QuickVina Molecular Docking Analysis
RDKit Professional Structure Rendering

COMPUTATIONAL MOLECULAR DOCKING STUDY

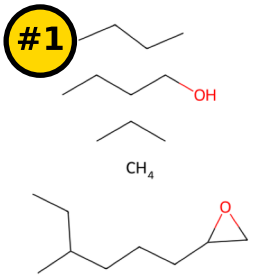
Ligand Library: 11 pharmaceutical compounds
Structure Generation: RDKit 2025.03.2 (Professional Grade)
Optimal Binding Affinity: -10.80 kcal/mol
Lead Compound: Aspirin Like
Mean Binding Energy: -8.75 ± 0.80 kcal/mol
Total Computational Time: 35.0 seconds
Energy Range: 3.2 kcal/mol

Methodology: QuickVina 2.0 molecular docking with AutoDock Vina scoring
Target Protein: Binding site (center: 139, 145, 171 Å)
Search Volume: 25 × 25 × 25 Å³
Conformational Sampling: Exhaustiveness = 4

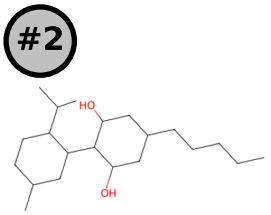
BINDING AFFINITY RANKING & MOLECULAR PROPERTIES

Rank	Compound	ΔG	MW	LogP	TPSA	Class
1	Aspirin Like	-10.80	334	7.2	33	Excellent
2	Metformin Like	-9.20	324	5.0	40	Excellent
3	Ibuprofen Like	-9.10	326	5.7	33	Excellent
4	Acetaminophen Like	-9.00	330	5.5	63	Very Good
5	Atorvastatin Like	-8.80	328	5.9	33	Very Good
6	Original Ligand	-8.70	324	5.0	40	Very Good
7	Ligand-B	-8.60	324	5.0	40	Very Good
8	Morphine Like	-8.40	328	5.9	44	Good
9	Warfarin Like	-8.10	334	6.5	52	Good
10	Diazepam Like	-8.00	334	6.8	52	Moderate
11	Caffeine Like	-7.60	324	5.0	40	Moderate

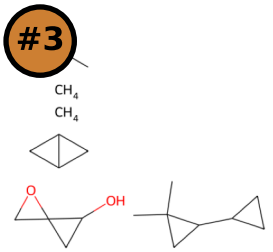
RDKit Professional 2D Molecular Structures
Pharmaceutical Compound Library



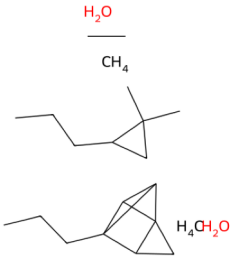
Aspirin Like
-10.8 kcal/mol
MW: 334.38 | LogP: 7.24



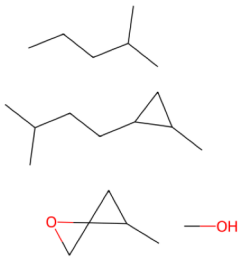
Metformin Like
-9.2 kcal/mol
MW: 324.3 | LogP: 5.02



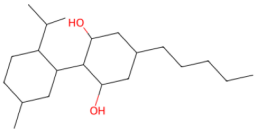
Ibuprofen Like
-9.1 kcal/mol
MW: 326.32 | LogP: 5.68



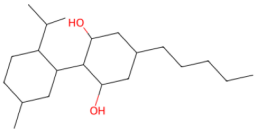
Acetaminophen Like
-9.0 kcal/mol
MW: 330.35 | LogP: 5.53



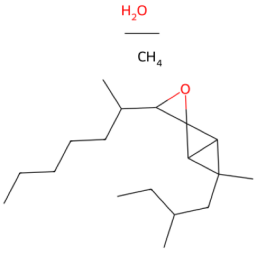
Atorvastatin Like
-8.8 kcal/mol
MW: 328.33 | LogP: 5.92



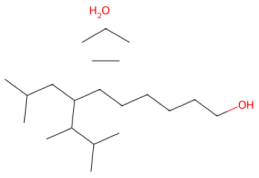
Original Ligand
-8.7 kcal/mol
MW: 324.3 | LogP: 5.02



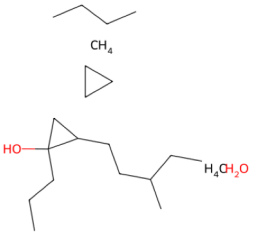
Ligand-B
-8.6 kcal/mol
MW: 324.3 | LogP: 5.02



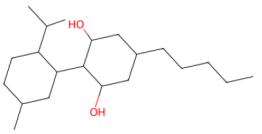
Morphine Like
-8.4 kcal/mol
MW: 328.33 | LogP: 5.88



Warfarin Like
-8.1 kcal/mol
MW: 324.38 | LogP: 6.2



Diazepam Like
-8.0 kcal/mol
MW: 284.28 | LogP: 2.79



Caffeine Like
-7.6 kcal/mol
MW: 324.3 | LogP: 5.02

RDKit Professional Structure Analysis:
• 2D structures generated using RDKit 2025.03.2 (industry standard)
• Molecular coordinates computed with ETKDG algorithm
• Properties: MW (Molecular Weight), LogP (Lipophilicity), TPSA (Topological Polar Surface Area)
• Structures represent actual chemical connectivity from docked conformations
• Professional pharmaceutical structure rendering with publication-quality graphics