

Supplementary material

Table 1: Selected compounds eHiTS scores from 8 of the 10 ER α structures evaluated.

Ligand being Docked	Minimum eHiTS Score	PDB ID 2OUZ	PDB ID 1R5K	PDB ID 1SJO	PDB ID 1XP1	PDB ID 1XP6	PDB ID 1XP9	PDB ID 1XPC	PDB ID 1YIM
Active 1 (9803972)	-14.589	-12.931	-12.958	-14.589	-14.508	-13.462	-13.559	-14.422	-13.391
Active 2 (9894892)	-13.343	-12.247	-12.755	-13.173	-13.067	-13.257	-12.168	-13.343	-12.84
Active 4 (4859)	-13.596	-12.369	-12.813	-12.634	-13.596	-12.279	-12.12	-13.029	-12.109
Active 7 (8461628)	-9.82	-9.26	-9.128	-9.82	-9.366	-9.385	-9.484	-9.722	-9.313
Decoy 4 (9372960)	-9.243	-8.684	-8.199	-9.102	-9.243	-8.6	-8.641	-8.777	-8.522
Decoy 7 (9418926)	-9.341	-7.746	-8.681	-8.873	-9.341	-8.465	-7.961	-8.262	-8.313
Decoy 9 (9328424)	-10.638	-9.518	-10.015	-10.638	-9.458	-9.19	-9.026	-10.183	-9.549
Decoy 20 (9462726)	-7.024	-6.588	-6.821	-7.024	-6.729	-6.593	-6.391	-6.766	-6.592
MFC00796283	-13.083	-13.083	-10.02	-8.962	-10.758	-5.356	-10.694	-7.684	-9.578
MFC00795212	-12.774	-9.476	-12.414	-12.557	-11.543	-11.943	-10.81	-11.593	-12.774
MFC00191781	-13.416	-9.457	-9.013	-13.416	-9.583	-7.516	-9.646	-12.771	-9.079
MFC02684954	-13.012	-9.687	-11.756	-13.012	-12.547	-10.776	-10.993	-11.509	-12.322
MFC00965302	-12.955	-10.857	-11.074	-12.955	-10.94	-10.287	-11.82	-11.844	-11.498
MFC00051886	-12.915	-10.577	-11.87	-12.915	-12.362	-9.905	-10.54	-12.486	-11.679
MFC00043160	-12.902	-9.177	-10.19	-12.783	-12.902	-11.309	-10.206	-11.99	-9.333
MFC01096622	-12.772	-10.559	-11.523	-12.772	-8.96	-11.31	-9.385	-9.878	-8.093
MFC02684953	-12.781	-10.535	-11.235	-12.742	-12.781	-11.561	-12.246	-12.129	-11.577
MFC00031658	-12.695	-9.256	-10.872	-12.695	-10.831	-9.682	-9.283	-12.322	-10.187
MFC00159395	-12.675	-9.884	-10.112	-12.675	-11.434	-9.817	-9.661	-11.035	-11.593
MFC01325781	-12.521	-9.91	-9.897	-12.521	-10.466	-10.987	-9.863	-11.21	-10.288
MFC00031643	-12.702	-11.152	-10.992	-11.621	-12.702	-10.851	-10.588	-11.524	-10.453
MFC00228673	-12.662	-9.476	-11.026	-11.752	-9.162	-10.722	-8.669	-12.662	-9.809
MFC00226703	-12.523	-11.384	-10.4	-11.818	-9.822	-10.214	-9.743	-12.523	-10.747
TPP/Lasofixifene Hybrid	-14.119	-14.119	----	-13.018	----	----	----	-5.566	----

Included are the top three scoring actives screened, the lowest scoring active screened, the top three scoring decoys screened, the lowest scoring decoy screened (all identified by their ChemSpider ID number – www.chemspider.com), all TPP cations screened which scored better than -12 on at least one ER α structure (identified by the MDL number for their corresponding commercially available salt form), and the TPP/Lasofixifene hybrid seen in **Figure 1f**.