Computational Biology and Chemistry 76 (2018) 202–209

Contents lists available at ScienceDirect

Computational Biology and Chemistry

journal homepage: www.elsevier.com/locate/cbac

Research Article

A non toxic natural food colorant and antioxidant 'Peonidin' as a pH indicator: A TDDFT analysis

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

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

ARTICLE INFO

Keywords:
Peonidin
Food colorant
pH indicator
Peony
Morning glory
TDDFT

ABSTRACT

A computational inestigation on the difference in colors of two plants 'Peony' and 'Morning glory' by the same pigment 'Peonidin' has been performed by means of absorption characteristics. Peonidin imparts purple color to the flowers in Peony and blue to that in Morning glory. TDDFT tool in Gaussian 09 software package has been employed to analyze the UV–vis spectra and has shown that in acidic media Peonidin exists in its flavylium cationic form where as in alkaline media it exists in the quinoidal base form. These two structural forms have colors red and blue respectively. TDDFT results of flavylium ion in acetic acid moves the absorption to higher wavelength and corresponds to purple color and is the color of Peony flower. One of the quinoidal bases in alkaline media gives violet-blue color to flowers in Morning glory. This is true as Peony grows in acidic soil only while Morning glory grows in alkaline soil only. The affinity towards pH values makes Peonidin to act as pH indicator besides its radical scavenging capacity. Further a good food colorant must be non toxic. The toxicological analysis has shown that Peonidin is non-irritant, non-mutagenic, non-carcinogenic and non-tumorigenic. The compound has sufficient solubility to use as a potential drug. Also the compound has a positive drug score. All these results confirm the potential druggability of Peonidin and its non toxicity.

1. Introduction

Chlorophyll, carotene, anthocyanidins, etc., imparts colors to plants. The shade in which a substance appeared is the complementary shade of the color that they have absorbed. Due to the instability of chlorophyll, its concentration decreases during summer resulting in the fading of color of leaves. Carotene absorbs blue-green light and looks like yellow. When plants have both chlorophyll and carotene, they could absorb red, blue-green and blue, and appear as green. During summer, chlorophyll decreases and carotene persists so that leaves changes their color to yellow. Unlike chlorophyll and carotene, the pigment anthocyanidins, a major class of flavonoids, are not membrane bound pigments, but dissolved in the cell sap. Their pH sensitivity makes them to use as pH indicators. At acidic pH they impart red and at basic pH they give blue or violet-blue color. In plants, in presence of light, the anthocyanidins are produced as a result of reaction between protein and sugar in the cell sap. As concentration of anthocyanidins increases, plants become bright colored. For example, apple appears red on the side where light falls and green on the other side.

Anthocyanidins are major constituents of vascular plants and are harmless water soluble natural pigments (Lu et al., 2014). This have been used as a good natural food colorant since historical times. Due to the wide range of uses there are a number of research articles available in literature about the anthocyanidins including its metal chelation (Asada et al., 2015; Horbowicz et al., 2011; Tachibana et al., 2014), antioxidant (Bueno et al., 2012; Elmastas and Aboul-enein, 2012; Guzmán et al., 2009; Mascayano et al., 2018), anticancer and antidiabetic (Castañeda-ovando et al., 2009) capacities. However the relationships of the structures of anthocyanidins with the properties that they have shown are not yet completely understood. In this scenario, a detailed structural analysis of anthocyanidins is particularly relevant.

The affinity towards pH, metal ions, temperature, concentration, light, etc., makes them unstable in the isolated state. The important feature of anthocyanidins is the presence of chromenylium/flavylium ion. Due to this, effective π-conjugation significantly enlarges in comparison to flan-3-ols. So HOMO-LUMO gap decreases than flavan-3-ols. This π-conjugation is responsible for its strong absorption around 500 nm (Castañeda-ovando et al., 2009) and thus they are brightly colored; this in turn enables them to be used as a natural food colorant. As the use of artificial colorants have been expanded to a splendid extent and become a extremely good risk to human fitness due to the fact of their toxicity so that the development of some herbal meals colorant are specially relevant in the area of food industry. Carotenoids and anthocyanidins are the broadly used herbal food colorants.

* Corresponding author.
E-mail addresses: vijirajan4@gmail.com (V.K. Rajan), kmuralika@gmail.com (K. Muraleedharan).

https://doi.org/10.1016/j.compbiolchem.2018.07.015
Received 19 March 2018; Received in revised form 21 July 2018; Accepted 22 July 2018
Available online 23 July 2018

Table 3
Aromaticity indices of isomers.

Isomer	HOMA	HOMT	AROM	λ_{max} (nm)
1	0.299	4.783	0.975	439.25
2	0.428	7.271	0.974	430.47
3	0.462	7.86	0.976	480.16
4	0.819	11.467	0.978	575.33
5	0.375	6.382	0.969	278.93
6	0.462	7.86	0.976	416.39
7	0.169	2.865	0.987	432.91
8	0.301	5.116	0.968	558.82

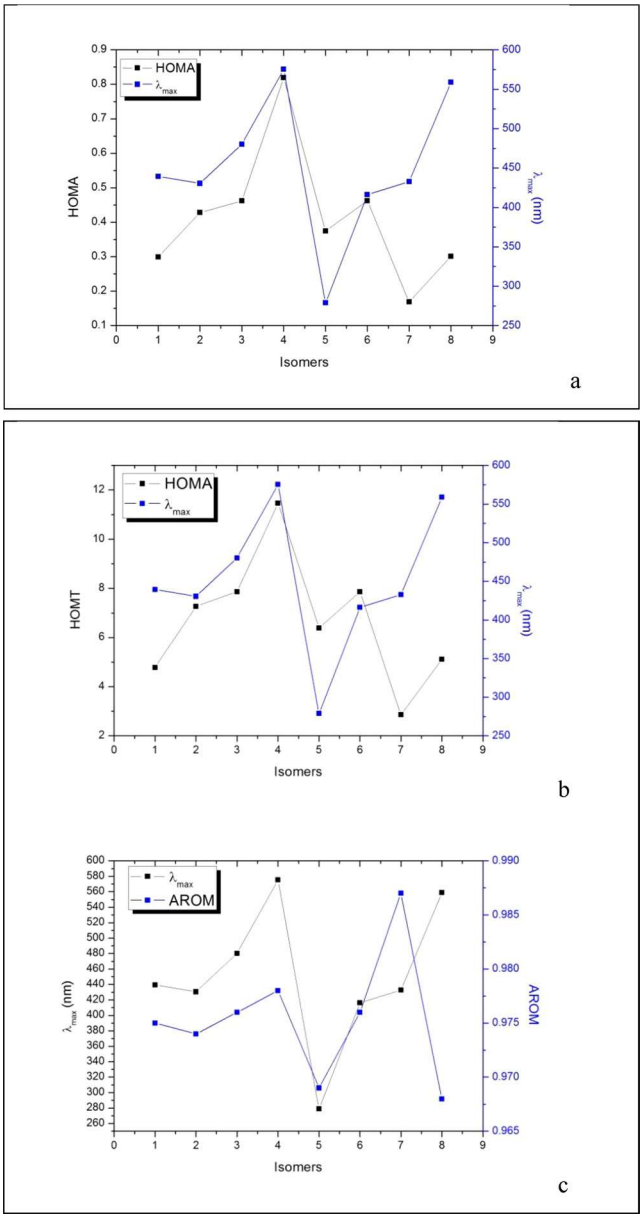

Fig. 7. Variation of λ_{max} values with a) HOMA, b) HOMT and c) AROM.

like as a leadlike molecule should satisfy the following criteria of xlogP ≤ 3.5, 250 ≤ MW ≤ 350 and number of rotatable bonds ≤ 7 (Teague et al., 1999). Its bioavailability is 0.55 (Martin, 2005). Peonidin shows drug likeness as per the Lipnski, Veber, Ghose, Egan and Muegge rules. It did not violate any of the Lipinsky rules of 5. It has 3 H-bond donors and 5 H-bond acceptors.

Table 4
Drug like properties of peonidin.

Property	Value
Mutagenic	None
Tumerogenic	None
Irritant	None
Carcinogenic	None
ClogP	2.28
Solubility	−2.54
Drug-likeness	1.07
Drug score	0.78
Bioavailability	0.55
Synthetic accesibility	2.96

4. Conclusion

A computational analysis of UV–vis spectrum of an anthocyanidin, Peonidin in two plants Peony and Morning glory has been evaluated. The results have shown that Peonidin can act as efficient pH indicator besides its radical scavenging capacity. The flowers of peony are purple colored while that in Morning glory is violet-blue in color, even though they contain the same color pigment Peonidin. TDDFT analysis has shown that in acidic media Peonidin exists in its flavylium cationic form where as in alkaline media it exists in the quinoidal base form. These two structural forms have colors red and blue respectively. TDDFT results of flavylium ion in acetic acid moves the absorption to higher wavelength and corresponds to purple color and is the color of Peony flower. One of the quinoidal bases in alkaline media gives violet-blue color to flowers in Morning glory. This is true as Peony grows in acidic soil only while Morning glory grows in alkaline soil only. Further the toxicological analysis has shown that Peonidin is non-irritant, non-mutagenic, non-carcinogenic and non-tumorigenic. It has a solubility −2.54 which is higher than −4.00, indicates that the compound has sufficient solubility to absorb in biological system. Also the compound has a positive drug score. All these results confirm the druggability of peonidin and its non toxicity. So Peonidin can be used as a pH indicator as well as a natural food colorant.

Acknowledgements

Author Vijisha KR acknowledges the 'University Grants Commision' (UGC), New Delhi, India (https://www.ugc.ac.in/), for the financial support through UGC-JRF (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-JRF [HRDG (CSIR) sanction letter No.09/043(0172)/2015-EMR-1]. We are also thankful to the colleagues Ajmala, Rinsha, Ragi and Kavitha for some fruitful discussions and to the Central Sophisticated Instrumentation Facility (CSIF) of University of Calicut for the Gaussian 09 software support (gaussian.com/glossary/g09/).

References

Alkorta, I., National, S., National, S., Proniewicz, L.M., 2011. Calculation of the HOMA model parameters for the carbon – boron bond calculation of the HOMA model parameters for the carbon – boron bond. Struct. Chem. 23, 595–600. https://doi.org/10.1007/s11224-011-9907-8.

Alves, V.M., Muratov, E.N., Zakharov, A., Muratov, N.N., Andrade, C.H., Tropsha, A., 2016. Chemical toxicity prediction for major classes of industrial chemicals: is it possible to develop universal models covering cosmetics, drugs, and pesticides? Food Chem. Toxicol. 1–9. https://doi.org/10.1016/j.fct.2017.04.008.

Asada, T., Koi, Y., Tamura, H., 2015. New technique to isolate anthocyanins from Delaware grapes by forming an aluminium complex using a Discovery DPA-6S. Food Chem. 166, 10–16. https://doi.org/10.1016/j.foodchem.2014.05.100.

Becke, A.D., 1993. Density-functional thermochemistry. III. The role of exact exchange. J. Chem. Phys. 5648–5652.

Birse, M.J., 2007. The Colour of Red Wine. The University of Adelaide.

Bridle, P., Bakker, J., Gate, E., Gate, E., 1994. The effect of pH on the formation of