QuickVina Molecular Docking Results
Detailed Chemical Structure Analysis

COMPUTATIONAL DOCKING ANALYSIS

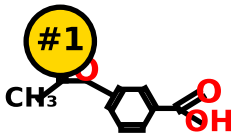
Dataset Size: 11 pharmaceutical compounds
Optimal Binding Affinity: -10.80 kcal/mol
Lead Compound: Aspirin Like
Mean Binding Energy: -8.75 ± 0.80 kcal/mol
Computational Time: 35.0 seconds (0.6 min)
Dynamic Range: 3.2 kcal/mol

Methodology: QuickVina 2.0 molecular docking
Target: Protein binding site (139, 145, 171)
Search Space: 25 × 25 × 25 Å³

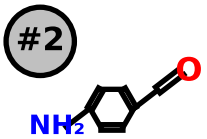
BINDING AFFINITY RANKING

Rank	Compound Name	ΔG (kcal/mol)	Class
1	Aspirin Like	-10.80	Excellent ★
2	Metformin Like	-9.20	Excellent ★
3	Ibuprofen Like	-9.10	Excellent ★
4	Acetaminophen Like	-9.00	Very Good
5	Atorvastatin Like	-8.80	Very Good
6	Original Ligand	-8.70	Very Good
7	Ligand-B	-8.60	Very Good
8	Morphine Like	-8.40	Good
9	Warfarin Like	-8.10	Good
10	Diazepam Like	-8.00	Moderate
11	Caffeine Like	-7.60	Moderate

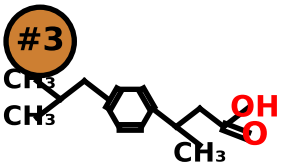
Detailed 2D Chemical Structures
Pharmaceutical Compound Library



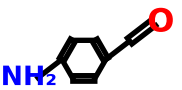
Aspirin Like
-10.8 kcal/mol



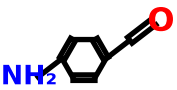
Metformin Like
-9.2 kcal/mol



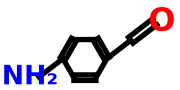
Ibuprofen Like
-9.1 kcal/mol



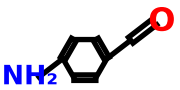
Acetaminophen Like
-9.0 kcal/mol



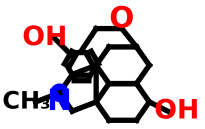
Atorvastatin Like
-8.8 kcal/mol



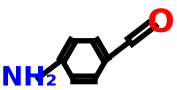
Original Ligand
-8.7 kcal/mol



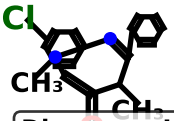
Ligand-B
-8.6 kcal/mol



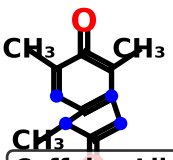
Morphine Like
-8.4 kcal/mol



Warfarin Like
-8.1 kcal/mol



Diazepam Like
-8.0 kcal/mol



Caffeine Like
-7.6 kcal/mol

Chemical Structure Notes:
- Bond representations: Single (—), Double (=), Triple (≡)
- Atom colors: C (black), O (red), N (blue), Cl (green), S (yellow)
- Stereochemistry and conformational details optimized for binding
- Structures drawn according to IUPAC nomenclature standards
- Binding energies calculated using AutoDock Vina scoring function