CHOLESTEROL ESTERASE-DETERGENT COMPLEX AT 1.4 Å RESOLUTION.

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The three dimensional structure of *Candida cylindracea* Cholesterol Esterase (ChE) in complex with the polymeric detergent $C_{12}H_{26}$-(O-CH_2-CH_2)$_n$ has been determined at 1.4 Å resolution in space group *P*1 using low temperature synchrotron data. The structure was refined by CNS and SHELX methods to R=0.14 and Rfree=0.17. The 8074 protein, 112 carbohydrate, 46 detergent, 1078 water nonhydrogen atoms and 8054 hydrogen atoms were localized. The ChE structure is a dimer with four spatially separated interfacial contact areas and four openings to an internal interfacial cavity. Carbohydrates were located in electron density maps on the side chains of Asn314 and Asn351 in both ChE monomers. There were two well defined N-acetyl-glucosoamine moieties at each site. For each monomer a 23 atom detergent fragment was unambiguously fitted to electron density in the elongated hydrophobic gorge of the enzyme acive site. Two alternative side chain conformations were detected for fourteen ChE residues with nearly equivalent occupancy values of 0.5+-0.1.
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Keywords: CHOLESTEROL ESTERASE CRYSTAL STRUCTURE HIGH RESOLUTION

HIGH RESOLUTION (1.45 Å) STRUCTURE OF THE COMPLEX BETWEEN CRYPTOGEIN AND CHOLESTEROL

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Cryptogein, a small 10kD elicitor produced by the parasitic oomycete *Phytophthora cryptogea* presents a strong sterol-carrier activity. Native protein crystallizes in the $P4_122$ with a diffraction limited to 2.1 Å. Its complex with cholesterol crystallizes in the *C*222 space group with an increased resolution to 1.4-1.5 Å. The large non-specific central cavity shows a strong hydrophobic character and is able to accommodate a large variety of 3β-hydroxyl sterols. As such, cryptogein acts as sterol shuttle for the parasitic oomycete to grow and complete its life cycle.

Figure: the electron density of the cholesterol molecule in the active site of cryptogein:

Keywords: CRYPTOGEIN CHOLESTEROL COMPLEX STEROL CARRIER PROTEIN

STRUCTURE OF C-PHYCOCYANIN FROM SPIRULINA PLATENSIS AT 2.2 Å RESOLUTION

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Phycobilisomes are light-harvesting complexes that associate with PSII in cyanobacteria and red algae. Phycobiliproteins in phycobilisomes can be divided into three groups: Phycoerythrin (PE), phycocyanin (PC) and allophycocyanin (APC). The crystal structure of C-phycocyanin (C-PC) from Spirulina platensis has been determined at 2.2 Å resolution. The crystals belong to monoclinic system, which has not been previously reported for phycobiliproteins in phycobilisomes. There are four C-phycocyanin trimers (ab)3 in the asymmetric unit, which associate face-by-face to form two hexamers (ab)6. The hexamers in the monoclinic crystals are arranged in layers rather than in columns that is often observed for phycobiliproteins. There are three different side-by-side packings of adjacent hexamers. The unique packing of the two hexamers in the asymmetric unit brings the chromophores b155 phycocyanobilin (PCB) very close together, and the possible lateral energy transfer is through b155-b155 route.

Keywords: STRUCTURE PHYCOBILIPROTEINS LIGHT-HARVESTING

NEUTRON CRYSTALLOGRAPHIC STUDY OF HUMAN LYSOZYNE

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The most important information from neutron crystallography is that from hydrogen atoms at physiological temperatures. Wild-type human lysozyme was chosen for our neutron structure determination because it has been studied by many other biophysical methods to reveal its nature as one of the most typical examples of stable globular proteins. Crystals were grown in D2O-based buffer solution. The size of the crystal used for the neutron structure determination was 3.0 mm x 1.0 mm x 0.7 mm. Diffraction data were collected with a monochromatic neutron diffractometer BIX-3 equipped with a neutron imaging plate. The total measuring time was 55 days. The neutron diffraction data have been analyzed up to 1.8 Å resolution. From the neutron structure analysis we obtained occupancies for hydrogen and deuterium atoms at each main chain amide position. These occupancies show a strong correlation with the averaged B-values of the main chain atoms. The results of the occupancy refinement were compared with those of hydrogen-deuterium (H-D) exchange experiment by nuclear magnetic resonance (NMR) spectroscopy which is another method utilizing the information from protons. In NMR spectroscopy, the H-D exchange experiment is popular to show the local flexibility of a protein molecule in solution.

Although both methods are known to have enough reliability to identify hydrogen atoms, some protons were observed to be protected against the H-D exchange by solution NMR where the neutron structure analysis reveals a high degree of exchange.

Keywords: NEUTORN NMR LYSOZYME