

Improvements of QSAR Class Names

| Before | After |
|---|---|
| CO_X alcohol less unreactive (EO mitigated) | CO_X alcohol unreactive w/ EO |
| CO_X alcohol unreactive Fish | CO_X alcohol unreactive w/o EO Fish |
| COS_X ketone unreactive | COns_X ketone unreactive |
| CO_X ketone unreactive aliphatic | COns_X ketone unreactive aliphatic |
| COS_X ketone unreactive aromatic fish | COS_X ketone unreactive aromatic |
| CNO_X aldehyde aliphatic general | CNO_X aldehyde general aliphatic |
| aldehyde aromatic general | CNO_X aldehyde general aromatic |
| COS_X ester unreactive | CNO_X ester unreactive |
| reactive phenol w/o 14- 12- (OH, NH2), w/o nito | phenol reactive w/o ortho,para-OH,NH2, w/o nitro |
| phenol unreactive | phenol unreactive unhindered |
| phenol unreactive w/o X | phenol unreactive unhindered w/o X |
| phenol unreactive excl. Diphenylether HRAC Ea | phenol unreactive unhindered excl. Diphenylether HRAC Ea |
| CNO_X amine NH2 reactive H (n, (OH, NH2) parent) | CNOS_X amine primary reactive w/o ortho,para-OH,NH2 |
| amine unreactive NH2 >1 | amine primary unreactive NH2 >1 |
| amine unreactive NH2 =1 aliphatic | amine primary unreactive NH2 =1 aliphatic |
| amine unreactive aromatic w/ NO2, SO2 w/o o-C | amine primary unreactive aromatic w/ NO2,SO w/o ortho-NH2 |
| CN_X amine NH, N< reactive (o-, p- N,OH) | amine sec, tert reactive w/ ortho,para-N,OH |
| CN_X amine unreactive NH, N< aromatic | CN_X amine sec, tert unreactive aromatic |
| CN_X amine unreactive NH, N< aliphatic | CN_X amine sec, tert unreactive aliphatic |
| CNO_X amine unreactive NH, N< aliphatic | CNO_X amine sec, tert unreactive aliphatic |
| CNOS_X basic aromatic n unreactive, excl. triazine | CNOS_X aromatic n unreactive, excl. triazine |
| CN_X nitril unreactive aliphatic | CN_X nitrile unreactive aliphatic |
| CN_X nitril unreactive | CN_X nitrile unreactive |
| CNOS_X amide unreactive | CNO_X amide unreactive |
| CNOSP_X phosphorus unreactive (no IRAC, HRAC, reactive alcohol) | CNOSP_X phosphorus unreactive |
| tentative CNOS_X halogen, unreactive | CNOS_X halogen unreactive |
| Cnos_X reactive fish, excl. n,cC=C | Cnos_X heteroaromatic reactive Fish |
| Cnos_X unreactive fish, daphnid | Cnos_X heteroaromatic unreactive Fish, Daphnid |
| Cnos_X unreactive excl. HC | Cnos_X unreactive |
| C_X HC aromatic w/ X (unreactive) | C_X unreactive aromatic w/ X |
| C_X aromatic HC wo X, R3=0 | C_X unreactive aromatic w/o X, fused R3=0 |
| C_X_aromatic w/o X, fused R=0 | C_X unreactive aromatic w/o X, fused R=0 |
| C_X HC w/ X (excl. Halomethane) | C_X unreactive aliphatic w/ X, excl. Halomethane |
| C_X HC w/ X (incl. Halomethane) | C_X unreactive halomethane |
| C_X HC aliphatic w/o X | C_X unreactive aliphatic w/o X |
| narcotic group (Fish acute) | narcotic group Fish Acute |
| primary alcohol SCAS | primary alcohol |
| CNOS_X amine aromatic lesstoxic | CNOS_X amine aromatic less toxic |
| CNOS_X amine sec, aliphatic or aromatic w/o n | CNOS_X amine sec, w/o n |
| ester mathacrylate | ester reactive methacrylate |
| CNOS_X N-hetero unreactive (w/o amine, aldoxime, carbamate) | CNOS_X N-hetero unreactive w/o amine, aldoxime, carbamate |
| CS_X thioether unreactive | CS_X sulfide unreactive |
| CO_X alcohol unreactive (w/o EO) (daphnid) | CO_X alcohol unreactive w/o EO Daphnid |
| CO_X alcohol unreactive | CO_X alcohol unreactive w/o EO Daphnid |
| COS_X ester unreactive | CNO_X ester unreactive |
| CNO_X ester unreactive (Daphnid) | CNO_X ester unreactive Daphnid |
| phenol hindered | phenol unreactive hindered |
| phenol unreactive | phenol unreactive unhindered |
| phenol unreactive w/o X | phenol unreactive unhindered w/o X |
| phenol unreactive excl. Diphenylether HRAC Ea | phenol unreactive unhindered excl. Diphenylether HRAC Ea |
| amine unreactive aromatic w/ NO2, SO2 w/o o-C | amine primary unreactive aromatic w/ NO2,SO w/o ortho-NH2 |
| CN_X amine unreactive NH, N< aromatic | CN_X amine sec, tert unreactive aromatic |
| CN_X amine unreactive NH, N< aliphatic | CN_X amine sec, tert unreactive aliphatic |
| CNOS_X aromatic n unreactive (daphnid) | CNOS_X aromatic n unreactive Daphnid |
| CNO_X amide unreactive (Daphnid) | CNO_X amide unreactive Daphnid |

| Before | After |
|---|---|
| CNO_X nitro >1 w/o 4-halogen, NO2 | CNO_X nitro >1 reactive w/o para-halogen,NO2 |
| CNO_X nitro mono unreactive (Daphnid) | CNO_X nitro mono unreactive Daphnid |
| Cnos_X unreactive fish, daphnid | Cnos_X heteroaromatic unreactive Fish, Daphnid |
| Cnos_X unreactive excl. HC | Cnos_X unreactive |
| C_X HC aliphatic (unreactive) w/ X | C_X unreactive aliphatic w/ X |
| C_X_aromatic w/o X, fused R=0 | C_X unreactive aromatic w/o X, fused R=0 |
| C_X w/ X, excl. gem-Cl2, 1,2-Cl2, TCE | C_X unreactive aliphatic w/ X, excl. gem,vic-Cl, TCE |
| narcotic group (Daphnid acute) | narcotic group Daphnid Acute |
| CNOS_X amine sec, aliphatic or aromatic w/o n S(Daphnid) | CNO_X amine sec w/o n Daphnid |
| ester mathacrylate | ester reactive methacrylate |
| CNOS_X N-hetero unreactive (w/o amine, aldoxime, carbamate) | CNOS_X N-hetero unreactive w/o amine, aldoxime, carbamate |
| CO_X alcohol unreactive C-OH w/o (acid, EO) | CO_X alcohol unreactive w/o halogen, acid, EO |
| CO_X ester unreactive (Alga) | CNO_X ester unreactive Alga |
| CO_X ether unreactive excl HRAC (Alga) | CO_X ether unreactive excl HRAC Alga |
| phenol unreactive excl. Diphenylether HRAC Ea | phenol unreactive unhindered excl. Diphenylether HRAC Ea |
| CNOS_X basic aromatic n unreactive | aromatic n reactive |
| C_X HC w/ X (excl. Halomethane) | C_X unreactive aliphatic w/ X, excl. Halomethane |
| Cos_X excl. HC, pyridine (Alga, Daphnid) | Cnos_X unreactive excl. pyridine Alga |
| narcotic group (Alga acute) | narcotic group Alga Acute |
| primary alcohol SCAS | primary alcohol |
| C_X HC w/ w/o X (unreactive) | C_X HC unreactive |
| Cnos_X w/o n+ unreactive (Fish chronic) | Cnos_X unreactive Fish Chronic |
| narcotic group (Fish chronic) | narcotic group Fish Chronic |
| CO_X alcohol unreactive (w/o EO) (daphnid) | CO_X alcohol unreactive w/o EO Daphnid |
| COS_X ketone unreactive | COns_X ketone unreactive |
| CNO_X ester unreactive (Daphnid) | CNO_X ester unreactive Daphnid |
| CN_X amine unreactive NH, N< | CNO_X amine sec, tert unreactive w/ N-Oxide,N-N=O |
| CNOS_X basic aromatic n unreactive | CNOS_X aromatic n unreactive |
| CNOS_X aromatic n unreactive (daphnid) | CNOS_X aromatic n unreactive Daphnid |
| CNO_X amide unreactive (Daphnid) | CNO_X amide unreactive Daphnid |
| Cnos_X unreactive fish, daphnid | Cnos_X heteroaromatic unreactive Fish, Daphnid |
| Cnos_X unreactive excl. HC | Cnos_X unreactive |
| C_X_aromatic w/o X, fused R=0 | C_X unreactive aromatic w/o X, fused R=0 |
| C_X w/ X, excl. gem-Cl2, 1,2-Cl2, TCE | C_X unreactive aliphatic w/ X, excl. gem,vic-Cl, TCE |
| CO_X alcohol unreactive C-OH w/o (acid, EO) | CO_X alcohol unreactive w/o halogen, acid, EO |
| CO_X ester unreactive (Alga) | CNO_X ester unreactive Alga |
| CO_X ether unreactive excl HRAC (Alga) | CO_X ether unreactive excl HRAC Alga |
| amine unreactive NH2 >1 Nv3 <3 (alga) | amine primary unreactive NH2 >1, Nv3 <3 |
| CNO_X amine unreactive NH, N< aliphatic | CNO_X amine sec, tert unreactive aliphatic |
| CN_X amine NH, N< reactive (o-, p- N,OH) | amine sec, tert reactive w/ ortho,para-N,OH |
| CN_X amine unreactive NH, N< | CNO_X amine sec, tert unreactive w/ N-Oxide,N-N=O |
| CNOS_X basic aromatic n unreactive | aromatic n reactive |
| CNOSP_X phosphorus unreactive (no IRAC, HRAC, reactive alcohol) | CNOSP_X phosphorus unreactive |
| CNOS_X N-hetero unreactive (w/o amine, aldoxime, carbamate) | CNOS_X N-hetero unreactive w/o amine, aldoxime, carbamate |