Cumhuriyet Science Journal
CSJ

e-ISSN: 2587-246X
ISSN: 2587-2680

Cumhuriyet Sci. J., Vol.39-1(2018) 66-70

Theoretical Study on Flavonoids Isolated from *Allium vineale*

TunayKARAN[1], Faik GOKALP[2], Ramazan ERENLER[3]*

[1]*Department of Molecular Biology and Genetics, Faculty of Arts and Sciences, Gaziosmanpasa University, 60240 Tokat, TURKEY*

[2]*Department of Mathematics and Science Education, Faculty of Education, Kırıkkale University, 71450 Kırıkkale, TURKEY*

[3]*Department of Chemistry, Faculty of Arts and Sciences, Gaziosmanpasa University, 60240 Tokat, TURKEY*

Received: 08.10.2017; Accepted: 11.12.2017 *http://dx.doi.org/10.17776/csj.342297*

Abstract: The chemical properties of chrysoeriol-7-*O*-[2"-O-E-feruloyl]-*β*-D-glucoside (**1**), chrysoeriol (**2**), and isorhamnetin-3-*β*-D-glucoside (**3**) from *Allium vineale* have been investigated as theoretical. RHF/STO-3G method was used for quantum calculations of chemical properties of these compounds. The structures of the compounds were fully optimized and then the results were evaluated by this method. The properties of compounds were presented and the utilization of these compounds in various fields was investigated by comparison of theoretical results with experimental ones. The experimental antioxidant effects were reported previously. The quantum calculations revealed that chrysoeriol (**2**) was unstable and was prone to react to the radical compounds. In brief, a good antioxidant can donate the electron to the radical compound easily.

***Keywords*:** Activity, flavonoids, theoretical calculation

Allium vineale Bitkisinden İzole Edilen Flavonoidler Üzerinde Teorik Çalışmalar

Özet: *Allium vineale*'dan izole edilen kiseriol-7-O-[2"-O-E-ferulil]-*β*-D-glukosit (**1**), kiseriol (**2**) ve isorhamnetin-3- *β*-D-glukosit (3) bileşiklerinin kimyasal özellikleri teorik olarak araştırıldı. Bu bileşiklerin kimyasal özellikleri hesaplanırken RHF/STO-3G metodu kullanıldı. Bileşiklerin optimizasyonu ve sonuçların değerlendirilmesi bu metodla gerçekleştirildi. Bileşiklerin özellikleri ortaya kondu, ayrıca teorik ve deneysel sonuçların karşılaştırılması ile ilgili bileşiklerin değişik alanlardaki kullanımları araştırıldı. Bileşiklerin antioksidan özellikleri daha önce rapor edildi. Hesaplamalar, kiseriol (**2**) bileşiğinin kararsız ve radikal bileşiklerle tepkime verme eğiliminde olduğunu gösterdi. Özetle, antioksidan bileşikler radikal bileşiklere kolaylıkla hidrojen vermektedir.

***AnahtarKelimeler*:** Aktivite, flavonoidler, teorik hesaplamalar

1. INTRODUCTION

Flavonoids are polyphenolic secondary metabolites produced by plants abundantly and play a significant role in plant physiology [1-5]. These compounds are also found in plant-related food including fruits, vegetables, herbs, oil nuts as well as in beverages such as tea and coffee [6].

Flavonoids protect plants against oxidative cell injury, ultraviolet radiation, pathogens and

* Corresponding author. *Email address:* *rerenler@gmail.com*

predators. In addition they control the transport of auxins and act as a function of pollination via coloration of flowers [7]. The amount of flavonoids in fruit and vegetables may vary due to the species variety, climatic condition, cultivation form, ripeness degree [8]. Moreover, storage and culinary process can also affect the content of flavonoids [9].

The estimation of daily dietary intake of flavonoids is difficult, due to the high number of food sources, their common distribution in plants, and diverse form of consumption [10]. Flavan-3-ols are generally found in tea, flavanones in citrus fruits, anthocyanidins in colored fruits such as cherries and grapes [11]. The blue, red and violet colours of fruits are gained from anthocyanidins that increase with the maturation [12]. Isoflavonoids (isoflavones, isoflavanones, and isoflavonols) are present in legumes [9]. Aromatic plants are outstanding source of flavonoids [13].

Phytochemical investigation on flavonoids revealed a large amount of biological effects such as anticancer [14, 15], antioxidant [3], anti-inflammatory, vasodilative, anticoagulative, proapoptotic activities [16] and against Alzheimer's disease [17].

Herein, we investigated the chemical properties of flavonoids isolated from *Allium vineale* theoretically and presented the relationship between the experimental results and theoretical calculation results.

2. MATERIAL and METHODS

The chemical properties of chrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**), chrysoeriol (**2**), and isorhamnetin-3-*β*-D-glucoside (**3**) from *Allium vineale* were determined as experimental and theoretical: The output dates of the molecule which was drawn on Chem Draw Ultra 11.0 is drawn in Chem 3D. It was calculated theoretically by using RHF/STO-3G bases in Gaussion 09W programme.These methods and fully optimized geometric structures of the compounds using this method were determined and evaluated.

3. RESULTS and DISCUSSION

It was resulted in Table 1 from the calculation on Gaussian 09 with RHF/STO-3G of chrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**), chrysoeriol (**2**), and isorhamnetin-3-*β*-D-glucoside (**3**) from *Allium vineale* (Figure 1).

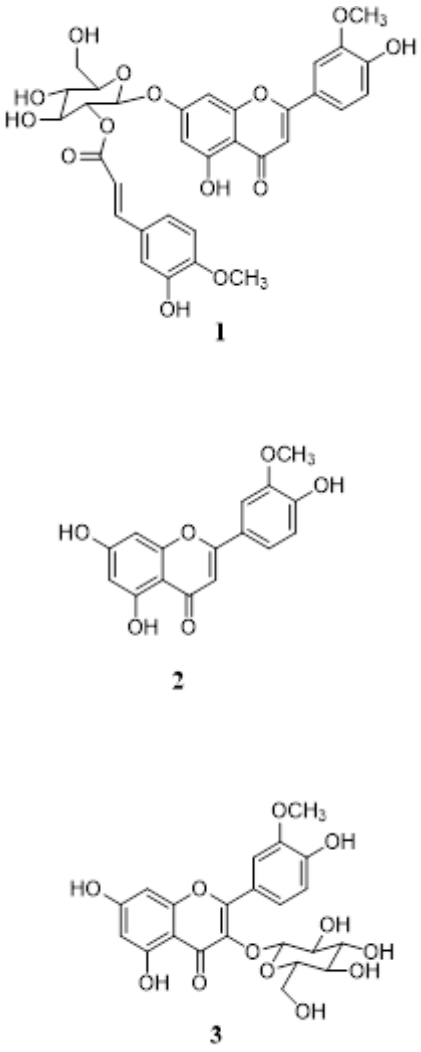

Figure 1. Theoretical calculation was executed for the compounds isolated from *A. Vinaleae.*

Table 1. The chrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**), chrysoeriol (**2**), and isorhamnetin-3- *β*-D-glucoside (**3**) values of HF, HOMO, LUMO, Δ (HOMO-LUMO) and dipole moment by using RHF/STO-3G.

	Chrysoeriol **2**	Isorhamnetin-3-*β*-D-glucoside **3**	Chrysoeriol-7-*O*-[2"-O-E-feruloyl]-*β*-D-glucoside **1**
HF	-1048.46704928	-1721.74847398	-2249.35232157
Dipol moment	4.8643	6.8876	7.7399
HOMO	-0.22449	-0.22647	-0.22664
LUMO	0.18575	0.19306	0.17866
η = εLUMO–εHOMO	0.41024	0.41953	0.40530

In previous work, we isolated chrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**), chrysoeriol (**2**), and isorhamnetin-3- *β*-D-glucoside (**3**) from *Allium vineale* and presented the antioxidant activities [18].

The order of metal chelating and DPPH free radical activity was as follow: chrysoeriol (**2**)>isorhamnetin-3- *β*-D-glucoside (**3**)> **c**hrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**). This result accorded with the theoretical study that HOMO values were -0.22449, -0.22647 and -0.22664 for compound **2**, compound **3** and compound **1** respectively. High HOMO value indicated the electron releasing ability of a compound. A good antioxidant can donate the electron to the radical compound easily.

E_{HOMO} is a quantum chemical parameter related to the electron donating ability of the molecule. If a molecule has high value of $E_{HOMO,}$ it will donate electrons to appropriate acceptor molecule of low empty molecular orbital energy [19].

Ionization potential (I) is defined as the amount of energy required to remove an electron from a molecule [20]. It is related to the energy of the E_{HOMO} through Eq. (1): $I = -E_{HOMO}$

The large HOMO–LUMO gap means high excitation energies for many of excited states, a good stability and a high chemical hardness [21]. A small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, Global hardness (η) can rewritten using Koopman's theorem: η = εLUMO – εHOMO.

Metal bond strength between interaction of acceptor (metal (II) halides) and donor (ligand) increases as the energy lowering [22]. In our theoretical calculations; chrysoeriol-7-*O*-[2"-*O*-E-feruloyl]-*β*-D-glucoside (**1**) has the lowest HOMO-LUMO gap, high polarity but a weak electron acceptor due to having lower LUMO. Isorhamnetin-3- *β*-D-glucoside (**3**) is the best electron acceptor because of having highest LUMO.

4. CONCLUSION

Asa result of theoretical calculations; we can assume that chrysoeriol (**2**) is unstable and tend to react to the radical molecules. In brief, a good antioxidant can donate the electron or hydrogen to the radical compound easily. It may be effective as destroying the cell structure of harmful microorganisms in the metabolism.

Conflicts of interest

The authors stated that did not have conflict of interests.

REFERENCES

[1] Erenler R., Telci I., Ulutas M., Demirtas I., Gul F., Elmastas M. and Kayir O., Chemical Constituents, Quantitative Analysis and Antioxidant Activities of *Echinacea purpurea* (L.) Moench and *Echinacea pallida* (Nutt.) Nutt., J. Food Biochem, 39 (2015) 622-630.

[2] Erenler R., Yilmaz S., Aksit H., Sen O., Genc N., Elmastas M. and Demirtas I., Antioxidant Activities of Chemical Constituents Isolated from *Echinops orientalis* Trauv., Rec. Nat. Prod., 8 (2014) 32-36.

[3] Erenler R., Meral B., Sen O., Elmastas M., Aydin A., Eminagaoglu O. and Topcu G., Bioassay-Guided Isolation, Identification of Compounds from *Origanum rotundifolium* and Investigation of Their Antiproliferative and Antioxidant Activities, Pharm. Biol., 55 (2017) 1646-1653.

[4] Erenler R., Sen O., Aksit H., Demirtas I., Yaglioglu A. S., Elmastas M. and Telci I., Isolation and Identification of Chemical Constituents from *Origanum majorana* and Investigation of Antiproliferative and Antioxidant Activities, J. Sci. Food Agr., 96 (2016) 822-836.

[5] Erenler R., Sen O., Yildiz I. and Aydin A., Antiproliferative Activities of Chemical Constituents Isolated from *Thymus praecox* Subsp *grossheimii* (Ronniger) Jalas, Rec. Nat. Prod., 10 (2016) 766-770.

[6] Codorniu-Hernández E., Mesa-Ibirico A., Montero-Cabrera L. A., Martínez-Luzardo F., Borrmann T., Stohrer W.-D. Theoretical Study of Flavonoids and Proline Interactions. Aqueous and Gas Phases, J. Mol. Struct., 623 (2003) 63-73.

[7] Kumar S., Pandey A. K. Chemistry and Biological Activities of Flavonoids: An Overview, Sci. World J., (2013); 1-16.

[8] Ross J. A., Kasum C. M. Dietary Flavonoids: Bioavailability, Metabolic Effects, and Safety, Annu. Rev. Nutr.,2002; 22: 19-34.

[9] Peterson J. and Dwyer J., Flavonoids: Dietary Occurrence and Biochemical Activity, Nutr. Res., 18 (1998) 1995-2018.

[10] Trischitta F. and Faggio C., Effect of the Flavonol Quercetin on Ion Transport in the Isolated Intestine of the Eel, *Anguilla anguilla*, Comp. Biochem. Physiol. C Toxicol. Pharmacol., 143 (2006) 17-22.

[11] Cook N. and Samman S., Flavonoids-Chemistry, Metabolism, Cardioprotective Effects, and Dietary Sources, J. Nutr. Biochem., 7 (1996) 66-76.

[12] Erlund I., Review of the Flavonoids Quercetin, Hesperetin, and Naringenin. Dietary Sources, Bioactivities, Bioavailability, and Epidemiology, Nutr. Res., 24 (2004) 851-874.

[13] Costa D. C., Costa H., Albuquerque T. G., Ramos F., Castilho M. C. and Sanches-Silva A., Advances in Phenolic Compounds Analysis of Aromatic Plants and Their Potential Applications, Trends Food Sci. Technol., 45 (2015) 336-354.

[14] Bie B., Sun J., Guo Y., Li J., Jiang W., Yang J., Huang C. and Li Z., Baicalein: A Review of Its Anti-Cancer Effects and Mechanisms in Hepatocellular Carcinoma, Biomed. Pharmacother., 93 (2017) 1285-1291.

[15] Gullón B., Lú-Chau T. A., Moreira M. T., Lema J. M., Eibes G. Rutin: A Review on Extraction, Identification and Purification Methods, Biological Activities and Approaches to Enhance Its Bioavailability, Trends Food Sci. Technol., 67 (2017) 220-235.

[16] Palacz-Wrobel M., Borkowska P., Paul-Samojedny M., Kowalczyk M., Fila-Danilow A., Suchanek-Raif R. and Kowalski J., Effect of Apigenin, Kaempferol and Resveratrol on the Gene Expression and Protein Secretion of Tumor Necrosis Factor alpha (TNF-α) and Interleukin-10 (IL-10) in Raw-264.7

Macrophages, Biomed. Pharmacother., 93 (2017) 1205-1212.

[17] Bakhtiari M., Panahi Y., Ameli J., Darvishi B. Protective Effects of Flavonoids against Alzheimer's Disease-Related Neural Dysfunctions, Biomed. Pharmacother., 93 (2017) 218-229.

[18] Demirtas I., Erenler R., Elmastas M., Goktasoglu A. Studies on the Antioxidant Potential of Flavones of *Allium Vineale* Isolated from Its Water-Soluble Fraction, Food Chem., 136 (2013) 34-40.

[19] Musa A. Y., Kadhum A. A. H., Mohamad A. B., Rahoma A. A. B., Mesmari H. Electrochemical and Quantum Chemical Calculations on 4, 4-Dimethyloxazolidine-2-Thione as Inhibitor for Mild Steel Corrosion in Hydrochloric Acid, J. Mol. Struct.: Theochem.,969 (2010) 233-237.

[20] Geerlings P., De Proft F. and Langenaeker W., Conceptual Density Functional Theory, Chem. Rev., 103 (2003) 1793-1874.

[21] Tanak H., Quantum Chemical Computational Studies on 2-Methyl-6-[2-(Trifluoromethyl) Phenyliminomethyl] Phenol, J. Mol. Struct.: Theochem., 950 (2010) 950: 5-12.

[22] Boukli-Hacene F., Merad M., Ghalem S. and Soufi W. Dft Study of the Interaction of Cu (Ii), Zn (Ii), Sn (Ii) with Carbohydrates in Aqueous Solution, J. Chem., 8 (2014) 1009-1017.