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Structural bioinformatics in the study of cold-active enzymes from marine organisms

Cold-active marine enzymes constitute an attractive resource for biotechnological applications. Some marine enzymes are important analytical tools. Enzymes from marine organisms with unique properties have been studied at the Pacific Institute of Bioorganic Chemistry: DNase from hepatopancreas of Kamchatka crab, specific for double-stranded DNA, alkaline phosphatase from marine bacteria, with the highest specific activity among known phosphatases, endo-glucanases of marine mollusks, showing transglycosylation activity and capable of synthesizing biologically active oligosaccharides, O-glycoside hydrolases from marine bacteria, modifying antigens of the blood group A and B. The spatial crystal structure of these enzymes is not currently established. Methods of structural bioinformatics were used for predicting three-dimensional (3D-) structure models of protein molecules from amino acid sequences. Fold recognitions of marine enzymes were carried out using 3D-PSSM, FUGUE and PHYRE servers. It was found that marine enzymes have folds with 100% confidence to enzymes having known crystal structures. Homology models of enzymes were generated by SWISS-MODEL, ModBase, I-TASSER servers and homology model module of program MOE™. The full-length structure models were constructed for nucleases duplex-specific nuclease (EC 3.1.30.2) from *Paralithodes camtschaticus* (Q8I9M9), S1/P1-type nuclease (EC 3.1.30.1) of marine fungus *Penicillium melinii* (D3JY17), endo-1,3-beta-D-glucanases (EC 3.2.1.39) of marine bacteria *Formosa algae* (A0A0B5GQL6) and from marine mollusks *Littorina sitkana* (C0KUK2), *Perna viridis* (B9W0H7), *Pseudocardium sachalinensis* (Q7Z0T2), *Chlamys albidus* (Q4FCS2), *Chlamys rosea* (Q4FCS1), *Mizuhopecten yessoensis* (Q5I6N3), alkaline phosphatase (EC 3.1.3.1) from marine bacterium *Cobetia marina* strain KMM 296 (Q1W622), alpha-galactosidase (EC 3.2.1.22) of the marine bacterium *Pseudoalteromonas* sp. KMM701

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(Q19AX0), alpha-N-acetylgalactosaminidase (EC 3.2.1.49) of the marine bacterium *Arenibacter latericius* KMM 426T (E1AXI3) and alginate lyases (EC 4.2.2.-) family PL7 of the marine bacterium *Zobellia* sp.

Marine enzyme models were used for active sites analysis, *in silico* mutagenes and for prediction of the enzyme-substrate and enzyme-inhibitor complexes structures by molecular docking approach. Models of complexes were building with programs GRAMM1.03, Docking module of MOE and Autodock4. Atomistic details of marine enzymes active sites, substrate binding subsites, inhibitors and metal binding sites were obtained. A comparison of the structure of psychrophilic marine enzymes and thermophilic enzymes was carried out by simulation molecular dynamics at various temperatures using the equipment of Shared Resource Center "Far Eastern Computing Resource" IACP FEB RAS (https://cc.dvo.ru). Marine enzymes 3D-structural data will allow an understanding better of the structure–function relationships and regulation activities of the marine cold-active enzymes.