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Data Article

Data on the phosphorylation state of the catalytic serine of enzymes in the α-D-phosphohexomutase superfamily

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ABSTRACT

Most enzymes in the α-D-phosphohexomutase superfamily catalyze the reversible conversion of 1- to 6-phosphosugars. They play important roles in carbohydrate and sugar nucleotide metabolism, and participate in the biosynthesis of polysaccharides, glycolipids, and other exoproducts. Mutations in genes encoding these enzymes are associated with inherited metabolic diseases in humans, including glycogen storage disease and congenital disorders of glycosylation. Enzymes in the superfamily share a highly conserved active site serine that participates in the multi-step phosphoryl transfer reaction. Here we provide data on the effects of various phosphosugar ligands on the phosphorylation of this serine, as monitored by electrospray ionization mass spectrometry (ESI-MS) data on the intact proteins. We also show data on the longevity of the phospho-enzyme under various solution conditions in one member of the superfamily from *Pseudomonas aeruginosa*, and present inhibition data for several ligands. These data should be useful for the production of homogeneous samples of phosphorylated or unphosphorylated proteins, which are essential for biophysical characterization of these enzymes.

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Specifications Table

Subject area	*Chemistry, Biology*
More specific subject area	*Biochemistry, Enzymology*
Type of data	*Tables, figures*
How data was acquired	*Mass spectrometry using a NanoLC-Nanospray QTOF (Agilent 6520) with C8 column chromatograph; enzyme inhibition assays*
Data format	*Analyzed*
Experimental factors	*Purified proteins were incubated with phosphosugar ligands and under different solution conditions; enzyme inhibition was assessed in presence of ligands*
Experimental features	*ESI-MS data on intact proteins were collected and the % phosphorylation of the catalytic serine calculated; enzyme activity was measured on a spectrophotometer using a colorimetric assay*
Data source location	*University of Missouri Charles W. Gehrke Proteomics Center, Columbia, MO USA*
Data accessibility	*The data is available within this article*

Value of the data

- The catalytic phosphoserine of enzymes in the α-D-phosphohexomutase superfamily plays an integral role in enzyme mechanism.
- We present data on the phosphorylation state of the serine under varying conditions.
- These data will be useful information for preparation of homogeneous samples of phospho- or dephospho-enzyme for future biophysical and kinetic studies.

1. Data

The data in this article show the effects of phosphosugar ligands and other variables on the phosphorylation state of the catalytic serine in several enzymes in the α-D-phosphohexomutase superfamily. Data were obtained by ESI-MS. Data on enzyme inhibition by several ligands is also presented.

2. Experimental design, materials and methods

2.1. Materials

Leuconostoc mesenteroides glucose 6-phosphate dehydrogenase (G6PDH), and all bis- and mono-phosphorylated sugars except xylose 1-phosphate (X1P) were obtained from Sigma-Aldrich. X1P was kindly synthesized by Dr. Thomas Mawhinney (University of Missouri).

2.2. Preparation of protein samples

Expression and purification of *Pseduomonas aeruginosa* PMM/PGM (PaPMM), *Bacillus anthracis* phosphoglucosamine mutase (BaPNGM), *Salmonella typhimurium* PGM (StPGM), *Francisella tularensis* PNGM (FtPNGM), and human phosphoglucosmutase 1 (hPGM1) were performed as described previously [1–4]. Purified proteins were dialyzed into 50 mM MOPS, pH 7.4, concentrated, and stored at −80 °C until use.