Data Article

Data on the UV filtering and radical scavenging capacity of the bitter masking flavanone Eriodictyol

Vijisha K. Rajan, Shameera Ahamed T.K., K. Muraleedharan *

Department of Chemistry, University of Calicut, Malappuram 673635, India

A R T I C L E   I N F O

Article history:
Received 29 June 2018
Accepted 24 August 2018
Available online 31 August 2018

A B S T R A C T

A computational analysis of UV filtering and radical scavenging capacity of a flavanone, Eriodictyol has been performed under DFT-B3LYP/6–31+G (d, p). Eriodictyol is nontoxic and nonirritant bitter masker used in wine and can be used for photo protection due to its potential UV filtering and radical scavenging capacity. The compound has an absorbance in the UV-A and UV-B region of electromagnetic spectrum, it can be used as a potential UV filter in sunscreen lotions and other cosmetic products. Eriodictyol is a potent antioxidant than the most commonly studied Quercetin. The most active site in the compound is 3’ position and is confirmed by NPA, NBO and pKa value analysis. The BDE values follow the order 3’<4’<7<5. The major transitions in the UV-visible spectrum of Eriodictyol are between HOMO and HOMO-1 with LUMO level and are well explained by NBO–NLMO tool in G09.

& 2018 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

S p e c i f i c a t i o n s   T a b l e

| Subject area         | Chemistry                  |
|----------------------|----------------------------|
| More specific subject area | Computational chemistry     |
| Type of data         | Table, image; word document |

DOI of original article: https://doi.org/10.1016/j.photobiol.2018.06.017
* Corresponding author. Fax: +91 494 2400269.
E-mail addresses: vijirajan4@gmail.com (V.K. Rajan), kmuralika@gmail.com (K. Muraleedharan).
How data was acquired

Computational analysis through results obtained from structural optimizations by using tools in Gaussian 09 software package like TDDFT, NBO-NLMO,NPA, etc.

Data format
Analyzed

Experimental factors
No experimental data, all results are computed.

Experimental features
–

Data source location
All data were computed through Gaussian 09 software package

Data accessibility
Data is with this article

Related research article
Vijisha. K. Rajan, Shameera Ahamed T.K, K. Muraleedharan: Studies on the UV filtering and radical scavenging capacity of the bitter masking flavanone Eriodictyol: JPHOTOBIOL: 2018. (in press)

Value of the data

- Eriodictyol can be used as potential UV filter in sunscreen lotions and other cosmetic products.
- Eriodictyol is a potential antioxidant than the most commonly studied Quercetin.
- The pKa values of all the possible sites are computed on the basis of free energy values.
- Its BDE values follow the order 3’ < 4’ < 7 < 5 position in the flavanone ring.
- Major transitions in the UV–visible spectrum are between HOMO and HOMO-1 with LUMO.
- The UV filtering capacity can be well explained by the combined NBO–NLMO study.

1. Data

The data include the structure and numbering of the optimized stable conformer of a flavanone called Eriodictyol (Fig. 1). A Density Functional Theory (DFT) based evaluation of the UV filtering and radical scavenging capacity of Eriodictyol has been described. All the computational calculations are carried out through Gaussian 09 software package and the Gaussview 5 graphical user interface [1,2]. The optimized structure contains a hydrogen bond between the carbonyl oxygen and the H30 at position 5 in ring A. the molecule has –OH groups in ring A and B and the conjugation is lost in ring C due to the presence of dihydrogens at position 3. This makes the ring B out of plane. Also it reduces the absorption wavelength and is falls in the UV-A and UV-B region so that the molecule can be effectively used as UV filter in sun screen lotions and other photo protective cosmetics. The Table 1 describes the donor–acceptor interactions of the molecule. This is obtained from the NBO analysis by the Gaussian 09 software package [3–5]. The presence of hydrogen bonding between the carbonyl oxygen and H30 has been confirmed through this analysis. It shows that both the lone pair of electrons in carbonyl oxygen donates to the σ* orbital of O3–H30. The higher interaction energy indicates that the hydrogen bond is strong enough to restrict the breaking of O3–H30 bond to form a radical at position 5. This makes the bond dissociation energy (BDE) at this position higher than that at position 7 [6].

2. Materials and method

The stable conformer (lowest energetic) obtained from the potential energy scanning (PES) of Eriodictyol has been optimized with DFT-B3LYP/6–31G+(d, p) [7–9]. The structure with numbering is shown in Fig. 1. The energy gap of the stable conformer and the related global reactive descriptors has been computed. The TDDFT tool [10] in Gaussian 09 software package has been implemented to study the excited state characteristics of the molecule and has found that the molecule can be used as an effective UV filter since it absorption falls in the UV-A–UV-B region. The results are confirmed by the combined NBO–NLMO analysis [10], which is done through Gaussian 09 software package. Besides this the mechanistic evaluation shows that the hydrogen atom transfer mechanism is suitable to explain
Table 1
Some important donor-acceptor interactions in Eriodictyol.

| Donor NBO | Acceptor NBO | $E(2)$ (Kcal/mol) | $E(j) - E(i)$ (HF) | $F(ij)$ (HF) |
|-----------|--------------|-------------------|-------------------|-------------|
| $\sigma$  | O6–H33       | C20–C21           | 4.64              | 1.31        | 0.07        |
| $\sigma$  | O6–C21       | C14–C19           | 1.6               | 1.47        | 0.044       |
| $\sigma$  | O6–C21       | C15–C20           | 1.28              | 1.46        | 0.039       |
| $\sigma$  | O6–C21       | C19–C21           | 0.67              | 1.43        | 0.028       |
| $\sigma$  | O6–C21       | C20–C21           | 0.93              | 1.47        | 0.033       |
| n1        | O6           | C19–C21           | 6.12              | 1.11        | 0.074       |
| n2        | O6           | $\pi^*$           | C20–C21           | 28.03       | 0.33        |
| $\sigma$  | O5–H32       | C19–C21           | 3.37              | 1.3         | 0.06        |
| $\sigma$  | O5–C19       | C9–C14            | 1.31              | 1.45        | 0.039       |
| $\sigma$  | O5–C19       | C14–C19           | 0.92              | 1.47        | 0.033       |
| $\sigma$  | O5–C19       | C20–C21           | 1.73              | 1.47        | 0.045       |
| n2        | O5           | $\sigma^*$        | O6–H33            | 2.65        | 1           |
| n1        | O5           | $\pi^*$           | C14–C19           | 5.87        | 1.17        |
| n1        | O5           | $\sigma^*$        | C19–C21           | 0.58        | 1.13        |
| n1        | O5           | $\pi^*$           | C14–C19           | 23.85       | 0.34        |
| $\sigma$  | O4–H31       | C16–C18           | 3.92              | 1.3         |
| $\sigma$  | O4–C18       | C12–C16           | 1.45              | 1.5         |
| $\sigma$  | O4–C18       | C13–C17           | 1.35              | 1.48        |
| $\sigma$  | O4–C18       | C16–C18           | 0.55              | 1.47        |
| $\sigma$  | O4–C18       | C17–C18           | 0.69              | 1.48        |
| n2        | O4           | $\sigma^*$        | C16–C18           | 5.75        | 1.14        |
| n1        | O4           | $\pi^*$           | C16–C18           | 29.09       | 0.33        |
| $\sigma$  | O3–H30       | C13–C17           | 4.72              | 1.3         |
| $\sigma$  | O3–C13       | C10–C12           | 1.66              | 1.44        |
| $\sigma$  | O3–C13       | C10–C13           | 0.82              | 1.43        |
| $\sigma$  | O3–C13       | C13–C17           | 0.97              | 1.47        |
| $\sigma$  | O3–C13       | C17–C18           | 1.46              | 1.47        |

Fig. 1. Numbering in the stable conformer of Eriodictyol.
the radical scavenging activity of eriodictyol and the position 3’ is the most reactive site in it. These are further confirmed by the charge analysis via Natural Population Analysis (NPA), pKa value [11] and bond order analysis. The donor acceptor interaction energy results from NBO have been given Table 1 and it confirms the presence of hydrogen bond between the carbonyl oxygen and the H30 at position 5.

Acknowledgements

Author Vijisha KR acknowledges the ‘University Grants Commision’ (UGC), New Delhi, India. (https://www.ugc.ac.in/), for the financial support through UGC-SRF (Ref.No: 22/12/2013(ii) EU-V Dated 1/7/2014). Author Shameera Ahamed acknowledges the ‘Council of Scientific and Industrial Research’ (CSIR), New Delhi, India (http://www.csir.res.in/) for financial support through CSIR-SRF [HRDG (CSIR) sanction letter No.09/043(0172)/2015-EMR-1]. The authors are thankful to colleagues Ajmala and Safna, for some fruitful discussions and to the Central Sophisticated Instrumentation Facility (CSIF) of the University of Calicut for the Gaussian 09 software support.

Transparency document. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.08.149.

References

[1] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, J.D. Fox, GAUSSIAN 09 (Revision A.2) Gaussian, Inc., Wallingford, CT, 2009.

Table 1 (continued )

| Donor NBO | Acceptor NBO | E(2) (Kcal/mol) | E(j)−E(i) (HF) | F(Ij) (HF) |
|-----------|--------------|----------------|----------------|------------|
| n2 O3 σ*  | C10–C13      | 7.16           | 1.06           | 0.078      |
| n1 O3 σ*  | C13–C17      | 0.51           | 1.1            | 0.021      |
| n1 O3 π*  | C13–C17      | 38.64          | 0.31           | 0.103      |
| σ O2–C11  σ* | O3–H30      | 0.57           | 1.42           | 0.026      |
| σ O2–C11  σ* | C7–C8        | 0.58           | 1.37           | 0.025      |
| σ O2–C11  σ* | C8–C11      | 0.86           | 1.41           | 0.031      |
| σ O2–C11  σ* | C10–C11     | 1.25           | 1.52           | 0.039      |
| σ O2–C11  σ* | C10–C12     | 1.51           | 1.55           | 0.044      |
| π O2–C11  σ* | C7–C8        | 0.71           | 0.71           | 0.02       |
| π O2–C11  σ* | C8–H23      | 1.68           | 0.79           | 0.033      |
| π O2–C11  σ* | C10–C12     | 4.84           | 0.37           | 0.043      |
| π O2–C11  σ* | C8–H23      | 1.2            | 0.44           | 0.056      |
| π O2–C11  π* | C10–C12      | 117.88         | 0.02           | 0.076      |
| n1 O2 σ*  | O3–H30      | 4.33           | 1.05           | 0.061      |
| n1 O2 σ*  | C10–C11     | 5.34           | 1.15           | 0.07       |
| n2 O2 σ*  | O3–H30      | 23.76          | 0.71           | 0.118      |
| n2 O2 σ*  | C7–C8       | 0.54           | 0.66           | 0.017      |
| n2 O2 σ*  | C8–C11      | 16.74          | 0.7            | 0.099      |
| n2 O2 σ*  | C10–C11     | 8.94           | 0.81           | 0.077      |
[2] J.M.M.R.D. Dennington, T.A. Keith, GaussView 5.0.8 Gaussian, 2008.
[3] J.P. Foster, F. Weinhold, Natural Bond Orbitals. J. Am. Chem. Soc. 102 (1980) 7211–7218.
[4] F. Weinhold, C.R. Landis, Natural bond orbitals and extensions of localized bonding concepts, Chem. Educ. Res. Pract. Eur. 2 (2001) 91–104. https://doi.org/10.1039/b1rp90011k.
[5] A. Reed, F. Weinhold, Natural localized molecular orbitals, J. Chem. Phys. 83 (1985) 1736–1740.
[6] R. Vijisha, T.K. Shameera Ahamed, K. Muraleedharan, Studies on the UV filtering and radical scavenging capacity of the bitter masking flavonone Eriodictyol, J. Photochem. Photobiol. B 185 (2018) 254–261.
[7] D. Becke A, Density-functional thermochemistry. III. The role of exact exchange, J. Chem. Phys. 98 (1993) 5648–5652.
[8] C. Lee, W. Yang, R.G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, Phys. Rev. B 37 (1988) 785–789.
[9] E. Lewars, Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers. New York, 2004.
[10] P. Ajmala Shireen, V.M. Abdul Mujeeb, K. Muraleedharan, Theoretical insights on flavanones as antioxidants and UV filters: a TDDFT and NLMO study, J. Photochem. Photobiol. B 170 (2017) 286–294. https://doi.org/10.1016/j.jphotobiol.2017.04.021.
[11] R. Vijisha K, K. Muraleedharan, The pKa values of amine based solvents for CO2 capture and its temperature dependence—an analysis by density functional theory, Int. J. Greenh. Gas Control 58 (2017) 62–70. https://doi.org/10.1016/j.ijggc.2017.01.009.