

Session: BP_training, Model: BP GPFixed

Sun September 11 2011, 13:17

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	3003	0.9919	7.302
VAL	751	0.9654	14.38

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: 119

Descriptors used in the model: 119

Model details:

Theta1: 4783.269043

Theta2: 4457.874512

Theta3: 0.400000006

Descriptor	Length scale
Vx	1759.238
MW	2313.916
PositiveCharge	20.72409
Flex	10.55044
AromaticRings	29.76101
logP	67.64646
ERTLNotPSA	730.0418
ERTLNoSPtPSA	757.0135
HBA-lip	49.80017
HBA-prof	44.7544
HBD-lip	24.09565
HBD-prof	18.96183
CH0Aa	10.51662
CH1Aa	23.96692
CH2Aa	121.2446
CH2hetero	39.89545
CH2link	132.6303
CH2long	110.1446
CH3Aa	57.49731
CH3hetero	22.44735
Ester	17.13491
HaloC	29.51943
NRB	152.1672
aliphOH-t6	14.05045
allylic-oxyd-t10	24.12119
anycarbonyl	26.19217
aromCl	16.61067
branchedCnotRing	33.92752
di-widhrow-cx4	50.03145
est-lact-latm-carbm-t7	18.56483
ether	20.67193
hydroxyA	15.3243
ketone-t14	10.87101

ketones	9.711635
lipovolume	155.3678
nonring-at	169.2998
ringat	170.9631
sp-carbons	17.45143
sp2-carbons	45.69707
nC(sp3)	155.2333
nOH	17.45023
nCO	23.27563
nOS	28.14171
nX	71.00064
nNprot	15.24666
dsCH	27.89742
aaCH	113.2876
sssCH	30.24619
tsC	14.19297
dssC	25.44952
aasC	51.80512
aaaC	27.73604
ssssC	28.50433
sNH2	11.76973
aaN	12.02355
sOH	19.20366
ssO	27.06325
sF	59.91794
sCl	32.91878
sBr	16.41156
nNneutral	21.51618
NnH	16.38343
NbN	25.27391
UB	163.2867
HAN	24.00653
HAS	10.21641
HAT	45.58996
HAO	44.39716
AliRingAttachment	25.02776
C4	31.13834
C10	14.91015
C6	39.6538
C3	47.35054
C8	21.50646
C1	147.1089
C2	28.04261
H3	12.05083
BasicGroup	14.35321
H2	18.35844
O3	25.51104
O9	21.42698
O10	11.90217
AroRingAttachment	57.81194
HydrophobicGroup	149.5631
H1a	39.79581
C5	23.89534
C21	32.52697
C22	12.72524
C23	14.65271
ed70	27.64362
ew10	26.80665
f004	36.75753
f007	30.06661
f015	25.81236
f147	27.43457

f244	82.68154
f245	77.10905
f390	68.83381
f393	105.0021
f407	54.79153
f413	26.04721
f440	71.64512
f441	85.68844
f443	52.17244
f444	65.747
f456	33.71245
q017	216.0044
q039	78.09913
q041	93.94803
q137	124.546
q192	49.4629
q257	63.58352
q300	30.87808
q358	46.30858
q453	76.56327
q457	22.16704
q458	115.0364
frg-8	10.36111
Nn	19.66002