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Type	Oral communication
Session	Structural Bioinformatics
Title	Bioinformatics study for the structural and functional characterization of lipoxygenases from diatoms
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Motivation

Diatoms are organisms at the base of trophic chain, which live in any aquatic ecosystem and play a very important ecological role. Diatoms, as many plants, animals, cyanobacteria, and some fungi, as consequence of abiotic or biotic stress, produce a wide variety of secondary metabolites, including oxylipins. These molecules, derived from the oxidation of poly-unsaturated fatty acids (PUFA) by lipoxygenase enzymes (LOX), influence not only the growth of phytoplankton, as the same diatoms, but also the growth of numerous organisms that make up zooplankton. Therefore, the study of the enzymes of the oxylipins pathway is a key point for a better knowledge of the mechanisms that regulate/dysregulate ecological and physiological process in marine ecosystem.
The purpose of this work is to explore the possible existence of different LOX in diatoms, classify and analyze them from the primary and 3D-structure's point of view.

Methods

Starting from sequence annotated as LOX in diatoms, a large-scale analysis of all diatoms' transcriptome and proteome have been performed by BLAST tool and database analysis. The cofactor coordination site typical of LOX (three His, one Asn and one Ile, coordination residues of Fe^{2+}) of all the protein sequences has been analyzed by a complex procedure including multiple sequence alignments, pairwise comparisons, database searches, pattern and domain searches, by BLAST, T-COFFEE, PROSITE, InterPro, and Clustal Omega tools and by visual inspection. The subgroup classification of LOX has been performed exploiting the construction of phylogenetic trees by MEGA 6.06 tool; while the analyses of the different patterns typical of each group have been executed by MEME tool. Moreover, 3D structural models have been created by ColabFold and Modeller10.2.

Results

Firstly, we detect the presence of hypothetic LOX domain in uncharacterized diatoms' sequences, predicted from transcriptomic experiments, and we collect the widest number of hypothetical LOX belonging to this species. After this screening, we find different features in terms of presence of domains, specific motifs, and position of amino acids with expectable functional roles. Therefore, based on these data, it was possible to make a preliminary classification that brings to the identification of at list six different groups, principally divisible in a few main classes.
The latters are splitted according to the presence or absence of a probable insertion or deletion between two different couples of coordination residues of the LOX cofactor.
In principle, our classification underline as there is a variability in the composition of the cofactor coordination site in some LOX groups: i.e. the substitution of the catalytic Asn in Ala, Ser, His and Gln, and a variability of the distance among these residues throw the sequence. These features seem to affect in different way the cofactor coordination, preserving or modifying it.
Finally, the 3D structure of LOX enzymes representative of each group were modelled, evaluated, and compared, revealing possible functional differences related to a different composition of the substrate-binding site.

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