Session: Rat Toxicity -log(LD50) M, Model: AMG_Rat Toxicity -log(LD50) M_Model_RBF Model

Fri May 13 2011, 18:52

Modeled property: Tox

Modeling technique: Radial Basis Function

Model statistics:

	Number	Rsqr	RMSE
TRN	5936	0.9928	0.08074
VAL	1484	0.6433	0.5719

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: 171

Descriptors used in the model: 171

Model details:

No GA performed

Descriptors

Vx
MW
NegativeCharge
PositiveCharge
Flex
AromaticRings
logP
ERTLNotPSA
ERTLNoSPtPSA
HBA-lip
HBA-prof
HBD-lip
HBD-prof
ACamideO-nh-nh2
CH0Aa
CH1Aa
CH2Aa
CH2hetero
CH2link
CH2long
CH3Aa
CH3hetero
CamideNH0
Ester
HaloC
NO
NRB
Ocarbamate
Pester
RSR
RbasicNH0
aliphOH-t6
allylic-oxyd-t10
aminoethanol0
aminoethanol1
anycarbonyl
aromCl
branchedCnotRing
carbamate-and-thio

dNO
di-widhraw-cx4
ertl-33
ertl-35
est-lact-latm-carbm-t7
ether
intraHbond6
ketone-t14
ketones
lipovolume
nonring-at
p-hetero-or-halo
phenol
phenolic-tautomer
ring-join
ring5-nH0
ringOdouble
ringat
sp-carbons
sp2-carbons
t-16-1
tert-amine-t11
nC(sp2)
nC(sp3)
nOH
nCO
nOS
nX
nNprot
ssCH2
dsCH
aaCH
sssCH
tsC
dssC
aasC
aaaC
ssssC
sNH2
ssNH
aaNH
dsN
aaN
sssN
sOH
ssO
sF
sssP
dS
sCl
nNneutral
NnH
N4
NbN
CamideNH
BasicNH02AroRings
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
N8
N2
H3
N1
BasicGroup
AcidGroup
H4
O3
O11
O5
O9
O10
AroRingAttachment
HydrophobicGroup
H1a
C5
C21
C22
C23
C24
ed70
ed20
ed40
ew10
ew100
f004
f007
f015
f147
f244
f245
f301
f390
f393
f407
f413
f440
f441
f443
f444
f456
q017
q039
q040
q137
q192
q257
q300
q358
q453
q457
q458
q481
frg-8
Nn