

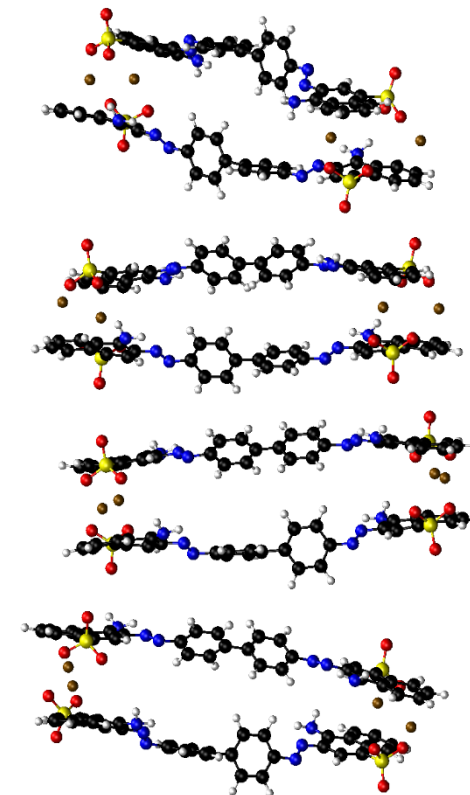
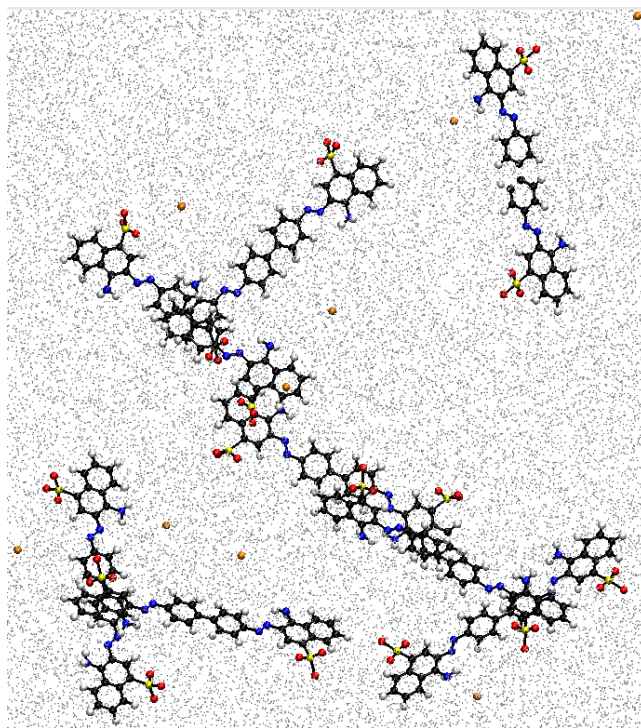
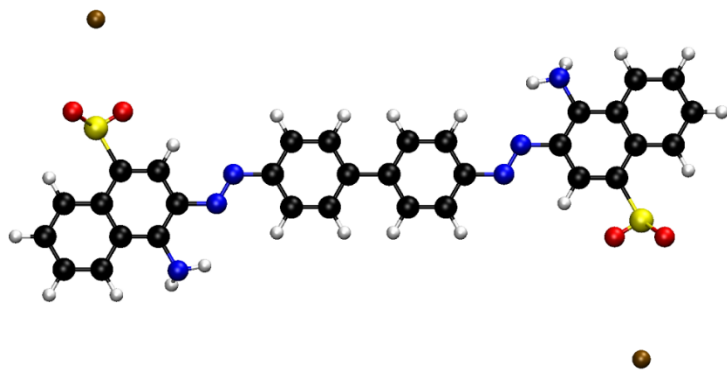
**The structural properties of
supramolecular ionic systems with
regard to understanding its interaction
with amyloids:
a molecular dynamics study**

OSKAR KLIMAS, MATEUSZ Z. BRELA, GRZEGORZ ZEMANEK, LESZEK KONIECZNY





The main area of interest – Congo Red and its properties





Literature

- ▶ A. Jagusiak, J. Rybarska, B. Piekarska, B. Stopa, L. Konieczny: Supramolecular Congo Red as Specific Ligand of Antibodies Engaged in Immune Complex. In: Roterman I., Konieczny L. (eds) Self-Assembled Molecules – New Kind of Protein Ligands. Springer, Cham. 2018.
- ▶ B. Stopa, L. Konieczny, B. Piekarska, et al. *Biochimie*, 79, 23-26, 1997.
- ▶ S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J Comp Phys*, 117, 1-19, 1995.
- ▶ M. J. Robertson, J. Tirado-Rives, W. L. Jorgensen, Improved α Peptide and Protein Torsional Energetics with the OPLS-AA Force Field. *J. Chem. Theory Comput.* 11 (7), 3499-3509, 2015.
- ▶ L. Martínez, R. Andrade, E. G. Birgin, J. M. Martínez. Packmol: A package for building initial configurations for molecular dynamics simulations. *Journal of Computational Chemistry*, 30(13):2157-2164, 2009.
- ▶ A. Kohlmeyer, TopoTools: Release 1.7, (2016), doi.org/10.5281/zenodo.50249.
- ▶ scheme.; *Mol. Phys.*, 1997, 92 (3), 477-487.
- ▶ Lippert, G; Hutter, J; Parrinello, M.; A hybrid Gaussian and plane wave density functional scheme.; *Mol. Phys.*, 1997, 92 (3), 477-487.

