

Molecular Dynamics of the Interaction of Pralidoxime and Deazapralidoxime with Acetylcholinesterase Inhibited by the Neurotoxic Agent Tabun

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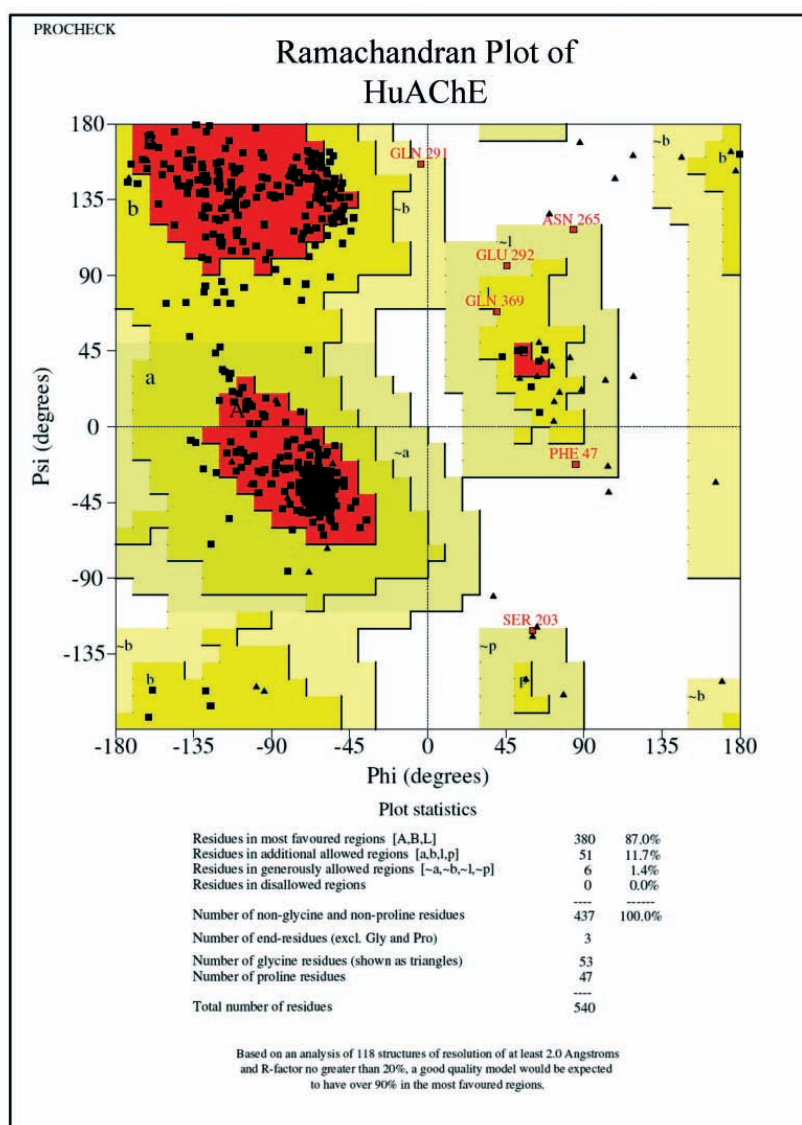


Figure S1. Ramachandran plot of HuAChE showing more than 98.00 % of the residues in the most favoured and additional allowed regions.

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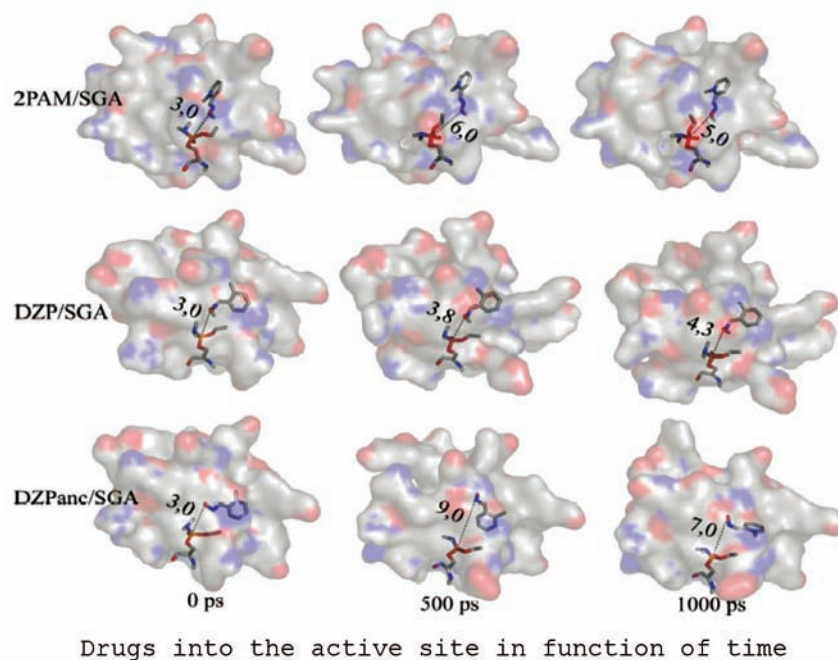


Figure S2. Distance variations between the phosphorous atom of GA and the oxygen of 2-PAM, DZP and DZPanion, along the MD simulations, when docked inside the HuAChE active site; Figures prepared with the software PyMOL.

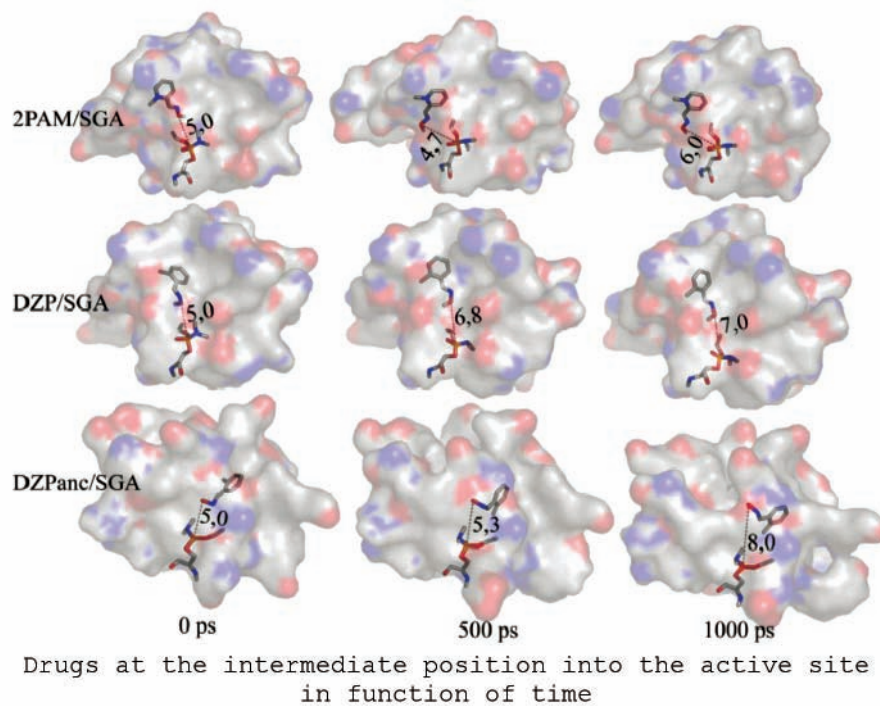


Figure S3. Distance variations between the phosphorous atom of GA and the oxygen of 2-PAM, DZP and DZPanion, along the MD simulations, when docked halfway inside the well that conducts to the active site of HuAChE; Figure prepared with the software PyMOL.

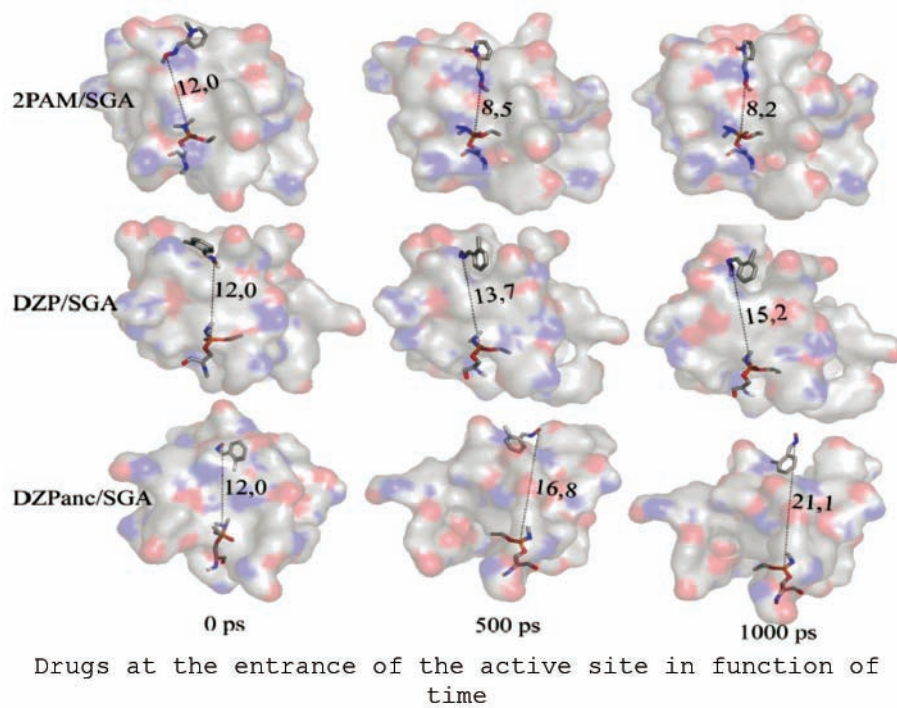


Figure S4. Distance variations between the phosphorous atom of GA and the oxygen of 2-PAM, DZP and DZPanion, along the MD simulations, when docked at the entrance of the well that conducts to the active site of HuAChE; Figure prepared with software PyMOL.