

## Session: Density\_training, Model: AMG\_Density\_training\_Model\_RBF Model

Sun September 11 2011, 12:59

Modeled property: Tox

Modeling technique: Radial Basis Function

### Model statistics:

|     | Number | Rsqr   | RMSE    |
|-----|--------|--------|---------|
| TRN | 6885   | 0.9983 | 0.01344 |
| VAL | 1722   | 0.9463 | 0.07718 |

### 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: 147

Descriptors used in the model: 147

### 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  
dNO  
di-widhraw-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  
dssC  
aasC  
aaaC  
ssssC  
sNH2  
ssNH  
aaN  
sssN  
sOH  
ssO  
sF  
dS  
sCl  
sBr  
nNneutral  
NnH  
NbN  
CamideNH  
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  
N11  
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