6TH EUROCC VILNIUS WORKSHOP ON USING HPC

Abstract book

January 22, 2026

Vilnius, Lithuania

Published by Vilnius University Press

https://doi.org/10.15388/EUROCC.2026.6

eISSN 2669-0233

Vilnius University Proceedings

Modeling Peptides in Aqueous Ionic Liquid Mixtures: a Quantum Mechanics/Molecular Dynamics Study of Structural and NMR Properties

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Ionic liquids (ILs) have been known as "green" and biocompatible solvents for quite some time and some of their possible biological uses include changing catalytic activity of enzymes, stabilizing or destabilizing various proteins, as well as making them permeate more easily through membranes [1]. The nature of ILs and proteins interactions varies and is difficult to evaluate, so smaller peptides are often used as a model system to discover how different ILs interact with said peptides and change their structure in the aqueous solution. The method most suited for recognizing intermolecular interactions is nuclear magnetic resonance (NMR) spectroscopy as atoms, especially hydrogen, chemical shift is very sensitive to changes of central molecule's close environment.

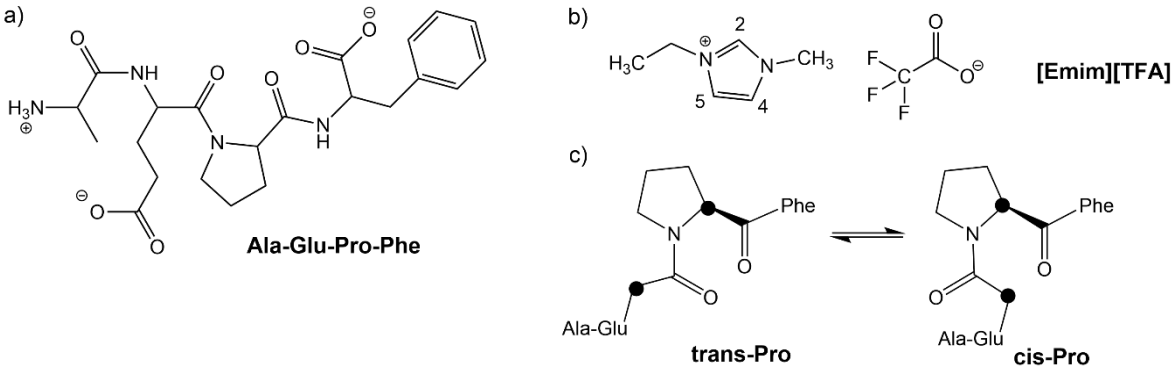

Fig. 1. Structural formulas of a) peptide Ala-Glu-Pro-Phe, b) ethyl-3-methylimidazolium trifluoroacetate, c) *trans/cis* isomeric forms of AEPF

In this work an Ala-Glu-Pro-Phe tetrapeptide (AEPF) was investigated using molecular dynamics (MD) simulations and quantum mechanics/molecular mechanics calculations, while in an aqueous environment and in IL/water mixture. An ionic liquid consisting of a popular imidazolium cation and trifluoroacetic acid – ethyl-3-methylimidazolium trifluoroacetate ([Emim][TFA]) was chosen. This peptide exists in two different isomers due to proline amino acid – *cis* or *trans,* both of them were evaluated. Theoretically computed chemical shift differences of peptide's hydrogen atoms were compared to experimental results [2] allowing us to evaluate the different interactions taking place in peptide/IL/water systems, while MD simulation data revealed some structural changes in the peptide's structure itself.

ACKNOWLEDGEMENTS

This study was supported by the Research Council of Lithuania, grant no. S-MIP-22-74. Computations were performed on resources provided by the High-Performance Computing Center "HPC Saulėtekis" at Vilnius University, Lithuania.

REFERENCES

[1] Gomes, J. M., Silva, S. S. & Reis, R. L. Biocompatible ionic liquids: fundamental behaviours and applications. *Chemical Society Reviews* **48**, 4317–4335 (2019)

[2] Richardt, A., Mrestani-Klaus, C. & Bordusa, F. Impact of ionic liquids on the structure of peptides proved by HR-MAS NMR spectroscopy. *Journal of Molecular Liquids* **192**, 9–18 (2014).