

Challenges Predicting Ligand-Receptor Interactions of Promiscuous Proteins:

The Nuclear Receptor PXR

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Table S4 – CoMFA Test Set Predictions

	Observed. Activity	Predicted Activity
Androstenedione	4.69	5.06
11-Ketoetiocholanone	4.39	5.19
Epitestosterone sulfate	5.47	3.97
5 α -Androstane	2.00	5.71
4,16-Androstadien-3-one	5.15	5.38
Corticosterone	5.00	4.82
Cortisone	4.16	2.92
Pregnenolone	5.64	3.42
Pregnanediol glucuronide	4.26	4.64
17 α ,20 β -Dihydroxyprogesterone	2.00	5.35
Dexamethasone	4.39	5.23
Chenodeoxycholic acid	2.00	4.08
Glycodeoxycholic acid	2.00	3.13
Taurocholic acid	2.00	2.06
5 β -cholestan-3 α ,7 α ,12 α ,-triol	2.00	2.94
23-Nordeoxycholic acid	4.79	4.55
Petromyzonol sulfate	4.55	1.41
Scymnol – sulfated	4.31	2.70
Taurolithocholic acid 3-sulfate, disodium salt	4.08	5.14
α -Cholestanol	2.00	3.50