

## Session: Fathead minnow -log(LC50) M, Model: AMG\_Fathead minnow -log(LC50) M\_Model\_GP2DSearch

Fri May 13 2011, 18:35

Modeled property: Tox

Modeling technique: Gaussian Processes

### Model statistics:

	Number	Rsqr	RMSE
TRN	652	0.8136	0.6435
VAL	164	0.6895	0.8114

### 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: 134

Descriptors used in the model: 134

### Model details:

Theta1: 48.7586441

Theta2: 38.08057404

Theta3: 0.5

Descriptor	Length scale
Vx	2525.004
MW	4029.793
PositiveCharge	33.75692
Flex	10.06039
AromaticRings	34.34966
logP	75.73994
OverallCharge	35.70981
ERTLNotPSA	1283.47
ERTLNoSPtPSA	1460.835
HBA-lip	98.70586
HBA-prof	69.15967
HBD-lip	43.34851
HBD-prof	29.15959
CH0Aa	11.66684
CH1Aa	19.45386
CH2Aa	83.3073
CH2hetero	58.64545
CH2link	107.8358
CH2long	70.7915
CH3Aa	53.46551
CH3hetero	31.54849
Ester	19.6313
HaloC	37.9715
NO	30.43041
NRB	200.8763
Pester	35.12154
RSR	14.46659
aldehydes	10.7549
aliphOH-t6	20.17391
allylic-oxyd-t10	28.67882
anycarbonyl	36.21817
aromCl	38.71242

branchedCnotRing	26.68095
dNO	25.78726
di-widhraw-cx4	35.27367
ertl-33	14.95334
est-lact-latm-carbm-t7	19.49432
ether	26.37831
intraHbond6	14.46659
ketone-t14	12.09539
lipovolume	130.7914
nonring-at	185.5626
p-hetero-or-halo	49.63956
phenol	18.64687
ringat	203.9229
sp-carbons	20.95007
sp2-carbons	54.84709
t-16-1	12.52218
nC(sp2)	188.2472
nC(sp3)	151.5827
nOH	26.73618
nCO	28.03731
nOS	49.90424
nX	71.31271
nNprot	19.28343
ssCH2	111.5215
dsCH	26.85908
aaCH	131.9322
sssCH	40.27164
tsC	15.04091
dssC	34.66475
aasC	78.9574
ssssC	35.70521
sNH2	18.41956
ssNH	15.73629
tN	10.67783
aaN	17.78262
sssN	19.48395
sOH	38.00216
ssO	44.48507
dS	11.60607
sCl	66.43625
nNneutral	48.37963
NnH	24.66186
NbN	49.78379
PRX-time1	35.29313
PRX-time-1	17.93943
UB	211.8735
HAN	41.89671
HAS	21.56
HAT	76.57531
HAO	64.27838
AliRingAttachment	50.54588
C12	10.98194
C4	43.00051
C10	14.82033
C6	43.6557
C3	64.92988
C8	19.68731
C1	118.2002
C2	32.6869
N6	27.87134
N7	18.36065
H3	29.23779
N1	14.04475

BasicGroup	22.40142
O3	37.63586
O9	23.83952
O10	18.89872
HydrophobicGroup	95.04674
H1a	51.02529
C5	30.6774
C21	34.94774
C22	31.40446
C23	31.5713
ed70	25.04154
ed20	24.43965
ed40	22.36407
ew10	41.32617
f004	60.50668
f007	47.91086
f244	105.8263
f390	139.0324
f393	116.7841
f407	68.28796
f413	32.51989
f440	75.40916
f441	96.01089
f443	50.31506
f444	68.64661
f456	49.18521
q017	233.7695
q039	133.3763
q040	156.4088
q137	302.5348
q192	122.9128
q257	80.94999
q300	49.96043
q358	82.23692
q453	235.6689
q457	54.59448
q458	166.023
frg-8	17.08862
Nn	39.72323