

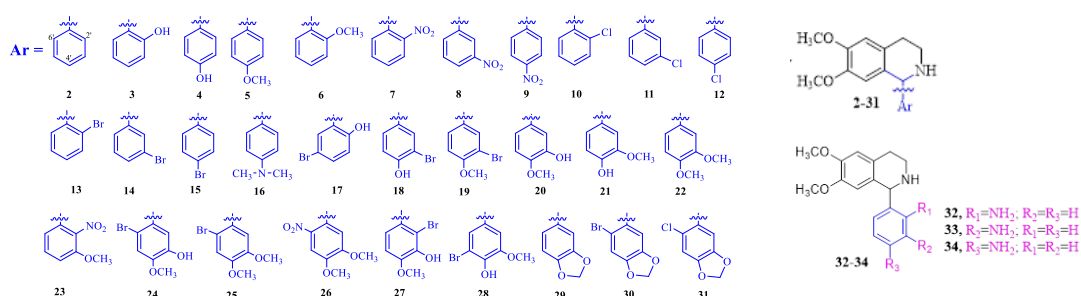
POSTER PRESENTATIONS

ANTI-ALCOHOL POTENTIAL OF 1-ARYL-6,7-DIMETHOXY-1,2,3,4-TETRAHYDROISOQUINOLINE DERIVATIVES: *IN SILICO* MODELING OF INTERACTION WITH ADH ORTHOSTERIC SITES

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Alcohol dehydrogenase (ADH) is an enzyme involved in ethanol metabolism by catalyzing its oxidation to acetaldehyde. The interaction of 34 derivatives of 1,2,3,4-tetrahydroisoquinoline with the orthosteric sites of alcohol dehydrogenase (PDB ID: 1HDX) were investigated *in silico*.



According to molecular docking results, the investigated ligands exhibited high binding affinity (ΔG) toward the orthosteric sites of alcohol dehydrogenase (PDB ID: 1HDX), forming specific and stable complexes via a non-competitive mechanism.

Molecular docking results of ligands with alcohol dehydrogenase enzyme (1HDX)

Ligands	ΔG (kcal/mol)	Ligands	ΔG (kcal/mol)	Ligands	ΔG (kcal/mol)	Ligands	ΔG (kcal/mol)
Cytisine	-6.5	9	-7.0	18	-6.7	27	-6.8
Ethanol	-2.5	10	-6.9	19	-6.9	28	-7.4
2	-7.0	11	-6.9	20	-7.0	29	-7.5
3	-6.8	12	-7.2	21	-6.8	30	-6.9
4	-7.0	13	-7.4	22	-7.0	31	-7.3
5	-6.7	14	-7.1	23	-6.8	32	-6.8
6	-7.0	15	-7.4	24	-6.6	33	-6.8
7	-6.9	16	-6.7	25	-6.5	34	-7.5
8	-7.6	17	-7.4	26	-7.0		

These *in silico* findings fundamentally support the ligands' capacity to influence ADH conformational stability, thereby modulating the neurotoxic and systemic pharmacological impacts of alcohol at the hepatocyte level.

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