**A simple approach for assessment of toxicity of nitroaromatic compounds without using complex descriptors and computer codes**

**Table S1-** Chemical abstract number (CAS#) and molecular structures of the training set

|  |  |  |  |
| --- | --- | --- | --- |
| No. | Name | CAS# | Molecular structure |
| 1 | 1,1'-Biphenyl, 2-nitro- | 86-00-0 |  |
| 2 | 1,5-Difluoro-2,4-dinitrobenzene | 327-92-4 |  |
| 3 | 1-Amino-2-chloro-4-nitrobenzene | 121-87-9 |  |
| 4 | 1-Chloro-2,4-dinitrobenzene | 97-00-7 |  |
| 5 | 1H-Isoindole-1,3(2H)-dione, 2-methyl-5-nitro- | 41663-84-7 |  |
| 6 | 1-Nitro-2,4-difluorobenzene | 446-35-5 |  |
| 7 | 1-Nitro-2-carboxyanthraquinone | 128-67-6 |  |
| 8 | 2,4,7-Trinitro-9H-fluoren-9-one | 129-79-3 |  |
| 9 | 2,5-dichloronitrobenzene | 89-61-2 |  |
| 10 | 2-Amino-4-nitrophenol | 99-57-0 |  |
| 11 | 2-Amino-5-nitrophenol | 121-88-0 |  |
| 12 | 2-Nitro-4-cresol | 119-33-5 |  |
| 13 | 2-Nitroaniline | 88-74-4 |  |
| 14 | 2-Nitroanisole | 91-23-6 |  |
| 15 | 2-Nitronaphthalene | 581-89-5 |  |
| 16 | 2-Nitro-p-phenylenediamine | 5307-14-2 |  |
| 17 | 3-Nitroaniline | 99-09-2 |  |
| 18 | 3-Nitrotoluene | 99-08-1 |  |
| 19 | 4,4'-Dinitro-2,2'-stilbenedisulfonic acid | 128-42-7 |  |
| 20 | 4-Amino-2-nitrophenol | 119-34-6 |  |
| 21 | 4-Amino-2-nitrotoluene | 119-32-4 |  |
| 22 | 4-Chloro-2-nitroaniline | 89-63-4 |  |
| 23 | 4-Chloro-3-nitrobenzoic acid | 96-99-1 |  |
| 24 | 4-Chloro-3-nitrobenzotrifluoride | 121-17-5 |  |
| 25 | 4-Nitroaniline | 100-01-6 |  |
| 26 | 4-Nitrobenzoyl chloride | 122-04-3 |  |
| 27 | 5-Nitro-o-anisidine | 99-59-2 |  |
| 28 | Acenocoumarol | 152-72-7 |  |
| 29 | Acifluorfen | 50594-66-6 |  |
| 30 | AI 3-25755 | 328-04-1 |  |
| 31 | Aristolochic acid | 313-67-7 |  |
| 32 | Azanidazole | 62973-76-6 |  |
| 33 | Benzenamine, 2-methoxy-4-nitro- | 97-52-9 |  |
| 34 | Benzene, 1-chloromethyl-4-nitro- | 100-14-1 |  |
| 35 | Benzene, 1-isocyanato-4-nitro- | 100-28-7 |  |
| 36 | Benzoic acid, 2,5-dichloro-3-nitro- | 88-86-8 |  |
| 37 | C.I. Disperse Blue 79:1 | 3618-72-2 |  |
| 38 | Chloramphenicol | 56-75-7 |  |
| 39 | Clonazepam | 1622-61-3 |  |
| 40 | Dinex | 131-89-5 |  |
| 41 | Dinitolmide | 148-01-6 |  |
| 42 | Dinoseb | 88-85-7 |  |
| 43 | DNOC | 534-52-1 |  |
| 44 | Fenitrothion | 122-14-5 |  |
| 45 | Flunitrazepam | 1622-62-4 |  |
| 46 | Fluorothion | 363-97-3 |  |
| 47 | m-(Trifluoromethyl)nitrobenzene | 98-46-4 |  |
| 48 | m-Nitroacetophenone | 121-89-1 |  |
| 49 | Moskene | 116-66-5 |  |
| 50 | Musk Ambrette | 83-66-9 |  |
| 51 | Musk Ketone | 81-14-1 |  |
| 52 | Musk tibetine | 145-39-1 |  |
| 53 | Musk Xylene | 81-15-2 |  |
| 54 | Nicardipine | 55985-32-5 |  |
| 55 | Niclosamide | 50-65-7 |  |
| 56 | Nifedipine | 21829-25-4 |  |
| 57 | Nitrazepam | 146-22-5 |  |
| 58 | Nitrofen | 1836-75-5 |  |
| 59 | Nitrofungin | 619-08-9 |  |
| 60 | Nitrothal-isopropyl | 10552-74-6 |  |
| 61 | Nitroxoline | 4008-48-4 |  |
| 62 | o-Cresol, 3,5-dinitro- | 497-56-3 |  |
| 63 | o-Phenylenediamine, 4-nitro- | 99-56-9 |  |
| 64 | o-Toluenesulfonyl chloride, 5-nitro- | 121-02-8 |  |
| 65 | Paraoxon | 311-45-5 |  |
| 66 | Parathion-methyl | 298-00-0 |  |
| 67 | Phenol, 2,4-dinitro-6-isopropyl- | 118-95-6 |  |
| 68 | Phenol, 4-((2,4-dinitrophenyl)amino)- | 119-15-3 |  |
| 69 | Phosphoric acid, bis(2-chloroethyl) p-nitrophenyl ester | 311-44-4 |  |
| 70 | Picric acid (Trinitrophenol) | 88-89-1 |  |
| 71 | p-Nitrobiphenyl | 92-93-3 |  |
| 72 | Pyrinuron | 53558-25-1 |  |

**Table S2-** Chemical abstract number (CAS#) and molecular structures of the test set

|  |  |  |  |
| --- | --- | --- | --- |
| No. | Name | CAS# | Molecular structure |
| 1 | 1,2-Epoxy-3-(p-nitrophenoxy)propane | 5255-75-4 |  |
| 2 | 2,4-Dinitroaniline | 97-02-9 |  |
| 3 | 4-Chloro-3,5-dinitrobenzotrifluoride | 393-75-9 |  |
| 4 | 4-Nitroanisole | 100-17-4 |  |
| 5 | 4-Nitrobenzaldehyde | 555-16-8 |  |
| 6 | 4-Nitrophenetole | 100-29-8 |  |
| 7 | 5-Nitrosalicylaldehyde | 97-51-8 |  |
| 8 | Benzenamine, 4-methoxy-2-nitro- | 96-96-8 |  |
| 9 | Benzenesulfonic acid, 5-amino-2-(2-(4-nitro-2-sulfophenyl)ethenyl)- | 119-72-2 |  |
| 10 | Binapacryl | 485-31-4 |  |
| 11 | Chlorothion | 500-28-7 |  |
| 12 | Dicloran | 99-30-9 |  |
| 13 | Ethanone, 1-(2-nitrophenyl)- | 577-59-  3 |  |
| 14 | Fenitrooxone | 2255-17-6 |  |
| 15 | Flutamide | 13311-84-7 |  |
| 16 | Nimesulide | 51803-78-2 |  |
| 17 | Nitromide | 121-81-3 |  |
| 18 | Pyrrolnitrin | 1018-71-9 |  |