Analysing bulk- and microviscosity effects from multilevel computation results of the properties of BODIPY-based molecular sensors

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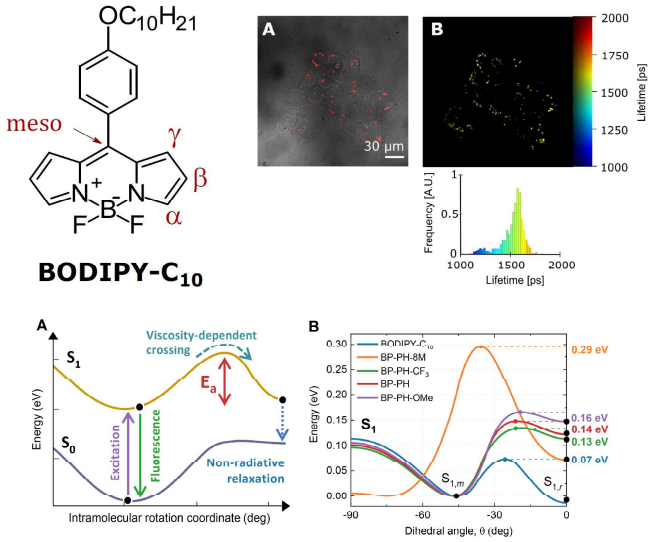
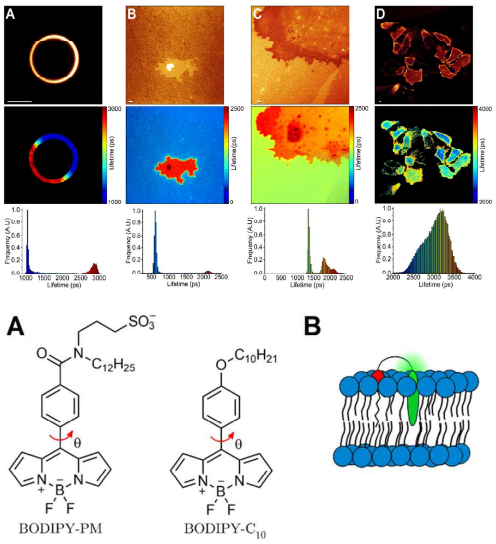
BODIPY viscosity sensors [1]



Membrane-specific BODIPY derivative [2]

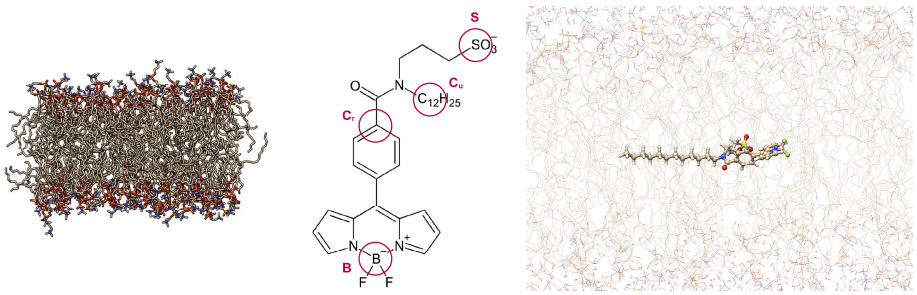


Hardware and simulations

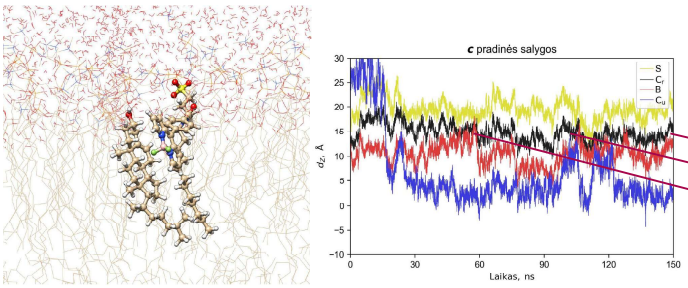
- **GROMACS** molecular dynamics (MD) package
  - *Lipid14/21*, *gaff* (sensor) force fields
- **Gaussian16** electronic structure package
  - Sensor parametrization (PM6, HF, MP2)

- **CPU**: Bull Sequana X1000 (**VU HPC Saulėtekis**)
  - **191** ns/day, 2400 h CPU time (19 h wall)
- **GPU**: NVIDIA RTX 3070
  - **167** ns/day, 43 h GPU time

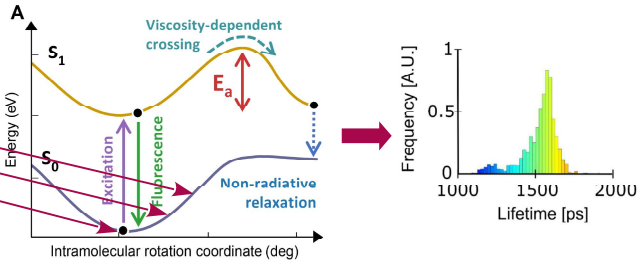
Sensor in a lipid bilayer membrane [3]



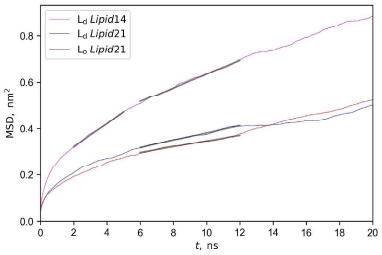
MD simulation run in ordered phase (L_o)



Model of BODIPY signal change from the membrane



Diffusion of membrane-inserted sensor



BODIPY-PM	601	L_d	Lipid14	2 – 5 ns	12,56 ± 2,03
				6 – 12 ns	7,43 ± 1,41
		L_o	Lipid21	6 – 12 ns	3,97 ± 0,31
				6 – 12 ns	3,08 ± 0,03
1 (BODIPY-C_{10})	424	L_d	Lipid14	2 – 5 ns	10,22
2	512			2 – 5 ns	7,52
3	629			2 – 5 ns	7,06

–
10,52
8,75
7,25

Outlook

- Sensor successfully sets in the membrane
- Planar **drift** itself is too slow to affect the fluorescence-lifetime measurements

- QM modeling and analysis of the changes in viscosity-sensing signal by membrane **fluctuations** is **still** in progress

References

1. K. Maleckaitė *et al.*, *Molecules* **27**, 23 (2022).
2. A. Polita *et al.*, *RSC Advances* **13**, 19257 (2023).
3. D. Narkevičius, *master thesis*, Vilnius University (2024).

Acknowledgments

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