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, Isorhamnetorhamnosyl-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 is used 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 with antimicrobial 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 structures of the constituents like Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetolrhamnosyl-hexoside and Stigmasterol were drawn in GaussView 5.0. The binding energy was 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 and Table-II.

**Table-1 Binding energy of compounds in B3LYP method**

<table>
<thead>
<tr>
<th>S. No</th>
<th>Compounds name</th>
<th>Basis sets</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>STO-3G</td>
</tr>
<tr>
<td>1</td>
<td>Quercetin</td>
<td>-1098.641</td>
</tr>
<tr>
<td>2</td>
<td>Epilupeol</td>
<td>-1231.708</td>
</tr>
<tr>
<td>3</td>
<td>Quercetintrihexose</td>
<td>-2220.678</td>
</tr>
<tr>
<td>4</td>
<td>Isorhamnetolrhamnosyl-hexoside</td>
<td>-2219.277</td>
</tr>
<tr>
<td>5</td>
<td>Stigmasterol</td>
<td>-1193.828</td>
</tr>
</tbody>
</table>

**Table-2 Binding energy of compounds in HF method**

<table>
<thead>
<tr>
<th>S. No</th>
<th>Compounds name</th>
<th>Basis sets</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>STO-3G</td>
</tr>
<tr>
<td>1</td>
<td>Quercetin</td>
<td>-1083.665</td>
</tr>
<tr>
<td>2</td>
<td>Epilupeol</td>
<td>-1223.366</td>
</tr>
<tr>
<td>3</td>
<td>Quercetintrihexose</td>
<td>-2208.715</td>
</tr>
<tr>
<td>4</td>
<td>Isorhamnetolrhamnosyl-hexoside</td>
<td>-2207.189</td>
</tr>
<tr>
<td>5</td>
<td>Stigmasterol</td>
<td>-1185.917</td>
</tr>
</tbody>
</table>

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 -2249.565 a.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 -1185.917 a.u. for Quercetin, Epilupeol, Quercetintrihexose, Isorhamnetol rhamnosyl-hexoside and Stigmasterol compounds. 321-G basis sets predicted -1091.672, -1231.488, -2225.029, -2236.484 and -1193.650 a.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 forthe above work Quercetintrihexose to have a good binding energy.

**REFERENCES**


