In Silico ADME Prediction and Molecular Docking of 1,2,3-Triazole-based Compounds Against Human Aromatase Cytochrome P450

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Table S1. Violations to medicinal chemistry rules and bioavailability score.

Molecule	Number of Violations to Rules					Bioavailability Score
	Lipinski	Ghose	Veber	Egan	Muegge	
Letrozole	0	0	0	0	0	0.55
Anastrozole	0	0	0	0	0	0.55
Compound 1	0	0	0	0	0	0.55
Compound 2	0	0	0	0	0	0.55
Compound 3	0	0	0	0	0	0.55
Compound 4	0	0	0	0	0	0.55
Compound 5	0	0	0	0	0	0.55
Compound 6	0	0	0	0	0	0.55
Compound 7	0	0	0	0	0	0.55
Compound 8	2	2	1	1	2	0.17
Compound 9	0	0	0	0	0	0.55
Compound 10	0	0	0	0	0	0.55
Compound 11	0	0	0	0	0	0.55

Table S2. Select pharmacokinetic properties.

Molecule	GI Absorption	BBB Permeant	P-gp Substrate	CYP1A2 Inhibitor	CYP2C19 Inhibitor	CYP2C9 Inhibitor	CYP2D6 Inhibitor	CYP3A4 Inhibitor
Letrozole	High	Yes	No	Yes	Yes	Yes	Yes	No
Anastrozole	High	Yes	No	No	No	Yes	No	No
Compound 1	High	Yes	No	Yes	Yes	Yes	No	No
Compound 2	High	Yes	No	Yes	Yes	Yes	No	No
Compound 3	High	Yes	No	Yes	Yes	Yes	No	No
Compound 4	High	No	No	No	No	Yes	No	Yes
Compound 5	High	No	No	No	No	Yes	No	Yes
Compound 6	High	No	No	No	No	Yes	No	Yes
Compound 7	High	No	No	No	No	Yes	No	Yes
Compound 8	Low	No	No	No	Yes	No	No	No
Compound 9	High	Yes	No	Yes	Yes	No	No	No
Compound 10	High	No	No	Yes	No	No	No	No
Compound 11	High	Yes	No	Yes	Yes	Yes	No	No

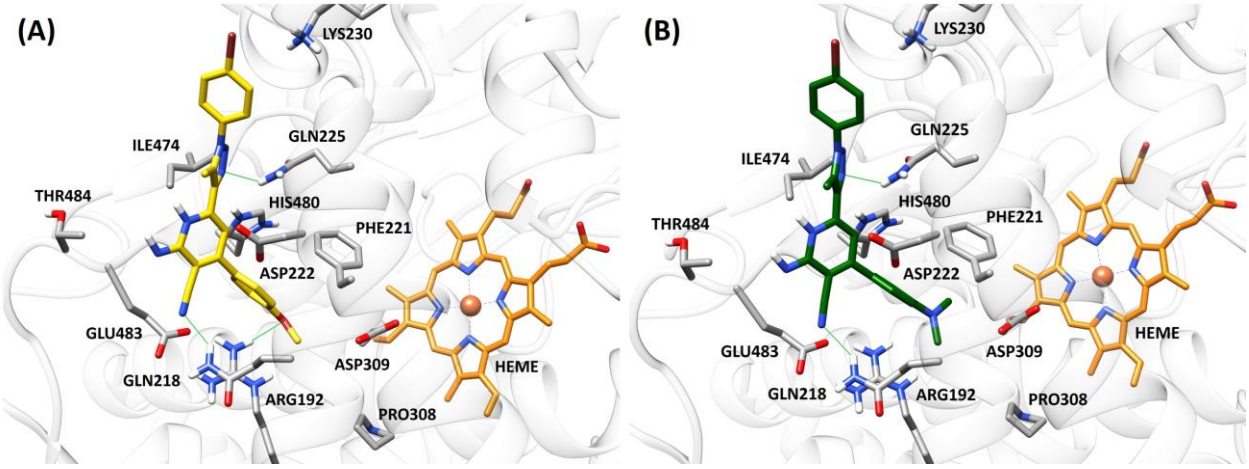

Figure S1. Docked poses of **(A)** compound **6** and **(B)** compound **7** in the potential allosteric site 1 of the enzyme.

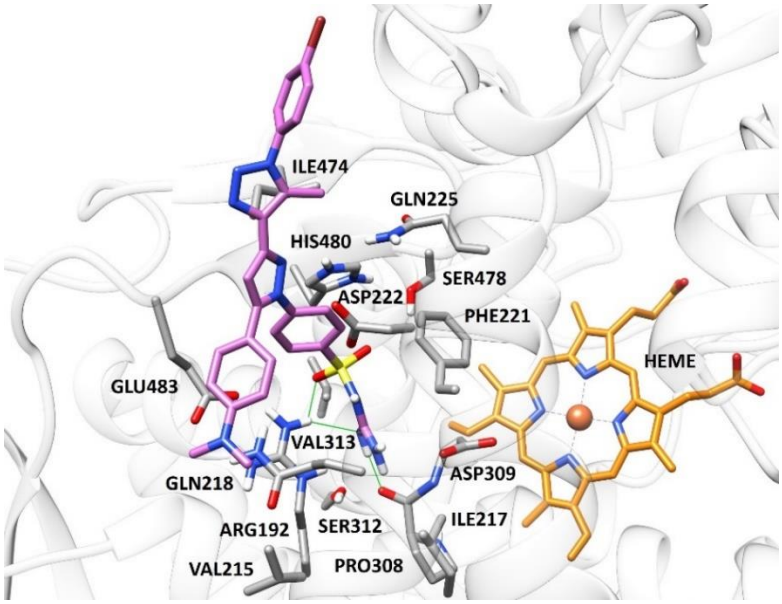

Figure S2. Compound **8** in the allosteric site 1 of the enzyme.

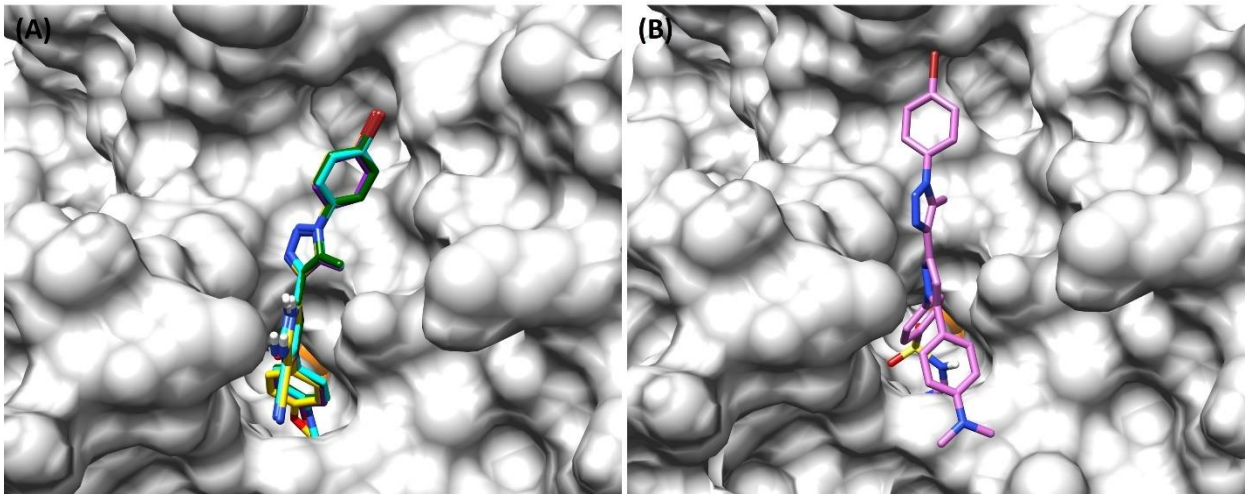

Figure S3. Potential allosteric site 1 of the enzyme with bound ligands: **(A)** Overlaid compounds **4** (purple), **5** (cyan), **6** (gold), and **7** (forest green). **(B)** Compound **8** (orchid).

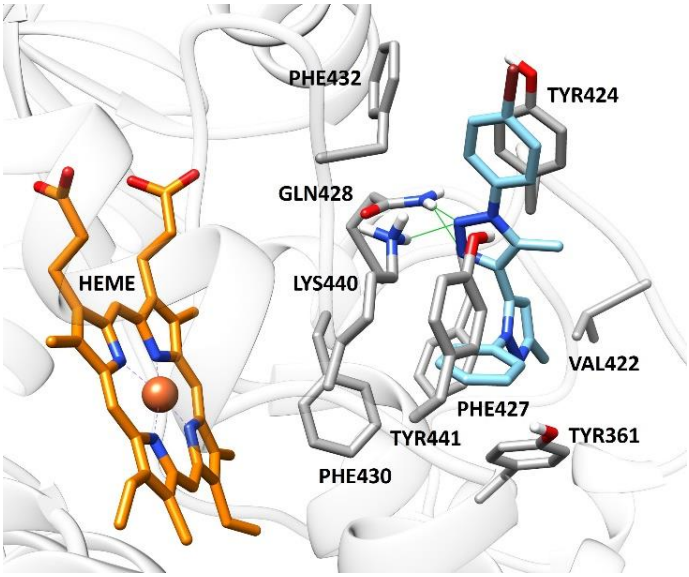

Figure S4. Compound **11** in the allosteric site 2 of the enzyme.

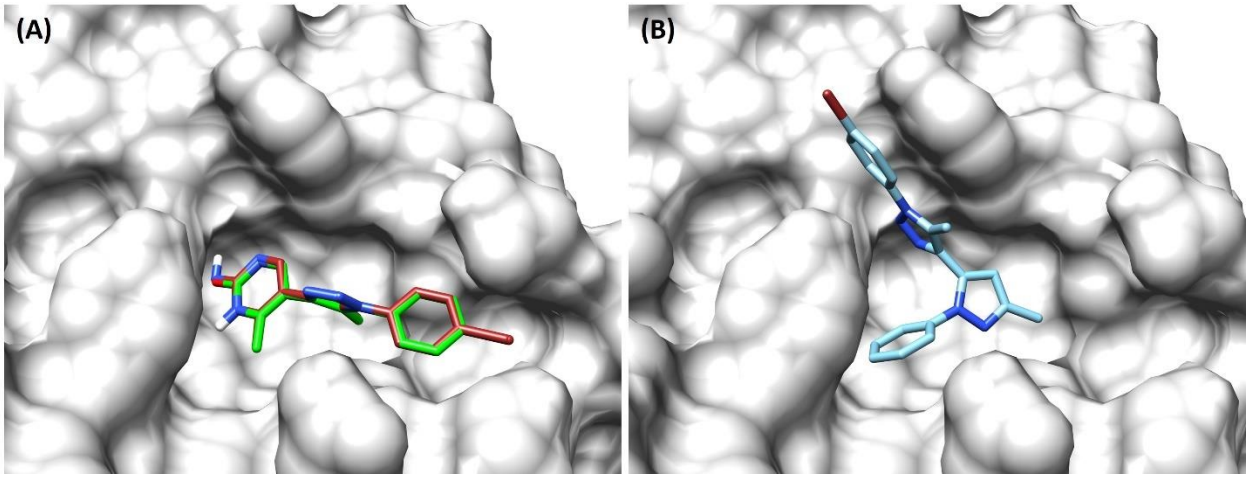

Figure S5. Potential allosteric site 2 of the enzyme with bound ligands: **(A)** Overlaid compounds **9** (green) and **10** (brown). **(B)** Compound **11** (sky blue).