

Session: Shen BBB Training Test and External merged

Created: Fri May 10 2013, 20:08

Classification model session

Data set: Shen BBB Training Test and External merged (1838 compounds)

Modeled property: Class

Summary of model results

	Trn		Val		Test	
Model	Kappa	Accuracy	Kappa	Accuracy	Kappa	Accuracy
RF Classification	0.9975	0.9992	0.8106	0.9309	0.8613	0.9455
DTModel1	0.6752	0.9154	0.6058	0.8655	0.7255	0.8945
DTModel2	0.6561	0.9107	0.6058	0.8655	0.7424	0.9018
DTModel4	0.6611	0.9107	0.6183	0.8691	0.7255	0.8945
DTModel5	0.6514	0.9092	0.6058	0.8655	0.7424	0.9018
DTModel7	0.5696	0.8936	0.4819	0.8327	0.6724	0.88
DTModel8	0.4518	0.8719	0.35	0.8	0.5426	0.84
DTModel10	0.5455	0.889	0.4678	0.8291	0.6382	0.8691
DTModel13	0.8534	0.9573	0.7876	0.92	0.8654	0.9455
DTModel14	0.8592	0.9589	0.7876	0.92	0.8569	0.9418
DTModel15	0.836	0.9534	0.7444	0.9055	0.8341	0.9345
DTModel16	0.8403	0.9534	0.7333	0.9018	0.8243	0.9309
DTModel17	0.7351	0.9286	0.7258	0.9018	0.8329	0.9345
DTModel18	0.7517	0.9325	0.7372	0.9055	0.8526	0.9418
DTModel19	0.8268	0.9503	0.7707	0.9164	0.9186	0.9673
DTModel20	0.7418	0.9301	0.6761	0.8873	0.8515	0.9418

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, NegativeCharge, PositiveCharge, Flex, AromaticRings, ERTLNotPSA, HBA-prof, HBD-lip, HBD-prof, ACamideO-nh-nh2, ACamideO-nh0, AbasicNH0, AbasicNH1, CH0Aa, CH1Aa, CH2Aa, CH2hetero, CH2link, CH2long, CH3Aa, CH3hetero, CamideNH0, Ester, HaloC, Michael-accept, NRB, 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-widhraw-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, ringOdoube, 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, aasN, 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, ew10, ew100, f004, f007, f015, f244, f245, 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 Shen BBB Training Test and External merged

Training (1288 compounds)

Shen BBB Training Test and External merged_0, Shen BBB Training Test and External merged_1, Shen BBB Training Test and External merged_2, Shen BBB Training Test and External merged_3, Shen BBB Training Test and External merged_4, Shen BBB Training Test and External merged_5, Shen BBB Training Test and External merged_7, Shen BBB Training Test and External merged_9, Shen BBB Training Test and External merged_10, Shen BBB Training Test and External merged_11, Shen BBB Training Test and External merged_12, Shen BBB Training Test and External merged_13, Shen BBB Training Test and External merged_14, Shen BBB Training Test and External merged_15, Shen BBB Training Test and External merged_16, Shen BBB Training Test and

merged_1821, Shen BBB Training Test and External merged_1823, Shen BBB Training Test and External merged_1825, Shen BBB Training Test and External merged_1826, Shen BBB Training Test and External merged_1829, Shen BBB Training Test and External merged_1830, Shen BBB Training Test and External merged_1831, Shen BBB Training Test and External merged_1832, Shen BBB Training Test and External merged_1833, Shen BBB Training Test and External merged_1834, Shen BBB Training Test and External merged_1837

[illegible]

[illegible][illegible]

[illegible]

Shen BBB Training Test and External merged_1591, Shen BBB Training Test and External merged_1598, Shen BBB Training Test and External merged_1600, Shen BBB Training Test and External merged_1602, Shen BBB Training Test and External merged_1616, Shen BBB Training Test and External merged_1617, Shen BBB Training Test and External merged_1633, Shen BBB Training Test and External merged_1634, Shen BBB Training Test and External merged_1637, Shen BBB Training Test and External merged_1642, Shen BBB Training Test and External merged_1653, Shen BBB Training Test and External merged_1654, Shen BBB Training Test and External merged_1660, Shen BBB Training Test and External merged_1671, Shen BBB Training Test and External merged_1673, Shen BBB Training Test and External merged_1686, Shen BBB Training Test and External merged_1688, Shen BBB Training Test and External merged_1690, Shen BBB Training Test and External merged_1692, Shen BBB Training Test and External merged_1695, Shen BBB Training Test and External merged_1712, Shen BBB Training Test and External merged_1717, Shen BBB Training Test and External merged_1718, Shen BBB Training Test and External merged_1739, Shen BBB Training Test and External merged_1767, Shen BBB Training Test and External merged_1771, Shen BBB Training Test and External merged_1778, Shen BBB Training Test and External merged_1788, Shen BBB Training Test and External merged_1792, Shen BBB Training Test and External merged_1796, Shen BBB Training Test and External merged_1800, Shen BBB Training Test and External merged_1804, Shen BBB Training Test and External merged_1812, Shen BBB Training Test and External merged_1815, Shen BBB Training Test and External merged_1822, Shen BBB Training Test and External merged_1827, Shen BBB Training Test and External merged_1835