Challenges Predicting Ligand-Receptor Interactions of Promiscuous Proteins: The Nuclear Receptor PXR

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Table S8. Best model training set correlation (r) values and model statistics (total cost and null cost) for Catalyst Hypogen hypotheses.

Compounds	Without excluded volumes	2 excluded volumes	Variable weight/tolerance	2 excluded volumes and variable weight/ tolerance
Bile Acids	0.65 (302.4 – 371.9)	0.79 (272.5-371.9)	0.71 (314.0-371.9)	0.81 (294.5-371.9)
Estratrienes	0.84 (73.9-82.8)	0.86 (66.9-82.8)	0.84 (96.3-82.8)	0.92 (89.5-82.8)
Androstanes	0.75 (127.7-149.2)	0.75 (127.7-149.2)	0.83 (141.7-149.2)	0.83 (141.7-149.2)
Pregnanes	0.62 (150.2-159.6)	0.81 (141.9-159.6)	0.83 (159.2-159.6)	0.92 (153 – 159.6)