

**Agnieszka Szumna** is an associate professor at the Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland. She received her M.Sc. degree from Warsaw University (crystallography, 1996) and completed her Ph.D. in supramolecular chemistry (2001) working on neutral anion receptors under the supervision of prof. J. Jurczak. She was a postdoctoral fellow with Prof. Jerry L. Atwood at University of Missouri, Columbia, USA (2001-2003). In 2004 she was appointed an assistant professor at the Institute of Organic Chemistry Polish Academy of Sciences and in 2010 she completed her habilitation (awarded as an outstanding habilitation by the Prime Minister and the III Department of Polish Academy of Sciences). Since 2012 she has worked as an associate professor at the Institute of Organic Chemistry. Szumna's research program is focused on various aspects of molecular recognition with a special emphasis on chiral recognition and separation, inherent chirality, dynamic covalent chemistry, encapsulation, reactivity and dynamics in confined spaces and mechanochemistry. She has reported in *Angewandte Chemie* on a chiral self-sorting of peptide-based capsules and in *Chemistry - A European Journal* on an unexpected process of mechanochemical molecular encapsulation.

**The scientific achievement** that received attention refers to the synthesis and studies of peptidic porous structures. The use of peptides for construction of porous structures offers numerous benefits including functionality, chirality, biocompatibility, availability and synthetic tuneability. However, such systems are very rare mainly due to conformational lability of peptide strands that implies low predictability and high tendency to collapse of the resulting porous structure. Szumna and her group have presented an ordering and rigidifying strategy that utilizes macrocyclic scaffolds for pre-positioning of peptides. The resulting semi-open cavitands further self-assemble through hydrogen bonds mimicking natural eight-stranded  $\beta$ -barrels to give stable molecular capsules. The capsules with cavity sizes up to 2280 Å<sup>3</sup> are formed in a dynamic way and present a high degree of sequence-dependent self-sorting. The groups of Szumna has also demonstrated the advantages of using mechanochemical methods over classical solution methods to enforce encapsulation in kinetically resistant capsules. In the further perspective, the combination of inherent features in peptidic molecular capsules opens various possibilities for applications, e. g. in chiral recognition, separation, delivery and catalysis or in construction of catalytic supramolecular frameworks.

Selected references:

- 1) "Mechanochemical Encapsulation of Fullerenes in Peptidic Containers Prepared by Dynamic Chiral Self-Sorting and Self-Assembly"  
M. Szymański, M. Wierzbicki, M. Gilski, H. Jędrzejewska, M. Sztylko, P. Cmoch, A. Shkurenko, M. Jaskólski, A. Szumna, *Chem. Eur. J.*, 2016, **22**, 3148–3155.

- 2) "Dynamic Formation of Hybrid Peptidic Capsules by Chiral Self-sorting and Self-assembly"  
H. Jędrzejewska, M. Wierzbicki, P. Cmoch, K. Rissanen, A. Szumna, *Angew. Chem. Int. Ed.*, 2014, **53**, 13760-13764.
- 3) "On the mechanism of mechanochemical molecular encapsulation in peptidic capsules"  
M. P. Szymański, H. Jędrzejewska, M. Wierzbicki, A. Szumna, *Phys. Chem. Chem. Phys.*, 2017, **19**, 15676-15680.
- 4) "A chiral member of the family of organic hexameric cages"  
M. Wierzbicki, A. A. Głowacka, M. P. Szymański, A. Szumna, *Chem. Commun.*, 2017, **53**, 5200-5203
- 5) "The templation effect as a driving force for the self-assembly of hydrogen-bonded peptidic capsules in competitive media"  
M. Grajda, M. J. Lewińska, A. Szumna, *Org. Biomol. Chem.*, **2017**, DOI:10.1039/C7OB01925D