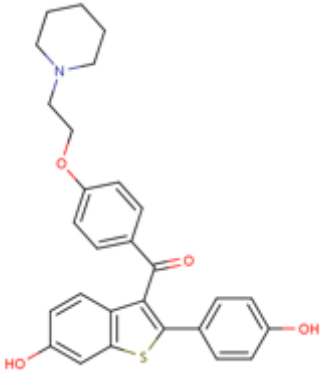
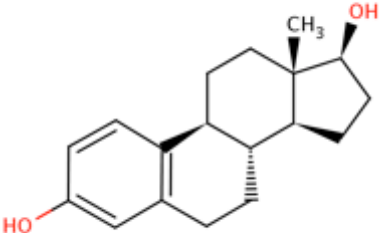
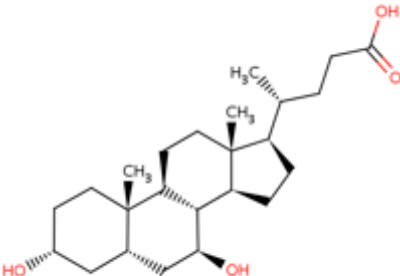
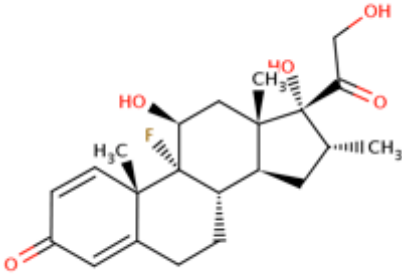
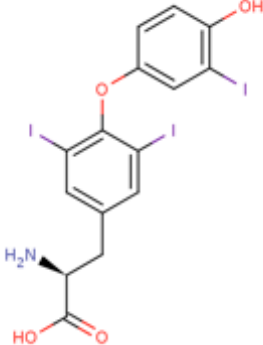
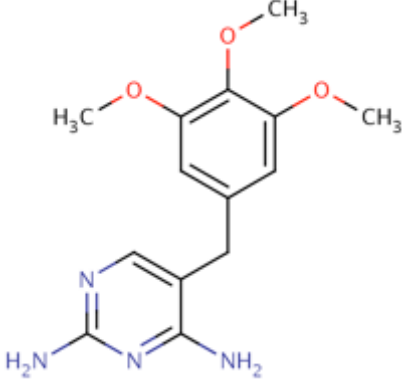
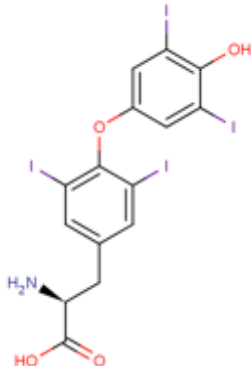
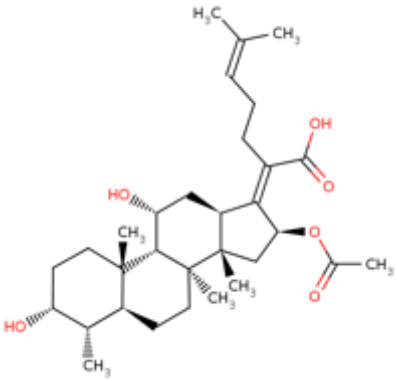
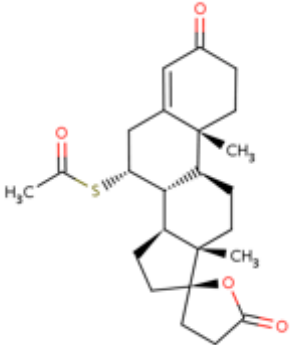


**Table S2 – Drugs predicted to bind PhzB2**

ID	Name	Structure	SMAP p-value	Glide Score
RAL	Raloxifene: Estrogen agonist	 <p>The chemical structure of Raloxifene consists of a central thiophene ring. At the 2-position of the thiophene ring, there is a 4-hydroxyphenyl group. At the 3-position, there is a 4-(2-(pyrrolidin-1-yl)ethoxy)phenyl group. At the 4-position, there is a 5-hydroxy-1H-benzofuran-2-yl group.</p>	2.65e-05	-6.04
EST	Estradiol: Steroid hormone	 <p>The chemical structure of Estradiol is a steroid nucleus with a phenolic A ring. It features a hydroxyl group at C3, a methyl group at C10, and a methyl group and a hydroxyl group at C13. The D ring is saturated, and the E ring is a five-membered ring with a methyl group at C14.</p>	7.06e-07	-5.79
JN3	Chenodeoxycholic acid: Cholagogues and Choloretics	 <p>The chemical structure of Chenodeoxycholic acid is a steroid nucleus with a hydroxyl group at C3 and a methyl group at C10. It has a methyl group at C13 and a methyl group and a hydroxyl group at C14. At C17, there is a propionic acid side chain.</p>	7.08e-05	-5.57

DEX	Dexamethasone: Glucocorticoid steroid drug	 <p>The image shows the chemical structure of Dexamethasone, a synthetic glucocorticoid. It features a four-ring steroid nucleus with a ketone group at C3, a double bond between C4 and C5, a methyl group at C10, a fluorine atom at C9, and a methyl group at C13. At C17, there is a side chain consisting of a methyl group, a hydroxyl group, and a 2-hydroxyethyl group.</p>	3.45e-05	-5.29
T3	3,5,3'-Triiodothyronine: Peptide hormone agonist	 <p>The image shows the chemical structure of 3,5,3'-Triiodothyronine (T3). It consists of a tyrosine derivative where the phenolic ring is substituted with three iodine atoms at the 3, 5, and 3' positions. The tyrosine side chain is shown with a primary amine group and a carboxylic acid group.</p>	2.36e-05	-5.25
TOP	Trimethoprim: Folic acid antagonist; anti-infective agent	 <p>The image shows the chemical structure of Trimethoprim. It features a pyrimidine ring with amino groups at the 2 and 4 positions, connected via a methylene bridge to a benzene ring. The benzene ring is substituted with three methoxy groups at the 3, 4, and 5 positions.</p>	3.63e-05	-4.96
T44	3,5,3',5'-Tetraiodo-L- thyronine: Peptide hormone	 <p>The image shows the chemical structure of 3,5,3',5'-Tetraiodo-L-thyronine (T44). It is similar to T3 but has an additional iodine atom at the 5' position of the phenolic ring, resulting in four iodine atoms in total.</p>	2.18e-05	-4.52

FUA	Fusidic acid: Antibacterial agent; protein synthesis inhibitor	 <p>The chemical structure of Fusidic acid is a complex polycyclic molecule. It features a pentacyclic steroid-like core with several methyl groups (CH<sub>3</sub>) and hydroxyl groups (OH) attached. A long side chain is attached to the core, ending in a carboxylic acid group (COOH) and a methyl group (CH<sub>3</sub>).</p>	3.24e-05	-4.32
SNL	Spironalactone: aldosterone (steroid) agonist	 <p>The chemical structure of Spironalactone is a steroid derivative. It features a pentacyclic core with a ketone group (C=O) at the 3-position and a methyl group (CH<sub>3</sub>) at the 13-position. A side chain is attached to the core, ending in a sulfur atom (S) bonded to a methyl group (CH<sub>3</sub>).</p>	9.86e-05	-4.52

The Glide score estimates the protein-ligand binding affinity for each drug predicted to bind to PhzB2. The more negative the score, the greater the predicted ability to interact.