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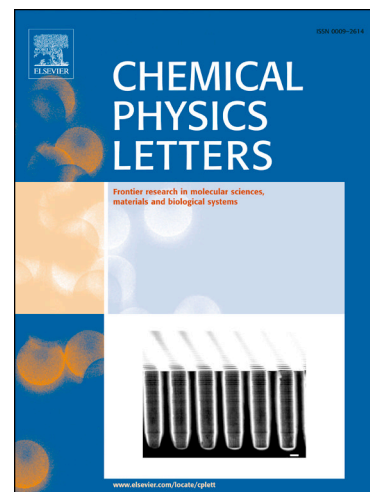
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Theoretical investigations of Human Acetylcholinesterase inhibition efficiency by neurotoxic organophosphorus compounds

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Abstract

Quantum chemistry calculations were done for four nerve agents (NAs): VX, tabun, sarin and soman to correlate their physicochemical and electronic properties with intention to clarify the reason of their high lethality. For isolated NAs, it was observed an excellent correlation between the energy gap values with their lethality and volatility. The water-octanol transference enthalpy is unfavorable for NAs indicating that human body absorption, which it was supported by the TPSA calculated here, is driven by entropic effects. The electronic results for NAs-serine adduct are similar implying that the reactivation mechanism of the acetylcholinesterase can be the same.

Keywords: Acetylcholinesterase, neurotoxic organophosphorus, lethality, theoretical studies

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