Evaluation of Stability of the Medicinally Important Compounds in Coleus aromaticus plant by DFT method

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Abstract - *Medicinal important compounds like were selected for their stability determination via binding energy calculation. The binding energy 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 binding energy proved that Rosmarinic acid was recognized to be more stable among other seven compounds. Binding energy byST03-G (-1280.016), 32-1G (-1289.780) and 63-1G (-1296.548) were observed by B3LYP method. HF method binding energies were found to be STO-3G (-1272.803), 321G (-1282.173) and 63-1G (-1288.805). These results showed that among the medicinal compounds present in the Coleus aromaticus plant, Rosmarinic acid 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**: **Coleus aromaticus plant, DFT, B3LYP and HF method.

1. INTRODUCTION:

Coleus aromaticus is basically the family of Lamiaceae. The leaves of the plant are bitter, acrid and were being widely used traditionally for various purposes. The plant has been reported various biological properties [1]. Coleus aromaticus plants of medicinal uses are antiepileptic and antioxidant activities. The Coleus aromaticus leaves are also used for medicinal uses are antiepileptic and antioxidant activities. The Coleus aromaticus leaves are also used for treatment of cough, throat infection and nasal congestion [2-6]. Coleus aromaticus reported antimicrobial activity and oil against pathogenic and non-pathogenic fungi and bacteria [7]. It is also reported to possess remarkable diuretic property and food additive properties. Antioxidant activity is reported to be mainly due to rosmarinic acid, chlorogenic acid and caffeic acid. The essential oil of Coleus aromaticus has great anti-microbial activity on Gram negative as well as Gram positive bacteria, drug resistant microorganism,phytopathogenic microorganism and fungi [8]. It is also reported to possess therapeutic efficacy to treat malarial fever, chronic asthma, cancer, bronchitis, helminthiasis, convulsions and epilepsy [9-10]. It has been reported that the essential oils extracted from these plants have potent activity against microorganisms [11]. In our present work, binding energies of eight constituents were computated using the B3LYP and HF methods by DFT approach.

2. Experimental Methods

2.1 Materials

The medicinal important compounds present in the Coleus aromaticus plant were selected for our work from the literature as given the structures below in **Fig.1-8.**

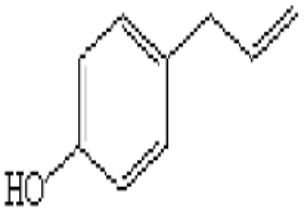

Fig -1: Chavicol

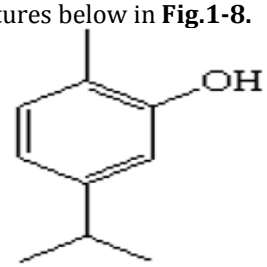

Fig -2: Carvacrol

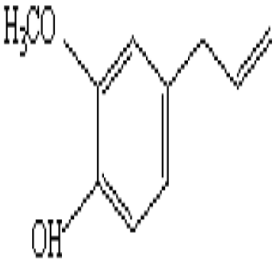

Fig -3: Eugenol

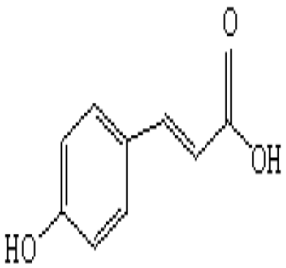

Fig -4: Coumaric acid

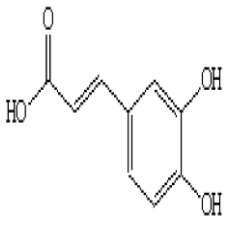

Fig -5: Caffeic acid

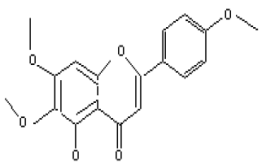

Fig -6: Salvigenin

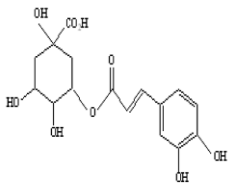

Fig -7: Chlorogenic acid

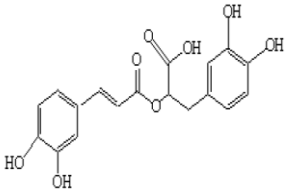

Fig -8: Rosmarinic acid

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 and 6-31G [12].

Table- 1 Binding energy of compounds in B3LYP method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
	Chavicol	-418.681	-421.690	-423.912
2.	Carvacrol	-458.938	-462.168	-464.592
3.	Eugenol	-531.683	-535.572	-538.381
4.	Coumaric acid	-565.735	-569.999	-573.004
5.	Caffeic acid	-639.883	-644.788	-648.184
6.	Salvigenin	-1131.982	-1140.441	-1146.406
7.	Chlorogenic acid	-1279.691	-1289.660	-1296.403
8.	Rosmarinic acid	-1280.016	-1289.780	-1296.548

Table- 2 Binding energy of compounds in HF method

S. No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
	Chavicol	-416.032	-418.942	-421.126
2.	Carvacrol	-456.037	-459.125	-461.506
3.	Eugenol	-528.441	-532.180	-534.936
4.	Coumaric acid	-562.433	-566.546	-569.492
5.	Caffeic acid	-636.264	-640.978	-644.304
6.	Salvigenin	-1125.510	-1133.613	-1139.461
7.	Chlorogenic acid	-1272.635	-1282.135	-1288.736
8.	Rosmarinic acid	-1272.803	-1282.173	-1288.805

Result and Discussion

2.2 DFT Calculation

2.2.1 B3LYP Method

The binding energy determination by three basis sets by B3LYP method as given in **Table-1** showed that whereas other compounds like Chavicol and Carvacrol were found have poor binding energy (-418.681 and – 458.938 a.u. by STO-3G), (-421.690 and -462.168 a.u. by 3-21G) and 6-31G method (-423.912 and -464.592 a.u.). The compounds Eugenol, Coumaric acid, Caffeic acid and Salvigenin were found to be less stable as per the binding energy in the range STO-3G method (-531.683, -565.735, -639.883 and -1131.982) a.u. 3-21G method (-535.572, -569.999, -644.788 and -1140.441) a.u. & 6-31G method (-538.381, -573.004, -648.184 and -1146.406) a.u. Chlorogenic acid and Rosmarinic acid were found to have good binding energy STO-3G (-1279.691 & -1280.016 a.u.), 3-21G (-1289.660 & -1289.780 a.u.) 6-31G (-1296.403 & -1296.548 a.u.) respectively.

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 -416.032, -456.037, -528.441, -562.433, -636.264, -1125.510, -1272.635 & -1272.803 a.u. for Chavicol, Carvocrol, Eugenol, Coumaricacid, Caffeicacid, Salvigenin, Cholrogenicacid and Rosmarinic acid compounds. 3-21G basis sets predicted –418.942, -459.125, -532.180, -566.546, - 640.978, -1133.613, -1282.135 & -1282.173 a.u. and 6-31G basis sets showed -421.126, -461.506, -534.936, -569.492, -644.304, -1139.461, -1288.736 & -1288.805 a.u. as binding energies for the above compounds as given in the same order.

4. Conclusion

Among the eight compounds selected for the determination of binding energy to predict their stability. The Rosmarinic acid was found to have good binding energy by B3LYP and HF methods Chavicol and Carvacrol were found to be very poor binding energy values less than -500 a.u. The compounds Eugenol, Coumaric acid and Caffeic acid were found to be less stable as per the binding energy values less than -1000 a.u. The Rosmarinic acid was found to have very good binding energy by both the B3LYP method (-1280.016, -1289.780 & -1296.548 a.u.) and by HF method (-1272.803, -1282.173 & -1288.805a.u.) compared to other compounds. Prediction of binding energy revealed that Rosmarinic acid was found to be more stable than Chavicol, Carvocrol, Eugenol, Coumaricacid, Caffeic acid, Salvigeinin, and

Cholrogenic acid. Hence Rosmarinic acid can be used as stable drug compared to other compounds.

Reference

1. Om Prakash Rout, Rabinarayan Acharya, Sagar Kumar Mishra,ss Rashmibala Sahoo Pathorchur (coleus aromaticus): a review of the medicinal evidence forits phytochemistry and pharmacology properties, 2012; 3(4), 0976-4550.
2. Murthy PS, Ramalakshmi K and Srinivas P, Fungitoxic activity of Indian borage (Plectranthus amboinicus) volatiles, Food Chemistry 2009; 114: 1014–1018.
3. Ragasa CY, Sangalang V, Pendon Z and Rideout JA, Antimicrobial flavones from Coleus amboinicus Philippine J. of Sci. 1999; 128: 347-351.
4. Pritima RA, Selvaraj R and Pandian RS, Antimicrobial activity of Coleus aromaticus (Benth) against microbes of reproductive tract infections among women, Afr. J. Infect. Diseases 2008; 1: 18 – 24.
5. Gurgel APAD, da Silva JG, Grangeiroa ARS, Oliveira DC, Limaa CMP, da Silvaa ACP, Oliveira RAG and Souzac IA, In vivo study of the anti-inflammatory and antitumor activities of leaves from Plectranthus amboinicus (Lour.) Spreng (Lamiaceae), J. of Ethnopharmacol, 2009; 125: 361–363.
6. Buznego MT and Perez-Saad H. Antiepileptic effect of Plectranthus amboinicus (Lour.), Spreng. Rev. Neurol. 1999; 29: 229-32.
7. Rao A, GSJG, Baby P and Prasad RY. Leaf oil of Coleus amboinicus Lour: the in vitro anti-microbial studies. Perfume and Kosmetik. 1991; 72(11): 744-45.
8. Rashmi Sahay Khare, Shanta Banerjee and Kanika Kundu Coleus aromaticus benth – a nutritive medicinal plant of Potential therapeutic value International Journal of Pharma and Bio Sciences.2011; 488-500.
9. Mohammad MS, Alireza SD, Mahnaz K, Mohammad RA, Fatemeh M, Hassan V. Chemical composition and larvicidal activity of essential oil of Cupressus arizonica E.L. Greene against malaria vector Anopheles stephensi Liston (Diptera: Culicidae). Pharmacognosy Res 2011; 3(2):135-139.
10. S. K. Gangai Abirami and Dr.P.Nirmala A comparative – invitro study of anticancer effect of menthe piperita, ocimum basilicum and coleus aromaticus against human laryngeal epidermoid carcinoma (HEP-2) cell lines. Journal of Medicinal Plants Studies 2014, 3(1); 6-9.
11. Shipradeep and Sourish Karmakar et al, Development of Probiotic Candidate in Combination with Essential Oils from Medicinal Plant and their Effect on Enteric Pathogens. Gastroenterology Research and Practice 2012; 1-6.
12. G.Valli* & M.Suganya computation of binding energy of bioactive constituents present in cassia fistula species by DFT approach 2015; 119-125.