

## Session: Nordquist CACO2\_training\_set\_5

Created: Sun October 14 2012, 14:12

Continuous model session

Training set: Nordquist CACO2\_training\_set (77 compounds)

Validation set: Nordquist CACO2\_test\_set (23 compounds)

Modeled property: caco2

### Summary of model results

Model	Trn		Val		Test	
	Rsqr	RMSE	Rsqr	RMSE	Rsqr	RMSE
PLS Model	0.468	0.5446	0.6556	0.4995		
RBF Model	1	2.258e-06	0.4487	0.6319		
RBF Model (no GA)	1	2.258e-06	0.4487	0.6319		
Random Forest	0.907	0.2277	0.6456	0.5067		
Regression Model						
GPFixed	0.6389	0.4487	0.6335	0.5152		
GP2DSearch	0.6155	0.463	0.6479	0.505		
GPFVS	0.6019	0.4711	0.6554	0.4996		
GPRFVS	0.6102	0.4662	0.6528	0.5015		
GPOPT	0.879	0.2597	0.07416	0.8189		
GPNEST	0.5522	0.4996	0.6446	0.5074		

### 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: 10

logP, Vx, HBD-prof, OverallCharge, HBA-prof, Flex, AromaticRings, NegativeCharge, ERTLNotPSA, PositiveCharge

### Compound IDs for split sets for session Nordquist CACO2\_training\_set\_5

Training (77 compounds)

acebutolol, acebutolol\_ester, acetylsalicylic\_acid, acyclovir, alprenolol, alprenolol\_ester, aminopyrine, artemisinin, artesunate, atenolol, betazolol, betazolol\_ester, bremazocine, caffeine, chloramphenicol, chlorothiazide, chlorpromazine, cimetidine, clonidine, corticosterone, desipramine, dexamethasone, dexamethasone\_b\_D\_glucoside, dexamethasone\_b\_D\_glucuronide, diazepam, dopamine, doxorubicin, erythromycin, estradiol, felodipine, ganciclovir, griseofulvin, hydrochlorothiazide, hydrocortisone, ibuprofen, imipramine, indomethacin, labetalol, mannitol, meloxicam, methanol, methotrexate, methylscopolamine, metoprolol, nadolol, naproxen, nevirapine, nicotine, olsalazine, oxprenolol, oxprenolol\_ester, phencyclidine, phenytoin, pindolol, pirenzepine, piroxicam, pnu200603, practolol, prazocin, progesterone, propranolol, propranolol\_ester, quinidine, ranitidine, salicylic\_acid, scopolamine, sucrose, sulphasalazine, telmisartan, terbutaline, tesosterone, timolol, timolol\_ester, uracil, urea, warfarin, zidovudine

Validation (23 compounds)

furosemide, guanabenz, fleroxacin, mibefradil, verapamil, guanoxan, saquinavir, lidocaine, enalapril, theophylline, cyclosporine, antipyrine, proscillaridin, coumarin, nitrendipine, epinephrine, tiacrilast, amoxicillin, diltiazem, remikren, sulpiride, bosentan, ceftriaxone