

Prof. Agnieszka Szumna (nee Pęczak)
Curriculum Vitae

Full name Agnieszka Szumna
ORCID 0000-0003-3869-1321
Nationality Polish
Present position Professor
Professional research field Structural, Synthetic and Supramolecular Organic Chemistry
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Education and employment history

2019 Full professor title awarded by the President of the Republic of Poland
2012 Started new research group "Molecular recognition" at the Institute of Organic Chemistry, PAS
2010-2011 Maternity leave
2010 Habilitation, April 16, Institute of Organic Chemistry, PAS
2005-2006 Maternity leave
2004 Start of independent research as a habilitation candidate (position: adiunct)
2001-2003 Post-doctoral stay, University of Missouri, Columbia, USA (Jerry L. Atwood)
1996 – 2001 Ph.D., with distinction, Institute of Organic Chemistry, PAS (supervisor prof. J. Jurczak)
1996 M.Sc., with distinction, Warsaw University, Chemistry Department (supervisor prof. J. Jurczak)
1992 – 1996 Warsaw University, Chemistry Department

Main experience abroad

Postdoc at the Chemistry Department, University of Missouri, Columbia, USA, Jerry L. Atwood (2001- 2003),
supramolecular chemistry

Professional activities

1. Published papers 52 (2020)
 2. Indeks Hirsha 19 (2020)
 3. Number of citations (Scopus, without self-citations) 1050 (2020)
 4. Reviews of papers 30/year
(*Nature Chemistry, Chemical Science, Chemical Society Reviews, Angewandte Chemie, Chemical Communications, Journal of the American Chemical Society, European Journal of Organic Chemistry, Chemistry- a European Journal, Organic & Biomolecular Chemistry.*)
 5. Member of grant evaluation panels in Polish National Science Center, reviews international grants and PhDs.
 6. Head of the Scientific Council (Exact and Technical Sciences) of The Nicolaus Copernicus University in Toruń
 7. Scientific Council member of the Polish Society of Autoimmunological
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Awards:

- 1996 MSc with distinctions
- 2001 PhD with distinctions
- 2011 Prime Minister award for outstanding habilitation
- 2011 Scientific Award of the III Department of Polish Academy of Sciences (Nagroda Naukowa III Wydziału PAN im. Włodzimierza Kołosa)
- 2017 Marie Skłodowska-Curie - Wilhelm Klemm-Vorlesung Lectureship by GDCh/PTChem

Research interest

- molecular recognition
- self-assembly and self-sorting in dynamic systems
- non-covalent and covalent control of aggregation of peptidic structures
- new types of chirality
- chiral recognition and separation
- dynamics and reactivity in confined spaces
- application of macromolecular crystallographic methods for X-ray structural studies of large supramolecular assemblies

External Funding – total number of former and current grants

1. Marie Curie ITN grant within HORIZON 2020 – 1 (PI in the consortium)
2. The Polish National Agency For Academic Exchange (NAWA) – 1 (PI)
3. Polish National Science Centre (NCN) general/advanced grants (OPUS) – 4 (PI)
4. Polish National Science Centre interdisciplinary grants (SYMFONIA) – 1 (consortium leader)
5. Foundation for Polish Science , grant after maternity leave (BRIDGE) – 1 (PI)
6. Polish National Science Centre individual grants for PhDs (PRELUDIUM) – 3 (PhD supervisor)
7. Ministry of Science and Higher Education, grant for talented students (DIAMOND) – 1 (PhD supervisor)

Supervising

- 3 PhD theses defended
- 10 MSc theses defended (4 of them with distinctions)
- 10 BSc theses defended
- currently supervising 8 PhD students, 2 MSc students and many undergraduate students and scholars of the Polish Children's Fund (Krajowy Fundusz na Rzecz Dzieci)

List of publications (2020)

1. "Porous Molecular Capsules as Non-Polymeric Transducers of Mechanical Forces to Mechanophores"
H. Jędrzejewska, E. Wielgus, S. Kaźmierski, H. Rogala, M. Wierzbicki, A. Wróblewska, T. Pawlak, M. J. Potrzebowski, A. Szumna, *Chem. Eur. J.*, **2020**, *26*, 1558-1566.
2. "Complexation of chiral amines by resorcin[4]arene sulfonic acids in polar media – circular dichroism and diffusion studies of chirality transfer and solvent dependence"
B. Setner, A. Szumna, *Beilstein J. Org. Chem.*, **2019**, *15*, 1913-1924.
3. "Peptide-based capsules with chirality-controlled functionalized interiors – rational design and amplification from dynamic combinatorial libraries"
H. Jędrzejewska, A. Szumna, *Chem. Sci.*, **2019**, *10*, 4412-4421.
4. "Chiral chromane[4]arenes synthesised by cycloaddition reactions of o-quinomethine resorcin[4]arenes"
K. Stefańska, A. Szafranec, M. P. Szymański, M. Wierzbicki, A. Szumna, W. Iwanek, *New J. Chem.*, **2019**, *43*, 2687-2693.
5. "Self-assembly and ordering of peptide-based cavitands in water and DMSO – the power of hydrophobic effects combined with neutral hydrogen bonds"
K. Eichstaedt, K. Szpotkowski, M. Grajda, M. Gilski, S. Wosicki, M. Jaskólski, A. Szumna, *Chem. Eur. J.*, **2019**, *25*, 3091-3097.
6. "Interlaced capsules by self-assembly of cavitands substituted with tripeptides and tetrapeptides"
M. P. Szymański, J. S. Czajka, P. Cmoch, W. Iwanek, A. Szumna, *Supramol. Chem.*, **2018**, *30*, 430-437.
7. "Pillar[4]pyridinium: a square-shaped molecular box"
S. Kosiorek, B. Rosa, T. Boinski, H. Butkiewicz, M. P. Szymański, O. Danylyuk, A. Szumna, V. Sashuk, *Chem. Commun.*, **2017**, *53*, 13320-13323.
8. "The templation effect as a driving force for the self-assembly of hydrogen-bonded peptidic capsules in competitive media"
M. Grajda, M. J. Lewińska and A. Szumna, *Org. Biomol. Chem.*, **2017**, *15*, 8513-8517.

9. "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.
10. "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.
11. "Hybrid[4]arenes with anthracene units and tuneable cavities"
T. Boinski, A. Szumna, *New J. Chem.*, **2017**, *41*, 3387-3391.
12. "Making a Right or Left Choice: Chiral Self-Sorting as a Tool for the Formation of Discrete Complex Structures"
H. Jędrzejewska, A. Szumna, *Chem. Rev.*, **2017**, *117*, 4863–4899.
13. "Calixarenes with naphthalene units: calix[4]naphthalenes and hybrid[4]arenes"
T. Boinski, A. Cieszkowski, B. Rosa, B. Leśniewska, A. Szumna, *New J. Chem.*, **2016**, *40*, 8892-8896.
14. "Chiral Calixarenes and Resorcinarenes"
M. Wierzbicki, H. Jędrzejewska, A. Szumna in *Calixarenes and Beyond*, ed. P. Neri, J. L. Sessler, M.-X. Wang, Springer Int. Publ., Switzerland, **2016**, *2*, 13-42
15. "The inverse demand oxa-Diels-Alder reaction of resorcinarenes: experimental and theoretical analysis of regioselectivity and diastereoselectivity"
K. Stefańska, H. Jędrzejewska, M. Wierzbicki, A. Szumna, W. Iwanek, *J. Org. Chem.*, **2016**, *81*, 6018–6025.
16. "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.
17. "Inherently chiral heterocyclic resorcinarenes using a Diels–Alder reaction"
W. Iwanek, K. Stefańska, A. Szumna, M. Wierzbicki, *RSC Adv.*, **2016**, *6*, 13027-13031.
18. "Synthesis of resorcinarene phosphonium salts and the effect of counteranion on their structure"
W. Iwanek, K. Stefańska, A. Szumna, M. Wierzbicki, *Tetrahedron*, **2016**, *72*, 142-147.
19. "Switching of inherent chirality driven by self-assembly"
H. Jędrzejewska, M. Kwit., A. Szumna, *Chem. Commun.*, **2015**, *51*, 13799-13801.
20. "New triazole appended tert-butyl calix[4]arene conjugates: synthesis, Hg²⁺ binding studies"
R. Rusu, A. Szumna, N. Rosu, C. Dumea, R. Danac, *Tetrahedron* **2015**, *71*, 2922–2926.
21. "Solvent-free synthesis and structure of 2-naphthol derivatives of resorcinarenes"
W. Iwanek, K. Stefańska, A. Szumna, M. Wierzbicki, *Tetrahedron* **2015**, *71*, 2222-2225.
22. "Hybrid [n]Arenes through Thermodynamically Driven Macrocyclization Reactions"
T. Boinski, A. Cieszkowski, B. Rosa, A. Szumna, *J. Org. Chem.* **2015**, *80*, 3488-3495.
23. "Concomitant polymorphs of p-iso-propylcalix[4]arene"
V. J. Smith, C. G. Marais, K. Suwińska, J. Lipkowski, A. Szumna, C. Esterhuysena, L. J. Barbour, *CrystEngComm*, **2015**, *17*, 5129-5133.
24. "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.
25. "Experiences with applications of macromolecular tools in supramolecular crystallography"
M. Wierzbicki, M. Gilski, K. Rissanen, M. Jaskólski, A. Szumna*, *CrystEngComm*. **2014**, *16*, 3773-3780.
26. "Chiral Calixarenes"
M. Wierzbicki, H. Jędrzejewska, A. Szumna in *Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, Waltham, MA, **2014**
27. "Inherently Chiral Iminoresorcinarenes through Regioselective Unidirectional Tautomerization"
M. Grajda, M. Wierzbicki, P. Cmoch, A. Szumna*, *J. Org. Chem.* **2013**, *78*, 11597–11601.
28. "Assembly-driven synthesis of hybrid molecular capsules controlled by chiral sorting"
M. Wierzbicki, A. Szumna*, *Chem. Commun.* **2013**, *49*, 3860-3862.

29. "A facile, moisture-insensitive method for synthesis of pillar[5]arenes-the solvent templation by halogen bonds"
T. Boinski, A. Szumna*, *Tetrahedron* **2012**, 68, 9419-9422.
30. "Inherently chiral concave molecules—from synthesis to applications"
A. Szumna,* *Chem. Soc. Rev.* **2010**, 39, 4274-4285.
31. "Chiral encapsulation by directional interactions"
A. Szumna,* *Chem. Eur. J.* **2009**, 2009, 15, 12381 – 12388.
32. "Water co-encapsulation in an inverted molecular capsule"
A. Szumna,* *Chem. Commun.* **2009**, 4191-4193.
33. "A self-assembled chiral capsule with polar interior"
B. Kuberski, A. Szumna, * *Chem. Commun.* **2009**, 1959-1961.
34. "A chiral "frozen" hydrogen bonding in C_4 -symmetric inherently chiral resorcin[4]arenes: NMR, X-ray, circular dichroism, and theoretical study"
B. Kuberski, M. Pecul, A. Szumna,* *Eur. J. Org. Chem.* **2008**, 3069-3078.
35. "Cyclochiral conformers of resorcin[4] arenes stabilized by hydrogen bonds"
A. Szumna,* *Org. Biomol. Chem.* **2007**, 5, 1358-1368.
36. "Diastereoselective formation of cyclochiral amino acids' substituted resorcin[4]arenes"
A. Szumna,* M Górski., O. Lukin, *Tetrahedron Lett.* **2005**, 46, 7423-7426.
37. "Structure-driven design and synthesis of chiral dioxocyclam derivatives"
M. Achmatowicz, A. Szumna, T. Zieliński, J. Jurczak, *Tetrahedron* **2005**, 61, 9031-9041.
38. "Structural studies of new chiral nickel (II) complexes of cyclams: the influence of systematically varied number of amide groups"
A. Szumna, M. Achmatowicz, T. Zieliński, J. Jurczak, *Polyhedron* **2005**, 24, 2981-2987.
39. "A charge transfer-type fluorescent molecular sensor that "lights up" in the visible upon hydrogen bond-assisted complexation of anions"
A. Kovalchuk, J. L. Bricks, G. Reck, K. Rurack, B. Schulz, A. Szumna, H. Weisshoff, *Chem. Commun.* **2004**, 1946-1947.
40. "Anion induced conformational switch of a macrocyclic amide receptor"
M. J.Chmielewski, A. Szumna, J. Jurczak, *Tetrahedron Lett.* **2004**, 45, 8699-8703.
41. "A new strategy for the synthesis of pendant benzodiazacoronands and their use as components of chromatographic stationary phases"
P. Piątek, D. T. Gryko, A. Szumna, J. Jurczak, *Tetrahedron* **2004**, 60, 5769-5776.
42. "Anion-sealed single-molecule capsules"
J. L. Atwood, A. Szumna, *Chem. Commun.* **2003**, 940-941.
43. "Hydrogen bonds seal single-molecule capsules"
J. L. Atwood, A. Szumna, *J. Am. Chem. Soc.* **2002**, 124, 10646-10647.
44. "Cation – π interactions in neutral calix[4]resorcinarenes"
J. L. Atwood, A. Szumna, *J. Supramol. Chem.* **2002**, 2, 479-482.
45. "Unusual encapsulation of two anions in the cavity of neutral macrocyclic octalactam - Preliminary communication"
A. Szumna, J. Jurczak, *Helv. Chim. Acta.* **2001**, 84, 3760-3765.
46. "A new macrocyclic poly lactam-type neutral receptor for anions - Structural aspects of anion recognition"
A. Szumna, J. Jurczak, *Eur. J. Org. Chem.* **2001**, 4031-4039.
47. "The synthesis and structure of macrocyclic pyridinophanes - Potential anion receptors"
A. Szumna, D. T. Gryko, J. Jurczak, *Heterocycles* **2002**, 56, 361-368.
48. "Calcium complexes of macrocyclic lactams: their structure and calcium induced conformational changes"
A. Szumna, D. T. Gryko, J. Jurczak, *J. Chem. Soc. Perk.. Trans. 2* **2000**, 1553-1558.
49. "H-1, C-13, N-15 NMR and X-ray diffractometry in structural studies of macrocyclic lactams containing pyridine moiety"

D. T. Gryko, A. Pęczak, W. Koźminski, P. Piątek, J. Jurczak, *Supramol. Chem.*, Sp. Iss. SI **2000**, 12, 229-235.

50. "Competition between pi-pi stacking and hydrogen bonding in (1 : 2) picrates of 1,5-diamino-3-oxapentane, 1,8-diamino-3,6-dioxaoctane and 1,5-diamino-3-azapentane - solid state studies"
A. Szumna, J. Jurczak, Z. Urbanczyk-Lipkowska, *J. Mol. Struct.* **2000**, 526, 165-175.
 51. "Tetracyclohexyloxaquaterene"
R. Pajewski, A. Pęczak, R. Ostaszewski, J. Jurczak, *Acta Cryst. Sect. C.* **1999**, 55, 1862-1864.
 52. "Synthetic and crystallographic studies on pyridinophanes"
D. T. Gryko, P. Piątek, A. Pęczak, M. Pałys, J. Jurczak, *Tetrahedron* **1998**, 54, 7505-7516.
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