Session: Viscosity_training, Model: Viscocity GP2DSearch

Thu September 15 2011, 18:30

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	346	0.9127	0.1563
VAL	87	0.9045	0.1646

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: 107

Descriptors used in the model: 107

Model details:

Theta1: 6.673535347

Theta2: 9.851138115

Theta3: 0.1000000015

Descriptor	Length scale
Vx	2216.636
MW	2702.914
PositiveCharge	15.4432
Flex	10.71257
AromaticRings	21.1616
logP	71.12737
OverallCharge	16.9858
ERTLNotPSA	766.2559
ERTLNoSPtPSA	791.4485
HBA-lip	54.0533
HBA-prof	43.38676
HBD-lip	27.05999
HBD-prof	24.35183
CH1Aa	25.30267
CH2Aa	140.9714
CH2hetero	30.02941
CH2long	109.9323
CH3Aa	44.37334
CH3hetero	22.67982
Ester	12.48243
HaloC	33.50912
NRB	189.7522
RSR	9.43963
aliphOH-t6	22.36237
allylic-oxyd-t10	21.08284
anycarbonyl	25.40901
aromF	10.48754
branchedCnotRing	38.43689
di-widhraw-cx4	57.60357
est-lact-latm-carbm-t7	14.41131
ether	14.88664
ketone-t14	8.702044
lipovolume	159.9459

nitro	8.95626
nonring-at	187.4484
ringat	142.2311
sp-carbons	10.00319
sp2-carbons	32.24781
nC(sp3)	175.7481
nOH	23.24538
nCO	17.71487
nOS	26.19169
nX	75.53754
nNprot	11.61652
dsCH	19.62459
sssCH	34.56443
dssC	18.07869
aasC	37.4222
ssssC	32.54795
sNH2	11.79722
ssNH	8.702044
sOH	25.00877
sF	70.6581
sCl	21.89606
sBr	14.34548
nNneutral	20.24157
NnH	14.37744
NbN	22.04229
PRX-time1	20.20327
UB	131.2929
HAN	19.51466
HAT	44.04048
HAO	42.61296
AliRingAttachment	30.34889
C4	40.48456
C10	13.99529
C6	28.73691
C3	36.78986
C8	15.72436
C1	163.4086
C2	25.91203
N6	13.33837
H3	11.974
O3	23.06856
O5	19.65928
O9	16.6097
H1a	37.21544
C5	20.78861
C21	25.30976
C22	11.18118
C23	13.74036
ed70	22.37519
ed40	12.00928
ew10	13.09749
f004	19.09266
f007	11.974
f015	23.22964
f244	93.22461
f407	38.10128
f413	18.65919
f440	44.2957
f441	52.35614
f443	34.38367
f444	41.00008
f456	22.59588

q017	251.5375
q039	61.51223
q041	82.62429
q137	108.022
q192	39.19653
q257	48.82673
q300	27.83361
q358	47.67103
q453	61.06809
q457	17.57506
q458	84.411
Nn	18.65919