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Evaluation of Stability of the Medicinally important compounds in Vitex Negundo plant by DFT method

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Abstract: Medicinal important compounds like Sabinine, Vanilic acid, Spathulenol, Luteolin, Vitexilactone, Betulinic acid, Urosilicacid, and Vitexin 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 Vitexin was recognized to be more stable among other seven compounds. Binding energy by STO-3G (-1543.087), 32-1G (-1554.960) and 63-1G (-1563.105) were observed by B3LYP method. HF method binding energies were found to be STO-3G (-1534.527), 32-1G (-1545.839) and 63-1G (-1553.820). These results showed that among the medicinal compounds present in the Vitex negundo plant, Vitexin 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.
Keywords: Vitex negundo plant, DFT, B3LYP and HF.

Introduction

Vitex negundo plant belongs to verbenaceae family commonly known as Nirkundi or Nallanocci[1]. The leaves and the bark of V.negundo are used in medicine as analgesic[2], anticonvulsant, antioxidant[3], insecticide, pesticides[4]. Vitex negundo plant parts are used to cure Asthma, Cancer[5], Jaundice[6&7], urticaria, cellulitis, Abcesses, Carbuncles, Eczema[8], Liver disorders[9], kwashiorkor[10], eye pain[11] and as an antidote for snake bite[12]. Leaves of Vitex were used as a mosquito repellent[13], antiulcerogenic[14], anti-parasitic[15], antimicrobial[16] and heaptoprotective[17] potentials. Vanilic acid and Luteolin isolated from bark were used in verminosis and opthalmopathy[18]. Compounds like Sabinine, Spathulenol, Vitexilactone Betulinic acid, Urosilic acid reported to have antibacterial and antifungal activities [19]. Crushed leaf is applied on forehead to relieve headache[20].

Binding energies of eight medicinal compounds, has been computed using the B3LYP and HF methods by DFT approach to predict the most stable drug.

Experimental Methods

Materials

The Medicinal important compounds present in the vitex negundo plant were selected for our work from the literature [19] as given below in figure.1-8.

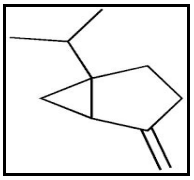

Figure.1 Sabinene

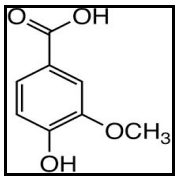

Figure.2 Vanilic acid

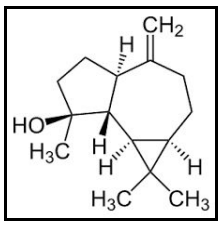

Figure.3 spathulenol

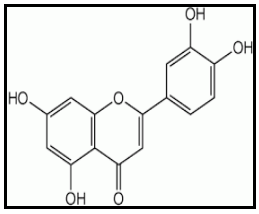

Figure.4 Luteolin

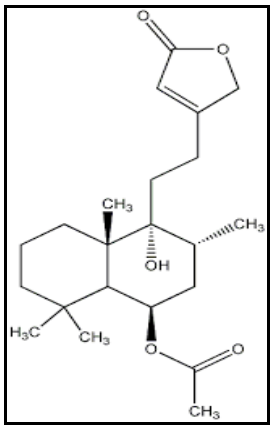

Figure.5 Vitexilactone

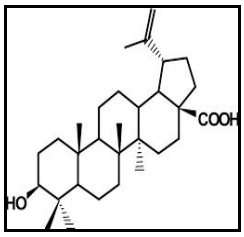

Figure.6 Betulinicacid

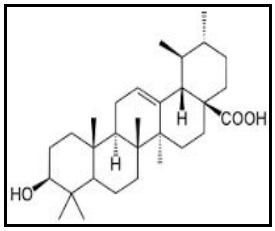

Figure.7 Ursolicacid

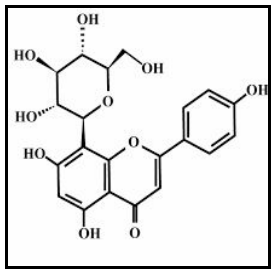

Figure.8 Vitexin

DFT Methods

The GaussView 5.0 software was used to draw the structures of the compounds. Binding energy of the above compounds were determined using Gaussian software, binding energy by B3LYP and HF methods using three basis sets STO-3G, 3-21G, 6-31G [21 & 22].

Table- 1 Binding energy of compounds in B3LYP method

S.No	Compounds name	Basis sets		
		STO-3G	**3-21G**	**6-31G**
1	Sabinine	-385.593	-388.208	-390.226
2	Vanilic acid	-602.456	-607.067	-610.254
3	Spathulenol	-652.335	-656.930	-660.340
4	Luteolin	-1015.466	-1023.186	-1028.568
5	Vitexilactone	-1141.884	-1150.436	-1156.450
6	Betulinic acid	-1377.652	-1387.605	-1394.794
7	Ursolic acid	-1377.734	-1387.716	-1394.908
8	Vitexin	-1543.087	-1554.960	-1563.105

Table- 2 Binding energy of compounds in HF method

S.No	Compounds name	Basis sets		
		STO-3G	**3-21G**	**6-31G**
1	Sabinine	-382.842	-385.369	-387.355
2	Vanilic acid	-599.102	-603.522	-606.640
3	Spathulenol	-647.849	-652.282	-655.633
4	Luteolin	-1009.800	-1017.208	-1022.485
5	Vitexilactone	-1134.620	- 1142.779	-1148.706
6	Betulinic acid	-1368.568	-1378.037	-1385.089
7	Ursolic acid	-1368.660	-1378.166	-1385.220
8	Vitexin	-1534.527	-1545.839	-1553.820

Result and Discussion

DFT Calculation

1) B3LYP Method

The binding energy determination by three basis sets by B3LYP method as given in table-1 showed that where as other compounds like Sabinine, Vanilic acid and Spathulenol were found have poor binding energy (-385.593, -602.456 and -652.335 by STO-3G), (-388.208, -607.067 and -656.930 by 3-21G) and 6-31G (-390.226, -610.254 and -660.340). Betulinic acid and Ursolic acid were found have moderate binding energy (-1377.652 and -1377.734) by STO-3G, (-1387.605 and -1387.716) 3-21G and (-1394.794 and 1394.716) by 6-31G. Vitexin was found to have good binding energy STO-3G (-1543.087) 3-21G (-1554.960) and 6-31G (-1563.105) respectively.

2) HF Method

The binding energy calculated to the above compounds given in Table-2 for the three basis sets. Binding energy calculated by STO-3G basis sets were -382.842, -599.102, -647.849, -1009.800, -1134.620, -1368.568, -1368.660 and -1534.527 a.u. for Sabinine, Vanilicacid, Spathulenol, Luteolin, Vitexilactone, Betulinic acid Ursolic acid and Vitexin compounds. 321-G basis sets predicted -385.369, -603.522, -652.282, -1017.208, -1142.779, -1378.037, -1378.166 and -1545.839 a.u. 6-31G basis sets showed -387.355, -606.640, -655.633, -1022.485, -1148.706, -1385.089, 1385.220 and -1553.820 a.u. as binding energies for the above compounds as given in the same order.

Conclusion

Among the eight compounds selected for the determination of binding energy to predict their stability. The Vitexin was found to have good binding energy by B3LYP and HF methods Sabinine, Spathulic acid and Vanilic acid were found to be less stable as per the binding energy values less than -1000 a.u. The compounds Betulinic acid and Ursolic acid were found to have moderate binding energy in the range -1377 to -1394.908. The Vitexin was found to have good binding energy by both method. The B3LYP method (-1543.087, -1554.960 and -1563.105 a.u.) and by HF method STO-3G(-1534.527), 3-21G(1545.839) and 6-31G (-1553.820 a.u.) compared to other compounds. Prediction of binding energy revealed that vitexin was found to be more stable than Sabinine, Vanilic acid, Spathulenol, Luteolin, Vitexilactone, Betulinic acid and Ursolic acid. Hence Vitexin can be used as stable drug compared to other compounds.

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