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

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ABSTRACT

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.

Specifications Table

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Table 1 (*continued*)

	Donor NBO		Acceptor NBO	$E(2)$ (Kcal/mol)	$E(j)-E(i)$ (HF)	$F(I,j)$ (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

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.

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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.

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