

Session: BBB_TrainingSet1

Created: Fri May 10 2013, 20:07

Classification model session

Training set: BBB_TrainingSet1 (1093 compounds)

Validation set: BBB_TestSet1 (499 compounds)

Test set: BBB_ExternalSet (246 compounds)

Modeled property: Class

Summary of model results

Model	Trn		Val		Test	
	Kappa	Accuracy	Kappa	Accuracy	Kappa	Accuracy
RF Classification	1	1	0.8506	0.976	0.2646	0.6992
DTModel1	0.7875	0.9286	0.7128	0.9579	0.05722	0.6423
DTModel2	0.745	0.9122	0.7189	0.9579	0.04643	0.6341
DTModel4	0.7814	0.9268	0.7128	0.9579	0.03039	0.6341
DTModel7	0.7172	0.9076	0.6137	0.9459	0.02524	0.626
DTModel8	0.7043	0.9039	0.5947	0.9439	-0.01494	0.6138
DTModel13	0.9351	0.9771	0.8257	0.9719	0.3242	0.7236
DTModel14	0.9433	0.9799	0.8257	0.9719	0.3737	0.7398
DTModel15	0.8918	0.9625	0.8366	0.9739	0.2409	0.6951
DTModel16	0.8927	0.9625	0.8644	0.978	0.158	0.6707
DTModel17	0.8472	0.9469	0.8008	0.9679	0.1385	0.6585
DTModel18	0.8668	0.9543	0.8114	0.9699	0.1385	0.6585
DTModel19	0.8838	0.9597	0.8257	0.9719	0.1744	0.6789
DTModel20	0.8972	0.9634	0.8187	0.9699	0.1832	0.6789

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: 172

logP, Vx, NegativeCharge, PositiveCharge, Flex, AromaticRings, ERTLNotPSA, HBA-prof, HBD-lip, HBD-prof, ACamideO-nh-nh2, AbasicNH0, AbasicNH1, CH0Aa, CH1Aa, CH2Aa, CH2hetero, CH2link, CH2long, CH3Aa, CH3hetero, CamideNH0, Ester, HaloC, Michael-accept, NRB, OHCHCdO, Ocarbamate, RCamideO-nh-nh2, RCamideO-nh0, RSR, RbasicNH0, aliphOH-t6, allylic-oxyd-t10, aminoethanol0, aminoethanol1, anycarbonyl, aromCl, aromF, basic-NH2, benzylicOH, branchedCnotRing, carbonate-carbamate, ch2-lipo-t9, di-widhrow-cx4, ertl-33, ertl-35, est-lact-latm-carbm-t7, ether, hydroxylation-t8, intraHbond5, intraHbond6, ketone-t14, ketones, lipovolume, nonring-at, p-hetero-or-halo, phenol, phenolic-tautomer, pyridine, ring-join, ring5-nH0, ring5nH, ringOdouble, ringat, sp2-carbons, spiroC, t-16-1, tert-amine-t11, urea-thio, xccn-t12, nC(sp2), nC(sp3), nOH, nCO, nOS, nX, nNprot, ssCH2, dsCH, aaCH, sssCH, dssC, aasC, aaC, sssC, sNH2, ssNH, aaNH, dsN, aaN, sssN, ssO, sF, dS, aaS, sCl, nNneutral, NnH, N4, NbN, fg5, CamideNH, BasicNH0R2AroRings, BasicNH02AroRings, BasicNH12AroRings, PRX-time1, PRX-time-1, UB, HAS, HAT, HAO, AliRingAttachment, C12, C4, C10, C6, C3, C8, C1, C11, C2, C26, N6, N7, N8, N2, N1, BasicGroup, AcidGroup, H4, O3, O11, O9, O10, AroRingAttachment, HydrophobicGroup, C5, C21, C22, C23, C24, S3, ed70, ed20, ed40, ed80, ew100, ew100, f004, f007, f015, f244, f301, f390, f407, f440, f441, f443, q017, q039, q040, q137, q192, q257, q300, q453, q457, q458, q481, frg-8, frg-26

Compound IDs for split sets for session BBB_TrainingSet1

Training (1093 compounds)

BBB_TrainingSet1_0, BBB_TrainingSet1_1, BBB_TrainingSet1_2, BBB_TrainingSet1_3, BBB_TrainingSet1_4, BBB_TrainingSet1_5, BBB_TrainingSet1_6, BBB_TrainingSet1_7, BBB_TrainingSet1_8, BBB_TrainingSet1_9, BBB_TrainingSet1_10, BBB_TrainingSet1_11, BBB_TrainingSet1_12, BBB_TrainingSet1_13, BBB_TrainingSet1_14, BBB_TrainingSet1_15, BBB_TrainingSet1_16, BBB_TrainingSet1_17, BBB_TrainingSet1_18, BBB_TrainingSet1_19, BBB_TrainingSet1_20, BBB_TrainingSet1_21, BBB_TrainingSet1_22, BBB_TrainingSet1_23, BBB_TrainingSet1_24, BBB_TrainingSet1_25, BBB_TrainingSet1_26, BBB_TrainingSet1_27, BBB_TrainingSet1_28, BBB_TrainingSet1_29, BBB_TrainingSet1_30, BBB_TrainingSet1_31, BBB_TrainingSet1_32, BBB_TrainingSet1_33, BBB_TrainingSet1_34, BBB_TrainingSet1_35, BBB_TrainingSet1_36, BBB_TrainingSet1_37, BBB_TrainingSet1_38, BBB_TrainingSet1_39, BBB_TrainingSet1_40, BBB_TrainingSet1_41, BBB_TrainingSet1_42, BBB_TrainingSet1_43, BBB_TrainingSet1_44, BBB_TrainingSet1_45, BBB_TrainingSet1_46, BBB_TrainingSet1_47, BBB_TrainingSet1_48, BBB_TrainingSet1_49, BBB_TrainingSet1_50, BBB_TrainingSet1_51,

[illegible]

[illegible]

[illegible]

Test (246 compounds)

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