Self-organized supramolecular structures of oppositely charged block copolymers and bile salts

The purpose of this research project is to provide fundamental understanding of the intermolecular interactions and co-assembly in aqueous mixtures of cationic block copolymers and oppositely charged bile salts (BSs) surfactants. BSs are biosurfactants that have an unconventional steroidal amphiphilic structure showing a different self-behavior with respect to common head-tail surfactants. They are some of the most important surfactants in many living organisms where they work as dispersing agents of dietary lipids to regulate their uptake in the small intestine. The interaction between some BSs and cationic block copolymers leads to the formation of self-organized supramolecular structures [1–3]. We study the structural hierarchy of these complexes, which are based on bundles of BS nanowires mediated by the block copolymer, and the factors that determine their structure, morphology and chirality. We have found that it is possible to tune the growth of these supramolecular structures by varying different parameters, e.g., the relative block lengths, BS/copolymer charge ratio or the chemical composition of the block copolymer. The possibility to tune properties of these complexes will provide a unique opportunity for developing new polymeric BS sequestrants (binding agents) that are used in the treatment of hypercholesterolemia and BS related diseases or as carriers of different active molecules. We employ state-of-the-art techniques, such as cryo-transmission electron microscopy and cryo-electron tomography, small angle X-ray scattering, dynamic and static light scattering, high-sensitivity differential scanning and isothermal titration calorimetry, NMR and measurements of the electrophoretic mobility.

[1] Schillén, K.; Galantini, L.; Du, G.; Del Giudice, A.; Alfredsson, V.; Carnerup, A. M.; Pavel, N. V.; Masci, G.; Nyström, B., Block Copolymers as Sequestrants: Intriguing Structures Formed in a Mixture of an Oppositely Charged Amphiphilic Block Copolymer and Bile Salt. Phys. Chem. Chem. Phys. 2019, 21, 12518–12529.
[2] Du, G.; Del Giudice, A.; Alfredsson, V.; Carnerup, A. M.; Pavel, N. V.; Loh, W.; Masci, G.; Nyström, B.; Galantini, L.; Schillén, K., Effect of Temperature on the Association Behavior in Aqueous Mixtures of an Oppositely Charged Amphiphilic Block Copolymer and Bile Salt. Polymer 2020, 206, 122871.
[3] Du, G.; Belić, D.; Del Giudice, A.; Alfredsson, V.; Carnerup, A. M.; Zhu, K.; Nyström, B.; Wang, Y.; Galantini, L.; Schillén, K., Condensed Supramolecular Helices: The Twisted Sisters of DNA. Angew. Chem. Int. Ed. 2022, 61, e202113279.

People: Guanqun Du, Karin Schillén, Luciano Galantini (Sapienza University of Rome, Italy), Viveka Alfredsson, Bo Nyström (University of Oslo, Norway), Yilin Wang (Chinese Academy of Sciences, China), Domagoj Belić (Josip Juraj Strossmayer University of Osijek, Croatia), Watson Loh (University of Campinas (UNICAMP), Brazil), Lennart Piculell.

Contact person: Karin Schillén