Session: Gombar_Hall_Suppl_Vdss, Model: log(VDss) GPFixed

Sun May 12 2013, 21:12

Data set: Gombar_Hall_Suppl_Vdss

Modeled property: log(VDss)

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	399	0.7338	0.3232
VAL	85	0.6174	0.3805
TEST	85	0.6405	0.3743

Parameters used:

Set split:

- Training set size: 70%
- Validation set size: 15%
- Clustering with tanimoto level: 0.7

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: 173

Descriptors used in the model: 173

Model details:

Theta1: 35.4431572

Theta2: 29.52980042

Theta3: 0.400000006

Descriptor	Length scale
logP	102.9964
Vx	3715.013
MW	5145.927
NegativeCharge	25.07148
PositiveCharge	74.01628
Flex	6.64795
AromaticRings	53.35299
OverallCharge	79.8783
ERTLNotPSA	2272.794
HBA-lip	132.8142
HBA-prof	110.9841
HBD-lip	83.51141
HBD-prof	60.22785
ACamideO-nh-nh2	21.68985
ACamideO-nh0	13.00158
ASamideO-nh-nh2	12.33989
AbasicNH0	16.50044
AbasicNH1	21.65365
CH0Aa	18.34335
CH1Aa	40.68374
CH2Aa	112.8592
CH2hetero	87.25342
CH2link	146.3043
CH3Aa	63.1274
CH3hetero	49.77417

CamideNH0	20.606
Ester	24.60976
HaloC	16.56054
NRB	363.5866
RCamideO-nh-nh2	17.89312
RCamideO-nh0	16.75829
RSR	18.19068
RbasicNH0	22.9366
aliphOH-t6	44.14641
allylic-oxyd-t10	36.48661
aminoethanol0	32.26052
aminoethanol1	29.39914
anycarbonyl	61.38792
aromCl	21.21123
aromF	21.80526
arylNHCO	10.33509
benzylicOH	15.76686
branchedCnotRing	43.12096
ch2-lipo-t9	21.29816
ertl-33	24.29828
ertl-35	34.98928
est-lact-latm-carbm-t7	29.05202
ether	50.56321
hydroxylation-t8	19.73316
intraHbond5	20.13192
intraHbond6	35.05497
ketone-t14	16.62567
ketones	12.02367
lipovolume	171.2842
nHindole-like	10.63925
nonring-at	245.3802
p-hetero-or-halo	36.82045
phenol	29.80543
phenolic-tautomer	19.41975
pyridine	14.98116
pyridones	17.96021
ring-join	56.79792
ring5-nH0	50.57906
ring5nH	14.24399
ringOdouble	35.70382
ringat	309.9764
sp2-carbons	97.03965
t-16-1	18.64588
tert-amine-t11	26.46362
xccn-t12	26.42011
nC(sp2)	243.5741
nC(sp3)	253.746
nOH	57.23996
nCO	45.73011
nOS	58.70393
nX	46.49143
nNprot	39.74052
ssCH2	154.2493
dsCH	41.04587
aaCH	160.8203
sssCH	110.2715
dssC	77.70074
aasC	111.3615
aaaC	68.25381
ssssC	38.88031
sNH2	33.01144
ssNH	39.02127
aaNH	17.88435

dsN	18.64588
aaN	61.34418
sssN	37.11749
sOH	64.08733
ssO	54.83237
sF	39.37302
sCl	24.32337
nNneutral	87.7691
NnH	54.43036
N4	20.35407
NbN	87.29097
fg5	14.58619
CamideNH	25.28539
BasicNH0R2AroRings	39.7278
BasicNH02AroRings	46.07642
BasicNH12AroRings	27.87628
PRX-time1	33.68
PRX-time-1	53.96241
UB	269.0899
HAS	25.07565
HAO	105.6745
AliRingAttachment	136.319
C12	17.9301
C4	99.06144
C10	38.5313
C6	58.83443
C3	101.1352
C8	21.99627
C1	149.9081
C11	23.24609
C2	62.92662
N6	21.85716
N7	32.04747
N8	17.47819
N2	33.7978
N1	29.14547
BasicGroup	46.0889
AcidGroup	46.57122
H4	26.16154
H2	60.80678
O3	42.03778
O11	15.24871
O5	21.19479
O9	52.28577
O10	23.63426
AroRingAttachment	141.5495
HydrophobicGroup	118.9498
C5	59.34446
C21	62.90667
C22	36.52815
C23	52.58594
C24	18.19068
S3	12.83155
ed70	45.58351
ed20	20.1475
ed40	41.26822
ed80	32.91203
ew75	15.05544
ew10	31.73045
ew100	23.9951
f004	86.24313
f007	58.13344
f015	43.94974

f244	154.7588
f301	210.7866
f393	54.63652
f407	110.8333
f440	97.35438
f441	156.771
f443	60.82914
f444	107.5276
q017	325.3761
q039	233.8803
q040	395.2505
q137	450.5138
q155	219.2079
q192	324.6213
q257	117.3179
q300	112.8864
q358	114.8648
q453	456.7432
q457	124.7325
q458	295.8939
frg-8	22.63135
frg-26	12.52496