

EFFECT OF DEEP EUTECTIC SOLVENTS ON THE STRUCTURAL STABILITY AND CONFORMATIONAL DYNAMICS OF CYTOCHROME C STUDIED BY SINGLE-MOLECULE AND ENSEMBLE-BASED TECHNIQUES

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Deep Eutectic Solvents (DESs) have received great attention in recent years as new environment-friendly green media in various fields such as bio-catalysis, extraction and preservation of various biomolecules like protein, DNA, lipids etc.[1] Few theoretical and experimental studies have been performed to explore the structure, stability and activity of some selected protein molecules in DESs.[2,3] Moreover, all the studies are conducted in ensemble conditions, without any reports at the single-molecule level, which give better information about the structure and conformational dynamics of the biomolecules. However, there are no studies so far on the conformational dynamics of any protein in these novel solvents. Here, we describe the effect of two DESs (based on betaine and ethylene glycol or glycerol) and their aqueous mixtures on the structural stability and conformational dynamics of a well-known protein, cytochrome c, both in single-molecule and ensemble conditions employing fluorescence correlation spectroscopy (FCS) and other biophysical methods such as steady-state absorption, emission, circular dichroism, and time-resolved fluorescence spectroscopy. This study reveals how small change in the structure of one of the constituents of the DESs drastically varies the structural stability and conformational dynamics of the protein in the selected DESs.

References

- [1] E. L. Smith; A. P. Abbott, and K. S. Ryder. Deep eutectic solvents (DESs) and their applications, *Chem. Rev.* **114**, 11060- 11082 (2014).
- [2] H. Monhemi; M. R. Housaindokht; A. A. Moosavi-Movahedi, and M. R. Bozorgmehr. How a protein can remain stable in a solvent with high content of urea: insights from molecular dynamics simulation of *Candida antarctica* lipase B in urea:choline chloride deep eutectic solvent, *Phys. Chem. Chem. Phys.* **16**, 14882- 14893 (2014).
- [3] A. Sanchez-Fernandez; K. J. Edler; T. Arnold; D. A. Venero, and A. J. Jackson. Protein conformation in pure and hydrated deep eutectic solvents, *Phys. Chem. Chem. Phys.* **19**, 8667-8670 (2017).