Session: Tetrahymena pyriformis -log(IGC50) M, Model: AMG_Tetrahymena pyriformis -log(IGC50) M_Model_GPRFVS

Fri May 13 2011, 11:20

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	867	0.9188	0.2956
VAL	217	0.884	0.3746

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: 46

Model details:

Theta1: 38.87514877

Theta2: 30.56957245

Theta3: 0.1000000015

Descriptor	Length scale
Vx	805.2439
MW	1394.785
logP	33.70524
ERTLNoSPtPSA	561.0958
HBD-prof	17.7921
CH2Aa	49.4558
CH3Aa	26.98215
Ester	12.18628
HaloC	8.474995
aliphOH-t6	11.96614
anycarbonyl	22.50468
aromBr	9.218918
est-lact-latm-carbm-t7	11.66237
ether	7.766674
ketone-t14	7.781804
ketones	7.361299
lipovolume	66.25507
p-hetero-or-halo	26.03682
phenol	14.2498
sp-carbons	14.31972
sp2-carbons	22.37708
nC(sp3)	75.25906
nOH	17.12507
nCO	15.64916
nX	23.52065
tsC	11.91713
dssC	15.266
tN	7.215097
dS	5.920647
sCl	17.5811
sBr	11.82564
HAS	6.81604

HAT	25.75062
C4	10.02556
C10	8.337981
C6	13.69457
C3	22.94471
N6	13.07266
HydrophobicGroup	53.91481
H1a	17.65849
C5	18.07557
C23	16.51429
ew10	21.68972
f393	24.28039
f407	28.95544
Nn	15.13386