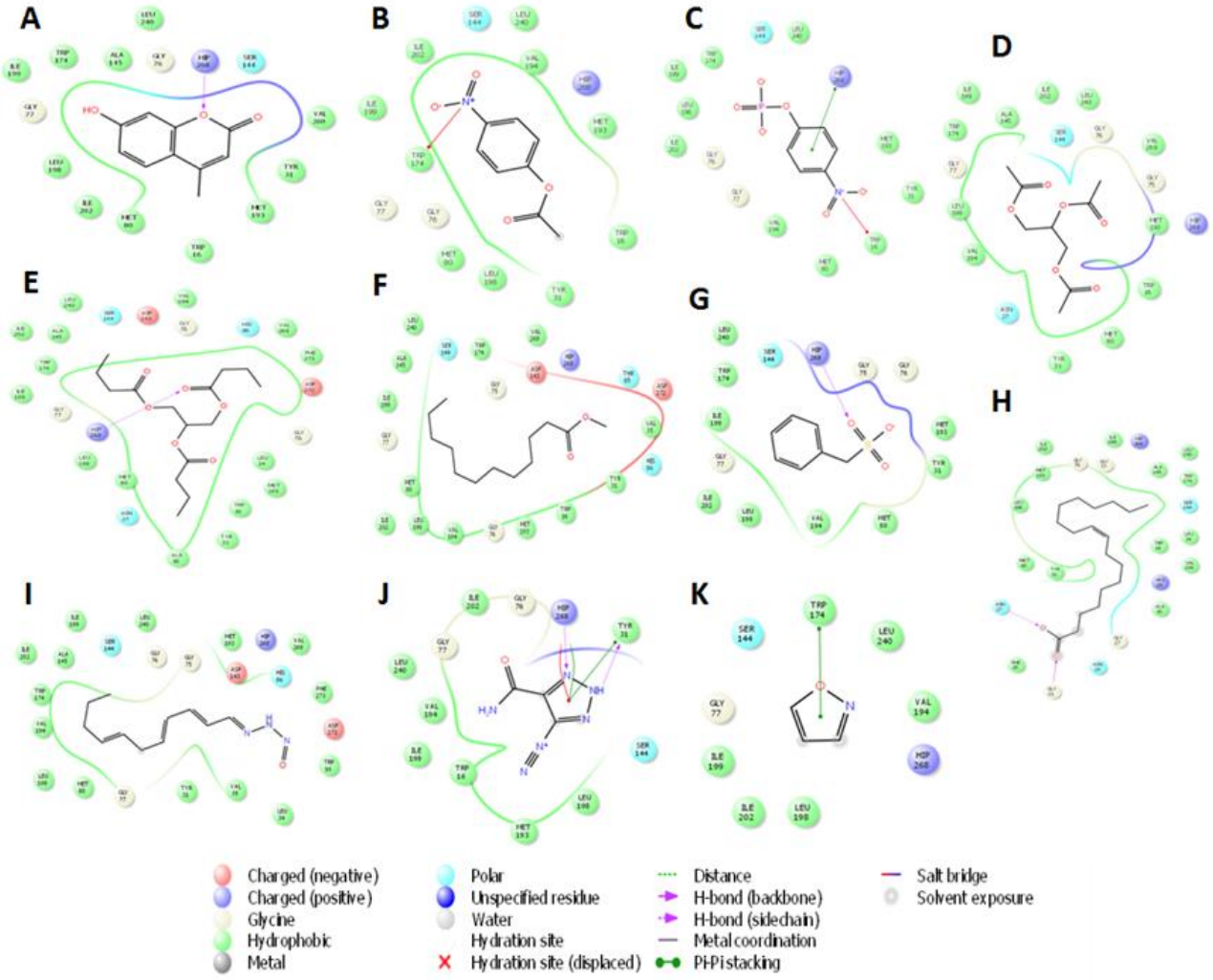
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Cartlann Taighde Oscailte Chorcaí

Title	A novel cold active esterase from a deep sea sponge Stelletta normani metagenomic library
Authors	Borchert, Erik;Selvin, Joseph;Kiran, Seghal G.;Jackson, Stephen A.;O'Gara, Fergal;Dobson, Alan D. W.
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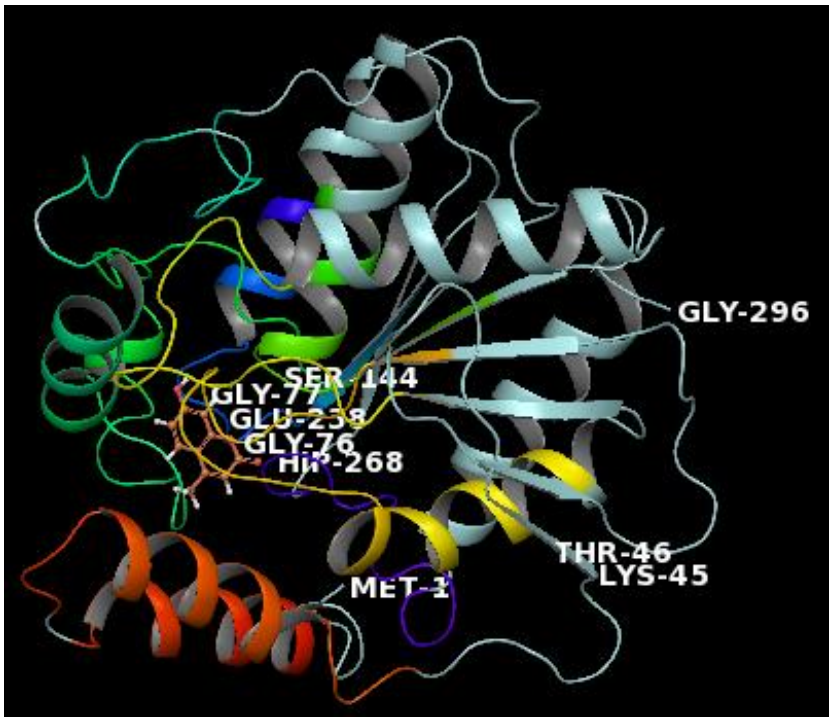
Supplementary file 1

1.1 Docking of different substrates and inhibitors to the active site of the esterase

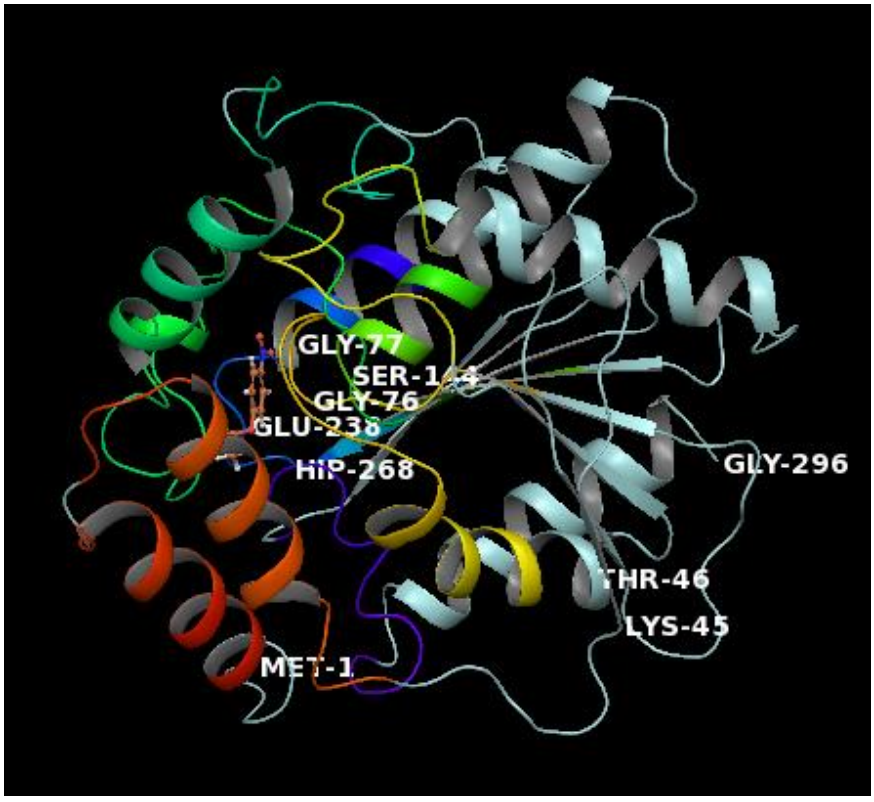


Docking of different substrates and inhibitors to the active site of the esterase. A) 4-methylumbelliferone B) 4-Nitrophenylacetate C) 4-Nitrophenylphosphate D) Triacetin E) Tributyrin F) Methylaurate G) Phenylmethansulfonic acid H) Oleic acid I) Triacsin C J) 5-Carbamoyl-2H-1,2,3-triazole-4-diazonium K) Isoxazole

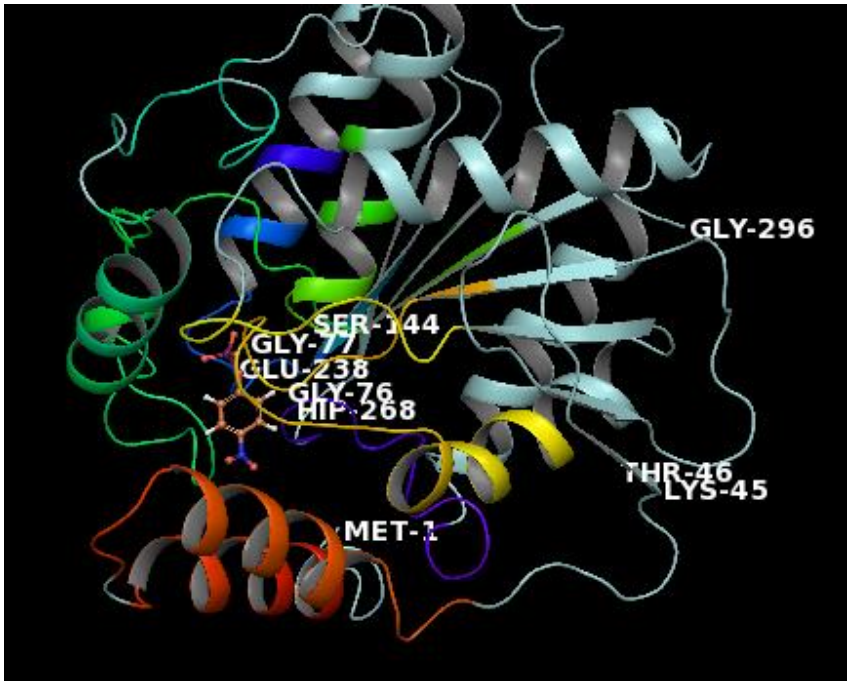
1.2 3D binding models: Substrates



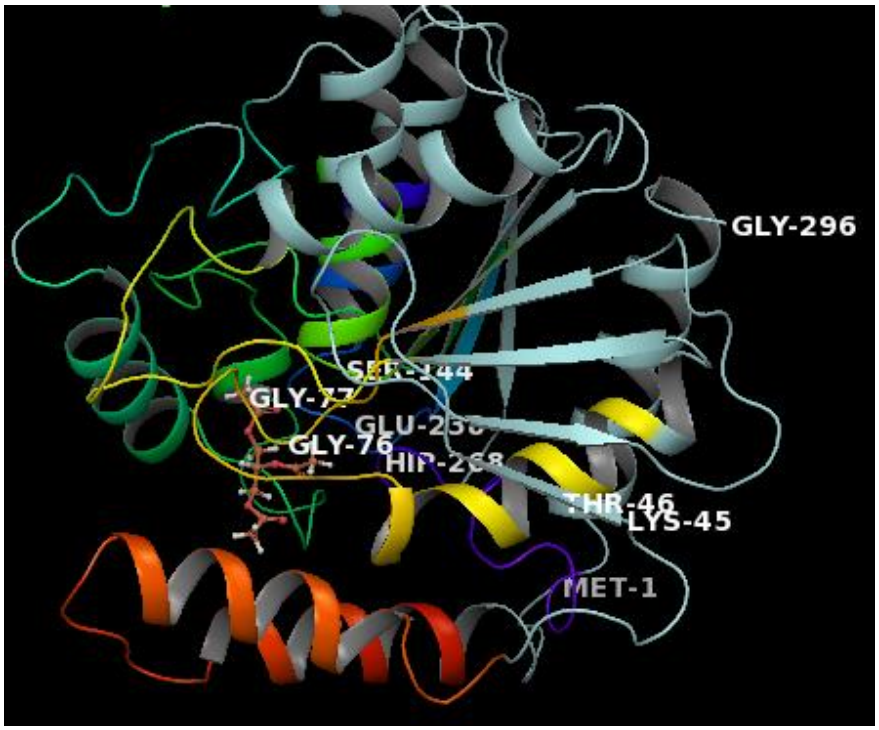
4-Methylumbelliferone



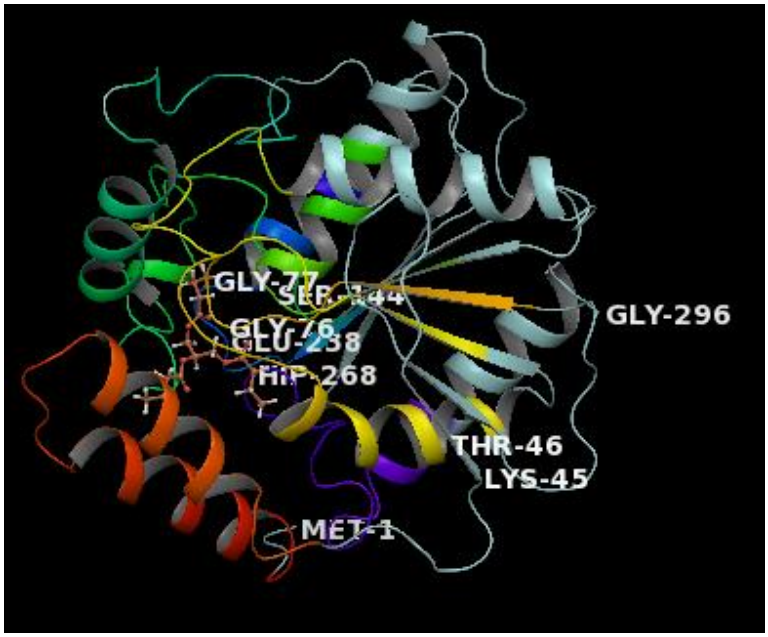
4-Nitrophenyl acetate



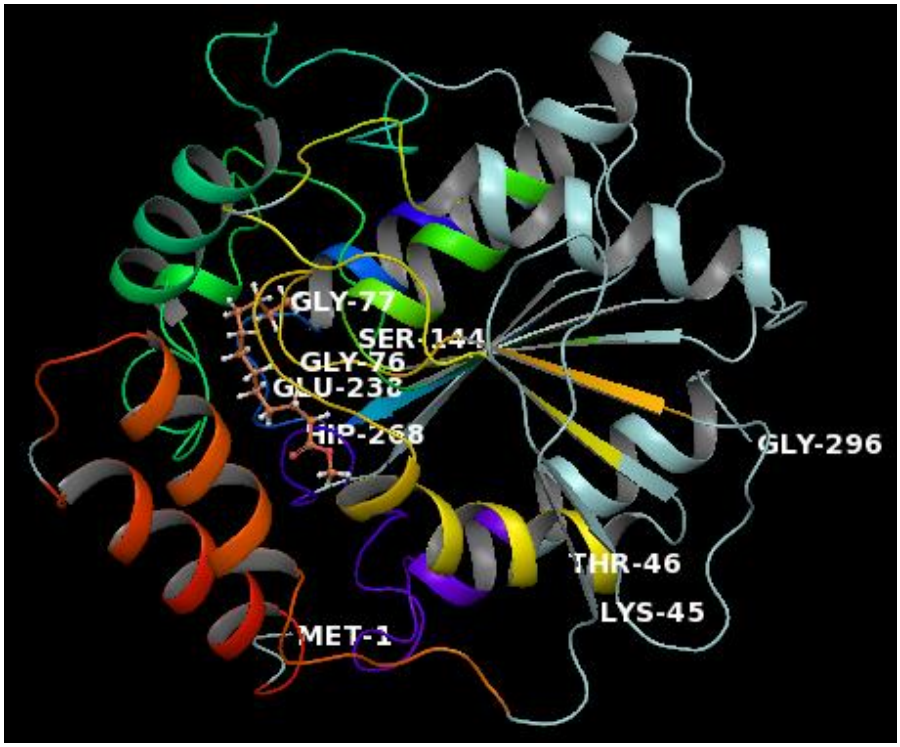
4-Nitrophenyl phosphate



Triacetin

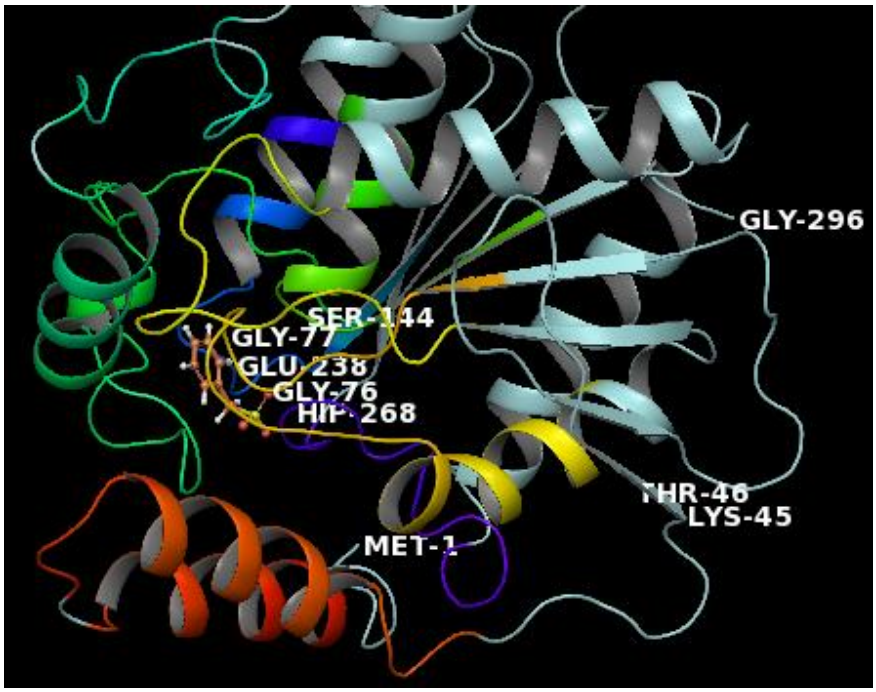


Tributyrin

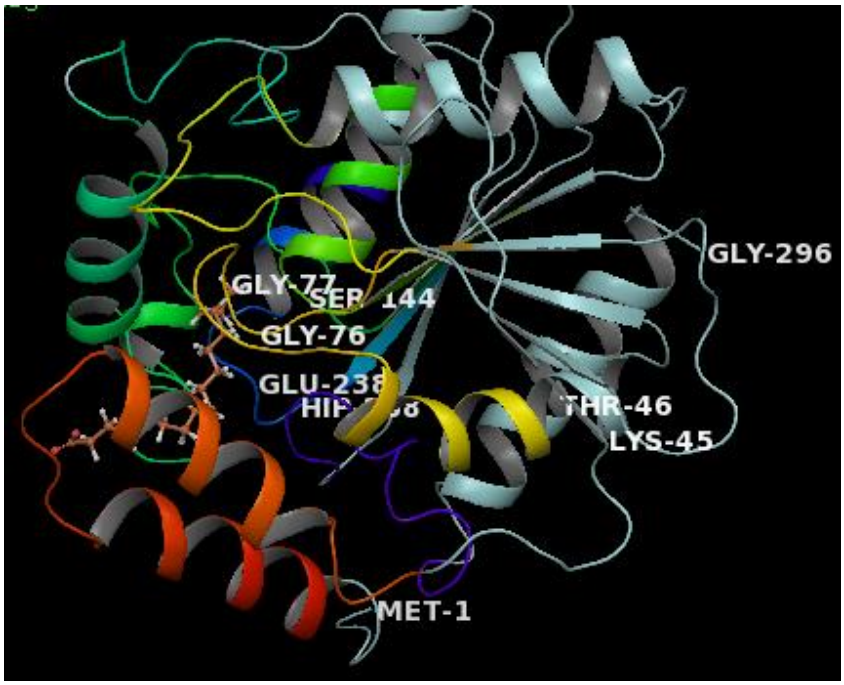


Methyl laurate

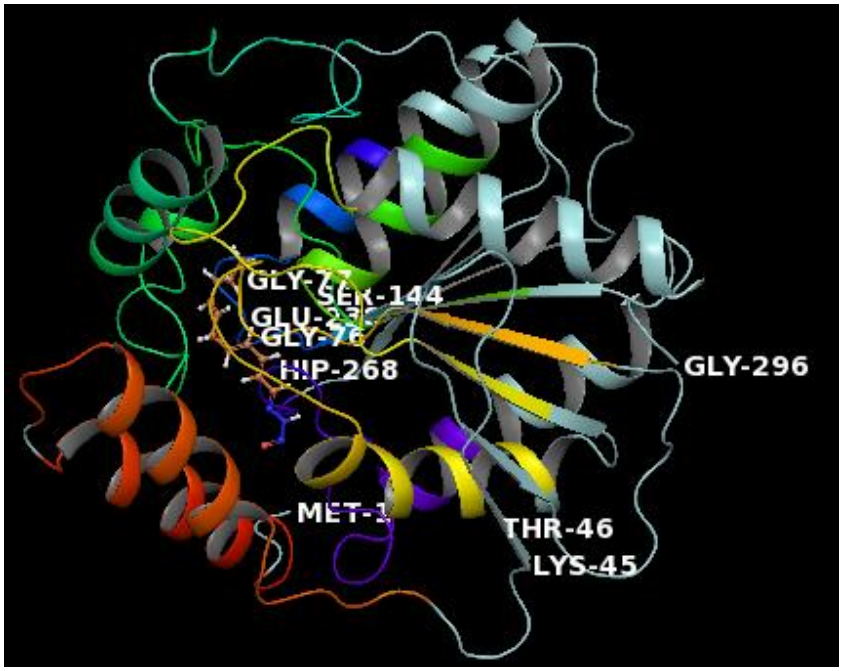
1.3 3D binding models: Inhibitors



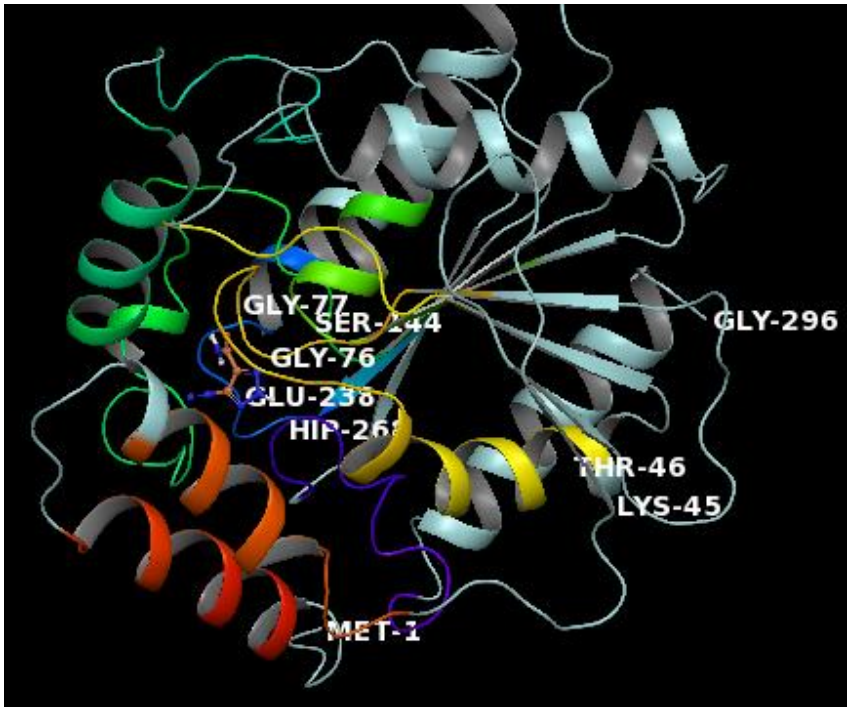
Phenylmethansulfonic acid



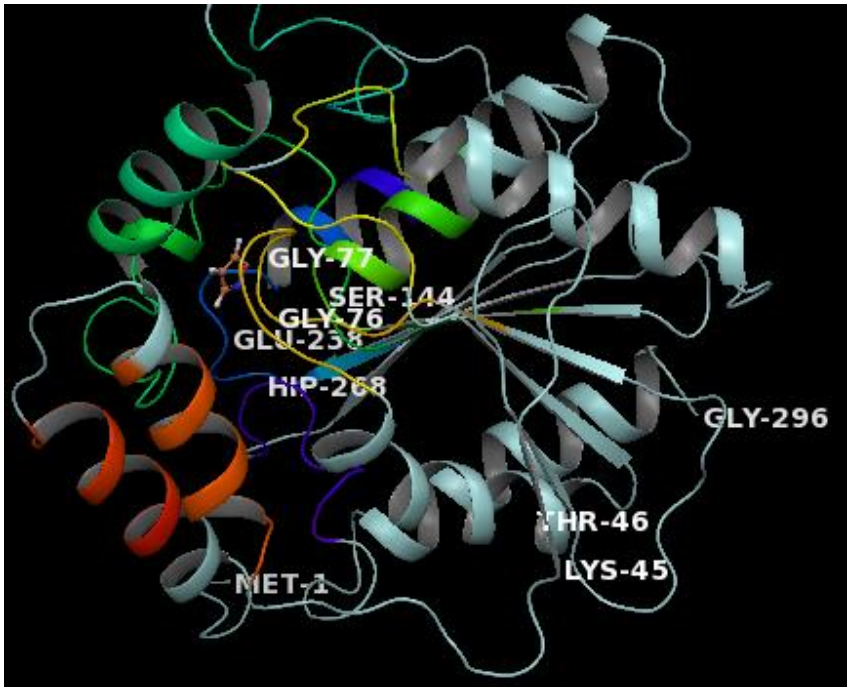
Oleic acid



Triacsin C



5-Carbamoyl-2H-1,2,3-triazole-4-diazonium



Isoxazole