National Academy of Sciences **2009**, *106*, 8824-8829. [4]Y. Yuan, S. Fuse, B. Ostash, P. Sliz, D. Kahne, S. Walker, *ACS Chem Biol* **2008**, *3*, 429-436. [5]A.L. Lovering, L.H. de Castro, D. Lim, N.C.J. Strynadka, *Science* **2007**, *315*, 1402-1405. [6] H. Heaslet, B. Shaw, A. Mistry, A.A. Miller, in *Journal of Structural Biology*, **2009**, *167*, 129-135.

Keywords: lipid II, moenomycin, transglycosylase

MS36.P09

Acta Cryst. (2011) A67, C473

Structural analysis of Toll-like receptor 2-activating lipoprotein Sangheon Yu,^a Na Yeon Lee,^b Soon-Jung Park,^b Sangkee Rhee,^a ^aDepartment of Agricultural Biotechnology, Seoul National University, Seoul 151-921, (Korea). ^bDepartment of Environmental Medical Biology and Institute of Tropical Medicine, Yonsei University College of Medicine, Seoul 120-752, (Korea). E-mail: shyu@snu.ac.kr

IlpA, a surface protein of the human pathogen Vibrio vulnificus, is the first lipoprotein to be characterized in Vibrio spp. as a major immunostimulant. Previously, it was characterized that IlpA was subject to lipidation at its N-terminal cysteine residue. The resulting IlpA then activates Toll-like receptor 2 in human cells, and induces overproduction of proinflammatory cytokines closely associated with septic shock in infected individuals. To identify structural features of IlpA, we determined the crystal structure of IlpA at 2.6 Å resolution. Specifically, IlpA consists of two homologous domains, each with α/β topology, similar to the structure of substrate-binding protein which is a component of ATP-binding cassette transporter. In fact, binding of L-methionine was observed in the pocket between the two domains, suggesting that IlpA is an L-methionine-binding protein. The structural features of IlpA in this study, along with the immunological properties of IlpA identified previously and other substrate-binding proteins, suggest that substrate-binding lipoproteins of ATP-binding cassette transporter present at the bacterial cell surface could serve as pathogenassociated molecular patterns to Toll-like receptor 2, causing host immune responses against infection.



[1] S. Yu, N.Y. Lee, S.J. Park, S. Rhee, Proteins 2011, 79, 1020-1025.

Keywords: lipoprotein, structure, substrate-binding

MS36.P10

Acta Cryst. (2011) A67, C473

Structure of the catalytic domain of H. pylori cholesterol- α -glucosyltransferase

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 α -Glucosyl cholesterol and its derivatives are the major cell wall components of Helicobacter pylori, also playing an important role in immune evasion and survival. *H. pylori* makes α-glucosyl cholesterol by glucosylating cholesterol extracted from the plasma membranes of human gastric mucosa cells, using the enzyme cholesterol-aglucosyltransferase. Here we present the crystal structure of the catalytic domain of cholesterol-a-glucosyltransferase from H. pylori at 1.50 Å resolution, providing a platform for discovering specific inhibitors of *H. pylori* cholesterol-a-glucosyltransferase that could be developed as novel antibiotics. This work was funded by Korea Ministry of Education, Science, and Technology, National Research Foundation of Korea; Basic Science Outstanding Scholars Program, World-Class University Program, and Innovative Drug Research Center for Metabolic and Inflammatory Disease; Korea Ministry of Health, Welfare & Family Affairs (Korea Healthcare Technology R&D Project, Grant no. A092006).

Keywords: cholesterol-a-glucosyltransferase, HP0421, helicobacter pylori

MS36.P11

Acta Cryst. (2011) A67, C473

Structure of the *Streptococcus pyogenes* β-NAD+ glycohydrolaseinhibitor complex

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Streptococcus pyogenes (group A streptococcus; GAS) secretes several extracellular proteins which contribute to pathogenesis. Among them, β -NAD⁺ glycohydrolase (SPN) is an important virulence factor. The mechanism for pathogenesis is intracellular β -NAD⁺ depletion within the host cell due to the β -NAD⁺ hydrolytic activity of SPN. SPN is also toxic to the bacterium itself; therefore, GAS encodes the *ifs* gene, whose product (IFS) is an endogenous inhibitor of the NAD⁺ glycohydrolase. In order to understand the inhibition mechanism of SPN by IFS, we have determined the crystal structure of the SPN-IFS complex at 1.8 Å resolution. SPN is an atypical member of the ADP-ribosyltransferase superfamily, lacking a canonical binding site for the protein substrate. The SPN-IFS complex is stabilized by numerous hydrogen bonds and electrostatic interactions. In the complex structure, IFS covers the active site of SPN and blocks the binding of β -NAD⁺.

Keywords: β-NAD+ glycohydrolase, IFS, streptococcus pyogenes

MS36.P12

Acta Cryst. (2011) A67, C473-C474

Crystal structures of Eis proteins from *M. tuberculosis* and *M. smegmatis*

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