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Role of the solvophobic effect in protein-ionic liquid interactions

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Biological applications which utilise enzymes, or other proteins, require the tertiary structure of the protein to be retained. However, many proteins readily undergo aggregation or denaturation when outside their native environment, and/or over longer timescales. The stability of proteins in solvents other than water is usually considered unappealing due to an assumption that the protein will be insoluble or denatured. However, a few solvents, such as glycerol and dilute alcohols have been shown to have protein stabilising properties, such as in cryopreservation.

Previously we have developed extensive structure-property relationships between the chemical structures and mesostructures of non-aqueous solvents and the solvophobic effect experienced by amphiphiles for molecular solvents [1] and protic ionic liquids [2]. Here we have extended this to develop a greater understanding of what solvent features are important for protein stability. We have utilised a series of small polar non-aqueous molecular solvents and protic ionic liquids consisting of the four acid-base combinations of ethyl- and ethanolammonium cations paired with formate or nitrate. Solutions were prepared of these solvents combined with water, and with added formate or nitrate for the ionic liquids to explore a broad range of pH effects. For this initial work egg white lysozyme (HEWL) was used. These solvent systems enabled us to explore the effect of pH, solvent concentration, solvent cohesive energy density and polarity towards protein stability [3]. The activity of the lysozyme was assessed based on its lytic activity towards *Micrococcus lysodieticus* using UV-Vis spectroscopy. The secondary and tertiary structures of the lysozyme were determined using Small angle X-Ray scattering (SAXS) and IR spectroscopy. Protein crystallisation studies have been successfully conducted for many of these protic ionic liquid solvent systems, with significant differences in the crystal structures formed.

This work extends our understanding of protein stability in a wide variety of solvent environments, and has enabled structure-property relationships to be developed for a protein in concentrated molecular solvent and protic ionic liquid solvent systems. This work has the potential to lead to the development of tailored solvent systems to optimise protein stability.

[1] E. C. Wijaya, T. L. Greaves and C. J. Drummond, *Faraday Discuss.*, 2013, 167, 191-215.

[2] T. L. Greaves, C. J. Drummond, *Chem. Soc. Rev.*, 2013, 42, 1096-1120

[3] Emmy C. Wijaya, Frances Separovic, Calum J. Drummond, Tamar L. Greaves, *Phys. Chem. Chem., Phys.* 2016, DOI: 10.1039/c6cp03334b.

Keywords or phrases (comma separated)

protein stability, ionic liquids, solvophobic effect, amphiphile, self-assembly

Are you a student?

No

Do you wish to take part in the Student Poster Slam?

No

Are you an ECR? (<5 yrs</br>since PhD/Masters)

No

What is your gender?

Female

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