

# Review of: "Comparative Modeling And Enzymatic Affinity of Novel Haloacid Dehalogenase From Bacillus Megaterium Strain BHS1 Isolated From Alkaline Blue Lake In Turkey"

NIRAN AEKSIRI<sup>1</sup>

<sup>1</sup> Naresuan University

**Potential competing interests:** The author(s) declared that no potential competing interests exist.

1. The 3D-structure prediction, the researcher should explain what is the protein template that they use to predict the 3D structure.

2. The researcher should compare the quality of the structure before and after MD simulation.

From the Figure 2 Structure topology of DehLBHS1 model and top threading templates, the researchers should create the superimpose structure to compare the structure.

1. Why the researcher uses 3CP, 2,2DCP, D2CP and L2CP for Docking calculation? Please explain

2. Table 3: Model evaluation of DehLBHS1 before and after refinement using different tools. Why the score from VERIFY3D after refinement is lower than before? Should explain?

3. The figure 5, The researchers should draw the hydrogen bond interaction and increase the resolution of the figure

4. The figure 6, the researchers should identify what is the importance of the residues in the box, please explain?

5. Why the researchers performed MD simulations of only DehLBHS1-3CP, DehLBHS1-2,2DCP complex and non-complex structural of DehLBHS1, not all of the complex structures from docking? please explain?

6. Figure 9 RMSF plot, the researchers should identify or draw or compare the main residues that this research focuses.

7. All the figure should be cleared or high resolution

8. The common comment, the researchers should check spelling and grammar again.