Journal of the Turkish Chemical Society, Section A: Chemistry
Owned by the Turkish Chemical Society
Correspondence e-mail: jotcsa@turchemsoc.org
Founded in February, 2014

A SEMI-EMPIRICAL STUDY OF CERTAIN FLAVONOIDS

BAZI FLAVONOİDLERİN YARI-DENEYSEL ÇALIŞMASI

Gürkan KURT[1], Ulku Dilek UYSAL[2*], Halil BERBER[2]

[1]ETİ Gıda San. Tic. A.Ş. Eskişehir, Turkey

[2] Anadolu University, Science Faculty, Department of Chemistry, 26470 Eskişehir, Turkey

*Corresponding author. duysal@anadolu.edu.tr

ABSTRACT

In this study, certain theoretical properties of six flavonoles-glucosides, and their tautomers (Table 1) such as stability, reactivity, geometry, nucleophilicity, possible H-bonds, and energy have been calculated by MOPAC2012 packet program [1] at the Restricted Hartree-Fock level using both PM6 and PM7 semi-empirical SCF-MO methods to understand the basic principles to understand their antioxidant behaviors [2].

Table 1. Name and abbreviations of flavonoles (The name of the tautomers are not given here)

Name	IUPAC Name	Abbreviation
Isoquer-citin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-((2S,3R,4R,5S)-3,4,5-trihydroxy-6-(hydroxymethyl)-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molecule 1
Kaempferitrin	5-hydroxy-2-(4-hydroxyphenyl)-3,7-bis((3R,4S,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molecule 2
Myricitrin	5,7-dihydroxy-3-((3R,4S,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one	Molecule 3
Quercitrin	2-(3,4-Dihydroxyphenyl)-5,7- dihydroxy-3-[[(2*S*,3*R*,4*R*,5*R*,6*S*)-3,4,5-trihydroxy-6-methyl-2- tetrahydropyranyl]oxy]-4-chromenone	Molecule 4
Rutin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyloxy]-4*H*-chromen-4-one	Molecule 5
Isorhamnetin-3-O[6-O rhamnosylgalactoside]-7-O-rhamnoside	5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-tetrahydro-2H-pyran-2-yloxy)-7-((2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molecule 6

Keywords

Flavonoid, PM6, PM7, antioxidant, semi-empirical, theoretical calculation.

ÖZET

Bu çalışmada, altı flavonol-glikozit ve tautomerlerinin (Tablo 1) kararlılık, reaktivite, geometri, nükleofilisite, muhtemel H-bağları ve enerji gibi bazı teorik özellikleri MOPAC 2012 paket programı ile [1] PM6 ve PM7 yarı deneysel SCF-MO metotları kullanılarak ve bu maddelerin antioksidan davranışlarını anlamak için hesaplanmıştır [2].

Tablo 1. Flavonollerin isim ve kısaltmaları (Tautomer isimleri burada verilmemiştir)

İsim	IUPAC Adlandırması	Kısaltma
Isoquercitin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-((2S,3R,4R,5S)-3,4,5-trihydroxy-6-(hydroxymethyl)-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molekül 1
Kaempferitrin	5-hydroxy-2-(4-hydroxyphenyl)-3,7-bis((3R,4S,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molekül 2
Myricitrin	5,7-dihydroxy-3-((3R,4S,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one	Molekül 3
Quercitrin	2-(3,4-Dihydroxyphenyl)-5,7- dihydroxy-3-[[(2*S*,3*R*,4*R*,5*R*,6*S*)-3,4,5-trihydroxy-6-methyl-2- tetrahydropyranyl]oxy]-4-chromenone	Molekül 4
Rutin	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyloxy]-4*H*-chromen-4-one	Molekül 5
Isorham-netin-3-O[6-O rhamnosylgalactoside]-7-O-rhamnoside	5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-tetrahydro-2H-pyran-2-yloxy)-7-((2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydro-2H-pyran-2-yloxy)-4H-chromen-4-one	Molekül 6

Anahtar Kelimeler

Flavonoid, PM6,PM7, antioksidan, yarı deneysel, teorik hesaplama.

Kaynaklar / References

[1] J. Stewart MOPAC2012, Stewart Computational Chemistry, Version 14.128W, 2012.

[2] N. Masuoka, M. Matsuda and I. Kubo, Food. Chem., 131, 541-545, 2012.