NINETH CRISTOFOR I. SIMIONESCU SYMPOSIUM
FRONTIERS IN MACROMOLECULAR AND SUPRAMOLECULAR SCIENCE
12 – 14 June 2017

SYMPOSIUM PROGRAM

June 12 • Romanian Academy, Bucharest, Romania
June 13 – 14 • "Petru Poni" Institute of Macromolecular Chemistry Iasi, Romania

This Symposium is part of a project that has received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreement No 667387 WIDESPREAD 2-2014 SupraChem Lab

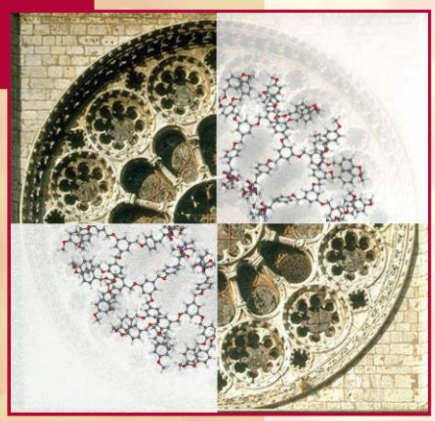
LRSM
The Laboratory for Research on the Structure of Matter

ACADEMIA ROMANA

Institutul de Chimie Macromoleculara
PETRU PONI

Frontiers in Macromolecular and Supramolecular Science

Nineth Cristofor I. Simionescu Symposium



Featuring:

David M. Haddleton
Warwick University

Michael L. Klein
Temple University, Philadelphia

Virgil Percec
University of Pennsylvania

Martin Möller
RWTH, Aachen

Peter H. Seeberger
MPI, Potsdam-Golm and
Free University of Berlin

Doron Shabat
Tel Aviv University

Conference Location
Romanian Academy
Calea Victoriei 125
Bucharest, Romania

date: June 12, 2017
time: 9:30am-3:00pm
place: Romanian Academy Bucharest

NSF

NSF-DMR05-1120901

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MRSEC Penn

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Calin Deleanu: calin.deleanu@yahoo.com, tel. +40-744-340456

ROMANIAN ACADEMY

Calea Victoriei 125, Bucharest, Romania

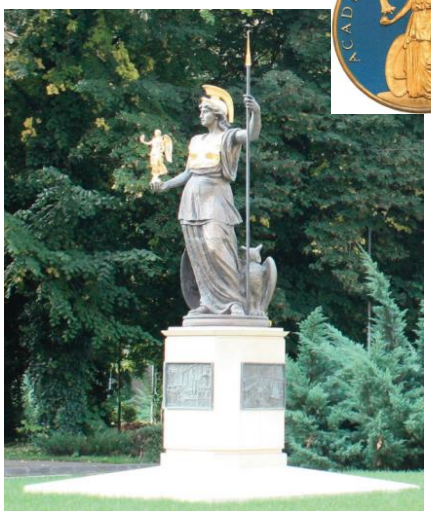
Sunday, June11

	Registration of Participants
	Team building activities

Monday, June 12

Location • *Academy Hall*, Romanian Academy, Bucharest, Romania

	$09^{00} – 09^{30}$
	Opening Ceremony
$09^{00} – 09^{15}$	**Welcome Address** **Ionel Valentin VLAD** *President of Romanian Academy*
$09^{15} – 09^{30}$	**Evocation of Cristofor I. Simionescu** **Virgil PERCEC** *University of Pennsylvania, Philadelphia, USA*
	$09^{30} – 11^{00}$
	Session 1. CONFERENCES Chair: Bogdan C. SIMIONESCU, Virgil PERCEC
$09^{30} – 10^{15}$	**Liquids, Crystals, Liquid Crystals, Plastic Crystals, and More … ?** **Michael L. KLEIN** *Temple University, Philadelphia, PA, USA*
$10^{15} – 11^{00}$	**Soft Microrobots** **Martin MÖLLER** *RWTH, Aachen, Germany*
$11^{00} – 11^{20}$	Coffee Break
	$11^{20} – 12^{50}$
	Session 2. CONFERENCES Chair: Simona PERCEC, Bogdan C. SIMIONESCU
$11^{20} – 12^{05}$	**SET LRP of Acrylamide in Aqueous Media and Sulfur Free RAFT in Emulsion** **David M. HADDLETON** *Warwick University, UK*
$12^{05} – 12^{50}$	**Creating Carbohydrate Materials from Scratch** **Peter H. SEEBERGER** *MPI, Potsdam-Golm and Free University of Berlin, Germany*
$12^{50} – 13^{30}$	Lunch
	$13^{30} – 15^{00}$
	Session 3. CONFERENCES Chair: Michael L. KLEIN, Calin DELEANU
$13^{30} – 14^{15}$	**Programming Protocells with Sequence Defined Self-Organizing Building Blocks** **Virgil PERCEC** *University of Pennsylvania, Philadelphia, PA, USA*
$14^{15} – 15^{00}$	**Unlocking the Potential of Chemiluminescence** **Doron SHABAT** *Tel Aviv University, Israel*
$16^{00} – 19^{00}$	Transfer to Iasi
$20^{00} – 22^{00}$	Dinner



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Institutul de Chimie Macromoleculara "Petru Poni"

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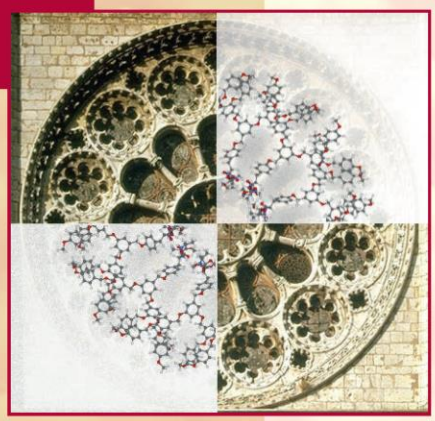

Featuring:

David M. Haddleton
Warwick University

Michael L. Klein
Temple University, Philadelphia

Andrei Neamtu
"Petru Poni" IMC, Iasi

Virgil Percec
University of Pennsylvania

Mariana Pinteala
"Petru Poni" IMC, Iasi

Alexandru Rotaru
"Petru Poni" IMC, Iasi

Peter H. Seeberger
MPI, Potsdam-Golm and
Free University of Berlin

Doron Shabat
Tel Aviv University

Conference Location
"Petru Poni" Institute of
Macromolecular Chemistry
Aleea Grigore Ghica Voda 41ª
700487 Iasi, Romania

date: June 13 June 14, 2017
time: 9:30am-5:00pm 9:30am-3:00pm
place: "Petru Poni" Institute of Macromolecular Chemistry, Iasi

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PETRU PONI" INSTITUTE OF MACROMOLECULAR CHEMISTRY,

41A Grigore Ghica Voda Alley, 700487 Iasi, Romania

Tuesday, June 13

Location • *Conference hall* "Petru Poni" Institute of Macromolecular Chemistry, Iasi

$09^{30} – 10^{00}$

Opening Ceremony

$09^{30} – 9^{45}$ **Welcome Address**
Valeria HARABAGIU
"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania

$09^{45} – 10^{00}$ **Evocation of Cristofor I. Simionescu**
Virgil PERCEC
University of Pennsylvania, Philadelphia, USA

$10^{00} – 12^{15}$

Session 4. CONFERENCES

Chair: Mariana PINTEALA, Virgil PERCEC

$10^{00} – 10^{45}$ **Liquids, Crystals, Liquid Crystals, Plastic Crystals, and More ... ?**
Michael L. KLEIN
Temple University, Philadelphia, PA, USA

$10^{45} – 11^{05}$ Cafee break

$11^{05} – 11^{50}$ **From Light Empowered to Self-Oscillating Microgel Objects – Rate and Directional Control of Microscopic Morphing out of Equilibrium**
Martin MÖLLER
RWTH, Aachen, Germany

$11^{50} – 12^{35}$ **Cell Imaging: from New Non-toxic Fluorescent Dyes to Raman Probes based on Metal Nanoparticles – Carbon Nanotube Nanoconjugates**
Alexandru ROTARU
"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania

$12^{35} – 13^{30}$ Lunch – *Library Hall*

$13^{30} – 15^{45}$

Session 5. CONFERENCES

Chair: Valeria HARABAGIU, Michael L. KLEIN

$13^{30} – 14^{15}$ **Design of Gene-Activated Matrix for Bone Repair**
Geta DAVID,[1] Cristina URITU,[2] Bogdan C. SIMIONESCU,[1,2] Mariana PINTEALA[2]
[1]"Gh. Asachi" Technical University of Iasi, Romania
[2]"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania

$14^{15} – 15^{00}$ **Programming Protocells with Sequence Defined Self-Organizing Building Blocks**
Virgil PERCEC
University of Pennsylvania, Philadelphia, PA, USA

$15^{00} – 15^{45}$ **Creating Carbohydrate Materials from Scratch**
Peter H. SEEBERGER
MPI, Potsdam-Golm and Free University of Berlin, Germany

$15^{45} – 16^{15}$ Coffee Break

$16^{15} – 17^{45}$

Session 6. ORAL COMMUNICATIONS

Chair: Doron SHABAT, Calin DELEANU

$16^{15} – 16^{40}$ **Nanostructured Electrochemical Sensors for Biomedical Applications**
Adina ARVINTE
"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania

16^{40} – 17^{05}	**Adsorbtion of Anionic Dyes on Amphiphilic Cationic Hydrogels based on Crosslinked Dextran** **Cristina STANCIU, Marieta NICHIFOR** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
17^{05} – 17^{30}	**Evaluation of Polymer-based Fibrous Materials as Oil Pill Sorbents: Experimental Design, Modeling and Optimization** **Corneliu COJOCARU, Petronela PASCARIU DORNEANU, Petrisor SAMOILA, Lucia PRICOP, Liviu SACARESCU** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
17^{30} – 17^{55}	**Phenothiazine Dyes as Efficient Luminescent Materials** **Andrei BEJAN,[1] Bogdan C. SIMIONESCU,[1,2] Luminita MARIN[1]** *[1]"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania* *[2]"Gh. Asachi" Technical University of Iasi, Romania*
19^{00} – 21^{00}	Dinner

Wednesday, June 14

Location • *Conference hall* "Petru Poni" Institute of Macromolecular Chemistry, Iasi

09^{30} – 11^{00}

Session 7. CONFERENCES

Chair: Simona PERCEC, Marcela MIHAI

09^{30} – 10^{15}	**SET LRP of Acrylamide in Aqueous Media and Sulfur Free RAFT in Emulsion** **David M. HADDLETON** *Warwick University, UK*
10^{15} – 11^{00}	**Unlocking the Potential of Chemiluminescence** **Doron SHABAT** *Tel Aviv University, Israel*
11^{00} – 11^{30}	Coffee Break

11^{30} – 12^{40}

Session 8. CONFERENCES

Chair: David M. HADDLETON, Alexandru ROTARU

11^{30} – 12^{15}	**Modelling and Simulation of Ion and Water Channels in Phospholipid Membranes** **Andrei NEAMTU,[1,2] Tudor VASILIU[1]** *[1]"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania* *[2]"Gr. T. Popa" University of Medicine and Pharmacy of Iasi, Romania*
12^{15} – 12^{40}	**Thiosemicarbazone Derivatives as Potential Ribonucleotide Reductase R2 Inhibitors** **Mirela ZALTARIOV, Maria CAZACU, Sergiu SHOVA** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
12^{40} – 13^{40}	Lunch – *Library Hall*

13^{40} – 14^{55}

Sessions 9. ORAL COMMUNICATIONS

Chair: Luminita MARIN, Peter SEEBERGER

13^{40} – 13^{55}	**Self-assembled Polymeric Vectors for Gene Delivery** **Bogdan Florin CRACIUN, Lilia CLIMA** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*

13^{55} – 14^{10}	**1,3-Dithiolium Flavonoids with Antibacterial Properties** **Lucian Gabriel BAHRIN**[1,2] **Lucian Mihail BIRSA**[2] [1]*"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania* [2]*"Alexandru Ioan Cuza" University of Iasi, Romania*
14^{10} – 14^{25}	**Experiment Design and Molecular Dynamics Simulations in Polyplex Formation** **Tudor VASILIU, Mariana PINTEALA** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
14^{25} – 14^{40}	**Zinc Oxide Nanocrystals Growth on Cellulose Acetate Butyrate Ultrafine Fiber Mats for Photocatalytic Degradation of Organic Dyes** **Petronela PASCARIU, Ana Lavinia VASILIU, Niculae OLARU** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
14^{40} – 14^{55}	**Removal of Anionic Dye by Novel Chitosan Functionalized Samarium Doped Cobalt Ferrite** **Andra Cristina HUMELNICU, Corneliu COJOCARU, Petronela PASCARIU DORNEANU, Petrisor SAMOILA, Valeria HARABAGIU** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
14^{55} – 15^{00}	**Closing of the Symposium** **Virgil PERCEC** *University of Pennsylvania, Philadelphia, USA* **Valeria HARABAGIU** *"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
15^{30} – 17^{30}	***Visit at The Palace of Culture – "Moldova" National Museum Complex***
19^{00} – 21^{00}	Dinner

The Palace of Culture – "Moldova" National Museum Complex

INVITED SPEAKERS

(ALPHABETICAL ORDER)

David M. HADDLETON obtained his PhD under the supervision of Professor Robin Perutz in York and joined the faculty at the University of Warwick in 1993 after 6 years at ICI/Zeneca. He was promoted to full Professor of Chemistry in 1998. His research focuses on controlled living radical polymerisation to give macromolecules of designed, desired, and targeted structure for biosciences and material applications. Professor Haddleton is a coauthor of 400 peer-reviewed scientific papers, 20 patents, and 5 book chapters and has mentored 55 successful Ph.D. candidates. His work has been cited in the scientific literature 13,000 times (Hirsch Index = 68, according Scopus – 07.06.2017) and has been the recipient of multiple awards including the Macro Group UK Medal, the Chemistry World, "Entrepreneur of the Year" Royal Society of Chemistry Prize, the Lord Stafford award for "Best University Spin-off" company, and the Medema Metal from the Dutch polymer community. He is currently the editor-in-chief of Polymer Chemistry, a high impact factor Royal Society of Chemistry journal.

Michael L. KLEIN is Laura H. Carnell Professor of Science and Director of the Institute for Computational Molecular Science in the College of Science and Technology at Temple University in Philadelphia, USA. He was previously the Hepburn Professor of Physical Science in the Center for Molecular Modeling at the University of Pennsylvania. Klein obtained a B.Sc. from the University of Bristol in 1961, followed by a Ph.D. in 1964. He was a researcher at the National Research Council 1968-1987, and joined the faculty of the University of Pennsylvania in 1987.

Professor Klein's research in computational chemistry, particularly statistical mechanics, intermolecular interactions, and modelling of condensed phases and biophysical systems, is among the most highly cited in the field. He received the Aneesur Rahman prize in 1999, which is the highest honor given by the American Physical Society for work in computational physics, and was elected to the United States National Academy of Sciences in 2009. Publications: 638 papers and 4 books (Edited); Hirsch Index = 90 (according Scopus – 07.06.2017).

Martin MÖLLER is Scientific Director, Chair of Textile and Macromolecular Chemistry, at the Institute for Textile Chemistry and Macromolecular Chemistry at RWTH Aachen University and is known for his research into polymer chemistry and functional nanotechnology. Möller studied chemistry in Hamburg and Freiburg and the doctorate 1981 in Freiburg. As post-doctoral candidate, he was a Fedor-Lynen student at the University of Massachusetts at Amherst. He then returned to Freiburg as a research associate at the Institute for Macromolecular Chemistry, where he habilitated in 1989 and subsequently became professor of Polymer Technology and Macromolecular Materials at the University of Twente, professor and head of the Department of Organic and Macromolecular

Chemistry at the University of Ulm (1993) and professor of Textile Chemistry and Macromolecular Chemistry at RWTH Aachen University (2002). Since 2003 he is the director of the Deutsches Wollforschungsinstitut (DWI). The research of Möller's group is directed towards oligomer and polymer building blocks that can undergo self-assembly to complex nanostructures and functional systems. Emphasis is laid on water-soluble and water-born polymers. This involves the synthesis of ultra-small particles, as well as synthesis of uniform linear and branched macromolecules with functional and reactive side and end groups. He is a member of the Academy of Sciences of North Rhine-Westphalia (since 2005) and the German Academy of Engineering (Acatech). In 2003, he received the Körber Prize for European Science for working on a light-driven molecular engine, focusing on surfaces. For 2014 Möller was awarded the Hermann-Staudinger-Prize. (Hirsch Index = 65, according Scopus – 07.06.2017)

Andrei NEAMȚU studied physics at „Al. I. Cuza" University and medicine at „Gr. T. Popa" University of Medicine and Pharmacy (UMF) of Iași. He received his PhD in 2007 at the UMF Iasi, Romania where now is associate professor at the Physiology Department of UMF Iasi. Scientific fields of interests: molecular modelling and simulations of membrane proteins, nucleic acids and glycosaminoglycans, inclusion complexes of cyclodextrins/modified cyclodextrins with different drugs, artificial membrane structures, biomaterials. Coauthor of more than 30 publications, 5 books, 2 book chapters and many participations at national and international conferences. Project leader of 1 national project and member in other 4 projects. Five awards at national/international scientific meetings.

Virgil PERCEC received his B.S. in organic and macromolecular chemistry from the Polytechnic Institute in Iasi and his PhD in macromolecular chemistry from "P. Poni" Institute of Macromolecular Chemistry, Iasi, Romania. After short postdoctoral stays at the Institute of Macromolecular Chemistry, Hermann Staudinger Hause of the University of Freiburg, Germany (July and August, 1981) and the Institute of Polymer Science of the University of Akron, USA (September, 1981 to March, 1982) he joined the Department of Macromolecular Science of Case Western Reserve University, Cleveland, USA in March, 1982 as an Assistant Professor. He was promoted to Associate Professor in 1984, to Full Professor in 1986 and to Leonard Case Jr. Chair in 1993. In 1999 he joined the Department of Chemistry at the University of Pennsylvania, Philadelphia as the inaugural P. Roy Vagelos Chair and Professor of Chemistry where he is leading a research group of undergraduate, graduate and postdoctoral students performing fundamental studies at the interface between organic, catalysis, supramolecular, macromolecular chemistry, liquid crystals, nanoscience and biology where he contributed over 700 refereed publications (Hirsch Index = 89, according Scopus – 07.06.2017), 80 patents, 18 books and Special Issues and over 1140 Endowed, Plenary and Invited Lectures. He is the editor of the Journal of Polymer Science: Part A: Polymer Chemistry (since 1996) and of the Book Series "Liquid Crystals" (since 2007). Professor Percec serves on the Editorial and Advisory Boards of 20 International Journals, on the Scientific Advisory Board of Symyx Company, Henkel Company, Molecular Foundry, Berkeley and Lawrence Berkeley National Laboratory. He is a consultant to numerous US and International Companies and Governmental Offices.

Mariana PINTEALA studied organic chemistry at Polytechnic Institute, Iasi, Romania and received her PhD in 1995 at the "Gh. Asachi" Technical University of Iasi, Romania. She is senior researcher at "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania and from 2011 is the Leader of the IntelCentre Department (www.intelcentru.ro). For periods of time she held research/postdoctoral positions at CNRS – Universite d'Evry-Val d'Essonne, France and University of Detroit Mercy, USA. Scientific fields of interest: synthesis of nanoconjugates with biomedical application, inclusion complexes of cyclodextrins/modified cyclodextrins with different drugs, pseudo- and polyrotaxanes of cyclodextrins with (co)polymers, synthesis and characterization of polymers and copolymers, cationic, anionic and radical copolymerization, structure-property relationship evaluation, data analysis and interpretation, interpolymer complexes between hydrophobic – hydrophylic copolymers, blend and networks containing silicon-based polymers, aggregation of block copolymers in solution by fluorescene, purification and analysis of antibiotics, synthesis and characterization of silicone resins, PEO membranes. More than 100 publications in ISI journals, 1 book, 10 book chapters and more than 50 participations at national and international conferences. Project leader of numerous European and national projects. "Nicolae Teclu" award of Romanian Academy in 1994 and 2015 Award of Romanian Chemical Society. (Hirsch Index = 15, according Scopus – 07.06.2017)

Alexandru ROTARU studied organic chemistry at State University of Moldova (Rep. Moldova) and received his PhD in 2005 at the "Al. I. Cuza" University of Iasi, Romania. He is senior researcher at "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania since 2012. During his PhD studies Alexandru Rotaru spent twelve moths DAAD scholarship at Department of Organic Chemistry, Heidelberg University, Germany. After the completion of his PhD studies he continued with postdoctoral position at Inorganic Chemistry Department, Heidelberg University, Germany, followed by another postdoctoral position at Aarhus University, Denmark. Scientific fields of interest include: organic synthesis, oligonucleotide chemistry, preparation and characterization of DNA-based nanostructures, supramolecular chemistry, metal nanoparticles and nanoconjugates of metal nanoparticles with carbon nanotubes. Alexandru Rotaru is author and co-author of 35 publications and multiple participations at national and international conferences. He is project member and group leader in European and national projects. Since 2015 he is the director of a national project for the development of young research groups. Member of the Romanian Chemical Society. (Hirsch Index = 11, according Scopus – 07.06.2017)

Doron SHABAT is professor at Tel Aviv University, Israel. He studied chemistry at the Technion-Israel Institute of Technology between 1987 and 1990. After obtaining his B.Sc. degree, he continued toward his Ph.D. degree under the supervision of Prof. Ehud Keinan in the field of catalytic antibodies. Upon the completion of his Ph.D. thesis in 1997, he joined a group led by Profs. Richard A. Lerner and Carlos F. Barbas, III at The Scripps Research Institute in La Jolla, California as a postdoctoral fellow. There, he continued to work in the area of catalytic antibodies. In 2000, he returned to Israel to start his independent career in the School of Chemistry at Tel Aviv University as a senior lecturer. He was promoted

to the rank of associate professor in 2005 and to full professor in 2008. His research is focused in bioorganic chemistry with particular interests in self-immolative molecular systems and long-wavelength fluorescent dyes for in vivo imaging. He is the recipient of the Juludan Prize for 2005, administered by the Technion-Israel Institute of Technology, the Israel Chemical Society's Prize (2005) for Outstanding Young Chemists and the Frost Fellowship (2012 and 2014) administrated by The Scripps Research Institute. Prof. Shabat is the author and coauthor of over 100 peer-review publications, book chapters and patent applications. (Hirsch Index = 37 according Scopus – 07.06.2017)

Peter H. SEEBERGER studied chemistry in Erlangen (Germany) and completed a PhD in biochemistry in Boulder (USA). After performing research at the Sloan-Kettering Cancer Center Research in New York he built an independent research program at MIT where he was promoted to Firmenich Associate Professor of Chemistry with tenure. After six years as Professor at the Swiss Federal Institute of Technology (ETH) Zurich he assumed positions as Director at the Max-Planck Institute for Colloids and Surfaces in Potsdam and Professor at the Freie University of Berlin in 2009. He is honorary Professor at the University of Potsdam. Professor Seeberger's research on the chemistry and biology of carbohydrates, carbohydrate vaccine development and continuous flow synthesis of drug substances spans a broad range of topics from engineering to immunology and has been documented in over 400 peer-reviewed journal articles (Hirsch Index = 65, according Scopus – 07.06.2017), four books, more than 35 patents, over 170 published abstracts and more than 700 invited lectures. This work was recognized with more than 25 international awards from the US (e.g. Arthur C. Cope Young Scholar Award, Horace B. Isbell Award, Claude S. Hudson Award from the American Chemical Society), Germany (e.g. Körber Prize for European Sciences), Holland (Havinga Medal), Israel (Honorary Lifetime Member Israel Chemical Society), Japan (Yoshimasa Hirata Gold Medal), Switzerland ("The 100 Most Important Swiss") and international organizations (Whistler Award 2012, Int. Carboh. Soc.). In 2013 he was elected to the Berlin-Brandenburg Academy of Sciences.

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