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NmrLineGuru: Fast 1D NMR Lineshape Simulation & Analysis with Multi-State Equilibrium Binding Models

Standalone software, NMRLineGuru, simulates and analyzes complex multi-state protein interactions using NMR line shape data, accounting for both kinetic and thermodynamic parameters.

Researchers at Purdue University have developed nuclear-magnetic resonance (NMR)-related software for simulation and analysis of protein interactions across multiple states detected with NMR chemical shifts. Proteins can have complex interactions; accordingly, multi-state equilibria involve complex mathematical models with simultaneous equations and matrix manipulations. Nonetheless, most existing tools for fitting NMR line shape data can only support a simple 2-state binding model. The Purdue researchers' software, called NMRLineGuru, simulates and fits NMR line shapes with two-, three-, and four-state binding models. It is a standalone and user-friendly software for simulating and fitting NMR line shapes. In fitting NMR line shape data, the Purdue system accounts for both thermodynamic and kinetic interaction parameters among proteins.

Related Publication: Feng, C., Kovrigin, E.L. & Post, C.B. NmrLineGuru: Standalone and User-Friendly GUIs for Fast 1D NMR Lineshape Simulation and Analysis of Multi-State Equilibrium Binding Models. Sci Rep 9, 16023 (2019). https://doi.org/10.1038/s41598-019-52451-8

Technology Validation: https://github.com/stonefonly/NmrLineGuru

Advantages:

- Simulates up to four protein interactions

- Accounts for both kinetic and thermodynamic interaction parameters

- User-friendly interface

Applications

Technology ID
2019-POST-68616

Category
Biotechnology & Life Sciences/Bioinformatics & Computational Biology
Pharmaceuticals/Computational & Software Tools
Pharmaceuticals/Research Tools & Assays

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- Simulating protein interactions

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Intellectual Property:

Keywords: nuclear-magnetic resonance, NMR, protein interactions, multi-state equilibrium, NMR chemical shifts, NMRLineGuru, NMR line shape simulation, two-state binding model, multi-state binding models, thermodynamic parameters, kinetic parameters