Data in Brief 6 (2016) 249–252

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

NOE distance and dihedral angle restraints to calculate the solution structure of the NDH-1 complex subunit CupS from *Thermosynechococcus elongatus*

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ARTICLE INFO

Article history:
Received 23 September 2015
Received in revised form
23 November 2015
Accepted 6 December 2015
Available online 15 December 2015

Keywords:
Bioenergetics/electron Transfer Complex CupS
Cyanobacteria
Membrane Proteins
NMR Protein Structure
NOE Distance And Dihedral Angle Restraints

ABSTRACT

Here, we have compiled a nuclear magnetic resonance (NMR)-derived set of nuclear Overhauser enhancement (NOE) distance and dihedral angle restraints that allow for the calculation of the structure of the NDH-1 complex subunit CupS from *Thermosynechococcus elongatus* in solution. These restraints to calculate the structure in solution of CupS have been deposited to the Protein Data Bank (www.rcsb.org) under PDB-ID accession number **2MXA**. This is the first experimental data set published to compute the three-dimensional structure of CupS. This structure is presented in the research article "Solution structure of the NDH-1 complex subunit CupS from *Thermosynechococcus elongatus*" published by Korste et al. in Biochim. Biophys. Acta 1847(2015)1212–1219 [1]. The cyanobacterial multi-subunit membrane protein complex NDH-1 structurally and functionally relates to Complex I of eubacteria and mitochondria. The NDH-1 complex is mechanistically involved in respiration and cyclic electron transfer around photosystem I (PSI) as well as in a unique mechanism for inorganic carbon concentration.

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http://dx.doi.org/10.1016/j.dib.2015.12.004

Specifications table

Subject area	Biochemistry, structural biology
More specific subject area	Nuclear magnetic resonance (NMR), protein structure calculation
Type of data	NMR distance restraints, dihedral angle restraints
How data was acquired	Multidimensional solution NMR spectroscopy
Data format	ARIA and CNS input files
Experimental factors	The NMR experiments were performed on a sample containing 0.5 mM protein in 50 mM Tris–HCl (pH 8.0), 50 mM NaCl, 10 mM deuterated dithiothreitol (DTT), and 10% D2O.
Experimental features	All NMR spectra were acquired at 298 K on BrukerBioSpin Avance-III 950, Avance-I 800, DRX-600, and DRX-500 spectrometers and processed using NMRPipe [2].
Data source location	Bochum, Germany and Osaka, Japan
Data accessibility	These restraints to calculate the structure in solution of CupS have been deposited to the Protein Data Bank (www.rcsb.org) under PDB-ID accession number **2MXA**.

Value of the data

- the very first NMR experimental data set to compute the three-dimensional structure of CupS in solution;
- this data set might help to elucidate the function of CupS not fully understood to date;
- this data set might serve as a reference for future studies of CupS molecular complexes.

1. Data

We have extracted a total of 2089 NOE distance restraints from three-dimensional ^{15}N-edited and ^{13}C-edited NOESY spectra, which were processed using NMRPipe [1,2]. Spectra exhibit substantial chemical shift dispersion – a feature also observed for the one-dimensional ^{1}H NMR spectrum of CupS (Fig. 1). In total, this data set consists of 929 intra-residual, 448 sequential, 281 medium range, and

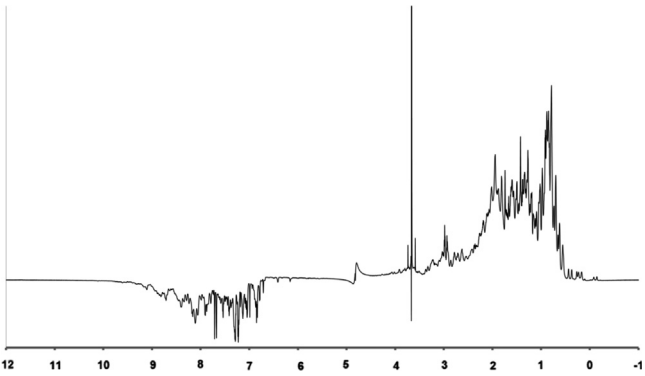

Fig. 1. One-dimensional ^{1}H NMR spectrum (with signal intensities plotted *versus* ppm values) of [^{15}N]-CupS recorded on a BrukerBioSpin Avance-III 950 spectrometer at pH 8.0 and at 293 K. Proton chemical shifts in the amide region were detected without the application of decoupling pulses to ^{15}N.