March 30, 2023

Modification of QSAR Class Names

Before (KATE2020 ver. 3.0)	After (KATE2020 ver. 4.0)
phenol not reactive - acid	phenol unreactive w/ acid
aldehyde F-D	aldehyde
ester alcohol reactive	ester reactive
ester acrylate	ester reactive acrylate
phenol bisphenol	phenol unreactive bisphenol
CNO_X phenol reactive, w/o o-formyl, OH,NH2	CNO_X phenol reactive, w/o ortho-CHO, ortho/para-OH,NH2
CNO_X phenol reactive, w/o o-formyl, w/ OH,NH2	CNO_X phenol reactive, w/ ortho-CHO, ortho/para-OH,NH2
phenol unreactive w/o X	phenol unreactive w/o X, HRAC Ea
phenol unreactive w X	phenol unreactive w/ X, w/o HRAC Ea
CNO_X reactive phenol w/ 14- 12- (OH, N)	CNO_X reactive phenol w/ ortho/para-OH, NH2
reactive phenol w/o 14- 12- (OH, NH2) w/ nitro	phenol reactive w/ ortho,para-OH,NH2, w/o nitro
CO_X ether reactive (epoxide)	CO_X ether reactive, epoxide
CNO_X reactive phenol w/ 14- 12- (OH, N)	CNO_X reactive phenol w/ ortho/para-OH,NH2
C_X HC unreactive	C_X hydrocarbon unreactive
Cnos_X unreactive	Cnos_X heteroaromatic unreactive
C_X unreactive aliphatic w/ X	C_X hydrocarbon unreactive aliphatic w/ X
C_X unreactive aromatic w/ X	C_X hydrocarbon unreactive aromatic w/ X
C_X unreactive aromatic w/o X, fused R3=0	C_X hydrocarbon unreactive aromatic w/o X, fused R3=0
C_X aromatic wo X, R3>0	C_X hydrocarbon unreactive aromatic w/o X, R3=0
C_X_aromatic HC w/o X, fused R>1	C_X hydrocarbon unreactive aromatic w/o X, fused R>1
C_X unreactive aromatic w/o X, fused R=0	C_X hydrocarbon unreactive aromatic w/o X, fused R=0
C_X unreactive aliphatic w/ X, excl. Halomethane	C_X hydrocarbon unreactive aliphatic w/ X, excl. Halomethane
C_X unreactive halomethane	C_X hydrocarbon unreactive halomethane
CO_X alcohol reactive C-OH w/ proMichael	CO_X alcohol reactive w/ proMichael 8
CO_X alcohol unreactive (w/ EO) (daphnid), not acute toxic	CO_X alcohol unreactive w/ EO daphnid
CNO_X ketone reactive (KP)	CNO_X ketone reactive
COS_X ester reactive alcohol	CO_X ester reactive
COS_X other reactive ester(malonate)	CO_X ester reactive malonate
CO_X alcohol reactive C-OH w/o proMichael	CO_X alcohol reactive w/o proMichael 8
CO_X alcohol reactive C-OH w/o pinacol	CO_X alcohol reactive w/o pinacol
CO_X alcohol reactive C-OH w/ pinacol	CO_X alcohol reactive w/ pinacol
CO_X other unreactive(peroxy)	CO_X peroxy unreactive
CNO_X aldehyde aliphatic reactive	CNO_X aldehyde reactive aliphatic
CNO_X aldehyde aromatic reactive	CNO_X aldehyde reactive aromatic
C_X w/ X, w/ gem-Cl2, 1,2-Cl2, TCE	C_X w/ X, incl. gem/vic Cl,TCE
COS_X C-thiol	COS_X thiol
CSO-X -SO3H, Sulfonic Acid, sulfo-, -sulfonic acid (not QSAR use)	COS-X sulfonic acid
CSO-X sulfoxide, sulfone unreactive	CSO-X sulfoxide unreactive
C_X unreactive aliphatic w/o X	C_X hydrocarbon unreactive aliphatic w/o X
C_X reactive HC	C_X hydrocarbon reactive
Cnos_X reactive excl. HC	CNOSP_X reactive
C_X reactive HC, excl. ClC=CCCl	C_X hydrocarbon reactive excl. 1,3-Dichloropropene
Cnos_X reactive excl. HC, nC=C	CNOSP_X reactive excl. n-vinyl
N_X amine aliphatic NH2=1	amine primary unreactive NH2=1
amine mitigated or acid	amine hindered or acid
CNO_X amine NH2 reactive (ecld. hydrazine)	CNOS_X amine primary reactive excl. hydrazine
CN_X amine unreactive aromatic w/o NO2, SO2 w/ o-C	amine primary unreactive aromatic w/o NO2, SO, ortho-NH2
amine primary unreactive aromatic w/ NO2,SO w/o ortho-NH2	amine primary unreactive aromatic w/ NO2,SO
CNO_X NH2 reactive (OH,NH2, hetero-NH2)	CNOS_X amine primary reactive w/ ortho,para-OH,NH2
amine NH2 reactive (hydrazine)	amine primary reactive (hydrazine)
NH2 reactive (w/o OH, Nv3X3) Daphnid	CNOS_X amine primary reactive w/o OH, Daphnid
NH2 reactive (w/ OH, Nv3X3) Daphnid chronic	CNOS_X amine primary reactive w/ OH, Daphnid Chronic
CNO_X amine sec, tert unreactive w/ N-Oxide,N-N=O	CNO_X amine sec, tert unreactive w/ N-Oxide,Nitroso

Before (KATE2020 ver. 3.0)	After (KATE2020 ver. 4.0)
COS_X ketone unreactive aliphatic	CNO_X aldehyde, ketone
CNOS_X basic aromatic n reactive, excl CN n+	CNOS_X aromatic n reactive, excl nitrile
CNOS_X SH unreactive	CNOS_X sulfur unreactive w/o thiol
CNOS_X S reactive	CNOS_X sulfur reactive
CNOS_X hydrazine general	CNOS_X hydrazine
CN_X C=N unreactive	CN_X imine
CNO_X nitro >1	CNO_X nitro >1 reactive
CNO_X nitro mono unreactive (Alga)	CNO_X nitro mono unreactive Alga
CNO_X nitro >1 w/ 4-halogen, NO2	CNO_X nitro >1 reactive w/o para-halogen,NO2
CNOS_X carbamate unreactive	CNOS_X carbamate unreactive Fish
CNOS_X carbamate reactive (incl isocyanate)	CNOS_X carbamate unreactive incl. isothiocyanate Fish
CNOS_X amine NH2 w/ C=O	CNOS_X amine primary w/ C=O
CNOS_X amine aromatic less toxic	CNOS_X amine aromatic w/ aliphatic carbon
CNOS_X amine aromatic slight toxic	CNOS_X amine aromatic w/o aliphatic carbon
CNOS_X amine sec, w/o n	CNOS_X amine sec, tert w/o n
CNOS_X amine sec w/ n	CNOS_X amine sec, tert w/ n
CNOS_X amine sec, di-functional	CNOS_X amine sec, tert multi
CNO_X amine sec w/o n Daphnid	CNO_X amine sec mono w/o n Daphnid
CNOS_X amine tert, unreactive w/ C=O	CNOS_X amine tert unreactive w/ C=O
CN_X nitril unreactive aromatic	CN_X nitrile unreactive aromatic
CN_X nitril reactive	CN_X nitrile reactive
CNO_X nitril reactive	CNO_X nitrile reactive
CNO_X nitril unreactive	CNO_X nitrile reactive
amide reactive, excl. a-C=O	amide reactive, excl. C=O,S,N
amide reactive (other class) (not QSAR use)	amide reactive (Oxamyl, Strychnine hemisulphate salt)
amide reactive (Daphnid)	CNO_X amide reactive Daphnid
CNO_X amide unreactive (Alga), not acute toxic, may >100mg/L	CNO_X amide unreactive Alga
CNO_X amide reactive (Alga)	CNO_X amide reactive Alga
CNOS_X urea unreactive	CNOS_X ether aromatic
CNOS_X hydrazine NH,NH0	CNOS_X hydrazine NH
CNO_X azo -N=N-	CNO_X azo
tentative CNOS_X halogen, reactive	CNOS_X halogen reactive
CNOSP_X phosphorus reactive (IRAC, HRAC, reactive alcohol) w/o N,n	CNOSP_X phosphorus reactive w/o N,n
CNOSP_X phosphorus reactive (IRAC, HRAC, reactive alcohol) w/ N,n	CNOSP_X phosphorus reactive w/ N,n
CNO_X unreactive (Fish chronic), excl. (CnosX w/o n+)	CNO_X unreactive Fish Chronic, w/ N,O
CNO_X reactive (Fish chronic)	CNO_X reactive Fish Chronic
CNOS_X acid general	CNOS_X acid unreactive
CNOS_X oxoacid general, carboxylic, not hindered	CNOS_X oxoacid unreactive, carboxylic, unhindered
CNOS_X acid reactive w/o N+	CNOS_X oxoacid unreactive, carboxylic, unhindered
CNOS_X acid not carboxylic general	CNOS_X acid sulfonic unreactive
alcohol unreactive (w EO) alga	alcohol unreactive w/ EO alga
CO_X alcohol reactive C-OH w/o acid alga not acute toxic	CO_X alcohol reactive w/o acid alga
CO_X ether unreactive excl HRAC Alga	CO_X ether unreactive excl. HRAC Ea Alga
C_X HC (all HC)	C_X hydrocarbon Alga Chronic
Cnos_X unreactive excl. pyridine Alga	Cnos_X heteroaromatic excl. pyridine Alga
MLR:C_X HC aromatic w/o X, excl. biphenyl	C_X aromatic hydrocarbon w/o X, excl. biphenyl
amine unreactive NH2 =1 aliphatic (alga)	amine primary unreactive aliphatic NH2=1 alga
CNOS_X aromatic n unreactive (alga)	CNOS_X aromatic n unreactive Alga
CNOS_X aromatic n reactive (alga)	CNOS_X aromatic n reactive Alga
aromatic n reactive	aromatic n reactive Alga
CNOS_X SH unreactive alga	CNOS_X sulfur unreactive Alga
CNOS_X S reactive alga excl. SS	CNOS_X sulfur reactive excl. disulfide Alga
CNOS_X S reactive alga incl. SS	CNOS_X sulfur reactive disulfide Alga
CNOS_X carbamate reactive alga	CNOS_X carbamate reactive incl. isothiocyanate Alga
narcotic group (Alga chronic)	Narcotic group Alga Chronic
CNO_X alcohol unreactive (wo EO) alga	CNO_X alcohol unreactive w/o EO Alga
Cnos_X reactive alga, excl. pyrole	Cnos_X heteroaromatic reactive excl. pyrrole Alga

Before (KATE2020 ver. 3.0)	After (KATE2020 ver. 4.0)
Cnos_X reactive alga, pyrole	Cnos_X heteroaromatic reactive pyrrole Alga
CNOS_X aromatic n reactive (daphnid)	CNOS_X aromatic n reactive Daphnid
CNOS_X hydrazine w/o NH2 or in ring	CNOS_X hydrazine w/o NH2 or in ring Daphnid
CNOS_X carbamate unreactive	CNOS_X carbamate unreactive Daphnid
narcotic group (Daphnid chronic)	narcotic group Daphnid Chronic
CNOS_X aromatic n unreactive, excl. triazine	CNOS_X aromatic n unreactive, excl. triazine Fish
CNOS_X aromatic n unreactive (fish) triazine	CNOS_X aromatic n unreactive triazine Fish
CNOS_X S reactive fish excl. thiophenol	CNOS_X sulfur reactive excl. thiophenol Fish
CNOS_X S reactive fish incl. thiophenol	CNOS_X sulfur reactive thiophenol Fish
Cnos_X reactive alga, n,cC=C	Cnos_X heteroaromatic reactive w/ vinyl Fish, Daphnid
primary alcohol	CO_X primary alcohol
amine NH2 reactive	amine primary reactive
phenol reactive Daphnid	phenol reactive
Cnos_X reactive alga	Cnos_X heteroaromatic reactive Alga
phenol not reactive, w/o acid	phenol unreactive w/o acid
ester unreactive	ester unreactive w/o acid
Cnos_X unreactive argae	Cnos_X heteroaromatic unreactive Alga