

## Session: 2\_2, Model: RBF\_T\_Half\_Life

Fri November 9 2012, 10:44

Modeled property: HTL

Modeling technique: Radial Basis Function

### Model statistics:

	Number	Rsqr	RMSE
TRN	998	1	0.000147
VAL	244	0.463	0.3207

### 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: 181

Descriptors used in the model: 181

### Model details:

No GA performed

### Descriptors

logP  
Vx  
MW  
NegativeCharge  
PositiveCharge  
Flex  
AromaticRings  
ERTLNotPSA  
HBA-lip  
HBA-prof  
HBD-lip  
HBD-prof  
ACamideO-nh-nh2  
ACamideO-nh0  
ASamideO-nh-nh2  
ASamideO-nh0  
AbasicNH0  
AbasicNH1  
CF3  
CH0Aa  
CH1Aa  
CH2Aa  
CH2hetero  
CH2link  
CH2long  
CH3Aa  
CH3hetero  
CamideNH0  
Ester  
HaloC  
NRB  
RCamideO-nh0  
RSamideO-nh0  
Ramidine  
RbasicNH0  
RbasicNH1  
SamideNH0  
aliphOH-t6  
allylic-oxyd-t10  
aminoethanol0

aminoethanol1  
anycarbonyl  
aromCl  
aromF  
aromO  
arylNHCO  
basic-NH2  
branchedCnotRing  
ch2-lipo-t9  
ertl-33  
est-lact-latm-carbm-t7  
ether  
hetero-halo-di-n-arom  
hydroxyA  
hydroxylation-t8  
intraHbond5  
intraHbond6  
lipovolume  
nH0indole-like  
nHindole-like  
nonring-at  
p-hetero-or-halo  
phenol-pyr2r  
phenol  
phenolic-tautomer  
pyridine  
pyridones  
ring-join  
ring5-nH0  
ring5nH  
ringOdouble  
ringat  
sp-carbons  
sp2-carbons  
sulphates  
t-16-1  
tert-amine-t11  
urea-thio  
xccn-t12  
nC(sp2)  
nC(sp3)  
nOH  
nCO  
nOS  
nX  
nNprot  
ssCH2  
dsCH  
aaCH  
sssCH  
dssC  
aasC  
aaaC  
ssssC  
sNH2  
ssNH  
tN  
dsN  
aaN  
sssN  
sOH  
ssO  
sF  
nNneutral  
NnH  
N4  
NbN  
fg5  
BasicNH0R2AroRings  
BasicNH02AroRings  
BasicNH12AroRings  
PRX-time1

PRX-time-1  
UB  
PRX-time2  
HAS  
HAO  
AliRingAttachment  
C12  
C4  
C10  
C6  
C9  
C8  
C1  
C11  
C2  
C26  
N7  
N8  
N2  
N1  
BasicGroup  
AcidGroup  
H4  
H2  
O3  
O11  
O9  
O10  
AroRingAttachment  
HydrophobicGroup  
C5  
C21  
C22  
C23  
C24  
S3  
ed70  
ed40  
ed80  
ew70  
ew60  
ew75  
ew10  
ew100  
f004  
f007  
f015  
f244  
f245  
f301  
f407  
f440  
f441  
f443  
f444  
q017  
q039  
q040  
q137  
q155  
q192  
q257  
q300  
q453  
q457  
q458  
q481  
frg-8  
frg-26