

Challenges Predicting Ligand-Receptor Interactions of Promiscuous Proteins:

The Nuclear Receptor PXR

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Table S7. Test set predictions for CoMFA ($R^2 = 0.11$) and CoMSIA ($R^2 = 0.04$) models (Bold = outliers).

Compound	Experimental Activity	Predicted Activity (CoMFA)	Predicted Activity (CoMSIA)
ANDROSTANES			
Androstenedione	4.69	4.84	4.74
11-Ketoetiocholanone	4.39	5.38	5.17
Epitestosterone sulfate	5.47	4.17	3.95
5 α -Androstane	2.00	5.49	5.85
4,16-Androstadien-3-one	5.15	5.87	5.84
PREGNANES			
Corticosterone	5.00	4.56	4.48
Cortisone	4.16	5.17	4.81
Pregnenolone	5.64	5.13	5.08
Pregnanediol glucuronide	4.26	2.42	2.24
17 α ,20 β -Dihydroxyprogesterone	2.00	5.57	5.15
Dexamethasone	4.39	3.69	3.82
BILE ACIDS / SALTS			
Chenodeoxycholic acid	2.00	4.02	4.27
Glycodeoxycholic acid	2.00	2.95	3.67
Taurocholic acid	2.00	2.35	1.92
5 β -cholestan-3 α ,7 α ,12 α ,-triol	2.00	2.00	2.58
23-Nordeoxycholic acid	4.79	4.66	4.03
Petromyzonol sulfate	4.55	2.26	2.14
Scymnol – sulfated	4.31	2.55	2.21
Taurolithocholic acid 3-sulfate, disodium salt	4.08	4.26	4.02
α -Cholestanol	2.00	2.04	2.58