molecules

MDPI

Supplementary Information

Mechanistic Insight into Binding of Huperzine A with Human Serum Albumin: Computational and Spectroscopic Approaches

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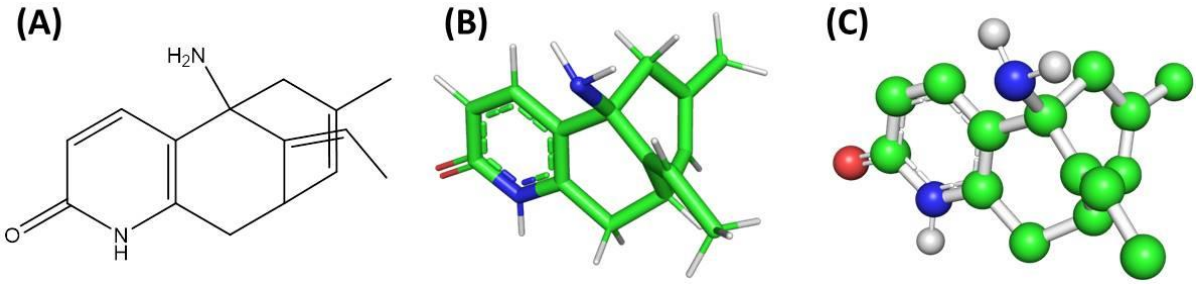

Figure S1. Molecular structure of Huperzine A. (A) 2D, (B) 3D stick, and (C) 3D ball and stick model of Huperzine A.

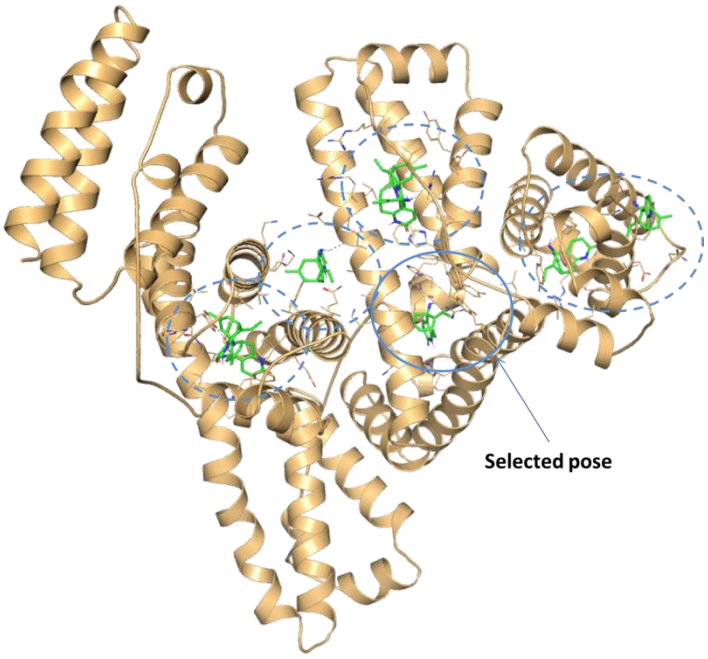

Figure S2. Different docked conformations of HpzA with HSA.

Huperzine_A_log - Notepad

File Edit Format View Help

```
# This is an auto-generated log file through InstaDock employing QuickVina-W #
Output will be Huperzine_A_out.pdbqt
Detected 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1452432156
Performing search ... done.
Refining results ...
searching finished in 3.277 seconds
done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   1         -7.2      0.000      0.000
   2         -6.5     22.367     24.175
   3         -6.4     52.114     53.432
   4         -6.4     52.192     53.557
   5         -6.4     17.159     19.166
   6         -6.3     18.023     20.214
   7         -6.3     19.911     22.341
   8         -6.2     13.667     15.987
   9         -6.1     13.894     16.503
Writing output ... done.
```

Figure S3. Energy table of different docked conformations of HpzA with HSA.