Poster Sessions


Keywords: human aldose reductase, protein-ligand complex, interaction energies

P08.08.68


X-ray visualization of protein biotinylation

Bagautdin Bagautdinov, Naoki Kunishima
RIKEN SPring-8 Center, Advanced Protein Crystallography Research Group, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, E-mail: bagautdi@spring8.or.jp

Biotin-dependent carboxylases play essential roles in the metabolism of all organisms. Their activation by biotinylation is catalysed by biotin protein ligase (BPL). The crystal structures of the archaeal BPL (PhBPL), the biotinyl domain of archaeal biotin carboxyl carrier protein (PhBCCP) and the PhBPL:PhBCCP complex have been determined by X-ray diffraction. The structural feature of the intermediate (biotinyl-5'-AMP) formation was studied using the PhBPL structures liganded with biotin, ATP and biotinyl-5'-AMP [1]. The BPL:BCCP complex was obtained using two BPL mutants R48A and R48A&K111A [2]. The mutants retain functionality as an enzyme but likely with lower activity, thereby providing the complex crystals. Structural funding of the transient BPL:BCCP complexes at formation (BPL:apo-BCCP) and product (BPL:holo-BCCP) stages allow us to visualize the biotinylation process. The catalytic N- and C-terminal domains of BPL and the biotinyl domain of BCCP act as three rigid-body parts of the complex. The C-terminal domain of BPL shows large conformational motions to accommodate BCCP, suggesting its functional importance. Additionally, the C-domain has a flexible loop that must open every time when BCCP attaches to BPL, and it allows the specific lysine of BCCP to enter the active site of BPL with the intermediate biotinyl-5'-AMP. These structural details are useful to understand the protein biotinylation which is widely used in purification, quantum dots targeting as well as in the design of anti-obesity drugs.


Keywords: biotinylation, protein-protein complex, X-ray diffraction

P08.08.69


Optical and electric properties depending on molecular arrangement of dehydro[12]annulene derivative

Hiroyuki Senga, Yuu Sakamoto, Hajime Shigemitsu, Ichiro Hisaki, Norimitsu Tohnai, Mikihi Miyata
Graduate School of Engineering, Osaka University, Department of Material and Life Science, 2-1 Yamadaoka, Suita, Osaka, 565-0871, Japan, E-mail: senga@molrec.mls.eng.osaka-u.ac.jp

To develop a novel π-conjugated molecule-based supramolecular assembly, we designed and synthesized trisdehydrotribenzo[12]-annulene ([12]DBA) derivative 1 which has three carboxyl groups at the periphery. Recrystallization of 1 from DMSO gave a crystal of the solvate 1/DMSO. Crystallographic analysis revealed that a face-to-face π-stacked one-dimensional (1D) assembly of 1 was achieved and that the DMSO molecule played a significant role as a “structure-dominant element” in the crystal. This is the first example of [12]DBA to stack completely orthogonal to the columnar axis. To reveal its superstructure-dependent optical and electrical properties, 1 and its parent molecule 2, which crystallizes in a herringbone fashion, were subjected to fluorescence spectroscopic analysis and charge-carrier mobility measurements in crystalline states. The 1D stacked structure of 1 provides a red-shifted, structureless, weakened fluorescence profile compared to 2, due to strong interactions between the π-orbitals of the stacked molecules. The charge-carrier mobility of the single crystal of 1/DMSO, as well as 2, was determined by flash photolysis time-resolved microwave conductivity measurements. The single crystal of 1/DMSO revealed significantly-anisotropic charge mobility along the columnar axis. This value is 12 times larger than that along the orthogonal axis.

Keywords: methionine γ-lyase, X-ray structure analyses, gamma-elimination