

Session: ST_training, Model: AMG_ST_training_Model_RBF Model (no GA)

Sun September 11 2011, 13:02

Modeled property: Tox

Modeling technique: Radial Basis Function

Model statistics:

	Number	Rsqr	RMSE
TRN	1136	0.9989	0.2261
VAL	285	0.8701	2.257

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: 100

Descriptors used in the model: 100

Model details:

No GA performed

Descriptors

Vx
MW
PositiveCharge
Flex
AromaticRings
logP
ERTLNotPSA
ERTLNoSPtPSA
HBA-prof
HBD-lip
HBD-prof
CH1Aa
CH2Aa
CH2hetero
CH2link
CH2long
CH3Aa
CH3hetero
Ester
HaloC
NRB
aliphOH-t6
allylic-oxyd-t10
anycarbonyl
branchedCnotRing
ch2-lipo-t9
est-lact-latm-carbm-t7
ether
hydroxyA
ketone-t14
lipovolume
nonring-at
pyridine
ring-join
ringat
sp-carbons
sp2-carbons
nC(sp3)
nCO
nOS

nX
dsCH
sssCH
dssC
aasC
ssssC
tN
aaN
sOH
ssO
sCl
sBr
nNneutral
NnH
NbN
NonOrganicAtom
PRX-time1
UB
HAN
HAS
HAT
HAO
AliRingAttachment
C4
C10
C6
C3
C2
N6
H3
H2
O9
O10
HydrophobicGroup
H1a
C5
C21
ed70
f147
f244
f245
f393
f407
f413
f440
f441
f443
f456
q039
q137
q139
q192
q257
q300
q358
q453
q457
q458
q481
Nn