

Studies on the Energy Transfer Pathways in the Light-Harvesting Complex II and the Key Regulatory Enzymes in *Calvin Cycle* of Cyanobacteria Photosystem

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2014年2月13日(木) 15:00–17:00

創成科学研究棟4階セミナー室C

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In the first part, the energy transfer pathways in trimeric and hexameric aggregation state of cyanobacteria C-phycoyanin (C-PC) were investigated in the framework of Förster model. Only when the protonation of phycocyanobilins and their long- and short-range interactions were properly taken into account, the calculated energy transfer rates were in good agreement with the experimental results of C-PC monomer and trimer. In C-PC hexamer, an additional energy flow was predicted to be from β -155 in top trimer to adjacent β -155 in bottom trimer. Fructose-1,6-/sedoheptulose-1,7-bisphosphatase (C-FBP/SBPase) is a unique enzyme for cyanobacteria with essential roles in *Calvin Cycle*. With a systematically structure-centric approach, in the second part, we identified the first set of novel inhibitors that selectively inhibit the active site of C-FBP/SBPase instead of the AMP allosteric site. The obtained inhibitors show micromolar-range activities *in vitro* and *in vivo*, and may open a promising route towards developing environmentally acceptable chemical control for cyanobacteria blooms treatment.

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Professor Jian Wan received his PhD at Kyoto University, Japan, on studies with the quantum chemistry. After post doctorate studies at York University, Canada, on molecular modeling he returned to China and initiated research academic activity at the CCNU to study the biological physical chemistry, chemical biology, and biochemistry with emphasis on the photosynthesis system. Prof. Jian Wan has more than 40 publications mostly on aspects related to molecular spectroscopic studies of photosynthesis system and molecular bases for various target enzymes and structure-based inhibitor design.