

## ESR 6 position

### Project title: Biomimetic peptide-based chiral molecular capsules through dynamical approach

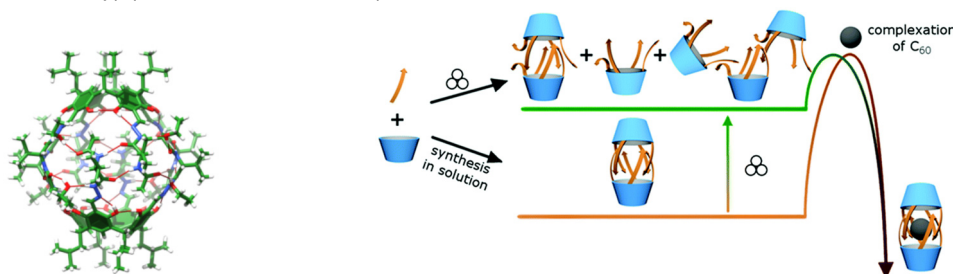
Location: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland

Supervisor: Prof. Agnieszka Szumna

#### Objectives of the individual project and expected results

ESR is expected to obtain a series of biomimetic peptidocalixarenes, having various polarity (ranging from hydrophobic to water-soluble), capable of self-assembling and encapsulation of chiral guest molecules. Various synthetic strategies will be tested including solution synthesis and mechanochemical approaches. She/he will characterize thermodynamic parameters of formation of dynamic assemblies and encapsulation and evaluate chiral self-sorting abilities. She/he will also check the possibilities of photoswitching of photoactive azine linkers and tests formation of new molecular containers by metal-coordination (experience in these areas will be gained through participation in ETN educational activities). The most promising containers will be characterized for catalysts' and drugs' complexation in the solution and by solid state mechanochemical methods.

The objectives of the training will be: 1) Acquisition of expertise in organic synthesis and characterization of peptide-based self-assembled dynamical structures by classical and mechanochemical methods, 2) Evaluate and study encapsulation processes of chiral biologically relevant molecules, with particular emphasis on chiral recognition by different techniques (i.e. NMR, CD, UV-Vis) 3) Gain experience in synthesis of new macrocyclic scaffolds – calix[4]pyrroles and test the possibilities to obtain hybrid capsules (*Academic secondment*), 4) Learn various design strategies by means of computational chemistry methods (*Industrial Secondment*), 5) Learn the “applicational way of thinking” by interactions with the industrial sector in non-classical approaches to product formulations (mechanochemistry) (*Industrial Secondment*).



#### References of the research group related to the subject:

1. M. Grajda, M. J. Lewińska and A. Szumna, *Org. Biomol. Chem.*, 2017, 15, 8513-8517.
2. M. P. Szymański, H. Jędrzejewska, M. Wierzbicki, A. Szumna, *Phys. Chem. Chem. Phys.*, 2017, 19, 15676-15680.
3. M. Wierzbicki, A. A. Głowacka, M. P. Szymański, A. Szumna, *Chem. Commun.*, 2017, 53, 5200-5203.
4. M. Szymański, M. Wierzbicki, M. Gilski, H. Jędrzejewska, M. Sztlyko, P. Cmoch, A. Shkurenko, M. Jaskólski, A. Szumna, *Chem. Eur. J.*, 2016, 22, 3148–3155.
5. H. Jędrzejewska, M. Wierzbicki, P. Cmoch, K. Rissanen, A. Szumna, *Angew. Chem. Int. Ed.*, 2014, 53, 13760-13764.

#### Planned secondments

**Academic Secondment:** Four month secondment is planned at **ICIQ, Tarragona, Spain** devoted to synthesis of hybrid macrocyclic scaffolds and capsules consisting of calixarenes and calix[4]pyrroles, training in ITC technique for binding constants determination.



**Industrial Secondment:** Six-month secondment is planned at **Mind the Byte, Spain** in order to apply different computational chemistry methods to evaluate binding potential of his/her chiral capsules and look for real applications and possible exploitation.

### Hosting Institution

Institute of Organic Chemistry is an independent, non-profit governmental research institute operated by Polish Academy of Sciences. In an official classification, it is ranked no. 1 in organic chemistry in Poland (no. 2 in general chemistry in Poland). It possesses state of the art equipment, the oldest PhD-study system in the country and employs several internationally recognized group leaders (16 research groups). For educational purposes ICHO PAS offers a set of 9 courses for PhD students (modern organic chemistry and spectroscopy), a course on scientific presentation and grant writing, and weekly seminars with distinguished invited speakers. Szumna is a group leader since 2012. She coordinates research activities funded by national funding agencies and teaches upper-level graduate courses outside the parent organization. She has experience in hosting international students (ERASMUS). (<http://ww2.icho.edu.pl/z09/index.php>).

### Eligibility requirements

**EU eligibility criteria for candidates:** Candidates of any nationality but in order to be eligible for the positions the following criteria applies to all applicants:

- The applicant shall at the time of recruitment be in the **first four years of his/her research career** and have **not been awarded a doctoral degree**.
- The applicant must not have resided or carried out his/her main activity in the Poland **for more than 12 months in the 3 years immediately prior to the recruitment**.

**Candidates profile:** candidates must hold a **Master's degree in Chemistry** with excellent academic transcripts. We are looking for **highly motivated** students with **good communication skills**

All candidates must **prove full proficiency in spoken and written English** (B2 certificate, TOEFL).

*Questions regarding the recruitment can be sent to: [noah@noah-itn.eu](mailto:noah@noah-itn.eu)*

*Questions regarding the project can be sent to: [agnieszka.szumna@icho.edu.pl](mailto:agnieszka.szumna@icho.edu.pl)*

