Institute of Organic Chemistry
Polish Academy of Sciences

Accelerating Sustainable Chemistry

Synthesis - Catalysts - AI

Warsaw 2021

Institute of Organic Chemistry
Polish Academy of Sciences

Kasprzaka 44/52
01-224 Warsaw
Poland

The history & the future

The Institute of Organic Chemistry of the Polish Academy of Sciences (IOC PAS) was established in 1964, when the Department of Organic Synthesis of the Polish Academy of Sciences was advanced to the rank of a Research Institute. Soon after, the Warsaw facility of the Institute received its present location on Kasprzaka street. Since the end of the sixties the process of disconnecting 'external' laboratories began; these units were transformed into independent institutions: Centre of Molecular and Macromolecular Studies in Łódź (CBMiM PAS) and Institute of Bioorganic Chemistry in Poznań (IChB PAS).

The Institute of Organic Chemistry PAS is an A-class scientific institution in all official rankings. It has the right to confer PhD and DSc (habilitation) degrees in the field of organic chemistry and to conduct applications for the title of professor.

In the international ranking of the quality of scientific institutions *SCImago Institutions Rankings* covering the years 2007–2011, in the most prestigious category of Q1 (taking into account only publications in the highest ranked scientific journals in the world), the Institute of Organic Chemistry was located in second place among all scientific institutions in Poland.

HR EXCELLENCE IN RESEARCH

On July 24, 2017, the Institute of Organic Chemistry received the HR Excellence in Research award from the European Commission, confirming the presence of excellent conditions for employment and conducting scientific research by scientists. The distinction is awarded to scientific institutions with internal staff policies and recruitment procedures that are compatible with activities including the "European Charter for Researchers and a Code of Conduct for the Recruitment of Researchers."

For dozens of years globally innovative synthesis technologies have been developed and elaborated on, such as: methods for the synthesis of simple sugars (Zamojski, 1970s), vicarious nucleophilic substitution of hydrogen (Mąkosza, 1978–2005), the synthesis of aza-crown ethers (Jurczak, 1980–2000), elaboration of new catalysts for olefin metathesis (Grela, 2000–2005), the synthesis of corroles (Gryko, 2000–2006) and the planning of organic syntheses through the software program CHEMATICA (Grzybowski, 2016) etc. These findings have helped cement the institute's place at the forefront of both Polish and European science, where it remains to this day.

Key areas of research activity within the Institute are: methodology of organic synthesis, supramolecular chemistry, chemistry of materials with specific properties, the structure and spectroscopy of organic compounds, and the study of reaction mechanisms. Recently, the development of computer-assisted organic synthesis routes has been undertaken.

Needless to say the focus of research has changed many times over the last 60 years, consistent with the changing visions of the international scientific community. The new directions prevalent in worldwide organic chemistry have been quickly applied within the Institute, which are exemplified by photo-redox catalysis (D. Gryko and M. Giedyk), supramolecular chemistry (J. Jurczak and A. Szumna), organocatalysis (J. Młynarski), functional dyes (D. T. Gryko, M. Grzybowski, M. Lindner), and CH-activation (W. Chaładaj). While the development of synthetic methodologies dominates, other directions play increasingly important roles. Within supramolecular chemistry studies, synthetic receptors for cations and anions are synthesized, including those capable of enantioselective differentiation. Along similar lines, self-assembling capsules are being prepared and studied. Somewhere in between both of these areas is the application of enzymes for organic synthesis (R. Ostaszewski) – one of the newer research trends at the IOC PAS. Within photo-redox catalysis the application of porphyrins as photo-sensitizers and studies on diazo compounds are worth mentioning. Studies of the structure and spectral properties of organic compounds are focused on the development of applications using modern spectroscopic techniques to determine the constitution and stereochemical structure of organic molecules. The same problems, together with predicting the physical and chemical properties and reactivity of organic compounds, are studied theoretically using the most recent methods of computational quantum chemistry. The software program CHEMATICA for planning organic syntheses, developed by Prof. Grzybowski, was recognized by the journal *Chemistry World* as one of the 10 most important discoveries of 2016.

The results of the research work conducted within the Institute are published in approximately 90 to 120 scientific papers per year.

Sciencific Council of The Institute of Organic Chemistry of the Polish Academy of Sciences in 1967.

Besides the basic research programs, the Institute conducts various projects related to applied organic chemistry and technology. These are often aligned with, and involve collaboration with the pharmaceutical industry. These collaborations have produced the kidney stone treatment *Debelizyna* (manufactured by Herbapol Pruszków) as well as two β-lactam antibiotics; generic cephalosporin *Tarcefoksym* and a new original cephalosporin named *Tarcevis* (both in collaboration with Tarchomin Pharmaceutical Company Polfa SA). The institute offers a doctoral research program which can be pursued in combination with industrial partners. Graduates are internationally recognized and have gone on to work at prestigious universities and companies around the world.

The modest size of the Institute has enabled rapid responses to the changing scientific environment within Poland and on the global scale. It has also made it possible to instigate critical reforms such as the beneficial introduction of a fast-track process for young assistant professors in 2000. Another pivotal change was the replacement of departments and laboratories by a system of research and service groups established according to the current program pursued at the Institute (1988). These critical changes, initiated by Prof. M. Mąkosza, have streamlined the use of instrumentation and increased research speed which is a foundation for the Institute's current standing.

The Institute is successful in applying for research grants, both domestic and international. One of the most important and the biggest was the project: "Sugars as renewable raw materials in the synthesis of products with high added value" (2010–2015; 25.5 mln PLN) which was conducted by a consortium of six Institutions: Institute of Organic Chemistry PAS (Leader), Institute of Physical Chemistry PAS, Gdańsk University, Łódź University, Warsaw Polytechnic, and Silesian Polytechnic.

Other notable international projects include:
1) Center of Excellence in Development of New Therapeutics from Sugars (CEDNETS) 2003–2006;
2) ERA-Chemistry (European Research Era in Chemistry 2006–2008);
3) Maria Skłodowska-Curie Innovative Training Networks (REVCAT and NOAH).

Group leaders from within our Institute won three prestigious TEAM grants (funded by Foundation for Polish Science) in the first series (2009–2014) in addition to three in the second series (2015–2017). The Institute's PIs are equally successful in winning grants from the National Science Centre. Indeed, during the last 5 years MAESTRO grants (3), HARMONIA grants (3), SYMFONIA grants (3) and OPUS grants (28) have been realized.

The Institute's employees can boast of numerous awards received from Polish and foreign institutions. Three scientists from our Institute; Professor Mieczysław Mąkosza, Professor Karol Grela, and Professor Daniel Gryko have been awarded with the highest Polish prize for science: The Award of the Foundation for Polish Science (2012, 2014, and 2017 respectively).

Scientists from the Institute have recently obtained other notable awards including:
- Professor Janusz Jurczak: Doctor Honoris Causa of the Poznań University and Warsaw University;
- Professor Marek Chmielewski: Doctor Honoris Causa of the Lublin Polytechnic;
- Professor Mieczysław Mąkosza: Doctor Honoris Causa of the Warsaw University of Technology.

Among the foreign awards, it is worth mentioning the title of Fellow ChemPubSoc Europe awarded in 2018 to Professors K. Grela and D.T. Gryko. It is a distinction awarded to scientists who particularly support the publishing activity of their national chemical associations, as well as contribute to raising the scientific level and recognition of publications in the field of chemistry in Europe.

Prof. Bartosz Grzybowski received the Feynman Award (Foresight Institute, 2016) in the field of nanotechnology for Chematica – a "chemical calculator" allowing the optimization of chemical synthesis. In October 2019, Professor B. Grzybowski represented the Institute at the 25th Solvay Conference on Chemistry regarding the use of computers in chemistry. The Solvay Conferences have been held in every three years in Brussels since 1911 and gather 30–40 invited scientists.

In 2018, the Polish Academy of Sciences honored two of our scientists. The Maria Skłodowska-Curie Scientific Award in chemistry went to Prof. Daniel Gryko and the Włodzimierz Kołos Scientific Award to Dr. Wojciech Chaładaj. Over the past 4 years, the employees have received five Wojciech Świętosławski prizes (the award of the Polish Chemical Society).

Board of Directors: Deputy Director Dr. Piotr Lipkowski, Director Prof. Daniel Gryko and Research Director Prof. Jacek Młynarski

Among the scientific activities of the Institute, the organization of the international and countrywide scientific conferences and seminars has to be noted. The most important of these is the series of symposia entitled "Poland-Korea Joint Organic Chemistry Conference" organized every 4 years and gathering the best specialists from Poland and Republic of Korea. Other conferences organized periodically are "Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences", "Symposium on Asymmetric Synthesis", "The Polish-German Conference on Organic Chemistry" and "Conference of the Polish Mass Spectrometry Society".

The Institute is equipped with state of the art instruments in a number of spectroscopic laboratories. These include NMR, MS, CD, and many others. A unique laboratory for high pressure organic synthesis (up to 10–20 kbar) is also present.

The Institute runs a four-year PhD study program, which has operated continuously since 1966 and was the oldest of its kind in the country. Over this time, the PhD degree in chemical sciences has been granted to more than 400 students.

In 2019 the IOC PAS became a member of the *Warsaw Doctoral School in Natural and Biomedical Sciences* (Warsaw-4-PhD) which is comprised of the nine Warsaw institutions:
- Nencki Institute of Experimental Biology, Polish Academy of Sciences (leader),
- Institute of Organic Chemistry, PAS,
- Institute of Physical Chemistry, PAS,
- Institute of Physics, PAS,
- Center of Theoretical Physics, PAS,
- Institute of High Pressure Physics, PAS,
- Maria Sklodowska-Curie National Research Institute of Oncology
- Institute of Psychiatry and Neurology
- The International Institute of Molecular and Cell Biology in Warsaw (IIMCB).

The Institute is also active in teaching students (summer training, internships in laboratories in IOC) and schoolchildren (workshops for high school students under the auspices of the National Children's Fund).

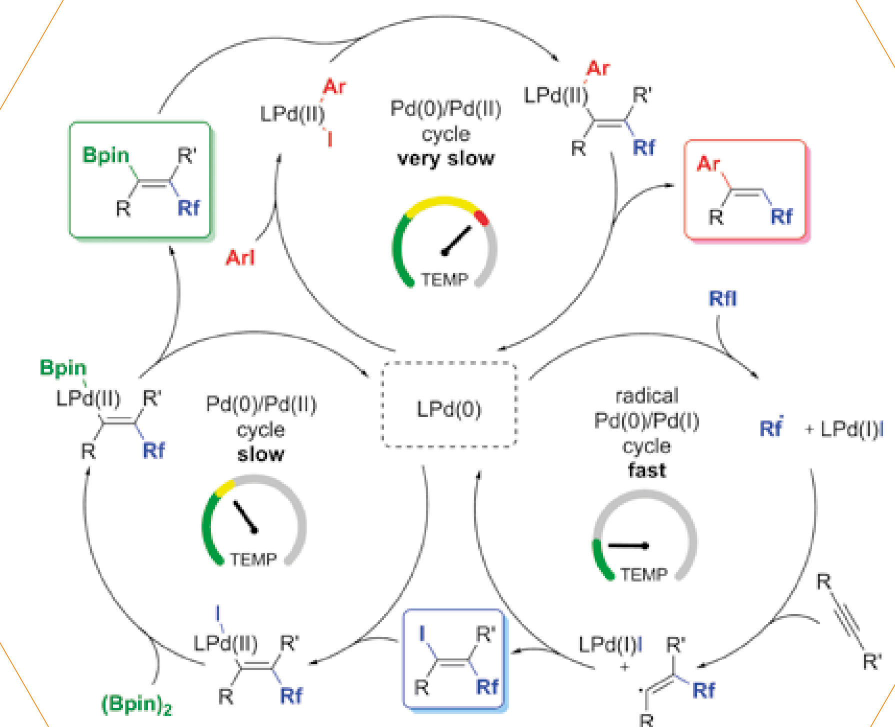
Research Groups

Assoc. Prof. Wojciech Chaładaj

Chaładaj Research Group

Current research:

- discovery of new Pd-catalyzed multicomponent transformations of alkynes enabling efficient direct assembly of simple building blocks into an elaborate target molecule.
- development of methods for fluoroalkylation of organic compounds, especially through tandem or sequential catalysis
- development of tandem reactions involving additions to alkynes and subsequent functionalization via cross-coupling
- investigation of the mechanisms of transition metal-catalyzed reactions



Selected publications:

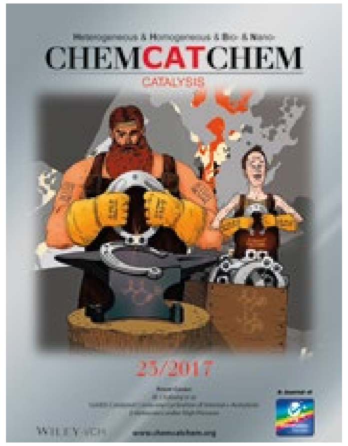
1 › Broadly Applicable Method for Pd-Catalyzed Carboperfluoro-Alkylation of Terminal and Internal Alkynes: A Convenient Route to Tri- and Tetrasubstituted Olefins, S. Domański, W. Chaładaj, *ACS Catal.* **2016**, *6*, 3452–3456

2 › Pd-Catalyzed Boroperfluoroalkylation of Alkynes Opens a Route to One-Pot Reductive Carboperfluoroalkylation of Alkynes with Perfluoroalkyl and Aryl Iodides, S. Domański, B. Gatlik, W. Chaładaj, *Org. Lett.* **2019**, *21*, 5021–5025

3 › Pd-Catalyzed Carbonylative Carboperfluoroalkylation of Alkynes. Through-Space 13C–19F Coupling as a Probe for Configuration Assignment of Fluoroalkyl-Substituted Olefins, S. Domański, O. Staszewska-Krajewska, W. Chaładaj, *J. Org. Chem.* **2017**, *82*, 7998–8007

4 › Tandem Palladium-Catalyzed 6-Exo-Dig Oxocyclization Coupling of δ-Acetylenic β-Ketoesters with Aryl Bromides and Chlorides: Route to Substituted Dihydropyrans, A. Kołodziejczyk, S. Domański, W. Chaładaj, *J. Org. Chem.* **2018**, *83*, 12887–12896

5 › Gold(I)-Catalyzed Conia-Ene Cyclization of Internal ϵ-Acetylenic β-Ketoesters under High Pressure. W. Chaładaj, A. Kołodziejczyk, S. Domański, *ChemCatChem* **2017**, *9*, 4334–4339

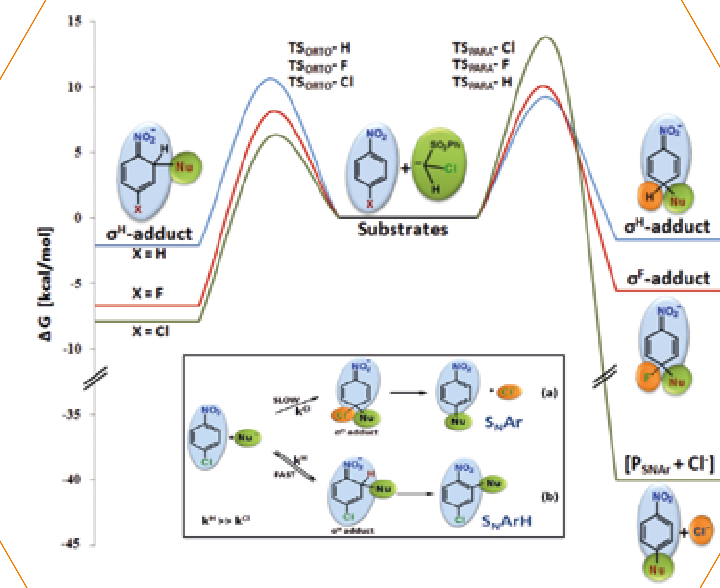


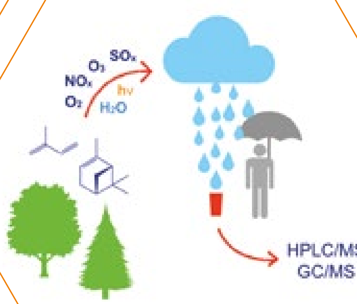
Prof. Witold Danikiewicz

Danikiewicz Research Group

Current research:

- identification and quantification of organic compounds in atmospheric precipitates and secondary organic aerosols. Elucidation of the synthetic pathways leading to these compounds
- studies on the mechanisms of the reactions of organic anions with neutral molecules in the gas phase and in solution using mass spectrometry and computational methods
- applications of ion mobility – mass spectrometry method for studying noncovalent complexes and other ion – molecule interactions





Selected publications:

1 › Radical oxidation of methyl vinyl ketone and methacrolein in aqueous droplets: Characterization of organosulfates and atmospheric implications, P. Wach, G. Spolnik, K.J. Rudzinski, K. Skotak, M. Claeys, W. Danikiewicz, R. Szmigielski, *Chemosphere*, **2019**, *214*, 1–9

2 › Chemical composition of isoprene SOA under acidic and non-acidic conditions: effect of relative humidity, K. Nestorowicz, M. Jaoui, K.J. Rudzinski, G. Spolnik, W. Danikiewicz, R. Szmigielski, *Atmos. Chem. Phys.*, **2018**, *18,* 18101–18121

3 › Improved UHPLC-MS/MS Methods for Analysis of Isoprene-Derived Organosulfates, G. Spolnik, P. Wach, K.J. Rudzinski, K. Skotak, W. Danikiewicz, R, Szmigielski, *Anal. Chem.*, **2018**, *90*, 3416–3423

4 › Gas-Phase Reactions of Dimethyl Disulfide with Aliphatic Carbanions – A Mass Spectrometry and Computational Study, B. Franczuk, W. Danikiewicz, *J. Am. Soc. Mass Spectrom.*, **2018**, *29*, 588–599

5 › How Does Nucleophilic Aromatic Substitution Really Proceed in Nitroarenes? Computational Prediction and Experimental Verification, K. Blaziak, W. Danikiewicz, M. Makosza, *J. Am. Chem. Soc.*, **2016**, *138*, 7276–7281

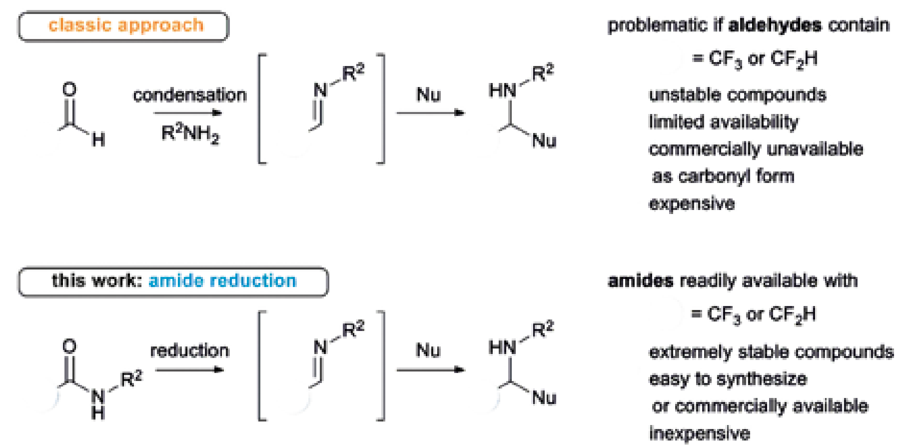
6 › Competition between Nucleophilic Substitution of Halogen (S_NAr) versus Substitution of Hydrogen (S_NArH)-A Mass Spectrometry and Computational Study, K. Blaziak, M. Makosza, W. Danikiewicz, *Chem. Eur. J.*, **2015**, *21*, 6048–6051

Prof. Bartłomiej Furman

Furman Research Group

Current research:

- chemoselective activation of amide carbonyls towards nucleophilic reagents
- kinugasa reaction as a stereoselective method of β-lactams synthesis: advanced applications
- studies on the rearrangement of vinyl ethers and alkoxydienes
- the synthesis, and chemical reactivity of tetroxanes



Selected publications:

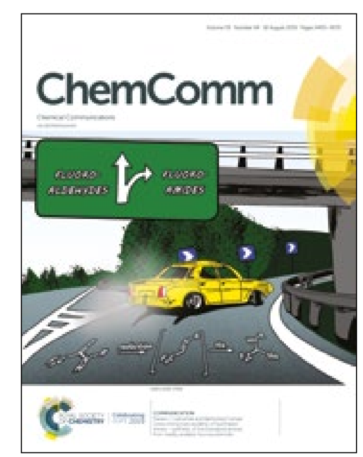
1 Synthesis of polyhydroxylated piperidine and pyrrolidine peptidomimetics via one-pot sequential lactam reduction/Joullié–Ugi reaction, P. Szcześniak, S. Stecko, E. Maziarz, B. Furman, *J. Org. Chem.* **2015**, *80*, 3621–3633

2 Schwartz's reagent-mediated regiospecific synthesis of 2,3-disubstituted indoles from isatins, A. Ulikowski, B. Furman, *Org. Lett.* **2016**, *18*, 149–153

3 Overcoming inaccessibility of fluorinated imines – synthesis of functionalized amines from readily available fluoroacetamides, P.J. Czerwiński, B. Furman, *Chem. Commun.*, **2019**, *55*, 9436–9439

4 Bypassing the stereoselectivity issue: transformations of Kinugasa adducts from chiral alkynes and non-chiral acyclic nitrones, R. Kutaszewicz, B. Grzeszczyk, M. Górecki, O. Staszewska-Krajewska, B. Furman, M. Chmielewski, *Org. Biomol. Chem.*, **2019**, *17*, 6251–6268

5 A new synthesis of highly functionalized cyclohexenes via a vinylogous Ferrier-Petasis cyclization reaction, A. Domżalska, E. Maziarz, B. Furman, *Tetrahedron* **2017**, *73*, 7030–7041



6 Chemoselective activation of amide carbonyls towards nucleophilic reagents P.J. Czerwiński, B. Furman*, *"Overcoming inaccessibility of fluorinated imines – synthesis of functionalized amines from readily available fluoroacetamides" Chem. Commun.*, **2019**, *55*, 9436–9439

Prof. Karol Grela

Grela Research Group

Current research:

- applications of olefin metathesis and other catalytic reactions in organic synthesis
- chemoselective C–C double bond hydrogenation applying formic acid as a hydrogen donor
- selective C–C triple bond semi-hydrogenation

Selected publications:

1. In tandem or alone: a remarkably selective transfer hydrogenation of alkenes catalyzed by ruthenium olefin metathesis catalysts, G.K. Zieliński, C. Samojłowicz, T. Wdowik, K. Grela, *Org. Biomol. Chem.*, **2015**, *13*, 2684–2688

2. Tandem Catalysis Utilizing Olefin Metathesis Reactions, G.K. Zieliński, K. Grela, *Chem. – Eur. J.*, **2016**, *22*, 9440–9454

3. E- and Z-Selective Transfer Semihydrogenation of Alkynes Catalyzed by Standard Ruthenium Olefin Metathesis Catalysts, R. Kusy, K. Grela, *Org. Lett.*, **2016**, *18*, 6196–6199

4. A Selective and Functional Group-Tolerant Ruthenium-Catalyzed Olefin Metathesis/Transfer Hydrogenation Tandem Sequence Using Formic Acid as Hydrogen Source, G.K. Zieliński, J. Majtczak, M. Gutowski, K. Grela, *J. Org. Chem.* **2018**, *83*, 2542–2553

Prof. Dorota Gryko

D. Gryko Research Group

Current research:

- photocatalysis – new catalysts and new reactions
- novel transformations of diazo compounds
- bioinspired Co-catalysis for sustainable processes
- vitamin B_{12} – synthesis and biomedical applications

Selected publications:

1 › Porphyrins as Photoredox Catalysts – Experimental and Theoretical studies, K. Rybicka-Jasińska, W. Shan, K. Zawada, K. Kadish, D. Gryko, *J. Am. Chem. Soc.*, **2016**, *138*, 15451–15458

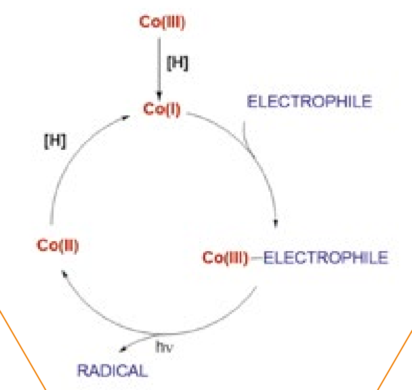
2 › Redox-activated amines in C(sp3)-C(sp) and C(sp3)-C(sp)2 bond formation enabled by metal-free photoredox catalysis, M. Ociepa, J. Turkowska, D. Gryko, *ACS Catalysis,* **2018**, *8*, 11362–11367

3 › Photocatalytic Alkylation of Pyrroles and Indoles with α-Diazo Esters, Ł.W. Ciszewski, J. Durka, D. Gryko, *Org. Lett.*, **2019**, *21*, 7028–7032

4 › Vitamin B_{12} transports modified RNA into E. coli and S. Typhimurium cells, M. Giedyk, A. Jackowska, M. Równicki, M. Kolanowska, J. Trylska, D. Gryko, *Chem. Comm.*, **2019**, *55*, 763–766

5 › A multicolor riboswitch-based platform for imaging of RNA in live mammalian cells, E. Braselmann, A.J. Wierzba, J.T. Polaski, M. Chromiński, Z.E. Holmes, S. Hung, D. Batan, J.R. Wheeler, R. Parker, R. Jimenez, D. Gryko, R.T. Batey, A.E. Palmer, *Nat. Chem. Bio.*, **2018**, *14*, 964–971

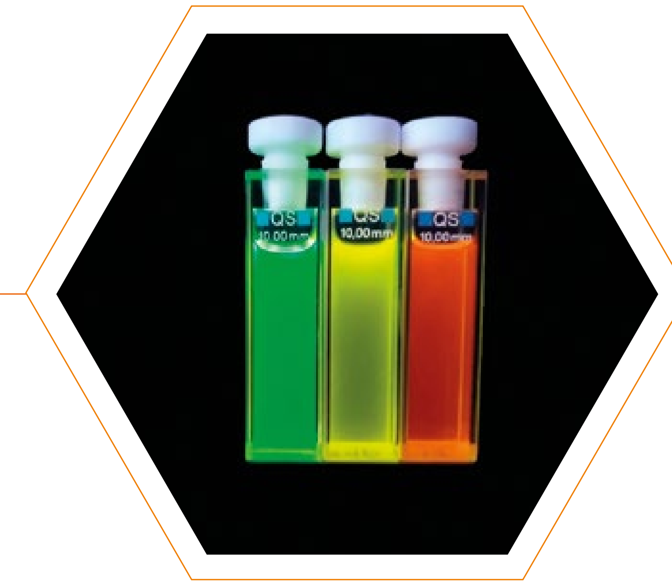
Co-CATALYSIS



6 › Vitamin B_{12} as a carrier of peptide nucleic acid (PNA) into bacterial cells, M. Równicki, M. Wojciechowska, A.J. Wierzba, J. Czarnecki, D. Bartosik, D. Gryko, J. Trylska, *Scientific Reports,* **2017**, *7*, 7644

Prof. Daniel T. Gryko

D.T. Gryko Research Group



Current research:

- new generation of fluorescent probes for stimulated emission depletion microscopy
- quadrupolar, two-photon absorbing dyes
- chemistry of diketopyrrolopyrroles and pyrrolo[3,2-*b*]pyrroles
- solvatochromism of fluorescence and symmetry breaking in the excited state
- curved aromatic architectures

Selected publications:

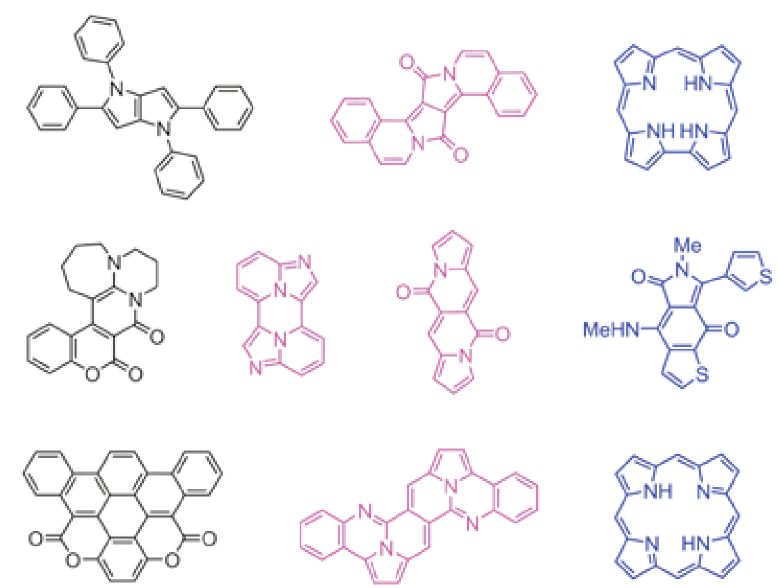
1 › Bright, color-tunable fluorescent dyes based on π-expanded diketopyrrolopyrroles
M. Grzybowski, E. Glodkowska-Mrowka, T. Stoklosa, D.T. Gryko, *Org. Lett.* **2012**, *14*, 2670–2673

2 › Oxidative aromatic coupling versus Scholl reaction, M. Grzybowski, K. Skonieczny, H. Butenschön, D.T. Gryko, *Angew. Chem. Int. Ed.* **2013**, *52*, 9900–9930

3 › The tetraarylpyrrolo[3,2-*b*]pyrroles – from serendipitous discovery to promising heterocyclic optoelectronic materials, M. Krzeszewski, D. Gryko, D.T. Gryko, *Acc. Chem. Res.* **2017**, *50*, 2334–2345

4 › On-surface synthesis of a nitrogen-embedded buckybowl with inverse Stone-Thrower-Wales topology, S. Mishra, M. Krzeszewski, C.A. Pignedoli, P. Ruffieux, R. Fasel, D.T. Gryko, *Nat. Commun.* **2018**, *9*, 1714

5 › Dipole effects on charge transfer are enormous, M. Krzeszewski, E.M. Espinoza, C. Červinka, J.B. Derr, J.A. Clark, D. Borchardt, G.J.O. Beran, D.T. Gryko, V.I. Vullev, *Angew. Chem. Int. Ed.* **2018**, *57*, 12365–12369



Prof. Bartosz Grzybowski

Grzybowski Research Group

Current research:

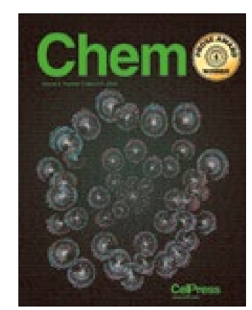
- we developed first-ever experimentally validated algorithms for planning multistep organic syntheses of complex targets, including natural products
- we are the pioneers of using Artificial Intelligence for the discovery of new organic reactions
- we design and validate networks of reactions synchronized in time and space; from reaction sequences to autocatalytic cycles
- we are at the forefront of using computers to predict properties of organic molecules, including pharmaceuticals, agrochemicals, organic-electronic materials, and more.
- we transform organic synthesis from trial-and-error to an algorithmic science!

Selected publications:

1 › Computer-assisted synthetic planning: the end of the beginning, S. Szymkuć, E. P. Gajewska, T. Klucznik, K. Molga, P. Dittwald, M. Startek, M. Bajczyk, B.A. Grzybowski, *Angew. Chem. Int. Ed.* **2016**, *55*, 5904–5937

2 › Prediction of major regio-, site-, and diastereoisomers in Diels-Alder reactions by using machine-learning: the importance of physically meaningful descriptors, W. Beker, E.P. Gajewska, T. Badowski, B.A. Grzybowski, *Angew. Chem. Int. Ed.* **2019**, *58*, 4515–4519

3 › Efficient syntheses of diverse, medicinally relevant targets planned by computer and executed in the laboratory, T. Klucznik, B. Mikulak-Klucznik, M.P. McCormack, H. Lima, S. Szymkuć, M. Bhowmick, K. Molga, Y. Zhou, L. Rickershauser, E.P. Gajewska, et al., *Chem* **2018**, *4*, 522–532

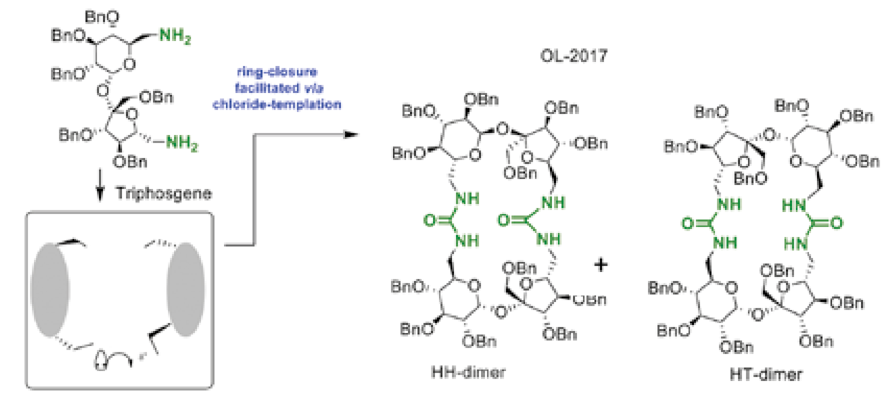


4 › Navigating around patented routes by preserving specific motifs along computer-planned retrosynthetic pathways, K. Molga, P. Dittwald, B.A. Grzybowski, *Chem* **2019**, *5*, 460–473

5 › Automatic mapping of atoms across both simple and complex chemical reactions, W. Jaworski, S. Szymkuć, B. Mikulak-Klucznik, K. Piecuch, T. Klucznik, M. Kaźmierowski, J. Rydzewski, A. Gambin, B.A. Grzybowski, *Nat. Commun.* **2019**, *10*, 1434

Prof. Sławomir Jarosz

Jarosz Research Group



1:1 ratio, 90% yield

Current research:

- stereoselective synthesis of sugar mimetics
- macrocyclic receptors with sucrose scaffold (including sucrose cryptands)
- modification and biological activity of lupane triterpenoids

Selected publications:

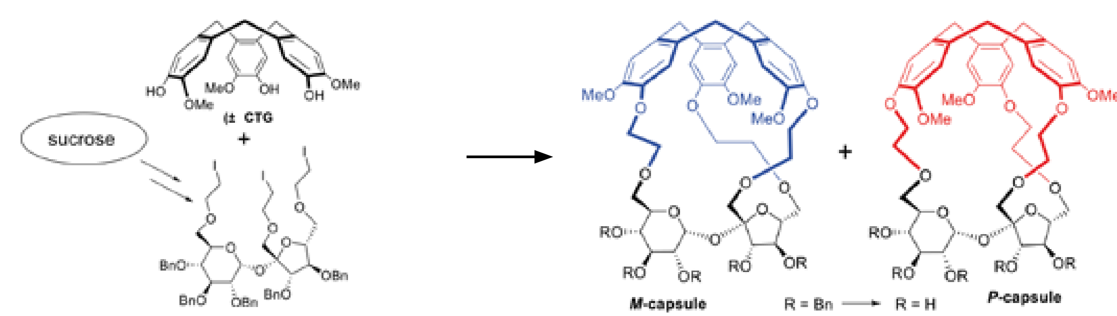
1 › Synthesis of polyhydroxylated quinolizidines and azaspiro-[4.5]decanes from D-xylose, M. Malik, G. Witkowski, M. Ceborska, S. Jarosz, *Org. Lett.*, **2013**, *15*, 6214–6217

2 › Chloride-Templated Macrocyclization and Anion-Binding Properties of C_2-Symmetric Macrocyclic Ureas Derived from Sucrose, K. Łęczycka-Wilk, K. Dąbrowa, P. Cmoch, S. Jarosz, *Org. Lett.*, **2017**, *19*, 4596–4599

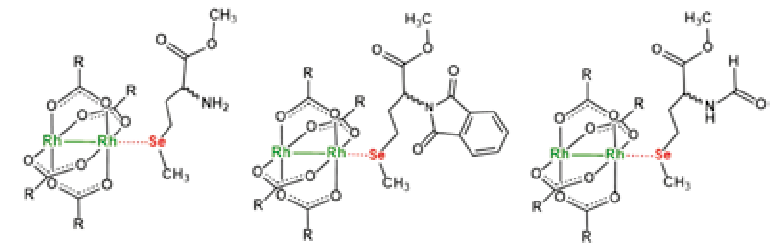
3 › "Choose-a-Size" Control in the Synthesis of Sucrose Based Thiourea Macrocycles, K. Łęczycka-Wilk, F. Ulatowski, P. Cmoch, S. Jarosz, *Org. Biomol. Chem.* **2018**, *16*, 6063–6069

4 › Synthesis of Cyclotriveratrylene-Sucrose-Based Capsules, Ł. Szyszka, P. Cmoch, A. Butkiewicz, M.A. Potopnyk, S. Jarosz, *Org. Lett.*, **2019**, *21*, 6523–6528

5 › Stereoselective Synthesis of Sugar Mimetics from Simple Monosaccharides, S. Jarosz, K. Tiara, M. Potopnyk, *Pure Appl. Chem.*, **2019**, *97*, 1137–1148



Prof. Jarosław Jaźwiński



Jaźwiński Research Group

Current research:

- application of nuclear magnetic resonance spectroscopy (NMR) in the liquid and solid phase to studies of transition metal complexes, hydrogen bonds and tautomeric equilibria
- molecular modelling and calculations of nuclear magnetic resonance (NMR) parameters by theoretical methods

Selected publications:

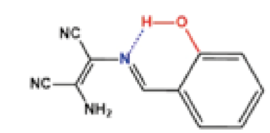
1 › In situ complexation of rhodium(II) tetracarboxylates with some derivatives of cysteine and related ligands studied by ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy, R. Głaszczka, J. Jaźwiński, *J. Coord. Chem.* **2016**, *69*, 3703–3714

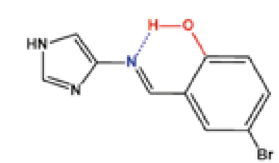
2 › Spectroscopic studies of the intramolecular hydrogen bonding in o-hydroxy Schiff bases, derived from diaminomaleonitrile, and their deprotonation reaction products, Szady-Chełmieniecka, B. Kołodziej, M. Morawiak, B. Kamieński, W. Schilf, *Spectrochim. Acta A,* **2018**, *189*, 330–341

3 › Ternary complexes consisting of chiral rhodium(II) tetracarboxylate, derivatives of amino acid and triphenylphosphine: The P-31 NMR, R. Głaszczka, A. Leniak, J. Jaźwiński, *J. Mol. Struct.,* **2019**, *1178*, 45–51

4 › Structure investigations of Schiff bases derived from 3-amino-1H-1,2,4-triazole, B. Kołodziej, M. Morawiak, W. Schilf, B. Kamieński, *J. Mol. Struct.,* **2019**, *1184*, 207–218

5 › Theoretical aspects of indirect spin–spin couplings, J. Jaźwiński, *Nuclear Magnetic Resonance,* **2015**, *44*, 150–169





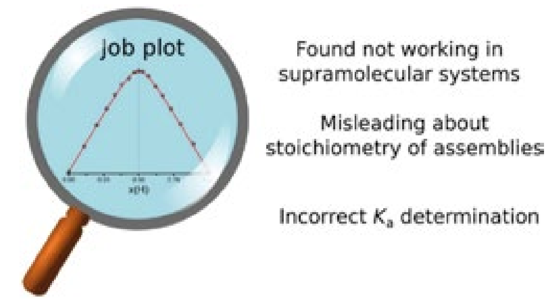
Prof. Janusz Jurczak

Jurczak Research Group

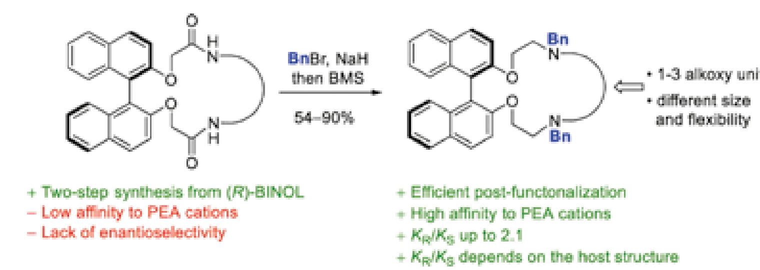
Current research:

- new macrocyclic and chain molecular receptors, and their application for recognition of ionic guests
- dynamic combinatorial chemistry
- new chiral catalysts and organocatalytic processes
- enantioselective reactions under PTC conditions
- the use of high pressure techniques in organic synthesis

Recognizing the limited applicability of Job plots in studying host-guest interactions in supramolecular chemistry, F. Ulatowski, K. Dąbrowa, T. Bałakier, J. Jurczak, *J. Org. Chem.*



Late-Stage Functionalization of (R)-BINOL-Based Diazacoronands and Their Chiral Recognition of α-Phenylethylamine Hydrochlorides, A. Tyszka, G. Pikus, K. Dąbrowa, J. Jurczak, *J. Org. Chem*



Selected publications:

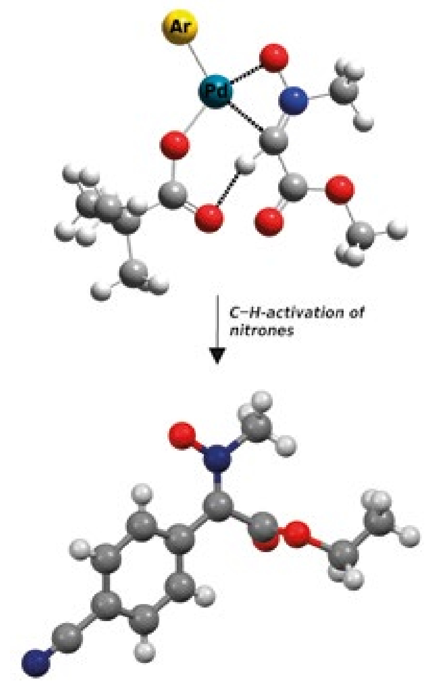
1. Late-Stage Functionalization of (R)-BINOL-Based Diazacoronands and Their Chiral Recognition of α-Phenylethylamine Hydrochlorides, A. Tyszka, G. Pikus, K. Dąbrowa, J. Jurczak, *J. Org. Chem.*, **2019**, *84*, 6502–6507
2. The Influence of Binding Site Geometry on Anion-Binding Selectivity: A Case Study of Macrocyclic Receptors Built on the Azulene Skeleton, D. Lichosyt, S. Wasiłek, P. Dydio, J. Jurczak, *Chem.: Eur. J.*, **2018**, *24*, 11683–11692
3. 8-Propyldithieno[3,2-b:2′,3′-e]pyridine-3,5-diamine (DITIPIRAM) derivatives as neutral receptors tailored for binding of carboxylates, A. Cholewiak, A. Tycz, J. Jurczak, *Org. Lett.*, **2017**, *10*, 3001–3004
4. Recognizing the limited applicability of Job plots in studying host-guest interactions in supramolecular chemistry, F. Ulatowski, K. Dąbrowa, T. Bałakier, J. Jurczak, *J. Org. Chem.*, **2016**, *81*, 1746–1756
5. A General Method for Synthesis of Unclosed Cryptands via H-Bond Templated Macrocyclization and Subsequent Mild Postfunctionalization, K. Dąbrowa, P. Niedbała, M. Majdecki, P. Duszewski, J. Jurczak, *Org. Lett.*, **2015**, *17*, 4774–4777

Assoc. Prof. Rafał Loska

Loska Research Group

Current research:

- transition metal-catalyzed C–H activation of nitrones
- new methods of allene synthesis
- new variants of Vicarious Nucleophilic Substitution of hydrogen in aromatic systems
- cycloaddition reactions of aromatic N-oxides



Selected publications:

1 › Transition Metal Free Nucleophilic Benzylation of Nitroarenes. Umpolung of the Friedel Crafts Reactions, K. Kisiel, J. Brześkiewicz, R. Loska, M. Mąkosza, *Adv. Synth. Catal.* **2019**, *361*, 1641–1646

2 › C–H-Alkenylation of Arenes in a One-Pot VNS – Julia-Kocienski Reaction, R. Loska, *Eur. J. Org. Chem.* **2018**, 6649–6656

3 › A-Chlorobenzylation of Nitroarenes via Vicarious Nucleophilic Substitution with Benzylidene Dichloride: Umpolung of the Friedel–Crafts Reaction, J. Brześkiewicz, R. Loska, M. Mąkosza, *J. Org. Chem.* **2018**, *83*, 8499–8508

4 › Azine-imidazole aza-BODIPY analogues with large Stokes shift, R. Loska, *Dyes and Pigments* **2017**, *137*, 312–321

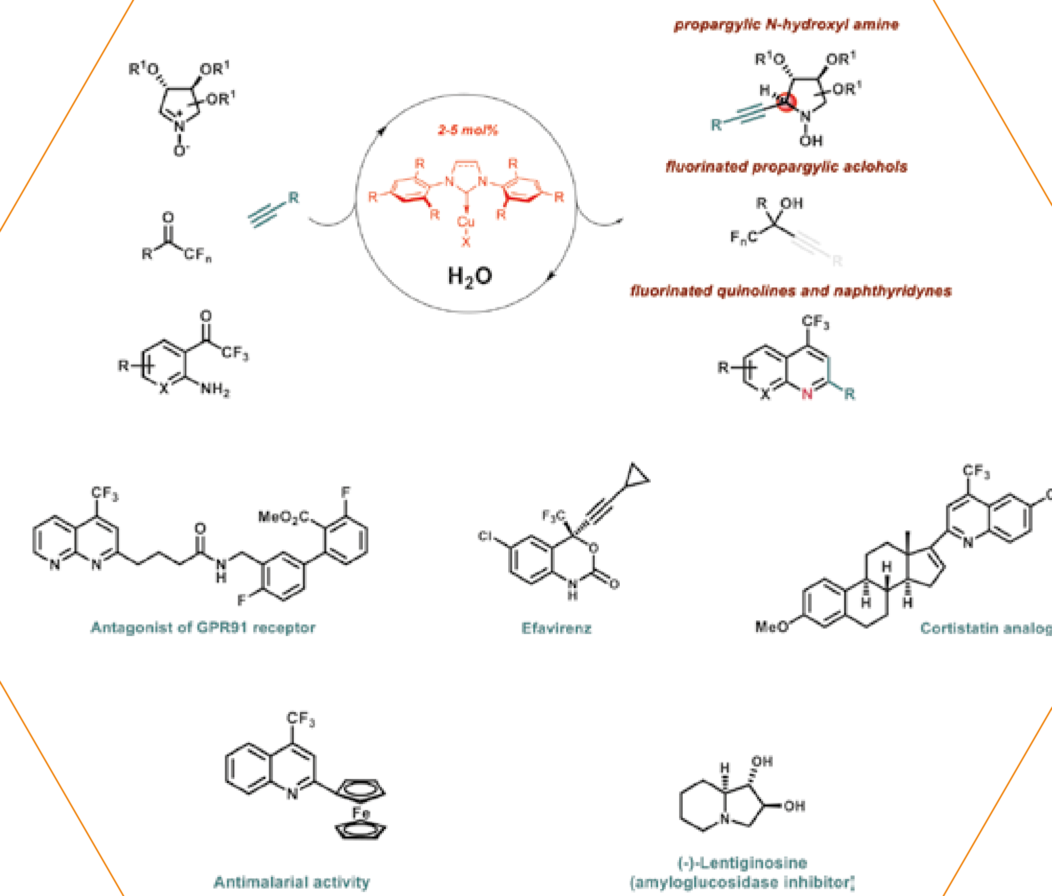
5 › Synthesis of Alkyl Aryl(heteroaryl)acetates from N-Oxides, R. Loska, K. Szachowicz, D. Szydlik, *Org. Lett.* **2013**, *15*, 5706–5709

Assoc. Prof. Michał Michalak

Michalak Research Group

Current research:

- synthesis of fluorinated azaheterocycles and propargylic alcohols via direct catalytic alkynylation on water catalyzed by N-heterocyclic carbene copper(I) complexes
- immobilization of N-heterocyclic carbene copper(I) and copper(II) complexes on magnetic nanoparticles and its applications for the synthesis of heterocyclic compounds
- new chiral C1-symmetric N-heterocyclic carbene gold(I) and gold(III) complexes and its applications in enantioselective catalysis
- synthesis of natural products and biologically relevant molecules



Selected publications:

1 › Diastereoselective synthesis of propargylic N-hydroxylamines via NHC-copper(I) halide-catalyzed reaction of terminal alkynes with chiral nitrones on water, L. Wozniak, O. Staszewska-Krajewska, M. Michalak, *Chem. Commun.* **2015**, *51*, 1933–1936

2 › NHC–Copper(I) Halide-Catalyzed Direct Alkynylation of Trifluoromethyl Ketones on Water, P. Czerwiński, E. Molga, L. Cavallo, A. Poater, M. Michalak, *Chem. Eur. J.* **2016**, *22*, 8089–8094

3 › NHC-Cu(I)-Catalyzed Friedländer-Type Annulation of Fluorinated o-Aminophenones with Alkynes on Water: Competitive Base-Catalyzed Dibenzo[b,f][1,5]diazocine Formation, P. Czerwiński, M. Michalak, *J. Org. Chem.* **2017**, *82*, 7980–7997

4 › The synthesis of cardenolide and bufadienolide aglycones, and related steroids bearing a heterocyclic subunit M. Michalak, K. Michalak, J. Wicha, *Nat. Prod. Rep.* **2017**, *34*, 361–410

5 › NHC-copper complexes immobilized on magnetic nanoparticles: synthesis and catalytic activity in the CuAAC reactions, I. Misztalewska-Turkowicz, K.H. Markiewicz, M. Michalak, A.Z. Wilczewska, *J. Catal.* **2018**, *362*, 46–54

6 › Synthetic approach to chiral non-C2-symmetric N-heterocyclic carbene precursors, P. Czerwiński, M. Michalak, *Synthesis* **2019**, *51*, 1689–1714

Prof. Jacek Młynarski

Młynarski Research Group

Current research:

- asymmetric catalysis with zinc- and magnesium chiral Lewis acids
- asymmetric reduction of prochiral ketones and imines promoted by zinc complexes
- stereocontrolled synthesis of natural products
- direct aldol reaction of hydroxyacetone and dihydroxyacetone
- light-induced transformations.

Selected publications:

1 › Chiral Amplification in Nature: Cell-extracted Chiral Carotenoid Microcrystals Studied Via RROA of Model Systems, M.A. Dudek, E. Machalska, T. Oleszkiewicz, T. Grzebelus, R. Baranski, P. Szcześniak, J. Mlynarski, G. Zajac, A. Kaczor, M. Baranska, *Angew. Chem. Int. Ed.*, **2019,** *58*, 8383–8388

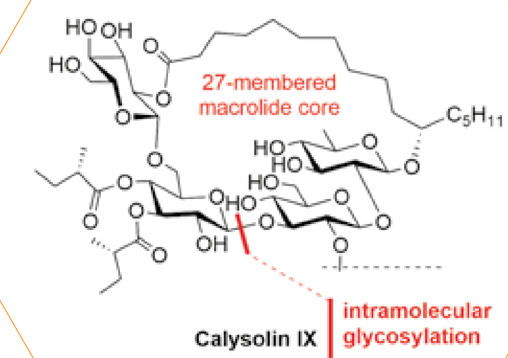
2 › Visible-Light-Mediated α-Oxygenation of 3-(N,N-Dimethylaminomethyl)-Indoles to Aldehydes, F. Stanek, R. Pawłowski, J. Mlynarski, M. Stodulski, *Eur. J. Org. Chem.*, **2018**, 6624–6628

3 › Application of the EF and GH Fragments to the Synthesis of Idraparinux, G. Łopatkiewicz, S. Buda, J. Mlynarski, *J. Org. Chem.*, **2017**, *82*, 12701–12714

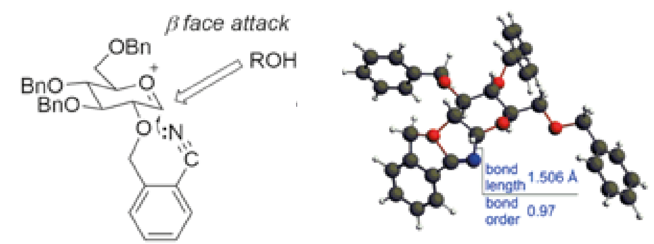
4 › Zinc Acetate-Catalyzed Highly Enantioselective Hydrosilylation of Ketones, M. Szewczyk, F. Stanek, A. Bezłada, J. Mlynarski, *Adv. Synth. Catal.*, **2015**, *357*, 3727–3731

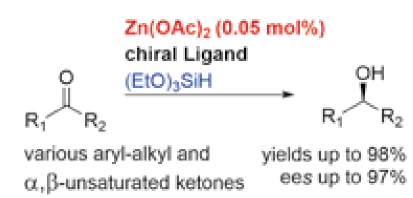
5 › Amine-Catalyzed Direct Aldol Reactions of Hydroxy- and Dihydroxyacetone: Biomimetic Synthesis of Carbohydrates, O. Popik, M. Pasternak-Suder, K. Leśniak, M. Jawiczuk, M. Górecki, J. Frelek, J. Mlynarski, *J. Org. Chem.*, **2014,** *79*, 5728–5739

Intramolecular glycosylation as an efficient tool for the synthesis of 27-membered macrocyclic ring of the most complex resin glycoside isolated to date – Calysolin IX.



The use of 2-nitrobenzyl and 2-cyanobenzyl groups control stereoselective formation of 1,2-trans-glycosidic linkage via arming participation effect.





Prof. Ryszard Ostaszewski

Ostaszewski Research Group

Current research:

- biocatalysis, the studies on the new types of enzymatically catalysed reactions (promiscuity), stereocontrolled synthesis – kinetic resolution, dynamic kinetic resolution of racemates
- the design of the chemoenzymatic cascade reactions
- multicomponent reactions, the synthesis of biologically active compounds
- design and synthesis of new hydrogen sulphide donors (in cooperation with prof. M. Ufnal, WUM) and anti-cancer active compounds (in cooperation with prof. J. Malejczyk, prof. J. Gołąb, WUM)
- the application of soft matter, micellar systems as an effective medium in chemical and enzymatic reactions

Selected publications:

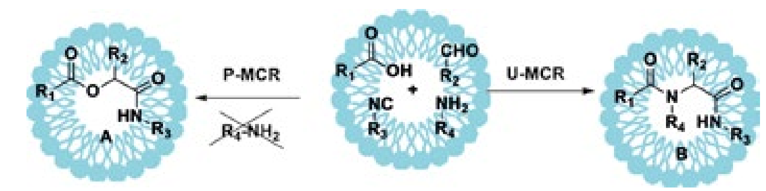
1 Evaluation of thioamides, thiolactams and thioureas as hydrogen sulfide (H_2S) donors for lowering blood pressure, *E. Zaorska, T. Hutsch, M. Gawrys-Kopcz*ynska, R. Ostaszewski, M. Ufnal, D. Koszelewski, *Bioorg. Chem.* **2019**, *88*, 102941

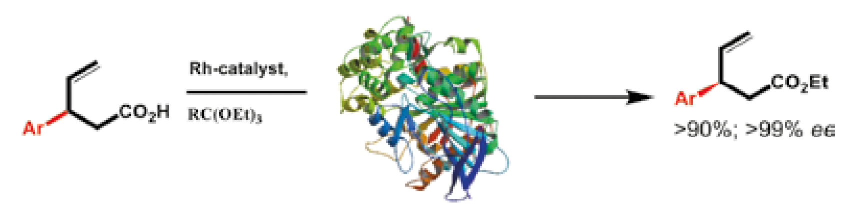
2 Biocatalytic Promiscuity of Lipases in Carbon-Phosphorus Bond Formation, D. Koszelewski, R. Ostaszewski, *ChemCatChem.* **2019**, *11*, 2554–2558

3 Soft and dispersed interface-rich aqueous systems that promote and guide chemical reactions, S. Serrano--Luginbühl, K. Ruiz-Mirazo, R. Ostaszewski, F. Gallou, P. Walde, *Nature Rev. Chem.* **2018**, *2*, 306–327

4 Studies on the Synthesis of Endocyclic Enol Lactones via a RCM of Selected Vinyl Esters, A. Brodzka, F. Borys, D. Koszelewski, R. Ostaszewski, *J. Org. Chem.* **2018**, *83*, 8655–8661

The application of soft matter concept for the synthesis of biologically active compounds through multicomponent reactions carried out in micellar systems leading to peptidomimetics A or B as products of Passerini and Ugi reactions.





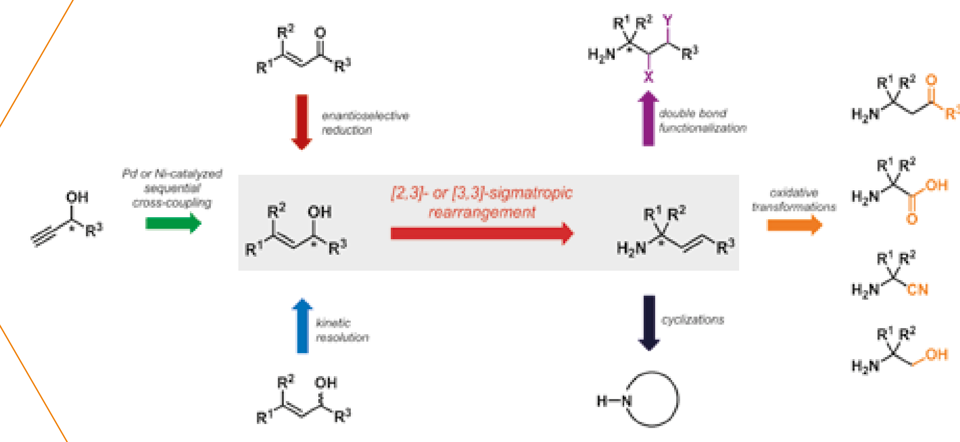
We have developed the new method for the synthesis of enantiomerically pure esters of unsaturated carboxylic acids based on chemoenzymatic catalysis

5 Dynamic Kinetic Resolution of 3-Aryl-4-pentenoic Acids, D. Koszelewski, A. Brodzka, A. Żądło, D. Paprocki, D. Trzepizur, M. Zysk, R. Ostaszewski, *ACS Catal.* **2016**, *6*, 3287–3292

6 Enzyme-Promoted Asymmetric Tandem Passerini Reaction, A. Żądło-Dobrowolska, D. Koszelewski, D. Paprocki, A. Madej, M. Wilk, R. Ostaszewski, *ChemCatChem.* **2017**, *9*, 3047–3053

Assoc. Prof. Sebastian Stecko

Stecko Research Group



Current research:

- [2,3]- and [3,3]-Sigmatropic rearrangements as a tool in organic synthesis
- Pd- and Ni-catalyzed or visible light induced cross-coupling reactions
- functionalization of allylamines and allyl alcohols
- stereocontrolled organic synthesis: synthesis of unnatural amino acids, carbohydrate derivatives, alkaloids and bioactive compounds
- heterocyclic chemistry

Selected publications:

1 › Total synthesis of levetiracetam, A. Narczyk, M. Mrozowicz, S. Stecko, *Org. Biomol. Chem.* **2019**, *17*, 2770–2775

2 › The synthesis of non-racemic β-alkyl-β-aryl-disubstituted allyl alcohols and their transformation into allylamines and amino acids bearing a tertiary stereocenter, A. Narczyk, M. Pieczykolan, S. Stecko, *Org. Biomol. Chem.* **2018**, *16*, 3921–3946

3 › The Synthesis of chiral β,β-diaryl allylic alcohols and their use in the preparation of α-tertiary allylamines and quaternary α-amino acids, M. Pieczykolan, A. Narczyk, S. Stecko, *J. Org. Chem.* **2017**, *82*, 5636–5651

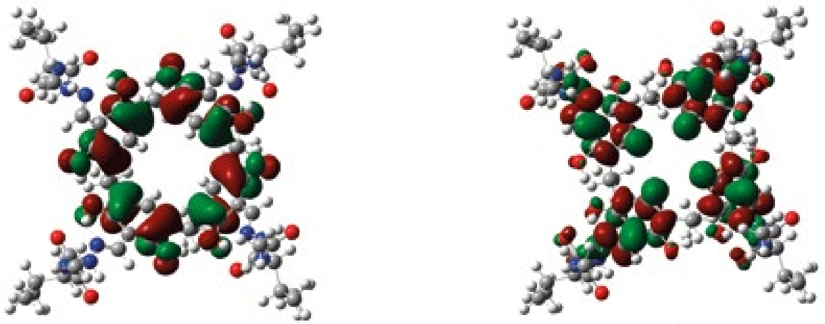
4 › The synthesis of α,α-disubstituted α-amino acids via Ichikawa rearrangement, P. Szcześniak, M. Pieczykolan, S. Stecko, *J. Org. Chem.* **2016**, *81*, 1057–1074

5 › The synthesis of 5-amino-dihydrobenzo[b]oxepines and 5-amino-dihydrobenzo[b]azepines via Ichikawa rearrangement and ring-closing metathesis, M. Chwastek, M. Pieczykolan, S. Stecko, *J. Org. Chem.* **2016**, *81*, 9046–9074

6 › An approach to asymmetric synthesis of β-aryl alanines by Pd(0)-catalyzed cross-coupling and cyanate-to-isocyanate rearrangement, P. Szcześniak, S. Stecko, *RSC Adv.* **2015**, *5*, 30882–30888

7 › Total synthesis of lacosamide, S. Stecko, *J. Org. Chem.* **2014**, *79*, 6342–634

Prof. Agnieszka Szumna

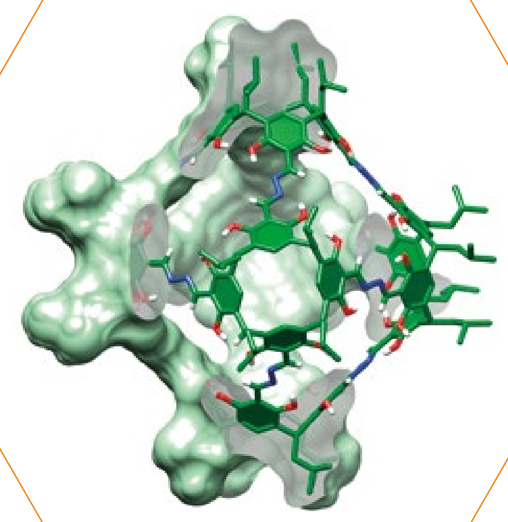


conf-1 HOMO conf-1 LUMO

Szumna Research Group

Current research:

- molecular recognition between peptide-type molecules and proteins
- bio-inspired self-assembly of functional molecular containers
- new macrocyclic scaffolds
- mechanochemistry of porous structures
- dynamic covalent chemistry



Selected publications:

1 › 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

2 › 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

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

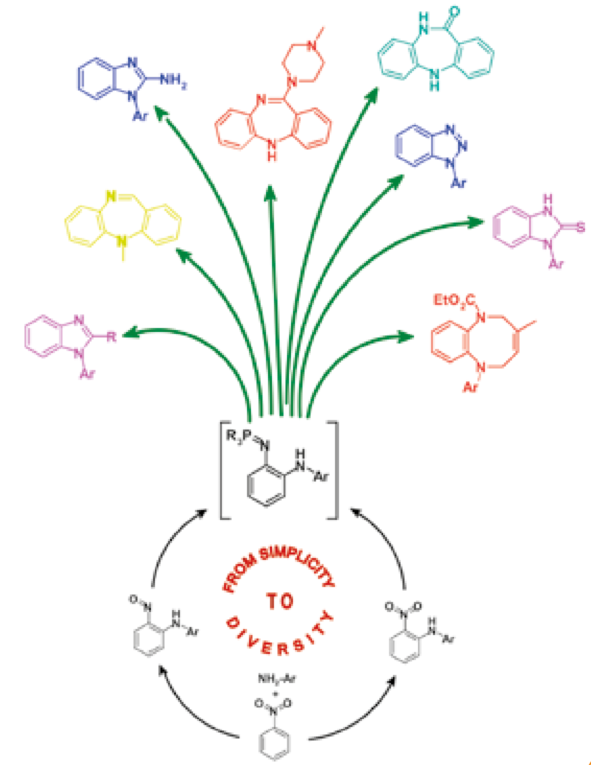
4 › Dynamic formation of hybrid peptidic capsules by chiral self-sorting and self-assembly, H. Jędrzejewska, M. Wierzbicki, P. Cmoch, K. Rissanen, A. Szumna, *Angew. Chem. Int. Ed.*, **2014**, *53*, 13760–13764

Assoc. Prof. Wróbel Zbigniew

Wróbel Research Group

Current research:

- synthesis of fused heterocyclic nitrogen compounds, particularly phenazines, indoles and quinolines, from nitroaromatic starting materials
- formation of σH adducts from nitroarenes and carbon- and nitrogen-centered anions; their reactivity towards nucleophilic and electrophilic reagents, and further transformations
- the use of aryliminophosphoranes, derived from nitrodiarylamines, as either starting materials or intermediates, for the synthesis of various classes of nitrogen heterocyclic compounds
- novel methods for the synthesis of dibenzodiazepine scaffolds based on cyclocondensation of nitro- and nitroso- diarylamines



Selected publications:

1 › Direct Reductive Cyclocondensation of the Nitro Group with the Amido Group: Key Role of the Iminophosphorane Intermediate in the Synthesis of 1,4-Dibenzodiazepine Derivatives, M. Tryniszewski, R. Bujok, P. Cmoch, R. Gańczarczyk, I. Kulszewicz-Bajer, Z. Wróbel, *J. Org. Chem.* **2019**, *84*, 2277–2286

2 › Simple synthesis of 2-alkylidene- and 2-keto-7-triazolylquinoxaline systems from 2-nitrosodiarylamines Z. Wróbel, R. Bujok, M. Tryniszewski, A. Kwast, *Arkivoc* **2019**, *v*, 60–72

3 › A general and convenient method for the synthesis of 2,4-dinitrobenzyl ketones. Almost unlimited access to 2-substituted 6-nitroindoles from 2,4-dinitrotoluene and aldehydes, R. Bujok, M. Wiszniewski, P. Cmoch, Z. Wróbel, *New J. Chem.* **2018**, *42*, 3260–3269

4 › Transition-metal-free synthesis of 3-(1-pyrrolidinyl)quinolines and 3-(1-pyrrolidinyl)quinoline 1-oxides via a one-pot reaction of 3-(1-pyrrolidinyl)crotonates with nitrobenzenes, R. Bujok, P. Cmoch, Z. Wróbel, K. Wojciechowski, *Org. Biomol. Chem.* **2017**, *15*, 2397–2402

5 › Reactivity and substituent effects in the cyclization of N-aryl-2-nitrosoanilines to phenazines Z. Wróbel, K. Plichta, *A. Kwast Tetrahedron* **2017**, *73*, 3147–3152

Emeritus Professors

Prof. Marek Chmielewski

Current research:

- Synthesis of β-lactams via Kinugasa reaction
- Gycosyl hydroperoxides, synthesis and properties

Selected publications:

1 Kinugasa reaction employing chiral alkynes; stereocontrolled transformations of adducts, R. Kutaszewicz, B. Grzeszczyk, M. Górecki, O. Staszewska-Krajewska, B. Furman, M. Chmielewski, *Org. Biomol. Chem.*, **2019**, *17*, 6251–6268

2 The synthesis of monobactams through diastereoselective Kinugasa reaction, K. Kabala, B. Grzeszczyk, B. Furman, M. Chmielewski, *J. Solecka,* A. Guspiel, *Synthesis* **2018**, *50*, 1991–2000

3 Glycosyl Hydroperoxides, *B. Szechner, B. Grzeszczyk,* B. Furman, M. Chmielewski, *J. Carbohydr. Chem.*, **2018**, *37*, 104–116

4 Formal synthesis of Thienamycin, M. Pieczykolan, B. Furman, M. Chmielewski, *J. Antibiot.* **2017**, *70*, 781–787

Prof. Mieczysław Mąkosza

Current research:

- synthetic application of nucleophilic aromatic substitution of hydrogen
- mechanism of nucleophilic aromatic substitution.

Selected publications:

1 Transition Metal Free Nucleophilic Benzylation of Nitroarenes, Umpolung of the Friedel Crafts Reaction, K. Kisiel, J. Brześkiewicz, R. Loska, M. Mąkosza, *Adv. Synth. Catal.*, **2019**, *361*, 1641–1646

2 Nucleophilic substitution in nitroarenes: a general corrected mechanism, M. Mąkosza, *ChemText*, **2019**, 9–15

3 Interfacial Generation of Carbanions, the Key Step of PTC Reactions Directly Observed by Second Harmonic Generation, M. Hamkało, P. Fita, M. Fedoryński, M. Mąkosza, *Chem. Eur. J.*, **2018**, *24*, 3975–3979

Laboratory for the Analysis of Bioactive Compounds

Laboratory for the Analysis of Bioactive Compounds provides analytical measurements for organic compounds, pharmaceuticals, cosmetics and other products of the chemical industry.

The laboratory offers comprehensive, high-quality analysis of:

- nuclear magnetic resonance (NMR),
- mass spectrometry (MS),
- optical spectroscopy (UV-VIS-NIR, IR, ECD, VCD, ORD, LD),
- X-ray crystallography (X-ray),
- elemental analysis (EA).

We perform comprehensive work which involves the identification of unknown samples components or processes e.g. identification of impurities in drugs. We prepare complete spectral documentation for structure confirmation for drugs or chemicals registration purposes.

Our approach is based on advanced measurement techniques and broad scientific knowledge. We are open to cooperate in scientific projects requiring analytical measurements in the fields of chemistry, biology, medicine or environmental science.

Contact:

Head of the Laboratory for the Analysis of Bioactive Compounds
Assoc. Prof. Wojciech Schilf
lasb@icho.edu.pl
tel. 22-343-22-11

Nuclear Magnetic Resonance Lab

The history of NMR measurements in the Institute dates back to 1962 when the first 60 MHz resolution spectrometer was installed. It was the first NMR spectrometer in Poland.

Instruments:

- Varian Mercury 400 MHz
- Bruker DRX 500 MHz
- Varian VNMRS 500 MH
- Varian VNMRS 600 MHz

Our offer includes a full range of one- and two-dimensional nuclear magnetic resonance experiments in the liquid phase and CPMAS measurements in the solid phase for most of nuclei with non-zero spin. We perform the measurements in a whole range of deuterated solvents in the range of temperatures from −120 to +120°C.

Contact:

Head of the Nuclear Magnetic Resonance Laboratory
Assoc. Prof. Wojciech Schilf
wojciech.schilf@icho.edu.pl

Mass Spectrometry Lab

Mass Spectrometry Laboratory of the Institute of Organic Chemistry PAS has been providing high quality services for 25 years.

Instruments:

- AutoSpec Premier (Waters) + HP 7890 (Agilent) gas chromatograph
- SYNAPT G2-S (Waters) + ACQUITY I-Class (Waters) liquid chromatograph
- GCT Premier (Waters) + 6890N gas chromatograph (Agilent)
- 7890A & 5975C GC/MS system (Agilent)
- 4000 Q-TRAP (SCIEX) + LC-20 Prominence (Shimadzu) liquid chromatograph
- API 3000 (SCIEX)

We offer standard and high resolution mass spectrometry measurements using EI, CI, ESI, APPI, APCI, ASAP ionization techniques. We perform also GC-MS (together with identification of known compounds using NIST and Wiley databases) and HPLC-MS (also UPLC-MS) qualitative and quantitative analyses. Our specialty are structural studies using MS/MS and MS3 fragmentation spectra and application of multiple interfaces and ionization techniques for the analysis of difficult samples

Contact:

Head of the Mass Spectrometry Laboratory
Dr. Dorota Staszek
dorota.staszek@icho.edu.pl

Optical Spectroscopy Lab

Laboratory of Optical Spectroscopy carries out analytical service using modern spectrometers with an extensive range of accessories and attachments which allow recording the high quality spectra for a wide range of liquid and solid samples in variable temperature range.

We perform measurements in a broad spectral range from UV-Vis-NIR to IR, using both transmission and reflectance (ATR) techniques.

We offer advanced chiroptical analysis services for any chiral compounds, in particular we carry out electronic and vibrational circular dichroism (ECD/VCD), optical rotatory dispersion (ORD) and linear dichroism (LD) spectra. Additionally, we perform HPLC chiral separations using both optical and chiroptical detectors, i.e. UV-VIS, RI, ECD and OR.

Using our unique blend of expertise and resources, that brings together experimental spectroscopy and computational simulations, we offer also determination of absolute configuration of synthetic/ natural products, and also advancing the understanding the role which chirality plays in studied systems and processes.

Instruments:

- Spectropolarimeter ECD Jasco J-715
- Spectropolarimeter ECD Jasco J-815, for solid-phase measurements
- Spectropolarimeter ORD Jasco J-815
- Chiral *IR*-2X DualPEM BioTools spectrometer
- Jasco V-670 UV-VIS-NIR spectrophotometer
- UV-VIS Varian spectrophotometer Carry 100E
- Spectrophotometer FTIR Jasco 6200
- Spectrophotometer FTIR Shimadzu IRTracer-100

Contact:

Head of the Optical Spectroscopy Laboratory
Dr. Marcin Górecki
marcin.gorecki@icho.edu.pl

X-ray Crystallography Lab

The X-Ray Diffraction Laboratory provides high quality structural characterization of organic compounds. The laboratory is equipped with modern Bruker AXS diffractometer with area detector APEX II which allows for advanced X-ray diffraction characterization of monocrystalline organic and metalloorganic materials. Application of Cu-radiation is particularly useful in studies of small to medium size (10-500 atoms) organic molecules, including assignement of absolute configuration.

Low temperature device designed by Oxford Cryosystems provides opportunity to study structure and phase transitions in the 100–373 K temperature range.

Another availavle option is possibility of measurement of crystal size and face indexing that makes sit useful for some solid phase physiscs.

Contact:

Head of the X-ray Crystallography Laboratory
Dr. Marcin Górecki
marcin.gorecki@icho.edu.pl

Elemental Analysis Lab

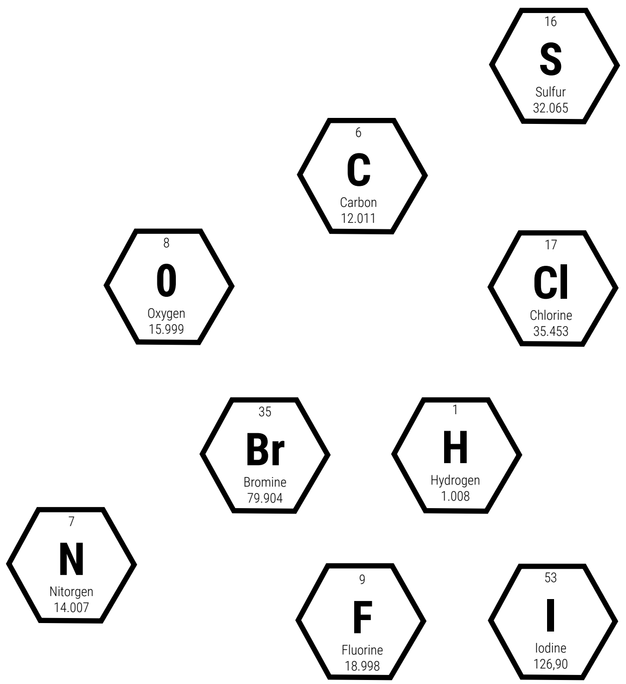
Laboratory of Elemental Analysis measures elemental composition of organic substances and compounds, including following elements: C, H, N, O, S, Cl, Br, I and F.

UNICUBE (Elementar) is used for determination of C, H, N, S and O content is determined with an Vario EL III (Elementar Analysensysteme) contents. The method is based on the catalytic combustion at 1150°C in helium/oxygen atmosphere.

Halogens and sulfur are determined using the Schőniger method. After mineralization of the analyzed substance on the platinum catalyst in the flask filed with oxygen the resulting halide and sulfide ions are determined by titration.

Contact:

Head of the Elemental Analysis Laboratory
Krystyna Markucińska
krystyna.markucinska@icho.edu.pl



Young Investigators

Dr. Kajetan Dąbrowa

Current research:

- light-controllable azobenzene-based switches for binding and transport of charged and neutral guests
- anion receptors exhibiting anti-Hofmeister selectivity
- development of post-macrocyclization synthetic strategies

Research grant: Sonata 2016/23/D/ST5/03301 NATIONAL SCIENCE CENTRE POLAND
„Development of novel light-controllable azobenzene switches as molecular receptors for selective sensing and transport of biologically relevant salts"

Dr. Cina Foroutan-Nejad

Current research:

- Chemical Bond Theory
- Magnetic Response Properties
- Molecular Electronics
- Smart Catalysis

Dr. Przemysław Gaweł

Current research:

- Organic Electronics,
- Synthetic Functional Materials,
- Physical Organic Chemistry,
- Supramolecular Chemistry

Research grant: Polish Returns – NAWA PPN/PPO/2020/1/00012 NAWA
„Cyclophane-based organic semiconductors"

Dr. Maciej Giedyk

Current research:

- photocatalysis
- microheterogenous solutions
- organic synthesis at interfaces

Research grant: Sonata 2018/31/D/ST5/00306 NATIONAL SCIENCE CENTRE POLAND
„Photocatalysis at interfaces: self-assembled microheterogenous solutions as reaction media for visible-light-induced transformations"

Dr. Marcin Górecki

Current research:

- Applications of chiroptic methods (ECD, ORD, VCD, ROA, CPL) in stereochemical analysis (absolute configuration, conformation, intermolecular interactions) of natural and synthetic compounds
- Development of solid-state circular dichroism (CD) spectroscopies for applications in medical and materials chemistry.

Research grant: Sonata 2019/35/D/ST4/00394 National Science Centre
„Solid-state circular dichroism (CD) spectroscopies as a tool for supporting the development of medicinal chemistry"

Dr. Jarosław Granda

Current research:

- asymmetric synthesis;
- machine learning and deep learning;
- organocatalysis;
- computer aided reaction discovery;
- reactants design; chirality;
- chemical space

Research grant: Polish Returns – NAWA PPN/PPO/2020/1/00034 NAWA
„Artificial intelligence-driven design and discovery of chiral phosphoric acid catalysed reactions"

Dr. Marek Grzybowski

Current research:

- synthesis of strained and curved polycyclic aromatic hydrocarbons

Research grant: Sonata 2018/31/D/ST5/00432 National Science Centre
„Synthesis of curved derivatives of acenes – towards bottom-up synthesis of zig-zag carbon nanotubes"

Dr. Marcin Lindner

Current research:

- aromatic curved functional materials
- heteroatom-doped nanographeness
- donor-acceptor organic nanoarchitectures

Research grant: Sonata 2018/31/D/ST5/00426 National Science Centre
„Modular, cycalzine-based polycyclic aromatic hydrocarbons (PAHs): novel materials for optoelectronic applications"
Research grant: Lider XI 0077/L-11/2019 The National Centre for Research and Development
„Synthesis of novel class of organic emitters for TADF OLED materials embracing curved nanographene fragments"

Dr. Piotr Szcześniak

Current research:

- Photochemical rearrangement of lactams.
- A ring-expansion approach towards structurally diverse heterocycles.

Research grant: Sonata 2019/35/D/ST4/00028
„Photochemical rearrangement of N-substituted lactams.
Ring expansion towards heterocyclic systems"

Dr. Mateusz Woźny

Current research:

- synthesis and properties of catenane and rotaxane molecular switches

Research grant: Sonata 2017/26/D/ST5/00361
„Synthesis and properties of zwitterionic rotaxanes and molecular switches"

Assoc. Prof. Bartosz Zambroń

Current research:

- development of new synthetic methodology
- application of chiral organoindiums in asymmetric synthesis
- studies of remote acyclic stereocontrol

Research grant: Sonata 2015/19/D/ST5/00713
"An application of new catalytic reactions of chiral 4-vinyl- and 4-ethynyl-azetidin-2-ones in the stereodivergent synthesis of nonracemic heterocyclic compounds."

Dr. Magdalena Maja Zimnicka

Current research:

- structural properties (3D shape, conformational differentiation, stability, thermochemical properties) of small and medium sized molecules and their noncovalent associates investigated by mass spectrometry and mass spectrometry-based techniques
- macrocyclic anion receptors exhibiting anti-Hofmeister selectivity
- post-macrocyclization strategies for efficient functionalization of macrocyclic systems

Research grant: Sonata 2011/03/D/ST4/03067
„Examination of properties of non-covalent complexes of melanocortin receptor ligands"

Fundacja na rzecz Nauki Polskiej

Laureates of Foundation for Polish Science Prize

Laureates:

- Professor Mieczysław Mąkosza
- Professor Karol Grela
- Professor Daniel Gryko

Professor Mieczysław Mąkosza

Prof. Mieczysław Mąkosza (b. 1934 in Cieszewla near Baranovichi, present-day Belarus) is an organic chemist. Retired professor from the Warsaw University of Technology and the Institute of Organic Chemistry of the Polish Academy of Sciences. He has gained worldwide recognition for his pioneering research with a fundamental significance for organic chemistry and wide-reaching practical applications in the chemical and pharmaceutical industries. Some of his greatest achievements include groundbreaking work in phase transfer catalysis, and subsequent research into nucleophilic aromatic substitution.

He graduated with distinction in chemistry from the University of Leningrad (present-day Saint Petersburg) in 1956. He has always had close ties with the Warsaw University of Technology, where he obtained his PhD (1963) and habilitation (1967). He rose to the rank of professor in 1984. He was the director of the Institute of Organic Chemistry of the Polish Academy of Sciences for 25 years (1979–2004). He successfully combined research work with numerous official functions at scientific institutions at the Polish Academy of Sciences: he was a member of the board of the Academy, president of the Committee of Chemistry, president of the scientific board of the Centre for Molecular and Macromolecular Studies, and member of the Central Committee for Degrees and Titles. He continues to be an active participant in the Academy's structures as the president of the scientific board of the Institute of Organic Chemistry for the period 2011–2014.

He is a member of four academies of sciences: the Polish Academy of Sciences, the Polish Academy of Arts and Sciences, the German Academy of Sciences Leopoldina, and Academia Europaea. He has been awarded six honorary degrees. He has also received numerous prizes and medals for his scientific achievements, including the Polish State Award 1st Class, the Award of the Prime Minister of Poland, the Order of Merit of the Republic of Poland, the Kostanecki Medal, and the Śniadecki Medal of the Polish Chemical Society.

Prof. Mąkosza has published over 300 research papers and 70 patents. He has also supervised over 200 Master's degrees and close to 50 PhDs.

Prof. Mąkosza's method has become the accepted standard in organic synthesis, and remains in widespread use in the synthesis and production of numerous chemical compounds such as medicines, agricultural products, dyes, etc.

Prof. Mieczysław Mąkosza from the Institute for Organic Chemistry of the Polish Academy of Sciences received the FPS prize 2012 in the field of Chemical and Material Sciences for discovery and introduction of vicarious nucleophilic substitution into the canon of organic chemistry.

The reaction involves aromatic compounds, a large and significant group of chemical compounds with a great significance in our everyday lives (they are widely used in the pharmaceutical industry, agricultural products and electronics). Greatly simplified, the compounds have the basic shape of a honeycomb cell, comprising carbon and hydrogen, with a cloud of free electrons trapped within the hexagonal ring.

Nucleophilic aromatic substitution was first described in the mid-20th century, and has been used for various purposes in organic synthesis ever since. For many years, scientists believed that only chlorides and other nucleophilic groups underwent nucleophilic substitution. Prof. Mąkosza demonstrated that this view is incorrect, and showed that under certain conditions, the reaction can take place as substitution of a hydrogen atom, although the process occurs at a much faster rate than the better-known substitution of chloride.

Prof. Mąkosza's main achievement was the discovery and description of detailed features of vicarious nucleophilic substitution, such as orientation, range and limitations, as well as the more subtle details of its mechanism. This had a significant impact on the development of organic chemistry, both on the theoretical and practical levels.

Professor Karol Grela

Professor Karol Grela, from the University of Warsaw and the Institute of Organic Chemistry of the Polish Academy of Sciences in Warsaw received the FNP Prize 2014 in the chemical and materials sciences for developing new catalysts for olefin metathesis reactions and applying them in industrial practice.

Professor Karol Grela, (b. 1970 in Warsaw) is a chemist working on the synthesis of organic and organometallic compounds. A graduate of the Faculty of Chemistry at the Warsaw University of Technology (1994), he obtained his PhD (1998), postdoctoral degree (2003) and the title of professor (2008) at the Institute of Organic Chemistry of the Polish Academy of Sciences. He spent 1999–2000 on a postdoctoral fellowship at the Max Planck Institute in Mülheim an der Ruhr.

He heads the Organometallic Synthesis Laboratory of the Biological and Chemical Research Centre of the Faculty of Chemistry at the University of Warsaw as well as working part-time at the Institute of Organic Chemistry of the Polish Academy of Sciences. He is a member of the Polish Chemical Society and an honorary member of the Israel Chemical Society.

He has received numerous awards and honours for scientific achievement, including a stipend for young researchers from the Foundation for Polish Science (1998), the Prime Minister's Prize for the best PhD (1999), an Alexander von Humboldt Fellowship (1999), the Polish Academy of Sciences' Włodzimierz Kołos Award (2003), the Prime Minister's Prize for the best postdoctoral degree (2004), the Polish Chemical Society's Maria Skłodowska-Curie Prize and the German Chemical Society's Wilhelm Klemm Prize (2007), the FNP's MISTRZ academic grant for professors (2007) and TEAM programme grant (2009), the Minister of Science and Higher Education Prize in the "research for scientific development" category (2009), the Prime Minister's Prize for scientific achievement (2010).

Professor Karol Grela's output includes over 120 scientific publications and 12 patents protected in a few dozen countries around the world. His research has found many practical applications. He works closely with the pharmaceutical industry, for example, and is a member of Polpharma S.A.'s Scientific Advisory Board among other posts.

International recognition for Professor Grela's achievements is proved, among other things, by the fact that one of the catalysts he developed and commercialized is known in the literature as the "Grela catalyst" while his team is considered a world leader among research groups working in this field.

The carbon-carbon double bond in olefins is one of the most useful elements in the structure of organic compounds. It can be used to build all kinds of organic skeletons and, due to its high chemical reactivity, is one of the most important functional groups used in numerous chemical transformations. Due to these extensive possibilities, over the past 150 years chemists have sought new ways of obtaining olefins. A completely new way of obtaining these extremely important chemical compounds was invented in recent decades: metathesis (for this achievement, three chemists – Yves Chauvin, Robert Grubbs and Richard Schrock – received the Nobel Prize in 2005).

Professor Grela and his associates have focused on the optimization of olefin metathesis reactions, i.e. seeking ways to conduct them in a way that is safe for the environment, combines high efficiency with the possibility of conducting them in mild conditions (at ambient or lower temperature or in a water solution, for example) and with tolerance for numerous, often very reactive functional groups. A catalyst, meanwhile, should be as cheap as possible, easy to recover after a reaction as well as being highly active and stable.

All these important problems and challenges have been identified and in many cases also solved by Professor Grela's group. The research he leads has resulted in many new catalysts: complex ruthenium compounds thanks to which the metathesis process can be individually regulated ("tuned") for countless applications, both in academic organic chemistry and in industry (e.g. in the production of new drugs, new polymer materials and recipes for new fuels based on renewable input materials).

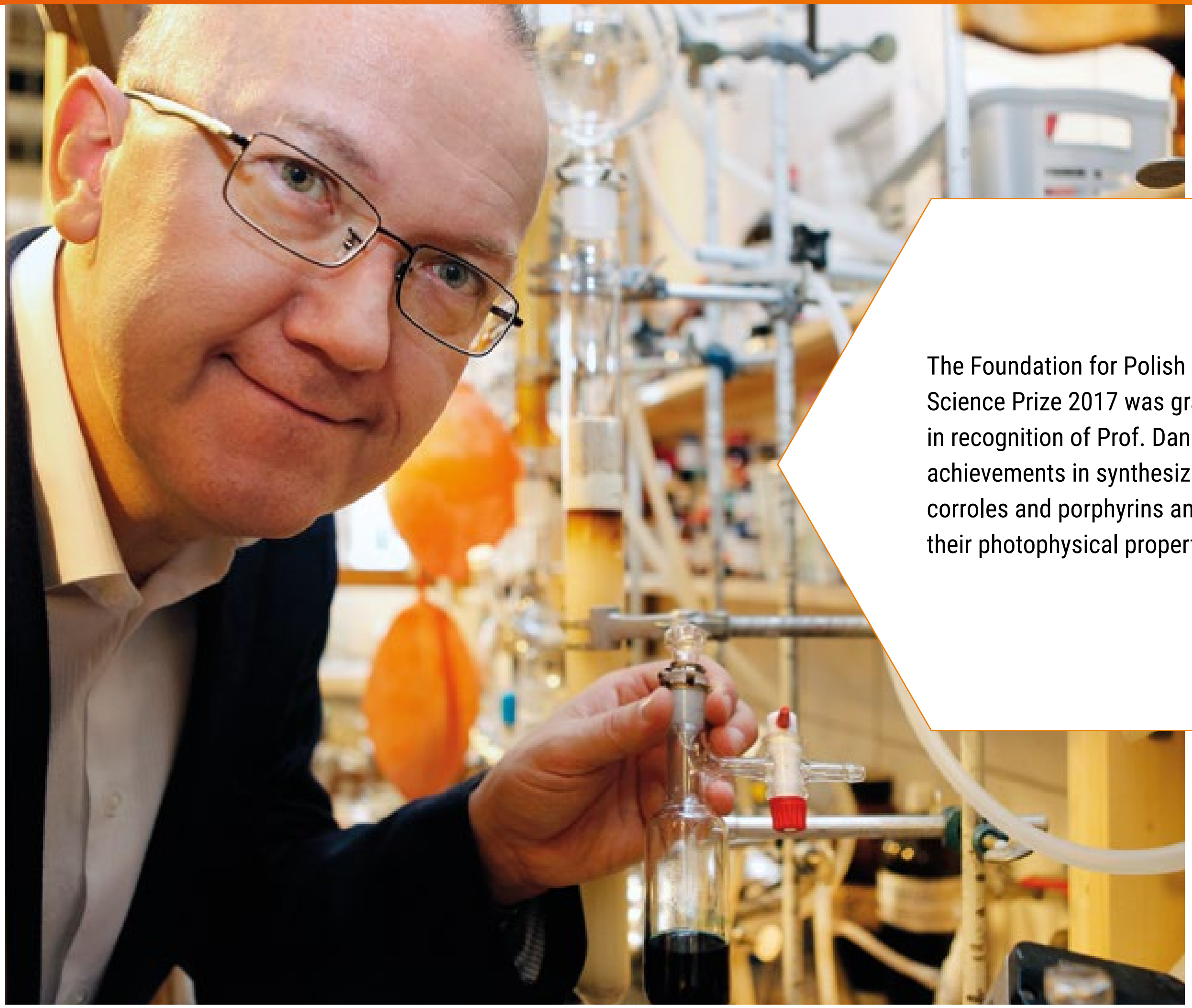
Professor Daniel Gryko

Prof. Daniel Gryko from the Institute of Organic Chemistry of the Polish Academy of Sciences in Warsaw has received the Foundation for Polish Science Prize 2017 in the chemical and material sciences for the development of an original method for synthesis and characterization of porphyrinoids.

Born in 1970, Daniel Gryko graduated from the Faculty of Chemistry at the University of Warsaw. He obtained his PhD at the Institute of Organic Chemistry of the Polish Academy of Sciences, where he also obtained his postdoctoral degree at the age of 33. He completed a postdoctoral fellowship at North Carolina State University in the United States in 1998-2000. He has worked as a visiting professor at the University of Burgundy in France and as a visiting researcher at Texas State University in Austin. He received the title of full professor in 2008. During this period he also worked at the Warsaw University of Technology for five years. Today he is a research worker of the Polish Academy of Sciences and heads a research group at the PAS Institute of Organic Chemistry. Although he takes part in many international projects, he has consistently carried out his research in Poland. Young scientists from other countries come here to work with him.

His great scientific achievements have won him an award from the Society of Porphyrins and Phthalocyanines (2008), the Prize of the Minister of Science and Higher Education (2012), the Wojciech Świętosławski Prize awarded by the Polish Chemical Society (2013). He was a beneficiary of the Foundation for Polish Science's MISTRZ academic grant for professors (2013). In addition, he has twice received a grant in the FNP's TEAM programme.

The professor has published about 240 scientific papers in journals such as Angewandte Chemie, Journal of the American Chemical Society and Chemical Communications, including a dozen or so overviews. His works have been cited almost 4,700 times. He has delivered over 40 lectures at conferences and about 70 at university-level schools, including Harvard and Caltech. He has registered many patents.



The Foundation for Polish Science Prize 2017 was granted in recognition of Prof. Daniel Gryko's achievements in synthesizing corroles and porphyrins and studying their photophysical properties.

Prof. Daniel Gryko's field of research is the chemistry of porphyrins, particularly corroles, which are organic dyes with multiple applications. Prof. Gryko designs and synthesizes such compounds. He has developed an effective method to obtain them, opening up new prospects for their application. Prof. Daniel Gryko's main achievement is a method of synthesizing meso-substituted corroles, especially ones that contain two different types of substituent around a macrocyclic core. This offers access to corroles whose properties can be changed and adjusted to different needs. They can also be attached to a surface or another chromophore in a specifically defined location. Thanks to this research, the coordination chemistry of corroles is seeing unprecedented development. Over the past six years scientists have obtained complexes with seventeen new metals. If it weren't for Prof. Gryko's work, such progress would have been impossible, because a sufficient amount of corroles would not have been available for research.

Prof. Gryko's achievements have opened the way to many potential applications. Water-soluble corrole complexes are raising hopes in medicine, as they could serve as catalysts for the decomposition of reactive nitrogen compounds in cells (related to Huntington's, Parkinson's and Alzheimer's diseases). It was recently also proved that corrole complexes effectively destroy cancer cells. Some corrole complexes have been patented and are undergoing clinical trials.

Porphyrins and their "relatives" corroles are strong light emitters. This is especially true of complexes with gallium and phosphorus. This property is invaluable when it comes to studying intracellular processes in molecular biology and also in medical diagnostics. The strong red fluorescence of corroles means there is a possibility they could be used as fluorescent probes.
Porphyrinoids are responsible for two crucial life processes: reversible binding of oxygen in the blood and photosynthesis.

Corroles prepared using Prof. Daniel Gryko's methodology have also been used in research on carbon monoxide detection, oxygen reduction, photoelectrochemical cells etc.

Although synthesis is Prof. Gryko's field, he initiated a lot of research that resulted, among other things, in checking the usefulness of corroles in research on electron transfer and water oxygenation, their two-photon absorption, in obtaining the first lanthanide corrole complexes etc.

Prof. Daniel Gryko's methodology has become popular with researchers all over the world. He has expanded his field of interest to include chlorites, artificial photosynthesis, two-photon absorption and intramolecular excited-state proton transfer. His work has contributed to further research in all these fields.