

RMSE

5

4

3

2

1

0

NMethylaniline

Quinalbarbitone

4Iodophenol

Pentobarbitone

Phenol

Ketoprofen

3Chlorophenol

Phenobarbitone

Amylobarbitone

Butobarbitone

4Propoxyphenol

4Pentoxyphenol

35Dichlorophenol

Quinoline

4Chlorophenol

34Dichlorophenol

4Ethoxyphenol

4Methoxyphenol

3Bromoquinoline

Sulfamethazine

4Butoxyphenol

Benzoicacid

rPropanolol

Chlorpromazine

Pericyazine

Acebutolol

Celiprolol

Molecule ID

