

## Supplementary material:

**Table 1:** Interaction properties of compounds found predicted to bind with FSH

LIGANDS	G SCORE	HYDROGEN BONDING	RESIDUES INVOLVED IN H BONDS
<b>STANDARD LIGANDS</b>			
Estradiol	-5.4	-1.2	GLN 123
Centchroman	-3.8	0.0	LYS 46, TYR 88
Levonogestral	-4.2	-0.9	LYS 46, GLN 123
<b>ZINC DATABASE LIGANDS</b>			
ZINC00193616	-9.1	-1.4	ASP 36, LYS 46, THR 86
ZINC03294620	-9.2	-1.9	THR 86, GLN 48, TYR 65, GLN 123
ZINC13598214	-8.7	-1.7	THR 86, GLN 48, LYS 46, TYR 65
ZINC02497690	-6.8	-1.9	LYS 46, GLU 77, GLN 123

**Table 2:** ADME parameters calculated for the Zinc Database compounds

Molecule	CNS	MW (g/mol)	HB		QPlog Po/w	QPlogS	QPPCac o	QPlogBB	% Human Oral Absorption	Rule Of Five
			Donor	Acceptor						
ZINC00193616	0	279.341	4	3.5	2.385	-2.677	238.533	-0.373	83.466	0
ZINC03294620	-2	389.41	2.25	6.25	3.317	-5.521	199.795	-1.568	87.545	0
ZINC13598214	-2	350.373	1.25	6.25	3.019	-4.89	337.653	-1.304	89.875	0
ZINC01834978	1	230.309	1	2.5	2.765	-2.751	365.645	-0.233	89.012	0
ZINC02497690	0	279.341	4	3.5	2.35	-2.667	208.848	-0.428	82.226	0