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DFT calculations and insilico drug activity predictions for the Bioactive constituent present in Delonix regia Plant

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Abstract - *Medicinal important compounds like Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetolrhamnosyl-hexoside and Stigmasterol were selected for their stability determination via binding energy calculation. The binding energy of these were determined by the Gaussian software 5.0. DFT were accomplished B3LYP and HF methods using three basis set be found of STO-3G, 3-21G, 6-31G. The DFT calculations of binding energy proved that Quercetin trihexose was recognized to be more stable among other four compounds. Binding energy by STO-3G (-2220.678), 32-1G (-2237.858) and 63-1G (-2249.565) were observed by B3LYP method. HF method binding energies were found to be STO-3G (-2208.715), 32-1G (-2225.029) and 63-1G (-2236.484). These results showed that among the medicinal compounds present in the Delonix regia plant, Quercetin trihexose was found to have very good binding energy. Because of its good binding energy and stability it may find as potential medicine for the treatment of disease.*

Key Words: **Delonix regia plant, DFT, B3LYP and HF.**

1.INTRODUCTION

Delonixregia plant with orange-red flowers belongs to the family of Ceasalpiniaceae, also known as Gulmohar royal Poinciana regia or Flamboyant [1]. The extract of Delonixregia is known to have medicinal properties.This plant isused in several countries to prepare extracts with antimicrobial and antifungal activities [2-5]. The Delonixregia plant is used in medicine as antiviral, anti-inflammatory and cytotoxic activity [1]. This plant is used in several countries to prepare extracts withantimicrobial and antifungal activities and used as antibiotics [6]. Binding energies of eight medicinal compounds has been computed using the B3LYP and HF methods by DFT approach to predict the most stable drug.

2. Experimental Methods

2.1 Materials

The medicinal important compounds present in the Delonix regia plant were selected for our work from the literature [1-6] as given below the structures Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetolrhamnosyl-hexoside and Stigmasterol in **Figure.1-5.**

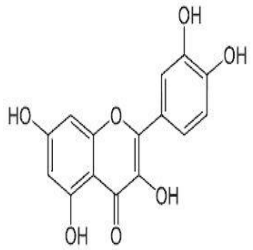

Fig -1: Quercetin

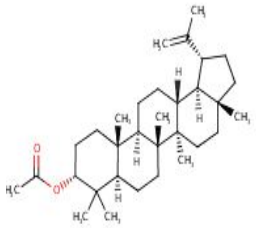

Fig -2: Epilupeol

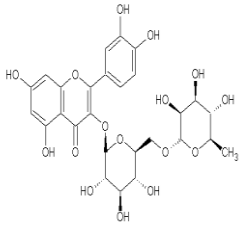

Fig -3: Quercetin tihexose

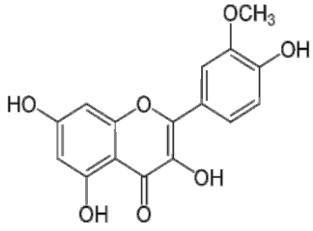

Fig -4: Isorhamnetinrhamnosyl-hexoside

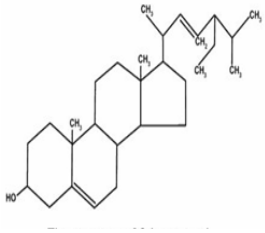

Fig -5: Stigmasterol

DFT Methods

The structures of the constituents like Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetolrhamnosyl-hexoside and Stigmasterol were drawn in GaussView 5.0 the binding energies were calculated by B3LYP and HF methods using three basis sets STO-3G, 3-21G, 6-31G [7-10]. The binding energy of the above compounds predicted by B3LYP and HF method were given in **Table-I &Table-II.**

Table- 1 Binding energy of compounds in B3LYP method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Quercetin	-1089.641	-1098.001	-1103.765
2.	Epilupeol	-1231.708	-1240.293	-1246.712
3.	Quercetintrihexose	-2220.678	-2237.858	-2249.565
4.	Isorhamnetolrhamnosyl-hexoside	-2219.277	-2236.520	-2248.197
5.	Stigmasterol	-1193.828	-1202.024	-1208.262

Table- 2 Binding energy of compounds in HF method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Quercetin	-1083.665	-1091.672	-1097.322
2.	Epilupeol	-1223.366	-1231.488	-1237.661
3.	Quercetintrihexose	-2208.715	-2225.029	-2236.484
4.	Isorhamnetolrhamnosyl-hexoside	-2207.189	-2223.548	-2234.96
5.	Stigmasterol	-1185.917	-1193.650	-1199.778

Result and Discussion

2.2 DFT Calculation

2.2.1 B3LYP Method

The binding energy calculation by using three basis sets (STO-3G, 3-21G & 6-31G) listed in **Table- I** showed the following result

STO-3G

The binding energy for the selected five compounds were found to be -1089.641, -1231.708, -2220.678, -2219.277 and -1193.828a.u. and it was found that Quercetintrihexose have good binding energy.

3-21G

From above compounds were found to be Quercetintrihexose have a good binding energy as -2237.858 a.u among the other bioactive constituents using 3-21G basis sets, other compounds binding energies were found to be -1098.001, -1240.293, -2236.520 and -1202.024 a.u.

6-31G

The binding energies of the above five compounds by 6-31G basis sets were found to be -1103.765, -1246.712, -2248.197 and -1208.262 a.u. From the above data it was ended with the intention of Quercetintrihexose was found to have a good binding energy as-2249.565a.u. among the other bioactive constituents.

2.2.1 HF Method

The binding energy calculated to the above compounds given in **Table- II** for the three basis sets. The binding energy calculated by STO-3G basis sets were -1083.665, -1223.366, -2208.715, -2207.189 and -1185.917a.u for Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetol rhamnosyl-hexoside and Stigmasterol compounds. 321-G basis sets predicted -1091.672, -1231.488, -2225.029, -2223.548 and -1193.650a.u. 6-31G basis sets showed -1097.322, -1237.661, -2236.484, -2234.96, and -1199.778 a.u. as binding energies for the above compounds as given in the same order.

3. CONCLUSIONS

The binding energy of five bioactive constituents were calculated by B3LYP and HF method using STO-3G, 3-21G & 6-31G. The B3LYP method revealed that Quercetintrihexose was found to have good binding energy (-2249.565) and compared to other bioactive constituents -1103.765, -1246.712, -2248.197 and -1208.262 a.u. The HF methods of calculation of binding energy showed that Quercetintrihexose was found to be good binding energy as -2236.484 compared to other bioactive compounds -1097.322, -1237.661, -2234.96 and -1199.778. The above computation of binding energy showed that five bioactive compounds selected for the above work Quercetintrihexose to have a good binding energy.

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