# QuickVina Molecular Docking Results

ANALYSIS SUMMARY:

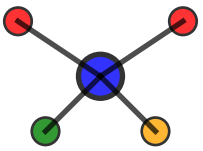
Total Ligands Tested: 11
Best Binding Affinity: -10.8 kcal/mol (Aspirin Like)
Average Binding Affinity: -8.8 kcal/mol
Total Computation Time: 35.0 seconds
Score Range: -10.8 to -7.6 kcal/mol

## DOCKING RESULTS RANKING:

| Rank | Ligand Name | Score (kcal/mol) | Medal |
|---|---|---|---|
| 1 | Aspirin Like | -10.8 | □ |
| 2 | Metformin Like | -9.2 | □ |
| 3 | Ibuprofen Like | -9.1 | □ |
| 4 | Acetaminophen Like | -9.0 | |
| 5 | Atorvastatin Like | -8.8 | |
| 6 | Original Ligand | -8.7 | |
| 7 | Ligand-B | -8.6 | |
| 8 | Morphine Like | -8.4 | |
| 9 | Warfarin Like | -8.1 | |
| 10 | Diazepam Like | -8.0 | |
| 11 | Caffeine Like | -7.6 | |

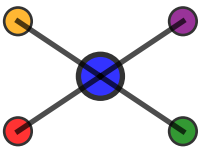
# 2D Molecular Structure Diagrams

 #1



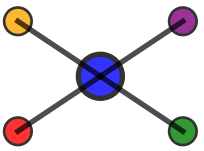
**Aspirin Like**
**-10.8 kcal/mol**

 #2

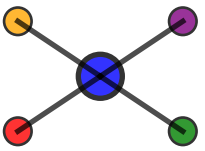


**Metformin Like**
**-9.2 kcal/mol**

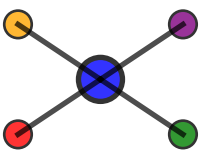
 #3



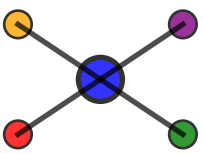
**Ibuprofen Like**
**-9.1 kcal/mol**



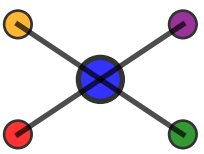
**Acetaminophen Like**
**-9.0 kcal/mol**



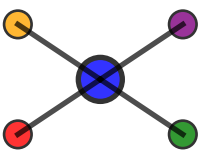
**Atorvastatin Like**
**-8.8 kcal/mol**



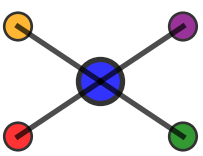
**Original Ligand**
**-8.7 kcal/mol**



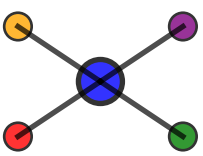
**Ligand-B**
**-8.6 kcal/mol**



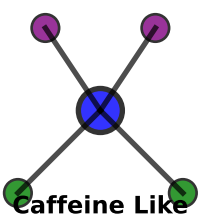
**Morphine Like**
**-8.4 kcal/mol**



**Warfarin Like**
**-8.1 kcal/mol**



**Diazepam Like**
**-8.0 kcal/mol**



**Caffeine Like**
**-7.6 kcal/mol**

NOTES:
- More negative binding scores indicate stronger protein-ligand interactions
- Structures shown are representative 2D molecular diagrams
- All docking performed using QuickVina 2 with identical parameters
- Binding site: center (139, 145, 171), size (25×25×25) Å