

RMSE

2.5
2.0
1.5
1.0
0.5
0.0

Quinoline
4Iodophenol
Amylobarbitone
Chlorpromazine
Phenobarbitone
4Methoxyphenol
4Ethoxyphenol
Butobarbitone
4Pentoxyphenol
Pentobarbitone
34Dichlorophenol
4Butoxyphenol
Sulfamethazine
4Propoxyphenol
rPropanolol
4Chlorophenol
35Dichlorophenol
3Chlorophenol
3Bromoquinoline
Quinalbarbitone
Phenol
Benzoicacid
NMethylaniline
Ketoprofen
Celiprolol
Acebutolol
Pericyazine

Molecule ID

