Structural Basis for the Methylation Mechanism in Methyl-Transferase BchU Involved in Bacteriochlorophyll *c* Biosynthesis

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An S-adenosylmethionine (SAM)-dependent methyltrasferase, BchU, is an enzyme in bacteriochlorophyll *c* (Bchl *c*) biosynthetic pathway, and catalyzes methylation at C-20 position of chlorin moiety. To shed light on the methylation mechanism underlying the Bchl *c* biosynthesis, we have determined the crystal structures of BchU and its complex with SAM.

Recombinant BchU from *Chlorobium tepidum* was overproduced in *E. coli*, purified, and crystallized. We collected diffraction data using synchrotron radiation at SPring-8 and determined the crystal structure at 2.3 Å resolution (R-factor=0.24, R_{free}=0.28). In addition, we also determined the BchU structure in complex with SAM at 2.6 Å resolution (R-factor=0.21, R_{free}=0.26). The structure of BchU consists of two domains; N-terminal domain and C-terminal domain. The N-terminal domain is involved in dimerizaion and the C-terminal domain has a typical Class I motif. The SAM binds to Glu147, Asp175, Asn200, Asp227, Cys242 and Arg243. The location and orientation of the SAM help define the second substrate (a precursor of the Bchl *c*) binding site. These structural features and analysis of putative substrate-binding pocket provide invaluable information for the methylation mechanism of BchU.

Keywords: methylases, enzymatic reaction mechanisms, substrate binding