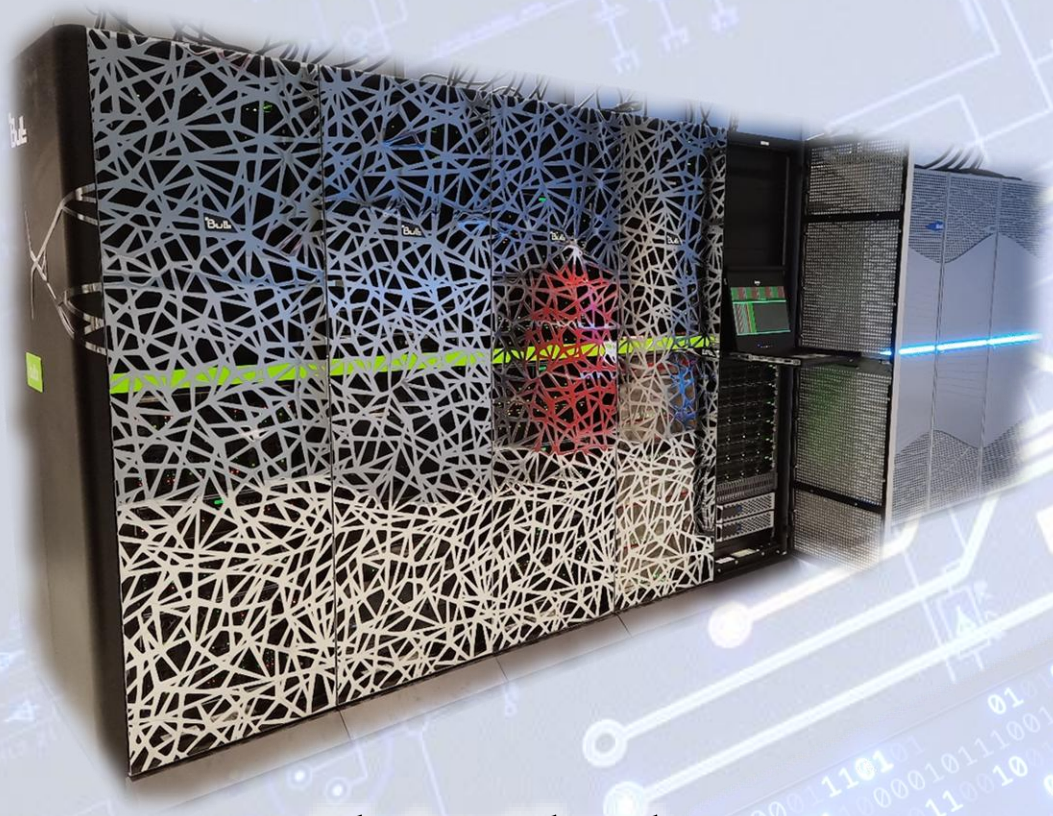
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

ktu kauno technologijos universitetas 1922

VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Nanoorganization in aqueous mixtures of choline lysinate studied by NMR and molecular dynamics / quantum mechanics modelling

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Choline lysinate (ChoLys) is a biocompatible ionic liquid (IL) that belongs to the family of choline-amino acid ILs (ChoAA). ChoAA ionic liquids have a capability to solubilize various drugs and other organic compounds (i.e. lignin in biomass processing) even when a small amount of IL is added to the water [1]. These properties are associated with complex intermolecular structure of ChoAA and water mixtures, ranging from small clusters of water surrounded by IL to intact network of water molecules, with a possible intermediate state – formation of water nanopackets (nanometer scaled clusters of water molecules) [1].

This study is aimed at structural characterization of ChoLys:water mixtures using a combination of molecular dynamics (MD) simulations and quantum mechanics / molecular mechanics calculations (QM/MM). This approach allows not only to characterize the intermolecular structure, but it also involves calculation of ^{1}H NMR shielding constants and validation of simulated structure by comparing calculated values to experimental data.

MD simulations of six ChoLys:H_2O mixtures, ranging from 0,025 % to 50 % ChoLys molar fraction, were simulated using „Amber“ package. Intermolecular structure was characterized by radial distribution functions between various atomic pairs, including N and O in Cho^+, O, Nα and Nε in Lys^- and O in H_2O. All these species participate in hydrogen bonding, forming a complex intermolecular network. Water cluster size distribution analysis showed that two water clusterization regimes (small clusters and water network) manifest in simulated trajectories. Trends of calculated diffusion coefficients support this result. Finally, ^{1}H NMR shielding constants were calculated for Cho+ CH_2 groups, Lys Hα, Hβ and Hε and water (Hw) protons. Results partially match with experimental data, with Hα and Hβ trends (with respect to variation of molar composition) being exceptionally accurate.

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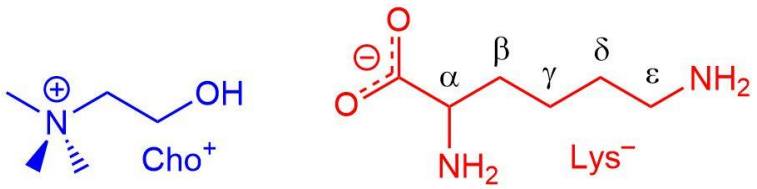

Fig. 1. ChoLys structural formula with positions in Lys^- anion denoted using Greek letters.

REFERENCES

[1] H. J. Jiang, S. Miao, S. Imberti, B. A. Simmons, R. Atkin, G. G. Warr; *Green Chem.* **23** (2021) pp. 856-866.