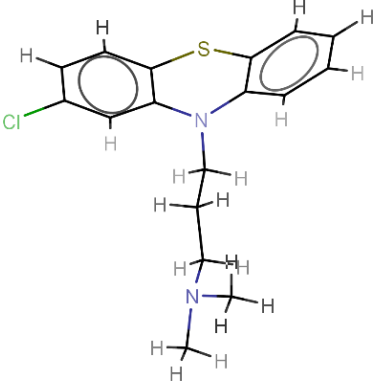
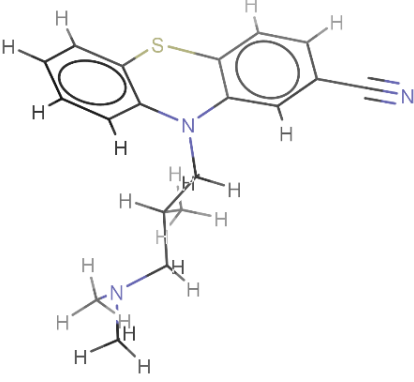
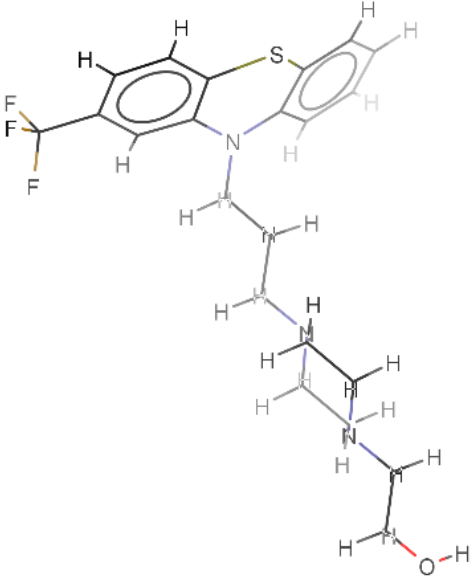
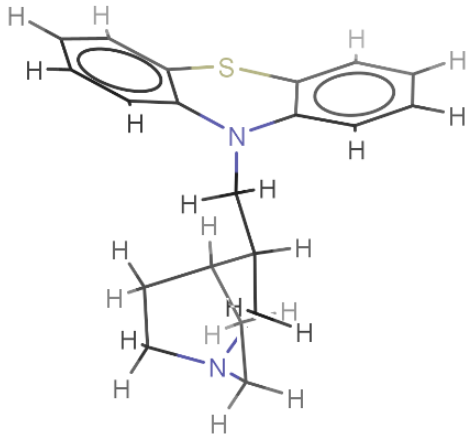


Modele de calcul și baze de date ale activităților biologice ale fenotiazinelor și fotoprodușilor identificați ai flufenazinei

Structurile chimice ale derivaților de fenotiazină și ale fotoprodușilor identificați din literatură ai flufenazinei ¹

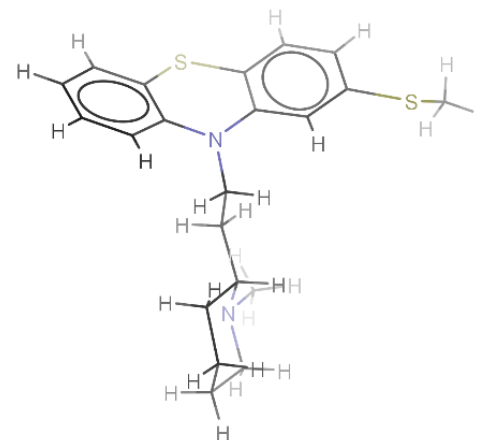
compus	SMILES	Structură chimică 3D optimizată
clorpromazină (CPZ)	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)Cl</chem>	
ciamemazină (CYA)	<chem>CC(CN1C2=CC=CC=C2SC3=C1C=C(C=C3)C#N)CN(C)C</chem>	

flufenazină (FLU)	<chem>C1CN(CCN1CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F)C(=O)O</chem>	
mequitazină (MEQ)	<chem>C1CN2CCC1C(C2)CN3C4=CC=CC=C4SC5=CC=CC=C53</chem>	

<p>levomepromazină (LEV)</p>	<chem>CC(CN1C2=CC=CC=C2SC3=C1C=C(C=C3)OC)CN(C)C</chem>	 <p>The structure shows a tricyclic core consisting of two benzene rings fused to a five-membered ring containing a sulfur atom and a nitrogen atom. One of the benzene rings has a methylamino group (-NH₂) attached. The central nitrogen atom is also bonded to a propylamine side chain (-CH₂-CH₂-CH₂-NH₂).</p>
<p>proclorperazină (PCPZ)</p>	<chem>CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)Cl</chem>	 <p>The structure is similar to levomepromazine but features a chlorine atom on the benzene ring that is fused to the five-membered ring. The side chain is a propylamine group (-CH₂-CH₂-CH₂-NH₂).</p>

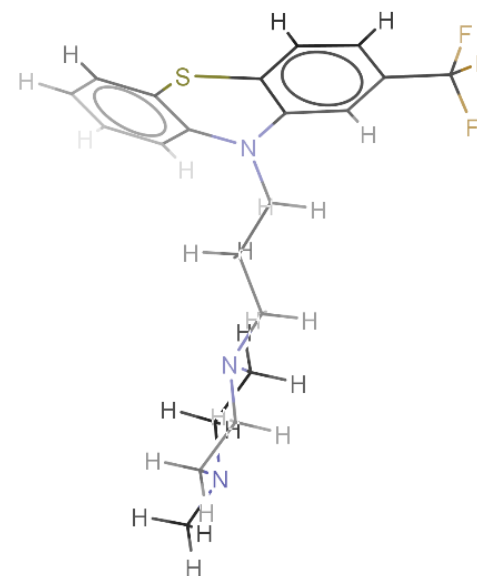
tioridazină (TZ)

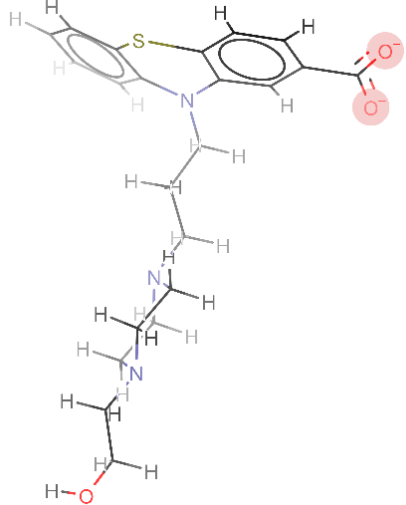
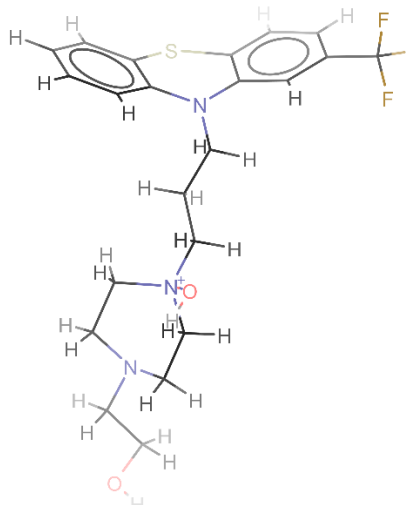
CN1CCCC1CCN2C3=CC=CC=C3SC4=C2C=C(C=C4)SC



trifluoperazină (TFPZ)

CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F



Fotoprodus	SMILES	Structură chimică 3D optimizată
F1	<chem>S1c2c(N(c3c1cccc3)CCC[NH+]1CCN(CC1)CCO)cc(cc2)C(=O)[O-]</chem>	
F2	<chem>S1c2c(N(c3c1cccc3)CCC[N+]1(O)CCN(CC1)CCO)cc(cc2)C(F)(F)F</chem>	

Cele mai mici energii de legare prezise utilizând andocarea moleculară pentru derivații de fenotiazină și fotoprodușii identificați ai FLU, F1 și F2 în interacție cu țintele terapeutice evaluate.

țintă	PDB	CPZ (kcal/mol)	CYA (kcal/mol)	FLU (kcal/mol)	F1 (kcal/mol)	F2 (kcal/mol)	MEQ (kcal/mol)	LEV (kcal/mol)	PCPZ (kcal/mol)	TZ (kcal/mol)	TFZ (kcal/mol)
RE α	3ERT	-9.26	-10.23	-12.24	-12.24	12.34	-10.62	-9.95	-10.51	-10.59	-10.97
RA	1E3G	-10.37	-11.17	-13.60	-14.13	-13.29	-10.54	-10.57	-12.37	-11.63	-12.63
TII	5GWK	-7.00	-8.07	-8.56	-9.37	-8.21	-7.65	-7.35	-8.34	-7.98	-8.50
RP	4OAR	-8.78	-9.75	-11.51	-11.83	-11.32	-9.01	-10.07	-10.30	-9.79	-10.60
CDK2	2FVD	-8.44	-8.98	-10.23	-11.02	-10.60	-9.08	-9.59	-9.59	-9.25	-9.95
EGFR	3W2S	-8.50	-8.78	-11.19	-11.61	-10.86	-9.08	-8.88	-9.77	-9.22	-10.13
HER-2	3PP0	-8.97	-9.36	-11.56	-13.53	-12.16	-10.25	-10.10	-11.66	-10.44	-11.74
PI3K	1E8Z	-8.85	-8.99	-11.29	-11.91	-11.29	-9.42	-9.00	-10.95	-10.13	-11.27
p38 α	1YQJ	-9.22	-9.81	-11.73	-12.28	-12.38	-9.60	-9.36	-10.77	-10.51	-11.28
BCL-2	6o0k	-8.13	-8.66	-10.04	-10.60	-10.31	-9.02	-8.26	-8.99	-8.93	-9.37

Țintele terapeutice:

receptorul de estrogen alpha uman =RE α

receptorul androgen =RA

topoisomeraza II = TII

receptorul de progesterone =RP

receptorul al factorului de creștere epidermal =EGFR

phosphoinositide 3-kinase =PI

Referințe

- (1) Trawiński, J.; Skibiński, R. Studies on Photodegradation Process of Psychotropic Drugs: A Review. *Environ Sci Pollut Res Int* **2017**, *24* (2), 1152–1199.
<https://doi.org/10.1007/s11356-016-7727-5>.