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From: **Royal Society Open Science** <onbehalf@manuscriptcentral.com>

Date: Wed, Dec 23, 2020 at 4:10 PM

Subject: Royal Society Open Science - Decision on Manuscript ID RSOS-201127.R1

To: <vera.khoirunisa@tf.itera.ac.id>

Cc: <vera.khoirunisa@tf.itera.ac.id>, <rusydi@fst.unair.ac.id>, <lusia_silfia@yahoo.co.id>, <ira-p@fst.unair.ac.id>, <h_rachmawati@fa.itb.ac.id>, <dipojono@gmail.com>, <journal-submit@datadryad.org>, <openscience@royalsociety.org>

This year has been very difficult for everyone, and we want to take the opportunity to thank you for your continued support in 2020.

The Royal Society Open Science editorial office will be closed from the evening of Friday 18 December 2020 until Monday 4 January 2021. We will not be responding during this time. If you have received a deadline within this time period, please contact us as soon as possible to allow us to extend the deadline. If you receive any automated messages during this time asking you to meet a deadline, we offer apologies and invite you to respond after the festive period or during normal working hours.

With our best for a peaceful festive period and New Year, and we look forward to working with you in 2021.

Dear Ms Khoirunisa:

Title: The significance of long-range correction to the hydroperoxyl radical-scavenging reaction of trans-resveratrol and gnetin C
Manuscript ID: RSOS-201127.R1

It is a pleasure to accept your manuscript in its current form for publication in Royal Society Open Science. The chemistry content of Royal Society Open Science is published in collaboration with the Royal Society of Chemistry.

The comments of the reviewer(s) who reviewed your manuscript are included at the end of this email.

Thank you for your fine contribution. On behalf of the Editors of Royal Society Open Science and the Royal Society of Chemistry, I look forward to your continued contributions to the Journal.

Yours sincerely,
Dr Laura Smith
Publishing Editor, Journals

Royal Society of Chemistry
Thomas Graham House
Science Park, Milton Road
Cambridge, CB4 0WF
Royal Society Open Science - Chemistry Editorial Office

On behalf of the Subject Editor Professor Anthony Stace and the Associate Editor Professor Kim Jelfs.

RSC Associate Editor:
Comments to the Author:
(There are no comments.)

RSC Subject Editor:
Comments to the Author:
(There are no comments.)

Reviewer(s)' Comments to Author:
Reviewer: 1

Comments to the Author(s)
The authors made the necessary revisions and addressed the comments and questions. The manuscript is recommended for publication.

Journal Name: Royal Society Open Science
Journal Code: RSOS
Online ISSN: [2054-5703](https://doi.org/10.1039/C9PY00000A)
Journal Admin Email: openscience@royalsociety.org
Journal Editor: Kim
Journal Editor Email: chemistryopenscience@rsc.org
MS Reference Number: RSOS-201127.R1
Article Status: ACCEPTED
MS Dryad ID: RSOS-201127.R1
MS Title: The significance of long-range correction to the hydroperoxyl radical-scavenging reaction of trans-resveratrol and gnetin C
MS Authors: Khoirunisa, Vera; Rusydi, Febdian; Boli, Lusia; Puspitasari, Ira; Rachmawati, Heni; Dipojono, Hermawan
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Keywords: radical-scavenging reaction, long-range correction, dispersion correction, density functional theory, hydrogen atom transfer
Abstract: Density functional theory has been gaining popularity for studying the radical scavenging activity of antioxidants. However, only a few studies investigate the importance of calculation methods on the radical-scavenging reactions. In this study, we examined the significance of (1) the long-range correction on the coulombic interaction and (2) the London dispersion correction to the hydroperoxyl radical-scavenging reaction of trans-resveratrol and gnetin C. We employed B3LYP, CAM-B3LYP, M06-2X exchange-correlation functionals, and B3LYP with the D3 version of Grimme's dispersion in the calculations. The results showed that long-range correction on the coulombic interaction had a significant effect on the increase of reaction and activation energies. The increase was in line with the change of hydroperoxyl radical's orientation in the transition state structure. Meanwhile, the London dispersion correction only had a minor effect on the transition state structure, reaction energy, and activation energy. Overall, long-range correction on the coulombic interaction had a significant impact on the radical-scavenging reaction.

EndDryadContent



Vera Khoirunisa <vera.khoirunisa@tf.itera.ac.id>

5:37 AM (39 minutes ago)



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From: **Royal Society Open Science** <onbehalfof@manuscriptcentral.com>

Date: Thu, Jun 25, 2020 at 1:38 PM

Subject: Royal Society Open Science - Manuscript ID RSOS-201127

To: <vera.khoirunisa@tf.itera.ac.id>

Cc: <vera.khoirunisa@tf.itera.ac.id>, <rusydi@fst.unair.ac.id>, <lusia_silfia@yahoo.co.id>, <ira-p@fst.unair.ac.id>, <h_rachmawati@fa.itb.ac.id>, <dipojono@gmail.com>

We hope you are keeping well at this difficult and unusual time. We continue to value your support of the journal in these challenging circumstances. If Royal Society Open Science can assist you at all, please don't hesitate to let us know at the email address below.

Dear Ms Khoirunisa,

Your manuscript entitled "The significance of long-range correction to the hydroperoxyl radical-scavenging reaction of trans-resveratrol and gnetin C" has been successfully submitted online to Royal Society Open Science.

Your manuscript ID is **RSOS-201127**. Please mention the above manuscript ID in all future correspondence or when calling the office for questions.

We aim to make the submission process as straightforward as possible, but we recognise there is always room for improvement. We would be grateful if you could please [complete a survey of 6 short questions](#) to help us improve the experience you and other authors have with the submission system. Responses will be anonymous.

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Thank you for submitting your manuscript to Royal Society Open Science.

Yours sincerely,

Royal Society Open Science Editorial Office

openscience@royalsociety.org