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Editorial

Crystallographic Studies of Enzymes (Volume II)

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Enzymes play a major role in the control of key biological processes by accelerating chemical reactions. It is for this reason that examining their structures and reaction mechanisms is essential for understanding not only the biological processes at a molecule level, but also their application in various fields, such as protein engineering and drug development. After the successful publication of twelve research articles in "Crystallographic Studies of Enzymes", we continue with the series. In the second Special Issue, "Crystallographic Studies of Enzymes (Volume II)", eleven research papers on the structural and functional aspects of enzymes were collected. A brief summary of each article is provided here. While collecting edited articles for this issue, Prof. Doohun Kim, the main editor, passed away. Without his contributions and efforts, it would not have been possible to complete this issue. His passion and insights into the structural and functional studies of enzymes are commemorated in this issue.

Dr. Doohun Kim at Sookmyung Women's University and Drs. Han-Woo Kim, Hackwon Do and Jun Hyuck Lee at the Korea Polar Research Institute published several papers on esterase on a continuum of their previous work [1–3]. They identified new esterases from various microbial sources and characterized their unique enzymatic properties. Furthermore, preliminary crystallographic studies of those esterases were provided [1–3]. In addition, they extended their research scope to the single-stranded DNA that binds protein from the psychrophilic bacterium, *Lacinutrix jangbogonensis*, and this provides an insight into the reaction mechanism of the cold-active enzymes, as well as novel strategies for protein engineering and the application on molecular biological techniques [4].

Drs. Hui-Woong Choe and Young Ju Kim reported the crystallization parameters that affect the space group and diffraction qualities of Ribulose-1,5-Bisphosphate Carboxylase/Oxygenase (RuBisCO) [5]. Based on their observation, a systematic approach required for improving the crystal quality of protein enzymes has been proposed.

Glideosome-associated connector protein (GAC) is a large cytosolic protein (286 kDa) protein that has a role in connecting the parasite F-action with transmembrane adhesin. To provide structural insights on the GAC interaction, Matthews et al. reported the studies on the secondary structure and crystallographic analysis of GAC from *Toxoplasma gondii* [6].

MobB is involved in the biosynthesis of the molybdenum cofactor present in many redox enzymes. Choe et al. proposed that MobB works as an enhancer of MobA activity, based on their structural and biochemical analyses of MobB *Bacillus subtilis* [7].

Schilde et al. reported a systematic analysis of the cross-linked enzyme crystals (CLECs), using halohydrin dehalogenase as an example [8]. They finally concluded that CLECs are suitable for industrial usage since they show good catalytic activities with enhanced mechanical properties.

Nit2, belonging to the nitrilase-like (Nit) branch of the nitrilase superfamily, is known to serve various functions, including as an amidase and a tumor suppressor. In this study, Chang et al. report the crystal structure of Nit2 from *Kluyveromyces lactis* [9]. Based on the structural comparison with other similar structures, they propose a structural relationship among broad spectrum nitrilases.

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Immune-responsive gene 1 (IRG1) is an enzyme that plays a role in producing itaconate, a multifunctional immune-metabolite. Dr. Park solved the high-resolution crystal structure of the active-site mutant IRG1 from *Bacillus subtilis* [10]. Based on a structural comparison with the wild-type protein, the author proposes the working mechanism of IRG1.

Wolny et al. in this study performed pico- and nanoscale molecular dynamic (MD) simulations using the high-resolution structure of Hyp-1, a pathogenesis-related class 10 (PR-10) protein from the medicinal herb *Hypericum perforatum*, and analyzed various structural parameters [11]. Based on the study, the authors concluded that MD methods can be used to verify experimental protein models and explain the structural ambiguities.

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