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Data article

Properties of substances inhibiting aggregation of oxidized GAPDH: Data on the interaction with the enzyme and the impact on its intracellular content

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ABSTRACT

This data is related to our paper "Small molecules preventing GAPDH aggregation are therapeutically applicable in cell and rat models of oxidative stress" (Lazarev et al. [1]) where we explore therapeutic properties of small molecules preventing GAPDH aggregation in cell and rat models of oxidative stress. The present article demonstrates a few of additional properties of the chemicals shown to block GAPDH aggregation such as calculated site for targeting the enzyme, effects on GAPDH glycolytic activity, influence on GAPDH intracellular level and anti-aggregate activity of pure polyglutamine exemplifying a denatured protein.

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Specifications Table

Subject area	Biology
More specific subject area	Biology of oxidative stress
Type of data	Text file, figure, images
How data was acquired	Molecular docking, Western blot, Dot blot, Microscope, Survey, Spectrometry
Data format	Analyzed
Experimental factors	Pure GAPDH and polyglutamine were used in *in vitro* experiments
Experimental features	Small molecules preventing GAPDH aggregation do not affect glycolytic activity of the enzyme, its intracellular level and do not suppress polyglutamine aggregation.
Data source location	St. Petersburg, Russia
Data accessibility	The data is supplied with this article

Value of the data

- The current paper presents a new GAPDH binders preventing its aggregation.
- To find the site of interaction between small molecules and GAPDH the molecular docking method was applied.
- This data article describes a set of methods to determine the specificity of interaction between protein and ligands, the impact of drugs on the state of the protein in the cell and the enzyme activity of target protein.

1. Data

The data presented in this article demonstrate the biochemical characteristics of the substances previously shown as blockers of GAPDH aggregation. Among other things, it contains data of molecular docking of these substances and the measurements of GAPDH enzymatic activity in the presence of the ligands.

2. Experimental design, materials and methods

2.1. Molecular docking

Early we found a group of substances that inhibit the aggregation of oxidized GAPDH [1]. To reveal the site of GAPDH molecule targeted by the selected substances (RX409, RX426, RX624, RX625, and RX648) the method of molecular docking was employed (Fig. 1). Molecular docking was performed using Lead Finder software [2]. The structures of ligands were built using ChemSketch (www.acdlabs.com).

2.2. Measurement of GAPDH enzymatic activity

Next we analyzed the effect of the five selected compounds on GAPDH enzymatic activity. Only RX648 was shown to reduce the enzymatic activity of GAPDH (Fig. 2). The effects of selected