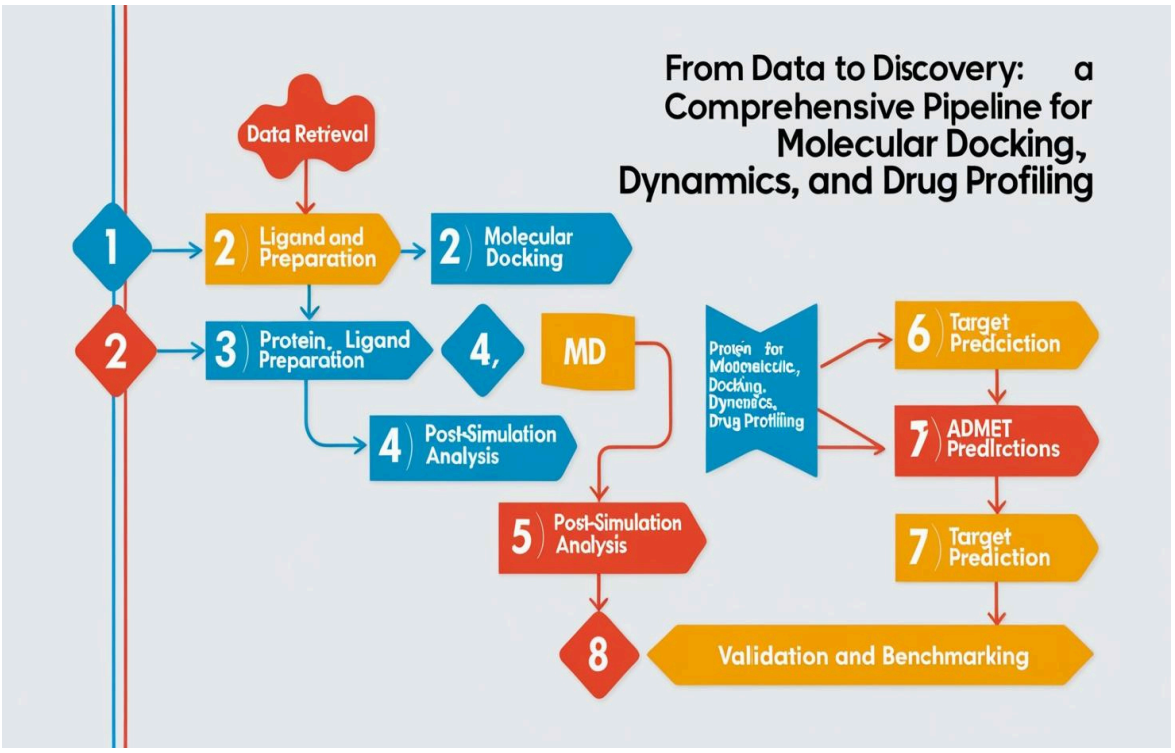
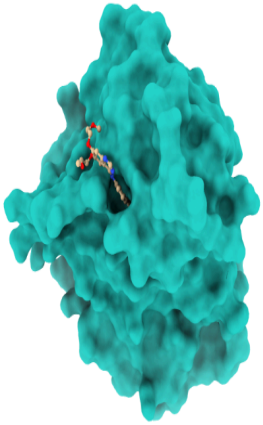
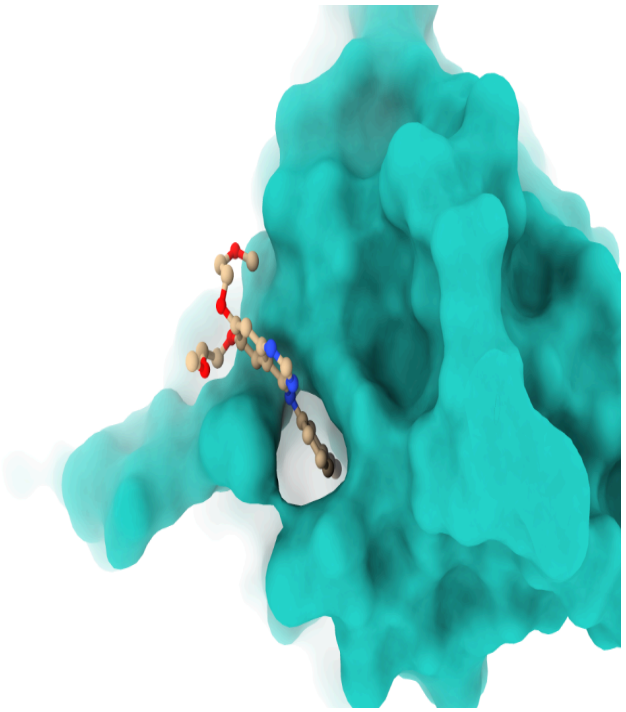
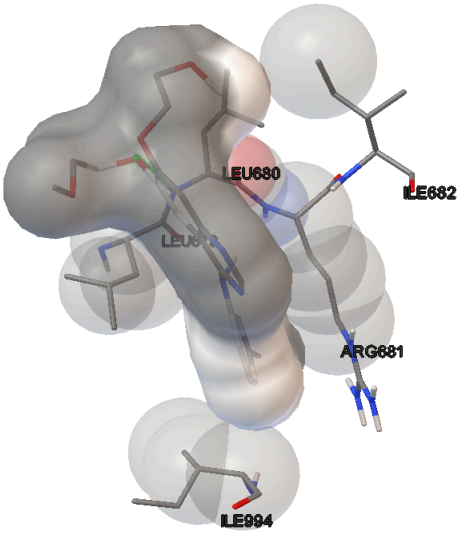
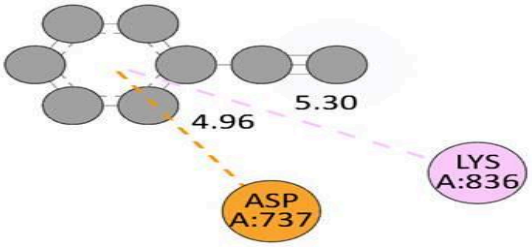
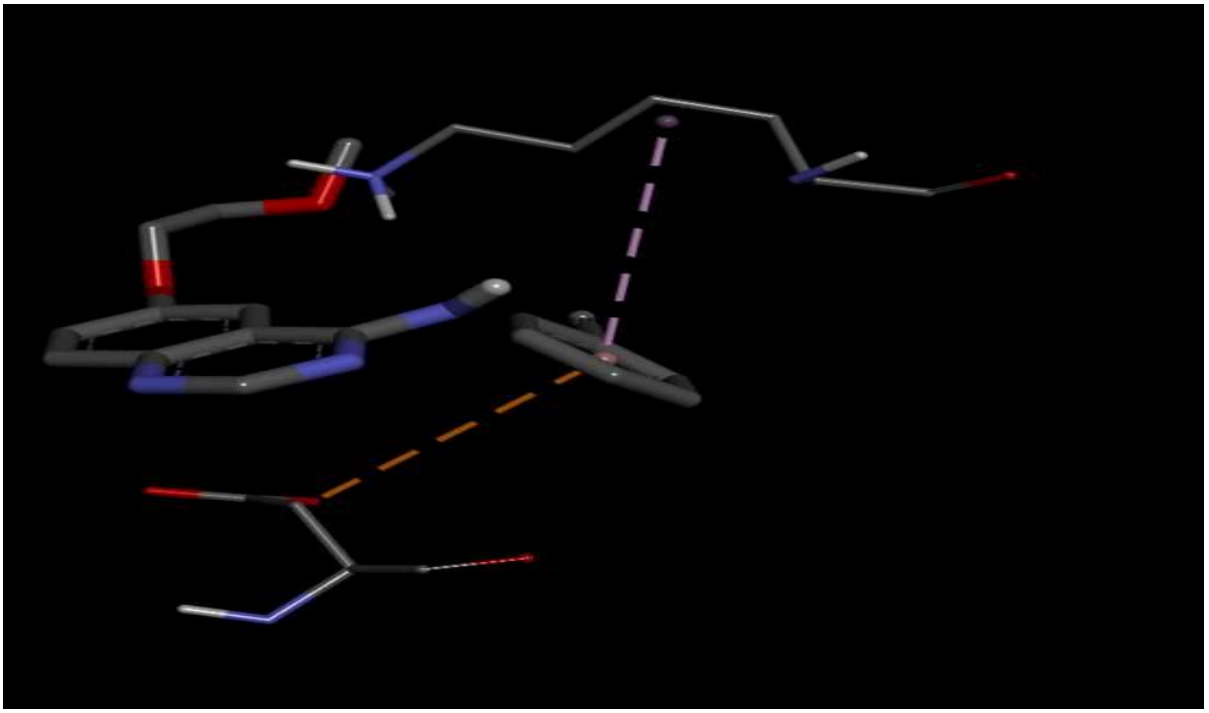

From Data to Discovery: a Comprehensive Pipeline for Molecular Docking, Dynamics, and Drug Profiling
Data Retrieval
1
2 Ligand and Preparation
2 Molecular Docking
2
3 Protein, Ligand Preparation
4,
MD
4 Post-Simulation Analysis
5 Post-Simulation Analysis
8
Validation and Benchmarking
6 Target Prediction
7 ADMET Predictions
7 Target Prediction

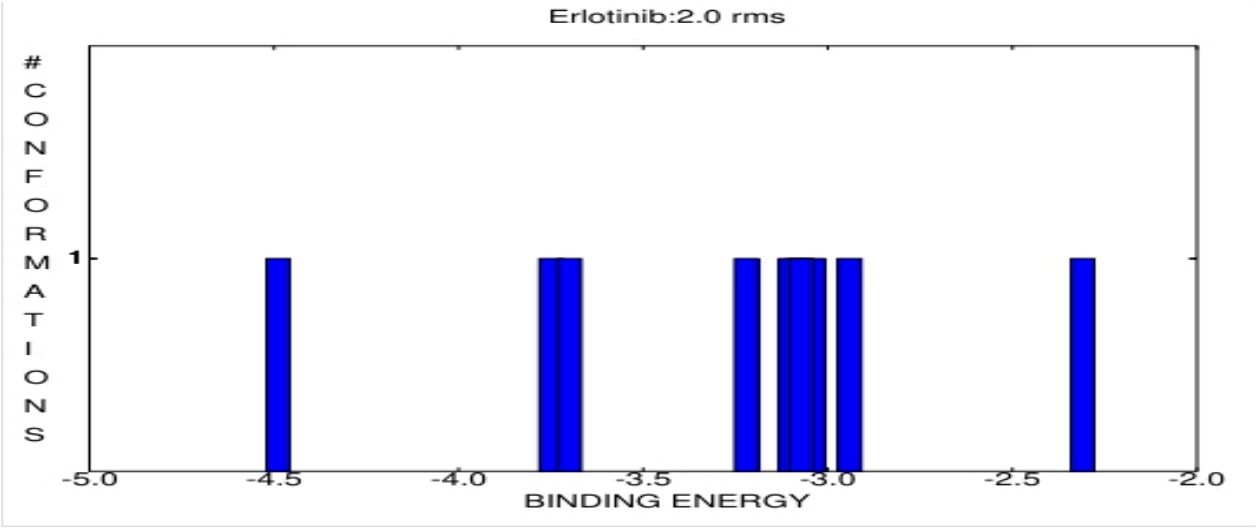


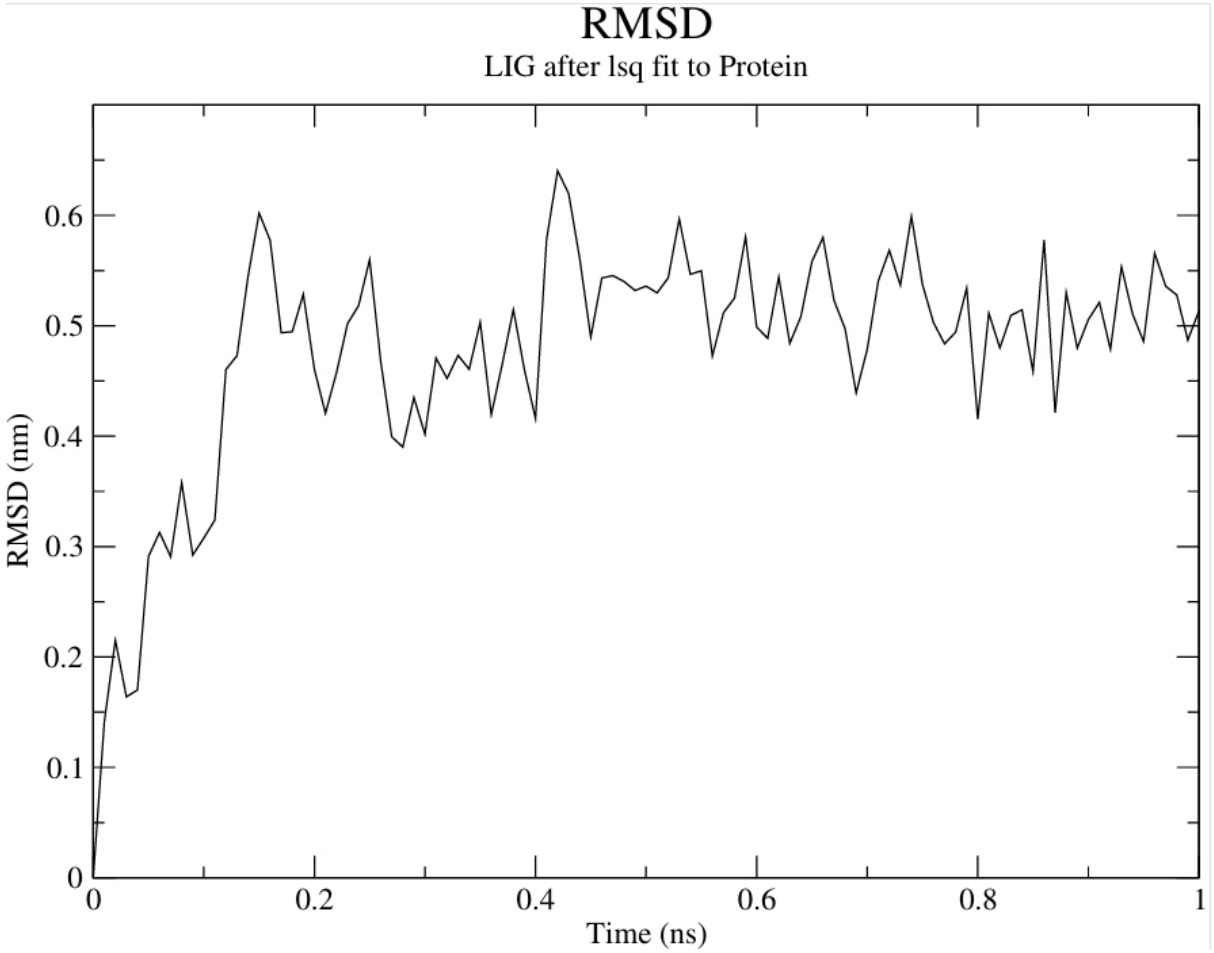


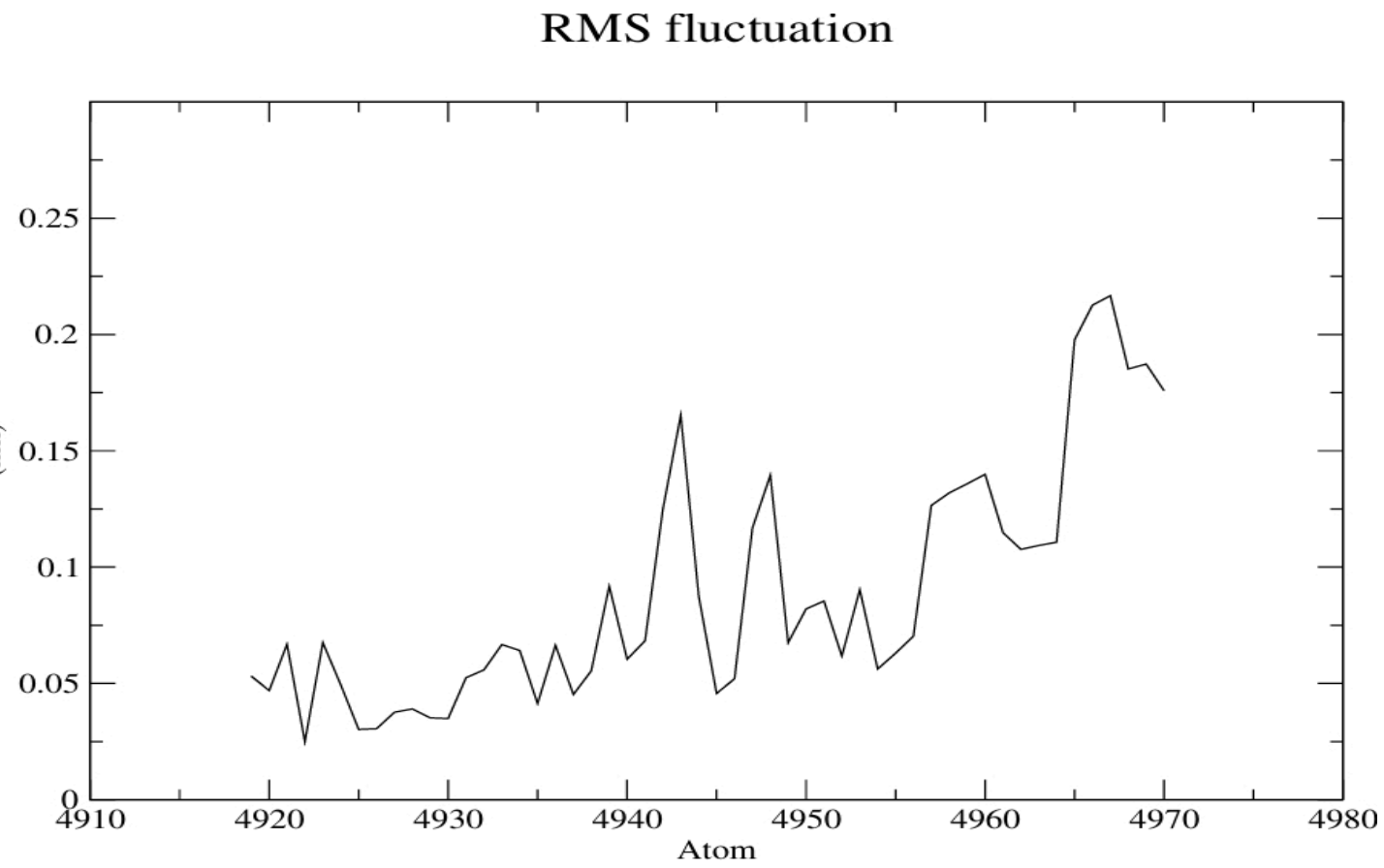

LEU680
ILE682
ARG681
ILE994

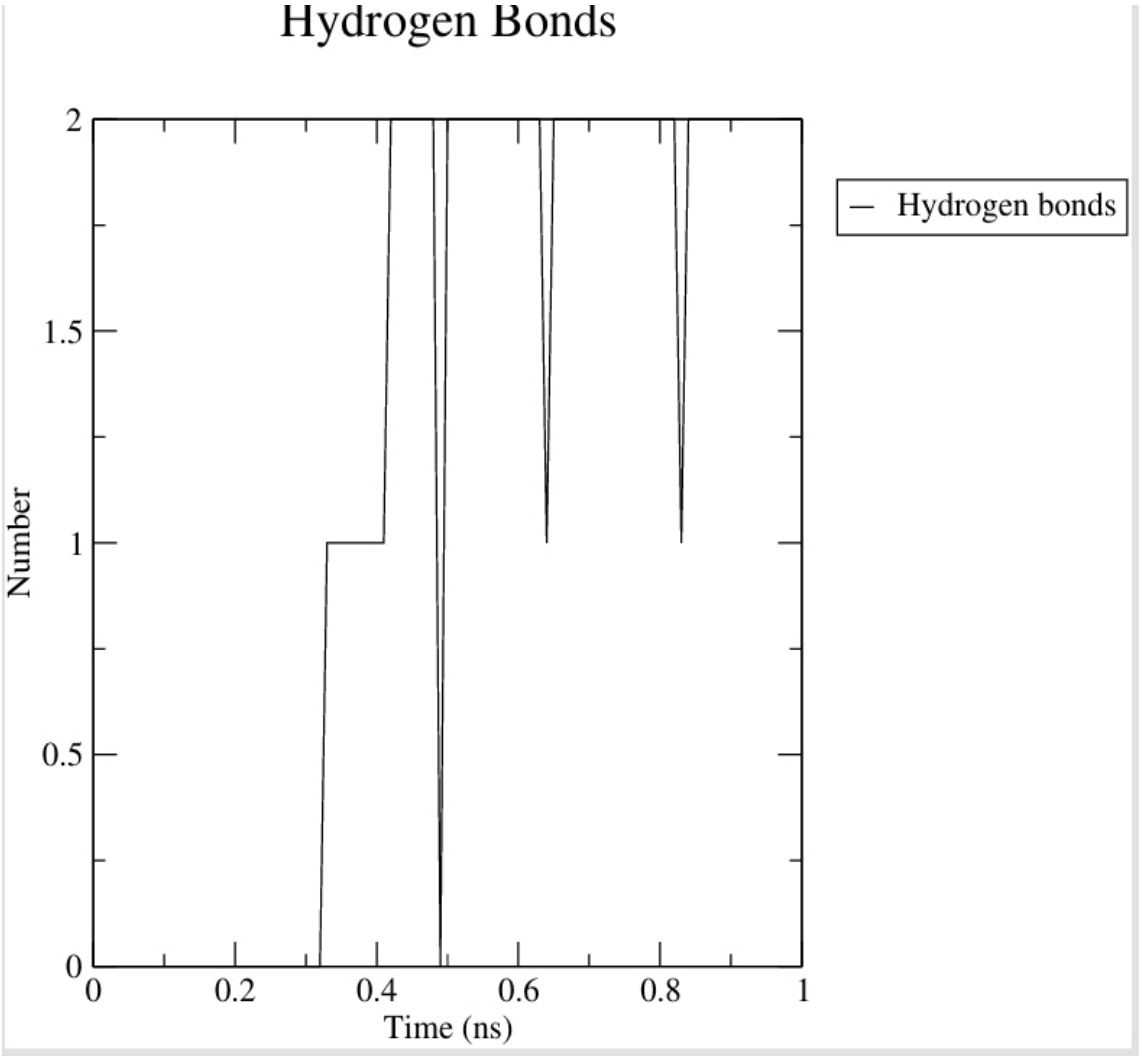

5.30
4.96
LYS
A:836
ASP
A:737

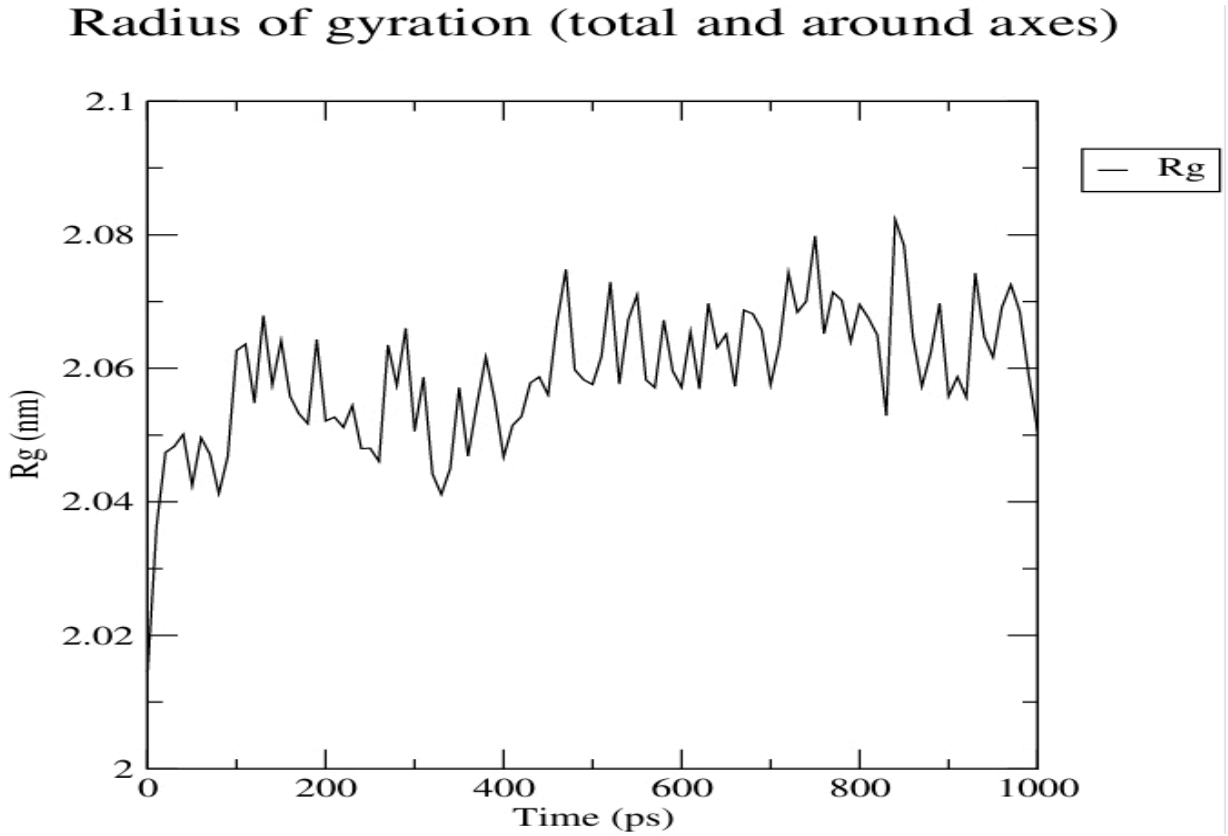


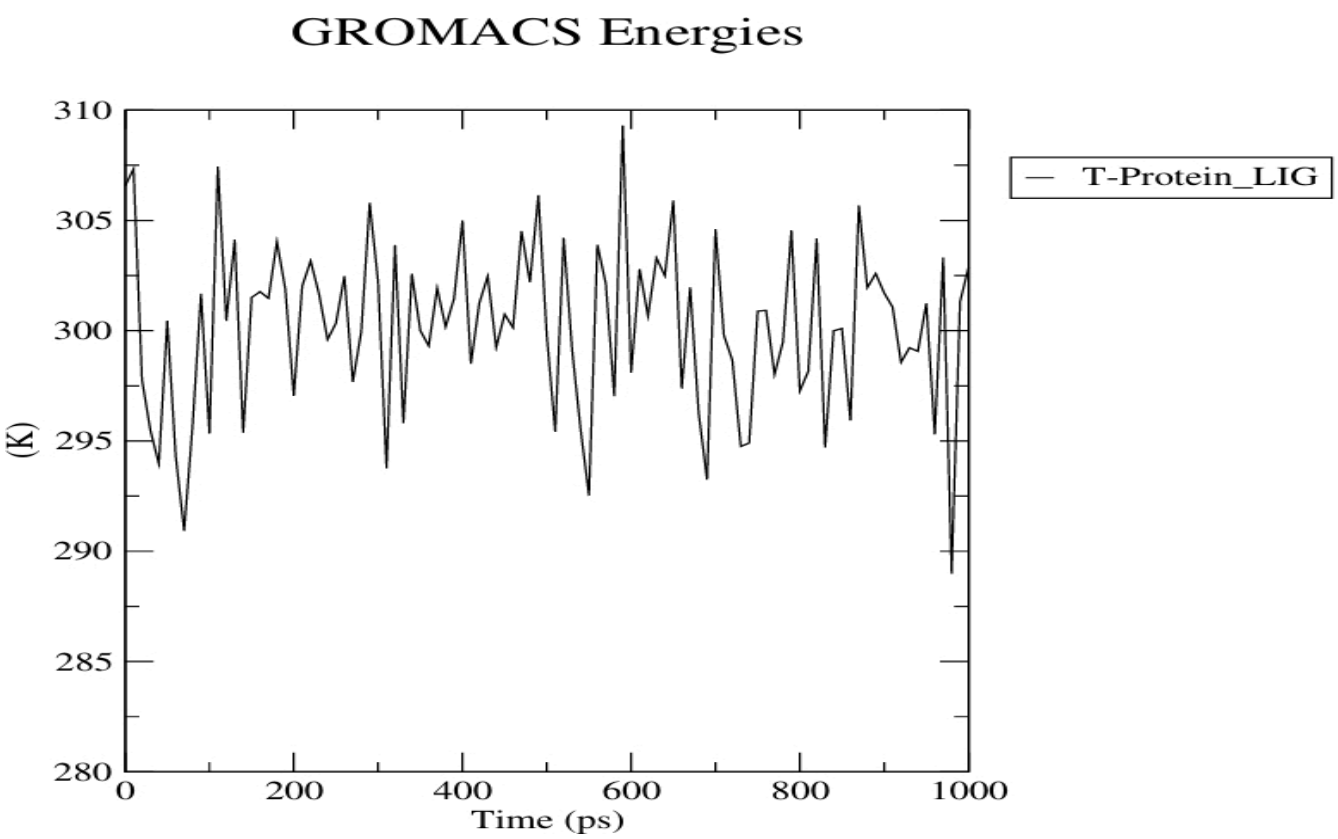

Erlotinib:2.0 rms
CONFORMATIONS
1
-5.0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
BINDING ENERGY

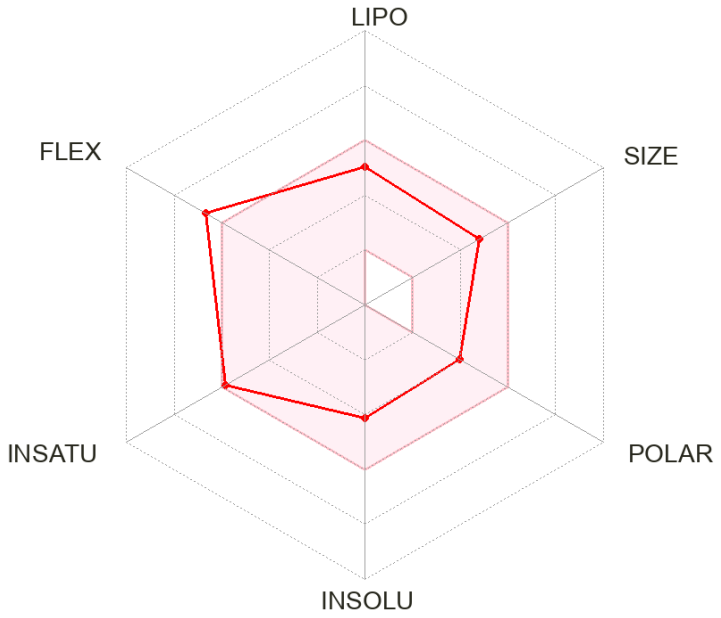

RMSD
LIG after lsq fit to Protein
RMSD (nm)
0
0.1
0.2
0.3
0.4
0.5
0.6
0
0.2
0.4
0.6
0.8
1
Time (ns)


RMS fluctuation
0.25
0.2
0.15
0.1
0.05
0
4910
4920
4930
4940
4950
4960
4970
4980
Atom


Hydrogen Bonds
Hydrogen bonds
Number
Time (ns)
0
0.5
1
1.5
2
0
0.2
0.4
0.6
0.8
1


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
2
2.02
2.04
2.06
2.08
2.1
0
200
400
600
800
1000


GROMACS Energies
310
305
300
295
290
285
280
(K)
0
200
400
600
800
1000
Time (ps)
T-Protein_LIG


LIPO
SIZE
POLAR
INSOLU
INSATU
FLEX