

# **3<sup>RD</sup> EUROCC VILNIUS WORKSHOP**

### ON USING HPC

### **Abstract book**

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#### **Project Implementers**









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## Simulation of molecular sensor insertion into a lipid membrane

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A recently-synthesized variant of boron-dipyrromethene (BODIPY)-based class of prospective molecular sensors, BODIPY-PM, was shown to preferentially aggregate in artificial and natural cell membranes [1]. To study the mechanism of sensor insertion and stabilization, molecular dynamics (MD) model containing the sensor, bilayer lipid membrane and water surroundings was constructed and run for a total simulation time of 450 ns [2]. The simulation confirmed successful sensor insertion into the membrane with two possible orientations, depending on the membrane properties (Fig. 1). Part of the computations was performed on resources at the supercomputer "VU HPC" of Vilnius University in Faculty of Physics location [3].



Fig. 1. Chemical structure of BODIPY-PM molecule (*left*) and evolution of the distance of its main functional groups from the center plane of a bilayer lipid membrane, as obtained by MD simulation (*right*).

#### REFERENCES

- [1] A. Polita et al., RSC Advances 13, 19257 (2023).
- [2] D. Narkevičius, masters thesis, Vilnius University (2024).
- [3] Supercomputer "VU HPC" Saulėtekis. [Online: https://sauletekis.ff.vu.lt/en/]