Session: Gombar_Hall_Suppl_Vdss, Model: log(VDss) PLS

Mon May 13 2013, 10:54

Data set: Gombar_Hall_Suppl_Vdss

Modeled property: log(VDss)

Modeling technique: PLS

Model statistics:

	Number	Rsqr	RMSE
TRN	399	0.4261	0.4746
VAL	85	0.4198	0.4686
TEST	85	0.5173	0.4337

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:

Number of PLS components: 2

Cross-validation Qsqr: 0.3335

Descriptor	Coefficient	Scaled Coefficient
logP	0.008467	0.02643
Vx	7.368e-005	0.008295
MW	-5.917e-006	-0.0009226
NegativeCharge	-0.06881	-0.05227
PositiveCharge	0.003797	0.008515
Flex	-0.01834	-0.003694
AromaticRings	0.001955	0.003161
OverallCharge	0.01004	0.0243
ERTLNotPSA	-0.0004118	-0.02836
HBA-lip	-0.006436	-0.0259
HBA-prof	-0.004607	-0.01549
HBD-lip	-0.003123	-0.007903
HBD-prof	-0.001732	-0.00316
ACamideO-nh-nh2	-0.01051	-0.006906
ACamideO-nh0	-0.0356	-0.01402
ASamideO-nh-nh2	-0.04013	-0.01501
AbasicNH0	0.08945	0.04472
AbasicNH1	0.04472	0.02934
CH0Aa	0.002181	0.001212
CH1Aa	0.007999	0.009861
CH2Aa	0.003686	0.0126
CH2hetero	0.01138	0.0301
CH2link	0.004575	0.02028
CH3Aa	0.004919	0.00941
CH3hetero	0.00756	0.0114
CamideNH0	-0.0324	-0.02023
Ester	0.002188	0.001632

HaloC	0.01279	0.00642
NRB	0.001077	0.01187
RCamideO-nh-nh2	0.005736	0.00311
RCamideO-nh0	-0.02638	-0.01339
RSR	-0.01651	-0.009103
RbasicNH0	0.01169	0.008125
aliphOH-t6	0.0063	0.008428
allylic-oxyd-t10	0.004134	0.004571
aminoethanol0	-0.005633	-0.005507
aminoethanol1	0.004811	0.004286
anycarbonyl	-0.02535	-0.04715
aromCl	0.004253	0.002734
aromF	0.01146	0.007574
arylNHCO	-0.002237	-0.0007004
benzylicOH	0.01895	0.009053
branchedCnotRing	0.004358	0.005694
ch2-lipo-t9	0.02506	0.01617
ertl-33	-0.03395	-0.025
ertl-35	-0.02121	-0.02249
est-lact-latm-carbm-t7	0.001056	0.0009293
ether	0.00192	0.002942
hydroxylation-t8	0.008573	0.005126
intraHbond5	-0.01912	-0.01166
intraHbond6	0.001092	0.00116
ketone-t14	0.03073	0.01548
ketones	0.03283	0.01196
lipovolume	0.001873	0.009722
nHindole-like	0.01307	0.004215
nonring-at	-0.0009495	-0.00706
p-hetero-or-halo	0.01835	0.02047
phenol	-0.008414	-0.007599
phenolic-tautomer	-0.02716	-0.01598
pyridine	0.008717	0.003957
pyridones	-0.02073	-0.01128
ring-join	0.006407	0.01103
ring5-nH0	-0.007255	-0.01112
ring5nH	-0.0003852	-0.0001663
ringOdouble	-0.002849	-0.003082
ringat	0.0009917	0.009314
sp2-carbons	-0.005724	-0.01683
t-16-1	0.003725	0.002105
tert-amine-t11	0.04308	0.03454
xccn-t12	-0.0004084	-0.000327
nC(sp2)	0.0009034	0.006668
nC(sp3)	0.002713	0.02086
nOH	0.003677	0.006378
nCO	-0.008907	-0.01234
nOS	-0.002588	-0.004603
nX	0.00762	0.01074
nNprot	0.03325	0.04005
ssCH2	0.004784	0.02236
dsCH	-0.00503	-0.006257
aaCH	0.0008147	0.00397
sssCH	-0.0007994	-0.002671
dssC	-0.007136	-0.0168
aasC	0.001457	0.004917
aaaC	0.002339	0.004838
ssssC	0.02083	0.02454
sNH2	0.003665	0.003666
ssNH	0.006943	0.00821
aaNH	-0.01928	-0.01045
dsN	-0.01556	-0.008791
aaN	-0.00319	-0.00593

sssN	0.009967	0.01121
sOH	-0.008324	-0.01616
ssO	0.005743	0.009543
sF	0.01322	0.01577
sCl	-0.004774	-0.003519
nNneutral	-0.006384	-0.01698
NnH	0.004187	0.006906
N4	0.01115	0.006878
NbN	0.0004974	0.001316
fg5	0.05483	0.02424
CamideNH	-0.004977	-0.003814
BasicNH0R2AroRings	0.009567	0.01152
BasicNH02AroRings	0.02997	0.04184
BasicNH12AroRings	0.02948	0.0249
PRX-time1	-0.001492	-0.001522
PRX-time-1	-0.01459	-0.02386
UB	-0.00216	-0.01761
HAS	-0.01161	-0.008819
HAO	-0.01013	-0.03244
AliRingAttachment	5.463e-005	0.0002257
C12	0.03753	0.02039
C4	0.0006629	0.00199
C10	-0.0003992	-0.0004661
C6	-0.001602	-0.002856
C3	0.009661	0.02961
C8	-0.02782	-0.01855
C1	0.003048	0.01385
C11	0.01633	0.01151
C2	0.0005061	0.000965
N6	-0.01665	-0.01103
N7	0.018	0.01748
N8	0.007232	0.00383
N2	0.005211	0.005337
N1	0.003178	0.002806
BasicGroup	0.02315	0.03233
AcidGroup	-0.02597	-0.03665
H4	-0.06302	-0.04996
H2	0.002762	0.005088
O3	0.004165	0.005306
O11	-0.02235	-0.01033
O5	-0.01239	-0.007958
O9	-0.01492	-0.02363
O10	-0.01013	-0.007255
AroRingAttachment	0.00119	0.005102
HydrophobicGroup	-0.00144	-0.005192
C5	-0.01392	-0.02504
C21	0.006206	0.01183
C22	0.007893	0.008737
C23	-0.000823	-0.001311
C24	-0.03368	-0.01856
S3	-0.007752	-0.003014
ed70	-0.002064	-0.002851
ed20	-0.002675	-0.001633
ed40	0.005817	0.007274
ed80	-0.009021	-0.008997
ew75	-0.03785	-0.01727
ew10	0.00613	0.005894
ew100	-0.0133	-0.00967
f004	-0.001058	-0.002765
f007	-0.0005326	-0.0009382
f015	0.001837	0.002447
f244	-0.001022	-0.00479
f301	0.0003314	0.002117

f393	0.009874	0.01635
f407	0.002964	0.009955
f440	-0.004882	-0.0144
f441	-0.0003424	-0.001627
f443	-0.009994	-0.01842
f444	-0.0008704	-0.002836
q017	-0.0006304	-0.006215
q039	0.003205	0.02271
q040	0.00218	0.02611
q137	-0.0005317	-0.007258
q155	0.0007872	0.005229
q192	-0.001676	-0.01648
q257	-0.006042	-0.02148
q300	-0.004824	-0.0165
q358	-0.01056	-0.03676
q453	-0.0002748	-0.003804
q457	-0.002602	-0.009833
q458	0.0007722	0.006924
frg-8	-0.01114	-0.007642
frg-26	-0.01957	-0.007428
Free term	0.07964	