

RMSE

3.0  
2.5  
2.0  
1.5  
1.0  
0.5  
0.0

4Iodophenol  
Chlorpromazine  
Quinoline  
Amylobarbitone  
3,4-Dichlorophenol  
Phenobarbitone  
4-Pentoxifyphenol  
3,5-Dichlorophenol  
Butobarbitone  
Pentobarbitone  
4-Ethoxyphenol  
4-Methoxyphenol  
r-Prananolol  
4-Butoxyphenol  
Sulfamethazine  
4-Propoxyphenol  
4-Chlorophenol  
Quinalbarbitone  
3-Chlorophenol  
3-Bromoquinoline  
Phenol  
Benzoic acid  
Ketoprofen  
N-Methylaniline  
Celiprolol  
Acebutolol  
Pericyazine

Molecule ID

