MODEL EXAM 2 – 21BBT035

PROTEIN : estrogen receptor alpha (5WGD)

LIGANDS: ZINC05632920 , ZINC05773243, ZINC12780336
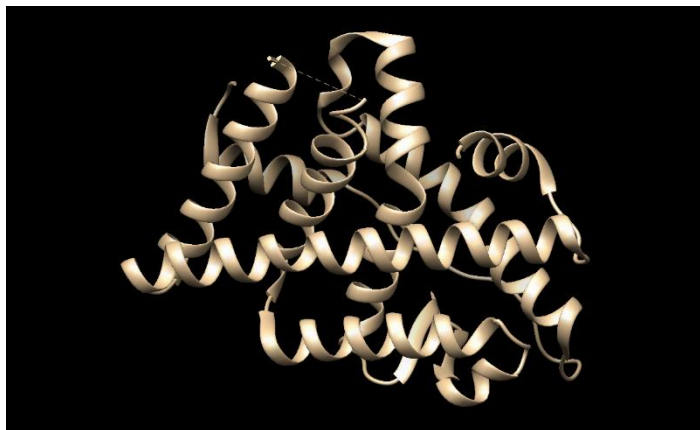

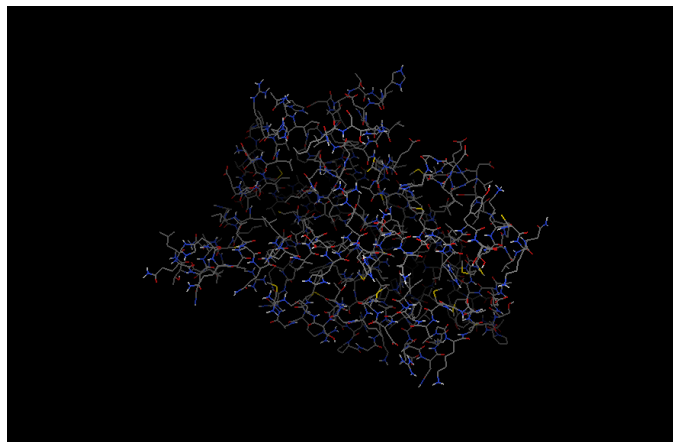*Figure 2: protein pdb file (after removing residues and chains)*
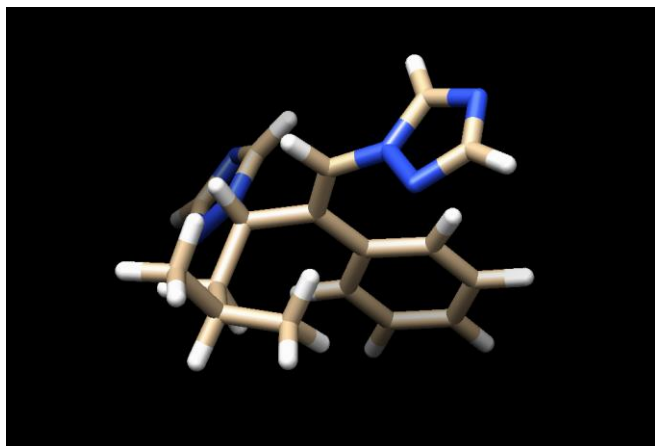

Figure 1 : protein . pdbqt file

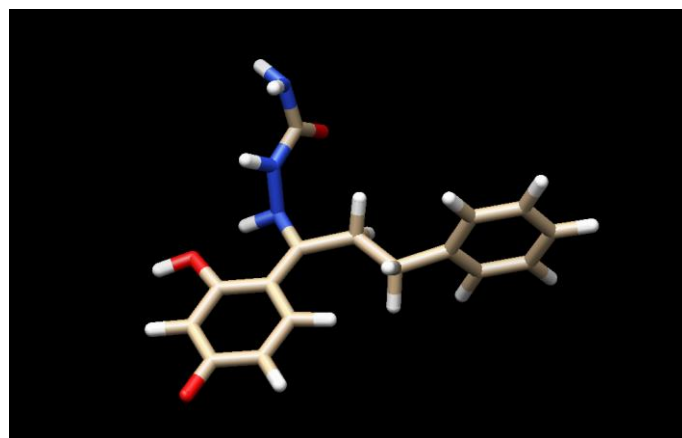*Figure 3: L1 minimized structure*
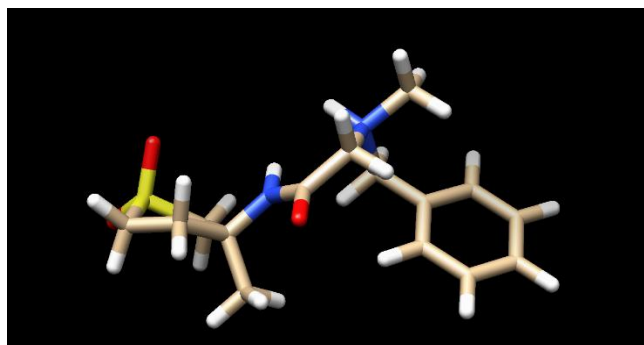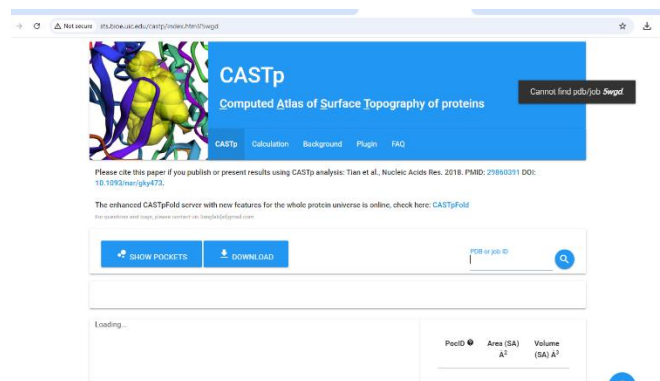

Figure 4: L2 minimized structure

Figure 5: L2 minimized structure

```
WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 12 CPUs
WARNING: at low exhaustiveness, it may be impossible to utilize all CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: 1053745336
Performing search ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************
done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -5.5      0.000      0.000
   2        -5.1      2.671      6.325
   3        -5.0     39.891     42.542
   4        -4.5     40.478     43.256
   5        -4.5     18.217     21.112
   6        -4.1     30.764     34.332
   7        -4.0     27.440     30.688
   8        -3.8      2.949      6.363
   9        -3.7     29.789     32.014
Writing output ... done.

G:\autodocking\03-run>
```

Figure 8: ligand 1 output file

```
WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 12 CPUs
WARNING: at low exhaustiveness, it may be impossible to utilize all CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -213877016
Performing search ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************
done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -5.3      0.000      0.000
   2        -5.3      5.675      7.664
   3        -5.2      4.878      6.332
   4        -4.9     35.308     37.284
   5        -4.8     32.231     33.956
   6        -4.5     32.386     34.282
   7        -4.5     29.042     31.103
   8        -4.4     32.155     33.830
   9        -4.4     32.024     34.332
Writing output ... done.

G:\autodocking\03-run2>
```

Figure 7 ligand 2.output file

```
WARNING: The search space volume > 27000 Angstrom^3 (See FAQ)
Detected 12 CPUs
WARNING: at low exhaustiveness, it may be impossible to utilize all CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -2143174392
Performing search ...
0%   10   20   30   40   50   60   70   80   90   100%
|----|----|----|----|----|----|----|----|----|----|
**************************************************
done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1        -5.0      0.000      0.000
   2        -4.6     20.803     23.760
   3        -4.6     21.988     24.919
   4        -4.5     14.335     16.913
   5        -4.5     17.354     19.420
   6        -4.4     13.820     16.625
   7        -4.4     22.954     25.295
   8        -4.3     33.861     35.494
   9        -4.3     35.890     38.338
Writing output ... done.
```

Figure 6 L3 output