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ORIGINAL ARTICLE

Computational Investigation on the •OOH Scavenging Sites of Gnetin C

Vera Khoirunisa[1,2,3] · Febdian Rusydi[1,4] · Lusia S. P. Boli[1,3] · Adhitya G. Saputro[3,5] · Heni Rachmawati[5,6] · Hiroshi Nakanishi[7] · Hideaki Kasai[7] · Hermawan K. Dipojono[3,5]

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Abstract

Melinjo seed extract contains melinjo resveratrol compounds that has antioxidant activity. The radical-scavenging sites required for the antioxidant activity, however, is yet to be located. We report a computational study that aims to locate scavenging sites of the simplest resveratrol dimer, gnetin C. We consider the reaction of gnetin C and hydroperoxyl radical energetically with the basis of density-functional calculations, to be compared with the reaction of the resveratrol monomer, trans-resveratrol, and hydroperoxyl radical. The results show that OH group at the para position is the most reactive scavenging site for both molecules. Besides the OH group, gnetin C also provides two CH groups in the furan ring that are favorable as scavenging sites. Therefore, furan ring plays an important role in the scavenging activity, which is contrary to the experimental speculation that propose resorcinol ring. Our study shows the prospect of density-functional calculation for studying the radical-scavenging reaction.

Keywords Gnetin C · Melinjo resveratrol · Radical-scavenging activity · Density-functional calculations

Introduction

Melinjo (Gnetum gnemon Linn) seeds carry bioactive compound with antioxidant [1, 2] and other beneficial pharmacological activities. In particular, the melinjo seed extract (MSE) confirms antimicrobial [1], anti-allergic [3], anti-angiogenesis [4], anti-melanogenesis [5], and anti-tumor [6] properties. Consuming MSE could reduce the serum uric acid levels [7] without serious adverse events both in the human [8] and toxicity studies [9]. It implies the potential of the seed for drugs, supplements, and functional foods that may benefit human health.

The main antioxidant in melinjo seed is resveratrol dimer (known as melinjo resveratrol). As antioxidants, melinjo resveratrol can act as radical scavengers. A study from Kato et al. [1] showed that melinjo resveratrol has comparable scavenging activity to dl-α-tocopherol. Their study also showed that melinjo resveratrol could maintain the scavenging activity longer than dl-α-tocopherol could. They proposed that resorcinol ring in resveratrol dimer plays an important role in the scavenging activity of melinjo resveratrol. However, no other studies have been reported to corroborate the findings. Further investigation in the radical-scavenging activity is needed to explain the antioxidant manner of melinjo resveratrol.

One preferred method to study the antioxidant activity is calculation method based on density functional theory (DFT) [10, 11]. DFT allows us to explore the chemical properties of molecules based on their quantum electronic

✉ Febdian Rusydi
rusydi@fst.unair.ac.id

✉ Hermawan K. Dipojono
dipojono@tf.itb.ac.id

1 Research Center for Quantum Engineering Design, Faculty of Science and Technology, Universitas Airlangga, Surabaya, 60115, Indonesia

2 Engineering Physics Study Program, Institut Teknologi Sumatera (ITERA), Lampung, 35365, Indonesia

3 Advanced Functional Materials Research Group, Institut Teknologi Bandung, Bandung, 40132, Indonesia

4 Department of Physics, Faculty of Science and Technology, Universitas Airlangga, Surabaya, 60115, Indonesia

5 Research Center for Nanosciences and Nanotechnology, Institut Teknologi Bandung, Bandung, 40132, Indonesia

6 School of Pharmacy, Institut Teknologi Bandung, Bandung, 40132, Indonesia

7 National Institute of Technology, Akashi College, Hyogo, 674-8501, Japan

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structures [12] as applied in the study of reactions with the basis of orbital interaction [13, 14]. DFT also allows us to predict the antioxidant activity from the thermodynamic parameters [15–21]. Furthermore, DFT can predict the reaction pathways, including the determination of transition state (TS) that is very challenging to observe in experimental methods. Once the TS is predicted, we can extend the method into the study of reaction kinetics of antioxidants [22–24]. Therefore, the density-functional calculations could be a reliable method for investigating the activity of melinjo resveratrol.

In this study, we utilize density-functional computations to locate the active scavenging site of melinjo resveratrol. We evaluate the possible site energetically by using gnetin C (the simplest melinjo resveratrol) to scavenge hydroperoxyl radical ($^{\bullet}$OOH). Here, we assume that the scavenging reaction undergoes a one-step reaction mechanism. Besides the energetic results, we can propose another ring apart from that of Kato et al. [1] speculated.

Computational Model

Scavenging Reaction Model

The one-step reaction mechanism models the $^{\bullet}$OOH scavenging by melinjo resveratrol (YH) has been suggested to be the preferable mechanism of phenolic antioxidants [25–27]. The reaction is as follows:

$$\mathrm{X} + \mathrm{YH} \rightarrow [\mathrm{X} - \mathrm{H} - \mathrm{Y}] \rightarrow \mathrm{XH} + \mathrm{Y}. \tag{1}$$

In our case, X is $^{\bullet}$OOH, YH is gnetin C, XH is H_2O_2, and Y is gnetin C radical. Besides gnetin C, we also consider trans-resveratrol as YH in the Eq. (1). The reasons are (1) trans-resveratrol is a well-studied monomer of resveratrol, and (2) the dimer form is gnetin C as shown in Fig. 1.

The [X - H - Y] activated complex is the TS. It is the state where the hydrogen atom transfer (HAT) from melinjo resveratrol to $^{\bullet}$OOH occurs. While the energy difference between product (XH and Y) and reactant (X and YH) describes the reaction energy (E_r), the energy difference between TS and reactant determine the barrier energy (E_b).

The H in [X – H – Y] activated complex may derive from 22 possible sites of gnetin C [see Fig. 1(c)] . We consider all H atoms from hydroxyl sites since they are essential for antioxidant activity of resveratrol [28]. The remains of the H atoms are evaluated based on their bond dissociation energy (BDE). BDE calculation from a site follows the generic dissociation,

$$\mathrm{YH} \rightarrow \mathrm{Y} + \mathrm{H}, \tag{2}$$

hence BDE is the energy difference between the product (Y and H) and the reactant (YH). The higher the BDE of a site means the least favor H donation from the site.

Density-Functional Calculation

The primary quantities here are E_r, and E_b. The ground state of reactants and products determines the first two energies. The optimization geometry calculation routine, based on DFT, obtains the geometry and energy of reactant (initial state) and product (final state) in the ground state. For E_b, we calculate the value from the energy difference between the TS and the reactant. The TS is obtained from the routine of optimization geometry at the saddle point of the potential surface [29]. We identify the appropriate TS from a particular vibrational mode, which has imaginary frequency and involves the motion of hydrogen between the 22-possible sites and the $^{\bullet}$OOH.

We couple DFT with vibrational mode calculations at 298.15 K. The energy calculated by DFT is electronic energy at 0 K. The vibrational mode calculations allow us to correct the electronic energy with thermal energy at 298.15 K. As for E_r and E_b, we use Gibbs free-energy correction to get the standard Gibbs energy of reaction ($\Delta_r G^0$) and activation ($\Delta^{\ddagger} G^0$), respectively. For BDE, we use enthalpy correction to get BDE*. In the current, the relevant quantity is BDE* of YH relative to BDE* of H-phenol C_6H_5OH, equated as

$$\Delta\mathrm{BDE}^* = \mathrm{BDE}^*{}_{(\mathrm{YH})} - \mathrm{BDE}^*{}_{(\mathrm{phenol})}. \tag{3}$$

BDE* of H-phenol is a standard reference value for the hydrogen atomic bond dissociation energy. Besides calculating ΔBDE*, we also calculate the spin density distribution as a qualitative method of checking the stability of Y. The more delocalized the spin density, the more stable the Y is, hence, the lower BDE* is. We also apply the spin density in term of single occupied molecular orbital (SOMO) at the TS to predict the reaction mechanism based on the Mayer's interpretation [30].

In using the DFT method, we employ M05-2X exchange-correlation functional and 6-31++G(d,p) basis set that are integrated into the Gaussian 09 software [31]. M05-2X functional has been recommended for thermochemistry and kinetic calculations [32, 33], and has performed well to predict internuclear distance at the TS, especially for hydrogen transfer reaction [34].

We couple DFT calculation with the polarized continuum model (PCM) [35, 36] for considering the solvent environment. PCM has been applied successfully to a significant number of systems in aqueous and non-aqueous media [36–39]. In this work, we consider water solvent since it is the primary cellular environment component.

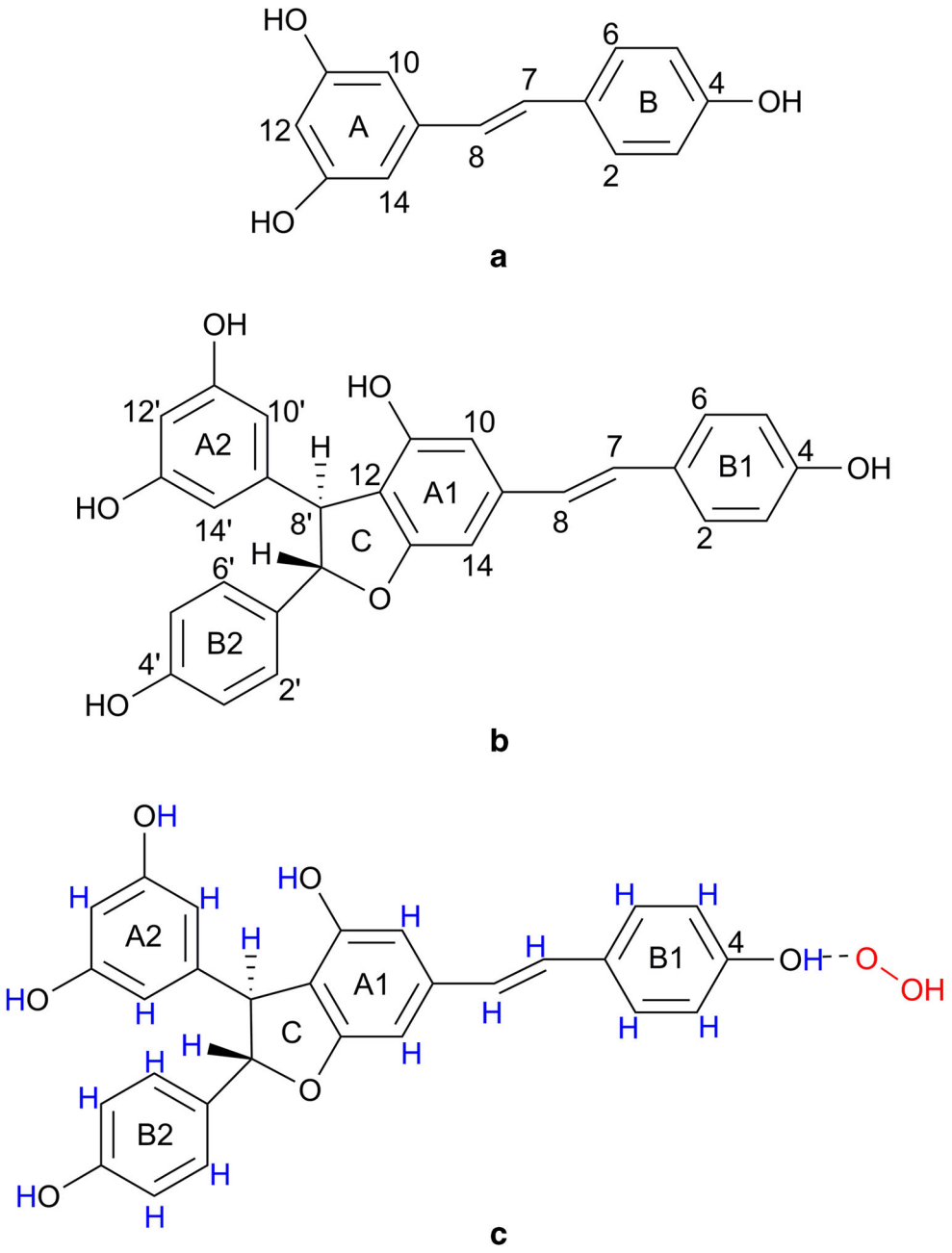

Fig. 1 Molecular model for **a** trans-resveratrol, **b** gnetin C, and **c** activated complex of gnetin C and •OOH for 4-OH site. The nomenclature is used throughout manuscript. A, B, C, are resorcinol, phenol, and furan rings in resveratrol system respectively. Red atom and blue atom labels indicate •OOH and the 22 possible scavenging sites respectively

Result and Discussion

The Bond Dissociation Energy

Figure 2 shows the optimized geometry for trans-resveratrol and gnetin C, while Table S1 (Supplementary Materials) lists the selected parameters. A gnetin C consists of one trans-resveratrol-like structure (ring A1 and B1) and one non-planar resveratrol structures (ring A2 and B2). Atom 13O and 12C of the planar trans-resveratrol are combined with atom 7′C and 8′C of non-planar resveratrol to form a new ring, namely furan ring (ring C).

Table 1 shows the ΔBDE* in all possible sites of trans-resveratrol and gnetin C based on Fig. 1. Overall, ΔBDE* in the O-H site is less than that in the C-H site in both molecules. Interestingly, 7′-CH and 8′-CH sites of gnetin C have comparable ΔBDE* with the O-H sites. The lower ΔBDE* in 7′-CH and 8′-CH sites is explained by the contribution of sp^n hybrid in their bonding orbital (as shown in Table S2, Supplementary Materials). The C-H bond in these sites has n≈3, instead of n≈2 as the other C-H bonds in gnetin C. It suggests that the weaker sp^3 bonding than sp^2 bonding is the reason of the lower ΔBDE* in 7′-CH and 8′-CH sites. Therefore, we consider 7′-CH and 8′-CH

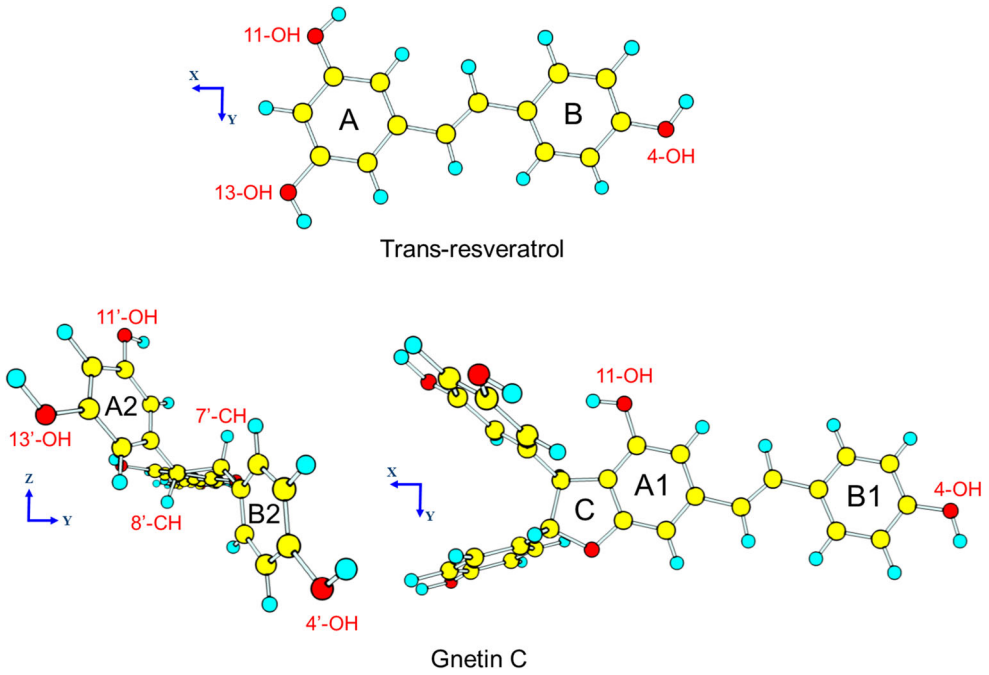

Fig. 2 Optimized structure of trans-resveratrol and gnetin C in water environment. Blue, red, and yellow atoms represent H, O, and C atom. Red marker indicates scavenging site

for the scavenging sites of gnetin C in addition to the OH sites.

The spin density plots in Fig. 3 shows the stability of gnetin C radical. The most stable radical is 8′-C gnetin C radical since the spin density covers two resorcinol and one furan ring. The stability of the radical reduces as the number of rings covered decreases. The second and third most stable radicals are 4′-O and 7′-C gnetin C radical. The former has two rings covered, while the latter has one and a half rings covered. The stability of 8′-C, 4′-O, and 7′-C radicals are inversely proportional to the ΔBDE* at site 8′-CH, 4′-OH, and 7′-CH. Therefore, the stability of gnetin C radical

Table 1 H-bond dissociation enthalpy of trans-resveratrol and gnetin C relative to H-phenol (ΔBDE*), at T=298.15 K

Reaction site	ΔBDE* (kcal/mol)	Reaction site	ΔBDE* (kcal/mol)
Trans-resveratrol			
4-OH	-4.95	6-CH	26.27
11-OH	1.13	7-CH	17.33
13-OH	1.47	8-CH	16.66
2-CH	25.14	10-CH	27.87
3-CH	27.48	12-CH	30.94
5-CH	28.12	14-CH	29.04
Gnetin C			
4-OH	-5.27	10-CH	27.75
11-OH	2.14	14-CH	29.80
4′-OH	-0.01	2′-CH	26.20
11′-OH	0.96	3′-CH	28.10
13′-OH	2.22	5′-CH	27.65
2-CH	24.99	6′-CH	26.39
3-CH	27.29	7′-CH	-3.98
5-CH	28.18	8′-CH	-6.56
6-CH	26.18	10′-CH	28.88
7-CH	16.53	12′-CH	30.22
8-CH	16.97	14′-CH	29.82

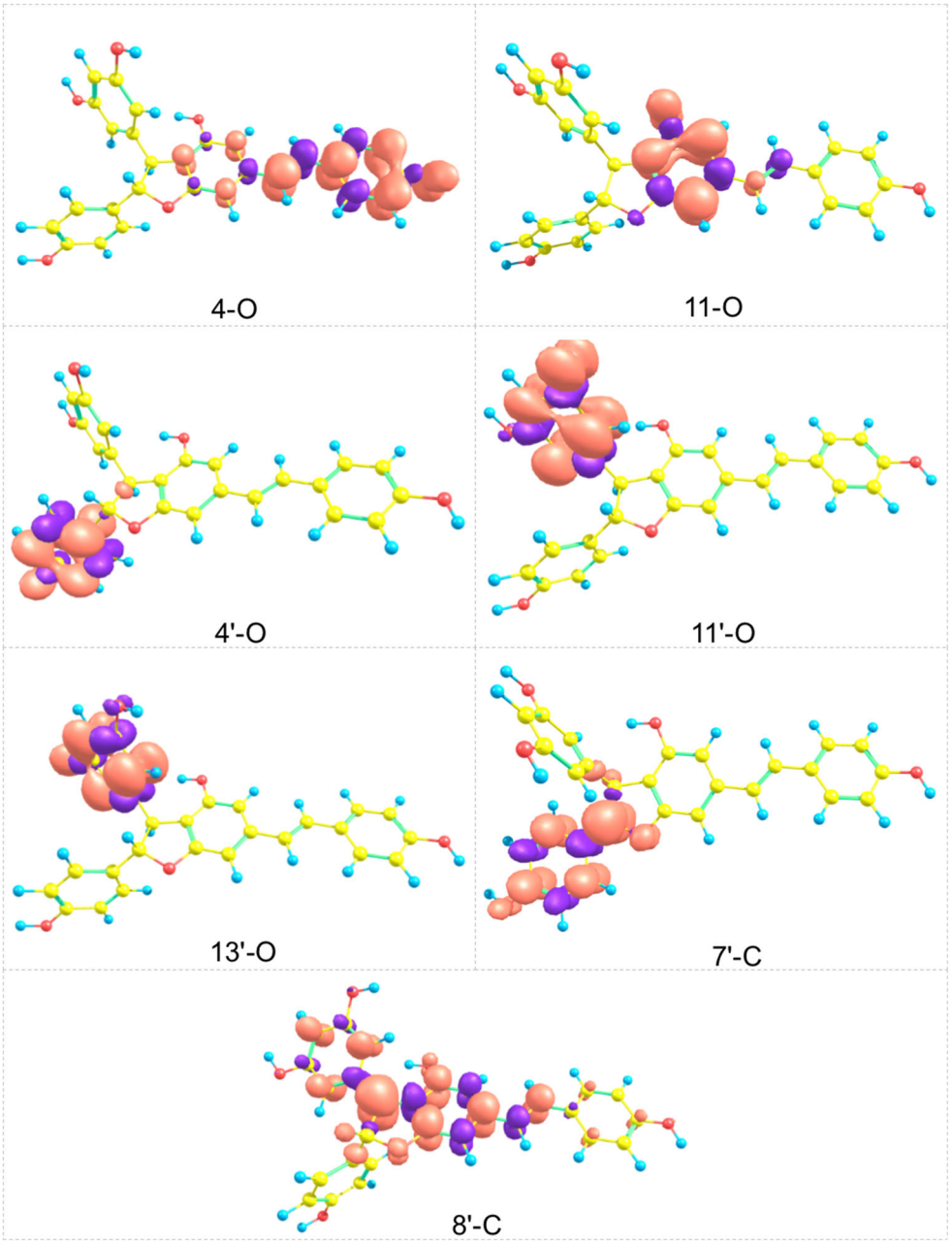

Fig. 3 The spin density distribution of gnetin C radical with isovalue 0.003. Orange and purple colors indicate α and β densities are dominant, respectively

supports the hydrogen atom transfer process in site 8′-CH, 4′-OH, and 7′-CH.

The Standard Gibbs Energy of Reaction

Table 2 provides the $\Delta_r G^0$ of the •OOH scavenging reaction by trans-resveratrol, according to Eq. (1). Out of three OH sites in trans-resveratrol, the •OOH scavenging reaction is exergonic only at site 4. Therefore, only the 4-OH site is favorable for scavenging •OOH. Another density-functional study on the identical system, employing the same exchange-correlation functional but 6-311++G(d,p) and solvation model based on density, concluded the same result [23]. It supports the recommendation by Zhao et al. [32, 33] that M05-2X is reliable for studying the scavenging reaction energetically.

As for gnetin C, Table 2 shows that the exergonic sites are not only at OH-group but also at CH-group. The scavenging sites of gnetin C are at 4-OH, 7′-CH, 8′-CH. Since gnetin C provides more scavenging site than trans-resveratrol does, the former is potent to have a higher antioxidant capacity than the later. These results support the experimental findings which reported that gnetin C has better antioxidant capacity than trans-resveratrol in ORAC assay [40]. Furthermore, by considering the ring in gnetin C, ring C provides more scavenging sites than other rings

Table 2 The calculation results of the standard Gibbs free energy of reaction ($\Delta_r G^0$, in kcal/mol) and activation ($\Delta^{\ddagger} G^0$, in kcal/mol) for the $^{\bullet}$OOH scavenging reaction based on Eq. (1)

Molecule	Reaction site	$\Delta_r G^{0a}$	$\Delta^{\ddagger} G^{0a}$	$\Delta^{\ddagger} G^{0b}$
Trans-resveratrol	4-OH	-3.59	18.69	17.96
	11-OH	2.09	21.31	20.25
	13-OH	1.83	20.70	19.77
Gnetin C	4-OH	-3.51	17.22	n/a[c]
	11-OH	2.69	21.55	n/a
	4′-OH	0.86	19.86	n/a
	11′-OH	4.03	21.29	n/a
	13′-OH	3.07	21.72	n/a
	7′-CH	-2.43	22.14	n/a
	8′-CH	-5.02	20.85	n/a

The values in column 3 and 4 are obtained from our calculations. The values from Iuga's calculations [24] in column 5 are used as benchmark for $\Delta^{\ddagger} G^0$

[a]Using M05-2X/6-31++G(d,p), this work.

[b]Using M05-2X/6-311++G(d,p), reported by Iuga et al. [24].

[c]n/a means not available value.

(A, phenol, and B, resorcin ring). It indicates that furan ring plays a more important role than other rings in the scavenging capacity of melinjo resveratrol.

Overall, ring A always provides the lowest $\Delta_r G^0$ value for OH site. It is valid for both trans-resveratrol and gnetin C. It implies, there is a relation between the position of the OH site and the $\Delta_r G^0$. Queiroz et al. [41] also reported this relation.

The Standard Gibbs Energy of Activation

We validate our work on reaction kinetics based on the trans-resveratrol case. Our predictions of $\Delta^{\ddagger} G^0$ are comparable with a theoretical work reported by Iuga et al. [24] (see Table 2), which computed the rate constants at room temperature with the basis of transition-state theory, whose results are comparable with the experimental results by Zinatullina et al. [42]. Consequently, our density-functional calculations on Eq. (1) is adequate to study $^{\bullet}$OOH scavenging by resveratrol system such as gnetin C.

Regarding gnetin C, Figure 4 shows the TS of $^{\bullet}$OOH scavenging according to Eq. (1). The activated complexes are at their optimized structure, where the syn arrangement exists as expected from phenolic antioxidants. The syn arrangement also exists in trans-resveratrol, which is also a group of phenolic antioxidants, as shown in the optimized structure in Fig. S1 (Supplementary Materials). It is also noteworthy that the distance between the H-atom of gnetin C and its scavenging site elongates to 0.16 $\AA$ on average (or at about 16%) relative to its ground state structure. It implies that H-atom's bonding to its scavenging site weakens at the TS for all scavenging sites. The reaction in Eq. (1) requires this condition.

The $\Delta^{\ddagger} G^0$ values of gnetin C in Table 2 show that the lowest $\Delta^{\ddagger} G^0$ is at site 4-OH. The site 4-OH in trans-resveratrol also has the lowest activation energy. These results agree with the previous experimental findings reporting that site 4-OH is the most reactive one in trans-resveratrol and its derivatives [43]. However, $\Delta^{\ddagger} G^0$ at site 4-OH of gnetin C is lower than that of trans-resveratrol. It implies that resveratrol in its dimer form is expected to react faster with $^{\bullet}$OOH than its monomer form.

As for $\Delta_r G^0$, the $\Delta^{\ddagger} G^0$ values at OH-group also has a relation with its location. Both site 4-OH and 4′-OH have the lowest $\Delta^{\ddagger} G^0$ in their respective resveratrol unit, and they are at para position of ring A1 and A2, respectively. The difference is that ring A1 is in the first unit, while ring A2 is in the second one. The resveratrol is planar in the first unit, but not in the second unit. It implies that the planarity of resveratrol in gnetin C increases the scavenging reactivity of an OH site.

Considering the $\Delta_r G^0$ value, it is also possible for site 7′-CH and 8′-CH to become a scavenging site. However, the reaction may be slower at these two CH sites than that of at 4-OH site due to their higher value of $\Delta^{\ddagger} G^0$. The high barrier is expected since geometrically ring A2 and B2 hinder $^{\bullet}$OOH to reach site 7′ and 8′. The various value of $\Delta^{\ddagger} G^0$ make the three sites scavenge three $^{\bullet}$OOH radicals at different rates. It is revealed that resveratrol dimer gradually scavenges one radical from ring A1 (phenol) and two more radicals from ring C (furan) to reach the maximum scavenging activity after a sufficient time. This gradual increase in scavenging activity was observed in the

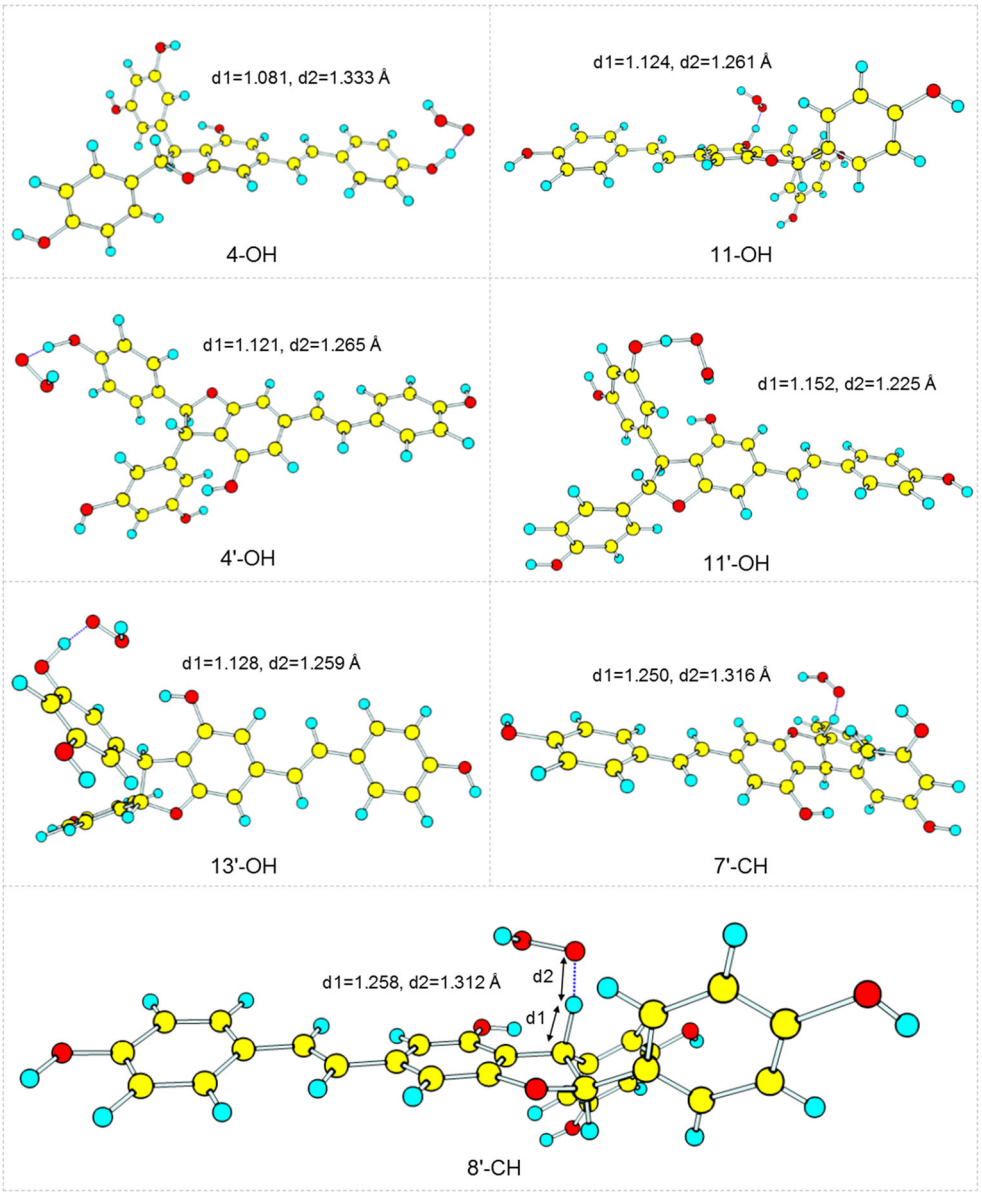

Fig. 4 TS structure for •OOH scavenging reaction by gnetin C on each site. Markers d1 is bond length of scavenging site, while d2 is the distance between O atom of •OOH with the nearest scavenging site

experiment done by Kato et al.[1]. However, this finding is contrary to their speculation proposing that it is ring B2 (resorcinol) that plays a crucial role in the scavenging activity of melinjo resveratrol.

All the three possible scavenging sites share similarities in their SOMO distribution. The 2p-like orbitals construct all SOMO distributions, as shown in Fig. S2 (Supplementary Materials). The orbital interaction forms sigma bonding between O or C (from the scavenging site) and at O (from •OOH). The sigma bond allows hydrogen atom (both the proton and the electron) to transfer from one side to another [30]. It implies that the •OOH scavenging at the three sites of gnetin C through the reaction in Eq. (1) is a hydrogen atom transfer.

Conclusion

We have demonstrated the use of a density-functional calculations to investigate the scavenging activity of gnetin C with trans-resveratrol as the comparison. We utilized density-functional calculations and used a one-step mechanism for the •OOH scavenging reaction model. The OH-group at the para position in a phenol ring turns out to be a common scavenging site for both trans-resveratrol and gnetin C. The scavenging reaction energy at this particular site, as observed in this study, is -3.59 kcal/mol and -3.51 kcal/mol for trans-resveratrol and gnetin C respectively, which makes the reaction at OH site is exergonic.

We have shown the role of the furan ring in relation to the antioxidant capacity and activity of melinjo resveratrol. Furan ring increases the antioxidant capacity of melinjo resveratrol by providing two more scavenging sites, namely site 7′-CH and 8′-CH. Such sites should have a slower reaction with •OOH as they require higher activation energy compared to 4-OH site. The activation energy differs as much as 4.92 kcal/mol between 7′-CH and 4-OH and 3.53 kcal/mol between 8′-CH and 4-OH. Our results suggested that gnetin C scavenge radicals gradually with the following sequence: 4-OH, 8′-CH, and 7′-CH, to reach its maximum scavenging activity. Thus, we propose the furan ring as the one playing a crucial role in the scavenging activity of melinjo resveratrol, not the resorcin ring as has been speculated in the experimental study. Finally, this work demonstrates that density-functional calculations are a prospective approach for studying the system in question.

Supplementary Information The online version contains supplementary material available at 10.1007/s11483-021-09666-y.

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Author Contributions Conceptualization: Febdian Rusydi; Methodology: Febdian Rusydi and Vera Khoirunisa; Formal analysis: Vera Khoirunisa, Lusia S. P. Boli; Investigation: Vera Khoirunisa; Writing - original draft preparation: Vera Khoirunisa; Writing - review and editing: Febdian Rusydi, Adhitya G. Saputro, Heni Rachmawati and Hermawan K. Dipojono; Resources: Hideaki Kasai and Hiroshi Nakanishi.

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Biophysical studies of foods and agricultural products involve research at the interface of chemistry, biology, and engineering, as well as the new interdisciplinary areas of materials science and nanotechnology. Such studies include but are certainly not limited to research in the following areas: the structure of food molecules, biopolymers, and biomaterials on the molecular, microscopic, and mesoscopic scales; the molecular basis of structure generation and maintenance in specific foods, feeds, food processing operations, and agricultural products; the mechanisms of microbial growth, death and antimicrobial action; structure/function relationships in food and agricultural biopolymers; novel biophysical techniques (spectroscopic, microscopic, thermal, rheological, etc.) for structural and dynamical characterization of food and agricultural materials and products; the properties of amorphous biomaterials and their influence on chemical reaction rate, microbial growth, or sensory properties; and molecular mechanisms of taste and smell. A hallmark of such research is a dependence on various methods of instrumental analysis that provide information on the molecular level, on various physical and chemical theories used to understand the interrelations among biological molecules, and an attempt to relate macroscopic chemical and physical properties and biological functions to the molecular structure and microscopic organization of the biological material.

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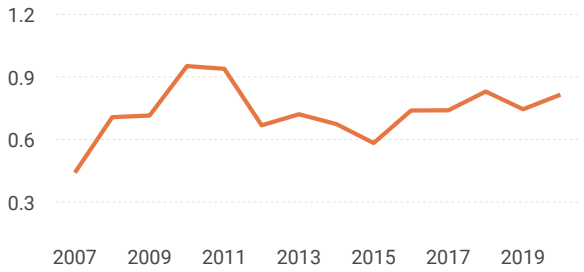

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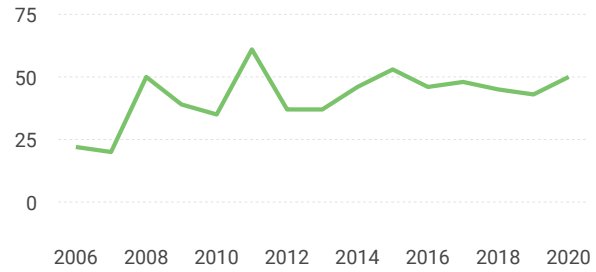

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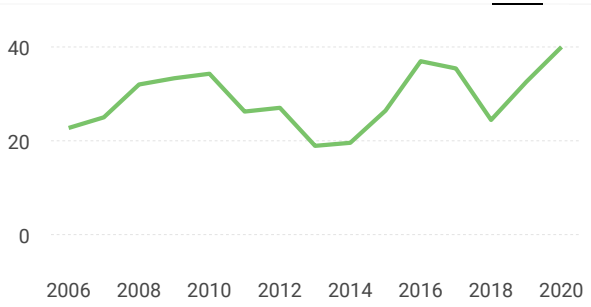

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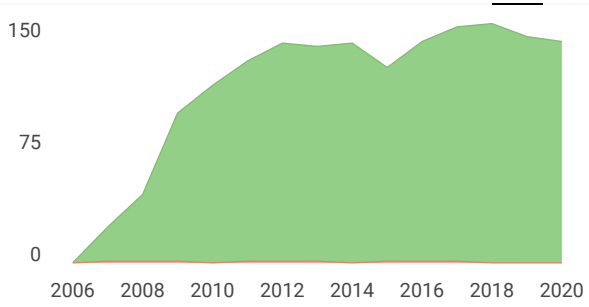

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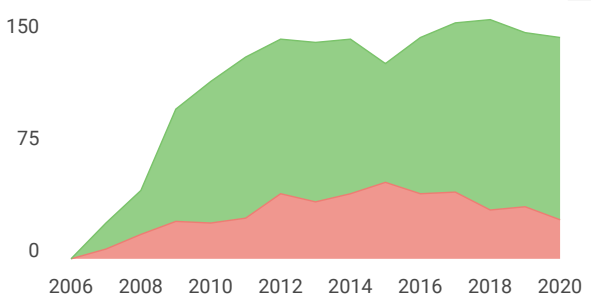

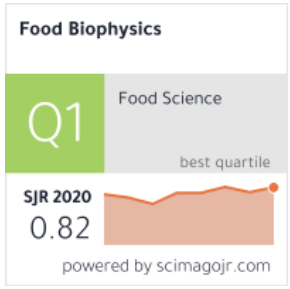

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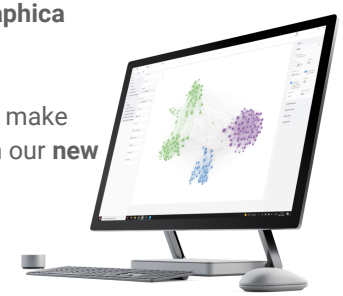

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