Dear reviewer,

We have done the corrections, changes, improvements as suggested by you. The corrections have been mentioned in bold letters.

Kindly go through it.

Thanking you.

**Reviewer 1**

Major issue:

- The isolation procedure of the compounds used for the present investigation is not included in the manuscript (defined as unpublished results in the Introduction and Methods sections). Since the compounds were used for experimental analysis, e.g. inhibition assays on the target enzymes, the description of their isolation procedures and their characterizations should be described (otherwise the authors should refer to published procedures).

Reference has been given for the procedure used for isolation.

Minor issues:

- Section 1. Introduction: lines 15-18, the sentence is too long (difficult to read), please simplify it (split in two shorter sentences).

Simplified the sentences.

- Error in section numbering: Renumber Section 3 (and subsections) as 2 and Section 2 (and subsections) as 3.

**Corrected numbering of sections**

- Table 1 and elsewhere in the manuscript: correct “Kcal/mol” in “kcal/mol”.

**- made the changes**

- Section 3.1 Molecular docking analysis: The section would benefit from a substantial shortening that could be supported by improved figures. The descriptions of the binding modes predicted from molecular docking analysis are poorly understandable in the current form. The author should consider to replace Table 2 and Figures 2-4 with figures showing the binding modes and the interactions predicted by their in-silico studies. A discussion of the role of the residues identified as crucial for the enzyme-compound interactions could help to explain their inhibition profiles. Furthermore, a comparison with formerly reported enzyme-inhibitor complexes could highlight the importance of the interactions predicted to stabilize the compound binding.

1. figures improved

2. Replaced table 2 and figures 2-4 with figures showing the binding modes

3. Role of residues and reported studies added

- Section 3.1 Molecular docking analysis (page 8, last three lines): since the inhibition data have not been displayed and discussed yet, the assessment “potent multi-target anti-amyloid agents” is not justified only by the docking results, please modify the sentence.

-Made the changes
Table 2: the interaction with Arg128 is reported as a Π - Π stacking interaction but, at physiological pH, arginine is usually protonated. Is this a real Π - Π stacking interaction or is this a cation - Π interaction?

- This is a cation - Π interaction. Corrections made in manuscript.

Section 3.3 Molecular dynamics (MD) and simulations: the subsection 3.3.1. RMSD would benefit from the introduction of a table the list all the values reported in the text. In this way, the extensive description of the obtained values could be avoided and the author could focus only on the most important results and their interpretation. Figure 5 and 6 are not called in the manuscript. Figure calls should be added in the appropriate positions within the section (and the subsections). In the second line of Subsection 3.3.1. RMSD, Fig. 1 is called but it should be Fig. 5 instead, please correct it.

- RMSD table introduced
- interpretation added
- figures 5 and 6 calls added at appropriate positions

- Figure 1 changed to Figure 5

Section 3.4 Enzyme inhibition: Figures 7-9 are not called in the manuscript. Figure calls should be added in the appropriate positions within the section (and the subsections). The author should discuss the inhibition properties reported for the three compounds in light of their predicted binding modes. Is there a correlation between the predicted binding modes and the inhibition properties of the compounds?

- Figures 7-9 calls added at appropriate positions in the manuscript.

- Inhibition properties in light of predicted binding modes were searched in the literature but could not find any information. Perhaps this is the first report of computational as well as in-vitro studies for these compounds. Because of these reasons we are not able to discuss the correlation between the predicted binding and inhibition properties of the compounds.

- Subsection 3.4.1. Cholinesterase inhibition (page 15, lines 7-8): change "exhibited in a much better manner" in "is more potent".

- changed the words

- Section 2. Methods: which procedure is the initial paragraph describing? If this is not describing any experimental procedure it should be removed from this section.

- It describes the initial literature review, collection of compound structures from the structure databases.

- Subsection 2.1 Protein preparation: correct "0.3°A" (penultimate line).

- corrected the word

- Subsection 2.6.2. In-vitro AChE and BChE activity assay: "Acetylcholinesterase (Amphiphilic), Butyrylcholinesterase (Human)" (lines 2-3 of the subsection), please check the term "Amphiphilic".

- changed the term, it is human