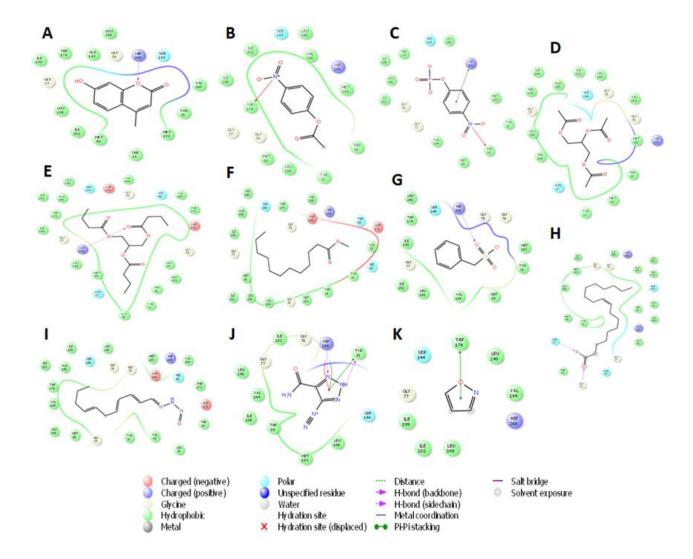


Title	A novel cold active esterase from a deep sea sponge Stelletta normani metagenomic library
Authors	Borchert, Erik;Selvin, Joseph;Kiran, Seghal G.;Jackson, Stephen A.;O'Gara, Fergal;Dobson, Alan D. W.
Publication date	2017
Original Citation	Borchert, E., Selvin, J., Kiran, S. G., Jackson, S. A., O'Gara, F. and Dobson, A. D. W. (2017) 'A novel cold active esterase from a deep sea sponge Stelletta normani metagenomic library', Frontiers in Marine Science, 4, 287 (13pp). doi: 10.3389/fmars.2017.00287
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://www.frontiersin.org/articles/10.3389/fmars.2017.00287/ full - 10.3389/fmars.2017.00287
Rights	© 2017, Borchert, Selvin, Kiran, Jackson, O'Gara and Dobson. This is an open-access article distributed under the terms of the Creative Commons Attribution License (CC BY). The use, distribution or reproduction in other forums is permitted, provided the original author(s) or licensor are credited and that the original publication in this journal is cited, in accordance with accepted academic practice. No use, distribution or reproduction is permitted which does not comply with these terms - https:// creativecommons.org/licenses/by/4.0/
Download date	2024-12-27 00:23:45
Item downloaded from	https://hdl.handle.net/10468/4898



University College Cork, Ireland Coláiste na hOllscoile Corcaigh

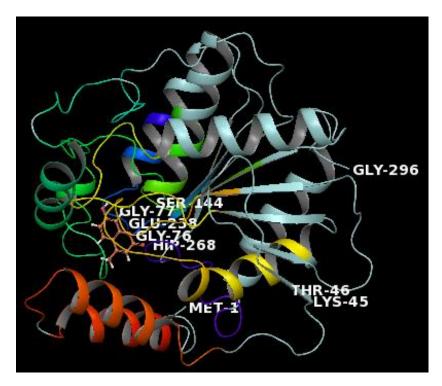
### Supplementary file 1



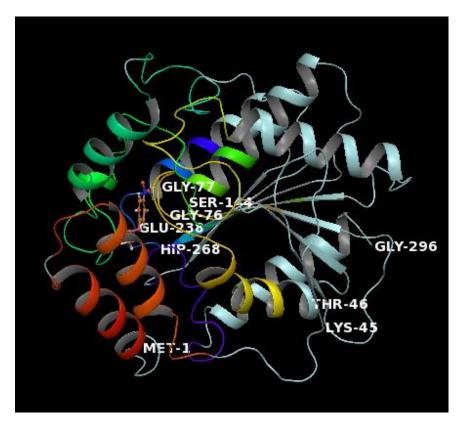
#### 1.1 Docking of different substrates and inhibitors to the active site of the esterase

**Docking of different substrates and inhibitors to the active site of the esterase.** A) 4methylumbelliferone 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-1,2,3triazole-4-diazonium K) Isoxazole

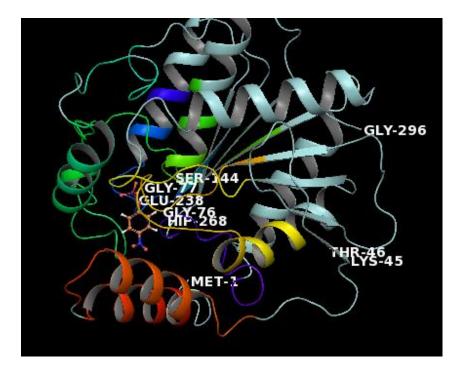
# 1.2 3D binding models: Substrates



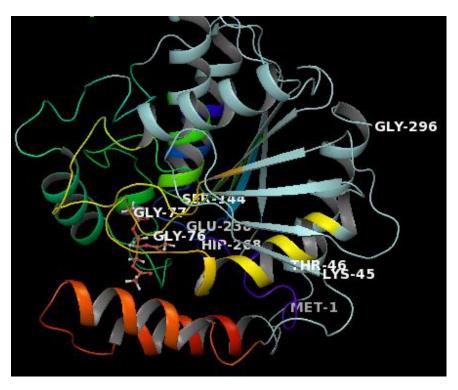
#### 4-Methylumbelliferone



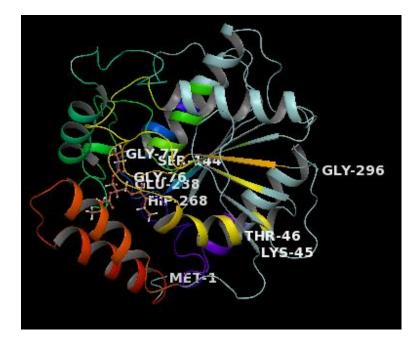
4-Nitrophenyl acetate



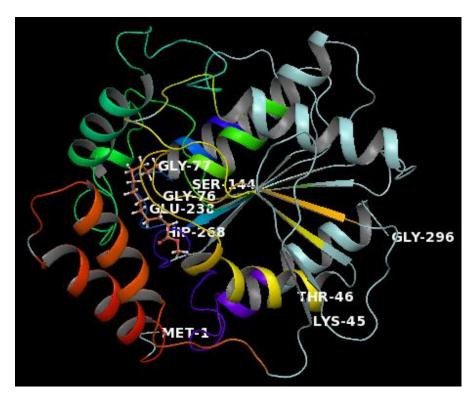
### 4-Nitrophenyl phosphate



Triacetin

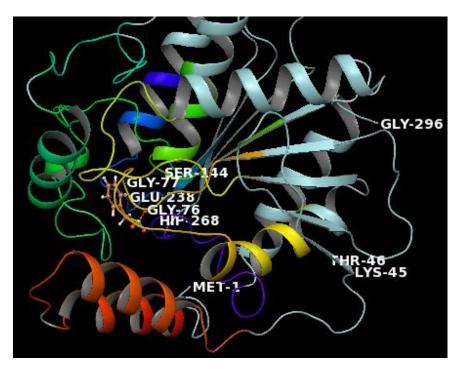


Tributyrin

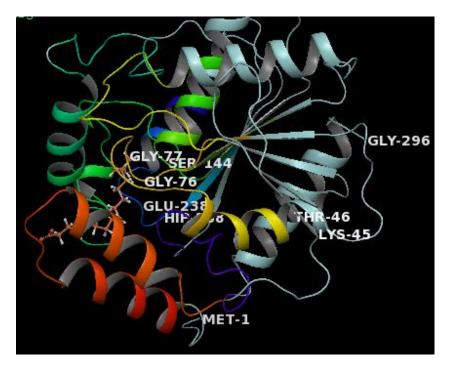


Methyl laurate

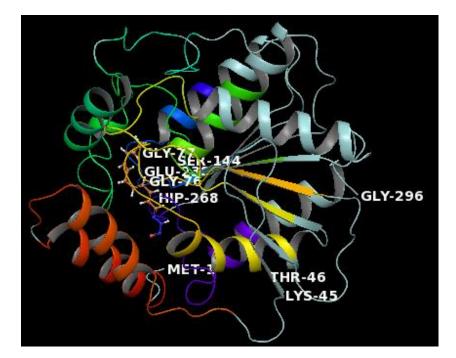
# 1.3 3D binding models: Inhibitors



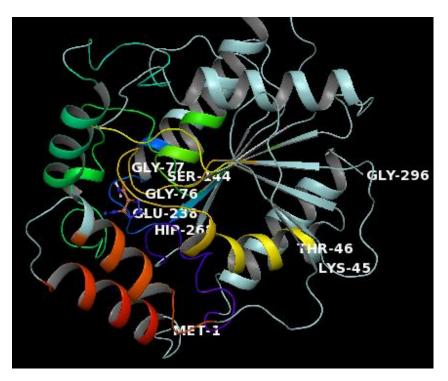
#### Phenylmethansulfonic acid



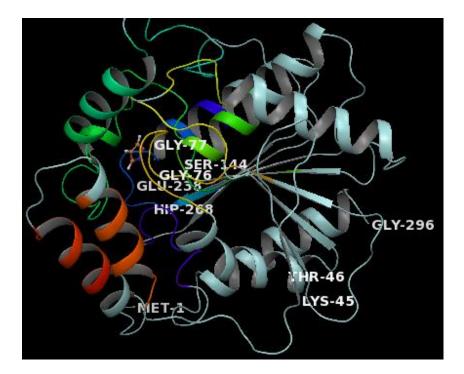
Oleic acid



Triacsin C



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



Isoxazole