Abstract

Today, due to urgent need for predictable models used for designing new drugs with improved properties and less side effects, it seems necessary to apply theoretical and computational methods which are able to predict activities of new compounds in a shorter time with no need for test. In this study, quantum mechanics calculations are used to optimize basic structure of some 6-amino, 4-phenyl tetrahydroquinoline derivatives in gaseous phase using b3lyp and mo6-2x methods with 6-31g ++ (d, p) base set by Gaussian 09 software package. Then, using both NBO calculations and AIM software, various properties of hydrogen bonding and its role on drug activity were evaluated. The results showed a desirable relationship between drug activity and hydrogen bond strength. The computation was also optimized using b3lyp method with base set 6-31g ++ (d, p) by Gaussian 09 software in polar and nonpolar solvents to evaluate drug-protein interactions. The results showed a strong interaction between polar solvents and the drug. The strongest interaction was observed in chloroform solvent. The final results also showed that the molecule acted through assembly of its own structure, and used electron-donor binding to move toward lipophilic state, so the compounds of 6-amino, 4-phenyl tetrahydroquinolines along with donor conjugates could be used as new drugs in FSH receptor inhibition.

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Theoretical investigation of inhibition effect of some 6-amino-4-phenyltetra hydroquinoline derivatives as antagonists for FSH receptor

Supervisors:
Dr. Hojat SamarehDelarami
Dr. Mahmood Sanchooli

Advisor:
Dr. Pouya Karimi

By:
Fatameh Rashki

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