Links to published DMSP-dependent protein structures for the apoenzyme DmdA from Pelagibacter ubique at NCBI's MMDB (En-Gen DMSP Cycling project)

Website: https://www.bco-dmo.org/dataset/3784
Version: 19 Nov 2012
Version Date: 2012-11-19

Project
» En-Gen: A Functional Genomics Approach to Organic Sulfur Cycling in the Ocean (En-Gen DMSP Cycling)

Contributors	Affiliation	Role
Moran, Mary Ann	University of Georgia (UGA)	Principal Investigator
Kiene, Ronald P.	Dauphin Island Sea Lab (DISL)	Co-Principal Investigator
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Dataset Description

Links are provided to published protein structures for the apoenzyme DmdA from *Pelagibacter ubique*, as well as for DmdA co-crystals soaked with substrate DMSP or the cofactor tetrahydrofolate (THF) accessible via NCBI's Molecular Modeling Database (MMDB).

Experimental design, methods, and results are further described in:
D. J. Schuller, C. R. Reisch, M. A. Moran, W. B. Whitman, and W. N. Lanzilotta (2012). Structures of dimethylsulfoniopropionate-dependent demethylase from the marine organism Pelegabacter ubique. Protein Science, vol. 21, p. 289. doi: 10.1002/pro.2015

Methods & Sampling

See Schuller et al. 2012 for detailed methods, which are paraphrased below:
"Expression and isolation of the dimethylsulfoniopropionate-dependent demethylase (DmdA) from recombinant E. coli that expressed the *P. ubique* DmdA (SAR11_0246) gene was performed as previously described in Reisch et al. (2008). Crystal screening of DmdA was performed in an anaerobic chamber consisting of an atmosphere of 95% nitrogen and 5% hydrogen using the microbatch diffusion technique and an IMPAX I-5 (Douglas Instruments, East Garston, United Kingdom) crystallization robot.

In addition to the native crystals, data was also collected on crystals that had been treated with either the substrate (2 mM DMSP) or the cofactor, tetrahydrofolate (2 mM THF). In both cases a solution of mother liquor was prepared, under anaerobic conditions,containing either DMSP or THF.

All data sets were collected at the Advanced Photon SER-CAT on beamline 22-ID (http://www.ser.aps.anl.gov/). Several programs from the CCP4 program suite (CCP4 website) were employed during structure determination and refinement. Various molecular replacement attempts were made using the program PHASER."

References:

Reisch CR, Stoudemayer MJ, Varaljay VA, Amster IJ, Moran MA, Whitman WB (2011). Novel pathway for assimilation of dimethylsulphoniopropionate widespread in marine bacteria. Nature 473:208–211. doi:10.1038/nature10078

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Data Files

File
DMSP_dependent_proteins.csv (Comma Separated Values (.csv), 542 bytes) MD5:2fb60b48f20f5d42d75862116839d6b7 Primary data file for dataset ID 3784

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Parameters

Parameter	Description	Units
protein_name	Name/description of the protein structure.	text
taxon	Scientific name of the organism of study.	text
strain	Name of the bacterial strain.	text
PDB_ID	Protein structure ID number at the Protein Data Bank (http://www.rcsb.org/pdb/home/home.do)	unitless
MMDB_ID	Protein structure ID number at NCBI's Molecular Modeling Database (MMDB).	unitless

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Project Information

En-Gen: A Functional Genomics Approach to Organic Sulfur Cycling in the Ocean (En-Gen DMSP Cycling)

Coverage: Sapelo Island, GA, USA, 31.4° N Lat, 81.3° W Lon / Dauphin Island, AL, USA, 30.3 ° N Lat, 88.1° W Lon

The recent discovery of key genes that mediate competing pathways at a critical juncture in the marine sulfur cycle has allowed biogeochemists to make rapid advances in understanding where and when sulfur transformations occur in the ocean, and most importantly, what factors regulate them. This project describes an environmental functional genomics project that will rapidly increase our knowledge of the role that bacterioplankton play in dimethylsulfoniopropionate (DMSP) cycling in ocean surface waters, focusing particularly on biological controls of volatile sulfur exchange across the ocean/atmosphere boundary.

The investigators have asked three critical hypotheses to explain the regulation of bacterial DMSP degradation: that involve investigations on the energy constraints of DMSP cycling, the role that DMSP concentration in the oceans plays, and the sulfur requirements for bacterial growth. These research areas serve as the focus for

hypothesis-driven laboratory and field studies using functional genomics approaches that will track patterns in gene expression in relation to sulfur metabolism. The hypotheses will be tested with:
1) chemostat systems with a model marine bacterium Silicibacter pomeroyi;
2) microcosm experiments with Gulf of Mexico seawater; and
3) field studies at various sites in the Gulf of Mexico. Marine bacterioplankton play a key role in regulating the flux of DMSP-derived sulfur to the atmosphere, a process of great importance for global climate regulation and marine productivity.

The investigators will also be involved in graduate and undergraduate student education, and two post-doctoral associates will be trained to address multidisciplinary challenges in environmental microbiology. High school biology students in Athens, GA will participate in marine microbial biology research that includes bacterial diversity and discovery studies in coastal Georgia, follow-up training in molecular tools and bioinformatics in their own classroom, and summer internships at the University of Georgia and Dauphin Island Sea Laboratory.

(The description above is from the NSF Award Abstract).

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Funding

Funding Source	Award
NSF Division of Ocean Sciences (NSF OCE)	OCE-0724017

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