

Review Form 3

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_128908
Title of the Manuscript:	Comparative Study of Epicatechin–Phenylalanine and Epicatechin–Alanine Interactions Using Quantum Chemistry Methods
Type of the Article	

General guidelines for the Peer Review process:

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guidelines for the Peer Review process, reviewers are requested to visit this link:

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PART 1: Comments

	Reviewer's comment	Author's Feedback <i>(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.	This manuscript presents a comparative quantum chemical analysis of epicatechin interactions with phenylalanine and alanine, providing insights into the non-covalent bonding mechanisms that influence these complexes. The findings enhance the understanding of polyphenol-protein interactions, relevant to pharmacological and food sciences. The detailed use of DFT, NBO, QTAIM, and NCI methods ensures robustness, making this study valuable for exploring the effects of structural variations in amino acids on bonding interactions.	
Is the title of the article suitable? (If not please suggest an alternative title)	The title is precise and accurately reflects the content of the manuscript. No changes are recommended.	
Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.	The abstract is clear and provides a comprehensive overview of the objectives, methods, results, and conclusions. Including a brief mention of the thermodynamic and spectroscopic parameters analyzed could further improve clarity.	
Is the manuscript scientifically, correct? Please write here.	The manuscript is scientifically sound. The methodology section thoroughly explains the computational techniques and parameters used. The results are well-supported with tables, figures, and appropriate discussion. However, the authors could enhance the discussion on the practical implications of their findings in biological and material science applications.	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.	The references are adequate and recent, covering a range of relevant studies. No additional references are required.	
Is the language/English quality of the article suitable for scholarly communications?	The language is clear and appropriate for scholarly communication. Minor edits for grammatical consistency and sentence structure will improve readability.	
<u>Optional/General</u> comments	<ol style="list-style-type: none">The tables and figures are well-structured but could benefit from additional explanatory captions.The authors should consider highlighting how their findings align or contrast with prior studies to strengthen the context of their results.Expanding on the potential implications for drug design or nutritional sciences would enhance the manuscript's impact.	

PART 2:

	Reviewer's comment	Author's comment <i>(if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
<u>Are there ethical issues in this manuscript?</u>	<i>(If yes, Kindly please write down the ethical issues here in details)</i>	

Reviewer Details:

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