Preface

PREFACE

It is with great pleasure that I introduce the proceedings of the 2019 5th International Conference on Smart Material Research (ICSMR 2019) which was held recently in Brisbane, Australia, 13-16, November 2019. ICSMR 2019 was dedicated to technical issues related to smart material research.

The objectives of the conference were not only to provide opportunities to the international scientists to present state of the art research in smart materials but also to provide a forum to discuss ideas for future directions in the field and explore possibilities for collaborative research projects.

The conference program included keynote, oral, and poster presentations from scholars working in the areas of materials science and engineering from all over the world. It covered recent trends and progress made in the field of materials engineering and manufacturing. Professors from Australia and USA were invited to deliver four keynote lectures regarding the latest information in their respective areas of expertise.

The proceedings present a selection of high quality papers submitted to the conference by researchers from universities, research institutes, and industry. All papers were subjected to peer-review by conference committee members and international reviewers. The papers were selected based on their quality and their relevance to the conference. The proceedings present recent advances in the fields of materials science and engineering and manufacturing as well as in other related areas including materials properties, measuring methods, analytical and numerical modeling and simulations among others.

I would like to express special gratitude to members of the conference committee and organizers of the conference. I would also like to thank the reviewers for their valuable time and advice which helped in improving the quality of the papers selected for presentation at the conference and for publication in the proceedings. Finally I want to thank the authors, the members of the organizing committee, the reviewers, the chairpersons, sponsors, and all other conference participants for their support of ICSMR 2019.

Prof. Ramesh K. Agarwal
Washington University in St. Louis, USA
January 21, 2020

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Theoretical investigation on electron transfer-based antioxidant activity of melinjo resveratrol

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Theoretical investigation on electron transfer-based antioxidant activity of melinjo resveratrol

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Abstract. We employ density functional calculations to study the electron transfer-based antioxidant activity of resveratrol derivatives from melinjo. The derivatives are monomer resveratrol which is trans-resveratrol, and dimer resveratrol which are gnetin C, gnetin L, and gnemonoside C. The results show that gnetin C has the lowest adiabatic ionization potential both in gas phase and water environment. Furthermore, our results demonstrate that dimer resveratrol is consistent to have better electron transfer ability than its monomer. This may due to the destabilization of the high occupied molecular orbital energy of resveratrol. However, the presence of glucoside in gnemonoside C does not affect the electron transfer-based antioxidant activity of dimer resveratrol.

1. Introduction

Resveratrol has gained great attention due to its prominent antioxidant properties. Through various *in vitro* assays, Gulcin has proven the resveratrol's excellent antioxidant activity compared to some standard antioxidant viz. trolox, BHA, BHT, and α-tocopherol [1]. Furthermore, some studies also support that resveratrol exhibits antioxidant effect in some physiological systems [2,3,4]. The antioxidant properties are linked to promote various health benefits such as protecting the brain [5] and lowering blood pressure [6]. Hence, resveratrol become a growing interest to be drug reference molecule.

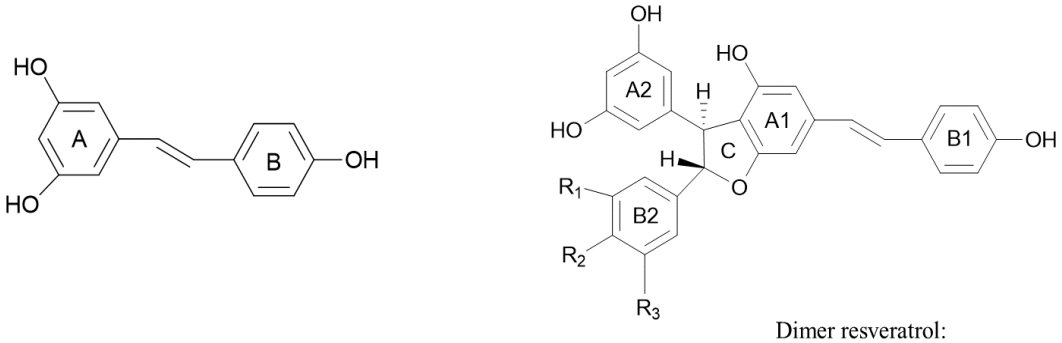
Resveratrol is a phenolic antioxidant that can deactivate radicals by two possible mechanisms, hydrogen atom transfer (HAT) and single electron transfer mechanism (SET) [7]. HAT is a direct mechanism, while SET is a stepwise mechanism. Both of them have the same net reaction in which antioxidant donate one of its hydrogen atoms to radical at the end of reaction. Even though HAT

mechanism is predominant mechanism, it is essential to investigate SET mechanism to explore antioxidant behaviour of molecules.

One of resveratrol derivatives sources is melinjo seed. The seed contains resveratrol mostly in the form of dimers [8] which are gnetin and gnemonoside. Gnetin is the simplest resveratrol dimer, and gnemonoside is a resveratrol dimer with additional glucoside. Experimental study performed by Kato et al. suggested that antioxidant activity of melinjo seed may associate with electron-donating ability of resveratrol dimer [9]. However, to the best of our knowledge, no further investigation is reported to confirm electron-donating ability of resveratrol dimer.

This paper address the relation between antioxidant activity of melinjo resveratrol and its structure based on SET mechanism; that contributes to a better understanding on the electron-donating ability of resveratrol dimer. Four chosen resveratrol derivatives are trans-resveratrol, gnetin C, gnetin L, and gnemonoside C (figure 1). The parameter used to examine the antioxidant activity of the four resveratrol derivatives is adiabatic ionization potential (AIP). This parameter is determined by performing density functional calculations.

Finally, the insightful discussion about the AIP values contribute to a better understanding on the electron-donating ability of resveratrol dimer.



Monomer Resveratrol:
A. Trans-resveratrol

Dimer resveratrol:
B. Gnetin C: R_1=H; R_2=OH; R_3=H
C. Gnetin L: R_1 =OH; R_2 =H; R_3 3=OCH3
D. Gnemonoside C: R_1 =H; R_2 =O-glucoside; R_3=H

Figure 1. Four resveratrol derivatives from melinjo seed.

2. Computational Model

We define our reaction model based on SET mechanism as it is shown in equation 1:

$$XH \rightarrow XH^{+} + e^{-}, \quad (1)$$

where XH and XH^{+} represent the parent molecules and the respective cation radical generated after electron transfer. We perform DFT calculations by using Gaussian 09 software package [10]. We use Becke three parameter exchange and Lee−Yang−Parr correlation (B3LYP) and 6-31++G(d,p) basis sets for geometry optimization of each resveratrol and respective cation structure in gas phase and water environment. The water solvation is considered using polarizable continuum model. We also perform vibrational frequency calculation to confirm that there is no imaginary frequency in the ground state structure, and to give thermal correction at 298.15 K. AIP is determined according to the formula,

$$AIP = (H_{XH^{+}} + H_{e-}) - H_{XH}, \quad (2)$$

where H_{e-} is enthalpy of the electron (0.00119787 hartree in gas phase and -0.0492478 hartree in water) [11].

3. Results and Discussion

Table 1 shows the AIP values of the resveratrol derivatives in gas phase and water environment. It shows that the AIP values of trans-resveratrol in gas phase and water environment are 160.7 and 93.7 kcal/mol, respectively. These values are close to the results of previous works [12,13]. Therefore, our model is reasonable for studying this case.

The values of AIP in water environment is lower than that in gas phase. We suspect that it is due to the polarity of the water that is higher than the gas phase. This result agrees with previous work done by Mikulski et al. [12]. They demonstrated that the AIP of molecules decreases with the increasing environment polarity. The lower AIP value in water environment indicates that the resveratrol derivatives are easier to transfer electron in water environment than in gas phase. The polar environment may facilitate the electron donation that is important for radical scavenging activity of the resveratrol derivatives [13].

We also find that all resveratrol dimers have lower AIP values than its monomer, trans-resveratrol. It implies that dimer structure of resveratrol has better electron-donating ability than the monomer. The sequence of AIP values of the resveratrol derivatives is as follows: **gnetin C < gnetin L or gnemonoside C < trans-resveratrol**. Thus, we propose gnetin C to be the most potential electron transfer-based antioxidant among the four resveratrol derivatives due to its highest electron-donating ability.

Table 1. AIP values of four resveratrol derivatives (see figure 1) in gas phase and in water environment in terms of enthalpy.

	AIP (kcal/mol)	
Resveratrol derivatives	Gas phase	Water
Trans-resveratrol	160.7	93.7
Gnetin C	152.8	92.3
Gnetin L	154.0	92.4
Gnemonoside C	154.0	N/A

Table 2 presents the HOMO energy of four resveratrol derivatives. We find that the stability of the HOMO energy corresponds to the AIP value. The more stable the HOMO energy, the higher the AIP value is. This relation is plotted in figure 2. By considering this relation, we may infer that the increasing electron transfer ability is associated with the destabilization of the HOMO energy. In this case, the destabilization in gas phase that is up to 0.18 eV corresponds to the decrement of AIP value by 7.9 kcal/mol.

Table 2. HOMO energy of four resveratrol derivatives in gas phase and in water environment.

	HOMO energy (eV)	
Resveratrol derivatives	Gas phase	Water
Trans-resveratrol	-5.63	-5.67
Gnetin C	-5.45	-5.60
Gnetin L	-5.51	-5.61
Gnemonoside C	-5.53	N/A

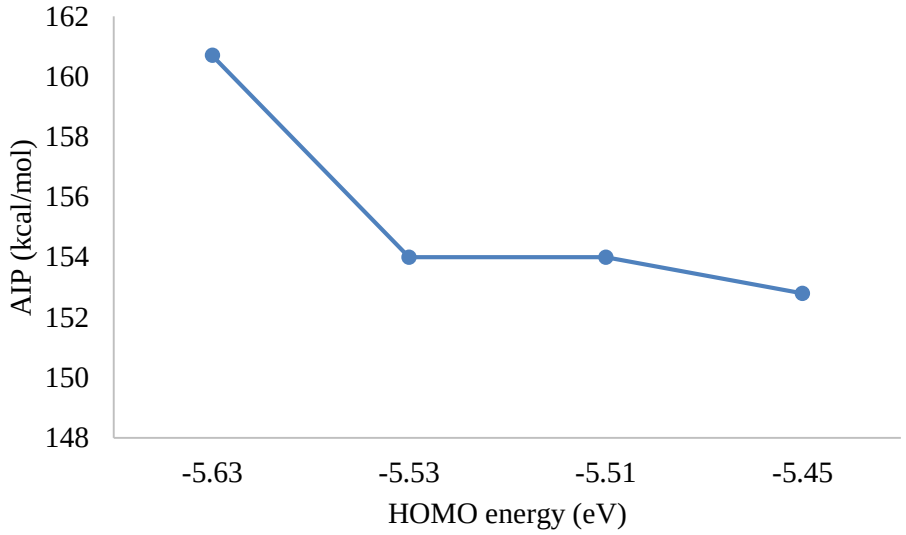


Figure 2. AIP values against HOMO energy of four resveratrol derivatives in gas phase. The HOMO energy is more stable towards the left side of the *x*-axis.

We also note that gnemonoside C has relatively close HOMO energy to gnetin C even though they are differed by the presence of glucoside. Based on our calculation results, the presence of glucoside slightly stabilizes the HOMO energy that leads to small changes of AIP value. Therefore, in this case, the presence of glucoside is not necessarily considered.

4. Conclusion

We have explored the electron-based antioxidant activity of four resveratrol derivatives: trans-resveratrol, gnetin C, gnetin L, and gnemonoside C. Trend of the AIP values has been found to be correlated with the trend of the HOMO energy. We suggest that the HOMO energy destabilization can enhance the antioxidant activity of resveratrol. Based on our finding, we propose that antioxidant activity of four melinjo resveratrols follows the order: **resveratrol dimer > resveratrol dimer with glucoside > resveratrol monomer**. To further our study, we are planning to investigate the reaction pathways of electron-donating precess from resveratrol dimer to radicals.

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