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SEMI EMPIRICAL AM1 CALCULATIONS OF A FLAVONE: "5,6,7-TRIHYDROXY-4'-METHOXY FLAVONE"

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ABSTRACT: Flavones are naturally occurring polyphenolic compounds known as non-toxic anti oxidants which mainly come from higher plants including seaweeds. These compounds possess a range of physiological properties and extensive literary information is available, but fewer theoretical insights of these compounds have been explored. In this paper, semi empirical Austin Model 1 (AM1) calculations has been reported for a flavone: "5,6,7-trihydroxy-4'-methoxy flavone" to predict the electronic structure and certain properties e.g. geometry optimization, total energy, dipole moments, and heat of formation etc.

KEY WORDS: Flavones, semi empirical calculations, molecular modeling.

INTRODUCTION

Marine algae are rich sources of structurally diverse bioactive compounds with various biological activities. Marine macro algae are important resource ecologically and commercially, being used as human food, animal feed and raw material for many industries, including pharmaceutical. Marine algae are rich in sulfated polysaccharides (SPs) such as carrageenans in red algae, fucoidans in brown algae and ulvans in green algae. These SPs exhibit many health beneficial nutraceutical effects such as antioxidant, anti-allergic, anti-human immunodeficiency virus, anticancer and anticoagulant activities. Generally algae shows higher antioxidant activity due to higher contents of nonenzymatic antioxidant components, such as ascorbic acid, reduced glutathione, phenols and flavonoids. Flavonoids are polyphenolic compounds known as non-toxic anti oxidants. Various studies revealed that high dietary intake of natural phenolics reduce the risk of developing some chronic diseases, carcinoma, blood pressure, diabetes and enhances life expectancy.

Over 4000 different flavoroids have been described. Flavonoids comprises of 15 carbon atom, two benzene rings joined by a linear three carbon chain. They are also known to serve a variety of important functions in plants including gene sequence and protein location. They are plant secondary metabolites, and the derivatives of 2-phenyl-benzyl-γ-pyrone are present throughout the plant kingdom, and a range of biological and physiological properties are associated with them (Sabina and Aliya, 2009). The figure. 1 shows the structure of 5,6,7-trihydroxy-4'-methoxy flavone.

Semi empirical methods are based upon parameterization of experimental and high level calculation data, hence they are able to execute calculations rapidly for smaller and medium sized systems (Arora and Kumar, 2001; Krossing and Slattery, 2006). Molecular properties, electronic structure and spectral information can be calculated nearly

accurately by these methods when the working system is similar to the parameterization of the method used. We have selected Austin Model 1 (AM1) Hamiltonian for this work.

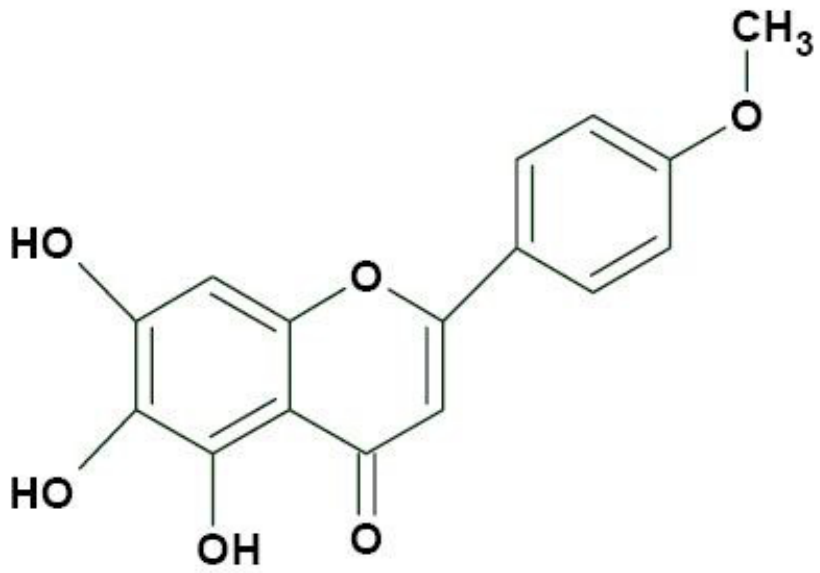

Fig. 1. Structure of 5,6,7-trihydroxy-4'-methoxy flavone.

COMPUTATIONAL DETAILS

All computations were performed on an Intel Pentium 4 computer with 1.0 GHz CPU and 2.0 GB of physical memory. Molecular modeling was done by ArgusLab 4.0.1 software (Thompson, 2004) and Merck Force Field (MMFF94) (Halgren, 1999) was used for initial geometry clean up. The geometry was optimized by semi-empirical AM1 Hamiltonian implemented in GAMESS software program (Schmidt *et al*., 1993). GAMESS was also used for calculating heat of formation, IR spectrum prediction, population analysis, total energy and dipole moments. Results of the computations were visualized by ChemCraft version 1.6 including high resolution image of the optimized structure and simulated IR spectrum (Zhurko and Zhurko, 2009).

RESULTS AND DISCUSSION

The starting geometry got smoothly optimized initially by MMFF94 molecular mechanics method followed by AM1 semi empirical method. The optimized geometry is given in *figure 2* with atomic labels and all bond lengths. The *table 1* lists some of the calculated properties and *table 2* lists Mulliken Charges. The *figure 3* shows the simulated IR spectrum of the title compound.

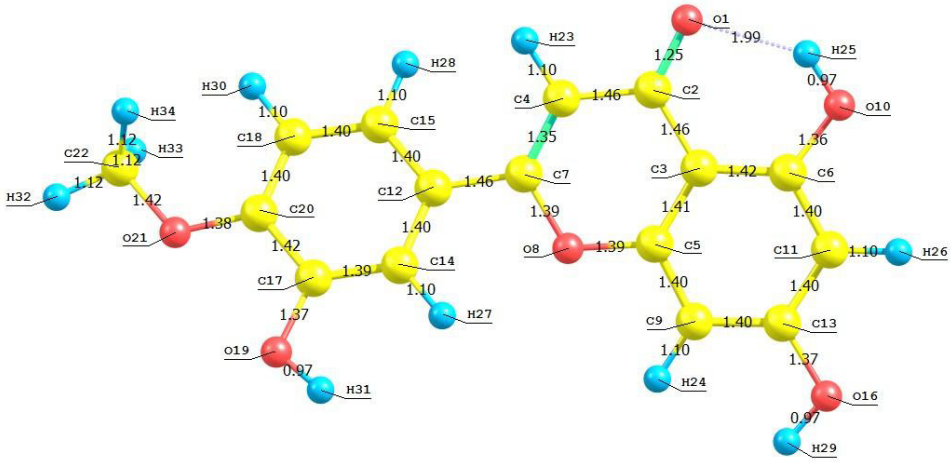

Fig. 2. Optimized geometry of 5,6,7-trihydroxy-4'-methoxy flavone.

Table 1. Calculated Properties.

Calculated Properties	**AM1**
Zero Point Energy (J/mol)	689624.8
Total Energy (kCal/mol)	-95345.8
Heat of Formation (kCal/mol)	-163.5
Dipole Moment (Debye)	4.0

Table 2. Mulliken Charges.

Calculated Mulliken Charges			
O1	-0.3728	C18	-0.24453
C2	0.367245	O19	-0.27762
C3	-0.33052	C 20	0.094636
C4	-0.35752	O21	-0.22128
C5	0.18561	C22	-0.21145
C6	0.225784	H23	0.24169
C7	0.152043	H24	0.223406
O8	-0.18224	H25	0.311477
C9	-0.34815	H26	0.249607
O10	-0.30469	H27	0.218566
C11	-0.28988	H28	0.210417
C12	-0.0762	H29	0.266608
C13	0.169543	H30	0.211872
C14	-0.20303	H31	0.256239
C15	-0.14251	H32	0.168255
O16	-0.29174	H33	0.122334
C17	0.056263	H34	0.122584

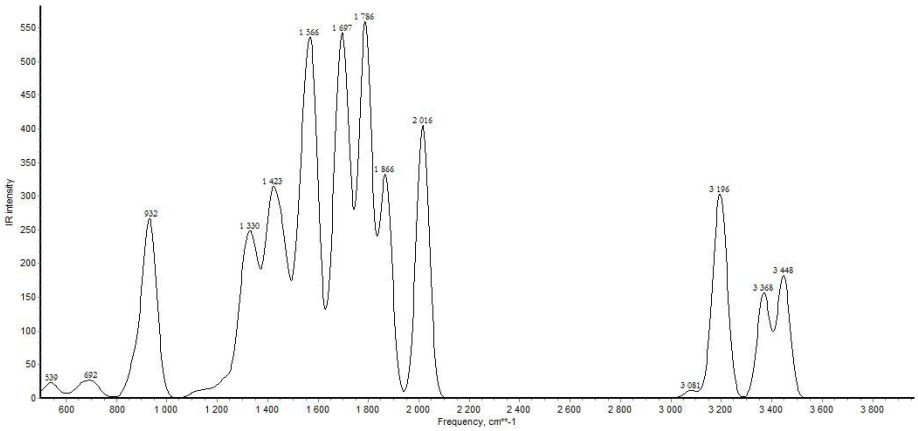

Fig. 3. Simulated IR Spectrum.

CONCLUSION

In this piece of work an attempt was made to explore some theoretically calculated properties e.g. geometry optimization, total energy, dipole moments, and heat of formation of "5,6,7-trihydroxy-4'-methoxy flavone", by using semi empirical method, and the results have been presented accordingly.

REFERENCES

Arora, K. and D. Kumar. 2001. *Semi-Empirical AM1 and PM3* Calculations for Electronic Structure of a Pyrazolone. *Asian J. Chem.* 13(4): 1325-1329.

Halgren, T.A. 1999. *MMFF VII.* Characterization of *MMFF94, MMFF94s,* and other widely available force fields for conformational energies and for intermolecular-interaction energies and geometries. *J. Computational Chem.* 20(7): 730-748.

Krossing, I. and J.M. Slattery. 2006. Semi-empirical methods to predict the physical properties of ionic liquids: An overview of recent developments. *Zeitschrift für Physikalische Chemie*. 220(10): 1343-1359.

Sabina, H. and R. Aliya. 2009. Seaweed as a New Source of Flavone, Scutellarein 4'-Methyl-Ether. *Pak. J. Bot.* 41(4): 1927-1930.

Schmidt, M.W., K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, Shyjun Su, T.L. Windus, M. Dupuis and J.A. Montgomery. 1993. General atomic and molecular electronic structure system. *J. Computational Chem.* 14(11): 1347-1363.

Thompson, M.A., 2004. *ArgusLab 4.0. 1.* Planaria Software LLC, Seattle, WA.

Zhurko, G. and D. Zhurko. 2009. Chemcraft—Graphical program for working with quantum chemistry computations. Version 1.6. 2009.