

RMSE

3.0
2.5
2.0
1.5
1.0
0.5
0.0

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

Molecule ID

