[4] DiMaio, F, et al. (2011) Improved molecular replacement by density- and energy-guided protein structure optimization. *Nature*. 26;473 (7348), 540-3.

[5] Sammito, M., et al. (2013) Exploiting tertiary structure through local folds for crystallographic phasing. *Nat Methods*. 10(11), 1099-101.

[6] http://www.sdsc.edu

**Keywords:** Fragment libraries, Local Folds, Supercomputing

## MS10-P9 Identification and structural modeling of a novel virulence factor from *H.pylori*

Burcu Kaplan-Türköz[1]

1. Ege University, Faculty of Engineering, Department of Food Engineering, Bornova, İzmir, Turkey

email: bkaplan@sabanciuniv.edu

Pathogens produce virulence factors, which help bacteria to invade the host, cause disease and evade host defenses. Recently a class of bacterial proteins which share homology with the Toll/IL-1 receptor (TIR) domain was identified. Those from pathogens; *Brucella* (BtpA and BtpB), uropathogenic *E. coli* (TcpC), *Salmonella* (TlpA) and *Yersinia* (YpTIR) were characterized and their effects on the immune system especially targeting TLR signaling was documented. (*1-5*) BtpA was shown to be directly involved in the virulence of *Brucella* (*5*) and the crystal structure of BtpA confirmed the presence of the TIR domain fold. (*6*). It is yet to be proven if other bacterial proteins with putative TIR domains also function in bacterial pathogenesis. *H. pylori* is a Gram-negative bacteria that colonizes the human stomach and associates with most gastric pathologies, including gastric cancer. *H.pylori* is known for its ability to achieve persistent infection with minimal immune response (7). *H.pylori* might possess a TIR domain containing virulence factor, which can play a role in supressing TLR signaling analogous to BtpA. In order to identify a putative *H.pylori* TIR domain protein, database were searched and HP1437 was found. HP1437, a 239 amino acid protein has a predicted C terminal TIR domain similar to BtpA/TlpA/TcpC and it contains the conserved TIR domain regions. In this study, HP1437 will be characterized using bioinformatic approaches in order to understand its possible role as a bacterial TIR domain protein. The tertiary structure of HP1437 and that of the C terminal TIR domain will be modelled using homology modeling. The structural models with the highest scores will be searched in protein structure database. The structural alignments will reveal the level of similarity of HP1437 to BtpA or other TIR domain protein structures. The results might contribute to our understanding of the reduced immune response to *H.pylori.*

**Acknowledgements**: This work is supported by TÜBİTAK-BİDEB (grant number: 114C095).

**References:** 1:Rana R.R. et al 2011, Microb Pathog, 51,89-95. 2: Salcedo, S.P. et al; 2008, PloS Pathog, 4, e21. 3: Cirl, C. et al., 2008, Nat Med, 14, 399-406. 4:Newman, R.M. et al.,2006, Infect Immun, 74, 594-601. 5:Salcedo, S.P. et al., 2013, Front Cell Infect Microbiol, 3,28. 6: Kaplan-Türköz, B. et al., FEBS Lett, 587 (21) 3412-16. 7: Salama, N. R. et al., 2013, Nat Rev Microbiol, 11(6)385-99.

**Keywords:** H.pylori, homology modeling, virulence factor