

RMSE

4

3

2

1

0

NMethylaniline

Phenol

Quinalbarbitone

Pentobarbitone

4Iodophenol

Ketoprofen

Quinoline

Amylobarbitone

Butobarbitone

Phenobarbitone

3Chlorophenol

4Propoxyphenol

4Pentoxyphenol

4Chlorophenol

35Dichlorophenol

4Ethoxyphenol

4Methoxyphenol

34Dichlorophenol

3Bromoquinoline

Sulfamethazine

4Butoxyphenol

Benzoicacid

Chlorpromazine

rPropranolol

Pericyazine

Acebutolol

Celiprolol

Molecule ID

