of the oligonucleotide in the presence of a variety of metal ions [2] (Mg^{2+}, Mn^{2+}, Ca^{2+}, Ni^{2+}, Sr^{2+}, Ba^{2+}, Cd^{2+}, Cu^{2+}, $Co(NH_3)_6^{3+}$, Zn^{2+} y Li^{+}) to stabilize the structure of the crystal. By X-ray diffraction we obtained patterns with low resolution from which in a first stage, it was only possible to determine the cell parameters and space group. The best crystals were obtained in presence of cadmium which has a high affinity for adenine bases. Contrary to common behavior of A-T rich oligonucleotides, when hairpin has been stabilized with cadmium the best crystals are obtained at 21°C, while using the other metal ions low temperatures is needed to obtain crystals; usually between 4 and 11°C. On the other hand, by performing DLS analysis was detected the influence of cadmium in the structure stabilization and in the intermolecular contacts stabilization, which compared to the magnesium interaction and the reference without metal ion is higher. Also by DLS analysis we confirmed the formation of the DNA hairpin by monitoring the diffusion coefficient and size of monomeric species. We constructed hairpin and duplex DNA theoretical structures and performed a simulation of the diffraction obtaining a model of molecular packing. We may assume the formation of a DNA hairpin from 100% A-T oligonucleotides and highlight the role of metal ions on the hairpin stabilization.

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Keywords: hairpin, oligonucleotide, crystallization

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Crystal structures of two CBSX proteins from *Arabidopsis thaliana*

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CBS (cystathionine-β-synthase) domain is a small intracellular module, mostly found in two or four copies within a protein, which has been identified in many proteins in all kingdoms of life. Tandem pairs of CBS domains can act as binding domains for adenosine derivatives and may regulate the activity of attached enzymes or other domains. Many proteins containing CBS domain are easily identified in plant genome. However, their exact physiological functions remain elusive. Two of them, AtCBSX1 and AtCBSX2 (CBS pair protein) from Arabidopsis thaliana have been cloned and analyzed. These encode 236 and 238 amino acid residues which contain two tandem CBS domains, respectively. Both proteins were over-expressed heterologously in E. coli and purified them as homogeneity. The structure of AtCBSX1 and AtCBSX2 determined at 2.2 and 1.9 Å resolution, respectively, reveals an unique architecture and a positively-charged pocket for AMP. The structure of AtCBSXs show that it is an anti-parallel dimer on its central two-fold axis and show a uniquely ~120º bent at the side whereas all the other parallel CBS domain proteins are approximately flat ~180º. However, the structure of dimeric AtCBSX2 with bound AMP is show approximately flat, which is significantly different from the apo form of that. This orientation, shape, molecular symmetry of AtCBSX protein and more importantly conformational change induced by ligand-binding might determine the interacting surface for binding molecules, which is related to its function.

Keywords: X-ray, structure, conformational change

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Structural and functional studies of the active-sites in four glycoside hydrolase β-jellyroll families

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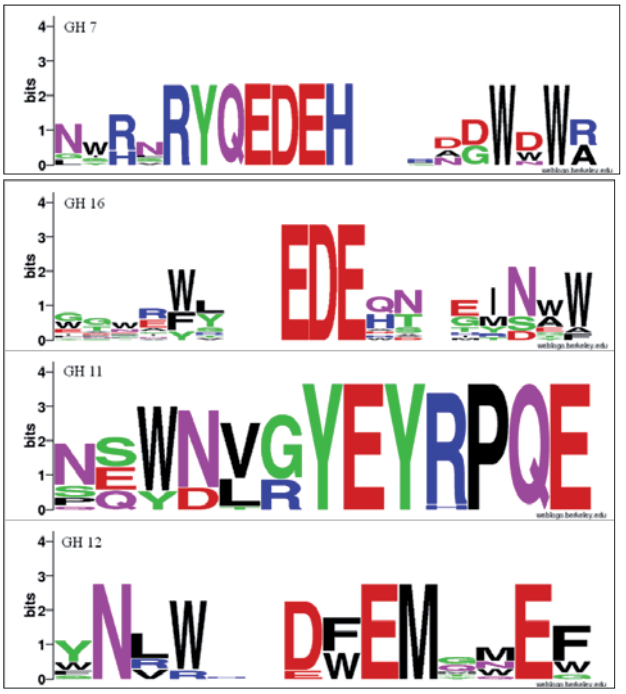
The three-dimensional (3D) structure of glycoside hydrolase family (GHF) 7, 11, 12 and 16 are collectively referred to as a jellyroll β-sandwich fold with a similar cleft catalytic active site, although the amino acid sequences of these four families are diverse. Based on the results of primary sequence alignment and 3D structural comparison, GHF 7 and 16 possess a conserved catalytic motif of RYQExDxEHWW and ExDxE/ExDxxE, whereas GHF11 and 12 share a general active site motif of $YE_nYPQE_{n+(88\sim94)}$ and $NE_nME_{n+(83\sim97)}$, respectively. The first and last glutamyl residues found in the catalytic motifs have been clearly identified as catalytic nucleophile and general acid/base for retention hydrolytic mechanism, respectively. A detailed structural comparison among the known structures reveals that they share a low level of amino acid sequence identity 5~20%, but the enzymes have a high degree of structural conservation at the active sites.



Keywords: glycoside hydrolase β-jellyroll family, conserved amino acid, structural and primary sequence comparison

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Crystal structures of symbiosis related lectin and its saccharide bound form

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