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.
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PART 1: Comments

	Reviewer's comment	**Author's Feedback** *(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
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.		
Is the title of the article suitable? (If not please suggest an alternative title)		
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.		
Is the manuscript scientifically, correct? Please write here.		
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.		

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Is the language/English quality of the article suitable for scholarly communications?		
Optional/General comments	**The work is devoted to a relevant and important topic, the study of weak interactions in polyphenol (epicatechin) complexes with components of protein molecules (alanine and phenylalanine), but there are a number of significant comments on its content.** **First, general comments.** **1) The density functional theory method and, in particular, globally hybrid functionals such as B3LYP are a fairly good compromise between accuracy and computational costs for many problems, but in this case, their use can significantly distort the results. In systems with the inclusion of a large number of non-polar groups, dispersion interaction can play a significant role (and in general, when studying systems with weak interaction, it cannot be neglected), but calculations using the B3LYP functional completely ignore the this interaction, which can lead to both an underestimation of the binding energy and incorrect geometry of the complexes. This problem is solved quite simply by including the Grimme corrections D3 (D3BJ) or D4 for this functional. The use of the 6-31+G(d,p) basis set also looks a bit strange in the presence of correlation-consistent basis sets (e.g. Dunning or Karlsruhe) which are more optimal for solving this problem, but this is not a mistake, just movetone.** **Next, on to the specifics.** **2) Item 2.4. Separation of bonds by interaction type (shared shell or closed shells depending on |V|/G) is convenient for understanding the covalent or ionic nature of bonds, but the approach proposed by the authors is somewhat outdated (in particular, the formula). I recommend studying the works 10.1002/jcc.26068, 10.1039/c4cp02585g, 10.1021/jp060571z to understand modern trends.** **3) In Fig. 3, it is advisable to leave only BCP for intermolecular interactions so as not to clutter the figure.** **4) There is no information on how BSSE is calculated, via gCP or according to the Boys & Bernardi method (10.1080/00268970110088901)**	

PART 2:

	Reviewer's comment	**Author's comment** ***(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)***
Are there ethical issues in this manuscript?	***(If yes, Kindly please write down the ethical issues here in details)***	

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