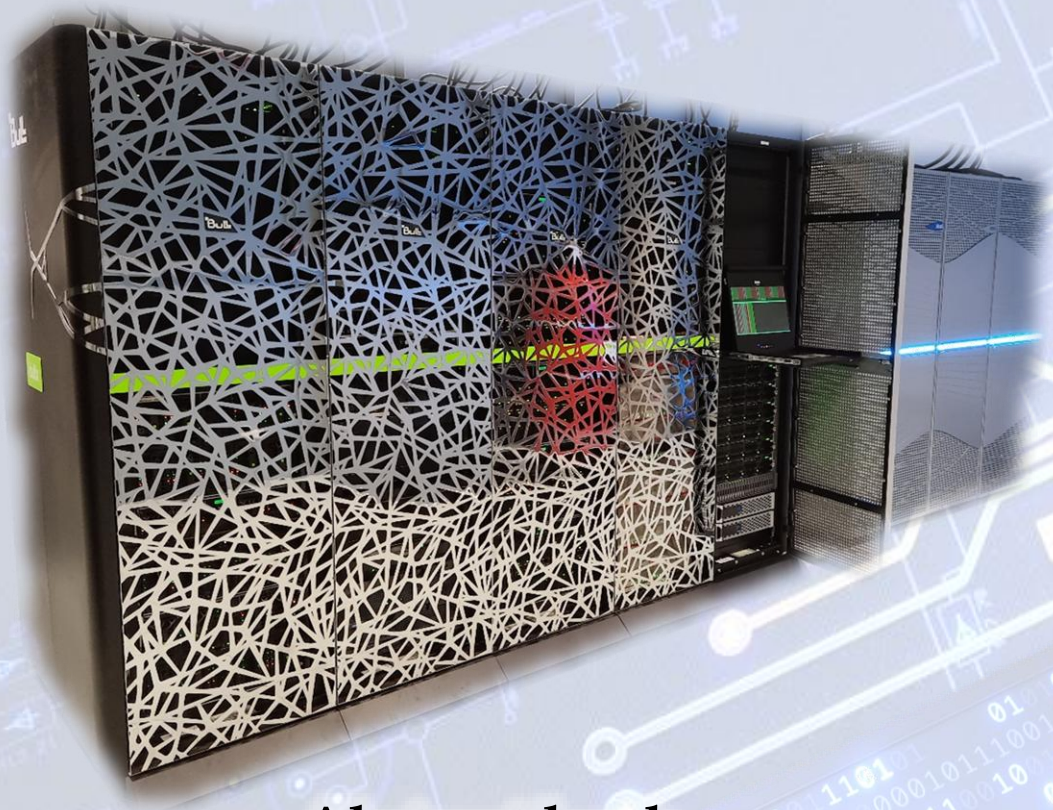
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

https://doi.org/10.5281/zenodo.15754592

https://www.eurocc-lithuania.lt/events_2025-06-27/

June 27, 2025

Vilnius, Lithuania

Hackathon & Workshop organizers

Local organizing committee

Mindaugas Mačernis
Laura Baliulytė

Scientific committee

Mindaugas Mačernis
Laura Baliulytė

Funding

Co-funded by the European Union

EuroHPC Joint Undertaking

Funded by the European Union. This work has received funding from the European High Performance Computing Joint Undertaking (JU) and Germany, Bulgaria, Austria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, Greece, Hungary, Ireland, Italy, Lithuania, Latvia, Poland, Portugal, Romania, Slovenia, Spain, Sweden, France, Netherlands, Belgium, Luxembourg, Slovakia, Norway, Türkiye, Republic of North Macedonia, Iceland, Montenegro, Serbia under grant agreement No 101101903.

Bendrai finansuoja Europos Sąjunga

Projektas bendrai finansuojamas 2021–2027 metų ES fondų investicijų programos (sutartis Nr. 10-051-P-0001).

EuroCC2-EuroCC4SEE
Project Organiser

Vilniaus universitetas 1579 Universitas Vilnensis

Project Implementers

Vilniaus universitetas 1579 Universitas Vilnensis — Fizikos fakultetas

Vilniaus universitetas 1579 Universitas Vilnensis — Matematikos ir informatikos fakultetas

ktu kauno technologijos universitetas 1922

VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

MODELING THE STRUCTURE AND NMR SPECTRA OF AMANTADINE ENCAPSULATED IN SUPRAMOLECULAR MATRICES

Amina Elkady[1], Kęstutis Aidas[2]

[1]*Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University*
[2]*Institute of Chemical Physics, Faculty of Physics, Vilnius University*

E-mail: amina.elkady@chgf.stud.vu.lt

Cavitands (or synthetic receptors) are supramolecular compounds with an enclosed cavity capable of binding small molecules—an attribute that makes them promising for diagnostic applications in biological fluids. Experiments reveal that carbohydrate-based cavitands selectively encapsulate certain alkylammonium compounds, such as drug amantadine, shifting its 1H NMR signals into the negative region (relative to tetramethylsilane) [1]. This distinct spectral shift highlights the potential of cavitands for metabolomic analyses.

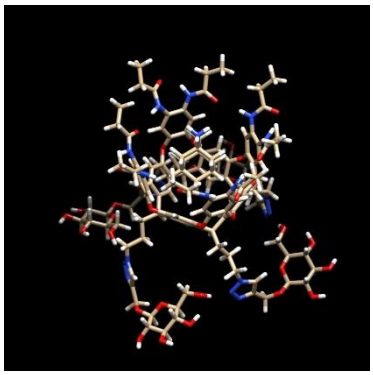


Fig. 1. tetrakis-β-D-glucosyl cavitand–protonated amantadine complex

In this project, the tetrakis-β-D-glucosyl cavitand–protonated amantadine complex is investigated using classical molecular dynamics (MD) simulations, combined with hybrid quantum mechanics/molecular mechanics (QM/MM) methods. Classical MD allows exploration of large-scale molecular behavior under defined thermodynamic conditions, while QM/MM calculations accurately capture electronic effects crucial for NMR shielding. By averaging over configurations from the MD trajectory, temperature-dependent influences are also included. Moreover, the computed NMR spectrum shows good agreement with experimental data, confirming the reliability of this modeling approach. This integrated approach advances our understanding of cavitand–drug interactions and underpins future applications of synthetic cavitands in biomedical diagnostics.

REFERENCES

[1] D. A. Ryan & J. Rebek, "1H NMR detection of small molecules in human urine with a deep cavitand synthetic receptor", Analyst,138, 1008-1010 (2013).