Theoretical modeling of two-photon fluorescent membrane probes (early results)

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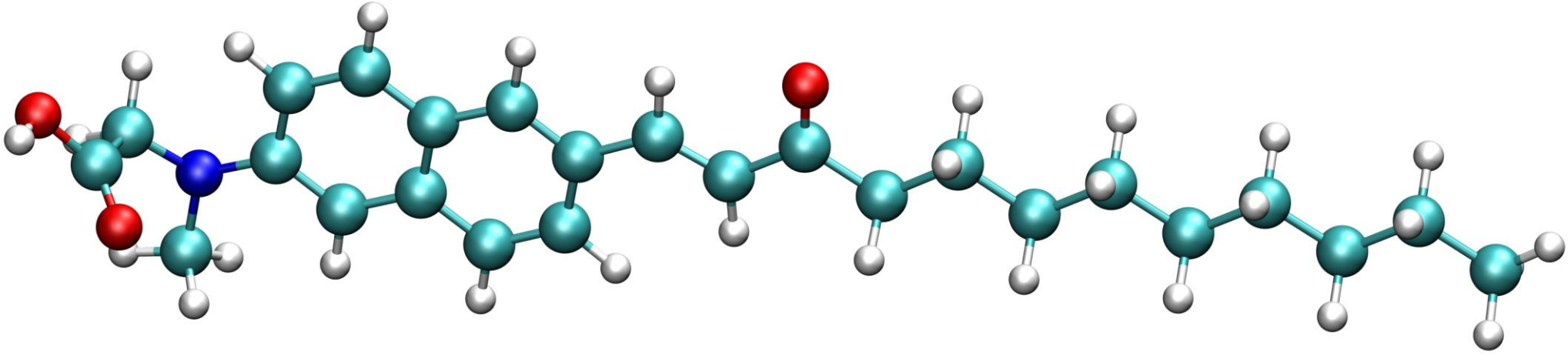
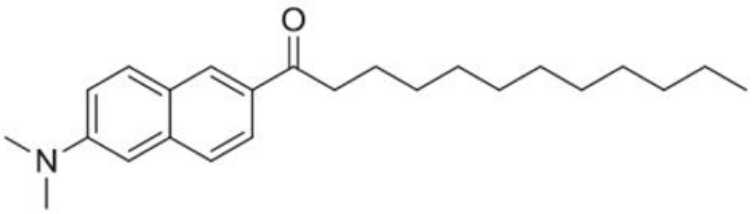
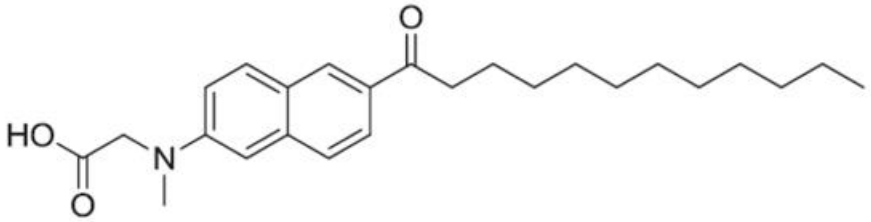


Quantum-chemical calculations

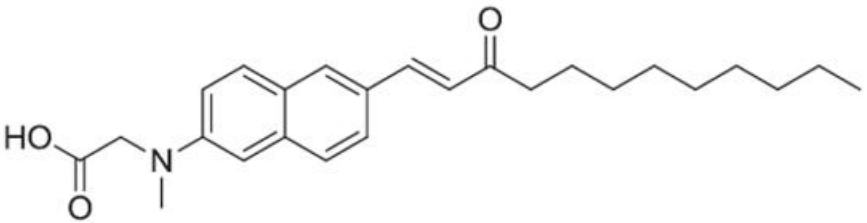
Investigated systems



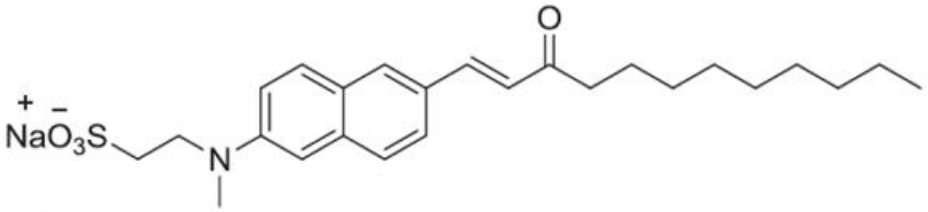
LAURDAN



CL



CL2



SL2

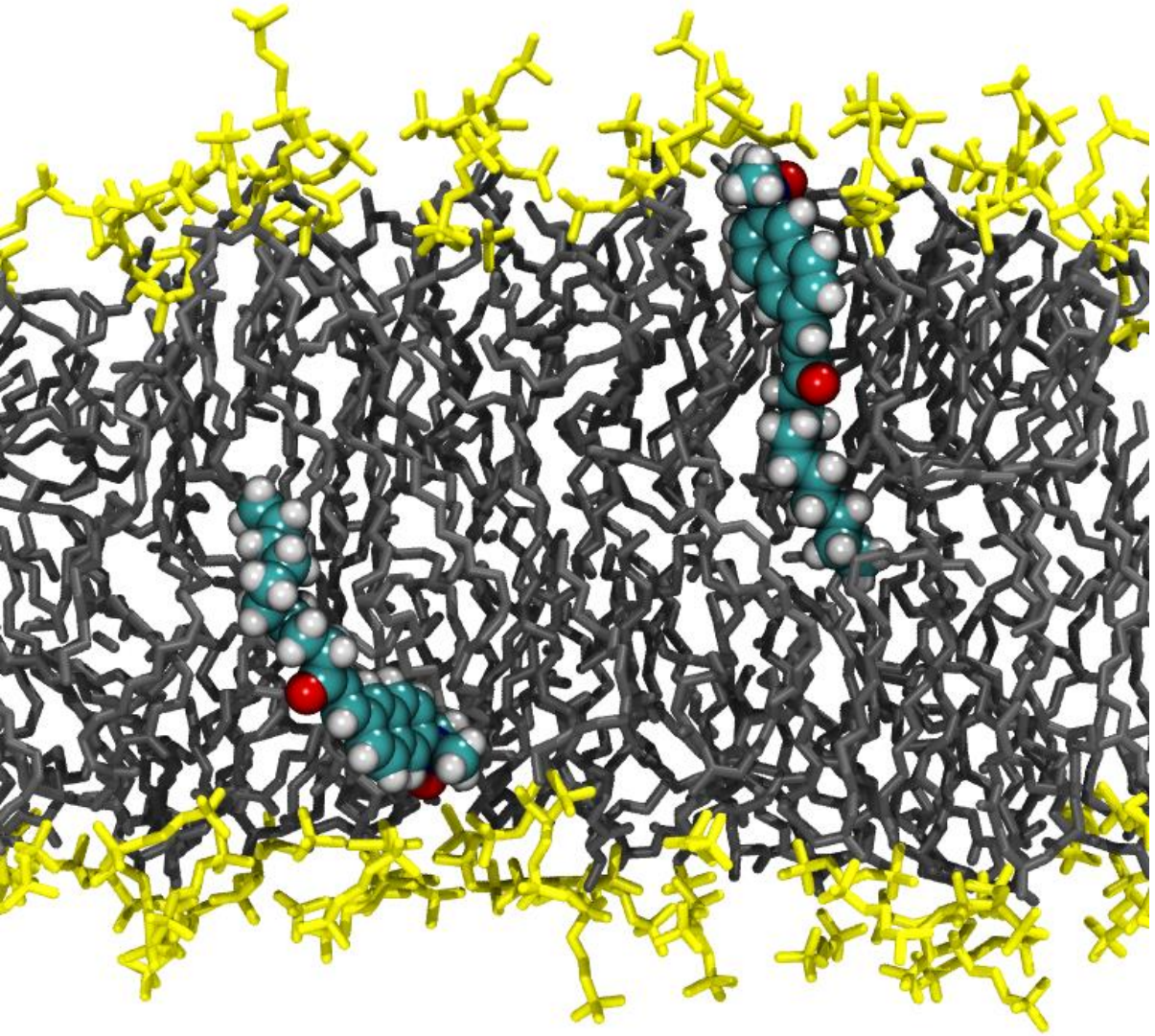
geometry optimization in vacuum and in PCM (water, ethanol, dimethylformamide, hexane)

one-photon absorption and emission spectra

two-photon excitation spectra

Gaussian 16 A03 and Dalton 2015.1 programs

Molecular dynamics simulations



tens of thousands of atoms in the investigated systems

up to 1 μs length of trajectory

GROMACS 5 package

information about probe's orientation and specific location in the cellular environment as well as its interactions with biological membranes