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A new approach to teach the stability of anethole in different solutions as theoretical

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Abstract

Anethole, having medical activity for a lot of diseases and used in the food industry, is changing solublity in different solutions (water, ethanole, methanol especially in blood). we prefer safe, cheap and time-saving materials to teach the properties of the most important effective substances in plants. We selected anethole to teach as a subject for this study to explain the properties in different solutions by using DFT method as theoretical.

Keywords: *Natural Product, Anethole, Ethanole, Methanol, Water, blood, DFT*

1. Introduction

Anothole is an aromatic compound (Soares, et al.,2007; Wang, et al.,2006; Fiori, et al.,2002) having anticancerogenic (Al-Harbi, et al.,1995), antioxidant (Freire, et al.,2005), anti-inflammatory (Chainy, et al.,2000), anaesthetic (Ghelardini, Galeotti, Mazzanti, 2001), properties. Trans-anethole formed the characteristic sweet aroma of anise (Pimpinella anisum, family Apiaceae) seeds and leaves (Takao et al., 2009). It was especially largely used in the food industry as flavors or odorant, for cakes, ice-creams, and a wide range of alcoholic beverages (Jurado, et al. 2006; Adam, et al.,2013; Andrzej, Dawidowicz, 2014).

Anethole strongly binds with plasma proteins. Only a small amount of anethole exists in free form. Anethole is a natural compound as the mainly component of the essential oil of star anise, comprising more than the others volatile components. The levels of nitric oxide (NO) and prostaglandins (PGE2) in the inflammatory in particular were reduced by treatment with anethole (Domiciano, et al.,2013). The higher levels of NO support pathways inducing cell cycle arrest, mitochondria respiration, senescence, or apoptosis (Napoli, et al.2013). Donati et al (2015) studies showed that Antioxidant capacity of anethole is higher according to TEAC values (Donatia, et al.2015). Anti-inflammatory and antidiarrheal activities with the common mechanism in both models by inhibition of PGE2 production, that makes a great contribution to understanding the pharmacological properties of this species (Beserra, et al.2016).

The neuroprotective effect of trans-anethole on neuronal injury might be due to its ability to inhibit excitotoxicity, oxidative stress and mitochondrial dysfunction. Considering these multiple

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pathways causing ischemic neuronal damage, the multifunctional effect of trans-anethole suggested that it may be effective in treating ischemic stroke (Ryu, Seol, Park, & Choi, 2014).

"This "oil" consists mainly of trans-anethol, which is an ester with a very specific odor that gives its unique anise smell to these beverages. Anethol is soluble in ethanol but extremely insoluble in water. When bottled, the ratio between the ethanol, water, and oil is chosen in such a way that the oil is still soluble in the mixture, so the mixture appears transparent. However, when the alcoholic beverage is poured into water, the oil is no longer soluble. This causes the oil droplets to form in the solution due to the supersaturation of the oil. The tremendous decrease in solubility due to the addition of water causes a very large supersaturation, so that many nuclei form from small fluctuations in concentration". When the visible light gets multiply scattered within the solution, as a result of this, the light makes the solution to appear milky white due to the forming a lot of droplets in the solution. If the amount of ethanol increases the stability of the emulsions in solution will also increase (Ganachaud, & Katz, 2005; Bouchemal, et al.2004; Scholten, Linden, & This, 2008)

Computer-aided programs can help the learner in several situtations and quite useful in the clssrooms. As a result of the increasing the demand fort he simulations programs, the scientist, programmer of them were increased, Moreover, a lot of learner reached them easily (Harrison, A.1989; Rutherford, F.J & Ahlgren, A.1996). If the students had problems about theoretical compherension. In this processes, students that had lack of knowledge of theory must be participant of the Project of computer aided simulations programmes step by step actively to compheresive the theory of the subject. The programmer of the Teacher of the theoretical subjects (Moursund, 1995; Yaşar, 2006) . Sanders (2014) emphasized that a new specialized developed software modules were integreated for all classroom especially graduate course cirriculum in future classrooms by the experts of this programs having experience and content knowledge (Sanders, Faesi, Goodman, 2014).

In this study, we prefer safe, cheap and time-saving materials to teach the properties of the most important effective substances in plants. Anethole is the mainly component of star anise (Illicium verum Hook.f., family Illiciaceae) and anise (Pimpinella anisum, family Apiaceae) seeds and leaves.

We selected anethole to teach as a subject for this study to explain the properties in different solutions.

2. Materyal and method

The electronic structures of Anethole are studied by DFT and HF, included in DFT and HF methods, containing Becke's gradient correction for exchange, and RB3LYP methods were used for quantum chemical calculations and geometry optimization. In the case of the RB3LYP functional, the non-local correlation was provided by the LYP expression, and the correction was carried out by means of the 6-31+g(d,p) functional (Gökalp, F.,2014). The thermodynamic values in blood were calculated by using DFT and HF method. The correction was carried out by means of the 6-31+g (d,p) functional. These methods and fully optimized geometric structure of the compounds using this method were determined and evaluated.

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3. Result and discussions

The extraction of limonene obtained from the orange peel was very successful, anethole (Fig 1) was nontoxic and the majority of the material getting from the extraction from fennel seed (Bodsgard, Lien, & Waulters, 2016).

The anethole's molecular structures are given in the Figure 1

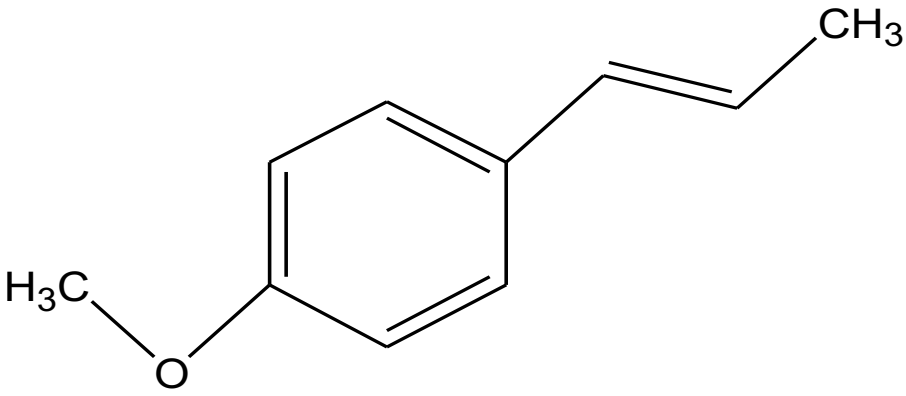

Figure 1 Molecular Structure of Anethole

The Anethole in different solutions (water, ethanol, methanol and blood) values of ΔG, HOMO, LUMO, Δ (HOMO-LUMO) and Dipol Moment by using DFT is given in Table 1.

Table 1. The Anethole in different solutions (water, ethanol, methanol and blood) values of ΔG, HOMO, LUMO, Δ (HOMO-LUMO) and Dipol Moment by using DFT

DFT	ΔG (Hartree)	HOMO (eV)	LUMO (eV)	Δ (HOMO-LUMO) (eV)	Dipol moment (Debye)
Anethole in water	-463.368590	-0.21344	-0.03590	-0.17754	1.5235
Anethole in ethanol	-463.368286	-0.21311	-0.03559	-0.17752	1.5034
Anethole in methanol	-463.368391	-0.21322	-0.03570	-0.17752	1.5103
Anethole in blood	-463.374710	-0.21108	-0.3521	-0.14102	1.5827

The gibbs energy, HOMO, LUMO, Δ (HOMO-LUMO) and Dipol Moment values of Anethole in Table 1 and Table 2 close to each other. For the water phase; the values are greater than ethanole and methanole. The stability of Anethole increase in the order of ethanole, methanole, water and blood. The solubility order of anethole for these phases; ethanole, methanol, water and blood. This event explained in literature (Ganachaud, & Katz, 2005; Bouchemal, et al., 2004; Scholten, Linden, & This, 2008).

The Anethole in different solutions (water, ethanol, methanol and blood) values of ΔG, HOMO, LUMO, Δ (HOMO-LUMO) and Dipol Moment by using DFT is given in Table 2.

ISSN: 2149-5939

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Table 2. The Anethole in different solutions (water, ethanol, methanol and blood) values of ΔG, HOMO, LUMO, Δ (HOMO-LUMO) and Dipol Moment by using HF

HF	ΔG (Hartree)	HOMO (eV)	LUMO (eV)	Δ (HOMO-LUMO) (eV)	Dipol moment (Debye)
Anethole in water	-460.362096	-0.28937	0.04200	-0.24737	1.6570
Anethole in ethanol	-460.361716	-0.28897	0.04202	-0.24695	1.6349
Anethole in methanol	-460.361846	-0.28911	0.04201	-0.24710	1.6425
Anethole in blood	-460.373074	-0.28896	0.07571	-0.21325	1.6074

Bodsgard et al. emphasized that Green chemistry had been increasingly the focus of a wide array of experiments at all levels of chemistry to impress upon students the importance of cleaner and less hazardous techniques (Bodsgard, Lien, & Waulters, 2016). . Therefore, we prefer cleaner, safe, cheap and time-saving techniques for teaching the activity of substances fort he medicinal plants. Anethole is an important example of them as calculated in this article.

4. Conclusions

As mentioned above as literatüre knowledge (Bodsgard, Lien, & Waulters, 2016); We can use the theoretical calculations by using DFT and HF to teach the stability and the solubility of Anethole for different phases because it is safe,time-saving and effective method to apply different active compounds of plants.

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