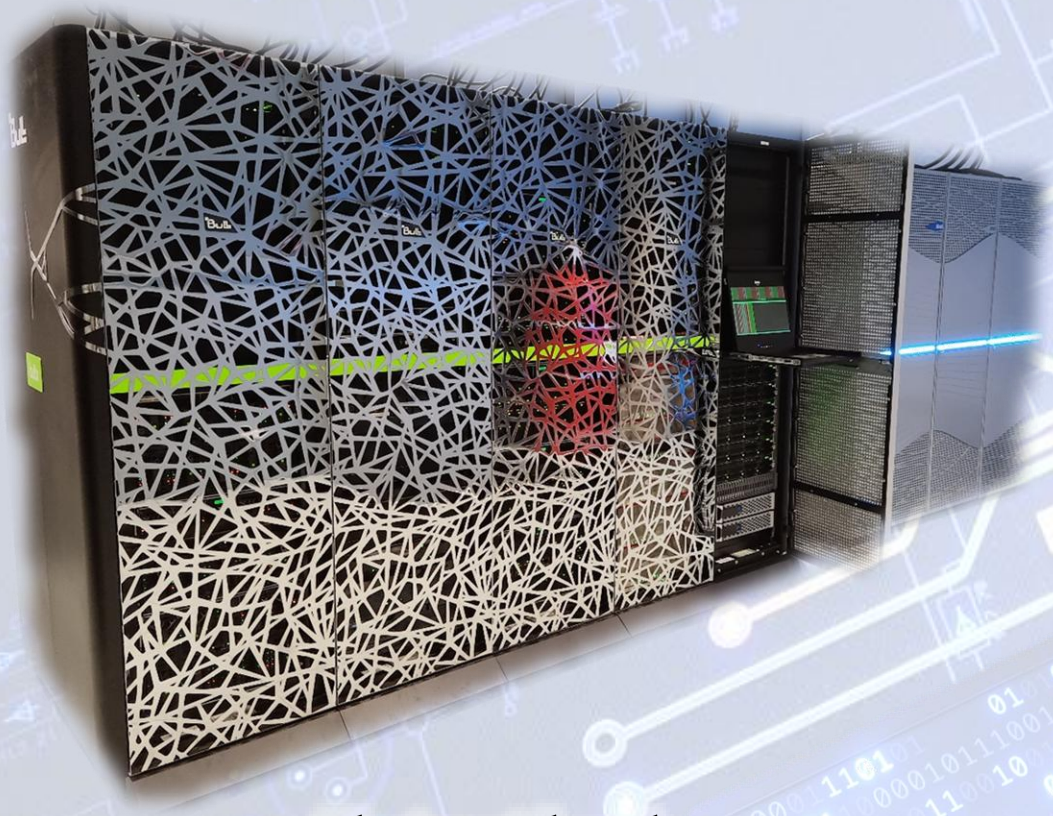
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

https://doi.org/10.5281/zenodo.14748386

January 20–21, 2025

Vilnius, Lithuania

Workshop organizers

Local organizing committee

Mindaugas Mačernis
Laura Baliulytė
Jonas Franukevičius

Scientific committee

Mindaugas Mačernis
Jevgenij Chmeliov
Andrius Gelžinis

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

Hydration free energy calculations using molecular dynamics for trans-stilbene and other compounds

Egidijus Vilčiauskas[1*], Mindaugas Mačernis[1]

[1]nstitute of Chemical Physics, Faculty of Physics, Vilnius University, Saulėtekio av. 3, LT-10257 Vilnius, Lithuania

E-mail: egidijus.vilciauskas@ff.stud.vu.lt

Organic molecules like diarylethylenes, exemplified by stilbene, are valued for their unique photochemical properties, including *trans-cis* isomerization and fluorescence lifetime variability, making them promising components for highly sensitive sensing applications. The structural Stilebene complexes modeling requires molecular dynamics (MD) analysis [1].Understanding of free energy calculations with MD simulations in context of other data provides insight into the reliability and accuracy of such methods.

In this work we present an overview of different ways for calculating hydration free energies while comparing our results against the FreeSolv database [2] and sources found within. Considering a thermal noise of 2.47 kJ/mol, we conclude that our findings correlate well with both experimental values calculated by other (non-MD) means (Fig. 1.) and with the findings of the Mobley group. Eight molecules were tested using two different methods, with different simulation lengths and solvated using different water models. The resulting difference in free energy values when using TIP4P or SPC/E water models is not significant and as such it is recommended to use the simpler and more efficient SPC/E model for further studies. We also find that extending the simulation length (BAR) past 10 ns and into 20 ns produces little change in the final value but significantly reduces the error. WHAM simulations are more efficient when computing resources are limited but are more prone to crashing and require multiple simulations to estimate an error value. All methods produce free energy values that are within 3 kJ/mol of each other (Fig. 2.). Default GROMACS simulation parameters results in producing accurate data.

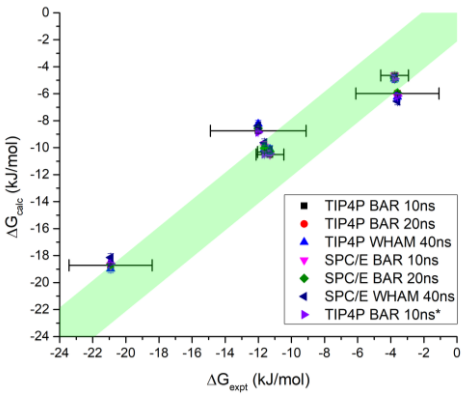


Fig.1. Calculated free energies (Y-axis) against Experimental values (X-axis).

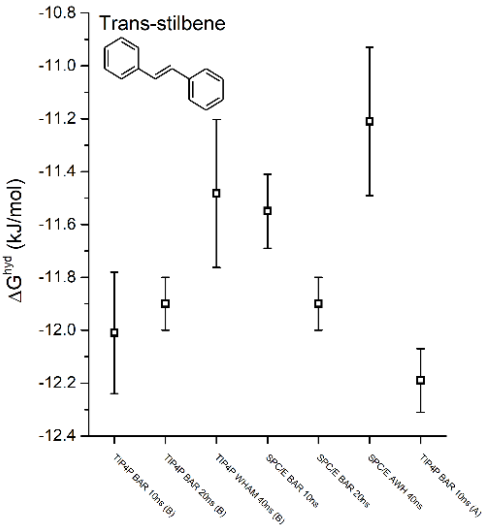


Fig. 2. Hydration free energies for trans-stilbene.

ACKNOWLEDGEMENTS

This work was partially supported by the Research Council of Lithuania (Grant No. S-MIP-23-48). Computations were performed on resources of the supercomputer "VU HPC" Saulėtekis in Vilnius University at Faculty of Physics.

REFERENCES

1. Halimski, I., Macernis, M., et al. (2024). PCCP, 26(36), 23692–23702. https://doi.org/10.1039/d4cp12345h
2. Matos, G. D. R., Kyu, D. Y., Loeffler, H. H., Chodera, J. D., Shirts, M. R., & Mobley, D. L. (2017). J. Chem. & Eng. Data, 62(5), 1559–1569. https://doi.org/10.1021/acs.jced.7b00104