A THEORETICAL STUDY ON THE ANTIOXIDANT ACTIVITY OF MAIN COMPOUNDS OF PEACH POMACE EXTRACT

Vorobyova V. I., Zaporozhets J. A., Chygyrynets O. E.

ТЕОРЕТИЧНІ ДОСЛІДЖЕННЯ АНТИОКСИДАНТНОЇ ЗДАТНОСТІ ОСНОВНИХ КОМПОНЕНТІВ ЖМИХА ПЕРСИКУ

Воробйова В. І., Запорожець Ю. А., Чигиринець О. Е.

ТЕОРЕТИЧЕСКИЕ ИССЛЕДОВАНИЯ АНТИОКСИДАНТНОЙ АКТИВНОСТИ ОСНОВНЫХ КОМПОНЕНТОВ ЖМЫХА ПЕРСИКА

Воробьева В. И., Запорожец Ю. А., Чигиринец Е. Э.

National Technical University of Ukraine
"Igor Sikorsky Kyiv Polytechnic Institute"
Kyiv, UKRAINE
vorobyovavika1988@gmail.com

A theoretical study on the primary antioxidant activity of main compounds of peach pomace extract has been carried out using the density functional theory (DFT). Their chemical behaviour is influenced by different parameters such as thermodynamics, orbital and structural properties.

***Keywords**: Antioxidant activity, DFT, apricot cake, extract*

Проведено теоретичне дослідження первинної антиоксидантної активності основних сполук екстракту жмиха персику з використанням теорії функціоналу густини (ТФГ). Досліджено вплив хімічної структури на різні параметри, такі як термодинаміка, орбітальні та структурні властивості.

***Ключові слова**: антиоксидантна активність, ТФГ, жмих персика, екстракт*

Теоретическое исследование первичной антиоксидантной активности основных соединений экстракта жмыха персика было проведено с использованием теории функционала плотности (DFT). Исследовано влияние химической структуры на различные параметры, такие как термодинамика, орбитальные и структурные свойства.

***Ключевые слова**: антиоксидантная активность, ТФГ, жмых абрикоса, экстракт*

Peach is the third most important deciduous tree fruits world-wide, ranking after apples and pears. A significant part of the harvested peaches is processed resulting in a substantial amount of waste stones. Peach (Prunus persicaL.) is a fruit rich in polyphenols that aremainly localized in the pulp and peel tissues. Chlorogenic acid, catechin, epicatechin, rutting, and cyanidin-3-glucoside represent the main phenolic compounds of this fruit [3]. Although it is rich in ascorbic acid and carotenoids, it was found that the phenolic content of the peach is the major contributor to the observed antioxidative activity. Phenolic compounds make important contributions to the nutritional properties, sensory characteristics.

Quantum chemical calculation was employed to gain insight into the antioxidant activity of PPE. Fig. 1 shows the frontier molecular orbital (FMO) density distributions, i.e., the HOMO and the LUMO. The calculated quantum chemical properties are summarized in Table 1-2. The EHOMO values for compounds increase in the following order: Thymol<Caffeic acid<Catechin<Linalool< Gallic acid<4-terpeniol<Cyclocitral< Benzaldehyde.

The analysis in Table 1 demonstrates that Cyclocitral and Benzaldehyde have near values of EHOMO, which are the highest. This revealed their enhanced electron-donating ability. This suggests that a decreased energy gap of ΔE H-L gives rise to an intensified charge sharing at the interface of inhibitor and metal, which in turn brings about strengthened interactions.

The calculated ΔE values of the compounds followed the order of Caffeic acid<Gallic acid<Thymol<Catechin<Cyclocitral< Benzaldehyde<Linalool<4-terpeniol, indicating that Caffeic acid probably played the most prominent role in retarding the corrosion process. The electronegativity (χ) is an indicator of the electron-attraction ability of amolecule.A higher χ corresponds to a lower chance of electron donationfrom the molecule and vice versa [1-6]. Thismeans higher electronegativity values correspond to higher inhibition efficiencies. According to Table 6, the electronegativity value of the compound increases in order Thymol > Catechin > Caffeic acid > Gallic acid>Linalool >4-terpeniol >Cyclocitra l> Benzaldehyde. Moreover, a higher value of global hardness (η) indicates a higher resistance of a molecule toward charge transfer [5-11]. The calculations indicate that Caffeic acid has the lowest value, which means the highest reactivity among the other inhibitor and accordingly the highest inhibition efficiency.

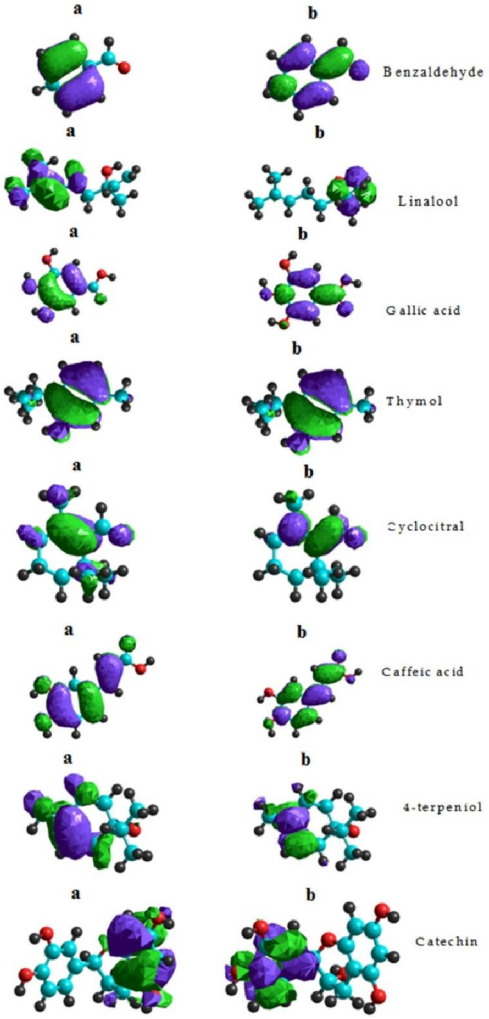

Fig. 1. The frontier molecule orbital density distributions of studied compounds; highest occupied molecular orbital (EHOMO) (a) and the lowest unoccupied molecular orbital (ELUMO) (b)

Table 1. Calculated quantum chemical properties for the most stable conformations of the major components of the PPE

Compounds	EHOMO	ELUMO	HOMO–LUMO gap (ΔE)
Benzaldehyde	-10.2236	-0.5566	9.6669
Linalool	-9.5938	0,8384	10.4322
Gallic acid	-9.61154	-0.7838	8.8277
Thymol	-8.83529	0.0601	8.8954
Cyclocitral	-10.1740	-0.5268	9.6472
Caffeic acid	-9.1764	-1.11589	8.0605
4-terpeniol	-9.8119	0.68560	10.4975
Catechin	-9.2143	-0.1269	9.0874

Table 2. Calculated quantum chemical properties for the most stable conformations of the major components of the PPE

Compounds	Electronegativity χ	Hardness η	Electrophilicity index ω	ΔN	ΔE
Benzaldehyde	5.3901	4.8334	1.3475	0.166	0.0168
Linalool	5.2161	4.3777	1.3040	0.203	0.0090
Gallic acid	5.1976	4.4138	1.2994	0.204	0.0081
Thymol	4.3875	4.4476	1.0969	0.293	0.0105
Cyclocitral	5.3504	4.8236	1.3376	0.171	0.0146
Caffeic acid	5.1461	4.0302	1.2865	0.230	0.0066
4-terpeniol	5.2487	4.5631	1.3122	0.191	0.0101
Catechin	4.6706	4.5436	1.1677	0.256	0.0012

Global electrophilicity index (ω) informs about the nucleophilic or electrophilic character of the molecule. The higher the value of electrophilicity index, the best the capacity of the molecule to accept electrons. Benzaldehyde has the greatest electrophilicity value (2,30659 eV/mol), which reflects its nucleophilicity, i.e. its good ability to donate electrons.

REFERENCES

[1] Okino Delgado, C. H., Fleuri, L. F.: Food Reviews International, 2015, 32(1), 1. doi:10.1080/87559129.2015.1041183
[2] Gullón B., Gullón P., Eibes G. et al.: Science of The Total Environment, 2018, 645. 533. https://doi.org/10.1016/j.scitotenv.2018.07.155
[3] Lemes A. C., Álvares G. T., Egea M. B. et al.: Bioresource Technology, 2016, 222, 210. https://doi.org/10.1016/j.biortech.2016.10.001
[4] Shakeel A., Mudasir A., Babu L. S. et al.: Journal of Advanced Research, 2016, 7, Is. 1, 17. https://doi.org/10.1016/j.jare.2015.02.007
[5] Skiba M., Vorobyova V., Pivovarov O. et al.: Eastern-European Journal of Enterprise Technologies, 2018, 2, 51.
[6] Kumar, K., Yadav, A.N., Kumar, V. et al.: Bioresour. Bioprocess., 2017, 4, 18. https://doi.org/10.1186/s40643-017-0148-6
[7] Maluf D. F., Gonçalves M. M., D'Angelo R. W. O. et al.: Cosmetics, 2018, 5(3), 46. https://doi.org/10.3390/cosmetics5030046
[8] Chyhyrynets, O.E., Fateev, Y.F., Vorobiova, V.I.: et al. Mater Sci., 2016, 51, 644. https://doi.org/10.1007/s11003
[9] Vorob'iova V., Chyhyrynets' O., Vasyl'kevych O.: Mater. Sci., 2015, 50, 726. https://doi.org/10.1007/s11003-015-9778-z
[10] Vorobyova V., Chygyrynets' O., Skiba M. International Journal of Corrosion and Scale Inhibition, 2018, 7, Is.2. P. 185. https://doi.org/10.17675/2305-6894-2018-7-2-6
[11] Vorobyova V., Chygyrynets' O., Skiba M. Journal of Chemical Technology and Metallurgy, 2018, 53, Is. 2, 336.