International Research Journal of Engineering and Technology (IRJET) e-ISSN: 2395-0056
Volume: 05 Issue: 01 | Jan-2018 www.irjet.net p-ISSN: 2395-0072

In Silico calculations of Dipole moment by DFT and Drug Activity Predictions for the bioactive constituent present in Coleus aromatics

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Abstract - *Medicinal important compounds like were selected for their stability determination via dipole moment calculation. The dipole moment of these was 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 proved that Chavicol was recognized to be more stable among other seven compounds. Dipole moment by ST0-3G (0.7485), 32-1G (0.8619) and 63-1G (1.1594) were observed by B3LYP method. HF method dipole moments were found to be STO-3G (1.0261), 321G (1.2176) and 63-1G (1.4305). These results showed that among the medicinal compounds present in the Coleus aromaticus plant, Chavicol was found to have very poor dipole moment. Because of it is more stability it may find as potential medicine for the treatment of disease.*

Key Words: Coleus aromaticus plant, DFT, B3LYP, HF, and Dipole moment.

1. INTRODUCTION

Coleus aromaticus belonging to the family Lamiaceae. Coleus aromaticus look as a green, perennial, shrub having oval shaped and succulent leathery leaves with scalloped edges. The plant grows to around 50 cm tall with horizontal stems up to 180 cm long potted plants. The leaves are highly aromatic with a strong flavor of mixed herbs [1]. Herbs and plant materials like stem, bark, resin, leaf, pollen, fruit, seed and roots find an important place in all forms of native and medicinal therapy all over the world [2-3]. Decoction of the leaves is administered in cases of chronic cough, asthma and is also reported to possess antilithotic, chemopreventive antioxidant potential, anti-inflammatory, antitumor, antimutagenic, anti-carcinogenic and diuretic activities [4-6]. Coleus aromaticus is used for seasoning meat dishes and in food products [7]. It is considered to be an antispasmodic, stimulant and stomachic and is used for the treatment of headache, fever, epilepsy and dyspepsia. It is used to treat conditions such as indigestion, diarrhea, nervous tension, insect bites, toothache, earache, rheumatism, whooping cough & bronchitis [8]. Leaf and stem are used to cure cold, tonsilities and urinary tract diseases. Cultivation of coleus is gaining importance, since there is a demand from ayurvedic pharmaceutical industries [9]. It is also known to be a very powerful painkiller, stimulates flow of bile aiding digestion. In our present work dipole moments have been calculated using B3LYP and HF methods [10].

VERNACULAR NAMES [11]

Sanskrit	:	Parnayavani
Bengal	:	Paatharchur,Paterchur
English	:	Country borage,Indian Borage
Gujarati	:	Ovvapaan
Hindi	:	Pattaajvaayana
Malayalam	:	Kannikurkka,panikkurukka
Oriya	:	Hemakedar,Amarpoi
Punjabi	:	Patharachur
Tamil	:	Karpuravalli
Telugu	:	Kapparillaku & Vamu-aku

Fig -1 Coleus aromaticus leaves

1.1 DFT Methods

The Gauss View 5.0 software was used to draw the structures of the compounds. Dipole moment of the above compounds were determined using Gaussian software, dipole moment by B3LYP and HF methods using three basis sets STO-3G, 3-21G, 6-31G.

1.2 Gaussian Software

Gaussian Software

Gauss View is a graphical user interface designed to help you prepare input for submission to Gaussian and to examine graphically the output that Gaussian produces.

Gauss View is not integrated with the computational module of Gaussian, but rather is a front-end/back-end processor to aid in the use of Gaussian. Gauss View provides three main benefits to Gaussian users.

First, through its advanced visualization facility, Gauss View allows you to rapidly sketch in even very large molecules, then rotate, translate and zoom in on these molecules through simple mouse operations. It can also import standard molecule file formats such as PDB files. You can also use Gauss View to launch jobs as well if Gaussian is installed on the same computer. Lastly, you can define default and named calculation templates—known as schemes—to speed up the job setup process.

1. Open the Gauss view software.
2. To start a new blank work space, go to **file -→ New--→ Create** molecular group.
3. Go to **"view"** menu and **L-click** the builder option **"builder"** window will open.
4. Choose the desired atom using the **L –click**. Make sure that the atom or fragment to be added one that is marked.
5. After adding all desired atoms (excluding hydrogen) you can start bonding them by using the **"Modified Bond"** option in the **"Builder".** The two chosen atoms change color and are marked as 1 and 2. In addition, a new window "Semichem Smart Slide" will open press the "OK" push button after choosing the bond.
6. Add hydrogen atoms by using the **"Add Valence"** option on the **"Builder"** window.
7. Remove atoms from the structure by using the **"Delete Atom"** icon on the **"Builder"** window.
8. The drawn structure looks like as given in figure. To save the structure, in Gaussian input file, File were Save as in "Gaussian input file" **as *gif*.**

The window will appear as given in **Figure2**.

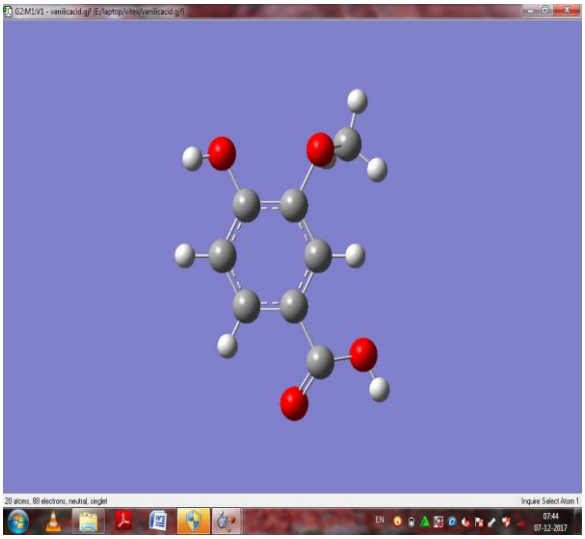

Fig -2: Structure of vanillic acid

1.3 Calculation set up

1. Click---→calculation option in the Gauss view main window menu, then open the Gaussian calculation setup window. Under Job Type, look at the various calculation options like **optimization, frequency, energy** and **dipole moment** calculations.

Choose optimization to calculate the optimum geometry.

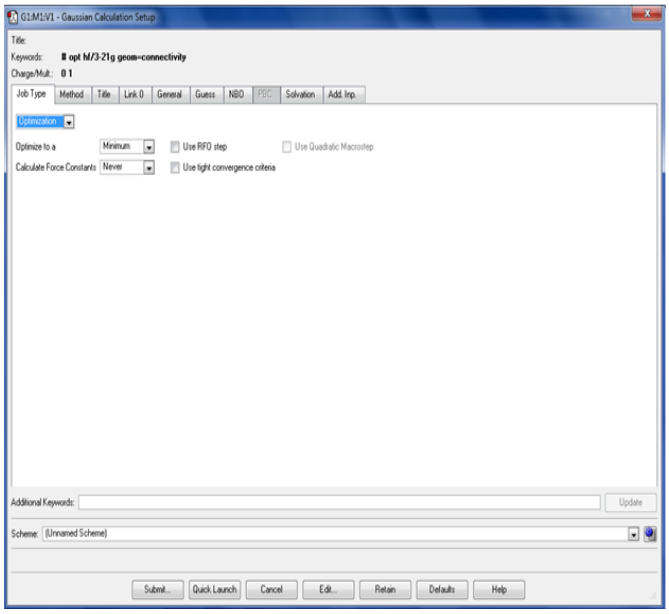

Fig -3: Calculation setup Window

To carry out energy calculation using an abinitio Hartree-Fock model.

1. Select the ground state, HF and set the basis set for 32-1G. The windows appears as Fig-4

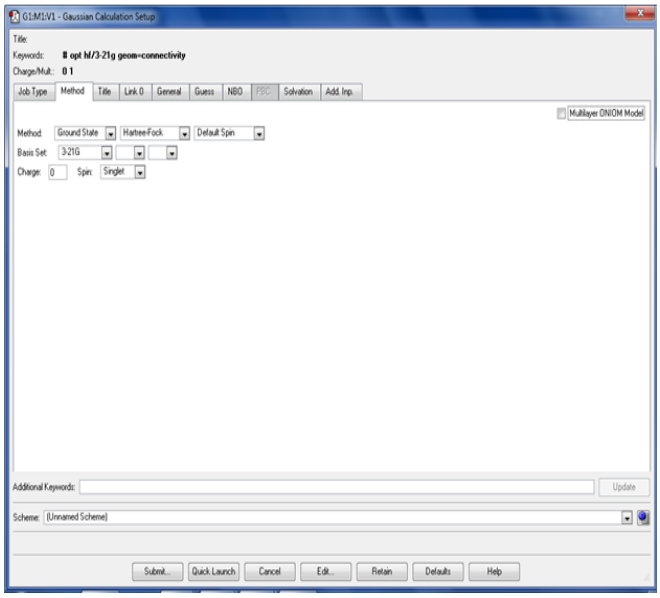

Fig -4: Calculation setup Window in HF method

1. On pressing submit button, it send the calculation from Gauss View to Gaussian. After finishing the calculation press OK to save the output file.

2. In the Gauss View menu bar, select Calculate-→Gaussian Calculation setup. Choose Energy to calculate the dipole moment and ensure that your window looks like the window below:

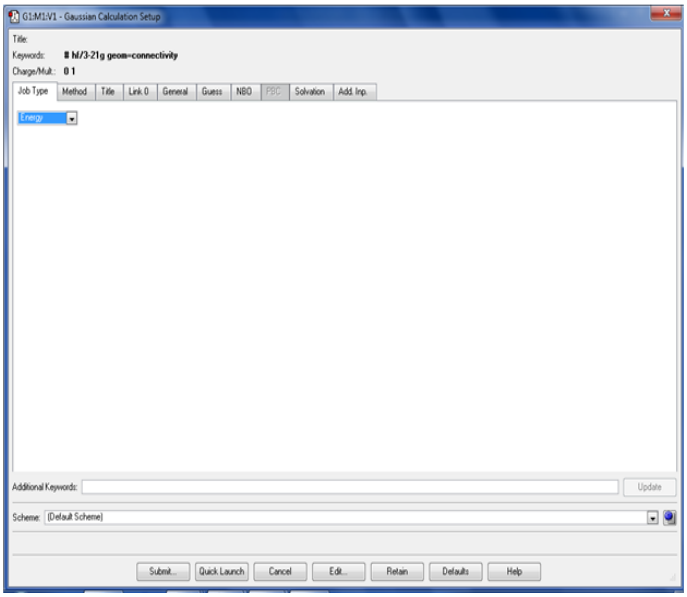

Fig -5: Energy Calculation setup Windows

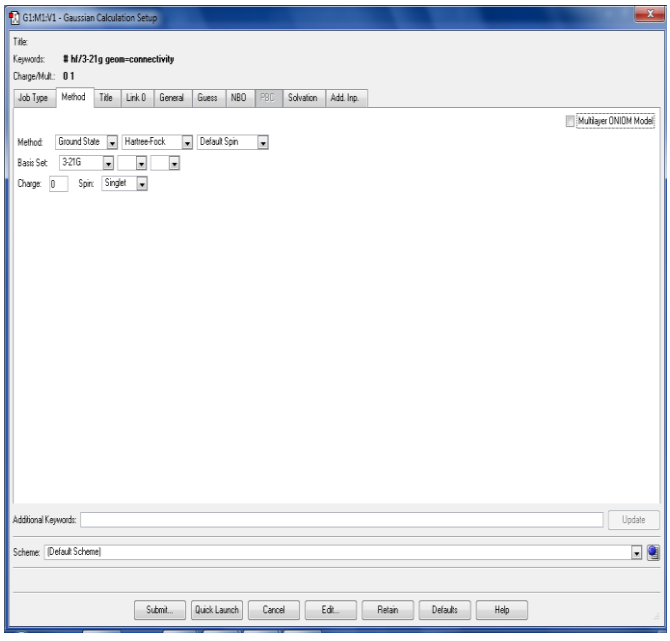

Fig -6: Energy Calculation Setup Windows in B3LYP Method

A new window should appear titled, Gaussian Job Completed, with a question asking if you would like to open your sen.log file. Click ok and a new window should appear titled, sen.chk.

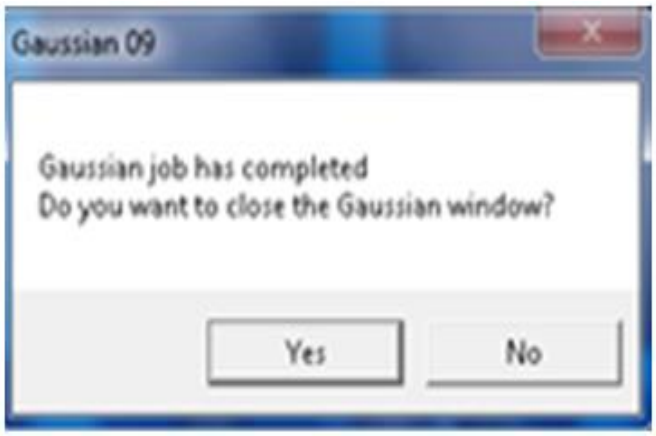

Fig -7: Gaussian Job Completed Window

2. Experimental Methods

2.1Materials

The Medicinal important compounds present in the Coleus aromaticus plant were selected for our work from the literature [12] as given below in **Figure.8-15.**

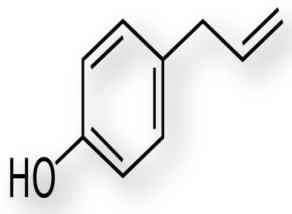

Fig -8: Chavicol

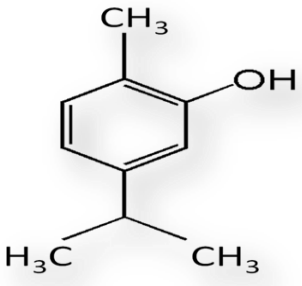

Fig -9: Carvocrol

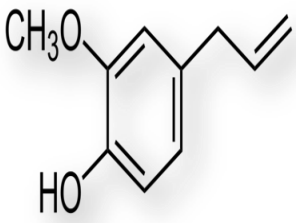

Fig -10: Eugenol

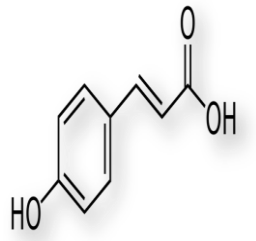

Fig -11: Coumaricacid

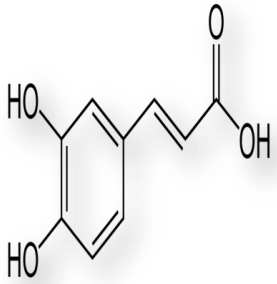

Fig -12: Caffeicacid

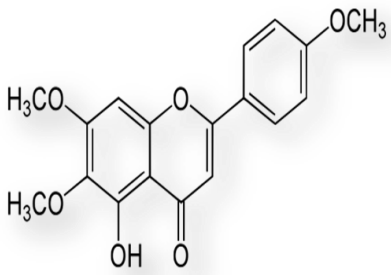

Fig -13: Salvigenin

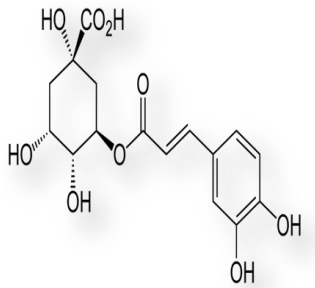

Fig -14: Chlorogenic acid

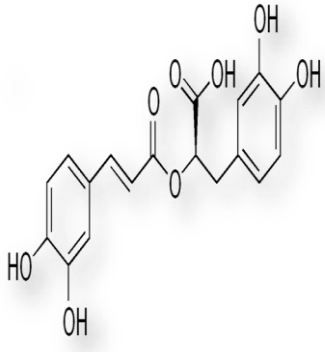

Fig -15: Rosmarinic acid

Table -1: Total Dipole moment (Debye) of compounds in (DFT) method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Chavicol	0.7485	0.8619	1.1594
2.	Carvacrol	1.2985	1.6879	1.9046
3.	Eugenol	1.4050	1.9465	2.3599
4.	Coumaric acid	1.8121	2.4873	3.0908
5.	Caffeic acid	2.8027	3.9856	4.7640
6.	Salvigenin	1.5015	2.2422	2.7262
7.	Chlorogenic acid	2.7062	3.4600	4.2921
8.	Rosmarinic acid	2.0920	2.2483	2.6411

Table -2: Total Dipole moment (Debye) of compounds in (HF) method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Chavicol	1.0261	1.2176	1.4305
2.	Carvacrol	1.4639	1.9634	2.1856
3.	Eugenol	1.9449	2.7802	3.1401
4.	Coumaric acid	2.3804	3.3886	3.9830
5.	Caffeic acid	3.6795	5.1947	5.9198
6.	Salvigenin	1.8496	3.1066	3.6174
7.	Chlorogenic acid	3.4008	5.2197	6.0345
8.	Rosmarinic acid	0.9584	1.8785	2.4003

3. RESULT AND DISCUSSION

DFT Calculation

3.1 B3LYP Method

The dipole moment determination by three basis sets by B3LYP method as given in **Table-1** showed that the compounds Eugenol, Coumaric acid, Salvigenin, Rosmarinic acid were found to be less stable as per the dipole moment in the range STO-3G method (1.4050, 1.8121, 1.5015 and 2.0920) 3-21G method (1.9465, 2.4873, 2.2422 & 2.2483) & 6-31G method (2.3599, 3.0908, 2.7262, and 2.6411) Chlorogenic acid and Caffeic acid were found to have very poor stability as per high dipole moment STO-3G (2.7062, 2.8027), 3-21G(3.4600 & 3.9856) 6-31G (4.2921& 4.7640) respectively. The other compounds like Chavicol and Carvacrol were found have poor dipole moment (0.7485and 1.2985 by STO-3G), (0.8619 and 1.6879 by 3-21G) and 6-31G method (1.1594 and 1.9046). From the above result, it was observed that Chavicol was found to have very low value of dipole moment as 0.7485 by STO-3G, 0.8619 by 3-21G & 1.1594 by 6-31G method and hence it was found to be more stable..

3.2 HF Method

The dipole moment calculated to the above compounds given in Table-2 for the three basis sets. Dipole moment calculated by STO-3G basis sets were 1.0261, 1.4639, 1.9449, 2.3804, 3.6795, 1.8496, 3.4008 & 0.9584 for Chavicol, Carvocrol, Eugenol, Coumaricacid, Caffeicacid, Salvigenin, Cholrogenicacid and Rosmarinic acid compounds respectively. 3-21G basis sets predicted as 1.2176, 1.9634, 2.7802, 3.3886, 5.1947, 3.1066, 5.2197 &1.8785 and 6-31G basis sets showed 1.4305, 2.1856, 3.1401, 3.9830, 5.9198, 3.6174, 6.0345 & 2.4003 as dipole moment values for the above compounds as given in the same order. In HF method also Chavicol compound having lowest dipole moment values as 1.0261 by STO-3G, 1.2176 by 3-21G & 1.4305 by 6-31G basis set. Hence it was found that Chavicol was the more stable compound in coleus aromaticus.

4. CONCLUSIONS

Among the eight compounds selected for the determination of dipole moment to predict their stability. The Caffeic acid was found to have good dipole moment by B3LYP and HF methods Chavicol found to be very poor dipole moment values less than 1500. The compounds Eugenol, Coumaric acid and Rosmarinic acid were found to be less stable. Prediction of dipole moment revealed that Chavicol was found to be more stable than Carvocrol, Eugenol, Coumaricacid, Rosmarinic acid, Salvigeinin, Caffeic acid and Cholrogenic acid. Hence Chavicol can be used as stable drug compared to other compounds

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