Session: Nordquist CACO2_training_set_5, Model: Caco2_log(Papp)_PLS

Sun October 14 2012, 21:29

Modeled property: caco2

Modeling technique: PLS

Model statistics:

	Number	Rsqr	RMSE
TRN	77	0.468	0.5446
VAL	23	0.6556	0.4995

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

Descriptors used in the model: 10

Model details:

Number of PLS components: 1

Cross-validation Qsqr: 0.3951

Descriptor	Coefficient	Scaled Coefficient
logP	0.08507	0.206
Vx	-0.0002965	-0.03121
HBD-prof	-0.09251	-0.2013
OverallCharge	-0.03839	-0.06782
HBA-prof	-0.03575	-0.1226
Flex	-0.1763	-0.035
AromaticRings	0.004036	0.005401
NegativeCharge	-0.1346	-0.07908
ERTLNotPSA	-0.00389	-0.24
PositiveCharge	-0.05323	-0.09407
Free term	-4.504	