

Poster

Protein thermodynamic properties, crystallisation, and the Hofmeister Series**E. Saridakis¹, K. Donta^{1,2}**

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The Hofmeister Series is a series of ions ordered according to their ability to precipitate proteins. It has also been linked to a host of (bio)chemical phenomena. Several attempts over the years to correlate the series to the varying success of different salts in crystallising proteins have been largely inconclusive.

We propose a correlation, based on published data and crystallisation conditions for several proteins, between thermodynamic properties of proteins and the position in the Hofmeister series of the salts from which they preferentially crystallise [1]. Namely, a high ratio between the entropic or enthalpic hydration (or, more accurately, protein-solvent interactions) contribution to thermodynamic stability and the total thermodynamic stability of a given protein ($|\Delta S_{unf}^{hyd}/\Delta G_{unf}|$ or $|\Delta H_{unf}^{p,s}/\Delta G_{unf}|$, where ΔG_{unf} is the Gibbs Free Energy of unfolding) indicate the protein's high propensity to crystallise in solutions of highly kosmotropic salts. Low such ratios on the other hand, indicate that chaotropic salts can be equally successful, i.e. that the protein in question is rather indifferent to the Hofmeister character of the salt.

Testing various model proteins for crystallisation against screens containing salts found at different points on the Hofmeister series, as well as further bibliographic analysis, have yielded results that appear to largely corroborate this hypothesis. These conclusions may conceivably be used as a crystallisation predictive tool [1].

[1] Saridakis, E., Donta, K. (2024). *ChemPlusChem*. e202300733. <https://doi.org/10.1002/cplu.202300733>