

## Session: BCF\_training, Model: AMG\_BCF\_training\_Model\_RBF Model

Fri May 13 2011, 10:56

Modeled property: Tox

Modeling technique: Radial Basis Function

### Model statistics:

	Number	Rsqr	RMSE
TRN	541	1	3.061e-05
VAL	136	0.7619	0.648

### 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: 139

Descriptors used in the model: 139

### Model details:

No GA performed

### Descriptors

Vx  
MW  
NegativeCharge  
PositiveCharge  
Flex  
AromaticRings  
logP  
ERTLNotPSA  
ERTLNoSPtPSA  
HBA-lip  
HBA-prof  
HBD-lip  
HBD-prof  
CH0Aa  
CH1Aa  
CH2Aa  
CH2hetero  
CH2link  
CH2long  
CH3Aa  
CH3hetero  
HaloC  
NO  
NRB  
Pester  
allylic-oxyd-t10  
anycarbonyl  
aromCl  
branchedCnotRing  
dNO  
di-withdraw-cx4  
ertl-33  
ertl-35  
ether  
hydroxyA  
intraHbond6  
lipovolume  
nonring-at  
p-hetero-or-halo  
phenol

ring-join  
ringOdouble  
ringat  
sp2-carbons  
t-16-1  
nC(sp3)  
nOH  
nCO  
nOS  
nX  
nNprot  
dsCH  
aaCH  
sssCH  
dssC  
aasC  
aaaC  
ssssC  
sNH2  
ssNH  
dsN  
aaN  
sssN  
sOH  
ssO  
dS  
sCl  
sBr  
nNneutral  
NnH  
N4  
NonOrganicAtom  
PRX-time1  
PRX-time-1  
UB  
HAN  
HAS  
HAT  
HAO  
AliRingAttachment  
C12  
C4  
C10  
C6  
C3  
C8  
C1  
C2  
N6  
N2  
H3  
BasicGroup  
AcidGroup  
O3  
O5  
O9  
O10  
AroRingAttachment  
HydrophobicGroup  
H1a  
C5  
C21  
C22  
C23  
C24  
ed70  
ed20  
ed40  
ed80  
ew10  
ew100  
f004

f007  
f015  
f244  
f245  
f301  
f390  
f393  
f407  
f413  
f440  
f441  
f443  
f444  
f456  
q017  
q039  
q041  
q137  
q192  
q257  
q300  
q358  
q453  
q457  
q458  
frg-8  
Nn