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

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Table S1. Molecular descriptors for PXR crystal structure ligands calculated with Discovery Studio ver 2.1 (Accelrys, San Diego, CA). MWT = molecular weight, Rotl Bonds = number of rotatable bonds, HBA = hydrogen bond acceptor, HBD = hydrogen bond donor, Polar surface area = polar surface area.

Compound	ALogP	MWT	Rotl. Bonds	Num_Rings	Num_Aromatic Rings	HBA	HBD	PSA
Estradiol	3.84	272.38	0	4	1	2	2	40.46
T1317	4.84	491.41	8	2	0	3	1	65.99
Colupulone	6.03	400.55	8	1	0	4	2	74.60
Hyperforin	10.11	542.83	13	1	0	4	1	71.44
Rifampicin	3.55	713.81	3	4	1	12	6	201.30
SR12813	4.89	504.53	13	1	1	7	1	110.91
Mean	5.54	487.59	7.50	2.17	0.50	5.33	2.17	94.12
SD	2.41	147.25	5.24	1.47	0.55	3.67	1.94	57.16