Contribution ID : **95** Type : **Poster Presentation**

# Molecular Dynamics Investigation of the Self-Assembly of Two-Antennary Oligoglycine in Aqueous Solution

Two-antennary oligoglycines represent a novel class of biocompatible amphiphilic compounds, rationally designed through preliminary molecular modelling [1]. These molecules consist of a central hydrophobic alkyl core bound to two hydrophilic oligoglycine chains, forming a symmetric bola-amphiphilic structure. In aqueous media, they spontaneously assemble into stable supramolecular structures called tectomers [2]. The size and shape of these assemblies can be tuned by adjusting conditions such as pH, temperature, ionic strength, and oligoglycines concentration [2,3]. Due to their unique structure and tunable properties, two-antennary oligoglycines bear great potential for applications in various fields such as nanotechnology, pharmaceutics, and medicine. Despite the growing experimental interest, their molecular-level self-assembly behaviour remains poorly understood from a theoretical point of view. In this work, we present an atomistic molecular dynamics study of the conduct of diantennary oligoglycine in bulk aqueous media solution. The self-assembly process of the amphiphilic molecule is thoroughly investigated, with detailed characterisation of the resulting supramolecular entities in terms of size and morphology. Key features such as self-assembly kinetics and secondary structure formation are analysed. The simulations reveal that within 500 ns the oligoglycine molecules form spherical aggregates. The tectomers are stabilised predominantly by intermolecular hydrogen bonds between the oligoglycine segments, accompanied by a reduction in intramolecular hydrogen bonding. Additionally, the zeta potential of the formed tectomers is calculated and is found to be in good agreement with available experimental data. These findings contribute to deeper understanding of the bulk self-assembly of two-antennary oligoglycines and offer new perspectives for their potential applications.

[1] N. Bovin et al., Nanotechnol. Russ., 2008, 3, 291–302. [2] D. Arabadzhieva et al., ChemSusChem, 2019, 12, 672–683. [3] D. Arabadzhieva et al., Colloids Surf., 2021, 630, 127591.

Acknowledgements: The present investigation is funded by the European Union-NextGenerationEU, project BG-RRP-2.012-0005-C01.

**Primary author(s) :** ENCHEVA, Eduarda (Institute of Physical Chemistry, Bulgarian Academy of Sciences)

**Co-author(s) :** ILIEV, Stoyan (Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski"); IVANOVA, Anela (Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski"); MILEVA, Elena (Institute of Physical Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Str.); TCHOUKOV, Plamen (Institute of Physical Chemistry, Bulgarian Academy of Sciences)

**Presenter(s) :** ENCHEVA, Eduarda (Institute of Physical Chemistry, Bulgarian Academy of Sciences)