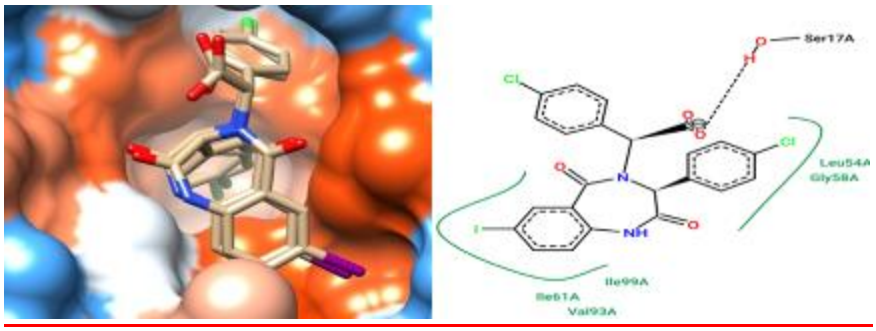
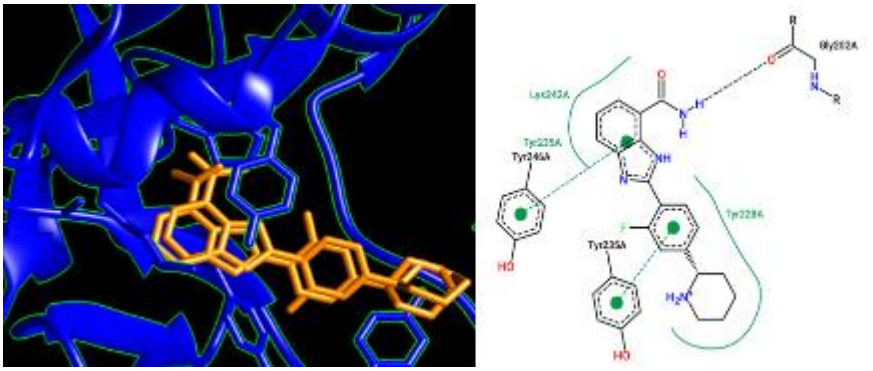


Appendix 1: Comparison of two bound conformations of DI-Chloro-benzo-diazepine the 3L3M active site: the left photo shows the crystal orientation and the redocked result. Chemical structure on the right side of 2-{2-fluoro-4-[(2S)-piperidin-2-yl] phenyl}-1.



Appendix 2: Comparison of two bound conformations of 2-{2-fluoro-4-[(2S)-piperidin-2-yl] phenyl}-1H-benzimidazole-7-carboxamidein the 3L3M active site: the left photo shows the crystal orientation and the redocked result. The Right The structure of 2-{2-fluoro-4-[(2S)-piperidin-2-yl] phenyl}-1.

Appendix 3: Molecule properties, drug likeness and ADMET of *Ergosta-14, 22-don-3-ol, (3β.5α, 22E).*

Property	Model Name	Predicted Value	Unit
Molecule properties	Molecular Weight	398.675	g/mol
	LogP	7.4107	
	Rotatable Bonds	4	
	Acceptors	1	
	Donors	1	
	Surface Area	179.984	$Å^2$
Drug likeness	Lipinski	Yes	1 violation: MLOGP>4.15
	Ghose	No	2 violations: WLOGP>5.6, atoms>70
	Veber	Yes	
	Egan	No	1 violation: WLOGP>5.88
	Muegge	No	2 violations: XLOGP3>5, Heteroatoms<2
	Bioavailability Score	0.55	
Absorption	Water solubility	-6.853	Numeric (log mol/L)
	Caco2 permeability	1.229	Numeric (log Papp in 10^{-6} cm/s)
	Intestinal absorption (human)	95.641	Numeric (% Absorbed)
	P-glycoprotein substrate	No	Categorical (Yes/No)
	P-glycoprotein I inhibitor	Yes	Categorical (Yes/No)
	P-glycoprotein II inhibitor	Yes	Categorical (Yes/No)
Distribution	VDss (human)	0.339	Numeric (log L/kg)
	Fraction unbound (human)	0	Numeric (Fu)

	BBB permeability	0.765	Numeric (log BB)
	CNS permeability	-1.765	Numeric (log PS)
Metabolism	CYP2D6 substrate	No	Categorical (Yes/No)
	CYP3A4 substrate	Yes	Categorical (Yes/No)
	CYP1A2 inhibitior	No	Categorical (Yes/No)
	CYP2C19 inhibitior	No	Categorical (Yes/No)
	CYP2C9 inhibitior	No	Categorical (Yes/No)
	CYP2D6 inhibitior	No	Categorical (Yes/No)
	CYP3A4 inhibitior	No	Categorical (Yes/No)
Excretion	Total Clearance	0.565	Numeric (log ml/min/kg)
	Renal OCT2 substrate	No	Categorical (Yes/No)
Toxicity	AMES toxicity	No	Categorical (Yes/No)
	Max. tolerated dose (human)	-0.561	Numeric (log mg/kg/day)
	hERG I inhibitor	No	Categorical (Yes/No)
	hERG II inhibitor	Yes	Categorical (Yes/No)
	Oral Rat Acute Toxicity (LD50)	2.16	Numeric (mol/kg)
	Oral Rat Chronic Toxicity (LOAEL)	0.904	Numeric (log mg/kg_bw/day)
	Hepatotoxicity	No	Categorical (Yes/No)
	Skin Sensitisation	No	Categorical (Yes/No)
	T.Pyriformis toxicity	0.567	Numeric (log ug/L)
	Minnow toxicity	-1.684	Numeric (log mM)