

Session: Gombar_Hall_Suppl_Vdss

Created: Fri May 10 2013, 20:09

Continuous model session

Data set: Gombar_Hall_Suppl_Vdss (569 compounds)

Modeled property: log(VDss)

Summary of model results

Model	Trn		Val		Test	
	Rsqr	RMSE	Rsqr	RMSE	Rsqr	RMSE
PLS Model	0.4261	0.4746	0.4198	0.4686	0.5173	0.4337
RBF Model	1	3.753e-06	0.6654	0.3558	0.6843	0.3507
Random Forest Regression Model	0.908	0.19	0.6233	0.3776	0.6347	0.3773
GPFixed	0.7338	0.3232	0.6174	0.3805	0.6405	0.3743
GP2DSearch	0.6233	0.3845	0.6164	0.381	0.6284	0.3805
GPRFVS	0.6213	0.3855	0.5039	0.4333	0.5796	0.4047
GPOPT	0.7294	0.3259	0.5662	0.4052	0.6661	0.3607

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

logP, Vx, MW, NegativeCharge, PositiveCharge, Flex, AromaticRings, OverallCharge, ERTLNotPSA, HBA-lip, HBA-prof, HBD-lip, HBD-prof, ACamideO-nh-nh2, ACamideO-nh0, ASamideO-nh-nh2, AbasicNH0, AbasicNH1, CH0Aa, CH1Aa, CH2Aa, CH2hetero, CH2link, CH3Aa, CH3hetero, CamideNH0, Ester, HaloC, NRB, RCamideO-nh-nh2, RCamideO-nh0, RSR, RbasicNH0, aliphOH-t6, allylic-oxyd-t10, aminoethanol0, aminoethanol1, anycarbonyl, aromCl, aromF, arylNHCO, benzylicOH, branchedCnotRing, ch2-lipo-t9, ertl-33, ertl-35, est-lact-latm-carbm-t7, ether, hydroxylation-t8, intraHbond5, intraHbond6, ketone-t14, ketones, lipovolume, nHindole-like, nonring-at, p-hetero-or-halo, phenol, phenolic-tautomer, pyridine, pyridones, ring-join, ring5-nH0, ring5nH, ringOdoube, ringat, sp2-carbons, t-16-1, tert-amine-t11, xccn-t12, nC(sp2), nC(sp3), nOH, nCO, nOS, nX, nNprot, ssCH2, dsCH, aaCH, sssCH, dssC, aasC, aaaC, sssC, sNH2, ssNH, aaNH, dsN, aaN, sssN, sOH, ssO, sF, sCl, nNneutral, NnH, N4, NbN, fg5, CamideNH, BasicNH0R2AroRings, BasicNH02AroRings, BasicNH12AroRings, PRX-time1, PRX-time-1, UB, HAS, HAO, AliRingAttachment, C12, C4, C10, C6, C3, C8, C1, C11, C2, N6, N7, N8, N2, N1, BasicGroup, AcidGroup, H4, H2, O3, O11, O5, O9, O10, AroRingAttachment, HydrophobicGroup, C5, C21, C22, C23, C24, S3, ed70, ed20, ed40, ed80, ew75, ew10, ew100, f004, f007, f015, f244, f301, f393, f407, f440, f441, f443, f444, q017, q039, q040, q137, q155, q192, q257, q300, q358, q453, q457, q458, frg-8, frg-26

Compound IDs for split sets for session Gombar_Hall_Suppl_Vdss

Training (399 compounds)

Gombar_Hall_Suppl_Vdss_0, Gombar_Hall_Suppl_Vdss_2, Gombar_Hall_Suppl_Vdss_3, Gombar_Hall_Suppl_Vdss_5, Gombar_Hall_Suppl_Vdss_6, Gombar_Hall_Suppl_Vdss_7, Gombar_Hall_Suppl_Vdss_8, Gombar_Hall_Suppl_Vdss_9, Gombar_Hall_Suppl_Vdss_12, Gombar_Hall_Suppl_Vdss_14, Gombar_Hall_Suppl_Vdss_15, Gombar_Hall_Suppl_Vdss_16, Gombar_Hall_Suppl_Vdss_17, Gombar_Hall_Suppl_Vdss_19, Gombar_Hall_Suppl_Vdss_20, Gombar_Hall_Suppl_Vdss_21, Gombar_Hall_Suppl_Vdss_22, Gombar_Hall_Suppl_Vdss_23, Gombar_Hall_Suppl_Vdss_24, Gombar_Hall_Suppl_Vdss_25, Gombar_Hall_Suppl_Vdss_26, Gombar_Hall_Suppl_Vdss_27, Gombar_Hall_Suppl_Vdss_29, Gombar_Hall_Suppl_Vdss_30, Gombar_Hall_Suppl_Vdss_32, Gombar_Hall_Suppl_Vdss_33, Gombar_Hall_Suppl_Vdss_34, Gombar_Hall_Suppl_Vdss_35, Gombar_Hall_Suppl_Vdss_36, Gombar_Hall_Suppl_Vdss_37, Gombar_Hall_Suppl_Vdss_39, Gombar_Hall_Suppl_Vdss_40, Gombar_Hall_Suppl_Vdss_42, Gombar_Hall_Suppl_Vdss_44, Gombar_Hall_Suppl_Vdss_48, Gombar_Hall_Suppl_Vdss_49, Gombar_Hall_Suppl_Vdss_50, Gombar_Hall_Suppl_Vdss_51, Gombar_Hall_Suppl_Vdss_52, Gombar_Hall_Suppl_Vdss_53, Gombar_Hall_Suppl_Vdss_54, Gombar_Hall_Suppl_Vdss_55, Gombar_Hall_Suppl_Vdss_57, Gombar_Hall_Suppl_Vdss_58, Gombar_Hall_Suppl_Vdss_59, Gombar_Hall_Suppl_Vdss_62, Gombar_Hall_Suppl_Vdss_63, Gombar_Hall_Suppl_Vdss_64, Gombar_Hall_Suppl_Vdss_67, Gombar_Hall_Suppl_Vdss_68, Gombar_Hall_Suppl_Vdss_70, Gombar_Hall_Suppl_Vdss_73, Gombar_Hall_Suppl_Vdss_74, Gombar_Hall_Suppl_Vdss_76, Gombar_Hall_Suppl_Vdss_77, Gombar_Hall_Suppl_Vdss_78, Gombar_Hall_Suppl_Vdss_80, Gombar_Hall_Suppl_Vdss_81, Gombar_Hall_Suppl_Vdss_83, Gombar_Hall_Suppl_Vdss_85,

[illegible]

