

# Supplementary Information

## Applications of Molecular Modeling in the Design of New Insect Repellents Targeting the Odorant Binding Protein of *Anopheles gambiae*

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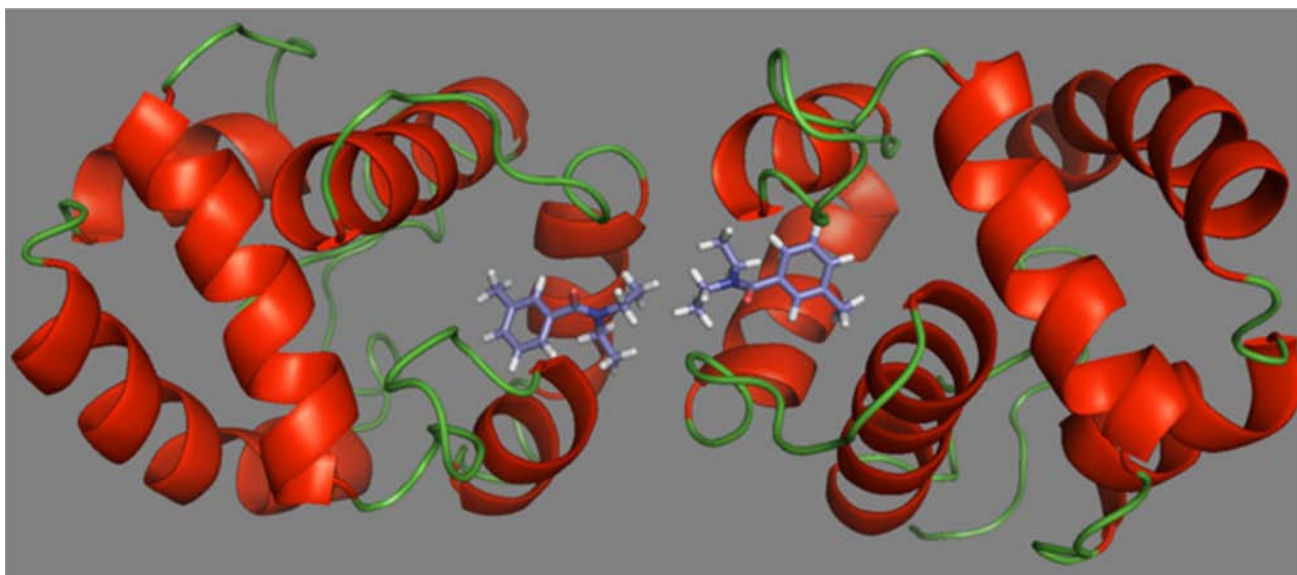
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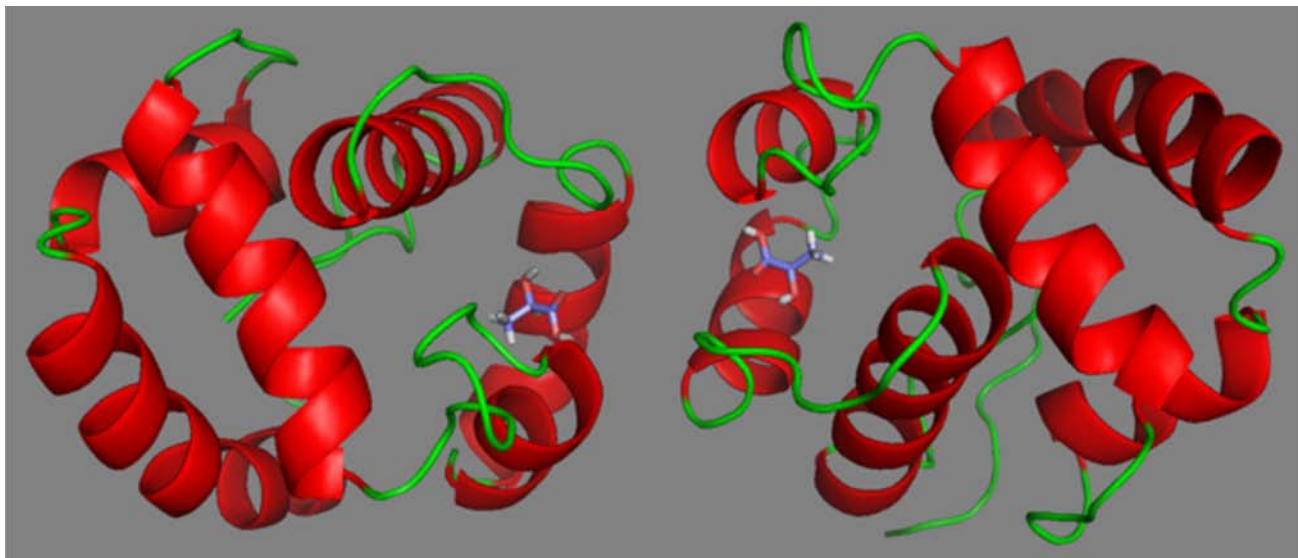
<sup>d</sup>National Institute of Industrial Property, Praça Mauá, 7, 20081-240 Rio de Janeiro-RJ, Brazil

Illustrations of the best poses of each ligand inside AgOBP<sub>1</sub>

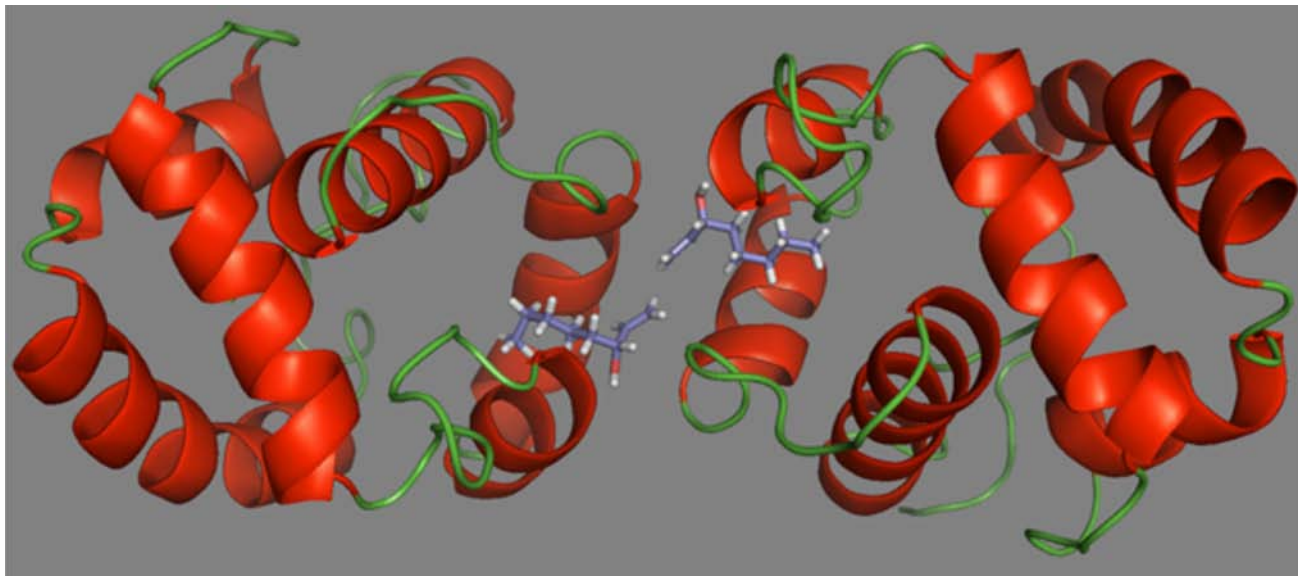
The files containing the 3D coordinates (.pdb format) can be requested by the e-mail [tanos@ime.eb.br](mailto:tanos@ime.eb.br)



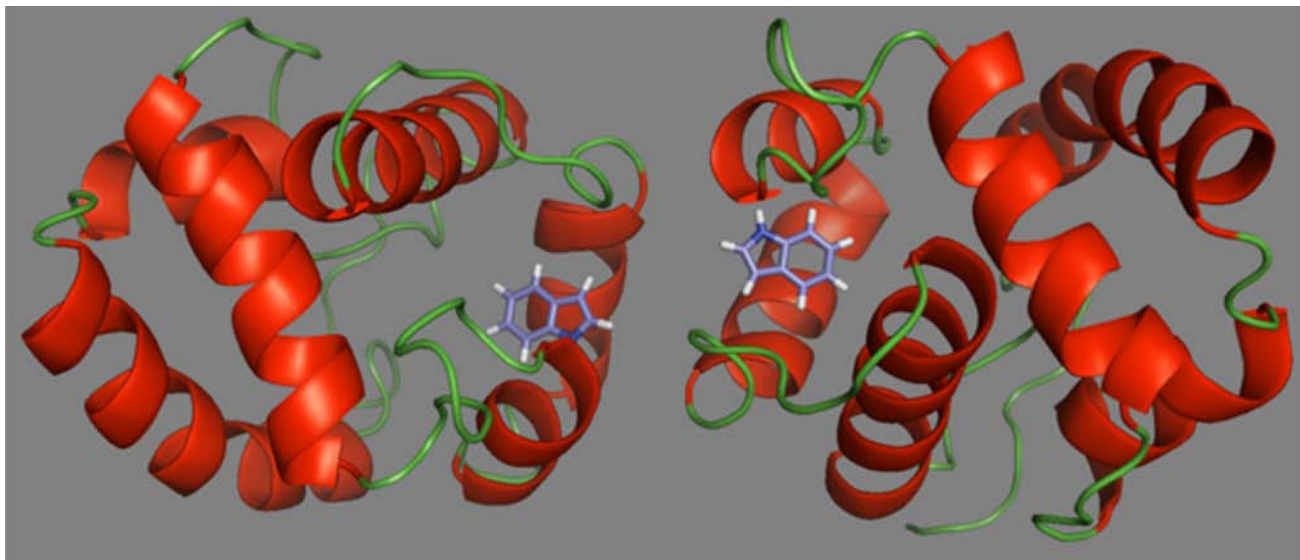
**Figure S1.** Best poses of DEET inside AgOBP<sub>1</sub>.



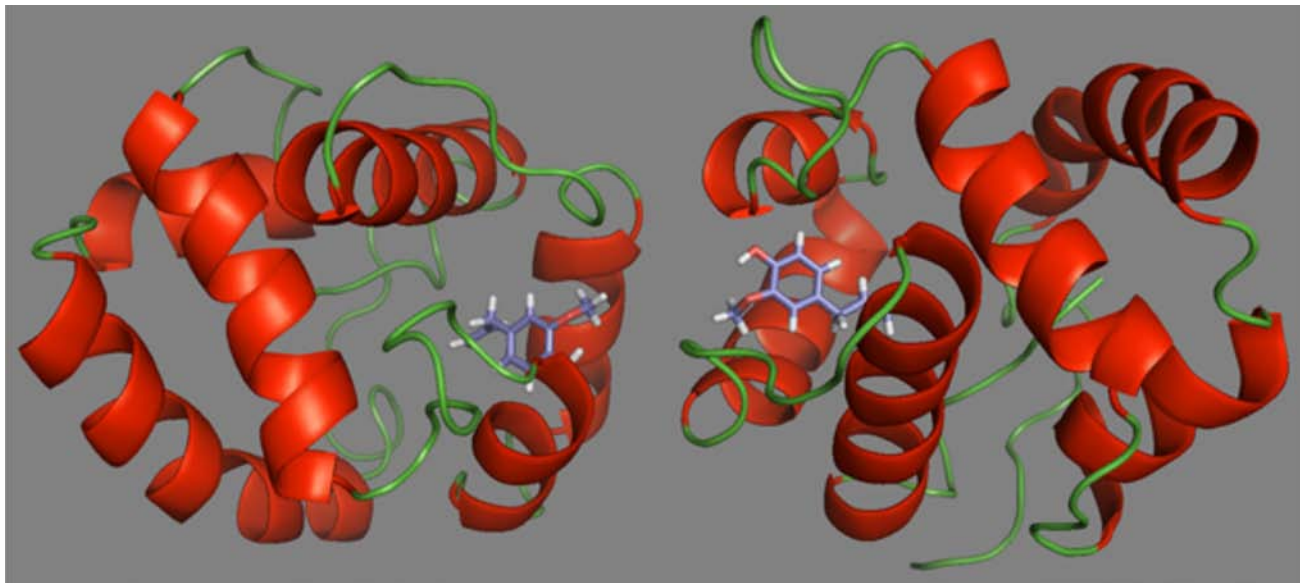
**Figure S2.** Best poses of lactic acid inside AgOBP<sub>1</sub>.



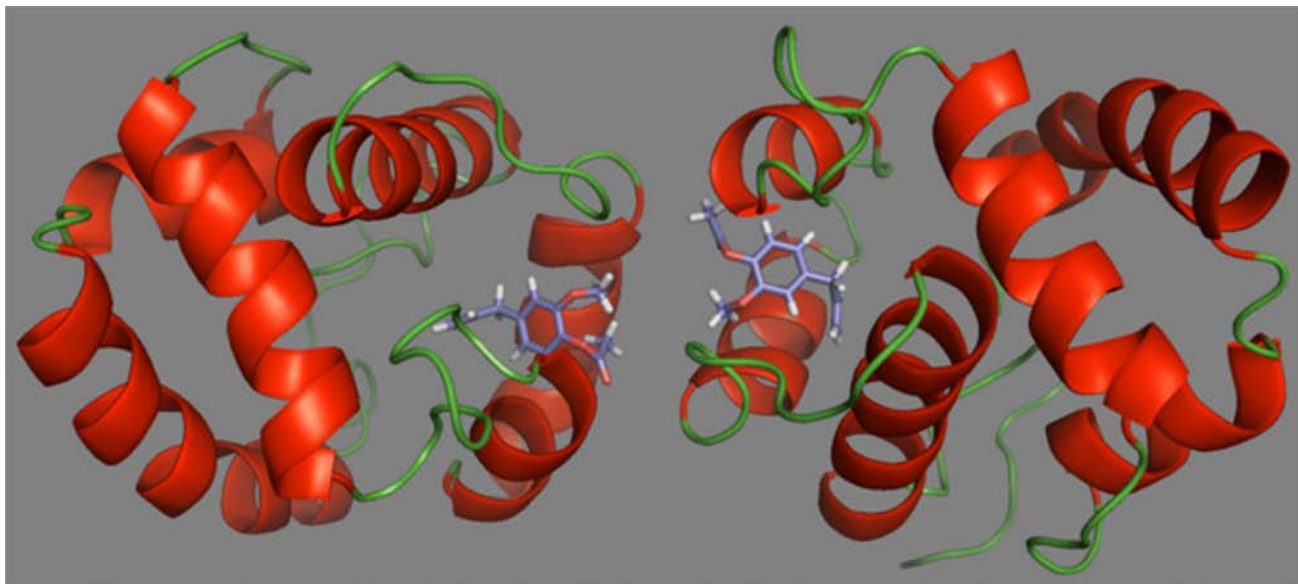
**Figure S3.** Best poses of 1-octen-3-ol inside AgOBP<sub>1</sub>.



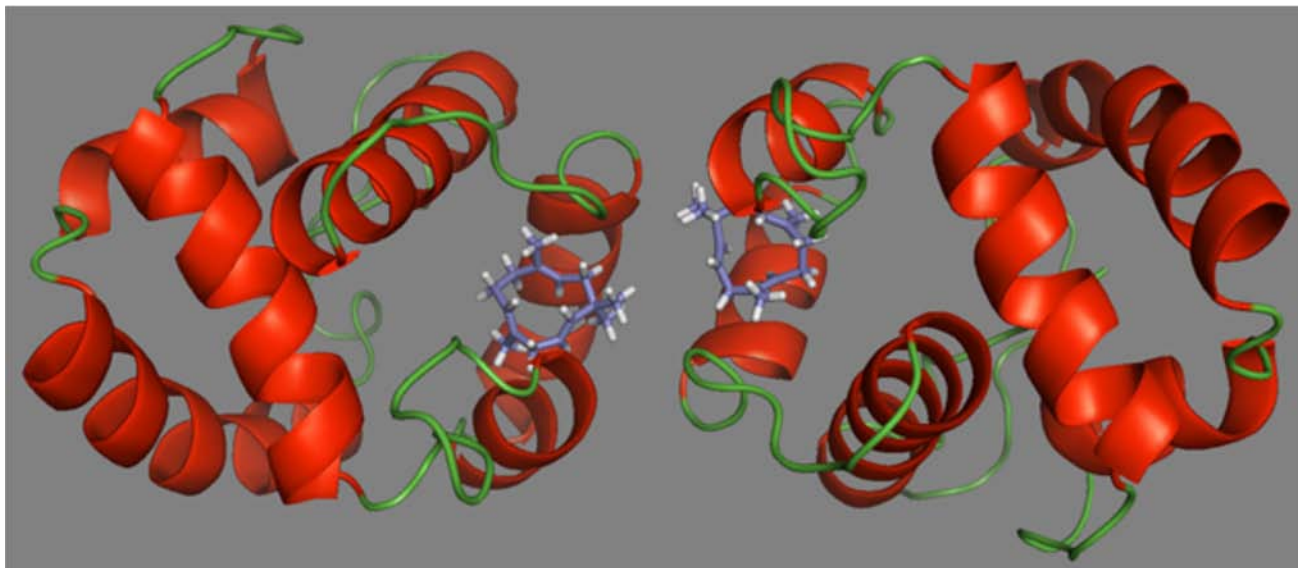
**Figure S4.** Best poses of indole inside AgOBP<sub>1</sub>.



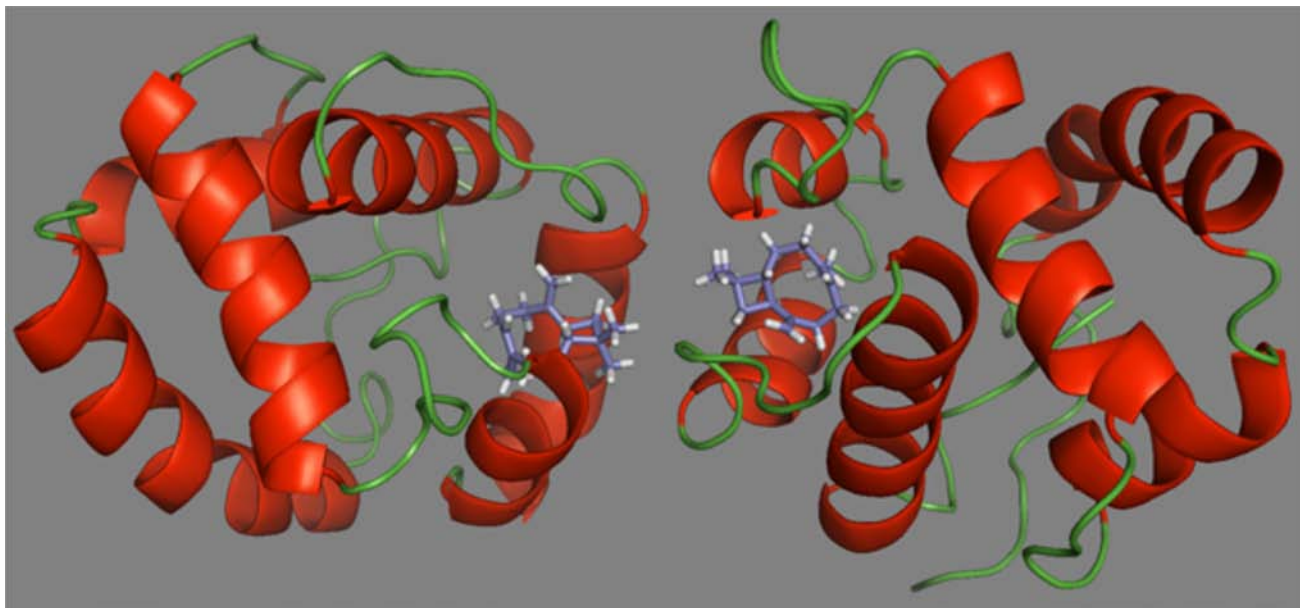
**Figure S5.** Best poses of eugenol inside AgOBP<sub>1</sub>.



**Figure S6.** Best poses of eugenyl acetate inside AgOBP<sub>1</sub>.



**Figure S7.** Best poses of  $\alpha$ -humulene inside AgOBP<sub>1</sub>.



**Figure S8.** Best poses of  $\beta$ -caryophyllene inside AgOBP.