

## Session: P-gp inhibitor classification\_2, Model: AMG\_P-gp inhibitor classification\_2\_Model\_RF Classification

Tue October 16 2012, 17:15

Data set: P-gp inhibitor classification no duplicates

Modeled property: Inhibitor

Modeling technique: Random Forests Classification

### Model statistics:

	Number	Kappa	Accuracy
TRN	134	1	1
VAL	28	0.8571	0.9286
TEST	28	0.7083	0.8571

### 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: 150

Descriptors used in the model: 150

### Model details:

Data was classified into 2 classes

- class Yes
- class No

### Confusion matrices

#### Training set

		Predicted	
		Yes	No
Observed	Yes	48	0
	No	0	86

- Sensitivity for Yes : 1
- Specificity for Yes : 1
- Sensitivity for No : 1
- Specificity for No : 1

#### Validation set

		Predicted	
		Yes	No
Observed	Yes	14	0
	No	2	12

- Sensitivity for Yes : 1
- Specificity for Yes : 0.875
- Sensitivity for No : 0.857
- Specificity for No : 1

#### Test set

		Predicted	
		Yes	No
Observed	Yes	10	2

- Sensitivity for Yes : 0.833
- Specificity for Yes : 0.833
- Sensitivity for No : 0.875
- Specificity for No : 0.875

Descriptor	Importance
logP	1
Vx	0.249919176
PositiveCharge	0
Flex	0.0237304773
AromaticRings	0.0450015888
ERTLNotPSA	0.0139460126
HBA-prof	0.00995961763
HBD-lip	-0.000385326974
HBD-prof	-0.00339103257
ACamideO-nh-nh2	0
ACamideO-nh0	0
AbasicNH0	0.00345827732
AbasicNH1	0.000858760788
CH0Aa	0.0033910356
CH1Aa	0.0148230335
CH2Aa	0.0597703755
CH2hetero	0.0370165668
CH2link	0.021009136
CH2long	0.00678206515
CH3Aa	0.0730108172
CH3hetero	0.44039309
CamideNH0	0.00357432663
Ester	0.0308637116
HaloC	0
NRB	-0.00498180417
RSR	-0.00367362029
RbasicNH0	0.0361640789
aliphOH-t6	-0.00565699814
allylic-oxyd-t10	0.0178414024
aminoethanol0	0.0381526798
aminoethanol1	0
anycarbonyl	0.128896043
aromCl	0.0220583286
aromO	0.00661251647
arylNHCO	0.0036736296
branchedCnotRing	-0.0127984341
ch2-lipo-t9	0.0105487984
di-widhraw-cx4	0
ertl-33	0
ether	0
hydroxylation-t8	0
intraHbond5	0
intraHbond6	-0.00367361843
ketone-t14	0.00629763352
ketones	0
lipovolume	0.267240167
nonring-at	0
ohccn-t17	0
p-hetero-or-halo	-0.00367361889
phenol	0
phenolic-tautomer	0.0803409591
pyridine	-0.0276459903
ring-join	0.0221862216
ring5-nH0	0.0250501353
ringOdouble	0.00734724756
ringat	0.0825938135

sp-carbons	0
sp2-carbons	0.016752366
spiroC	0
tert-amine-t11	0.0034802719
xccn-t12	0
nC(sp2)	0.119990826
nOH	0
nOS	0.0468123555
nX	0.0153836617
nNprot	-0.00857722759
ssCH2	0
dsCH	-0.0116250105
aaCH	0.0459716767
sssCH	0.0344491228
dssC	0.0170721076
aasC	0.0165684782
aaaC	0.0481471345
ssssC	0
ssNH	-0.0128051881
aaN	0.0200745538
sssN	0.0261669308
sF	0
sCl	0
nNneutral	0.00678206515
N4	0
NbN	0.0369307399
fg5	0.00314881676
CamideNH	0.0187055171
BasicNH0R2AroRings	0
BasicNH12AroRings	0
PRX-time1	-0.0132250385
PRX-time-1	0.00367361889
UB	0.150159791
HAS	0
HAT	-0.00502617564
HAO	0.00734724384
AliRingAttachment	-0.00426614098
C12	0
C4	0.022108689
C10	0.0149683198
C6	0.00552797224
C3	0
C8	0
C1	0.0294711459
C11	0.0491000079
C2	0.0112369685
C26	-0.00367361982
N6	0.078870751
N7	0.0135783814
N8	0
N2	-0.00734723825
BasicGroup	-0.00710008759
H2	0.00400758768
O3	0.0136664379
O9	0.034029685
O10	0.00348027027
AroRingAttachment	0
C25	0
HydrophobicGroup	0
C5	0.00867740624
C21	0.0463651456
C22	0
C23	0.0141183902

C24	0
S3	0
ed70	0.022967644
ed20	0
ed80	0.00348027027
ew10	0
ew100	0.0673689917
f004	0.0225702412
f007	0.0316910408
f015	0.0689511448
f244	0.0509829633
f245	0.00456036674
f301	0.01361515
f390	0.00283960439
f407	0.218383029
f440	-0.000242223978
f441	0.213564336
q017	0.0949956551
q039	0.172642961
q040	0.0711385608
q137	0.296550959
q139	0.0104177902
q192	0.0397921912
q257	0.207820207
q300	0.104043923
q453	0.0791292861
q457	0.00346594979
q458	-0.00426614098
q481	0.0382633768
frg-8	-0.0116691515
frg-26	0