In Silico calculations of Dipole moment predictions for the bioactive constituent present in Vitex negundo plant

M.Suganya[1], S.Sunmathi[2], L.Indumathy[2]

[1]*Assistant professor of Chemistry & Department of Chemistry and Physics Nadar Saraswathi College of Arts and Science, Theni, Tamilnadu, India*
[2]*II MSc Chemistry & Department of Chemistry and Physics Nadar Saraswathi College of Arts and Science, Theni, Tamilnadu, India*

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Abstract - *Medicinal important compounds like Vanilic acid, Luteolin, Vitexilactone, Betulinic acid, Urosilicacid, Vitexin, Gardenine B, Gardenine A, Heptamethoxy flaone, Hentriacontane, Negundin A and vitedoamine were taken for our studies. DFT calculations for the for stability determination of dipole moment calculation were carried out using Gaussian software. The dipole moments 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 dipole moment proved that Vanilic acid was recognized to be more stable among other twelve compounds. Because of its good dipole moment and stability it may find as potential medicine for the treatment of disease.*

Key Words: *Vitex negundo plant, Dipole moment, DFT, B3LYP and HF.*

1. INTRODUCTION

Vitex negundo plant belongs to verbenaceae family. Leaves are aromatic, bitter, acrid, astringent, anti- inflammatory, antipyretic or febrifuge, tranquillizer, bronchial smooth muscle relaxant, anti-arthritic, antihelmintic and also used as a mosquito repellent, antiulcerogenic, anti-parasitic, antimicrobial and heaptoprotective [1-6]. The flowers are used to cure fever, liver complaints, and diarrhea. The flowers are used in cholera, haemorrhages, hepatopathy, cardiac disorders, pneumonia and dysentery. Root are used in tonic, febrifuge, expectorant, diuretic, an antidote to snake venom, flatulence, urinary disorders, wounds, ulcers, cough, malarial fever, dysmenorrhoea, skin diseases and general debility [7-9]. Vanilic acid and Luteolin isolated from bark were used in verminosis and opthalmopathy. Compounds like Sabinine, Spathulenol, Vitexilactone Betulinic acid, Urosilic acid reported to have antibacterial and antifungal activities, Crushed leaf is applied on forehead to relieve headache. The leaves and the bark of V.negundo are used in medicine as analgesic, anticonvulsant, antioxidant, insecticide, pesticides. Vitex negundo plant parts are used to cure Asthma, Cancer, Jaundice, urticaria, cellulitis, Abcesses, Carbuncles, Eczema, Liver disorders, kwashiorkor, eye pain and as an antidote for snake bite [10-13]. In our present work dipole moments have been calculated using B3LYP and HF methods [14].

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 **Figure1-5**.

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 -1: 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-2

Fig -2: 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:
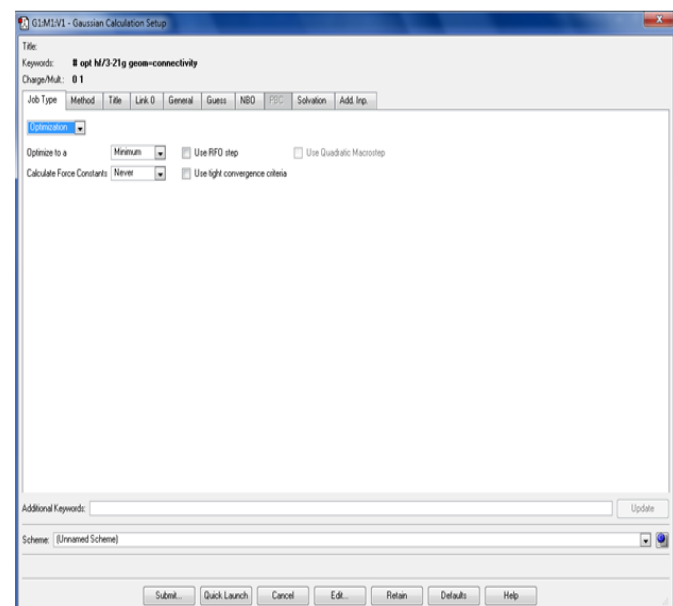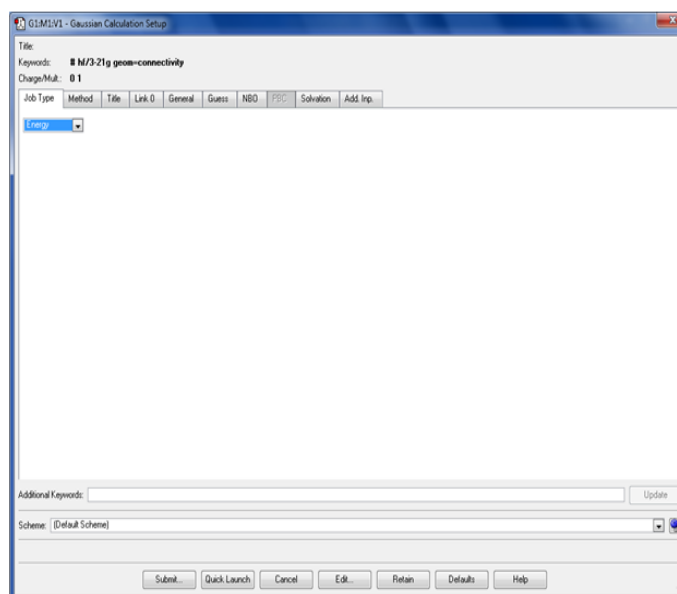

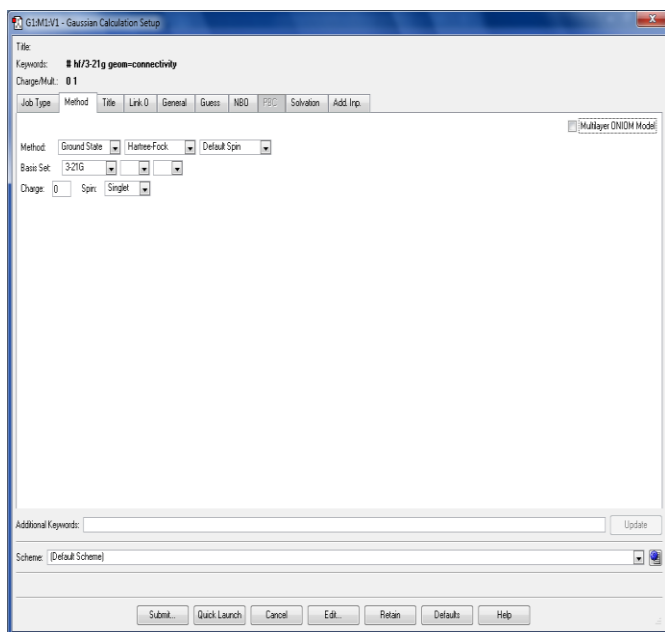**Fig -3**: Energy Calculation setup Windows

Fig -4: 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 -5: Gaussian Job Completed Window

2. Experimental Methods

2.1 Materials

The Medicinal important compounds present in the vitex negundo plant were selected for our work from the literature [9] as given below in **Figure.6-17**.
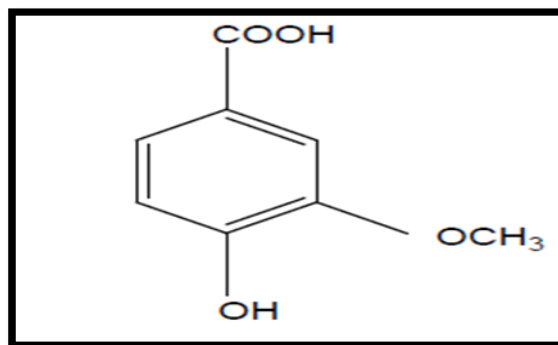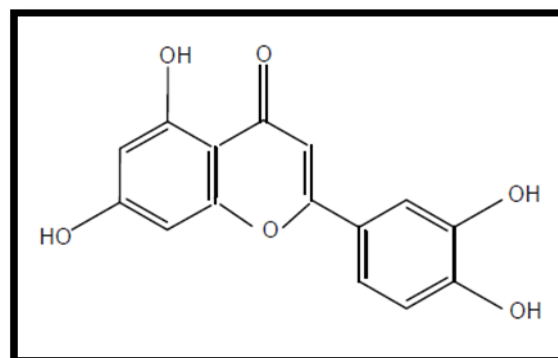

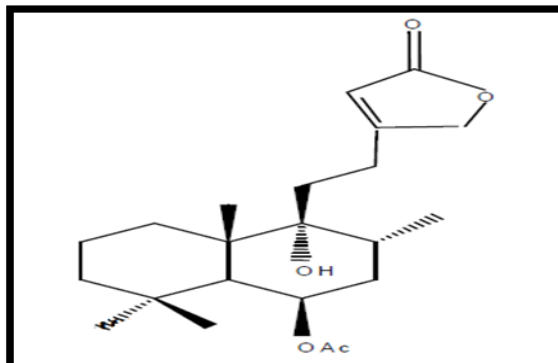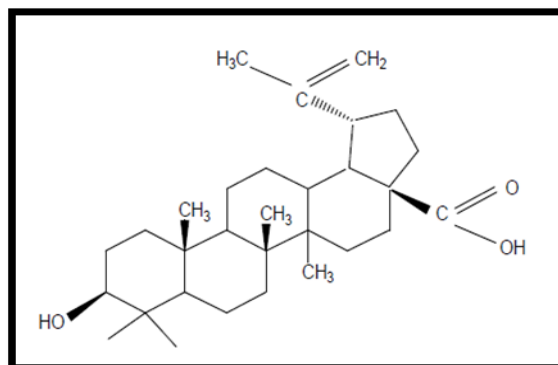**Fig -6**: Vanillic acid

Fig -7: Luteolin
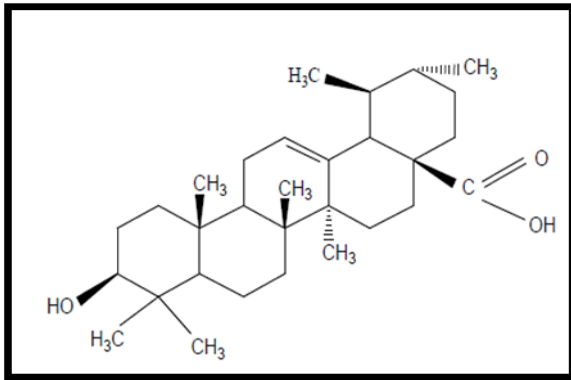

Fig -8: Vitexilactone
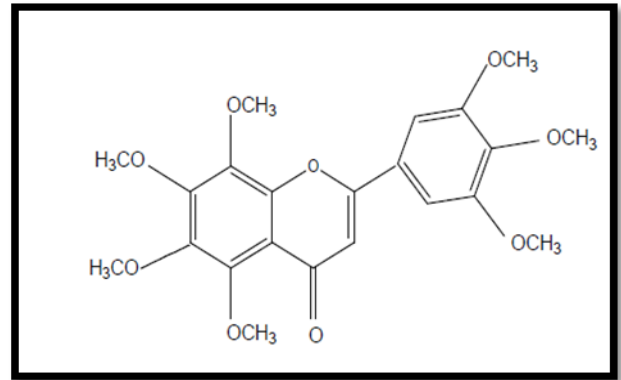

Fig -9: Betulinic acid

Fig -10: Ursolic acid

Fig -11: Vitexin

Fig -12: Gardenin B

Fig -13: Gardenin A

Fig -14: Heptamethoxy flavones
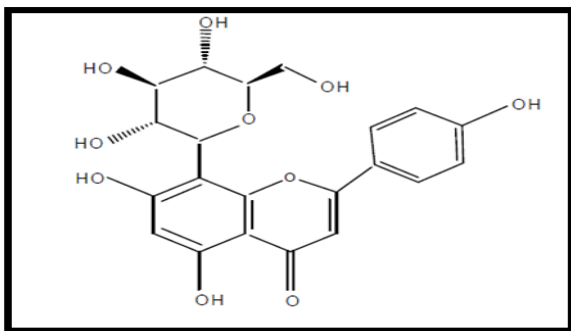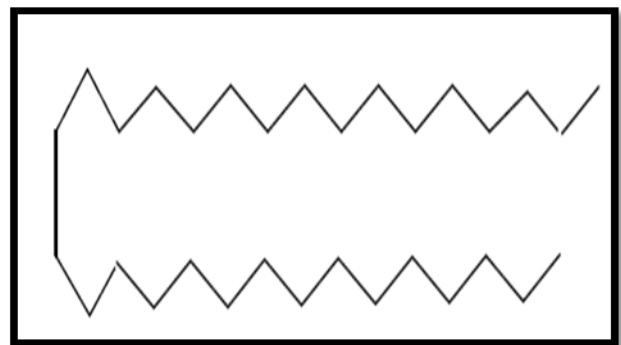
Fig -15: Hentriacontane

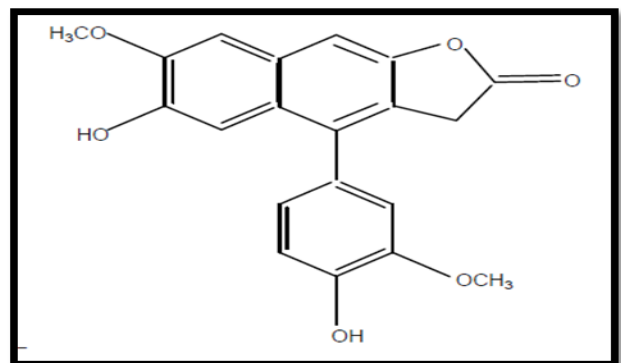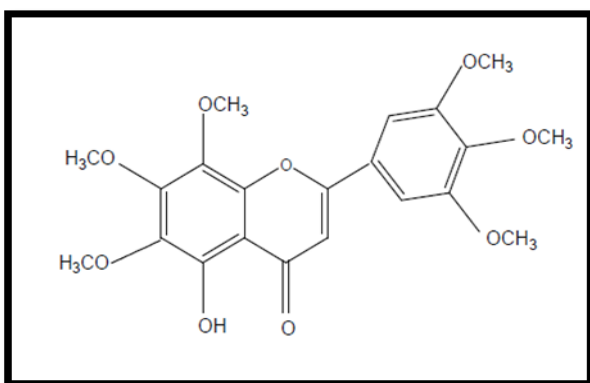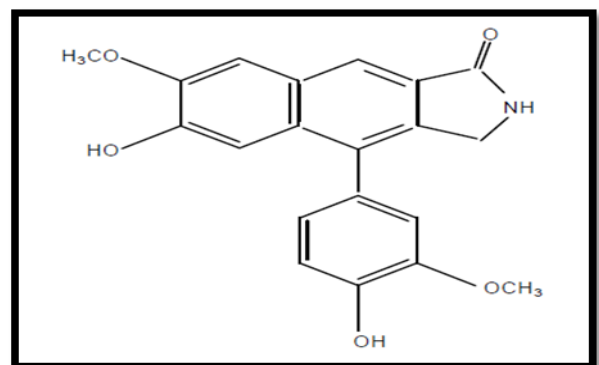**Fig -16**: Negundin A

Fig -17: Vitedoamine

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

S.No	Compounds Name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Vanilic acid	0.4255	0.2992	0.3420
2.	Luteolin	-	6.0536	6.7936
3.	Vitexilactone	-	12.1183	13.3615
4.	Betulinic acid	5.1309	8.1763	8.7068
5.	Ursolic acid	4.8389	7.3812	7.8663
6.	Vitexin	3.7653	5.1096	5.2650
7.	Gardenine B	2.5776	2.7718	3.1616
8.	Gardenine A	2.8057	3.0222	3.3921
9.	Heptamethoxy flaone	1.3744	1.5651	1.6795
10	Hentriacontane	1.3076	1.5624	1.7064
11	Negundin A	9.5100	12.4755	13.3869
12	Vitedoamine	1.9505	3.4022	3.7490

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

S.No	Compounds Name	Basis sets		
		STO-3G	3-21G	6-31G
1.	Vanilic acid	1.1261	0.9449	0.9808
2.	Luteolin	4.8985	7.5116	8.2837
3.	Vitexilactone	16.0907	-	-
4.	Betulinic acid	1.2946	4.0822	4.9535
5.	Ursolic acid	4.2214	5.3772	5.4540
6.	Vitexin	3.5156	5.5572	5.8988
7.	Gardenine B	1.8977	2.9597	3.4779
8.	Gardenine A	2.2951	3.1442	3.5818
9.	Heptamethoxy flaone	1.1843	1.8131	1.8212
10.	Hentriacontane	1.3890	1.7559	1.9194
11.	Negundin A	13.7166	16.3642	17.2466
12.	Vitedoamine	1.3219	3.5999	3.7490

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 where as other compounds like Vanilic acid, Heptamethoxy flaone and Hentriacontane were found have poor dipole moment (0.4255, 1.3744 and 1.3076 by STO-3G), (0.2992, 1.5651 and 1.5624 by 3-21G) and 6-31G (0.3420, 1.6795 and 1.7064). Gardenine A, Gardenine B, Betulinic acid and Ursolic acid were found have moderate dipole moment (2.2951, 2.5776, 5.1309, 4.8389) by STO-3G, (3.0222, 2.7718, 8.1763 and 7.3812) 3-21G and (3.3921, 3.1616, 8.7068 and 7.8663) by 6-31G. Negundin A has higher dipole moment value as 9.5100 by STO-3G, 12.4755 by 3-21G, 13.3869 by 6-31G, it was found to be less stable. From the above results, it was observed that Vanilic acid was found to have lowest dipole moment values STO-3G (0.4255) 3-21G (0.2992) and 6-31G (0.3420).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 1.1261, 4.8985, 16.0907, 1.2946, 4.2214, 3.5156, 2.2951, 1.8977, 1.1843, 1.3890, 13.7166 and 1.3219 for Vanilic acid, Luteolin, Vitexilactone, Betulinic acid, Ursolic acid ,Vitexin, Gardenine A, Gardenine B, Heptamethoxy flaone, Hentriacontane, Negundin A, vitedoamine compounds. 321-G basis sets predicted 0.9449, 7.5116, 4.0822, 5.3772, 5.5572, 2.9597, 3.1442, 1.8131, 1.7559, 16.3642 and 3.5999. 6-31G basis sets showed 0.9808, 8.2837, 4.9535, 5.4540, 5.8988, 3.4779, 3.5818, 1.8212, 1.9194, 17.2466, and 3.7490 as dipole moments for the above compounds as given in the same order. From the above results, it was observed that Vanilic acid was found to have lowest dipole moment values (1.1261, 0.9449, and 0.3420) in HF method & hence it was found to be more stable.

3. CONCLUSIONS

Among the thirteen compounds selected for the determination of dipole moment to predict their stability. The Vanilic acid was found to have lowest dipole moment value by B3LYP and HF methods. Prediction of dipole moment revealed that Vanilic acid was found to be more stable than Luteolin, Vitexilactone, Betulinic acid, Ursolic acid, Vitexin, Gardenine A, Gardenine B, Heptamethoxy flaone, Hentriacontane, Negundin A & vitedoamine compounds. Hence Vanilic acid can be used as stable drug compared to other compounds. Negundin A was found to be very less stability due to their higher dipole moment value (9.5100, 12.4755, & 13.3869 in B3LYP method) (13.7166,

16.3642 &17.2466 in HF method) and hence it was found to be less stable compound in vitex negundo plant.

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BIOGRAPHIES

Assistant professor of Chemistry, Department of Chemistry and Physics,
Nadar Saraswathi College of Arts and Science, Theni.