Structure of Cytokinin-specific Binding Protein in Complex with Plant Hormone

Oliwia Pasternak^a, Grzegorz D. Bujacz^{a,b}, Yasuyuki Fujimoto^c, Yuichi Hashimoto⁴, Michal M. Sikorski^a, Mariusz Jaskolski^{a,e}, ^aInstitute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland. ^bInstitute of Technical Biochemistry, Technical University of Lodz, Poland. ^cFaculty of Pharmaceutical Sciences, Teikyo University, Japan. ^aInstitute of Molecular and Cellular Biosciences, University of Tokyo, Japan. ^eDepartment of Crystallography, A. Mickiewicz University, Poznan, Poland. E-mail: yenefer@rose.man.poznan.pl

The high-resolution (1.2 Å) crystal structure a cytokinin-specific binding protein from mung bean (VrCSBP) complexed with zeatin reveals that the protein, structurally resembles plant pathogenesis related proteins of class 10 (PR-10), despite a low sequence conservation (below 20%). The four VrCSBP molecules present in the asymmetric unit assemble into two dimers. Between the concave face of the molecular β -sheet and the C-terminal helix, a binding pocket is formed where the zeatin molecules are located. Surprisingly, in three (out of the four) binding pockets two zeatin molecules are found, with excellent definition in the electron density maps. In one of the binding sites (observed also in the forth, single-site, VrCSBP molecule), the ligand molecules, located deep in the cavity, have identical conformation and hydrogen-bonding pattern. In the second binding site, at the entrance to the internal cavity, the ligand molecules show variable, but clearly defined, binding modes.

Keywords: protein-ligand complexes, plant hormones, high resolution x-ray structures macromolecules