

Session: FP_training, Model: AMG_FP_training_Model_RBF Model

Sun September 11 2011, 13:01

Modeled property: Tox

Modeling technique: Radial Basis Function

Model statistics:

	Number	Rsqr	RMSE
TRN	6480	0.9964	5.004
VAL	1620	0.898	26.83

Parameters used:

Descriptor pre-selection:

- Threshold for minimum occurrence: 4%
- Threshold for minimum standard deviation: 0.0005
- Threshold for maximum correlation between descriptors: 0.95

Descriptors remaining after pre-selection: 145

Descriptors used in the model: 145

Model details:

No GA performed

Descriptors

Vx
MW
NegativeCharge
PositiveCharge
Flex
AromaticRings
logP
OverallCharge
ERTLNotPSA
ERTLNoSPtPSA
HBA-prof
HBD-lip
HBD-prof
CH0Aa
CH1Aa
CH2Aa
CH2hetero
CH2link
CH2long
CH3Aa
CH3hetero
Ester
HaloC
NO
NRB
RSR
aliphOH-t6
allylic-oxyd-t10
anycarbonyl
aromCl
branchedCnotRing
di-withdraw-cx4
ertl-33
est-lact-latm-carbm-t7
ether
intraHbond6
ketone-t14
ketones
lipovolume
nonring-at

p-hetero-or-halo
phenol
ring-join
ringOdouble
ringat
sp-carbons
sp2-carbons
t-16-1
tert-amine-t11
nC(sp2)
nC(sp3)
nOH
nCO
nOS
nX
nNprot
dsCH
aaCH
sssCH
tsC
dssC
aasC
aaaC
ssssC
sNH2
ssNH
aaN
sssN
sOH
ssO
sF
dS
sCl
sBr
nNneutral
NnH
NbN
NonOrganicAtom
PRX-time1
PRX-time-1
UB
HAN
HAS
HAT
HAO
AliRingAttachment
C4
C10
C6
C3
C8
C1
C11
C2
N6
N7
N2
H3
N1
BasicGroup
AcidGroup
H4
O3
O5
O9
O10
AroRingAttachment
HydrophobicGroup
H1a
C5
C21
C22

C23
ed70
ed20
ed40
ew10
f004
f007
f015
f147
f244
f245
f301
f390
f407
f413
f440
f441
f443
f456
q017
q039
q040
q137
q192
q257
q300
q358
q453
q457
q458
q481
frg-8
Nn