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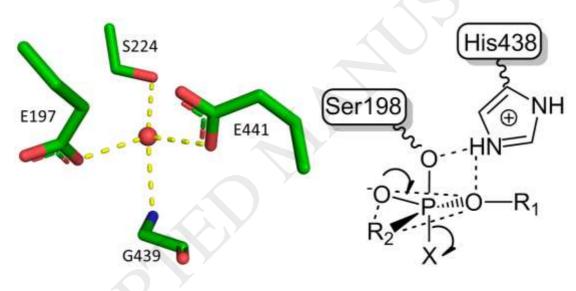
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Catalytic bioscavengers against organophosphorus agents: mechanistic issues of self-reactivating cholinesterases

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Graphical abstract



Highlights

- Rational design of novel ChE-based catalytic bioscavengers requires understanding of mechanisms
- However, there are discrepancies about mechanisms of inhibition, aging and reactivation of ChEs
- Knowledge of proton transfer pathways within active site are important for stability and reactivity
- Interplay between X-ray structure, molecular modeling and self-reactivation kinetics

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