Abstract Submitted for the TSF16 Meeting of The American Physical Society

The Structure of the N-terminal end (1-961 aa) of Txo2: an important player in the synthesis of the antibiotic teixobactin¹ RAUL HIGUERA, University of Texas at El Paso, DOMINKA BOREK, ZBYSZEK OTWINOWSKI, UT Southwestern Medical Center — Every year, 2 million people are infected with drug resistant bacteria and many die from infections. Understanding the sources of antibiotics is one important step to finding solutions to combat drug-resistant bacteria. E. terrae is a gram negative bacteria that produces the antibiotic teixobactin. A fragment (1-961 aa) of the Txo2 gene in E. terrae encodes the production of an important enzyme involved in the synthesis of teixcobactin. We are interested in the sites of the fragment that help synthesize necessary enzymes. Thus, we solved the 2.8Å crystal structure of the fragment at Argonne National Laboratory. The structure was processed using WinCoot and REFMAC and analyzed using programs and servers: -BLAST, Consurf, and DALI. We found that Txo2 contains three domains: a condensation domain, an HxxPF domain, and canonical fold of non-ribosomal peptide synthetases, or NRPS, domain. We analyzed several properties, e.g. the evolutionary conservation, to find molecular level components responsible for important actions. We found that the structure of the N-terminal end of Txo2 is responsible for adding the Ser residue to teixobactin.

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