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Data Article

Fluorescence-based thermal shift data on multidrug regulator AcrR from *Salmonella enterica subsp. entrica serovar Typhimurium str. LT2*

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ABSTRACT

The fluorescence-based thermal shift (FTS) data presented here include Table S1 and Fig. S1, and are supplemental to our original research article describing detailed structural, FTS, and fluorescence polarization analyses of the *Salmonella enterica subsp. entrica serovar Typhimurium str. LT2* multidrug transcriptional regulator AcrR (StAcrR) (http://dx.doi.org/10.1016/j.jsb.2016.01.008) (Manjasetty et al., 2015 [1]). Table S1 contains chemical formulas, a Chemical Abstracts Service (CAS) Registry Number (CAS no.), FTS rank (a ligand with the highest rank) has the largest difference in the melting temperature (ΔT_m), and uses as drug molecules

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AcrR
Salmonella enterica
High-throughout screening

against various pathological conditions of sixteen small-molecule ligands that increase thermal stability of StAcrR. Thermal stability of human enolase 1, a negative control protein, was not affected in the presence of various concentrations of the top six StAcrR binders (Fig. S1).

Specifications Table

Subject area	*Chemistry, Biology*
More specific subject area	*Protein-ligand interactions*
Type of data	*Tables, figure*
How data was acquired	*Fluorescence-based thermal shift (FTS) analysis. 384-well PCR plates; an Echo550 acoustic transfer robot (Labcyte, Sunnyvale, CA); real-time PCR machine CFX384 (Bio-Rad Laboratories, Hercules, CA); in-house ExcelFTS software.*
Data format	*Analyzed*
Experimental factors	*High concentration protein stocks were diluted in the FTS analysis buffer*
Experimental features	*The FTS analysis was performed in high-throughput mode using semi-automatic approach*
Data source location	*Chicago*
Data accessibility	*Data is within this article.*

Value of the data

- FTS data present potential StAcrR small-molecule binders that may affect the protein's structure and function.
- Researchers in the field may utilize employed high-throughput FTS approach in screening small-molecule binders for homologous multidrug regulators from the TetR family.
- Collectively, presented data could be exploited for the design of the StAcrR inhibitors.

1. Data

Here, we present FTS data featuring multidrug-binding nature of the transcriptional regulator StAcrR. The top sixteen binders of StAcrR, as shown in Table S1, were identified by the FTS analysis from a library of 320 unique ligands. Human enolase 1, a negative control protein (Fig. S1), did not bind the top six binders of StAcrR, while implying their specific interactions with StAcrR. The remaining compounds were not tested against human enolase 1. Theoretical data for Table S2 were obtained from National Center for Biotechnology Information PubChem Compound Database (https://pubchem.ncbi.nlm.nih.gov/compound/) and include chemical properties such as topological polar surface ($Å^3$), number of hydrogen bond donors/acceptors, XLogP3, and molecular weight (g/mol) of the top six StAcrR FTS hits, dequalinium chloride, proflavine, ethidium bromide and rhodamine 6G.

The latter three molecules were identified as the StAcrR binders employing a fluorescence polarization experimental approach (see our original publication [1]).

2. Experimental design, materials and methods

The FTS assay was run in 384-well PCR plates using an Echo550 acoustic transfer robot (Labcyte, Sunnyvale, CA) for dispensing a dimethyl sulfoxide stock of ligands to assay plates that contain 10 μl of a mixture of StAcrR (1 μg) and 2.5 × SYPRO Orange fluorescence dye (Invitrogen, Carlsbad, CA) in 100 mM HEPES buffer pH 7.5 and 150 mM NaCl. Thermal scanning (from 10 to 80 °C at 1.5 °C min^{-1} ramp rate) on a real-time PCR machine CFX384 (Bio-Rad Laboratories, Hercules, CA) was coupled with fluorescence detection every 10 s.

A test molecule, dequalinium, bound at 40 μM that prompted us to screen a 320-molecule subset of the Spectrum library (Micro Source Discovery, Gaylordsville, CT, hereafter referred as SPC2-ECH008), dequalinium belongs to. The best binders were selected based on ΔT_m, reduction of the background reading, and shape of the melting curve. The top six hits were further subjected to a dose-dependent response analysis using their 2.5, 5, 10, 25, 50, 75 and 100 μM concentrations. Human enolase 1 (1.2 μg in 10 μl assay mixture) was used as a negative control protein and tested against the top six binders at 10, 25 and 50 100 μM concentrations. FTS data were analyzed with the in-house ExcelFTS software.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.03.003.

References

[1] B.A. Manjasetty, A.S. Halavaty, C.H. Luan, J. Osipiuk, R. Mulligan, K. Kwon, W.F. Anderson, A. Joachimiak, Loop-to-helix transition in the structure of multidrug regulator AcrR at the entrance of the drug-binding cavity, J. Struct. Biol. 194 (2016) 18–28.