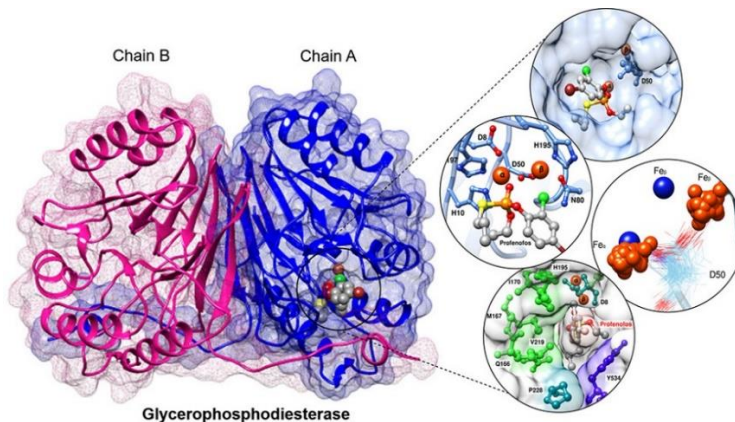




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### Computational study of the binding mechanism of organophosphate pesticides with glycerophosphodiesterase

Organophosphate (OP) pesticides are toxic substance as they irreversibly inhibit the acetylcholinesterase enzyme involved in neurotransmission and thereby leading to poisoning. In addition, the OP pesticides commonly contaminate water and soil. Occupational exposure and environmental contamination of OP pesticides affect both human health and environments. To solve such issues, a “green and clean” approach is introduced to break down these harmful agents. One of the most attractive strategies is the use of the OP-degrading enzymes. Specifically, glycerophosphodiesterase (GpdQ) has attracted recent attention as a promising enzyme for bioremediation since it can hydrolyze some OP pesticides. This work explored the binding interactions of three OP pesticides (*i.e.*, profenofos, diazinon and chlorpyrifos) to the GpdQ using computational techniques. The results showed that the binding of the pesticides could stabilize the enzyme structure in the active conformation, allowing the substrate to be catalyzed into less harmful products. The ability of *in silico* analysis presented here can be used as guidance for improving enzyme stability and activity toward OP pesticides in the future.



#### Reference:

Bhat N, Nutho B, Vangnai A, Takahashi K, Rungrotmongkol T. Substrate binding mechanism of glycerophosphodiesterase towards organophosphate pesticides. Journal of Molecular Liquids, 2021;329:115526. <https://doi.org/10.1016/j.molliq.2021.115526>



ความเชื่อมโยงกับเป้าหมาย SDGs:

เป้าหมายที่ 3: การมีสุขภาพและความเป็นอยู่ที่ดี

เป้าหมายที่ 9: อุตสาหกรรม นวัตกรรม โครงสร้างพื้นฐาน