

Session: WS_training, Model: AMG_WS_training_Model_RBF Model

Fri September 9 2011, 18:59

Modeled property: Tox

Modeling technique: Radial Basis Function

Model statistics:

	Number	Rsqr	RMSE
TRN	4064	0.998	0.0968
VAL	1015	0.8793	0.8085

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: 167

Descriptors used in the model: 167

Model details:

No GA performed

Descriptors

Vx
MW
NegativeCharge
PositiveCharge
Flex
AromaticRings
logP
OverallCharge
ERTLNotPSA
ERTLNoSPtPSA
HBA-lip
HBA-prof
HBD-lip
HBD-prof
ACamideO-nh-nh2
CH0Aa
CH1Aa
CH2Aa
CH2hetero
CH2link
CH2long
CH3Aa
CH3hetero
Ester
HaloC
NO
NRB
Pester
RSR
aliphOH-t6
allylic-oxyd-t10
aminoethanol0
aminoethanol1
anycarbonyl
aromCl
branchedCnotRing
dNO
di-withdraw-cx4
ertl-33
ertl-35

est-lact-latm-carbm-t7
ether
intraHbond5
intraHbond6
ketone-t14
lipovolume
nonring-at
p-hetero-or-halo
phenol
phenolic-tautomer
ring-join
ring5-nH0
ringOdouble
ringat
sp2-carbons
t-16-1
urea-thio
urea
nC(sp2)
nC(sp3)
nOH
nCO
nOS
nX
nNprot
ssCH2
dsCH
aaCH
sssCH
dssC
aasC
aaaC
ssssC
sNH2
ssNH
aaNH
dsN
aaN
sssN
sOH
ssO
sF
dS
ssS
sCl
nNneutral
NnH
N4
CamideNH
NonOrganicAtom
PRX-time1
PRX-time-1
UB
HAN
PRX-time2
HAS
HAT
HAO
AliRingAttachment
C12
C4
C10
C6
C3
C8
C1
C11
C2
N6
N7
N2
H3

N1
BasicGroup
AcidGroup
H4
O3
O11
O5
O9
O10
AroRingAttachment
N11
HydrophobicGroup
H1a
C5
C21
C22
C23
C24
ed70
ed20
ed40
ed80
ew10
ew100
f004
f007
f015
f147
f244
f245
f301
f390
f393
f407
f413
f440
f441
f443
f444
f456
q017
q039
q040
q137
q155
q192
q257
q300
q358
q453
q457
q458
q481
frg-8
Nn