

Session: ST_training, Model: AMG_ST_training_Model_GPFixed

Thu September 15 2011, 18:27

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	1136	0.9419	1.625
VAL	285	0.8209	2.65

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: 100

Descriptors used in the model: 100

Model details:

Theta1: 254.4570313

Theta2: 227.4622345

Theta3: 0.400000006

Descriptor	Length scale
Vx	2417.728
MW	2788.066
PositiveCharge	14.66585
Flex	10.6535
AromaticRings	23.23683
logP	67.94947
ERTLNotPSA	774.556
ERTLNoSPtPSA	812.2247
HBA-prof	55.29808
HBD-lip	17.69068
HBD-prof	13.29166
CH1Aa	21.04943
CH2Aa	139.0983
CH2hetero	48.76128
CH2link	165.5353
CH2long	134.5355
CH3Aa	50.00475
CH3hetero	16.06696
Ester	25.80014
HaloC	21.63234
NRB	191.3098
aliphOH-t6	10.86151
allylic-oxyd-t10	16.99786
anycarbonyl	27.46638
branchedCnotRing	28.38988
ch2-lipo-t9	8.301495
est-lact-latm-carbm-t7	23.69251
ether	19.67963
hydroxyA	12.02343
ketone-t14	8.363523
lipovolume	163.6179
nonring-at	219.5925
pyridine	8.208671

ring-join	15.77593
ringat	137.4087
sp-carbons	16.12571
sp2-carbons	38.5455
nC(sp3)	176.616
nCO	25.86701
nOS	37.34183
nX	40.1365
dsCH	17.91793
sssCH	26.05258
dssC	27.79614
aasC	27.77655
ssssC	19.34611
tN	9.508816
aaN	9.191894
sOH	15.83399
ssO	37.14671
sCl	18.79087
sBr	12.75657
nNneutral	18.75597
NnH	8.545235
NbN	20.27386
NonOrganicAtom	9.320128
PRX-time1	16.39673
UB	135.2597
HAN	18.6538
HAS	12.07842
HAT	54.09703
HAO	55.95977
AliRingAttachment	17.30173
C4	22.25125
C10	12.31945
C6	25.022
C3	51.06551
C2	24.80283
N6	12.14088
H3	10.68829
H2	13.33337
O9	25.46482
O10	9.722015
HydrophobicGroup	154.1691
H1a	31.71864
C5	26.5306
C21	22.06285
ed70	16.90588
f147	19.56935
f244	64.17525
f245	55.91935
f393	64.35846
f407	62.95473
f413	31.53204
f440	31.83596
f441	48.69676
f443	24.4438
f456	13.55641
q039	44.42168
q137	66.82005
q139	51.76946
q192	36.35798
q257	83.99712
q300	13.62612
q358	58.21988

q453	42.51917
q457	11.82691
q458	77.0518
q481	54.65289
Nn	18.48678