33-9 | 0.067 | 0.056 | -0.179 | 2 | 0 | - |
| Phenytoin | 57-41-0 | 0.104 | 0.056 | -0.206 | 2 | 0 | - |
| Pindolol | 13523-86-9 | -0.035 | 0.088 | -0.324 | 1 | 0 | - |
| Piperazine | 110-85-0 | -0.403 | 0.136 | -0.275 | 0 | 0 | - |
| Prazosin | 19216-56-9 | 1.756 | 0.171 | -0.752 | 5 | 0 | - |
| Prednisolone | 50-24-8 | -0.750 | 0.152 | -0.022 | 0 | 0 | - |
| Procaine | 59-46-1 | 0.302 | 0.060 | -0.350 | 2 | 0 | - |
| Progesterone | 57-83-0 | -0.172 | 0.144 | -0.444 | 0 | 0 | - |
| Promazine | 58-40-2 | 0.793 | 0.053 | -0.269 | 4 | 0 | - |
| Propylthiouracil | 51-52-5 | -0.440 | 0.136 | -0.248 | 0 | 0 | - |
| Quinine | 130-95-0 | 1.099 | 0.184 | -0.932 | 2 | 0 | - |
| Ranitidine | 66357-35-5 | 0.695 | 0.100 | -0.637 | 2 | 0 | - |
| Risperidone | 106266-06-2 | 0.607 | 0.088 | -0.573 | 2 | 0 | - |
| Sotalol | 3930-20-9 | 0.224 | 0.057 | -0.293 | 2 | 0 | - |
| Sulfaguanidine | 57-67-0 | -0.579 | 0.122 | 0.293 | 2 | 0 | - |
| Sulfaphenazole | 526-08-9 | 0.787 | 0.053 | -0.265 | 4 | 0 | - |
| Sulfasalazine | 599-79-1 | -0.186 | 0.154 | 0.259 | 6 | 1 | - |
| Sumatriptan | 103628-46-2 | 0.293 | 0.060 | -0.344 | 2 | 0 | - |
| Terazosin | 63590-64-7 | 1.437 | 0.134 | -0.739 | 4 | 0 | - |
| Terbinafine | 91161-71-6 | 0.439 | 0.132 | -0.670 | 1 | 0 | - |
| Testosterone | 58-22-0 | 0.013 | 0.160 | -0.579 | 0 | 0 | - |
| Theophylline | 58-55-9 | -0.271 | 0.077 | 0.068 | 2 | 0 | - |
| Timolol | 26839-75-8 | 0.759 | 0.111 | -0.684 | 2 | 0 | - |
| Tolazamide | 1156-19-0 | 0.070 | 0.056 | -0.181 | 2 | 0 | - |
| Tolbutamide | 64-77-7 | 0.030 | 0.057 | -0.152 | 2 | 0 | - |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Trenbolone acetate | 10161-34-9 | 0.097 | 0.170 | -0.640 | 0 | 0 | - |
| Triamterene | 396-01-0 | 0.824 | 0.076 | -0.072 | 5 | 0 | - |
| Triflupromazine | 146-54-3 | 1.373 | 0.104 | -0.473 | 5 | 0 | - |
| Warfarin | 81-81-2 | 0.253 | 0.046 | -0.095 | 3 | 0 | - |
| 2,6-Dichlorobenzonitrile | 1194-65-6 | 0.077 | 0.057 | 0.034 | 3 | 0 | - |
| Acetochlor | 34256-82-1 | 0.662 | 0.054 | -0.393 | 3 | 0 | - |
| Acroleine | 107-02-8 | -0.696 | 0.148 | -0.061 | 0 | 0 | - |
| Ametryn | 834-12-8 | 0.823 | 0.069 | -0.511 | 3 | 0 | - |
| Anilofos | 64249-01-0 | 0.359 | 0.063 | -0.392 | 2 | 0 | - |
| Azocyclotin | 41083-11-8 | 0.475 | 0.241 | -0.916 | 0 | 0 | - |
| Benalaxyl | 71626-11-4 | 1.276 | 0.103 | -0.622 | 4 | 0 | - |
| Benomyl | 17804-35-2 | -0.168 | 0.087 | -0.227 | 1 | 0 | - |
| Bensulfuron-methyl | 83055-99-6 | 1.315 | 0.097 | -0.430 | 5 | 0 | - |
| Beta-cyfluthrin | 68359-37-5 | 0.708 | 0.051 | -0.207 | 4 | 0 | - |
| Bromoxynil | 1689-84-5 | 0.338 | 0.063 | 0.063 | 4 | 0 | - |
| Chloridazon | 1698-60-8 | -0.483 | 0.102 | 0.003 | 1 | 0 | - |
| Chlorimuron-ethyl | 90982-32-4 | 0.776 | 0.078 | -0.037 | 5 | 0 | - |
| Chlorothalonil | 1897-45-6 | 0.661 | 0.155 | 0.267 | 6 | 0 | - |
| Chlorotoluron | 15545-48-9 | 0.369 | 0.044 | -0.179 | 3 | 0 | - |
| Chlorsulfuron | 64902-72-3 | 1.009 | 0.077 | -0.207 | 5 | 0 | - |
| Cyanazine | 21725-46-2 | 0.863 | 0.074 | -0.540 | 3 | 0 | - |
| Cyhexatin | 13121-70-5 | 0.288 | 0.201 | -0.780 | 0 | 0 | - |
| Decanoic acid | 334-48-5 | -1.262 | 0.175 | -0.275 | 0 | 1 | - |
| Diclofop methyl | 51338-27-3 | 1.109 | 0.080 | -0.280 | 5 | 0 | - |
| Diclofop P | 40843-25-2 | -0.023 | 0.089 | -0.080 | 5 | 1 | - |
| Dimethachlon | 24096-53-5 | -0.042 | 0.069 | 0.121 | 3 | 0 | - |
| Endosulfan | 115-29-7 | -0.595 | 0.141 | -0.135 | 0 | 0 | - |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Ethalfluraline | 55283-68-6 | 0.393 | 0.059 | 0.023 | 4 | 0 | - |
| Ethametsulfuron | 111353-84-5 | -0.012 | 0.089 | -0.088 | 5 | 1 | - |
| Ethoxyquin | 91-53-2 | 0.841 | 0.072 | -0.524 | 3 | 0 | 1.51 |
| Fenamiphos | 22224-92-6 | 1.090 | 0.111 | -0.706 | 3 | 0 | - |
| Fenhexamid | 126833-17-8 | 0.861 | 0.056 | -0.319 | 4 | 0 | - |
| Fenoxaprop | 95617-09-7 | -0.411 | 0.071 | -0.017 | 4 | 1 | - |
| Fenpropidin | 67306-00-7 | 1.084 | 0.180 | -0.921 | 2 | 0 | - |
| Fentin hydroxide | 76-87-9 | 0.408 | 0.044 | -0.208 | 3 | 0 | - |
| Fluazifop P | 83066-88-0 | 0.202 | 0.099 | -0.464 | 4 | 1 | - |
| Flumetsulam | 98967-40-9 | 0.947 | 0.076 | -0.162 | 5 | 0 | - |
| Fluroxypyr | 69377-81-7 | -0.283 | 0.099 | 0.110 | 5 | 1 | - |
| Iprodione | 36734-19-7 | -0.032 | 0.067 | 0.113 | 3 | 0 | - |
| Cybutryne | 28159-98-0 | 1.044 | 0.102 | -0.672 | 3 | 0 | - |
| Isoproturon | 34123-59-6 | 0.380 | 0.065 | -0.407 | 2 | 0 | - |
| Lindane | 58-89-9 | -0.381 | 0.136 | -0.291 | 0 | 0 | - |
| Mefenacet | 73250-68-7 | 0.554 | 0.081 | -0.534 | 2 | 0 | - |
| Metalaxyl | 57837-19-1 | 0.834 | 0.071 | -0.519 | 3 | 0 | - |
| Methabenzthiazuron | 18691-97-9 | -0.220 | 0.088 | -0.189 | 1 | 0 | - |
| Metolachlor | 51218-45-2 | 0.912 | 0.081 | -0.576 | 3 | 0 | - |
| Metribuzin | 21087-64-9 | -0.029 | 0.155 | -0.548 | 0 | 0 | - |
| Metsulfuron-methyl | 74223-64-6 | 1.131 | 0.082 | -0.296 | 5 | 0 | - |
| Molinate | 2212-67-1 | -0.390 | 0.136 | -0.285 | 0 | 0 | - |
| Nicosulfuron | 111991-09-4 | 1.327 | 0.098 | -0.439 | 5 | 0 | - |
| Oxadiargyl | 39807-15-3 | 0.764 | 0.052 | -0.248 | 4 | 0 | - |
| Oxadiazon | 19666-30-9 | 1.071 | 0.074 | -0.472 | 4 | 0 | - |
| Oxadixyl | 77732-09-3 | 0.689 | 0.056 | -0.413 | 3 | 0 | - |
| Pendimethalin | 40487-42-1 | 0.878 | 0.076 | -0.111 | 5 | 0 | - |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Phenmedipham | 13684-63-4 | 0.897 | 0.058 | -0.345 | 4 | 0 |  |
| Pretilachlor | 51218-49-6 | 1.092 | 0.111 | -0.707 | 3 | 0 | 2.11 |
| Prometryn | 7287-19-6 | 0.997 | 0.094 | -0.638 | 3 | 0 |  |
| Quinclorac | 84087-01-4 | -0.765 | 0.074 | 0.022 | 3 | 1 |  |
| Quizalofop P | 94051-08-8 | -0.067 | 0.074 | -0.268 | 4 | 1 |  |
| Tebuthiuron | 34014-18-1 | 0.839 | 0.125 | -0.742 | 2 | 0 |  |
| Terbumeton | 33693-04-8 | 1.031 | 0.100 | -0.663 | 3 | 0 |  |
| Terbutryn | 886-50-0 | 0.934 | 0.084 | -0.592 | 3 | 0 |  |
| Thiobencarb | 28249-77-6 | 0.588 | 0.085 | -0.559 | 2 | 0 | 2.30 |
| Thiophanate methyl | 23564-05-8 | 0.159 | 0.056 | -0.246 | 2 | 0 |  |
| Tribenuron | 106040-48-6 | 0.139 | 0.092 | -0.198 | 5 | 1 |  |
| 1,1,2,2-Tetrachloroethane | 79-34-5 | -0.657 | 0.145 | -0.090 | 0 | 0 |  |
| 1,1,2-Trichloroethane | 79-00-5 | -0.644 | 0.144 | -0.099 | 0 | 0 |  |
| 1,1-Dichloroethane | 75-34-3 | -0.597 | 0.141 | -0.134 | 0 | 0 |  |
| 1,1-Dichloroethylene | 75-35-4 | -0.725 | 0.150 | -0.040 | 0 | 0 | 0.33 |
| 1,2,3-Trichloropropane | 96-18-4 | -0.501 | 0.137 | -0.204 | 0 | 0 |  |
| 1,2-Dibromo-3-chloropropane | 96-12-8 | -0.572 | 0.140 | -0.152 | 0 | 0 | 0.78 |
| 1,2-Dichloroethane | 107-06-2 | -0.660 | 0.145 | -0.088 | 0 | 0 |  |
| 1,2-Dichloropropane | 78-87-5 | -0.564 | 0.140 | -0.158 | 0 | 0 | -0.15 |
| 1,3-Dibromopropane | 109-64-8 | -0.551 | 0.139 | -0.167 | 0 | 0 | **1.41** |
| 1,3-Dichloropropane | 142-28-9 | -0.580 | 0.140 | -0.146 | 0 | 0 |  |
| 1,3-Dichloropropene | 542-75-6 | -0.754 | 0.153 | -0.019 | 0 | 0 | **1.87** |
| 1-Chlorobutane | 109-69-3 | -0.561 | 0.139 | -0.160 | 0 | 0 |  |
| 3,4-Dichlorobut-1-ene | 760-23-6 | -0.562 | 0.140 | -0.159 | 0 | 0 | 0.67 |
| Acetic acid, bromo-, 2-butene-1,4-diyl ester | 20679-58-7 | -0.432 | 0.136 | -0.254 | 0 | 0 |  |
| Bromodichloromethane | 75-27-4 | -0.836 | 0.161 | 0.041 | 0 | 0 | 0.77 |
| Carbon tetrachloride | 56-23-5 | -0.949 | 0.176 | 0.123 | 0 | 0 | **1.31** |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Cyclohexane | 110-82-7 | -0.316 | 0.137 | -0.339 | 0 | 0 |  |
| Dibromochloromethane | 124-48-1 | -0.783 | 0.155 | 0.002 | 0 | 0 | 0.42 |
| Ethyl bromide | 74-96-4 | -0.581 | 0.140 | -0.145 | 0 | 0 |  |
| Ethylcyclohexane | 1678-91-7 | -0.268 | 0.139 | -0.374 | 0 | 0 | **2.18** |
| Methylcyclohexane | 108-87-2 | -0.132 | 0.146 | -0.473 | 0 | 0 | **1.67** |
| Pentachloroethane | 76-01-7 | -0.739 | 0.151 | -0.030 | 0 | 0 |  |
| Trichloroethylene | 79-01-6 | -0.877 | 0.166 | 0.071 | 0 | 0 | 0.54 |
| 1-(N-phenylamino)-naphthalene | 90-30-2 | -0.086 | 0.062 | -0.067 | 2 | 0 | **2.50** |
| 1,2-Dimethylnaphthalene | 573-98-8 | 0.307 | 0.060 | -0.354 | 2 | 0 | 1.83 |
| 1,3-Dimethylnapthalene | 575-41-7 | 0.110 | 0.056 | -0.210 | 2 | 0 | 1.94 |
| 1,5-Napthalenediamine | 2243-62-1 | -0.701 | 0.147 | 0.382 | 2 | 0 | 0.97 |
| 1,8-Naphthylenediamine | 479-27-6 | -0.701 | 0.147 | 0.382 | 2 | 0 | 1.45 |
| 1-Methylnaphthalene | 90-12-0 | -0.282 | 0.089 | -0.144 | 1 | 0 | **1.40** |
| 2,7-Dimethylnaphthalene | 582-16-1 | 0.319 | 0.061 | -0.363 | 2 | 0 | 1.94 |
| 2-Methylnaphthalene | 91-57-6 | -0.046 | 0.088 | -0.316 | 1 | 0 | 1.87 |
| 3-Hydroxy-2-naphthoic acid | 92-70-6 | -0.969 | 0.088 | -0.049 | 2 | 1 |  |
| Isopropylnaphthalene | 29253-36-9 | 0.012 | 0.090 | -0.358 | 1 | 0 | **2.36** |
| N-phenyl-2-naphthylamine | 135-88-6 | 0.082 | 0.056 | -0.190 | 2 | 0 |  |
| ß-Naphthol | 135-19-3 | -0.254 | 0.088 | -0.164 | 1 | 0 | 1.56 |
| ß-Naphthylamine | 91-59-8 | -0.419 | 0.097 | -0.044 | 1 | 0 | 1.56 |
| Tetralin | 119-64-2 | 0.035 | 0.057 | -0.155 | 2 | 0 | 1.34 |
| 1,2,3-Trichlorobenzene | 87-61-6 | -0.019 | 0.066 | 0.104 | 3 | 0 | 1.75 |
| 1,2-Dichlorobenzene | 95-50-1 | -0.186 | 0.069 | 0.006 | 2 | 0 | 1.59 |
| 1,3-Dichlorobenzene | 541-73-1 | -0.197 | 0.070 | 0.014 | 2 | 0 | 1.41 |
| 1,4-Benzenediamine, N,N'-bis(1-methylpropyl)- | 101-96-2 | 0.469 | 0.072 | -0.472 | 2 | 0 | **2.78** |
| 1,4-Dichlorobenzene | 106-46-7 | -0.189 | 0.069 | 0.008 | 2 | 0 | **1.82** |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 2,4,6-Trichlorophenylhydrazine | 5329-12-4 | 0.263 | 0.071 | 0.118 | 4 | 0 | 2.33 |
| 2,4-Diamino-6-nitrotoluene | 6629-29-4 | -0.093 | 0.125 | 0.378 | 4 | 0 |  |
| 2,4-Diaminotoluene | 95-80-7 | -0.195 | 0.089 | 0.232 | 3 | 0 |  |
| 2,4-Dichlorotoluene | 95-73-8 | 0.151 | 0.051 | -0.020 | 3 | 0 |  |
| 2,4-dinitrotoluene | 121-14-2 | -0.227 | 0.095 | 0.256 | 3 | 0 |  |
| 2,5-Diaminotoluene | 95-70-5 | -0.268 | 0.102 | 0.286 | 3 | 0 | **2.81** |
| 2,5-Dichlorotoluene | 19398-61-9 | 0.112 | 0.054 | 0.008 | 3 | 0 | 1.60 |
| 2,6-Diamino-4-nitrotoluene | 59229-75-3 | 0.014 | 0.105 | 0.300 | 4 | 0 |  |
| 2,6-Diaminotoluene | 823-40-5 | -0.174 | 0.086 | 0.217 | 3 | 0 |  |
| 2,6-dichlorotoluene | 118-69-4 | 0.112 | 0.054 | 0.008 | 3 | 0 | 1.85 |
| 2,6-Dinitrotoluene | 606-20-2 | -0.366 | 0.120 | 0.357 | 3 | 0 | **0.73** |
| 2-Amino-4,6-dinitrotoluene | 35572-78-2 | -0.025 | 0.112 | 0.328 | 4 | 0 |  |
| 2-Amino-4-nitrotoluene | 99-55-8 | -0.103 | 0.076 | 0.165 | 3 | 0 |  |
| 2-Amino-6-nitrotoluene | 603-83-8 | -0.208 | 0.091 | 0.242 | 3 | 0 |  |
| 2-Chlorohydroquinonedimethylether | 2100-42-7 | 0.593 | 0.049 | -0.343 | 3 | 0 | 0.79 |
| 2-Chlorotoluene | 95-49-8 | -0.056 | 0.060 | -0.089 | 2 | 0 | 1.22 |
| 2-methyl-4-chlorophenoxyacetic acid | 94-74-6 | -0.573 | 0.067 | -0.118 | 3 | 1 |  |
| 2-Phenylpropene | 98-83-9 | 0.101 | 0.095 | -0.423 | 1 | 0 | 1.21 |
| 3,4-Dichlorotoluene | 95-75-0 | 0.245 | 0.046 | -0.089 | 3 | 0 | 1.57 |
| 3,5-Bis(trifluoromethyl)benzylamine | 85068-29-7 | 0.406 | 0.044 | -0.206 | 3 | 0 | 1.34 |
| 3-Chlorotoluene | 108-41-8 | 0.009 | 0.058 | -0.136 | 2 | 0 |  |
| 4,6-Dichlororesorcinol | 137-19-9 | 0.271 | 0.070 | 0.112 | 4 | 0 |  |
| 4-Allyl-1,2-dimethoxybenzene | 93-15-2 | 0.449 | 0.044 | -0.238 | 3 | 0 | 1.10 |
| 4-Chlororesorcinol | 95-88-5 | 0.137 | 0.052 | -0.010 | 3 | 0 |  |
| 4-Chlorotoluene | 106-43-4 | 0.085 | 0.056 | -0.192 | 2 | 0 | 1.32 |
| 4-Nitrotoluene-2-sulphonic acid | 121-03-9 | -1.874 | 0.287 | 0.205 | 3 | 2 |  |
| 4-tert-Butyltoluene | 98-51-1 | 0.645 | 0.093 | -0.601 | 2 | 0 | 1.94 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 4-Toluenesulfonyl chloride | 98-59-9 | 0.018 | 0.057 | -0.143 | 2 | 0 | 0.39 |
| Atenolol | 29122-68-7 | 0.335 | 0.062 | -0.374 | 2 | 0 |  |
| Benzalacetone | 122-57-6 | -0.291 | 0.090 | -0.137 | 1 | 0 | 1.41 |
| Benzotrifluoride ((Trifluoromethyl)Benzene) | 98-08-8 | -0.405 | 0.096 | -0.054 | 1 | 0 | 1.01 |
| Benzyl alcohol | 100-51-6 | -0.298 | 0.090 | -0.132 | 1 | 0 |  |
| Benzyl cyanide | 140-29-4 | -0.231 | 0.088 | -0.181 | 1 | 0 |  |
| Benzylamine | 100-46-9 | -0.213 | 0.087 | -0.194 | 1 | 0 |  |
| Bromobenzene | 108-86-1 | -0.342 | 0.092 | -0.100 | 1 | 0 | 1.56 |
| Butylbenzene | 104-51-8 | -0.086 | 0.087 | -0.287 | 1 | 0 | 1.61 |
| Catechol | 120-80-9 | 0.058 | 0.056 | -0.172 | 2 | 0 |  |
| Chlorobenzene | 108-90-7 | -0.378 | 0.094 | -0.074 | 1 | 0 | 1.23 |
| Cyclohexylbenzene | 827-52-1 | 0.083 | 0.093 | -0.410 | 1 | 0 | **2.13** |
| Diisopropylbenzene | 25321-09-9 | 0.470 | 0.072 | -0.473 | 2 | 0 | 2.30 |
| Dimethyl phthalate | 131-11-3 | 0.062 | 0.056 | -0.175 | 2 | 0 |  |
| Diuron | 330-54-1 | 0.223 | 0.047 | -0.073 | 3 | 0 |  |
| Divinylbenzene | 1321-74-0 | 0.136 | 0.056 | -0.229 | 2 | 0 | 1.49 |
| Ethylbenzene | 100-41-4 | -0.102 | 0.087 | -0.275 | 1 | 0 |  |
| Fenobucarb | 3766-81-2 | 0.332 | 0.062 | -0.372 | 2 | 0 | 1.33 |
| Isopropylbenzene | 98-82-8 | -0.068 | 0.087 | -0.300 | 1 | 0 |  |
| Metaxylene hexafluoride | 402-31-3 | -0.335 | 0.084 | 0.115 | 2 | 0 | 1.47 |
| m-Phenylenebis(methylamine) | 1477-55-0 | 0.287 | 0.060 | -0.339 | 2 | 0 | **0.19** |
| m-Phenylenediamine | 108-45-2 | -0.548 | 0.117 | 0.270 | 2 | 0 |  |
| n-Propylbenzene | 103-65-1 | -0.121 | 0.087 | -0.261 | 1 | 0 |  |
| o-Phenylenediamine | 95-54-5 | -0.452 | 0.100 | 0.200 | 2 | 0 | 1.37 |
| o-Toluenesulfonamide | 88-19-7 | -0.350 | 0.086 | 0.126 | 2 | 0 |  |
| Oxyfluorfen | 42874-03-3 | 0.931 | 0.127 | 0.070 | 6 | 0 |  |
| p-Cymene | 99-87-6 | 0.433 | 0.069 | -0.446 | 2 | 0 | 1.83 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| p-Phenylenediamine | 106-50-3 | -0.526 | 0.113 | 0.254 | 2 | 0 | **3.21** |
| Propoxur | 114-26-1 | 0.678 | 0.098 | -0.625 | 2 | 0 |  |
| Resorcinol | 108-46-3 | 0.002 | 0.058 | -0.131 | 2 | 0 |  |
| Sulphanilamide | 63-74-1 | -0.497 | 0.108 | 0.233 | 2 | 0 |  |
| Thiamphenicol | 15318-45-3 | -0.068 | 0.061 | -0.080 | 2 | 0 |  |
| Toluene | 108-88-3 | -0.175 | 0.087 | -0.222 | 1 | 0 | 0.57 |
| Trans-cinnamic acid | 140-10-3 | -1.267 | 0.125 | -0.051 | 1 | 1 |  |
| 2-(1,1-Dimethyl)-4,6-dimethylphenol | 1879-09-0 | 1.411 | 0.128 | -0.720 | 4 | 0 | 1.85 |
| 2,3,4,5-tetrachlorophenol | 4901-51-3 | 0.391 | 0.112 | 0.244 | 5 | 0 |  |
| 2,3,5,6-tetrachlorophenol | 935-95-5 | 0.428 | 0.107 | 0.217 | 5 | 0 |  |
| 2,3,5-trichlorophenol | 933-78-8 | 0.264 | 0.070 | 0.117 | 4 | 0 |  |
| 2,3,5-trimethylphenol | 697-82-5 | 0.712 | 0.051 | -0.210 | 4 | 0 |  |
| 2,3,6-trichlorophenol | 933-75-5 | 0.264 | 0.070 | 0.117 | 4 | 0 |  |
| 2,3,6-trimethylphenol | 2416-94-6 | 0.734 | 0.051 | -0.226 | 4 | 0 |  |
| 2,3-dimethylphenol | 526-75-0 | 0.304 | 0.045 | -0.132 | 3 | 0 |  |
| 2,4,6-Tribromophenol | 118-79-6 | 0.344 | 0.063 | 0.059 | 4 | 0 | 2.34 |
| 2,4,6-trimethylphenol | 527-60-6 | 0.863 | 0.056 | -0.320 | 4 | 0 |  |
| 2,4-Dibromophenol | 615-58-7 | 0.178 | 0.050 | -0.040 | 3 | 0 | 1.84 |
| 2,4-di-tert-butylphenol | 96-76-4 | 1.410 | 0.185 | -0.939 | 3 | 0 | 2.48 |
| 2,5-dimethylphenol | 95-87-4 | 0.516 | 0.046 | -0.287 | 3 | 0 | 1.33 |
| 2,6-dimethylphenol | 576-26-1 | 0.418 | 0.044 | -0.215 | 3 | 0 | 0.91 |
| 2,6-Di-sec-butylphenol | 5510-99-6 | 1.079 | 0.108 | -0.698 | 3 | 0 | **3.14** |
| 2-Allylphenol | 1745-81-9 | 0.099 | 0.056 | -0.202 | 2 | 0 |  |
| 2-ethylphenol | 90-00-6 | 0.226 | 0.057 | -0.295 | 2 | 0 |  |
| 2-methoxyphenol | 90-05-1 | 0.065 | 0.056 | -0.177 | 2 | 0 |  |
| 2-n-propylphenol | 644-35-9 | 0.265 | 0.059 | -0.323 | 2 | 0 |  |
| 2-tert-butyl phenol | 88-18-6 | 0.499 | 0.075 | -0.494 | 2 | 0 | 1.61 |

Table S3. Continued

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | | pLC50 (mM)\*\* | |
| 2-tert-Butyl-p-cresol | 2409-55-4 | 0.973 | 0.090 | -0.620 | 3 | 0 | | 1.94 | |
| 3,4,5-trichloroguaiacol | 57057-83-7 | 0.684 | 0.083 | 0.030 | 5 | 0 | |  | |
| 3,4,5-trichlorophenol | 609-19-8 | 0.223 | 0.075 | 0.147 | 4 | 0 | |  | |
| 3,4-dimethylphenol | 95-65-8 | 0.355 | 0.044 | -0.169 | 3 | 0 | |  | |
| 3-ethylphenol | 620-17-7 | 0.254 | 0.058 | -0.315 | 2 | 0 | |  | |
| 3-Trifluoromethyl-4-nitrophenol | 88-30-2 | 0.211 | 0.048 | -0.064 | 3 | 0 | |  | |
| 4-(1-Methylethenyl)phenol | 4286-23-1 | 0.204 | 0.057 | -0.279 | 2 | 0 | | 1.16 | |
| 4-(2,4-dichlorophenoxy)-phenol | 40843-73-0 | 0.872 | 0.076 | -0.107 | 5 | 0 | |  | |
| 4,5,6-trichloroguaiacol | 2668-24-8 | 0.597 | 0.089 | 0.094 | 5 | 0 | |  | |
| 4,5-Dichloroguaiacol | 2460-49-3 | 0.361 | 0.062 | 0.046 | 4 | 0 | |  | |
| 4-Chloro-2-methylphenol | 1570-64-5 | 0.164 | 0.050 | -0.030 | 3 | 0 | |  | |
| 4-Chloro-2-nitrophenol | 89-64-5 | -0.111 | 0.077 | 0.171 | 3 | 0 | | 1.20 | |
| 4-ethylphenol | 123-07-9 | 0.166 | 0.056 | -0.251 | 2 | 0 | |  | |
| 4-n-Nonylphenol | 104-40-5 | 0.570 | 0.083 | -0.546 | 2 | 0 | |  | |
| 4-n-octylphenol | 1806-26-4 | 0.444 | 0.070 | -0.454 | 2 | 0 | | **3.37** | |
| 4-Pentylphenol | 14938-35-3 | 0.263 | 0.059 | -0.322 | 2 | 0 | | 2.07 | |
| 6-tert-Butyl-m-cresol | 88-60-8 | 0.955 | 0.087 | -0.607 | 3 | 0 | | 1.78 | |
| 6-Tert-butyl-o-cresol | 2219-82-1 | 0.729 | 0.060 | -0.442 | 3 | 0 | | 1.58 | |
| Methyl p-hydroxybenzoate | 99-76-3 | 0.147 | 0.056 | -0.237 | 2 | 0 | | 0.40 | |
| o-sec-Butylphenol | 89-72-5 | 0.348 | 0.063 | -0.384 | 2 | 0 | | 1.40 | |
| p-sec-Butylphenol | 99-71-8 | 0.191 | 0.057 | -0.269 | 2 | 0 | | 1.76 | |
| Tetrachloroguaiacol | 2539-17-5 | 0.951 | 0.126 | 0.055 | 6 | 0 | |  | |
| Thymol | 89-83-8 | 0.700 | 0.057 | -0.421 | 3 | 0 | | 1.50 | |
| Trichlorosyringol | 2539-26-6 | 0.972 | 0.125 | 0.040 | 6 | 0 | |  | |
| 1-Nitropyrene | 5522-43-0 | -0.790 | 0.143 | 0.227 | 1 | 0 | |  | |
| 2-acetamidophenoxazin-3-one | 1916-55-8 | -0.129 | 0.064 | -0.036 | 2 | 0 | |  | |
| 2-amino-7-methoxyphenoxazin-3-one |  | 0.408 | 0.044 | -0.208 | 3 | | 0 | |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 9-Vinylcarbazole | 1484-13-5 | -0.773 | 0.154 | -0.005 | 0 | 0 |  |
| Acenaphthene | 83-32-9 | 0.000 | 0.058 | -0.130 | 2 | 0 |  |
| Dibenzo[b,f]cyclohepten-1-one | 2222-33-5 | 0.474 | 0.054 | -0.036 | 4 | 0 |  |
| Dibenzothiophene | 132-65-0 | -0.727 | 0.150 | -0.039 | 0 | 0 | **2.12** |
| Fluorene | 86-73-7 | 0.457 | 0.055 | -0.024 | 4 | 0 |  |
| Phenanthrene | 85-01-8 | -0.638 | 0.143 | -0.104 | 0 | 0 | **2.10** |
| Phenothiazine | 92-84-2 | 0.523 | 0.052 | -0.072 | 4 | 0 | 2.41 |
| 1-Decanol | 112-30-1 | -0.097 | 0.149 | -0.499 | 0 | 0 | **1.75** |
| 1-Nonanol | 143-08-8 | -0.286 | 0.138 | -0.361 | 0 | 0 | **1.65** |
| 2-(2-Butoxyethoxy)ethanol | 112-34-5 | -0.290 | 0.138 | -0.358 | 0 | 0 |  |
| 2-Butoxyethanol | 111-76-2 | -0.406 | 0.136 | -0.273 | 0 | 0 |  |
| 2-Isoproxyethanol | 109-59-1 | -0.594 | 0.141 | -0.136 | 0 | 0 |  |
| 3-Pentanol | 71-41-0 | -0.653 | 0.144 | -0.093 | 0 | 0 |  |
| Cyclohexanol | 108-93-0 | -0.295 | 0.138 | -0.354 | 0 | 0 |  |
| Hexanol | 111-27-3 | -0.566 | 0.140 | -0.156 | 0 | 0 |  |
| Isodecyl alcohol | 25339-17-7 | -0.398 | 0.136 | -0.279 | 0 | 0 | **1.43** |
| 1,6-Hexanediamine | 124-09-4 | -0.572 | 0.140 | -0.152 | 0 | 0 | 0.21 |
| 2-(Dibutylamino)ethanol | 102-81-8 | -0.140 | 0.146 | -0.467 | 0 | 0 | 0.78 |
| 2,2'-Dimethyl-4,4'-methylenebis(cyclohexylamine) | 6864-37-5 | 0.045 | 0.163 | -0.602 | 0 | 0 | 1.04 |
| 2-Amino-2-ethylpropanediol | 115-70-8 | -0.699 | 0.148 | -0.059 | 0 | 0 |  |
| Cyclohexylamine | 108-91-8 | -0.350 | 0.137 | -0.314 | 0 | 0 | 0.48 |
| Dibutylamine | 111-92-2 | -0.129 | 0.146 | -0.475 | 0 | 0 |  |
| Diethanolamine | 111-42-2 | -0.560 | 0.139 | -0.161 | 0 | 0 |  |
| Diethylamine | 109-89-7 | -0.558 | 0.139 | -0.162 | 0 | 0 | 0.43 |
| Diethylnitrosamine | 55-18-5 | -0.369 | 0.136 | -0.300 | 0 | 0 |  |
| Diisopropylamine | 108-18-9 | -0.075 | 0.151 | -0.515 | 0 | 0 |  |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Dimethylamine | 124-40-3 | -0.450 | 0.136 | -0.241 | 0 | 0 |  |
| Piperidine | 110-89-4 | -0.249 | 0.140 | -0.388 | 0 | 0 |  |
| t-Butylamine | 75-64-9 | -0.412 | 0.136 | -0.269 | 0 | 0 |  |
| Triethylamine | 121-44-8 | -0.362 | 0.136 | -0.305 | 0 | 0 | 0.63 |
| 2-(Dimethylamino)ethyl methacrylate | 2867-47-2 | -0.147 | 0.145 | -0.462 | 0 | 0 | 0.92 |
| 2-Ethylhexyl methacrylate | 688-84-6 | 0.080 | 0.168 | -0.628 | 0 | 0 | 1.85 |
| 2-hydroxyethyl acrylate | 818-61-1 | -0.599 | 0.141 | -0.132 | 0 | 0 | 1.25 |
| 2-hydroxyethyl methacrylate | 868-77-9 | -0.480 | 0.137 | -0.219 | 0 | 0 |  |
| Ethyl trichloroacetate | 515-84-4 | -0.683 | 0.147 | -0.071 | 0 | 0 | 0.64 |
| Ethylacrylate | 140-88-5 | -0.503 | 0.138 | -0.202 | 0 | 0 | 1.92 |
| Isobutyl acetate | 110-19-0 | -0.334 | 0.137 | -0.326 | 0 | 0 | 0.83 |
| Methyl acrylate | 96-33-3 | -0.490 | 0.137 | -0.212 | 0 | 0 | 1.79 |
| Methyl methacrylate | 80-62-6 | -0.387 | 0.136 | -0.287 | 0 | 0 |  |
| n-Butyl acrylate | 141-32-2 | -0.472 | 0.137 | -0.225 | 0 | 0 | 1.73 |
| n-butyl methacrylate | 97-88-1 | -0.251 | 0.139 | -0.386 | 0 | 0 | 1.40 |
| Testosterone propionate | 57-85-2 | 0.475 | 0.241 | -0.916 | 0 | 0 |  |
| Tetracaine | 94-24-6 | 0.634 | 0.091 | -0.593 | 2 | 0 |  |
| Vinyl acetate | 108-05-4 | -0.731 | 0.151 | -0.036 | 0 | 0 | 1.55 |
| 2,3,4-trichloroaniline | 634-67-3 | 0.029 | 0.102 | 0.289 | 4 | 0 |  |
| 2,3-dichloroaniline | 608-27-5 | -0.170 | 0.086 | 0.214 | 3 | 0 |  |
| 2,3-Dimethylaniline | 87-59-2 | 0.147 | 0.052 | -0.017 | 3 | 0 |  |
| 2,4,5-Trichloroaniline | 636-30-6 | 0.063 | 0.097 | 0.264 | 4 | 0 |  |
| 2,4,6-trichloroaniline | 634-93-5 | 0.115 | 0.089 | 0.226 | 4 | 0 | 1.57 |
| 2,4,6-Trimethylaniline | 88-05-1 | 0.633 | 0.050 | -0.152 | 4 | 0 | **0.39** |
| 2,4-Dichloroaniline | 554-00-7 | -0.145 | 0.082 | 0.196 | 3 | 0 | 1.30 |
| 2,4-dimethylaniline | 95-68-1 | 0.173 | 0.050 | -0.036 | 3 | 0 |  |
| 2,5-dichloroaniline | 95-82-9 | -0.121 | 0.078 | 0.178 | 3 | 0 | 1.87 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 2,5-dimethylaniline | 95-78-3 | 0.163 | 0.050 | -0.029 | 3 | 0 |  |
| 2,6-dichloroaniline | 608-31-1 | -0.122 | 0.079 | 0.179 | 3 | 0 |  |
| 2,6-diethylaniline | 579-66-8 | 0.284 | 0.045 | -0.117 | 3 | 0 |  |
| 2,6-dimethylaniline | 87-62-7 | 0.162 | 0.051 | -0.028 | 3 | 0 |  |
| 2-Chloro-5-methylaniline | 95-81-8 | 0.097 | 0.055 | 0.019 | 3 | 0 | 1.11 |
| 2-Chloroaniline | 95-51-2 | -0.350 | 0.086 | 0.126 | 2 | 0 | 1.24 |
| 2-ethylaniline | 578-54-1 | -0.161 | 0.067 | -0.012 | 2 | 0 |  |
| 2-Methyl-4-nitroaniline | 99-52-5 | -0.116 | 0.078 | 0.175 | 3 | 0 |  |
| 2-Methylaniline | 95-53-4 | -0.286 | 0.078 | 0.079 | 2 | 0 | -0.15 |
| 2-Nitroaniline | 88-74-4 | -0.509 | 0.110 | 0.242 | 2 | 0 | 0.52 |
| 2-Nitro-p-anisidine | 96-96-8 | -0.070 | 0.072 | 0.141 | 3 | 0 | 0.61 |
| 3,4,5-Trichloroaniline | 634-91-3 | 0.090 | 0.093 | 0.244 | 4 | 0 |  |
| 3,4-Dichloroaniline | 95-76-1 | -0.079 | 0.073 | 0.148 | 3 | 0 | 1.17 |
| 3,4-Dimethylaniline | 95-64-7 | 0.129 | 0.053 | -0.004 | 3 | 0 |  |
| 3,5-dichloroaniline | 626-43-7 | -0.103 | 0.076 | 0.165 | 3 | 0 |  |
| 3,5-dimethylaniline | 108-69-0 | 0.274 | 0.045 | -0.110 | 3 | 0 | 0.55 |
| 3-chloroaniline | 108-42-9 | -0.313 | 0.082 | 0.099 | 2 | 0 | 1.16 |
| 3-ethylaniline | 587-02-0 | -0.035 | 0.059 | -0.104 | 2 | 0 |  |
| 3-methylaniline | 108-44-1 | -0.141 | 0.065 | -0.027 | 2 | 0 |  |
| 3-Nitroaniline | 99-09-2 | -0.322 | 0.083 | 0.105 | 2 | 0 | 0.19 |
| 4-Chloro-2-nitroaniline | 89-63-4 | -0.315 | 0.110 | 0.320 | 3 | 0 | 1.01 |
| 4-chloroaniline | 106-47-8 | -0.320 | 0.082 | 0.104 | 2 | 0 | 1.34 |
| 4-ethylaniline | 589-16-2 | -0.004 | 0.058 | -0.127 | 2 | 0 |  |
| 4-Fluoroaniline | 371-40-4 | -0.309 | 0.081 | 0.096 | 2 | 0 |  |
| 4-Isopropylaniline | 99-88-7 | 0.059 | 0.056 | -0.173 | 2 | 0 | 0.47 |
| 4-Methylaniline | 106-49-0 | -0.067 | 0.061 | -0.081 | 2 | 0 | -0.05 |
| 4-Nitroaniline | 100-01-6 | -0.348 | 0.086 | 0.124 | 2 | 0 | 0.21 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Aniline, p-(phenylazo)-(p-Aminoazobenzene) | 60-09-3 | -0.007 | 0.065 | 0.095 | 3 | 0 | 2.75 |
| Chlorfluoroaniline | 21397-08-0 | -0.138 | 0.081 | 0.191 | 3 | 0 |  |
| Dithiodianiline | 722-27-0 | 0.053 | 0.098 | 0.271 | 4 | 0 |  |
| N,N-Diethylaniline | 91-66-7 | 0.205 | 0.103 | -0.499 | 1 | 0 | 0.76 |
| N,N'-dimethylaniline |  | -0.360 | 0.093 | -0.087 | 1 | 0 |  |
| N,N-Dimethylaniline | 121-69-7 | -0.360 | 0.093 | -0.087 | 1 | 0 |  |
| N-Ethylaniline | 103-69-5 | -0.115 | 0.087 | -0.266 | 1 | 0 | 0.22 |
| p-Anisidine | 104-94-9 | -0.083 | 0.062 | -0.069 | 2 | 0 |  |
| 2-ethyl-Butanoic acid | 88-09-5 | -1.405 | 0.175 | -0.170 | 0 | 1 | 0.14 |
| 2-Methylbutanoic acid | 600-07-7 | -1.518 | 0.179 | -0.088 | 0 | 1 |  |
| 3-Methylbutanoic acid | 503-74-2 | -1.278 | 0.174 | -0.263 | 0 | 1 |  |
| Acrylic acid | 79-10-7 | -1.629 | 0.186 | -0.007 | 0 | 1 | 0.07 |
| A-fluoro-b-alanine | 3821-81-6 | -1.698 | 0.192 | 0.044 | 0 | 1 |  |
| Chloroacetic acid | 79-11-8 | -1.678 | 0.190 | 0.029 | 0 | 1 | 0.12 |
| Dansylglycine | 1091-85-6 | -0.885 | 0.085 | -0.110 | 2 | 1 |  |
| Flumequine | 42835-25-6 | -0.011 | 0.078 | -0.309 | 4 | 1 |  |
| Gentisic acid | 490-79-9 | -0.866 | 0.081 | 0.096 | 3 | 1 |  |
| Glyoxylic acid | 298-12-4 | -1.709 | 0.193 | 0.052 | 0 | 1 | 0.26 |
| Heptanoic acid | 111-14-8 | -1.272 | 0.174 | -0.267 | 0 | 1 | 0.24 |
| Isocyanuric acid | 108-80-5 | 0.303 | 0.045 | -0.131 | 3 | 0 |  |
| Malonic acid diethylester | 105-53-3 | -0.720 | 0.150 | -0.044 | 0 | 0 | 0.61 |
| Methacrylic acid | 79-41-4 | -1.570 | 0.182 | -0.050 | 0 | 1 |  |
| Octanoic acid | 124-07-2 | -1.140 | 0.179 | -0.364 | 0 | 1 | 0.45 |
| Orthoformic acid trimethylester | 149-73-5 | -0.387 | 0.136 | -0.287 | 0 | 0 |  |
| Oxolinic acid | 14698-29-4 | -0.168 | 0.070 | -0.194 | 4 | 1 |  |
| Perfluorooctanoic acid | 335-67-1 | -2.024 | 0.239 | 0.282 | 0 | 1 |  |
| Pivalic acid | 75-98-9 | -1.219 | 0.176 | -0.306 | 0 | 1 |  |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Pyridaphenthion | 119-12-0 | -0.198 | 0.087 | -0.205 | 1 | 0 |  |
| Sorbic acid | 110-44-1 | -1.640 | 0.187 | 0.001 | 0 | 1 | 0.17 |
| 2-Methylvaleraldehyde | 123-15-9 | -0.658 | 0.145 | -0.089 | 0 | 0 |  |
| Capronaldehyde | 66-25-1 | -0.491 | 0.137 | -0.211 | 0 | 0 |  |
| Crotonaldehyde | 4170-30-3 | -0.609 | 0.142 | -0.125 | 0 | 0 | **2.99** |
| Dodecanal | 112-54-9 | 0.121 | 0.174 | -0.658 | 0 | 0 |  |
| Glutaraldehyde | 111-30-8 | -0.725 | 0.150 | -0.040 | 0 | 0 | 1.06 |
| Propionaldehyde | 123-38-6 | -0.606 | 0.142 | -0.127 | 0 | 0 |  |
| 1,2,4-trichloro-5-nitrobenzene | 89-69-0 | -0.122 | 0.131 | 0.399 | 4 | 0 |  |
| 2-Chloro-1-fluoro-4-nitrobenzene | 350-30-1 | -0.001 | 0.064 | 0.091 | 3 | 0 | 1.94 |
| 2-Chloronitrobenzene | 88-73-3 | -0.452 | 0.100 | 0.200 | 2 | 0 |  |
| 2-Nitroanisole | 91-23-6 | -0.160 | 0.067 | -0.013 | 2 | 0 | 0.51 |
| 2-Nitrotoluene | 88-72-2 | -0.383 | 0.090 | 0.150 | 2 | 0 |  |
| 3,4-Dichloronitrobenzene | 99-54-7 | -0.100 | 0.076 | 0.163 | 3 | 0 | 1.61 |
| 3-Chloronitrobenzene | 121-73-3 | -0.237 | 0.073 | 0.043 | 2 | 0 |  |
| 3-Nitroanisole | 555-03-3 | 0.059 | 0.056 | -0.173 | 2 | 0 | 0.41 |
| 4-Amino-2,6-dinitrotoluene | 19406-51-0 | -0.159 | 0.139 | 0.426 | 4 | 0 |  |
| 4-Amino-2-nitrotoluene | 119-32-4 | -0.305 | 0.108 | 0.313 | 3 | 0 |  |
| 4-Chloro-3-methylnitrobenzene | 13290-74-9 | 0.088 | 0.056 | 0.026 | 3 | 0 |  |
| 4-Chloronitrobenzene | 100-00-5 | -0.261 | 0.076 | 0.061 | 2 | 0 |  |
| 4-Methylnitrobenzene | 99-99-0 | 0.010 | 0.058 | -0.137 | 2 | 0 | 0.57 |
| alpha-Chloro-4-nitrotoluene | 100-14-1 | -0.026 | 0.059 | -0.111 | 2 | 0 | **2.45** |
| Nitrobenzene | 98-95-3 | -0.415 | 0.097 | -0.047 | 1 | 0 |  |
| 1,3-Diphenylguanidine | 102-06-7 | -0.055 | 0.060 | -0.090 | 2 | 0 | 1.09 |
| 2,2-Bis[4-(2-hydroxyethoxy)phenyl]propane | 901-44-0 | 1.565 | 0.163 | -0.833 | 4 | 0 | 1.18 |
| 2,3,4,4'-Tetrahydroxybenzophenon | 31127-54-5 | 1.223 | 0.119 | -0.143 | 6 | 0 | 0.84 |
| 2,4-Diamino-6-phenyl-s-triazine | 91-76-9 | 0.426 | 0.057 | -0.001 | 4 | 0 |  |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 2-Hydroxy-4-methoxybenzophenone | 131-57-7 | 0.883 | 0.058 | -0.335 | 4 | 0 | 1.78 |
| 3,4,4'-Trichlorodiphenylurea | 101-20-2 | 0.641 | 0.085 | 0.062 | 5 | 0 |  |
| 4,4'-Diaminodiphenyl ether | 101-80-4 | 0.566 | 0.051 | -0.103 | 4 | 0 |  |
| 4,4'-Dihydroxydiphenylmethane | 620-92-8 | 0.501 | 0.053 | -0.056 | 4 | 0 | 1.19 |
| 4,4'-Methylenedianiline | 101-77-9 | 0.340 | 0.063 | 0.062 | 4 | 0 | 0.98 |
| Benzenamine,2,5-diethoxy-4-(4-morpholinyl)- | 51963-82-7 | 1.183 | 0.088 | -0.554 | 4 | 0 | 1.08 |
| Benzophenone | 119-61-9 | -0.187 | 0.069 | 0.007 | 2 | 0 |  |
| Bis(4-hydroxyphenyl)sulfone | 80-09-1 | 0.542 | 0.052 | -0.086 | 4 | 0 |  |
| Bisphenol A | 80-05-7 | 1.239 | 0.097 | -0.595 | 4 | 0 | 1.46 |
| Dibenzyl ether | 103-50-4 | 0.400 | 0.066 | -0.422 | 2 | 0 | 1.46 |
| Dibromocresyl glycidyl ether | 30171-80-3 | 0.121 | 0.056 | -0.218 | 2 | 0 | 2.39 |
| Diphenyl ether | 101-84-8 | 0.306 | 0.060 | -0.353 | 2 | 0 | **1.98** |
| Diphenylamine | 122-39-4 | -0.045 | 0.060 | -0.097 | 2 | 0 | 1.41 |
| Di-p-tolylamine | 620-93-9 | 0.908 | 0.059 | -0.353 | 4 | 0 | 2.66 |
| Hydrazobenzene | 122-66-7 | -0.226 | 0.072 | 0.035 | 2 | 0 | **3.63** |
| N,N'-Bis(2-methylphenyl)guanidine | 97-39-2 | 0.624 | 0.050 | -0.146 | 4 | 0 | 1.10 |
| Procymidone | 32809-16-8 | 0.221 | 0.047 | -0.071 | 3 | 0 |  |
| Pyrimethamine | 58-14-0 | 1.227 | 0.119 | -0.146 | 6 | 0 |  |
| Styrene-7,8-oxide | 96-09-3 | -0.449 | 0.099 | -0.022 | 1 | 0 | 1.14 |
| Sulfadiazine | 68-35-9 | 0.056 | 0.058 | 0.049 | 3 | 0 |  |
| Sulfadimethoxine | 122-11-2 | 0.809 | 0.077 | -0.061 | 5 | 0 |  |
| Sulfamethazine\_\_Sulfadimidine | 57-68-1 | 0.973 | 0.076 | -0.181 | 5 | 0 |  |
| Sulfamethoxazole | 723-46-6 | 0.357 | 0.062 | 0.049 | 4 | 0 |  |
| Tetrabromobisphenol A | 79-94-7 | 2.023 | 0.276 | -0.288 | 8 | 0 | 1.77 |
| Trimethoprim | 738-70-5 | 1.621 | 0.186 | -0.214 | 7 | 0 |  |
| 1,1'-oxybis-butane | 142-96-1 | -0.512 | 0.138 | -0.196 | 0 | 0 |  |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 1,5-Cyclooctadiene | 111-78-4 | -0.447 | 0.136 | -0.243 | 0 | 0 | 0.92 |
| 1-Benzo[b]thien-2-ylethan-1-one | 22720-75-8 | -0.528 | 0.107 | 0.036 | 1 | 0 | 1.25 |
| 1-Chloro-2,4-dinitrobenzene | 97-00-7 | -0.253 | 0.099 | 0.275 | 3 | 0 | **3.10** |
| 1-Cyclohexene-1-carbonitrile | 1855-63-6 | -0.544 | 0.139 | -0.172 | 0 | 0 | 0.42 |
| 1-Mercaptooctane [n-Octylmercaptan] | 111-88-6 | -0.227 | 0.140 | -0.404 | 0 | 0 | 2.65 |
| 1-Methoxy-2-propanol | 107-98-2 | -0.498 | 0.137 | -0.206 | 0 | 0 |  |
| 2-(1'-Cyclohexenyl)cyclohexanone | 1502-22-3 | -0.168 | 0.144 | -0.447 | 0 | 0 | 0.79 |
| 2,2,5,5,-Tetramethylhydrofuran | 15045-43-9 | -0.551 | 0.139 | -0.167 | 0 | 0 |  |
| 2,2,6,6-Tetramethylpiperidin-4-ol | 2403-88-5 | 0.025 | 0.161 | -0.588 | 0 | 0 |  |
| 2,2'-Dithiobisbenzothiazole | 120-78-5 | -0.323 | 0.083 | 0.106 | 2 | 0 |  |
| 2,3,3,3,2',3',3',3'-Octachlorodipropyl ether | 127-90-2 | -0.272 | 0.139 | -0.371 | 0 | 0 | **2.81** |
| 2,3-Dichloro-1,4-napthoquinone | 117-80-6 | -0.290 | 0.079 | 0.082 | 2 | 0 | **3.86** |
| 2,4,6-Trimethylbenzaldehyde | 487-68-3 | 0.782 | 0.053 | -0.261 | 4 | 0 | 1.09 |
| 2-acetoxy-1,4-naphthoquinone | 1785-65-5 | -0.271 | 0.077 | 0.068 | 2 | 0 |  |
| 2-aminophenol | 95-55-6 | -0.166 | 0.067 | -0.009 | 2 | 0 | 2.21 |
| 2-Aminopyridine | 504-29-0 | -0.364 | 0.093 | -0.084 | 1 | 0 | 0.93 |
| 2-Butanone oxime | 96-29-7 | -0.381 | 0.136 | -0.291 | 0 | 0 |  |
| 2-Butenedinitrile, (E)- | 764-42-1 | -0.780 | 0.155 | 0.000 | 0 | 0 | 2.34 |
| 2-Chlorobenzyl chloride | 611-19-8 | 0.036 | 0.057 | -0.156 | 2 | 0 | **2.78** |
| 2-Decanone | 693-54-9 | -0.281 | 0.138 | -0.364 | 0 | 0 |  |
| 2-hydroxy-1,4-naphthoquinone | 83-72-7 | -0.327 | 0.083 | 0.109 | 2 | 0 |  |
| 2-Mercaptobenzothiazole | 149-30-4 | -0.248 | 0.074 | 0.051 | 2 | 0 |  |
| 2-Mercaptoethanol | 60-24-2 | -0.690 | 0.147 | -0.066 | 0 | 0 | 0.43 |
| 2-methyl-1,4-naphthoquinone | 58-27-5 | -0.007 | 0.058 | -0.125 | 2 | 0 |  |
| 2-Methyl-4(5)-nitroimidazole | 696-23-1 | -0.071 | 0.061 | -0.078 | 2 | 0 |  |
| 2-methylthio-4-tert-butylamino-6-amino-s-triazine | 30125-65-6 | 0.807 | 0.068 | -0.499 | 3 | 0 |  |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl- | 470-82-6 | 0.049 | 0.164 | -0.605 | 0 | 0 |  |
| 2-Phenylindole | 948-65-2 | 0.043 | 0.057 | -0.161 | 2 | 0 | **2.85** |
| 2-Phenylphenol | 90-43-7 | 0.304 | 0.045 | -0.132 | 3 | 0 |  |
| 2-Propenenitrile, 2-chloro- | 920-37-6 | -0.709 | 0.149 | -0.052 | 0 | 0 | **3.02** |
| 2-Propenenitrile | 107-13-1 | -0.686 | 0.147 | -0.069 | 0 | 0 | 1.02 |
| 2-Undecanone | 112-12-9 | -0.229 | 0.140 | -0.402 | 0 | 0 |  |
| 2-Vinylpyridine | 100-69-6 | -0.146 | 0.087 | -0.243 | 1 | 0 | 1.21 |
| 3-(Methylthio)propionaldehyde | 3268-49-3 | -0.418 | 0.136 | -0.264 | 0 | 0 | 1.17 |
| 3,3'-Dichlorobenzidine | 91-94-1 | 0.718 | 0.148 | 0.225 | 6 | 0 | **2.70** |
| 3,4,5-Trichlorocatechol | 56961-20-7 | 0.447 | 0.105 | 0.203 | 5 | 0 |  |
| 3,4,6-Trichlorocatechol | 32139-72-3 | 0.406 | 0.110 | 0.233 | 5 | 0 |  |
| 3,4-Dichlorocatechol | 3978-67-4 | 0.315 | 0.065 | 0.080 | 4 | 0 |  |
| 3,5,5-Trimethyl-2-cyclohexen-1-one | 78-59-1 | -0.101 | 0.149 | -0.496 | 0 | 0 |  |
| 3,5-Dichlorocatechol | 13673-92-2 | 0.271 | 0.070 | 0.112 | 4 | 0 |  |
| 3,5-Di-tert-butylsalicylic acid | 19715-19-6 | 0.657 | 0.186 | -0.796 | 4 | 1 | 1.97 |
| 3a,4,7,7a-Tetrahydro-1H-indene | 3048-65-5 | -0.418 | 0.136 | -0.264 | 0 | 0 | 1.44 |
| 3-Amino-1,2,4-triazole | 61-82-5 | -0.472 | 0.101 | -0.005 | 1 | 0 |  |
| 3-amino-2-Butenenitrile | 1118-61-2 | -0.818 | 0.159 | 0.028 | 0 | 0 | 0.68 |
| 3-Amino-4-chlorobenzoic acid | 2840-28-0 | -1.040 | 0.101 | 0.223 | 3 | 1 |  |
| 3-Aminophenol | 591-27-5 | -0.185 | 0.069 | 0.005 | 2 | 0 | -0.04 |
| 3-Aminopyridine | 462-08-8 | -0.369 | 0.094 | -0.080 | 1 | 0 | 1.04 |
| 4,4,4-Trifluorocrotonitrile | 406-86-0 | -0.614 | 0.142 | -0.121 | 0 | 0 | **2.78** |
| 4,4'-Dihydroxy-biphenyl | 92-88-6 | 0.719 | 0.051 | -0.215 | 4 | 0 | 1.16 |
| 4,5-Dichlorocatechol | 3428-24-8 | 0.334 | 0.064 | 0.066 | 4 | 0 |  |
| 4,6-Dinitro-o-cresol | 534-52-1 | 0.268 | 0.070 | 0.114 | 4 | 0 | 2.26 |
| 4-Amino-2-nitrophenol | 119-34-6 | -0.212 | 0.092 | 0.245 | 3 | 0 |  |
| 4-Aminophenol | 123-30-8 | -0.256 | 0.075 | 0.057 | 2 | 0 | 2.07 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| 4-Aminopyridine | 504-24-5 | -0.430 | 0.098 | -0.036 | 1 | 0 | 1.44 |
| 4-Chlorocatechol | 2138-22-9 | 0.204 | 0.048 | -0.059 | 3 | 0 |  |
| 4-ethyl-1,1'-Biphenyl | 5707-44-8 | 0.570 | 0.048 | -0.326 | 3 | 0 | 2.48 |
| 4-Hydroxybenzoic acid | 99-96-7 | -1.021 | 0.090 | -0.011 | 2 | 1 | 0.17 |
| 4-Methylbenzoic acid | 99-94-5 | -0.884 | 0.085 | -0.111 | 2 | 1 | 0.33 |
| 4-Vinylpyridine | 100-43-6 | -0.131 | 0.087 | -0.254 | 1 | 0 | **2.02** |
| 5-Ethylidene-8,9,10-trinorborn-2-ene | 16219-75-3 | 0.180 | 0.182 | -0.701 | 0 | 0 | 1.23 |
| 6-Ethoxy-1,2-dihydro-2,2,4-trimethylquinoline | 91-53-2 | 0.841 | 0.072 | -0.524 | 3 | 0 | 1.51 |
| 6-Methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one | 2439-01-2 | 0.292 | 0.045 | -0.123 | 3 | 0 |  |
| 8-Hydroxyquinoline | 148-24-3 | -0.127 | 0.087 | -0.257 | 1 | 0 | 1.76 |
| Acetophenone | 98-86-2 | -0.360 | 0.093 | -0.087 | 1 | 0 |  |
| Acetylsalicylic acid | 50-78-2 | -0.992 | 0.089 | -0.032 | 2 | 1 |  |
| alpha,alpha-Dichlorotoluene | 98-87-3 | -0.335 | 0.092 | -0.105 | 1 | 0 | 0.85 |
| Anisol | 100-66-3 | -0.132 | 0.087 | -0.253 | 1 | 0 |  |
| Benazolin ethyl | 25059-80-7 | 0.225 | 0.047 | -0.074 | 3 | 0 |  |
| Benzaldehyde | 100-52-7 | -0.334 | 0.092 | -0.106 | 1 | 0 |  |
| Benzenethiol | 108-98-5 | -0.284 | 0.089 | -0.142 | 1 | 0 | **4.09** |
| Benzoyl-chloride | 98-88-4 | -0.434 | 0.098 | -0.033 | 1 | 0 |  |
| Benzyl-chloroformiate | 501-53-1 | -0.354 | 0.093 | -0.091 | 1 | 0 |  |
| Betariboacetate | 13035-61-5 | -0.549 | 0.139 | -0.169 | 0 | 0 |  |
| Biphenyl | 92-52-4 | 0.113 | 0.056 | -0.212 | 2 | 0 | 1.60 |
| Bis(2-chloroethyl) ether | 111-44-4 | -0.507 | 0.138 | -0.199 | 0 | 0 |  |
| Bismerthiazol | 79319-85-0 | -0.536 | 0.139 | -0.178 | 0 | 0 |  |
| Buparvaquone | 88426-33-9 | 0.525 | 0.078 | -0.513 | 2 | 0 |  |
| But-3-en-3-olide | 674-82-8 | -0.557 | 0.139 | -0.163 | 0 | 0 | 0.98 |
| Butachlor | 23184-66-9 | 0.853 | 0.073 | -0.533 | 3 | 0 | **3.05** |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Butylbenzyl phthalate | 85-68-7 | 0.485 | 0.045 | -0.264 | 3 | 0 |  |
| Captopril | 62571-86-2 | -1.094 | 0.182 | -0.397 | 0 | 1 |  |
| Chlorohydroquinone | 615-67-8 | 0.214 | 0.048 | -0.066 | 3 | 0 |  |
| Cinmethylin | 87818-31-3 | 0.910 | 0.139 | -0.794 | 2 | 0 |  |
| Cotinine | 486-56-6 | 0.013 | 0.090 | -0.359 | 1 | 0 |  |
| Cyclohexanone oxime | 100-64-1 | -0.299 | 0.138 | -0.351 | 0 | 0 |  |
| Cyclohexanone | 108-94-1 | -0.392 | 0.136 | -0.283 | 0 | 0 |  |
| Cyclosulfamuron | 136849-15-5 | 1.594 | 0.138 | -0.634 | 5 | 0 |  |
| Diallyl phthalate | 131-17-9 | 0.333 | 0.062 | -0.373 | 2 | 0 | **2.75** |
| Diethyl disulfide | 110-81-6 | -0.383 | 0.136 | -0.290 | 0 | 0 | 1.01 |
| Diethyl malonate | 105-53-3 | -0.709 | 0.149 | -0.052 | 0 | 0 | 0.61 |
| Diethyl phthalate | 84-66-2 | 0.117 | 0.056 | -0.215 | 2 | 0 |  |
| Diisobutyl phthalate | 84-69-5 | 0.265 | 0.059 | -0.323 | 2 | 0 | 1.92 |
| Dimethyl disulphide | 624-92-0 | -0.458 | 0.137 | -0.235 | 0 | 0 | **1.93** |
| Dimethylformamide | 68-12-2 | -0.487 | 0.137 | -0.214 | 0 | 0 |  |
| Dimethylnitrosamine | 62-75-9 | -0.657 | 0.145 | -0.090 | 0 | 0 |  |
| Dinitramine | 29091-05-2 | 0.355 | 0.062 | 0.051 | 4 | 0 |  |
| Diphenylpropanediol |  | 0.111 | 0.056 | -0.211 | 2 | 0 |  |
| Droperidol | 548-73-2 | 0.192 | 0.079 | 0.170 | 4 | 0 |  |
| Enrofloxacin | 93106-60-6 | 0.172 | 0.096 | -0.442 | 4 | 1 |  |
| Ethanethiol | 75-08-1 | -0.514 | 0.138 | -0.194 | 0 | 0 | 1.45 |
| Glycidyl methacrylate | 106-91-2 | -0.603 | 0.142 | -0.129 | 0 | 0 | 1.71 |
| Haloxyfop R | 72619-32-0 | 1.297 | 0.095 | -0.417 | 5 | 0 |  |
| Hexamethylene diacrylate | 13048-33-4 | 0.056 | 0.165 | -0.610 | 0 | 0 | **2.77** |
| Hydrogenatedbisphenol A | 80-04-6 | 0.295 | 0.202 | -0.785 | 0 | 0 | 1.10 |
| Hydroquinone | 123-31-9 | 0.048 | 0.057 | -0.165 | 2 | 0 |  |
| Isoprene | 78-79-5 | -0.314 | 0.137 | -0.340 | 0 | 0 | 0.66 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Maleic anhydride | 108-31-6 | -0.688 | 0.147 | -0.067 | 0 | 0 |  |
| Medazepam | 2898-12-6 | 0.975 | 0.064 | -0.402 | 4 | 0 |  |
| Methacrylonitrile | 126-98-7 | -0.569 | 0.140 | -0.154 | 0 | 0 |  |
| Methyl isothiocyanate | 556-61-6 | -0.605 | 0.142 | -0.128 | 0 | 0 | **2.78** |
| Methylhydrazine | 60-34-4 | -0.716 | 0.149 | -0.047 | 0 | 0 | 2.08 |
| m-Toluic acid | 99-04-7 | -0.926 | 0.086 | -0.080 | 2 | 1 | 0.22 |
| N-(tert-Butyl)-2-benzothiazolylsulfenamide | 95-31-8 | 0.024 | 0.090 | -0.367 | 1 | 0 | 2.23 |
| N,N-Dimethylhydrazine | 57-14-7 | -0.665 | 0.145 | -0.084 | 0 | 0 |  |
| N-Cyclohexyl-2-benzothiazolylsulfenamide | 95-33-0 | -0.272 | 0.089 | -0.151 | 1 | 0 | 2.10 |
| N-Methyl-N,N-bis(2-dimethylaminoethyl)amine | 3030-47-5 | 0.546 | 0.258 | -0.968 | 0 | 0 |  |
| o-Acetoacetotoluidide | 93-68-5 | -0.161 | 0.067 | -0.012 | 2 | 0 |  |
| o-Chlorobenzonitrile | 873-32-5 | -0.116 | 0.064 | -0.045 | 2 | 0 | 0.57 |
| Octanedinitrile | 629-40-3 | -0.277 | 0.138 | -0.367 | 0 | 0 | -0.61 |
| Olaquindox | 23696-28-8 | 0.178 | 0.056 | -0.260 | 2 | 0 |  |
| o-Tolidine | 119-93-7 | 0.788 | 0.140 | 0.174 | 6 | 0 | 1.21 |
| Pentane-1-thiol | 110-66-7 | -0.555 | 0.139 | -0.164 | 0 | 0 | **1.90** |
| Phenol,4,4',4''-ethylidynetris- | 27955-94-8 | 1.383 | 0.125 | -0.260 | 6 | 0 |  |
| Phthalic anhydride | 85-44-9 | -0.212 | 0.071 | 0.025 | 2 | 0 |  |
| Phthalonitrile | 91-15-6 | -0.107 | 0.063 | -0.052 | 2 | 0 | 0.75 |
| Pivaloyl chloride | 3282-30-2 | 0.042 | 0.163 | -0.600 | 0 | 0 |  |
| p-Methoxybenzaldehyde | 123-11-5 | 0.093 | 0.056 | -0.198 | 2 | 0 | 0.53 |
| p-Phenylphenol | 92-69-3 | 0.469 | 0.045 | -0.252 | 3 | 0 | 1.70 |
| Propyl gallate | 121-79-9 | 0.609 | 0.050 | -0.135 | 4 | 0 |  |
| Propyzamide | 23950-58-5 | 0.403 | 0.044 | -0.204 | 3 | 0 |  |
| Pyrazosulfuron ethyl | 93697-74-6 | 1.758 | 0.171 | -0.754 | 5 | 0 |  |
| Quinoline | 91-22-5 | 0.206 | 0.057 | -0.280 | 2 | 0 | 0.30 |

Table S3. Continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | CAS | Pred.  pEC50, MTT[PLHC-1] | HAT i/i (h\*=0.375) | Mor28e | NaasC | CATS2D\_01\_AN | pLC50 (mM)\*\* |
| Secobarbital | 76-73-3 | -0.058 | 0.152 | -0.527 | 0 | 0 |  |
| Simazine | 122-34-9 | 0.501 | 0.046 | -0.276 | 3 | 0 |  |
| Sulfaquinoxaline | 59-40-5 | 0.334 | 0.044 | -0.154 | 3 | 0 |  |
| tert-Butyl 2-ethylperoxyhexanoate | 3006-82-4 | 0.106 | 0.171 | -0.647 | 0 | 0 | 1.67 |
| tert-Butylhydroperoxide | 75-91-2 | -0.494 | 0.137 | -0.209 | 0 | 0 | -0.02 |
| Tetrachlorocatechol | 1198-55-6 | 0.557 | 0.171 | 0.343 | 6 | 0 |  |
| Tetrachlorohydroquinone | 87-87-6 | 0.679 | 0.153 | 0.254 | 6 | 0 |  |
| Tetrachlorophthalic anhydride | 117-08-8 | 0.735 | 0.146 | 0.213 | 6 | 0 |  |
| Tetrahydromethylphthalic anhydride | 11070-44-3 | -0.472 | 0.137 | -0.225 | 0 | 0 |  |
| Thiopental | 76-75-5 | -0.162 | 0.144 | -0.451 | 0 | 0 |  |
| Thiophene | 110-02-1 | -0.665 | 0.145 | -0.084 | 0 | 0 | 0.43 |
| Thiosemicarbazide | 79-19-6 | -0.990 | 0.182 | 0.153 | 0 | 0 | 0.64 |
| Thiourea dioxide | 4189-44-0 | -0.940 | 0.175 | 0.117 | 0 | 0 |  |
| Thiourea | 62-56-6 | -1.028 | 0.189 | 0.181 | 0 | 0 |  |
| Triclosan | 3380-34-5 | 1.027 | 0.122 | 0.000 | 6 | 0 | 2.64 |
| Trifluralin | 1582-09-8 | 0.753 | 0.052 | -0.240 | 4 | 0 |  |
| Trimethylquinone | 935-92-2 | -0.653 | 0.144 | -0.093 | 0 | 0 |  |
| Triphenyl phosphate | 115-86-6 | 0.823 | 0.069 | -0.511 | 3 | 0 | 2.40 |
| Tris-(2,3-dibromopropyl) phosphate | 126-72-7 | -0.369 | 0.136 | -0.300 | 0 | 0 | **2.56** |
| Tris(2-chloroethyl) phosphate | 115-96-8 | -0.525 | 0.138 | -0.186 | 0 | 0 |  |

\*\*pLC50 (mM) values were obtained from the literature [31]. Bold values indicate pLC50 data with very weak relationship with the pEC50, MTT[PLHC-1] prediction.

[31] *Results of aquatic toxicity tests of chemicals conducted by Ministry of the Environment in Japan (March 2018).* Available at <http://www.env.go.jp/en/chemi/sesaku/aquatic_Mar_2018.pdf>