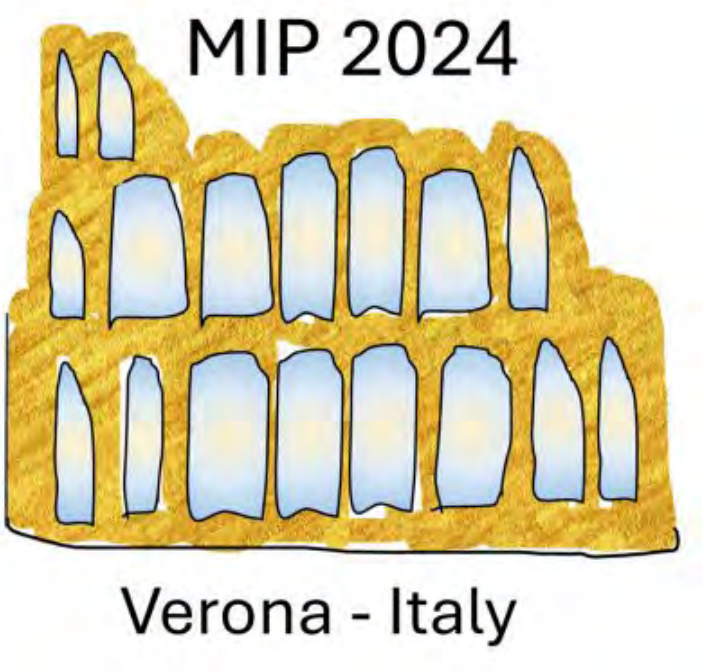
The 12th International Conference on Molecular Imprinting – MIP2024

Verona, Italy, 19-21 June 2024



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The University of Verona, Italy – Dept. of Biotechnology, in association with the Society for Molecular Imprinting are pleased to welcome you to the 12th International Conference on Molecular Imprinting – MIP2024, to be held in Verona, Italy on 19-21 June 2024.

The **main venue for the conference is the Conference Centre of the Polo Universitario Santa Marta (University of Verona, Polo Santa Marta, Via Cantarane, 24, 37129 Verona VR).** Registration and a welcome reception will be held at the venue on the afternoon/evening of Tueday 18 June.

The scientific program will be presented over two and a half days, and will cover advances in all aspects of the science, technology and applications of molecularly imprinted materials. Whilst the meeting will include in-depth talks by acknowledged experts in the field, it will also provide ample opportunity for younger or less experienced researchers to showcase their contributions, either through short oral or poster presentations.

The topics for the conference may include, but are not limited to:

- Synthesis of imprinted materials, monomers and templates
- Novel morphologies and formats of imprinted materials
- Molecular modelling aspects of imprinting
- Sensors, assays and other devices featuring imprinted materials
- Imprinted materials in separation science and sample preparation
- Imprinted materials in catalysis
- Imprinted materials in protein folding, enzyme inhibition and stabilisation
- Biologically-active imprinted materials
- Imprinted materials in biomedicine and drug delivery

This will be the first meeting under the auspices of the Society to be held in person since the pandemic and is therefore a golden opportunity to connect with other individuals and groups working in the field or to meet old friends for the first time in a number of years. While we hope that the pandemic is behind us, please take precautions with personal hygiene and wear a mask if you feel unsafe mixing with a group of people.

The meeting organization is curated by Sabiwork s.r.l. Padova (Italy), that will have representatives at the helpdesk to assist with any issue.

On behalf of the organisers, we wish you a safe and successful conference!

Organising Committee

- Alessandra Maria Bossi (University of Verona, Italy)
- Claudio Baggiani (University of Torino, Italy)
- Boris Mizaikoff, (Universität Ulm, Germany)
- Peter Lieberzeit, (University of Vienna, Austria)
- Karsten Haupt (University of Compiegne, France)
- Mike Whitcombe (President of the Society for Molecular Imprinting)
- Pınar Çakır Hatır (Istinye University, Turkey)

Scientific Advisory Board

- Alessandra Maria Bossi (University of Verona, Italy)
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- Sergey Piletsky (University of Leicester, UK)
- Börje Sellergren (Malmö University, Sweden)
- Zhen Liu (Nanjing University, P.R. China)
- Huiqi Zhang (Nankai University, P.R. China)
- Antonio Martín-Esteban (INIA-CSIC Madrid, Spain)
- Boris Mizaikoff, (Universität Ulm, Germany)
- Peter Lieberzeit, (University of Vienna, Austria)

Local Organisers

- Alessandra Maria Bossi (University of Verona, Italy)
- Mimimorena Seggio (University of Verona, Italy)
- Alice Marinangeli (University of Verona, Italy)
- Todd Cowen (University of Verona, Italy)
- Deniz Bayulgen (University of Verona, Italy)
- Daniel Moranduzzo (University of Trento, Italy)
- Reza Mahdavi (University of Trento, Italy)
- Devid Maniglio (University of Trento, Italy)
- Thea Serra (University of Torino, Italy)
- Valentina Testa (University of Torino, Italy)
- Claudio Baggiani (University of Torino, Italy)

SPECIAL JOURNAL ISSUE

iScience, the interdisciplinary open access journal published by Cell Press, is publishing a special issue on the topic of ''Translational and interdisciplinary advances of molecular imprinting technology''.

Molecular imprinting enables the creation of artificial, tailor-made, selective recognition sites in polymeric materials and is increasingly exploited for biomedical, environmental and translational applications.

This Special Issue, brought forth in collaboration with Prof. Alessandra Maria Bossi, Prof. Zhen Liu and Prof. Boris Mizaikoff, encompasses advances in the field of molecularly imprinted polymers (MIP) synthesis and formats, with emphasis on rational design by molecular modelling, linking simulations and experiments, 3D printing architectures and novel morphologies, and aims to highlight state-of-the-art research advances and review articles focusing on interdisciplinary work exploiting MIPs as well as strategies to overcome the existing challenges in the practical use, translational potential, and industrial applications of MIPs.

The scope of the Special Issue includes, but is not limited to:

- Biologically-active imprinted materials with functional properties, for pharmaceutical and drug delivery applications, theragnostics and imaging, protein folding, enzyme inhibition and stabilisation
- Molecular imprinting for biomedical applications, such as biomonitoring, disease diagnosis and therapy, viral inhibition, and poison/toxin neutralisation
- MIP-based (miniaturized) devices for sensing, wearable or other applications and assays
- Molecular imprinting technology for environmental or food applications such as environmental or food analysis, treatment and safety, or toxic compounds detection and removal
- Synthetic innovations in the field of green chemistry for molecular imprinting, challenges, and sustainable developments

Do you think your research fits the scope of the special issue? If so, we encourage you to discuss with our editor, Maria Mytiliniou (M.Mytiliniou@cell.com)

The special issue is scheduled for publication in 2025, and **the tentative deadline of submission is Dec. 31st, 2024**. iScience is a **fully open access** journal, so the standard APC will be charged for the paper if accepted. The standard editorial review and peer-review processes will be applied. With regard to manuscript type, we accept Original Research, Review, or Perspective.

MIP2024 Plenary, Invited and Keynote Speakers

The conference organisers are happy to announce the Plenary, Invited and Keynote speakers at MIP2024.

Plenary Speaker: János Vörös

The Plenary lecture will be delivered by János Vörös, Professor in the Institute for Biomedical Engineering of the University and ETH Zurich (Department for Information Technology and Electrical Engineering) heading the Laboratory for Biosensors and Bioelectronics since 2006.

János Vörös studied Physics at the Eötvös Loránd University in Budapest. After receiving a diploma in Physics in 1995, he was a doctoral student at the Department of Biological Physics of the Eötvös University (in collaboration with Microvacuum Ltd.) where he received his PhD in Biophysics in 2000. From 1998 he was a member of the BioInterface group in the Laboratory for Surface Science and Technology at the Department of Materials, ETH Zurich as a visiting scientist, postdoc, and from 2004, group leader of the Dynamic BioInterfaces group (until 2006).

Prof. Vörös is interested in research and teaching in the areas of Biosensors, Bioelectronics, and Bottom-up Neuroscience. His research group focuses on the development of novel biosensor techniques for diagnostics and drug discovery; on interacting with well-defined neural networks; as well as on stretchable bioelectronic devices.

Wulff Memorial Lecturer: Ken Shea

Kenneth J. Shea, Distinguished Professor of Chemistry at the University of California, Irvine.

Career: Postdoctoral Research Fellow, California Institute of Technology; Graduate Research, The Pennsylvania State University; Currently Distinguished Professor of Chemistry, University of California, Irvine

Professor Shea is a former chair and currently Distinguished Professor of Chemistry, Emeritus in the Department of Chemistry at the University of California, Irvine. He is a Cope Scholar, a Winston Churchill College Overseas Fellow, Cambridge University and is a Fellow of the American Chemical Society's Division of Polymeric Materials, Science and Engineering and of the American Chemical Society's Division of Polymer Chemistry. He is an Adjunct Professor, Beijing University of Chemical Technology, Beijing, China and Zhejiang University, Hangzhou, China.

He has served as a member of the Physical and Life Science Directorate External Review Committee of the Lawrence Livermore National Laboratory and a member of the Lawrence Livermore National Security, LLC Science & Technology Committee.

Professor Shea's research interests are in synthetic and mechanistic organic chemistry and polymer and materials chemistry. He has mentored over 150 graduate and postdoctoral students at the University of California.

Mosbach Memorial Lecturer: Chris Lowe

Professor Emeritus Christopher R. Lowe, OBE, FREng was trained as a biochemist and following postdoctoral positions in Liverpool and Lund and a lectureship at the University of Southampton, he was appointed to the University of Cambridge in 1984 to found the Institute of Biotechnology, which he ran for 23 years prior to subsequently merging it with the Department of Chemical Engineering to form the Department of Chemical Engineering & Biotechnology.

He is a Fellow of Trinity College, the Royal Academy of Engineering and a Life Member of the Royal Institution. He has over 420 peer-reviewed publications, 8 books and monographs, >100 patents and has supervised 99 PhD students.

He has won a number of National and International prizes: Pierce Award for Outstanding Contributions to the Field of Affinity Chromatography (1989), Queen's Award for Technological Achievement (1996), Queen's Anniversary Prize for Higher and Further Education (2007), Most Entrepreneurial Scientist of the UK, and an OBE in the Queen's New Year Honours.

He has been the driving force for the establishment of 12 spin-out companies, is involved with a number of national and international granting and governmental organisations. He established two pioneering Master's courses: Bioscience Enterprise (MBE) (2002) and Therapeutic Sciences (MTS) (2018). After formal retirement, he was re-employed by the University to establish the Cambridge Academy of Therapeutic Sciences (CATS) to promote research, translation, education and policy in therapeutic sciences.

Invited Keynote Speaker:

Zeynep Altintas, Kiel University, Germany.

Keynote Speakers:

Claudio Baggiani, University of Torino, Italy.

Alessandra Maria Bossi, University of Verona, Italy.

Mehmet Dinc, Hahn-Schickard, Ulm, Germany.

Karsten Haupt, Université de Technologie de Compiègne, Compiègne, France.

Wlodzimierrz Kutner, Polish Academy of Sciences, Warsaw, Poland.

Peter Lieberzeit, University of Vienna, Austria.

Zhen Liu, Nanjing University, China.

Antonio Martín-Esteban, Instituto Nacional de Investigación y Tecnología Agraria y Alimentaria, Madrid, Spain

Ian Nicholls, Linnaeus University, Sweden.

Sergey Piletsky, University of Leicester, UK.

Börje Sellergren, Malmö University, Sweden.

Michael Whitcombe, President of the Society for Molecular Imprinting, UK.

Huiqi Zhang, Nankai University, Tianjin, China

MIP2024 Day 0: Tuesday, 18th June 2024: Registration and Welcome Drinks Reception

16:00 - 18:00	**Conference Registration** - University of Verona, Polo Santa Marta, Via Cantarane, 24, 37129 Verona VR
17:00 - 19:00	followed by: **Welcome Reception**

MIP2024 Scientific Program Day 1: Wednesday, 19th June 2024

08:50-09:10	**Opening of the MIP2024 conference** by Prof. Alessandra Maria Bossi (Conference Chairman), Dr. Mike Whitcombe (SMI President), Prof. Karsten Haupt & Prof. Börje Sellergren (SMI Vice-Presidents) & Prof. Claudio Baggiani (Conference Co-Chairman).
09:10-10:45	**Session 1** - The legacy of non-covalent imprinting. Session Chairpersons: Karsten Haupt and Mike Whitcombe
09:10-09:45	Mosbach Lecture **Professor Klaus Mosbach: A Friend, Mentor and Visionary Scientist** Christopher R. Lowe *University of Cambridge, Trinity College, Cambridge, CB2 1TQ, UK*
09:45-10:45	Session 1 Keynote speakers
09:45-10:05	Keynote 1 **MIP nanoparticles for diagnostics – are we ready for the market?** Sergey Piletsky *Leicester Biotechnology Group, School of Chemistry, University of Leicester, Leicester, LE1 7RH, UK*
10:05-10:25	Keynote 2 **Recent receptors designed using imprinting and adaptable ligand displays** Börje Sellergren *Biofilms Research Center for Biointerphases, Department of Biomedical Sciences, Malmö University, Sweden*
10:25-10:45	Keynote 3 **3D-Printing Meets MIPs: A New Era of Precision and Scalability in MIP Manufacturing** Mehmet Dinc, *Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany*
10:45-11:15	Coffee break
11:15-13:15	**Session 2** - Fundamentals in molecular imprinting. Session Chairpersons: Sergey Piletsky and Huiqi Zhang
11:15-11:50	Wulff lecture **Synthetic Antibodies and Molecularly Imprinted Polymers, Next Generation Protein Affinity Reagents?** Kenneth J. Shea *Department of Chemistry, University of California, Irvine, USA*
11:50-12:10	Keynote 4 **Evidence of Positive Cooperativity in the Binding Behavior of nanoMIPs Prepared by Solid Phase Polymerization Synthesis** Claudio Baggiani, *Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, 10125 - Torino, Italy*
12:10-12:30	Keynote 5 **A Closer Look on the Surfaces of MIP Thin Films** Peter A. Lieberzeit, *University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria*

12:30-12:45	Oral 1 **Design and optimization of molecularly imprinted polymer nanoparticles from mechanistic principles** Todd Cowen *University of Verona, Dept. of Biotechnology, Strada Le Grazie 15, 37134 Verona, Italy*
12:45-13:00	Oral 2 **Unlocking new avenues: Solid-state synthesis of molecularly imprinted polymers** Ede Bodoki, *Analytical Chemistry Department, "Iuliu Haţieganu" University of Medicine and Pharmacy, 4, Louis Pasteur St., 400349, Cluj-Napoca, Romania*
13:00-13:12	IND1 **MIP-based SARS-CoV-2 sensors in POCT connected to the Internet as novel strategies to address challenges in COVID-19 Diagnosis and Treatments** Riccardo Rovida, *Moresense, Italy*
13:12-14:50	Buffet Lunch and Poster Session I
14:50-16:00	**Session 3** - Sensing with MIPs 1 Session Chairpersons: Claudio Baggiani and Boris Mizaikoff
14:50-15:10	Keynote 6 **Machine-Learning-Aided Molecularly Imprinted Materials for Biomedical Applications** Zeynep Altintas *Department of Bioinspired Materials and Biosensor Technologies, Faculty of Engineering, Kiel University, Germany*
15:10-15:30	Keynote 7 **Chemosensors with extended-gate field-effect transistors (EG-FETs) coupled with polymers molecularly imprinted with epitopes of protein biomarkers predictive for idiopathic pulmonary fibrosis (IPF) for selective chemosensing of these biomarkers in body fluids** Wlodzimierz Kutner, *Faculty of Mathematics and Natural Sciences. School of Sciences, Cardinal Stefan Wyszynski University in Warsaw, Wóycickiego 1/3, 01-938 Warsaw, Poland*
15:30-15:45	Oral 3 **Detection of *Pseudomonas aeruginosa* Infection Using A Polydopamine-based Molecularly Imprinted Electrochemical Sensor** Lei Ye, *Division of Pure and Applied Biochemistry, Department of Chemistry, Lund University, 22100, Lund, Sweden*
15:45-16:00	Oral 4 **Non-invasive detection of glucose with electroactive molecularly imprinted polymers (e-MIPs): Application in wearable sensors** Oliver Jamieson, *University of Manchester, School of Engineering, Manchester, M20 4BX, United Kingdom*
16:00-16:25	Coffee break
16:25-17:00	**Session 4** - Short oral presentations (6 minutes + 1 minute for questions) Session Chairpersons: Wlodzimierz Kutner and Iva Chianella
16:25-16:32	S1 **Imprinted hollow TiO_2 microspheres for selective photocatalysis** Manuel Azenha, *CIQ-UP, Institute of Molecular Sciences, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal*

16:32-16:39	S2 **Molecularly imprinted polymer (MIP) nanoparticles for targeted breast cancer therapy and controlled drug delivery** Perla Ben Ghouzi , *Sorbonne Université, CNRS, PHysico-chimie des Electrolytes et Nanosystèmes InterfaciauX, PHENIX, F-75005 Paris,France.*
16:39-16:46	S3 **A glycan shield-targeting broad-spectrum antiviral nanomedicine provides potent therapeutic and prophylactic effects** Jingran Chen, Jingran Chen, *Nanjing University, Xianlin Campus, School of Chemistry and Chemical Engineering, State Key Laboratory of Analytical Chemistry for Life Science, 210023, China.*
16:46-16:53	S4 **Towards a Computational Polymer Design Protocol for Biomarkers Detection: 1) Prostate-specific Antigen, Water and Cyrene interactions** Callum Donaldson, *Department of Chemical Engineering, University of Bath, Claverton Down, Bath, Somerset BA2 7AY, United Kingdom*
16:53-17:00	S5 **Molecularly imprinted nanoprobes and time-resolved fluorescence spectroscopy in a nanosensing device for the detection of ultralow protein concentrations** Alice Marinangeli, *Dept. of Biotechnology, University of Verona, Strada Le Grazie 15, 37134 Verona, Italy*
17:00-17:45	**Session 5** - Sensing with MIPs 2 Session Chairpersons: Wlodzimierz Kutner and Iva Chianella
17:00-17:15	Oral 5 **Dual Fluorescent Molecularly Imprinted Polymers (MIPs) for Detection of the Prevalent Anti-Inflammatory Drug Diclofenac** Michelle Buchholz, *Technische Universität Berlin, Institut für Chemie, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Straße des 17.Juni 124, 10623 Berlin, Germany*
17:15-17:30	Oral 6 **Photo-iniferter polymerization: a convenient approach for integrating Molecularly Imprinted Polymers with nanostructured sensors** Tiziano Di Giulio, *Dipartimento di Scienze e Tecnologie Biologiche e Ambientali, Università del Salento, Lecce, Italy*
17:30-17:45	Oral 7 **Design of turn-on fluorescent imprinted polymers for sensing of lead in complex water samples** Catherine Branger, *University of Toulon, MAPIEM, Toulon, France*
17:45-17:55	Day 1 Closing remarks and announcements

MIP2024 Scientific Program Day 2: Thursday, 20th June 2024

09:00-09:35	**Session 6** - Invited Plenary Lecture Session Chairpersons: Börje Sellergren and Peter Lieberzeit
09:00-09:35	Plenary **Why does non-specific binding limit diagnostically relevant biosensors?** Janos Vörös *Laboratory of Biosensors and Bioelectronics, ETH Zurich, Institute for Biomedical Engineering, Switzerland*
09:35-10:10	**Session 7** - MIPs in biomedical applications 1 Session Chairpersons: Börje Sellergren and Peter Lieberzeit
09:35-09:55	Keynote 8 **Hydrophilic Hairy Fluorescent Molecularly Imprinted Polymer Micro- or Nanocapsules for Bioanalytical and Biomedical Applications** Huiqi Zhang, *State Key Laboratory of Medicinal Chemical Biology, Key Laboratory of Functional Polymer Materials (Ministry of Education), Tianjin Key Laboratory of Functional Polymer Materials, and College of Chemistry, Nankai University, Tianjin 300071, P. R. China*
09:55-10:10	Oral 8 **Molecularly Imprinted Polymers as synthetic antibodies for therapeutic applications** Claudia Herrera-Leon, *Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, France*
10:10-10:25	Oral 9 **MUC 1 analogue imprinted nanogels effectively discriminate glycopeptide positional isomers: on the way to early detection of glycosylated biomarkers** A. Khalid, *Department of Drug Sciences, University of Pavia, Viale Taramelli 12, 27100, Pavia (PV), Italy*
10:25-10:55	Coffee break
10:55-12:35	**Session 8** - MIPs in biomedical applications 2 Session Chairpersons: Chris Lowe and Ian Nicholls
10:55-11:15	Keynote 9 **Polishing molecularly imprinted polymers for biomedical applications** Zhen Liu *Nanjing University, China*
11:15-11:30	Oral 10 **Evolution of molecularly imprinted polymer nanoparticles as antibody mimics through the characterization of the molecular recognition process by single-molecule microscopy** Alessia Di Fiore, *Université de Technologie de Compiègne, France*
11:30-11:45	Oral 11 **Molecularly imprinted polymers to target and inhibit Gram-negative efflux pump membrane transporter** Tiffany Auroy, *Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Rue du Docteur Schweitzer, 60203 Compiègne Cedex, France.*

11:45-12:05	Keynote 10 - **Molecularly imprinted polymers - new materials and applications in synthetic biology** Karsten Haupt, *Université de Technologie de Compiègne, France*
12:05-12:20	Oral 12 **Magnetic Molecularly Imprinted Polymer for Cancer Therapy** Nébéwia Griffete, *Sorbonne Université, CNRS, PHysico-chimie des Electrolytes et Nanosystèmes InterfaciauX, PHENIX, F-75005 Paris,France.*
12:20-12:35	Oral 13 **Snapshot Imprinting: Rapid Identification of Cancer Cell Surface Proteins and Epitopes using Molecularly Imprinted Polymers** Stanislav S. Piletsky, *Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, London, W12 0BZ, UK*
12:35-14:20	Buffet lunch and Poster Session II
14:20-15:40	**Session 9** - Novel materials and classical monomers Session Chairpersons: Zhen Liu and Mike Whitcombe
14:20-14:40	Keynote 11 **Hierarchical Imprinting with Biopolymers** Ian A Nicholls, *Bioorganic & Biophysical Chemistry Laboratory, Department of Chemistry & Biomedical Sciences, Linnaeus University, SE-391 82 Kalmar, Sweden*
14:40-14:55	Oral 14 **Molecular Imprinting of Lipid and Glycan Toward Biological Membranes** Lianghai Hu *Center for Supramolecular Chemical Biology, State Key Laboratory of Supramolecular Structure and Materials, School of Life Sciences, Jilin University, Changchun 130023, China*
14:55-15:10	Keynote 12 **BioMIPs biocompatible biomimetics: molecular imprinting ties the knot with natural polymers. Synthesis, properties and future of silk molecularly imprinted nanoparticles.** Alessandra Maria Bossi, *University of Verona, Dept. Biotechnology, Strada Le Grazie 15, 37134, Verona, Italy*
15:10-15:25	Oral 15 **Biobased molecularly imprinted polymers for the development of new biocontrol formulations** Cyrian Thaeder, *Université de Technologie de Compiègne, CNRS UMR 7025, UPJV, Enzyme and Cell Engineering Laboratory, Rue du Docteur Schweitzer, 60203 Compiègne Cedex, France*
15:25-15:40	Oral 16 **Exploring cationic C-H hydrogen bonding for the preparation of stoichiometric imprinted polymer targeting sulphonic/sulfated molecules** Sudhirkumar Shinde, *School of Consciousness, Dr Vishwanath Karad MIT World Peace University Kothrud 411038 Pune India*
15:40-15:55	Oral 17 **Design of host-guest anchored epitope imprinting polymers and application to sensitive detection of cancer biomarkers** Qiong Jia *College of Chemistry, Jilin University, China*
15:55-16:25	Coffee break

16:25-17:30	**Session 10** - Industrial and short presentations Session Chairpersons: Ken Shea and Elena Piletska
16:25-16:40	Joint presentation from Cell Press and Elsevier by Maria Mytiliniou for Cell Press and Annelies Voorhaar for Elsevier.
16:40-16:47	S6 **Gold screen-printed electrodes coupled with molecularly imprinted conjugated polymers for ultrasensitive detection of streptomycin in milk** Margaux Frigoli, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, the Netherlands*
16:47-16:54	S7 **Supercritical CO_2-assisted metal–Biomolecular Imprinting: Rational design using Molecular Dynamics** A. I. Furtado, *iBB-Institute for Bioengineering and Biosciences and i4HB–Institute for Health and Bioeconomy, Instituto Superior Técnico, University of Lisbon, Lisboa 1049–001, Portugal.*
16:54-17:01	S8 **Bispecific Immune Checkpoints nanoBlocker Reinvigorate Both Innate and Adaptive immunity against Triple Negative Breast Cancer** Peixin Guan, *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, China*
17:01-17:08	S9 **Electropolymerized Molecularly Imprinted Polymer-modified Interdigitated Electrodes: A proof-of-concept Testing for Cystatin-C Detection** Meriem Kassar, *Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Baden-Württemberg 76344, Germany*
17:08-17:15	S10 **NanoMIP as synthetic receptor for rabbit IgG: effect of different crosslinker amount** Valentina Testa, *University of Turin, Italy*
17:15-17:22	S11 **Adenosine detection using a molecularly imprinted polymer biosensor with incorporated modified thymidine monomers.** Molly Wild, *Department of Chemistry, University of Sheffield, Dainton Building, 13 Brook Hill, Sheffield, S3 7HF, UK.*
17:22-17:29	S12 **Detection of inflammatory biomarkers using core-shell imprinted nanocomposites** Rahil Radfar, *Department of Bioinspired Materials and Biosensor Technologies, Kiel University, Kaiserstraße 2, 24143, Germany*
17:30-17:35	Day 2 Closing remarks and announcements
20:00-00:00	Social Dinner

MIP2024 Scientific Program Day 3: Friday, 21st June 2024

09:10 - 10:35	**Session 11** - Analytical approaches in molecular imprinting 1 - Keynote and short oral presentations Session Chairpersons: Lei Ye and Catherine Branger
09:10 - 09:30	Keynote 13 **AGREEMIP – Analytical greenness metric for molecularly imprinted polymers synthesis** A. Martín-Esteban, *Department of Environment & Agronomy. INIA-CSIC.. Carretera de A Coruña km 7.5. 28040 Madrid, Spain*
09:30 - 09:37	S13 **Tailored Macroscopic Geometries of Porous Molecularly Imprinted Polymers via LCD-Based 3D Printing** B. Keitel, *Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany.*
09:37 - 09:44	S14 **Development towards a novel screening method for nipecotic acid bioisosteres using molecular imprinted polymers (MIPs) as alternative to in vitro cellular uptake assays** Niels Knippenberg, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, the Netherlands*
09:44 - 09:51	S15 **Glycan Shield-Targeting Nanoparticles for Pan-coronavirus Neutralization with a Dual Thermal-effect Virucidal Mechanism** Ying Li, *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China*
09:51 - 09:58	S16 **Hybrid light emitting array for the wireless electroanalysis of mycotoxins** Tamara Moya-Cavas, *Department of Analytical Chemistry, Chemical Optosensors & Applied Photochemistry Group (GSOLFA), Faculty of Chemistry, Complutense University of Madrid, 28040 Madrid, Spain*
09:58 - 10:05	S17 **Surface Imprinted Polymers for the Detection of Fungal Spores** Nathalie Philippaerts, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, the Netherlands*
10:05 - 10:12	S18 **MIPs for robust affinity-based capture of phosphorylated and methylated proteins** Kristin Sultan, *Biofilms Research Center for Biointerfaces, Department of Biomedical Sciences, Faculty of Health and Society, Malmö University, SE-21432 Malmö, Sweden*
10:12 - 10:19	S19 **Thermal Detection of Riboflavin in Fruit Juices Using Molecularly Imprinted Polymers** Gil van Wissen, *Department of Sensor Engineering, Faculty of Science and Engineering, Maastricht University, the Netherlands*
10:19 - 10:26	S20 **MIP-based SARS-CoV-2 sensors in POCT connected to the Internet as novel strategies to address challenges in COVID-19 Diagnosis and Treatments** Riccardo Rovida, *Department of Engineering, University of Campania Luigi Vanvitelli, Via Roma 29, 81031 Aversa, Italy*

10:26 - 10:33	S21 **Screen-printed electrodes coated with molecularly imprinted polymers for the detection of PFOA** Fatemeh Ahmadi Tabar, *Laboratory for Soft Matter and Biophysics, KU Leuven, 3001 Leuven, Belgium*
10:35 - 11:05	Coffee break
11:05 - 13:20	**Session 12** - Analytical approaches in molecular imprinting 2 Session Chairpersons: Antonio Martín-Esteban and Elisabetta Mazzotta
11:05 - 11:20	Oral 18 **Lateral Flow nanoMIP Assay: A Proof-of-concept** Thea Serra, *Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, Via Giuria 7, 10125 - Torino, Italy*
11:20 - 11:35	Oral 19 **Point-of-care and in-field electrochemical MIP sensors: advantages, challenges and possible solutions** Iva Chianella *Surface Engineering and Precision Centre, School of Aerospace, Transport and Manufacturing, Cranfield University, Cranfield, Beds, MK43 0AL, United Kingdom*
11:35 - 11:50	Oral 20 **Disposable Sensors using Carbon Paste Grafted with Molecularly Imprinted Polymers** Yasuo Yoshimi, *Dept. Applied Chemistry, Shibaura Institute of Technology, Japan*
11:50 - 12:05	Oral 21 **Molecularly imprinted polymer films grafted on gold electrodes as smart electrochemical receptors for the detection of PAH** Farah Ibrahim, *University of Toulon, MAPIEM, Toulon, France*
12:05 - 12:20	Oral 22 **A novel proteomics approach using molecular imprinting** Elena Piletska, *Leicester Biotechnology Group, School of Chemistry, University of Leicester, Leicester, LE1 7RH, UK*
12:20 - 12:35	Oral 23 **Synthesis of nanoMIP Beacons for the Detection of Methamphetamine** Jon Ashley, *Department of Pharmaceutical and Biomolecular Sciences, Liverpool John Moores University, UK*
12:35 - 12:50	Oral 24 **NanoMIPs Enable the Rapid and Highly Sensitive Detection of a Crucial Biomarker for Myocardial Infarction, Troponin I** Jake McClements, *Merz Court, School of Engineering, Newcastle University, NE17RU Newcastle upon Tyne, U.K.*
12:50 - 13:20	**Closing Session** Dr. Mike Whitcombe, SMI President, **MIP Technology - Art or Science? Looking forward to the next 24 years!** Prize Giving (prizes sponsored by Springer and Cell Press) Closure of the conference.

MIP2024 Scientific Program Day 1: Wednesday, 19th June 2024 Poster Session I

Poster Board	Poster Presentation
1	P1 **Electrochemical Sensor for Atrial Natriuretic Peptide Detection based on a MIP Thin Film Receptor** José A. Ribeiro, *CIQUP/IMS, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal*
2	S1 **Imprinted hollow TiO_2 microspheres for selective photocatalysis** Manuel Azenha, *CIQ-UP, Institute of Molecular Sciences, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal*
3	P2 **Enantioselective nanoMIPs toward Thyroid Hormones** Valentina Testa, *Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, 10125 - Torino, Italy*
4	P6 **Ionic Imprinted Polymers PEGDA-based for Selective Binding of Lithium Ions** Valentina Testa, *Department of Chemistry, University of Turin - Turin, Italy*
5	P4 **Magnetic Molecularly Imprinted Polymers in Organic Synthesis: From Standard to Dynamic Kinetic Resolution** Huiyin Liu, *Sorbonne Université, CNRS, Méthodes et Applications en Chimie Organique, IPCM, 75005 Paris, France.*
6	P22 **Molecularly imprinted polymer nanogels for the detection of the heart failure biomarker Troponin T** Grisel Palome Villezcas, *Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*
7	P3 **Grafting nanoMIPs onto Surfaces of ELISA Microplates for the Development of Biomimetic Assays** Thea Serra, *Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, Via Giuria 7, 10125 - Torino, Italy*
8	S4 **Preparation of Environment-friendly Magnetic Molecularly Imprinted Polymers for Selective Separation of Components in Chinese Medicine** Langxing Chen, *College of Chemistry, Tianjin Key Laboratory of Biosensing and Molecular Recognition, Nankai University, Tianjin 300071, China.*
9	S3 **A glycan shield-targeting broad-spectrum antiviral nanomedicine provides potent therapeutic and prophylactic effects** Jingran Chen, Jingran Chen, *Nanjing University, Xianlin Campus, School of Chemistry and Chemical Engineering, State Key Laboratory of Analytical Chemistry for Life Science, 210023, China.*

10	S2 **Molecularly imprinted polymer (MIP) nanoparticles for targeted breast cancer therapy and controlled drug delivery** Perla Ben Ghouzi , *Sorbonne Université, CNRS, PHysico-chimie des Electrolytes et Nanosystèmes InterfaciauX, PHENIX, F-75005 Paris,France.*
11	S5 **Molecularly imprinted nanoprobes and time-resolved fluorescence spectroscopy in a nanosensing device for the detection of ultralow protein concentrations** Alice Marinangeli, *Dept. of Biotechnology, University of Verona, Strada Le Grazie 15, 37134 Verona, Italy*
12	P5 **SPR Sensor based on Imprinted Nanogels for Detection of Bovine Serum Albumin in Milk** José A. Ribeiro, *CIQUP/IMS, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal*
13	S4 **Towards a Computational Polymer Design Protocol for Biomarkers Detection: 1) Prostate-specific Antigen, Water and Cyrene interactions** Callum Donaldson, *Department of Chemical Engineering, University of Bath, Claverton Down, Bath, Somerset BA2 7AY, United Kingdom*
14	P13 **A dust of gold to shine light on MIP** Ester Iatta, *University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria*
15	P7 **Evaluation of deep eutectic solvents in the synthesis of molecularly imprinted fibers for the solid-phase microextraction of triazines in soil** Antonio Martín-Esteban, *Department of Environment & Agronomy. INIA-CSIC. Carretera de A Coruña km 7.5. 28040 Madrid, Spain*
16	P8 **Screen-printed electrodes modified by electropolymerized Molecularly Imprinted Polymers (e-MIP) to develop voltammetric sensors** Giancarla Alberti, *Department of Chemistry, University of Pavia, via Taramelli, 12 – 27100 Pavia (Italy)*
17	P9 **Dual epitope imprinted QCM sensor for selective detection of Salmonella typhi bacterial protein** Akriti Srivastava, *Department of Chemistry, MMV, Banaras Hindu University, Varanasi-221005, India*
18	P11 **Molecularly Imprinting polymer nanoparticles for inhibition of β-Lactamase activity** Ammar Ibrahim, *School of Chemistry, The University of Leicester, University Road, Leicester, LE1 7RH, United Kingdom*
19	P12 **Solid phase synthesis with low molecular weight templates – challenges and approaches for imprinting of the mycotoxin deoxynivalenol (DON)** Julia Völkle, *Centre of Electrochemical Surface Technology, 2700 Wiener Neustadt, Austria*

20	P14 **Synthesizing Molecularly Imprinted Polymer Thin Films for Sensing Carbonaceous Nanoparticles** Houra Hadadi, *University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria*
21	P10 **Solid-Phase Extraction Using a Green Metal-Organic Framework MOF-808 Integrated Molecularly Imprinted Polymer for Selective Drug Adsorption from Wastewater Samples** Sherman Lesly Zambou Jiokeng, *Institute of Analytical and Bioanalytical Chemistry, University of Ulm, Ulm 89081, Germany*
22	P16 **Utilizing Cyclodextrin Inclusion Complexes During Additive Manufacturing of Molecularly Imprinted Polymers for Diclofenac-Contaminated Water Samples** Amelie Huber, *Institute of Analytical and Bioanalytical Chemistry - Ulm University*
23	P15 **Enrichment of diclofenac and carbamazepine from wastewater using molecularly imprinted polymers** Anika Kotyrba, *Institute of Analytical and Bioanalytical Chemistry, Ulm University, 89069 Ulm, Germany*
24	P17 **Novel Materials and Methods for Thyroid Hormone Bioanalysis** Turki Alfuhayr, *School of Chemistry and Chemical Engineering, Queen's University Belfast*
25	P19 **Systematic studies on surface imprinting on the micrometer scale** Chiara Luna Onorati, *University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria*
26	P25 **Rational Design of Non-Covalent Molecularly Imprinted Polymers Based on the Combination of Molecular Dynamics Simulation and Quantum Mechanics Calculation** Xue Yu, *Shandong Fuyang Biotechnology Co., Ltd*
27	P18 **Application of molecularly imprinted polymer nanoparticles for lung cancer cell surface proteomics** Kirabo Magumba, *Department of Chemistry, University of Leicester, University Road, Leicester, LE1 7RH, United Kingdom.*
28	P20 **In-situ synthesis of MIP to Detect Au Nanoparticles on QCM** M.Bagheri, *University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria*
29	P21 **Soft molecularly imprinted nanoparticles coupled with simultaneous lossy mode and surface plasmon multi-resonances optical platform for femtomolar sensing of proteins** Mimimorena Seggio, *Department of Biotechnology, University of Verona, Strada Le Grazie 15, 37134 Verona, Italy.*
30	S18 **MIPs for robust affinity-based capture of phosphorylated and methylated proteins** Kristin Sultan, *Biofilms Research Center for Biointerfaces, Department of Biomedical Sciences, Faculty of Health and Society, Malmö University, SE-21432 Malmö, Sweden*

31	P23 **A MIP based sensor for highly sensitive detection of Human Chorionic Gonadotropin (hCG): Towards a reusable pregnancy test** Radvile Zubryte, *Pharmista Technologies AB, Scheelevägen 3, Lund, 223 63, Sweden*
32	P24 **Molecularly imprinted polymers sensitive to S-metolachlor** Dominika Rapacz, *Wroclaw University of Science and Technology, Faculty of Chemistry, wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wroclaw, Poland*
33	P26 **Double surrogated imprinting for the preparation of virus-selective particles** Beatriz Fresco-Cala, *Affordable and Sustainable Sample Preparation (AS2P) research group, Departamento de Química Analítica, Instituto Químico para la Energía y el Medioambiente IQUEMA, Universidad de Córdoba, Campus de Rabanales, Edificio Marie Curie, E-14071, Córdoba, Spain.*
34	P44 **Tailoring Drug Delivery: Ellagic Acid Imprinted Polymer Nanoparticles-Entrapped Hydrogels for Enhanced Loading and Controlled Release** Necla Yucel Ayten, *Yildiz Technical University, Institute of Sciences, Department of Bioengineering, Istanbul / Turkey*
35	P34 **Cladded molecularly imprinted nanoparticles for fluorescence imaging of polysialic acid on tumor issues** Lingrui Huang, *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, 163 Xianlin Avenue, Nanjing 210023 P.R. China*
36	P35 **Molecularly-imprinted polymer synthesis for tramadol determination using venlafaxine as a dummy template** Beatriz Fresco-Cala, *Affordable and Sustainable Sample Preparation (AS2P) research group, Departamento de Química Analítica, Instituto Químico para la Energía y el Medioambiente IQUEMA, Universidad de Córdoba, Campus de Rabanales, Edificio Marie Curie, E-14071, Córdoba, Spain.*
37	P45 **Electrochemosensor based on molecularly imprinted poly o-phenylenediamine membranes for the ultrasensitive detection of cytochrome c** Najmeh Karimian , *Department of Molecular Sciences and Nanosystems, University Ca' Foscari of Venice, via Torino 155, 30172 Venice, Italy*
38	P56 **Molecularly Imprinted Polymers combined with Peptide Nucleic Acids as a Novel Hybrid Receptor for miRNA 21** Muhammed Abdel-Hamied, *Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert Einstein Allee, 11, 89081, Ulm, Germany*

MIP2024 Scientific Program Day 2: Thursday, 20th June 2024 Poster Session II

Poster Board	Poster Presentation
1	S8 **Bispecific Immune Checkpoints nanoBlocker Reinvigorate Both Innate and Adaptive immunity against Triple Negative Breast Cancer** Peixin Guan, *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University*
2	S7 **Supercritical CO_2-assisted metal–Biomolecular Imprinting: Rational design using Molecular Dynamics** A. I. Furtado, *iBB-Institute for Bioengineering and Biosciences and i4HB–Institute for Health and Bioeconomy, Instituto Superior Técnico, University of Lisbon, Lisboa 1049–001, Portugal.*
3	S6 **Gold screen-printed electrodes coupled with molecularly imprinted conjugated polymers for ultrasensitive detection of streptomycin in milk** Margaux Frigoli, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University*
4	S10 **NanoMIP as synthetic receptor for rabbit IgG: effect of different crosslinker amount** Valentina Testa, *University of Turin*
5	S11 **Adenosine detection using a molecularly imprinted polymer biosensor with incorporated modified thymidine monomers.** Molly Wild, *Department of Chemistry, University of Sheffield, Dainton Building, 13 Brook Hill, Sheffield, S3 7HF, UK.*
6	S13 **Tailored Macroscopic Geometries of Porous Molecularly Imprinted Polymers via LCD-Based 3D Printing** B. Keitel, *Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany.*
7	S15 **Glycan Shield-Targeting Nanoparticles for Pan-coronavirus Neutralization with a Dual Thermal-effect Virucidal Mechanism** Ying Li, *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China*
8	S12 **Detection of inflammatory biomarkers using core-shell imprinted nanocomposites** Rahil Radfar, *Department of Bioinspired Materials and Biosensor Technologies, Kiel University, Kaiserstraße 2, 24143, Germany*
9	S14 **Development towards a novel screening method for nipecotic acid bioisosteres using molecular imprinted polymers (MIPs) as alternative to in vitro cellular uptake assays** Niels Knippenberg, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University*

10	S19 **Thermal Detection of Riboflavin in Fruit Juices Using Molecularly Imprinted Polymers** Gil van Wissen, *Department of Sensor Engineering, Faculty of Science and Engineering, Maastricht University*
11	S17 **Surface Imprinted Polymers for the Detection of Fungal Spores** Nathalie Philippaerts, *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, the Netherlands*
12	S20 **Screen-printed electrodes coated with molecularly imprinted polymers for the detection of PFOA** Fatemeh Ahmadi Tabar, *Laboratory for Soft Matter and Biophysics, KU Leuven, 3001 Leuven, Belgium*
13	S16 **Hybrid light emitting array for the wireless electroanalysis of mycotoxins** Tamara Moya-Cavas, *Department of Analytical Chemistry, Chemical Optosensors & Applied Photochemistry Group (GSOLFA), Faculty of Chemistry, Complutense University of Madrid, 28040 Madrid, Spain*
14	P36 **Molecularly Imprinted polymers with bio-based monomers to adsorb carbamazepine from wastewater** Elettra Savigni, *Università di Bologna*
15	P27 **Molecularly Imprinted Nanoparticles for the Detection of Norovirus in Food** Amy Dann, *Department of Chemical Engineering and Analytical Science, School of Engineering, University of Manchester, Manchester M20 4BX, United Kingdom*
16	P38 **Combating the AMR Crisis: Utilizing Molecular Imprinting Technology for the Dual Detection of Antibiotics in Environmental and Food Samples.** Oliver Jamieson, *Newcastle University, School of Engineering, Merz Court, Claremond Road, NE1 7RU, Newcastle Upon Tyne*
17	P29 **Exploring the influence of the peptide length used as template on binding performance of nanoparticles produced by epitope imprinting** Ainhoa Elejaga-Jimeno, *Department of Analytical Chemistry, University of the Basque Country UPV/EHU, 01006, Vitoria-Gasteiz (Spain)*
18	P31 **Development of Hypoxanthine Sensor Using Molecularly Imprinted Polymer** Sato Yui, *Department of Applied Chemistry, Shibaura Institute of Technology, Tokyo, Japan*
19	P33 **Development of A Disposable Inosine-Molecularly Imprinted Polymer Carbon Paste Electrodes for Freshness Evaluation of Fish** Takumi Iwasaki, *Department of Applied Chemistry, Shibaura Institute of Technology, Tokyo, Japan*
20	P28 **Rational Design of MIPs for Precise Discrimination of Viral and Bacterial Infections** Soumya Rajpal, *Institute of Analytical and Bioanalytical Chemistry Ulm University Albert-Einstein-Allee 11, 89081 Ulm, Germany*

21	P39 **Sensing Clinically Relevant Proteins through Electrochemical Detection with Electrodes Decorated with Molecularly Imprinted Polymers** Vitali Syritski, *Department of Materials and Environmental Technology, Tallinn University of Technology, Estonia*
22	P37 **Development of a MIP-based fluorescent sensor for the detection of foodborne pathogenic bacteria** Rahil Radfar, *Department of Bioinspired Materials and Biosensor Technologies, Kiel University, Kaiserstraße 2, 24143, Germany*
23	P40 **Molecularly imprinted drug reservoir for targeted glioblastoma cell treatment: in vitro and in vivo characterization** Bogdan-Cezar Iacob, *Department of Analytical Chemistry, Faculty of Pharmacy, "Iuliu Haţieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania*
24	P41 **A versatile vapor-phase polymerization approach for molecularly imprinted polymers (MIPs) in optical sensing.** Tiziano Di Giulio, *Dipartimento di Scienze e Tecnologie Biologiche e Ambientali, Università del Salento, Lecce, Italy*
25	P30 **Influence of the cross-linker percentage on the thermoresponsive character and binding behaviour of peptide imprinted nanoparticles produced against the CB1 cannabinoid receptor** Alberto Gómez-Caballero, *Department of Analytical Chemistry, University of the Basque Country UPV/EHU, 01006, Vitoria-Gasteiz (Spain)*
26	P55 **Molecularly imprinted polymer nanogels for the detection of acute kidney injury biomarker KIM-1** Kyra Magdato, *Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*
27	P47 **Imaging of Neurotransmitter Secretion in Living Brain Probed by Fluorescent Molecularly Imprinted Nanoparticles** Yasuo Yoshimi *Dept. Applied Chemistry, Shibaura Institute of Technology*
28	P48 **On-Site Detection of Perfluoroalkyl Carboxylic Acids with Dual Fluorescent Molecularly Imprinted Particles Coupled to a Miniaturized Opto-Microfluidics Platform** Kornelia Gawlitza, *Bundesanstalt für Materialforschung und prüfung (BAM), Richard-Willstätter-Str. 11, 12489 Berlin, Germany*
29	P32 **Development of a Disposable Histamine Sensor Using Molecularly Imprinted Carbon Paste for Freshness Evaluation of Fish** Hina Sakurai, *Department of Applied Chemistry, Shibaura Institute of Technology, Tokyo, Japan*
30	P42 **Molecularly imprinted polymers in the process of gentamicin monitoring** Katarzyna Smolinska-Kempisty *Wroclaw University of Science and Technology, Faculty of Chemistry, wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wroclaw, Poland*

31	P43 **Integrated molecularly imprinted membranes for the monitoring of bisphenol A in the capacitive deionization process** Joanna Wolska, *Wroclaw University of Science and Technology, Faculty of Chemistry, Wyb. Wyspiańskiego 27, 50-370 Wroclaw, Poland*
32	P49 **Multi-functional nanocavity for specific sensing of small extracellular vesicles prepared by template polymerization using a polymerizable functional polymer** Hirobumi Sunayama, *Graduate School of Medicine, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
33	P50 **TROP2-molecular imprinting polymere nanoparticles for breast cancer targeting therapy** Lila Louadj, *CRSA, Sorbonne Université, UMR INSERM 938 France*
34	P51 **Fluorescent signaling molecularly imprinted polymer nanogels for assembly of a biotic/ abiotic sensing platform** Hirobumi Sunayama, *Graduate School of Medicine, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
35	P52 **Epitope imprinted polymers for sensing bacterial proteins** Meenakshi Singh, *Banaras Hindu University*
36	P53 **In silico models for the rational development of electrosynthesized MIP-based sensors** Tiziano Di Giulio, *Dipartimento di Scienze e Tecnologie Biologiche e Ambientali, Università del Salento, via per Monteroni, Lecce (73100), Italy.*
37	P54 **Molecularly imprinted polymers fighting antimicrobial resistance** Sara Spada, *Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*

Abstracts: Plenary and Founder Lectures

Plenary

Why does non-specific binding limit diagnostically relevant biosensors?

Janos Vörös

voros@ethz.ch

Laboratory of Biosensors and Bioelectronics, ETH Zurich, Institute for Biomedical Engineering, Switzerland

One of the main pillars of modern diagnostics is the precise quantification of disease markers using biosensors. Non-specific binding (NSB) is the archenemy of such diagnostically relevant biosensors, because it is not only inevitable but it is also the main factor that determines the limit of detection (LOD) of most existing systems.[1] Real samples, e.g. blood, plasma, serum, saliva, synovial fluid, urine, tissue biopsy, cell lysate, etc., have many orders of magnitude higher concentration of background molecules than disease markers, which makes molecular diagnostics equivalent to "finding Nemo" among all the fish in the ocean. (Figure 1)

I will systematically introduce and define NSB, discuss the thermodynamic and molecular reasons behind it and show its consequences in diagnostics. In addition, I will provide a detailed recipe for correctly assessing the LOD of new sensor technologies and explain the most common mistakes that occur in literature.

Referencing is a common practice to deal with NSB-related problems. I will also explain why referencing is seldom a solution; and show how and why sub-micron-scale, coherent referencing is needed to substantially reduce NSB-induced and other environmental noise.[2] With the example of focal molography, I also show how diffraction based read-out along with coherent referencing enables real-time, label-free measurements of molecular binding in complex samples, such as plasma[3] or live cells[4].

Stochastic sensing deals with NSB by statistical means. Nanopore based biosensors not only provide the possibility of detecting single molecules, but the characteristic peaks in translocation events also enable their identification. Here, I will introduce a force-controlled nanopore sensor with scanning capabilities that allows analysing the content of live cells and the characterization of cell-cell communication.[5,6]

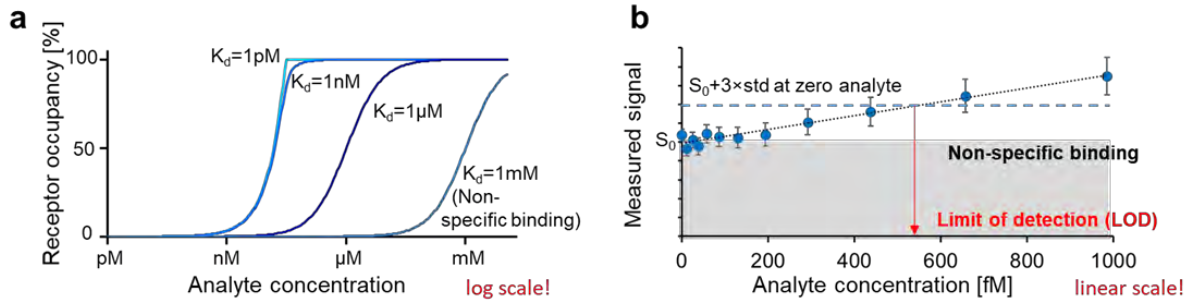

Figure 1: a) Dose response curves of a typical (ELISA) sandwich assay. The receptor occupancy saturates above the K_d value of the used receptors. b) The measured signal of typical biosensors is directly proportional to the amount of captured analytes. Here, the diagnostically relevant, linear part of a typical dose-response curve is shown along with the inevitable non-specific binding and the LOD. (Note the difference between the log and linear scale of the two curves.).

References

[1] Nonspecific Binding - Fundamental Concepts and Consequences for Biosensing Applications; A. Frutiger, et al.; *Chem. Rev.* **2021**, *submitted*.

[2] Ultra Stable Molecular Sensors by Submicron Referencing and Why They Should Be Interrogated by Optical Diffraction; A. Frutiger, et al.; *Sensors*, **2020**, DOI:10.3390/s21010009

[3] Focal molography is a new method for the in situ analysis of molecular interactions in biological samples; V. Gatterdam, et al.; *Nature Nanotechnology*, **2017**, DOI: 10.1038/nnano.2017.168

[4] Quantification of Molecular Interactions in Living Cells in Real Time using a Membrane Protein Nanopattern; A.M. Reichmuth, et al.; *Analytical Chemistry*, **2020**, DOI: 10.1021/acs.analchem.0c00987

[5] Localized detection of ions and biomolecules with a force-controlled scanning nanopore microscope; M. Aramesh, et al.; *Nature Nanotechnology,* **2019**, 14:791; DOI: 10.1038/s41565-019-0493-z

[6] Aptamer-Functionalized Interface Nanopores Enable Amino Acid-Specific Peptide Detection; T. Schlotter, et al.: *ACS Nano* 2024 18:6286, DOI: 10.1021/acsnano.3c10679

Mosbach Memorial Lecture

Professor Klaus Mosbach: A Friend, Mentor and Visionary Scientist

C R Lowe*
University of Cambridge, Trinity College, Cambridge, CB2 1TQ
*crl1@cam.ac.uk

This memorial lecture is a lasting tribute to my friend, mentor and visionary scientist, Klaus Mosbach, and describes his early life and educational background, international profile and academic achievements. His pioneering work on immobilised enzymes [1], coenzymes [2] and cells [3], affinity chromatography [4] and sensor technologies [5] will be described as a backdrop to his distinction style and latter major contributions to the field of non-covalent molecular imprinting [6]. The lecture will highlight some of his most cited work placed in appropriate context with that of others, particularly of Polyakov, Dickey and Wulff, and take a view on where this technology is heading, its limitations and potential alternative approaches. A brief collection of Laudatorial statements made by key internationally renowned scientists will complete the lecture.

[1] Mosbach, K. (1980) Immobilised enzymes. *Trends Biochem Sci* **5**, 1-3.
[2] Lindberg, M., Larsson, P.O. & Mosbach, K. (1973) A new immobilised NAD^+ analogue. Its application in affinity chromatography and a functioning coenzyme. *Eur J Biochem* **40**, 187-193.
[3] Brodelius, P., Deus, B., Mosbach, K. & Zenk, M.H. (1979) Immobilised plant cells for the production and transportation of natural products. *FEBS Lett* **103**, 93-97.
[4] Mosbach, K., Guilford, H., Ohlsson, R. & Scott, M. (1972) General ligands in affinity chromatography. *Biochem J* **127**, 625-631.
[5] Haupt, K. & Mosbach, K. (2000) Molecularly imprinted polymers and their use in biomimetic sensors. *Chem Rev* **100**, 2495-2504.
[6] Mosbach, K. (1994) Molecular Imprinting. *Trends Biochem Sci* **19**, 9-14.

Wulff Memorial Lecture

Synthetic Antibodies and Molecularly Imprinted Polymers, Next Generation Protein Affinity Reagents?

Kenneth J Shea
Department of Chemistry
University of California, Irvine
Irvine CA, 92617

kjshea@uci.edu

Abiotic protein affinity reagents, such as synthetic antibodies and molecularly imprinted polymers, offer alternatives to traditional, biological affinity reagents such as antibodies. There have been exceptional advances in these fields over the past 20 years. Using recent examples, [1-7] I will describe the current state of the art of abiotic synthetic antibodies (SAs) and explain our current understanding of why and how they work. I will also highlight differences and similarities between the two approaches and call attention to the remaining challenges that both technologies must overcome if they are to impact biotechnology.

1. *J. Am. Chem. Soc.*, **2023**, *145*, 23143–23151.
2. *Journal of Controlled Release, **2023**, 355, 745-759.*
3. *ACS Applied Materials & Interfaces, **2022**, 14, 19178-19191.*
4. *Nature Communications, **2021,** 12,1-14.*
5. *Nano Letters**, 2021**, 21, 13, 5663-5670.*
6. *J. Am. Chem. Soc, **2020**, 142, 5, 2338–2345.*
7. *Nature Chemistry, **2017**, 9, 715-722.*

Abstracts: Keynote Lectures

Keynote 1

MIP nanoparticles for diagnostics – are we ready for the market?

Sergey A. Piletsky
School of Chemistry
College of Science and Engineering
University of Leicester
LE1 7RH
E: sp523@le.ac.uk

Our team has made a major breakthrough in MIP technology developing solid-phase approach for preparation of soluble molecularly imprinted nanoparticles (nanoMIPs) - “plastic antibodies” with exquisite affinity and selectivity for their templates. The success came from combining controlled radical polymerisation with an affinity separation step performed on surface-immobilised template. This approach represents the state-of-the-art in nanoMIP synthesis: not only are soluble particles with defined size (20-200 nm) and a narrow size distribution produced in one hour, they possess subnanomolar dissociation constants for their respective targets, they can be easily functionalised with fluorescent, electrochemical or magnetic labels, and the immobilised template can be re-used. High affinity nanoMIPs were made for small molecules, proteins, whole cells, bacteria and virus particles.

The main practical niche for application of synthesised nanoMIPs in diagnostics has been a low hanging fruit for years. Members of our team have used nanoMIPs successfully as a replacement for antibodies in ELISA-type assays, electrochemical and optical sensors. The possibility to integrate recognition and sensing capabilities makes our materials particularly suitable for sensing but also for theranostics applications. Main progress was achieved by our team as well as by our colleagues worldwide in integration of MIPs with sensors by screen printing, ink jet printing and other tools suitable for large scale manufacturing. What is left to do to bring our MIPs to the market? This is still a difficult question to answer.

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2. Canfarotta F., Waters A., Sadler R., McGill P., Guerreiro A., Papkovsky D., Haupt K., Piletsky S. (2016). Biocompatibility and internalization of molecularly imprinted nanoparticles. *Nano Research*, **9**, 3463–3477.
3. Smolinska-Kempisty K., Guerreiro A., Canfarotta F., Caceres C., Whitcombe M., Piletsky S. (2016). A comparison of the performance of molecularly imprinted polymer nanoparticles for small molecule targets and antibodies in the ELISA format. *Sci. Reports*, **6**, 37638.
4. Canfarotta F., Lezina L., Guerreiro A., Czulak J., Petukhov A., Daks A., Smolinska-Kempisty K., Poma A., Piletsky S., Barlev N. (2018) Specific drug delivery to cancer cells with double-imprinted nanoparticles against EGFR membrane receptor. *Nano Letters*, **18**, 4641-4646.
5. Ekpenyong-Akiba A., Canfarotta F., Hatem B. A., Poblocka M., Casulleras M., Castilla-Vallmanya L., Kocsis-Fodor G., Kelly M. E., Janus J., Althubiti M., Piletska E., Piletsky S., Macip S. (2019). Detecting and targeting senescent cells using molecularly imprinted nanoparticles. *Nanoscale Horizons*, **4**, 757-768.
6. Garcia-Cruz A., Ahmad O. S., Alanazi K., Piletska E., Piletsky S. A. (2020). Generic sensor platform based on electro-responsive molecularly imprinted polymer nanoparticles (e-NanoMIPs). *Microsys. Nanoeng.*, **6**, 1-9.
7. Piletsky S. S., Piletska E., Poblocka M., Macip S., Jones D. J. L., Braga M., Cao T. H., Singh R., Spivey A. C., Aboagye E. O., Piletsky S. A. (2021). Snapshot imprinting: rapid identification of cancer cell surface proteins and epitopes using molecularly imprinted polymers. *Nano Today*, **41**, 101304.

Recent receptors designed using imprinting and adaptable ligand displays

Börje Sellergren
Biofilms Research Center for Biointerfaces, Department of Biomedical Sciences, Faculty of Health and Society, Malmö University, Sweden
Email: borje.sellergren@mau.se

The concepts of “lock-and-key” and multivalent interactions can be used to describe recognition phenomena in nature as well as the operating principles of most synthetic receptors. Molecular imprinting and multivalent receptor models are particularly effective in mimicking these events. This talk will discuss some recent examples of receptors designed according to these approaches.

Keynote 3

3D-Printing Meets MIPs: A New Era of Precision and Scalability in MIP Manufacturing

M. Dinc,[a,*] B. Keitel,[a,b] A. Huber,[a,b] K Junginger,[a,b] & B. Mizaikoff [a,b]

[a] *Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany.*

[b] *Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany.*

**Mehmet.Dinc@Hahn-Schickard.de*

Molecularly imprinted polymers (MIPs) stand out for their stability and specificity, presenting versatile applications in diagnostics, drug delivery, and environmental monitoring. Despite their straightforward synthesis and notable stability, the commercial scale-up of MIPs encounters significant challenges, particularly in achieving consistent scalability, homogeneity, and reproducibility - critical for industrial application.

To overcome these challenges, we utilize the synergistic potential of 3D printing and MIP technology, which enables an unprecedented level of manufacturing precision. The integration of photo-curing-based 3D-printing with polymerization-induced phase separation has been a key advancement enabling producing complex macroscopic polymer structures. With this method, the inherent porosity can be precisely controlled at the sub-micrometer level, while at the same time facilitating tailored "printed" macro-porosity via digital design (see Figure 1).

This hybridization of techniques marks a new era for MIPs facilitating the production of materials with carefully engineered properties that meet the demanding requirements of a wide variety of applications. The result is a robust and scalable approach that not only improves the reproducibility of MIPs, but also expands their applicability and promises a rapid transition from laboratory innovation to commercial reality.

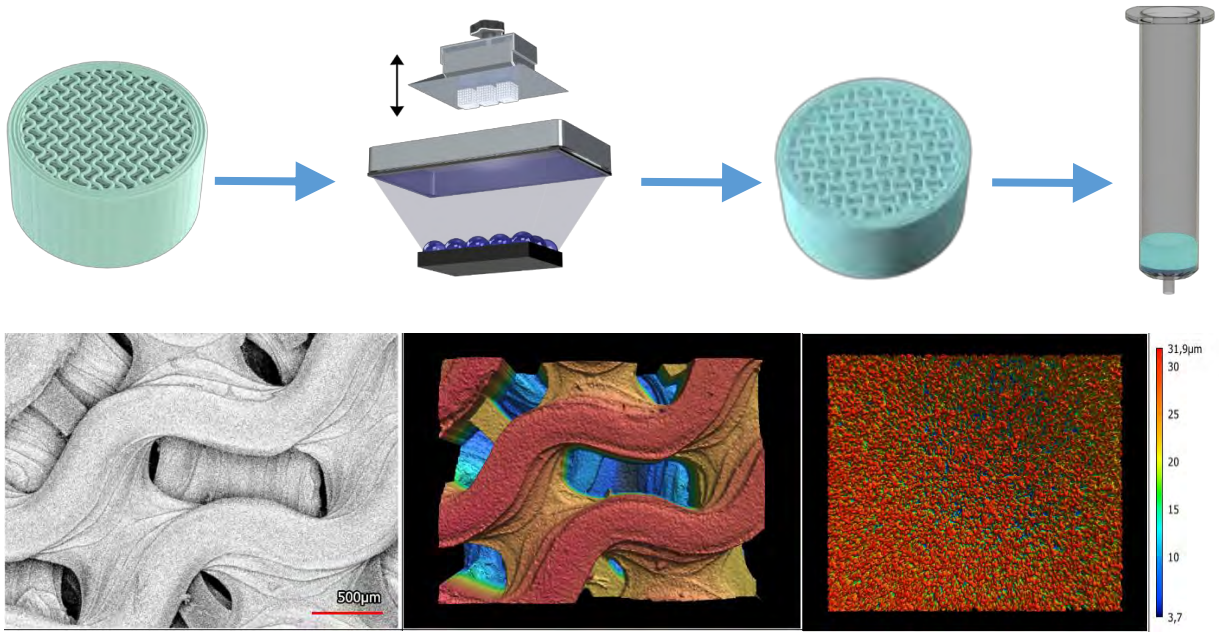

Figure 1. 3D printing of porous molecularly imprinted polymers with complex macroscopic geometries.

Keynote 4

Evidence of Positive Cooperativity in the Binding Behavior of nanoMIPs Prepared by Solid Phase Polymerization Synthesis

C. Baggiani,* L. Anfossi, S. Cavalera, F. Di Nardo, T. Serra, V. Testa

Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, 10125 - Torino, Italy

**claudio.baggiani@unito.it*

The Solid Phase Polymerization Synthesis (SPPS) is an innovative approach to prepare nanosized Molecularly Imprinted Polymers (nanoMIPs). It consists in the covalent immobilization of the template onto the surface of a solid support, the fast polymerization around the template, the removal of low binding materials and the final release of the imprinted nanoparticles by changing the medium conditions. The obtained nanoMIPs are virtually free of template and show good selectivity and very high affinity for the target molecule, making them low-cost and robust alternatives to antibodies in applications as immunoassay, sensoristics and complex sample purification by affinity chromatography.

NanoMIPs and polyclonal antibodies are assumed to share the same binding behavior, with very similar thermodynamic and kinetic properties, due to the presence of mutually independent binding sites and characterized by a continuous distribution of the binding affinity with respect to an average value. This assumption necessarily implies a behavior characterized by negative cooperativity, well described by the Freundlich-Langmuir (Hill) binding isotherm model and qualitatively represented by a convex Scatchard plot.

Nevertheless, some preliminary experimental indications suggest the possibility of a different binding behavior, characterized by positive cooperativity. Since this behavior would have significant repercussions on the practical use of nanoMIPs, we decided to thoroughly investigate the binding behavior of a nanoMIP with molecular recognition properties towards ciprofloxacin chosen as a well-known model system [1,2]. Repeated equilibrium binding experiments performed in pH 7 buffered solutions on nanoMIPs of different cross-linking degree (2% and 20% moles of methylene-bis-acrylamide as cross-linker) and with ciprofloxacin and danofloxacin as ligands allowed us to accurately determine the binding isotherms over a wide range of ligand concentrations. The consequent statistical treatment of the data showed the clear prevalence of binding isotherm models consistent with positive cooperativity (exponential term $n>1$ and concave Scatchard plot) when compared to all the other alternative binding models considered. Moreover, the exponential term of the selected model does not correlate with the degree of crosslinking of the nanoMIPs, suggesting that positive cooperativity is not related to the degree of stiffness of the nanopolymer. Further experimental data obtained from nanoMIPs prepared with a sterically bulky template (rabbit IgG) indicate that the positive cooperativity effect is presumably due to the structural proximity of the binding sites.

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Keynote 5

A Closer Look on the Surfaces of MIP Thin Films

P.A. Lieberzeit,* F. Thier, B. Bräuer, C.L. Onorati, M. Werner

University of Vienna, Faculty of Chemistry, Department of Physical Chemistry, 1090 Vienna, Austria
University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria

**Peter.Lieberzeit@univie.ac.at*

Even though molecularly imprinted polymers (MIP) have been the focus of intense research for 3-4 decades, they largely have not yet delivered on their promise of straightforward, polymer-based recognition in a commercially feasible way [1]. Whereas MIP nanobodies [2] are promising in that regard, this is not yet the case for MIP thin films, except for electropolymerized ones [3], which rely on a limited number of monomers.

A reason for this may be the statistical nature of radical polymerization: one (implicitly) assumes that MIP layers are homogeneous and on average represent the compositions of their monomer mixtures. However, nanomechanical measurements with AFM (Figure 1) clearly reveal that this is not the case: a flat styrene-co-divinyl benzene film contains areas of different elastic modulus.

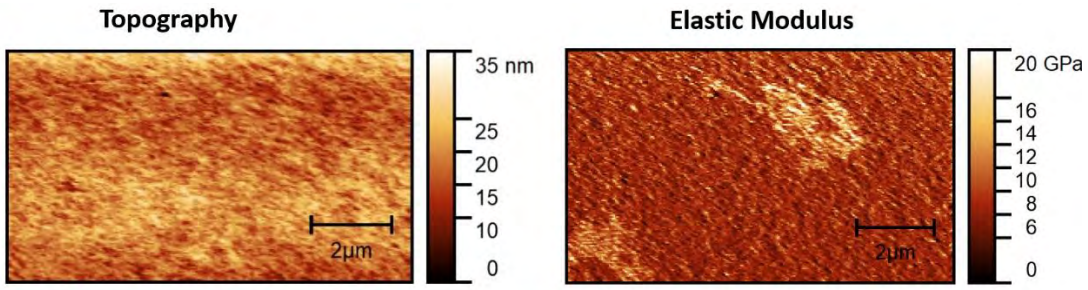

Figure 1: Topograpy and adhesion image of a Sty-co-DVB thin film

Furthermore, stamp imprinting of micrometer-sized templates such as bacteria or titania/silica nanoparticles shows another discrepancy: whereas the template species usually form dense layers on stamp surfaces, the resulting surface MIP show very uneven distribution of cavities. Both point at inhomogeneous distribution of surface properties and affinities, which may affect the reproducibility of MIP layers.

Addressing this issue requires understanding the surfaces of MIP better and, thus, analytical techniques to characterize them. Raman microscopy offers a tool for doing so, at least for imprints in the µm range: it allows for lateral resolutions of about 800*800nm^2. Indeed, it is possible to record spectra of bacteria MIP surfaces templated with different bacteria (e.g. *E. coli* and *B. subtilis*). Despite spectra being very similar, chemometry reveals differences between MIP and NIP surfaces as well as the cavities of different bacteria. Whether those are statistically significant depends on the respective polymer: it is for polyacrylates providing functional groups for binding sites, but not for polystyrenes.

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Keynote 6 - invited

Machine-Learning-Aided Molecularly Imprinted Materials for Biomedical Applications

Zeynep Altintas

Department of Bioinspired Materials and Biosensor Technologies, Faculty of Engineering, Kiel University, Germany
zeynep.altintas@tf.uni-kiel.de

Machine Learning (ML) algorithms excel at advancing complex datasets analysis to identify most relevant patterns and correlations. In molecularly imprinted polymer (MIP) design, ML can process vast amounts of data related to polymer characteristics: types of templates, monomers, cross-linking agents, and binding affinities, along with optimal synthesis conditions. Herein, we aim to design novel and advanced polymer compositions and structures for highly specific molecular targets. Moreover, the applications of our novel MIP recipes range from biomarker detection and disease diagnostics (cancer, chronic-wound diseases, infections, neurodegeneration, and genetic disorders), to potential therapeutic modalities.

In our research, we go beyond conventional recipes via using cutting-edge computational techniques. Our input datasets for ML combine both computational and experimental insights, with a primary focus on distinctive secondary structural (SS) components of the template molecules [1]. Different SS components affect the nanoMIP's imprinting affinity via leading to variations in formed H-bond patterns. Moreover, the orientation of the templates' functional groups is also dictated by the SS elements, therefore we considered key structural units for our template molecules, including α-helices, β-pleated sheets, and random coils, as well as specific combinations of these components. In addition to these parameters, other relevant nanoMIP features such as binding affinities, solvent exposures, H-bonds, atomic fluctuations, interaction energies, types of chemical bonds, particle size distributions, surface charges, nanoMIPs stability and their rebinding performance are also considered. Since Random Forest (RF) model is particularly suitable for making accurate predictions even with non-linear dependencies, and Gradient Boosting (GB) excels in feature relevance identification, we present a dual-model ML approach where RF is used to predict the most effective MIP components (templates, monomers and cross-linkers), while GB is deployed to analyze the same dataset, focusing however on identifying the most influential factors within our nanoMIPs synthesis process.

Consequently, our approach promises to significantly enhance the efficiency and efficacy of nanoMIPs development, paving the way for more precise and targeted biomedical applications, ranging from progressive biosensing purposes to advanced therapeutic strategies [1].

Keywords: Machine Learning, MIP, nanoMIP design, computational methods, Random Forest, Gradient Boosting, decision trees, novel materials, bio-inspired polymers.

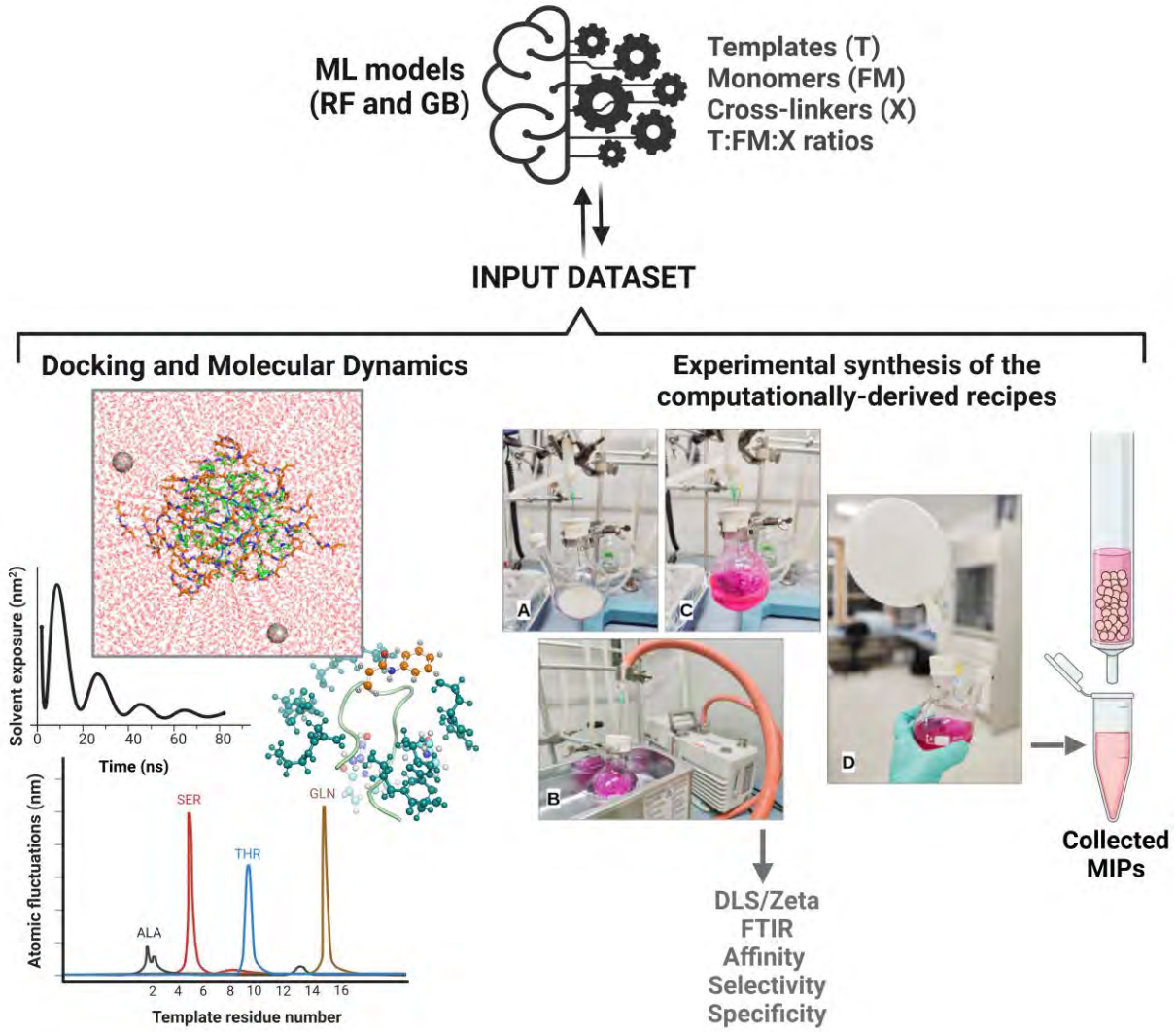

Figure 1. Overall workflow of our molecularly imprinted materials design strategy [1].

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Keynote 7

Chemosensors with extended-gate field-effect transistors (EG-FETs) coupled with polymers molecularly imprinted with epitopes of protein biomarkers predictive for idiopathic pulmonary fibrosis (IPF) for selective chemosensing of these biomarkers in body fluids

Wlodzimierz Kutner [a, b,*] Katarzyna Bartold [a], Zofia Iskierko [a], Pawel Borowicz [a], Krzysztof Noworyta [a], Chu-Yun Lin [c], Jakub Kalecki [a], Kostiantyn Nikiforow [a], Andrzej Ardasiewicz [a], Piyush Sindhu Sharma [a], Hung-Yin Lin [c]

[a] *Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland*
[b] *Faculty of Mathematics and Natural Sciences. School of Sciences, Cardinal Stefan Wyszynski University in Warsaw, Warsaw, Poland*
[c] *Department of Chemical and Materials Engineering, National University of Kaohsiung, Kaohsiung, Taiwan*
**E-mail address: wkutner@ichf.edu.pl; *phone: +48 506 679 485*

We have devised a rapid and easy procedure for quantifying the MMP-1 and SP-A protein biomarkers diagnostic for idiopathic pulmonary fibrosis (IPF) in bodily fluids [1-3]. For that, we integrated by electropolymerization thin molecularly imprinted polymer (MIP) film-based recognition units with the gates of extended-gate field-effect transistor (EG-FET) transducers to fabricate biomarker-selective chemosensors proper as point-of-care diagnostic tools. Using either MIAHDFPGIGHK (50–500 nM, 60 nM) [1,2], HGYPKDIYSS (50–500 nM, 20 nM) [1,2], AQDDIDGIQAI (10–250 nM, 7.5 nM) [2], or FKGNKYWAVQGQNV (10–250 nM, 2 nM) [2] single-epitope template imprinting, we ascertained the MMP-1 (linear dynamic concentration range and limit of detection). We designed, built, and evaluated a multi-gate EG-FET device (Figure 1) for that purpose [3]. Finally, we simultaneously imprinted three epitopes of MMP-1, lowering the MMP-1 LOD to 0.1 nM, thus enabling its determination in body fluids.

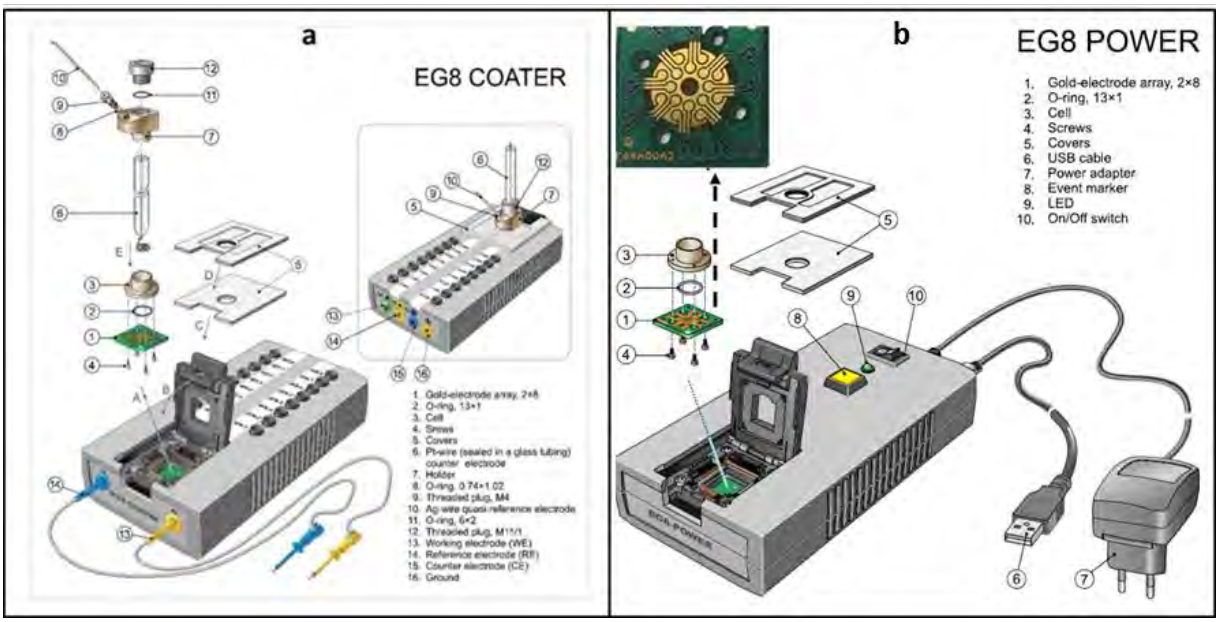

Figure 1. Expanded views of (a) the EG8 COATER module and (b) the EG8 POWER module with components numbered and described.

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Keynote 8

Hydrophilic Hairy Fluorescent Molecularly Imprinted Polymer Micro- or Nanocapsules for Bioanalytical and Biomedical Applications

Huiqi Zhang,* Yanyan Mu, Yang Liu and Yan Zhou

State Key Laboratory of Medicinal Chemical Biology, Key Laboratory of Functional Polymer Materials (Ministry of Education), Tianjin Key Laboratory of Functional Polymer Materials, and College of Chemistry, Nankai University, Tianjin 300071, P. R. China

**zhanghuiqi@nankai.edu.cn*

Molecularly imprinted polymers (MIPs) are tailor-made synthetic receptors with high affinity and selectivity towards the target analytes. They have drawn great attention over the past half century owing to their great potential as substitutes for biological receptors in a wide range of bioanalytical and biomedical applications. Particularly, the development of advanced functional hydrophilic MIP micro- or nanoparticles capable of selectively recognizing small organic analytes in the complex aqueous milieus is of significant importance because the food safety control, environmental monitoring, and biomedical applications are normally based on the aqueous systems.[1]

Over the past 15 years, our group has developed some versatile approaches for the controlled synthesis of hydrophilic hairy MIP micro- or nanoparticles that can selectively detect small organic analytes in the complex biological media based on our developed controlled/"living" radical precipitation polymerization techniques (CRPPs), which proved to hold much promise in various bioanalytical and biomedical applications.[1,2] To further improve their comprehensive performance, we have recently developed a facile and efficient strategy for preparing well-defined multifunctional hydrophilic hairy polymer micro- or nanocapsules, which involves first the synthesis of uniform "living" and easily etchable polymer micro- or nanoparticles via CRPPs, their controlled surface-grafting of crosslinked polymer shells and hydrophilic polymer brushes, and subsequent removal of the cores by solvent-washing.[3] Very recently, we have utilized this strategy to develop a series of hydrophilic hairy fluorescent MIP micro- or nanocapsules for different purposes.[4] In this lecture, I will present our progress in the development of some advanced hydrophilic hairy fluorescent MIP micro- or nanocapsules for bioanalytical and biomedical applications.

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Keynote 9

Polishing molecularly imprinted polymers for biomedical applications

Zhen Liu

State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, 163 Xianlin Avenue, Nanjing 210023, China

Email: zhenliu@nju.edu.cn

Abstract (500 words):

Molecularly imprinted polymers (MIPs), which are considered as plastic or artificial antibodies, are chemically synthesized by polymerization in the presence of a target compound. MIPs have exhibited great application potential in many important fields. However, conventional molecular imprinting approaches suffer from a dilemma; because non-imprinted surface is also constructed under the same imprinting conditions as those for the construction of binding cavities, non-imprinted surface contains plentiful functionalities and thereby inevitably results in apparent non-specific adsorption. Due to this reason, conditional optimization in conventional molecular imprinting usually fails to simultaneously provide the best affinity and the best specificity, but a compromise between the two aspects. To solve this bottle-neck issue, we have developed a new strategy called molecular imprinting and cladding (MIC) [1,2]. The principle is straightforward; after molecular imprinting, a chemically inert cladding thinlayer is generated to precisely cover non-imprinted area. The prepared cladded MIPs (cMIPs) exhibited significantly improved affinity and specificity and thereby enabled a range of challenging applications, including bioimaging, disease diagnosis, cancer therapy, viral inhibition and so on. This presentation will introduce the MIC strategy and the potential of cMIPs for biomedical applications.

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Keynote 10 **Molecularly imprinted polymers - new materials and applications in synthetic biology**

Karsten Haupt,[1,2] Carlo Gonzato[1] Christos Galanos[1]

[1]*Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*

[2]*Institut Universitaire de France*

Molecularly imprinted polymers (MIPs) [1] are synthetic antibodies that specifically recognize molecular targets. They are cross-linked polymers synthesized in the presence of a molecular template, which induces three-dimensional binding sites in the polymer that are complementary to the template in size, shape and chemical functionality. Here we present the use of MIPs in a synthetic biology application aiming at materials that are part of a solid-state cell factory. MIPs against a surface protein of photosynthetic cyanobacteria were obtained through a rational approach starting with in silico epitope design. Chemically synthesized peptide epitopes were then used as templates in a solid-phase protocol for MIP synthesis [2], resulting in thermoresponsive nanogels with an operation temperature around 25°C. Fluorescence binding assays and QCM studies demonstrate specific target binding. After interfacing the MIP with nanocellulose, surfaces allowing for the specific capture of the cyanobacteria were obtained.

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Keynote 11

Hierarchical Imprinting with Biopolymers

Subramanian Suriyanarayanan and Ian A. Nicholls

Bioorganic & Biophysical Chemistry Laboratory, Department of Chemistry & Biomedical Sciences, Linnaeus University, SE-391 82 Kalmar, Sweden

ian.nicholls@lnu.se

Hierarchical molecular imprinting is emerging as a powerful tool for the fabrication of imprinted materials for applications where both affinity and recognition kinetics are critical, ***e.g.***, surface-based sensing and catalysis. Here, efforts to develop hierarchically imprinted materials based upon renewable biomacromolecular "monomers" shall be presented, with a focus on studies using the maize-derived protein zein, crab shell-derived oligosaccharide chitosan and milk-derived protein casein. The design, synthesis and characterization of these materials shall be described, along with their application in quartz crystal microbalance (QCM)-based sensing platforms.

Keynote 12

BioMIPs biocompatible biomimetics: molecular imprinting ties the knot with natural polymers. Synthesis, properties and future of silk molecularly imprinted nanoparticles.

Alessandra Maria Bossi[1], Devid Maniglio[2]

1 University of Verona, Dept. of Biotechnology, LAStMolCAL, Strada Le Grazie 15, 37134 Verona, Italy. Email: alessandramaria.bossi@univr.it

2 University of Trento, Dept. of Industrial Engineering, BIOtech Research Center, Via delle Regole 101, Mattarello, 38123 Trento, Italy. Email: devid.maniglio@unitn.it

We report about the development of tailor-made biomimetics stemmed from merging biology with polymer chemistry and material science. Aqueous-soluble nanotraps that behave as biomimetic receptors were prepared in the form of proteinaceous disordered super-assemblies, fixed by non-natural crosslinking. The specific formation of the nanotrap started from the biocompatible, nontoxic material, already in use in regenerative medicine, that is silk fibroin [1].

Pioneering a paradigm change, the tailor-made molecular recognition was conveyed to the silk nanotrap by the unconventional exploitation of the molecularly imprinted polymers (MIPs) technique, that is a specifically designed strategy to entail molecular recognition to a nanomaterial by means of a template-assisted synthesis [2,3], but herein methacrylated silk fibroin polypeptides were used as macromolecular building blocks. Such MIP synthetic protocol was optimized with the aid of surface response method. The silk-nanotraps, called bioMIPs, were physically and functionally characterized, demonstrating high affinity binding (nM) for the targets and selectivity [4]. Enzymatic degradation of the bioMIPs was studied. The biocompatibility of the nanotraps was confirmed. The nanotraps were further labelled with fluorescent tags and tested for imaging in cell cultures [6]. The bioMIP's synthesis proved a general route for entailing recognition towards proteins or small molecules [4,5], which let foreseen applications in sequestering molecular players, thus counteracting effects of diseases.

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AGREEMIP – Analytical greenness metric for molecularly imprinted polymers synthesis

W. Wojnowski [a,b], M. Marć [b] , F. Pena-Pereira [c], A. Martín-Esteban [d,*] , M. Tobiszewski [b]

[a] *University of Oslo, Department of Chemistry, 0315 Oslo, Norway*

[b] *Gdańsk University of Technology, Faculty of Chemistry, Department of Analytical Chemistry, 80-233 Gdańsk, Poland*

[c] *Centro de Investigación Mariña, Universidade de Vigo, Departamento de Química Analítica e alimentaria, Grupo QA2, Edificio CC Experimentais, Campus de Vigo, As Lagoas, Marcosende, 36310 Vigo, Spain*

[d] *Department of Environment & Agronomy. INIA-CSIC.. Carretera de A Coruña km 7.5. 28040 Madrid, Spain*

[*] amartin@inia.csic.es

Molecular imprinting technology is well established in areas where a high selectivity is required, such as catalysis, sensing, and separations/sample preparation. However, according to the Principles of Green Chemistry [1], it results evident that the various steps required to obtain MIPs are far from ideal. In this regard, greener alternatives to the synthesis of MIPs have been proposed in recent years and thus further research in this field is expected in the coming years [2, 3]. However, although it is intuitively possible to design new green MIPs, it would be desirable to have a quantitative measure of the environmental impact of the different changes introduced for their synthesis.

This work proposes, for the first time, a metric tool to assess the greenness of MIP synthesis procedures. The developed metric (called AGREEMIP) is based on 10 categories of impacts, which were converted into sub-scores on a 0-1 scale and then used to calculate the final assessment score. The assessment criteria included the selection and use of solvents, materials and reagents (monomers, crosslinkers), waste generation and energy consumption. The assessment procedure is carried out using a user-friendly open access software that produces an easy-to-read pictogram with information on overall performance and hazard structure. The applicability of AGREEMIP will be successfully demonstrated in this presentation using different MIP synthesis case studies.

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Abstracts: Oral Presentation

Oral 1

Design and optimization of molecularly imprinted polymer nanoparticles from mechanistic principles

Todd Cowen

University of Verona, Dept. of Biotechnology, Strada Le Grazie 15, 37134 Verona, Italy.
Email: toddjames.cowen@univr.it

Improper models of natural processes severely limit their technological application. There are famous examples through the history of science, and countless less notable cases, of good theories being misapplied, corrected or replaced by more appropriate approximations. The mechanism used to describe the formation of molecularly imprinted polymer nanoparticles was adapted from that of an abstractly related but thermodynamically distance process. The aqueous synthesis of modern imprinted nanoparticles has little relation to the covalent imprinting process from which it descends, and so the adoption of its synthesis mechanism will limit the further development of MIP science and technology.

Biomimetic molecularly imprinted polymer nanoparticles develop by a dynamic growth process following subtle energy gradients [1]. With this modification, the diameter of polymer nanoparticles and nanoMIPs can be controlled by consideration of the competing intermolecular interactions, temperature and concentration [2]. The final affinity and selectivity of the resulting imprinted polymer can also be optimized through control of the environment in which the molecular imprinting occurs. Specific energy gradients can therefore be created to induce the desired properties in the resulting material, in a manner analogous to the synthesis, function and adaption of biological systems. This presentation will describe in detail the proposed synthetic mechanism, the evidence for its accuracy, and how it can be exploited for technological development.

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Oral 2

Unlocking new avenues: Solid-state synthesis of molecularly imprinted polymers

Bogdan-Cezar IACOB[1], Andreea-Elena BODOKI[2], Ede BODOKI[1]*

[1]Analytical Chemistry Department, "Iuliu Haţieganu" University of Medicine and Pharmacy, 4, Louis Pasteur St., 400349, Cluj-Napoca, Romania
[2]General and Inorganic Chemistry Department, "Iuliu Hatieganu" University of Medicine and Pharmacy, 12, Ion Creangă St., 400010, Cluj-Napoca, Romania
**bodokie@umfcluj.ro*

Molecular imprinting enables the fast, versatile, robust and cost-effective synthesis of biomimetic polymeric receptors with tailored selectivity for a wide variety of target molecules. In the last few decades, it has evolved into a mature process with well-established protocols and commercial applications. As a result, nowadays molecularly imprinted polymers (MIPs) are being widely used for separation, sensing, drug delivery and diagnostics. Nevertheless, there are continuous efforts around this topic in addressing existing challenges, seeking further improvements in their performance or identifying novel applications. While MIPs have been synthesized using various techniques, including bulk polymerization, precipitation polymerization, and emulsion polymerization, there is still a need for new and more efficient methods to develop MIPs with better properties, such as microfluidic synthesis and template-assisted polymerization, being some the more recently introduced.
Solvents are a critical component in the synthesis of MIPs, both as a porogen and reaction media, however their use comes with additional challenges. On a larger scale, especially the nonpolar ones, may imply environmental concerns. Some solvents can interfere with the binding of the target molecule to the polymer matrix, leading to reduced binding efficiency or selectivity. This can be especially problematic for polar or charged molecules, which may be solubilized only by certain solvents. Some template molecules may have limited solubility in common solvents, making it difficult to incorporate them into the polymer matrix. This can limit the range of target molecules that can be imprinted. The properties of solvents, such as polarity and viscosity, can vary depending on factors such as temperature, pressure, and impurities, which may translate into variation in MIP performance, which can be challenging to control. And last, but not least some polymerization methods, such as precipitation polymerization, require the use of specific solvents or solvent mixtures. This can limit the flexibility of MIP synthesis and may require additional optimization steps to achieve the desired properties.
To address some of the above-mentioned issues, but also to explore potential opportunities or further constrains, we report the first solvent-free mechanochemical synthesis of MIPs via liquid-assisted griding. The successful synthesis of the imprinted polymer has been functionally demonstrated measuring its template rebinding capacity, as well as the selectivity of the molecular recognition process in comparison with the ones obtained by the conventional, non-covalent molecular imprinting process in liquid media. The proof-of-concept study demonstrated similar binding capacities towards the template molecule and superior chemoselectivity compared to the conventional MIP synthesis method.
The adoption of green chemistry principles with all its inherent advantages in the synthesis of MIPs, not only alleviates potential environmental and health concerns associated with their analytical (e.g. selective adsorbents) and drug delivery (e.g. drug carriers or reservoirs) applications, but might also offer a conceptual change in the molecular imprinting technology. Future studies, besides gaining a deeper understanding on the chemical structure of the resulting imprinted polymer and different mechanochemical variables on the molecular recognition properties of, will also need to answer to a series of key questions, such as what is the range of template molecules compatible with the mechanochemical synthesis of MIPs, with a special emphasis on macromolecules (proteins, nucleotides, etc.), what is the extent of unwanted degradation of the employed monomers, cross-linkers and template depending on the employed experimental conditions, if and by which extent the template molecule is covalently biding to the polymeric scaffold, is mechanochemistry transferable to other MIP synthetic approaches.

Acknowledgements
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Oral 3

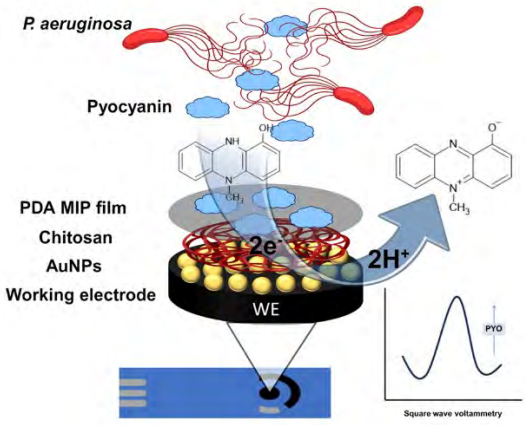
Detection of *Pseudomonas aeruginosa* Infection Using A Polydopamine-based Molecularly Imprinted Electrochemical Sensor

Pannawich Thirabowonkitphithan,[a,b] Solmaz Hajizadeh,[b]
Wanida Laiwattanapaisal,[a] & Lei Ye [b,*]

[a] *Department of Clinical Chemistry, Faculty of Allied Health Sciences, Chulalongkorn University, Bangkok, 10330, Thailand*
[b] *Division of Pure and Applied Biochemistry, Department of Chemistry, Lund University, 22100, Lund, Sweden*

**lei.ye@tbiokem.lth.se*

Pyocyanin, a redox-active secondary metabolite produced by *Pseudomonas aeruginosa*, serves as a crucial virulence factor and its quantification can aid early diagnosis of infection. A selective and sensitive molecularly imprinted electrochemical sensor was constructed by using a green polymerization technique to deposit an ultrathin polydopamine film on an electrode modified with gold nanoparticles and chitosan. The target recognition was enabled by the specific binding sites complementary to the pyocyanin structure in the imprinted polymer matrix. The electrochemical behavior of the sensor was characterized through various techniques, including cyclic voltammetry, electrochemical impedance spectroscopy and square wave voltammetry. The influence of fabrication components such as chitosan concentration, monomer concentration, electro-polymerization condition, pH, and rebinding time were investigated. The sensor exhibited a high degree of specificity and sensitivity for pyocyanin, with a wide linear detection range of 1 – 100 µM and a low detection limit of 0.74 µM. The proposed sensor was also used to detect pyocyanin in bacterial cultures, giving a recovery of the spiked standard ranging from 93 to 103%. The electrochemical sensor displayed satisfactory stability lasting for at least 5 weeks. Moreover, the applicability of the sensor for clinical measurement was demonstrated by detecting pyocyanin in infected burn wounds on an *ex vivo* skin model. By harnessing the synergistic advantages of molecularly imprinted polymer and the specific redox window for pyocyanin, the electrochemical sensor offers a promising avenue for early-stage detection of infection, thereby contributing to improved treatment and more effective healthcare for patients.



Oral 4

Non-invasive detection of glucose with electroactive molecularly imprinted polymers (e-MIPs): Application in wearable sensors

***Saweta Garg*[1,2]**, *Pankaj Singla*[1,2], *Shayan Seyedin*[2], *Marloes Peeters*[1,2]

[1]*Department of Chemical Engineering and Analytical Science, School of Engineering, University of Manchester, Manchester M20 4BX, United Kingdom.*
[2]*School of Engineering, Newcastle University, Newcastle Upon Tyne, United Kingdom*
Saweta.garg@manchester.ac.uk; S.garg5@newcastle.ac.uk

Effective diabetes management is crucial upon continuous glucose level monitoring (total 425 million individuals affected worldwide). [1,2] The current diagnostic methods have associated problems and challenges for instance finger prick tests are discomfortable and glucose monitoring devices are expensive. [3] Moreover, these devices are inaccessible to the patients specifically from the developing nations and poor population. [4] Therefore, there is still need for a cost-effective and non-invasive glucose monitoring solution.

This work focuses on the development of electroactive sensor using inexpensive material such as molecularly imprinted particles (e-MIPs) and screen-printed electrodes (SPEs). e-MIPs were synthesized using straightforward polymerization method via incorporating electroactive monomers (Pyrrole) with glucose as a template. These prepared e-MIPs were extensively characterized through dynamic light scattering (DLS), FTIR, and transmission electron microscopy (TEM). Cyclic voltammetry (CV) results of e-MIPs functionalized SPE sensor showed a linear response towards D-glucose (1 μM to 10 mM), with a limit of detection (LOD) of 0.622 μM and a limit of quantification (LOQ) of 1.88 μM. In addition, rigorous testing against similar compounds (fructose, galactose, ascorbic acid) and non-imprinted particles (NIPs) confirmed the sensor's selectivity and specificity [**Figure 1]**. This developed e-MIPs sensor is fast and provide the result within 30 seconds.

Furthermore, developed e-MIPs functionalized SPE sensor was assessed using samples obtained from diabetic patients. The results demonstrated promising potential for seamless integration into wearable sensor technology. This study introduces an innovative, cost-effective, and non-invasive glucose sensor, addressing a crucial gap in diabetes management.

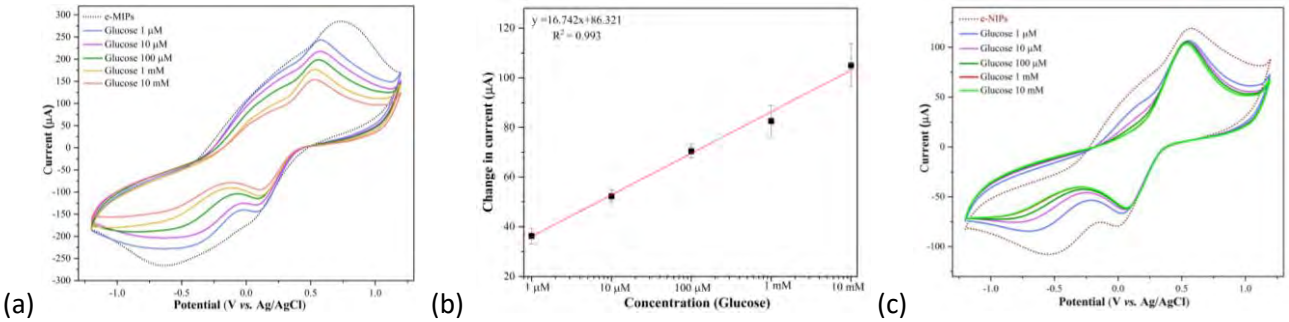


Figure *1*: The cyclic voltammogram (CV) of **(a)** e-MIPs, **(b)**, calibration curve of glucose concentration (1 μM-10 mM) versus current change (μA), **(c)** non-imprinted polymeric nanoparticles (NIPs) in the presence of different concentrations of glucose (1 μM-10 mM).

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Oral 5

Dual Fluorescent Molecularly Imprinted Polymers (MIPs) for Detection of the Prevalent Anti-Inflammatory Drug Diclofenac

Kornelia Gawlitza[1], Michelle Buchholz[2], Anna Gersdorf[1], Michael Gradzielski[2] and Knut Rurack[1]

[1]Bundesanstalt für Materialforschung und -prüfung (BAM), Chemical and Optical Sensing Division, Richard-Willstätter-Straße 11, 12489 Berlin, Germany

[2]Technische Universität Berlin, Institut für Chemie, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Straße des 17.Juni 124, 10623 Berlin, Germany

Ensuring the purity of air and water is essential for the overall well-being of life on earth and the sustainability of the planet's diverse ecosystems. To achieve the goal of zero pollution, as outlined in the 2020 European Green Deal by the European Commission,[1] significant efforts are in progress. A key aspect of this commitment involves advancing more efficient and economically viable methods for treating wastewater. This includes the systematic monitoring of harmful pollutants such as heavy metals, microplastics, pesticides, and pharmaceuticals.

One example is the presence of the anti-inflammatory drug diclofenac in water systems, primarily originating from its use as a gel or lotion for joint pain treatment. Diclofenac contamination in surface waters has been detected at approximately 10 µg L^{-1} (0.03 µM)[2] which is not solely due to widespread usage but also because of the drug's resistance to microbial degradation. Conventional wastewater treatment plants (WWTPs), which rely on biodegradation, sludge sorption, ozone oxidation, and powdered activated carbon treatment, struggle to efficiently remove diclofenac from wastewater.[3],[4] For instance, to enable WWTPs to efficiently monitor and optimize their processes, it would be advantageous to develop on-site detection and extraction methods for persistent pharmaceutical residues in aqueous samples.

In this work, a sol-gel process was used to prepare Nile blue-doped silica nanoparticles (*d*SiO_2-NPs) with a diameter of ca. 30 nm that were further functionalized to enable reversible-addition-fragmentation chain-transfer (RAFT) polymerization. To achieve fluorescence detection, a fluorescent monomer was used as a probe for diclofenac in ethyl acetate, generating stable complexes through hydrogen bond formation. The diclofenac/fluorescent monomer complexes were imprinted into thin molecularly imprinted polymer (MIP) shells on the surface of the *d*SiO_2-NPs. Thus, the MIP binding behaviour could be easily evaluated by fluorescence titrations to monitor the spectral changes upon addition of the analyte. Doping the core substrate with Nile blue generates effective dual fluorescent signal transduction. This approach does not solely depend on a single fluorescence emission band in response to analyte recognition. Instead, it enables the fluorescent core to function as an internal reference, minimizing analyte-independent factors such as background fluorescence, instrumental

fluctuation, and operational parameters.[5] Rebinding studies showed that the MIP particles have excellent selectivity towards the imprinted template and good discrimination against the competitor ibuprofen, with a discrimination factor of 2.5. Additionally, the limit of detection was determined to be 0.6 µM. Thus, with further optimization of the MIP, there is potential for the development of a MIP-based biphasic extract-&-detect fluorescence assay for simple, sensitive and specific sensing of diclofenac in aqueous samples down to the required concentrations of 0.03 µM.

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Oral 6

Photo-iniferter polymerization: a convenient approach for integrating Molecularly Imprinted Polymers with nanostructured sensors

T. Di Giulio[1], I. M. Asif[1], C. Malitesta[1], C. Gonzato[2], K. Haupt[2], M. Corsi[3], G. Barillaro[3], E. Mazzotta[1]*.

[1] *Dipartimento di Scienze e Tecnologie Biologiche e Ambientali, Università del Salento, Lecce, Italy.*
[2] *UMR 7025 CNRS Enzyme and Cell Engineering Laboratory, Sorbonne Universités, Université de Technologie de Compiègne, Compiègne, France.*
[3] *Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Pisa, Italy*

elisabetta.mazzotta@unisalento.it

Molecularly imprinted polymers (MIPs) have gained significant attention as artificial biomimetic materials due to their ease of synthesis and their ability to combine strength, durability, and molecular recognition capabilities akin to biological elements like antibodies and enzymes [1]. Functioning as "antibody mimics," MIPs find diverse applications, with their utility continually expanding through advancements in synthetic techniques. In this context, the photostructuring of MIPs holds particular appeal because it allows precise control over their properties, including size, morphology, and thickness [2]. In this study, we exploit photo-induced controlled radical polymerization to deposit MIPs on nanostructured porous silica ($PSiO_2$) photonic crystals with high aspect ratios (100) and columnar pores with dimensions around 50 nm, used as interferometer. $PSiO_2$ has gained prominence in biosensing and chemical sensing due to its large specific surface area, cost-effectiveness, and straightforward fabrication, which opens the door to mass-producing affordable biosensors for point-of-care applications [3]. Our research focuses on the development of tailor-made molecularly imprinted polymer films for propranolol, a model target, within nanoporous silica substrates. We employ low-intensity visible light to achieve the deposition of homogeneous thin polymer layers on $PSiO_2$ scaffolds (Figure 1), as verified through UV-Vis reflectance spectroscopy and X-ray photoelectron spectroscopy.

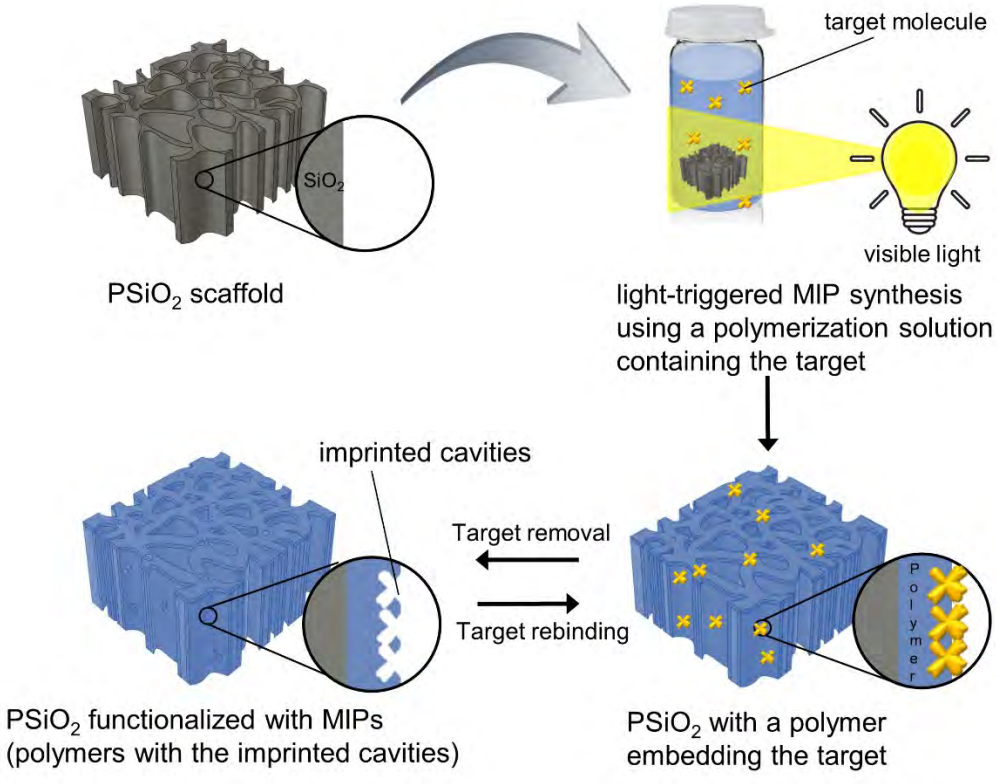

Figure 1: Schematic representation of photo-iniferter polymerization for MIP deposition on PSiO2 scaffolds.

Our resulting sensor demonstrates excellent linearity over a broad concentration range from 0.005 to 0.1 mM, with a low detection limit of 0.0012 mM. Furthermore, our propranolol detection tests conducted in tap water confirm the sensor's capability to detect the target in real-world matrices. Additionally, our versatile synthesis approach is demonstrated by imprinting another molecule, atenolol. The resulting MIPs exhibit high specificity for the imprinted target, selectivity against interfering molecules (other beta-blockers), and stability, enabling the sensors to be used for at least 60 days.

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Oral 7

Design of turn-on fluorescent imprinted polymers for sensing of lead in complex water samples

W. René[1,2], K. Laatikainen[3,4], V. Lenoble[2], C. Branger[1,*]

[1] *University of Toulon, MAPIEM, Toulon, France*

[2] *University of Toulon, Aix Marseille University, CNRS, IRD, MIO, Toulon, France*

[3] *Lappeenranta-Lahti University of Technology, LUT, School of Engineering Science, Department of Separation Science, Lappeenranta, Finland*

[4] *Finnish Defence Research Agency, Lakiala, Finland*

** branger@univ-tln.fr*

Molecularly imprinted polymers have proved their efficiency as specific receptors for sensing applications. In the field of trace metal sensing, fluorescent detection can be an advantageous alternative due to high sensitivity and miniaturization ability. Moreover, the analysis of a fluorescence signal can provide additional information through the analysis of excitation and emission spectra as well as fluorescence intensity, lifetime, and anisotropy. However, in the case of trace metals, their lack of intrinsic fluorescence properties means that alternative methods must be found. One such method is to introduce a fluorescent monomer into the MIP structure whose fluorescence will be sensitive to the complexation with the target metal ion. A « turn-on » mode is beneficial because of a lower optical background and higher signal-to-noise ratio.

Therefore, in the aim of preparing sensing receptor for Pb(II) detection in real water samples, we designed a new fluorescent monomer with a turn-on mode based on photoinduced electron transfer (PET). This fluorescent probe (named ANQ-ST) was prepared by combination of 5-amino-8-hydroxyquinoline and a styrene moiety [1]. Its binding ability was studied in the conditions of the polymerization step (solvent, counter-ion and temperature) in order to optimize the complex formation with Pb(II) and the binding properties of the associated MIP. Various synthesis parameters were explored for the preparation of the MIP particles, such as the porogen solvent, the crosslinker and the metal/functional monomer ratio [2]. After optimization of the solvent choice and the molar ratios of monomers, MIP particles were obtained by precipitation copolymerization of ANQ-ST with EGDMA as a crosslinker. They were characterized by solid-state ^{13}C NMR spectroscopy, SEM and nitrogen adsorption/desorption experiments. The study of the selectivity properties of the IIP towards Ag(I), Na(I), Ca(II), Cd(II), Co(II), Cu(II), Pb(II), Zn(II) and Al(III) ions was achieved by three-dimensional fluorescence. The best designed MIP presented a low limit of detection of 2.1 $\mu g \cdot L^{-1}$ in pure water with a linear range of 7.1−60 $\mu g \cdot L^{-1}$ [3]. It was evidenced that all the MIPs were only slightly sensitive to the pH and the nature of the aqueous matrix by the comparison of calibration curves obtained in different types of waters and at different pH: ultra-pure water (pH = 5.9), buffered waters (pH = 7.0 and 8.1), tap water and seawater. This was confirmed by the successful determination of Pb(II) in some real sample waters, including seawater.

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Oral 8

Molecularly Imprinted Polymers as synthetic antibodies for therapeutic applications

Claudia Herrera-Leon[a]*, Peyman Sakhaii[b], Helena Mora-Radó[b], Pradeep K. Dhal[c], Bernadette Tse Sum Bui[a], Karsten Haupt[a]

[a]*Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, France*
[b]*Global CMC Early Development, Synthetics Platform, Sanofi-Aventis Deutschland GmbH, Germany*
[c]*Global CMC Early Development, Synthetics Platform, Sanofi Global R&D, USA*

**claudia.herrera-leon@utc.fr*

Since the discovery of the first monoclonal antibody (MAb) more than 45 years ago, the MAbs industry has invested billions to meet the increasing demand for clinical diagnosis and therapies [1,2]. Currently, MAbs are approved for the treatment of a variety of diseases, including cancer, Alzheimer's disease, and auto-immune disorders such as rheumatoid arthritis [3,4]. However, there are still some limitations, mainly related to the lack of stability, side effects, and high costs [2]. To counteract these drawbacks, molecular imprinting has emerged as a promising alternative for the design and production of materials with antibody-like molecular recognition capabilities [5,6].

In the present work, we propose a synthetic antibody based on molecularly imprinted polymer nanogels (MIP-NGs) to target Tumor Necrosis Factor-alpha (TNF-α), a cytokine involved in a wide range of cell signaling events [3] and with a crucial role in the pathogenesis of inflammatory diseases [7]. MIP-NGs were prepared by epitope imprinting [8] using an *in silico* rational approach to identify potential epitopes of TNF-α. MIP synthesis was carried out using a solid-phase approach [9] in which the peptide epitope is covalently immobilized on glass beads as a solid support. The obtained MIP-NGs bind the template peptide and recombinant TNF-α with high affinity and selectivity and can block the binding of TNF-α to its receptor. Consequently, they were applied to neutralize pro-inflammatory TNF-α in the supernatant of human THP-1 macrophages, leading to a downregulation of the secretion of pro-inflammatory cytokines. Our results suggest that MIP-NGs, with qualities such as greater stability, ease of manufacturing, and cost-effectiveness compared to antibodies, are a promising alternative as next-generation TNF-α inhibitors for the treatment of inflammatory diseases.

Keywords: molecularly imprinted polymer, TNF-α, therapeutic antibody, biomimicry

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Oral 9

MUC1 analogue-imprinted nanogels effectively discriminate glycopeptide positional isomers: on the way to early detection of glycosylated biomarkers

C.Contardi,[1] A. Khalid,[1] L. Mavliutova,[2] M. Serra,[1] D. Rubes,[1] R.Dorati,[1] B. Sellergren,[2] & E De Lorenzi[1*]

[1]Department of Drug Sciences, University of Pavia, Viale Taramelli 12, 27100, Pavia (PV), Italy
[2]Department of Biomedical Sciences, Faculty of Health and Society, Per Albin Hanssons Väg 35, Malmö University, Malmö 21432, Sweden

*ersidelo@unipv.it

Cancer-related glycan modifications are protein-specific, site-specific and cell-specific, and give rise to a plethora of glycoforms featuring very high heterogeneity [1]. Although much knowledge has been gained on cancer-related early expressed epitopes, their accurate detection and selective discrimination is still strongly hindered by the lack of suitable diagnostic tools [2,3]. In the quest for water-compatible molecularly imprinted polymer nanogels (MIP NGs) targeting specific glycans, our work started with the exploration of three distinct phenylboronic acid (PBA) derivatives as potential monomers. Our initial focus centered on synthesizing MIP NGs designed to selectively target either α2,6- or α2,3-sialyllactose, chosen as simplified models representing cancer-related sT and sTn antigens. Based on boronate-sialyllactose interaction studies and mobility shift Affinity Capillary Electrophoresis (msACE) analysis, the o-aryl-amido phenylboronic acid was identified as an optimal monomer, for crafting polymers with the capability to target both sialyllactoses. Subsequently, we embarked on the synthesis of highly selective MIP NGs, employing the previously optimized o-substituted isomer of boronic acid against a glycopeptide template strategically designed to mimic aberrantly glycosylated cancer biomarkers. Then, we undertook the synthesis of crude mimics resembling cancer-related truncated O-glycans, serving as simplified models for mucin 1 (MUC1). Direct N-glycosylation of a pentapeptide epitope with both sugar isomers via reductive amination facilitated the generation of Fmoc-protected and deprotected glycosylated sequences. These sequences were then employed in imprinting acrylamide-based MIP NGs, with recognition abilities assessed through ELISA-like assays. Affinity experiments pointed out a poor imprinting for NGs obtained from protected sequences, possibly due to hydrophobic side interactions with Fmoc group. In contrast, the removal of the protecting group significantly enhanced imprinting efficiency, resulting in unprecedented discrimination between the two glycopeptide isomers. The selectivity of these polymers was further validated through msACE, confirming successful cavity tailoring with affinity constants of about 10^6 M^{-1}. Crucially, our findings demonstrated that peptide conjugation led to a substantial amplification of imprinting efficiency. We believe that this progress will pave the way for a new generation of tumor-specific glycan receptors, addressing the longstanding need in cell and tissue imaging and advancing glycomics research.

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Evolution of molecularly imprinted polymer nanoparticles as antibody mimics through the characterization of the molecular recognition process by single-molecule microscopy

Alessia Di Fiore,[a] Carlo Gonzato,[a] Chang Zhou,[b] Ignacio Izeddin,[b] Valentina Krachmalnikoff,[b] Yannick De Wilde,[b] Karsten Haupt[a,c]

[a] *Université de Technologie de Compiègne, France*
[b] *Institut Langevin, ESPCI Paris, PSL University, CNRS, France*
[c] *Institut Universitaire de France*
alessia.di-fiore@utc.fr

Molecularly imprinted polymers (MIPs) [1] are synthetic antibody mimics that specifically recognize molecular targets. They are cross-linked polymers synthesized in the presence of a molecular template, which induces three-dimensional binding sites in the polymer that are complementary to the template in size, shape, and chemical functionality. Here we describe the evolution of molecularly imprinted polymers, by applying a finer characterization for the study of the molecular interaction through a novel patented method capable of detecting simultaneously single fluorescent molecules with nanometric precision as well as their fluorescence lifetime in a wide-field optical configuration (smFLIM). We developed a method based on post-polymerization [2,3], allowing the synthesis of MIPs with a shell containing alkyne groups, and their subsequent immobilization on a flat surface by click-chemistry for single-molecule experiments, to obtain accurate statistics molecular characteristics of MIP nanogels.

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Oral 11

Molecularly imprinted polymers to target and inhibit Gram-negative efflux pump membrane transporter

T. Auroy,[1] B. Bihan-Avalle,[1] K. Haupt,[1]

[1] Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Rue du Docteur Schweitzer, 60203 Compiègne Cedex, France.

* tiffany.auroy@utc.fr

Antimicrobial resistance is considered by the World Health Organization (WHO) as one of the major health challenges of our time. Gram-negative bacteria, especially the ESKAPE pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter species*) head the list of pathogens having the highest resistance indices of all bacteria threatening human health [1]. One of the main mechanisms that leads these bacteria to acquire resistance is the efflux pump system. Indeed, efflux pumps confer resistance to multiple classes of antibiotics by their ability of expelling antibiotic molecules outside the bacteria cells [2]. The aim of this work is to face this health problem by synthesising Molecularly Imprinted Polymer nanogels able to target and bind in a specific and selective way a chosen epitope of the efflux pump and potentially affects its activity.

The synthesis of MIP nanoparticles was performed using a solid-phase approach relying on accessible epitopes as the template [3]. MIPs were characterized physico-chemically and for their specificity and affinity for the target. This interaction was studied both with the fluorescently labelled epitope peptide (used as template) through in batch binding assays, and with the whole native protein. In addition, flow cytometry and confocal microscopy were performed on *Escherichia coli* cells in the presence of fluorescently labelled MIPs. The activity of the efflux pump in presence of MIPs was also studied. Results obtained with this work revealed that synthetised MIPs are able to bind specifically to both the designed peptide (template) and the native protein on the surface of *E. coli* cells. Moreover, the MIP was able to inhibit the efflux pump system.

Acknowledgment

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Oral 12

Magnetic Molecularly Imprinted Polymer for Cancer Therapy

Nébéwia Griffete[1*], Aude Michel[1], Michèle Sabbah[2], Claire Wilhelm[3]

[a] *Sorbonne Université, CNRS, PHysico-chimie des Electrolytes et Nanosystèmes InterfaciauX, PHENIX, F-75005 Paris,France.*

[b] *Sorbonne Université, Saint-Antoine Research Center (CRSA), INSERM, CNRS, F-75012 Paris, France.*

[c] *Laboratoire Matière et Systèmes Complexes, France.*

Email: nebewia.griffete@sorbonne-universite.Fr, +0033-144273169

Research in nanotechnology prospered during the last decade and yielded several prerequisites for drug delivery systems. Among the broad spectrum of nanoscale materials being investigated for biomedical applications, magnetic nanoparticles have attracted significant attention due to their intrinsic magnetic properties [1]. The last 20 years have witnessed an important increase in the number of reports dedicated to magnetic hyperthermia. Magnetic hyperthermia is a type of thermal cancer treatment that takes advantage of the heat generated by magnetic nanoparticles when applying alternative magnetic field (AMF) [2]. An interesting field of research concerns the use of localized temperature around the magnetic nanoparticles (hot spot effect).

Molecularly imprinted polymers (MIPs) have been widely utilized as molecular-recognition and separation materials in different fields. The imprinting process involves the polymerization of a functional monomer in the presence of a molecule with a cross-linking agent. After the extraction of the molecule, the polymer matrix contains tailor-made binding sites, perfectly complementary to the molecule. In recent years, their use in nanomedicine has emerged [3-5]. In this context, we recently developed innovative molecularly imprinted polymers magnetic delivery nanomaterial for triggered cancer therapy showing active control over drug release using AMF [6-8]. Upon AMF, the magnetic nanoparticle locally heats and the drug, sequestered in the MIP, is released by disrupting hydrogen bonds existing with the polymer. As many anticancer drugs possess side effects, this novel material could be helpful to release the drug, with control, at the desired place.

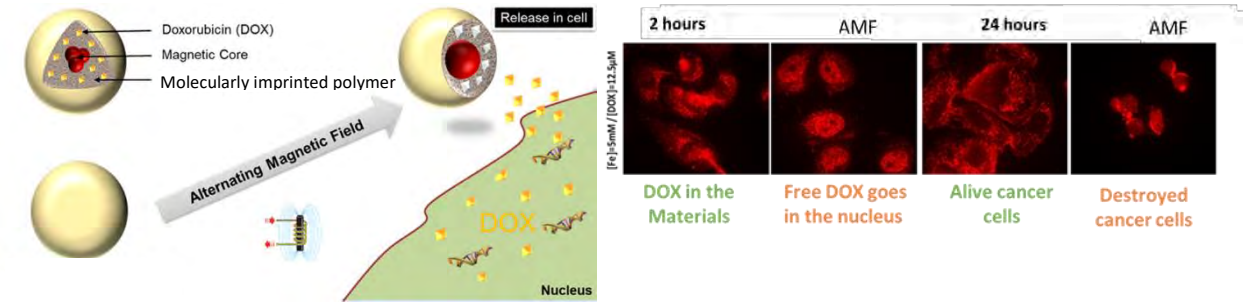

Figure 1. (a) MIP for controlled drug release through AMF. (b) Confocal microscopy of cancer cells with and without AMF application after 2 and 24 hours.

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Snapshot Imprinting: Rapid Identification of Cancer Cell Surface Proteins and Epitopes using Molecularly Imprinted Polymers

Stanislav S. Piletsky[a], Elena Piletska,[b] Marta Poblocka,[c] Salvador Macip,[c,d] Donald J. L. Jones,[e,f,g] Marta Braga,[h] Thong H. Cao,[f,g] Rajinder Singh,[e] Alan C. Spivey,[a] Eric O. Aboagye,[h] Sergey A. Piletsky [b]*

[a] *Department of Chemistry, Molecular Sciences Research Hub, White City Campus, Imperial College London, London, W12 0BZ, UK*
E-mail: stanislav.piletsky14@imperial.ac.uk
[b] *School of Chemistry, College of Science and Engineering, University of Leicester, Leicester, UK*
[c] *Mechanisms of Cancer and Ageing Laboratory, Department of Molecular and Cell Biology, University of Leicester, Leicester, UK*
[d] *FoodLab, Faculty of Health Sciences, Universitat Oberta de Catalunya, Barcelona, Spain*
[e] *Leicester Cancer Research Centre, Leicester Royal Infirmary, University of Leicester, Leicester, UK*
[f] *Department of Cardiovascular Sciences, University of Leicester, Leicester, UK*
[g] *National Institute for Health Research, Leicester Biomedical Research Centre, Glenfield Hospital, Leicester, UK*
[h] *Department of Surgery and Cancer, Imperial College London, Hammersmith Campus, Du Cane Road, London, UK*

Proteomic mapping of cell surfaces is an invaluable tool for drug development and clinical diagnostics. This work describes a new molecularly imprinted polymer-based cell surface mapping technique, dubbed 'snapshot imprinting'. The analysis of two cancer cell lines, HN5 and MDA-MB-468, was performed as a proof of concept, along with the selective targeting of three identified epitopes of epidermal growth factor receptor using molecularly imprinted polymer nanoparticles.

The major advantage of snapshot imprinting is the ability to analyse cell surface proteins without tedious fractionation, affinity separation or labelling. We believe that this system of protein analysis may provide a basic molecular diagnostics toolbox for precise, personalised treatment of cancer and other diseases.

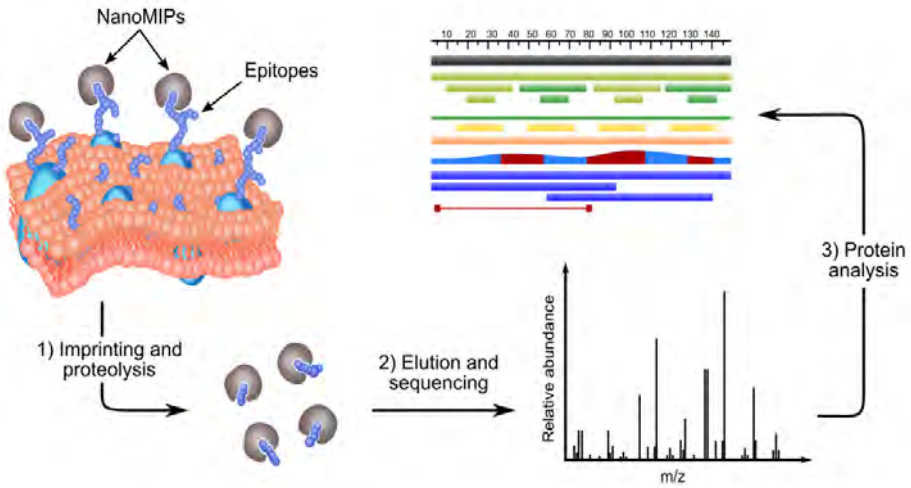

Fig. 1. Diagram depicting snapshot imprinting, wherein cell surface proteins are imprinted, the resultant nanoMIPs are collected, and the template peptides eluted and sequenced in order to identify novel biomarkers.

Oral 14

Molecular Imprinting of Lipid and Glycan Toward Biological Membranes

Lianghai Hu

Center for Supramolecular Chemical Biology,State Key Laboratory of Supramolecular Structure and Materials, School of Life Sciences, Jilin University, Changchun 130023, China.

E-mail: lianghaihu@jlu.edu.cn

Lipid and glycan are the key composition of membranes of cell, bacteria, virus and exosome et al., playing important roles for molecule transportation, recognition and communication. However, due to the structural diversity and amphipathic nature of glycan and lipid, there are lacking antibodies for specific recognition of them as compared to proteins. Herein, we developed molecular imprinting strategies for controllable imprinting toward the polar head of phospholipid exposed on the surface of cellular membranes for recognition. In addition, bunch of glycans from HIV virus were used as templates for preparation of the MIP, where it showed specific recognition and significant inhibition effect. Collectively, the synthesized molecularly imprinted materials have great potential for selective membrane recognition for targeted drug delivery and biomarker discovery.

Oral 15

Biobased molecularly imprinted polymers for the development of new biocontrol formulations

Cyrian Thaeder[1], Shruthi Meenakshisundaram[2], Elise Prost[1], Yolande Perrin[1], Antoine Fayeulle[2] & Aude Cordin[1]*

[1]*Université de Technologie de Compiègne, CNRS UMR 7025, UPJV, Enzyme and Cell Engineering Laboratory, Rue du Docteur Schweitzer, 60203 Compiègne Cedex, France*

[2]*Université de Technologie de Compiègne, ESCOM, Integrated Transformations of Renewable Matter, Rue du Docteur Schweitzer, 60203 Compiègne Cedex, France*

**aude.cordin@utc.fr*

The current applications of molecularly imprinted polymers (MIPs) mainly involve sensors and separation for different fields [1], but they also can be applied as drug delivery systems for therapeutic molecules, or more recently for biopesticides [2] to use them in crop protection. These natural substances are great alternatives for pest control but they often show low stability or solubility. MIPs can thus be used to stabilize the biopesticides and to control their release. In the context of a growing demand for sustainable agricultural practices and sustainable polymer production, the use of monomers derived from renewable sources represents a necessity and a new challenge. Since the cross-linker traditionally represents more than 80% of the MIP composition, its substitution by a biobased alternative is a first step towards greener MIPs. They are a promising and innovative tool for new environmentally friendly plant protection formulations.

New biobased MIPs were synthesized by precipitation free-radical polymerization using several biobased cross-linkers, derivate from plant oils, polyphenols and biopolymers instead of the conventional petroleum-based reagents traditionally used for molecular imprinting. Selected antifungal biopesticides were used as template to create new phytopathogen management solutions. The interaction between the biopesticides and several vinylic monomers was studied by NMR using a Job plot method to select the most adapted functional monomer. Nanoparticles were obtained with a size depending on the cross-linker and were characterized by SEM and FTIR. The binding properties and selectivity of MIPs were also determined and compared to EDMA-based polymer as reference. Finally, the biopesticides release by MIPs was examined and the antifungal properties of these new drug delivery systems were studied against 3 major crop phytopathogens: *S. sclerotiorum*, *B. cinerea* and *F. solani*.

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Oral 16

Exploring cationic C-H hydrogen bonding for the preparation of stoichiometric imprinted polymer targeting sulphonic/sulfated molecules

Sudhirkumar Shinde[a] Börje Sellergren[b], Panagiotis Manesiotis[c]*

[a]School of Consciousness, Dr Vishwanath Karad MIT World Peace University Kothrud 411038 Pune India; E-mail: sudhirkumar.shinde@mitwpu.edu.in
[b]Biofilm Research Center for Biointerfaces, Malmö University, 23014 Malmö, Sweden
[c]School of Chemistry and Chemical Engineering, Queen's University Belfast, David Keir Building, Stranmillis Road, Belfast BT9 5AG, U.K.

Sulfonated and sulfated molecules play crucial roles in many important chemical and biological processes. The design of sulfate and sulfated molecule receptors is complicated because of the high hydration energy ($-\Delta G_{hyd}$ = -1080 kJ mol^{-1} for sulfate), extreme hydrophilicity according to the Hofmeister series, and tetrahedral geometry of the sulfate groups.
Due to the lack of dedicated analytical methods for sulfated biomolecules, there is a rapidly growing need for receptors capable of recognizing sulfated molecules with high affinity and capable of discriminating anions. In this direction, only a few imprinted receptors are available for the recognition of sulfonate [1] and sulfated tyrosine.[2] which were prepared using diaryl urea host monomers.
In this abstract, we present the design and synthesis of high affinity and selective sulfonate-binding imprinted polymers using functional monomers based on combined ionic and C-H hydrogen bond. We have in-depth investigated pre-polymerization complex of monomers and templates by UV, ^{1}H NMR, and modelling and correlated it with the binding capacity and affinity of imprinted polymers prepared by stoichiometric imprinting. [3] We have demonstrated that the water compatibility and selectivity of binding pocket can be easily tuned by tailor-made imidazolium functional monomers with various geometries, architectures, and number of binding sites. Furthermore, we demonstrate the applicability of imprinted polymers for the solid phase extraction of sulphonated compounds from drinking water.

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Oral 17

Design of host-guest anchored imprinting polymers and application to sensitive detection of cancer biomarkers

Q. Jia*, R. Zhu, P. Zhang
College of Chemistry, Jilin University, Changchun 130012, China
*jiaqiong@jlu.edu.cn

Molecularly imprinted polymers (MIPs) are a kind of synthetic receptors possessing wide application prospects in cancer biomarkers recognition. However, there are still great challenges in protein cancer biomarkers imprinting due to their large size and easy conformation change. In this study, we explored novel MIPs based on host-guest interaction (hg-MIP) and constructed hg-MIP-SERS based approaches for efficiently recognizing the protein cancer biomarkers with transferrin (TRF) and neuron-specific enolase (NSE) as representatives, which are well-known biomarkers for some diseases such as small cell lung cancer, neuroblstom, diabetes, thalassemia, and liver disease.

Typically, β-cyclodextrin was selected as the host molecule due to its remarkable ability of constructing complexes with many molecules through noncovalent interactions containing hydrogen bond interaction, hydrophobic interaction, van der Waals force, and dipole-dipole interaction. The imprinted layer was formed by polymerization of various functional monomers. Combined with SERS detection, antibody-free sandwich assays based on hg-MIP were successfully used to detect the concentration of TRF or NSE in human serums, with the advantages of simple operation, small sample volume, and wide linear range. The developed hg-MIP-SERS approach can also be extended to the detection of other proteins cancer biomarkers.

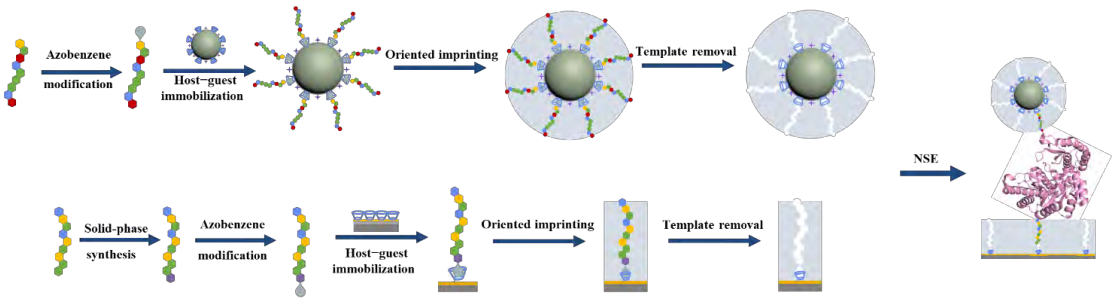


Figure 1. Schematic illustration of the synthesis of hg-MIP.

Oral 18

Lateral Flow nanoMIP Assay: A Proof-of-concept

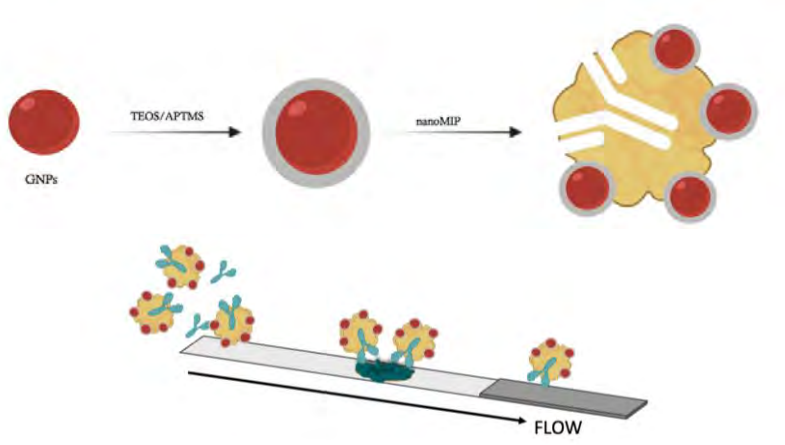
T. Serra,* S. Cavalera, F. Di Nardo, V. Testa, C. Baggiani, L. Anfossi

Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, Via Giuria 7, 10125 - Torino, Italy

** thea.serra@unito.it*

The solid-phase polymerization synthesis of nanoparticles (nanoMIPs) leads them to emerge as highly efficient mimics of natural receptors, offering a promising alternative to antibodies in sensors and bioanalytical applications [1]. In recent years, within the realm of immunodiagnosis, lateral flow (LFIA) devices have evolved into formidable instruments for modern diagnosis. Functioning as portable tools, they facilitate the rapid and precise assessment of a wide range of medical conditions. By utilizing a reactive strip, these tests provide real-time results without requiring sophisticated laboratory equipment. Their intuitive and user-friendly design, coupled with the ability for direct application at the point of care, has significantly transformed the diagnostic timeliness and efficiency. The combined advancements in both lateral flow tests and nanoMIPs represent a potential transformative shift in the landscape of medical diagnostics, marking a significant stride forward in the field, and promising more effective and efficient approaches to diagnostics and healthcare.

This study proposed a simple method for fabricating a new composite material that combines the molecular recognition properties of nanoMIP with the optical properties of the metallic nanoparticles. A hybrid material was synthesized by modifying the surface of the nanoMIP with silica-coated spherical gold nanoparticles (Au@SiO_2). Different synthetic approaches at Au@SiO_2 were investigated. All the methods have foreseen the use of TEOS (tetraethyl orthosilicate) as a silica source for the growth of the silica shell and APTMS (3-Aminopropyl trimethoxysilane) as the silanizing agent to provide a terminal amino function for covalent grafting onto nanoMIPs , allowing their covalent attachment onto the nano polymer's surface [2].



Highly selective nanoMIPs for immunoglobulin G (IgG) were prepared, and their binding properties were assessed through batch rebinding analysis. Subsequently, to assess translation to lateral flow pseudoimmuno-assay platform, nanoMIPs were covalently grafted onto modified gold-silica nanoparticles. The applicability of the hybrid material for LFA was thoroughly investigated by evaluating flow properties, binding kinetics, limit of detection for the target immunoglobulin, and selectivity, proving the suitability of the Au@SiO_2-nanoMIP as effective probes for developing LFA. Moreover, the newly synthesized materials were exhaustively characterized at the different synthesis stages by transmission electron microscopy (TEM), UV-visible spectroscopy, and dynamic light scattering (DLS), confirming the synthesis strategy as an efficient and reproducible way to produce a novel labeled synthetic receptor. This approach can be employed in lateral flow assays as a viable alternative to antibodies, enhancing the foundational aspects of rapid tests, including accessibility, robustness, and user-friendliness.

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Point-of-care and in-field electrochemical MIP sensors: advantages, challenges and possible solutions

Iva Chianella *

Surface Engineering and Precision Centre, School of Aerospace, Transport and Manufacturing, Cranfield University, Cranfield, Beds, MK43 0AL, United Kingdom

i.chianella.1998@cranfield.ac.uk

Electrochemical transducers are particularly suited to develop portable and inexpensive point-of-care (POC) and in-field sensors thanks to their low cost and their ability to be easily miniaturised. Among all the available receptors to render the sensors specific and selective, molecularly imprinted polymers (MIP) are highly promising for POC and in-field diagnostics because of their robustness as well as their ability to provide a highly specific recognition of target analytes. Several electrochemical techniques can be used to develop electrochemical sensors with electrochemical impedance spectroscopy (EIS) being among the most versatile, especially when performed in presence of redox probes. In here, examples of MIP based EIS sensors developed recently in our group for several environmental applications such as the detection of drugs of abuse (e.g., cocaine and morphine) and the detection of important concerning pollutants in wastewater such as 2-hydroxy-4-methoxybenzophenone, octocrylene, and oestradiol will be reported. Advantages and disadvantage of using electropolymerised MIP films, generated either with conductive (i.e., aniline) and non-conductive (i.e., dopamine) monomers, *versus* molecularly imprinted polymers nanoparticles immobilised on electrodes via the use of polymeric films will be presented. Finally, the importance of minimising the sensors' non-specific binding, especially when using a labeless and extremely sensitive technique such as EIS will be discussed and effective methods on how to do so for MIP based sensors will be presented.

Oral 20

Disposable Sensors using Carbon Paste Grafted with Molecularly Imprinted Polymers

Y. Yoshimi*[1] and Aaryashree[2]

1. Dept. Applied Chem. and 2. Innovative Global Program,
Shibaura Institute of Technology, 3-7-5 Toyosu Koto-ku, Tokyo, 135-8548, Japan

yosimi@sic.shibaura-it.ac.jp

The need for single-use disposable sensors is critical in the medical field, particularly for maintaining hygiene standards. These sensors, exemplified by the disposable blood glucose sensor using L. Clark's enzyme electrode [1], must be disposable, highly reproducible, and simple in their operation. Building on this concept, there's an emerging interest in exploring the potential of Molecularly Imprinted Polymers (MIPs). MIPs are specialized materials designed to mimic biological recognition processes. If we can harness the specific interaction between MIPs and analytes—substances used as templates—and translate this interaction into an electrical signal, it could revolutionize the development of disposable sensors. Such sensors could be tailored to detect biologically relevant substances, such as drugs and biomarkers.

Classical radical polymerization has the advantages of simple operation, low cost, and abundant usable materials (monomers). The authors found that the redox current at an electrode with a thin film of MIP formed by radical graft polymerization significantly depends on the specific binding to the target material as a template (gate effect) [2-4]. This electrode is expected to be an easily prepared sensor with a simple measurement method. However, the difficulty of controlling radical polymerization makes it hard to produce uniform sensors for disposable use.

To solve this problem, the authors have developed a new sensor method in which a MIP layer is formed on the surface of graphite particles by graft polymerization, and the electrode is made by kneading it with oil to form a paste [5]. This method can produce homogeneous electrodes because the paste can be kneaded well before the electrodes are made. A disposable sensor was fabricated by loading the carbon paste with fixed MIP onto the working electrode of a sensor chip that incorporates a reference electrode and a counter electrode (**Fig.**). This disposable sensor has a high repeatability, sufficient for single use. The disposable sensor has a high enough repeatability for single use and a measurement time of seconds to measure total blood concentrations of vancomycin [6], theophylline [7], and phenobarbital [8]. These drugs are classified as high-risk drugs and require careful drug dosing planning (Therapeutic Drug Monitoring: TDM) while monitoring blood levels. Monitoring various drugs in blood using this disposable sensor is expected to improve the therapeutic efficacy and safety of chemotherapy dramatically.

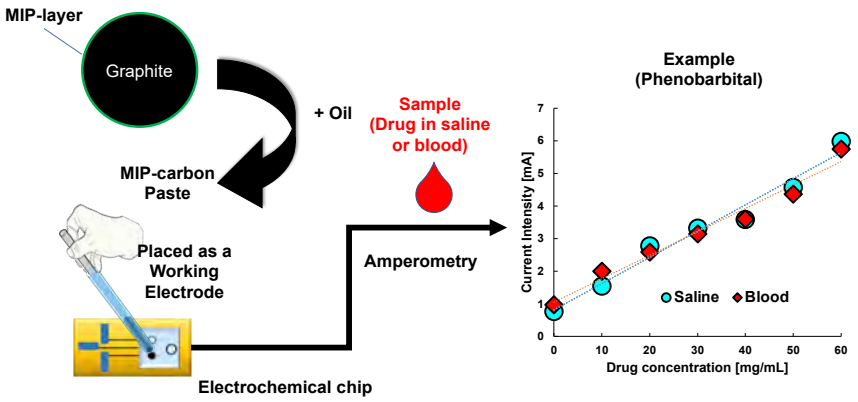

Fig. Fabrication of a disposable sensor using graphite particle on which MIP-layer is

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Molecularly imprinted polymer films grafted on gold electrodes as smart electrochemical receptors for the detection of PAH

F. Ibrahim[1,*], A. Sala[1], G.Laffite[2], C. Nanteuil[2], H. Brisset[1], C. Branger[1,**]

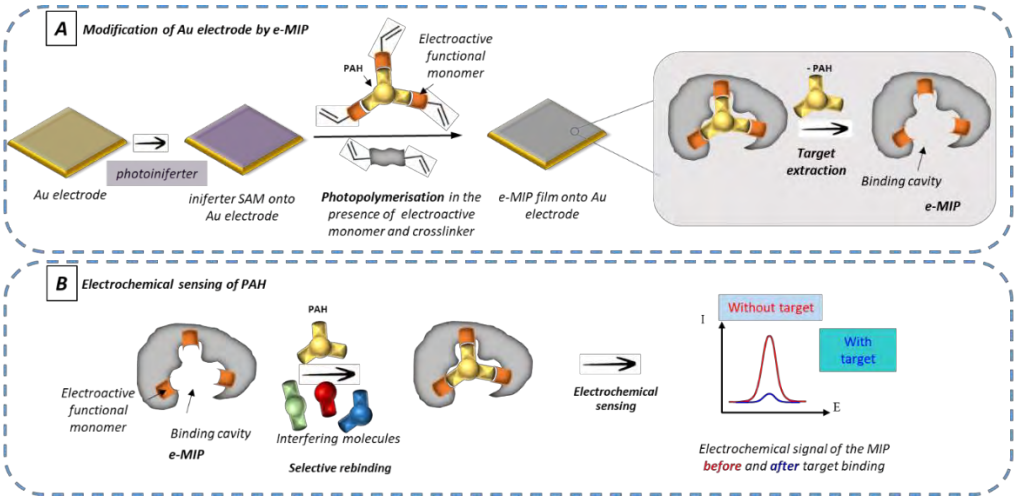
[1] *University of Toulon, MAPIEM, Toulon, France*

[2] *KLEARIA, Technopole Nice Méridia, Nice, France*

** farah.ibrahim@univ-tln.fr, ** branger@univ-tln.fr*

When designing electrochemical sensors based on molecularly imprinted polymers, an innovative strategy relies on the use of a redox probe as a functional monomer [1,2]. Indeed, this allows the detection of molecular targets that have no intrinsic electrochemical activity, without the need for competitive analytes. In the case of electrochemical MIPs (e-MIPs), the electrochemical signal measured is that of the redox probe, which is impacted by the interaction with the target bound in the imprinted cavities.

We previously reported e-MIPs for benzo[a]pyrene (BaP) and for bisphenol A in the format of microbeads, prepared by precipitation polymerization, that were respectively mixed with carbon paste in carbon-paste electrodes [1] or screen-printed electrodes [3]. In order to improve the sensitivity and reproducibility of the sensing elements based on e-MIPs, we now describe the modification of gold electrodes by grafting an e-MIP polymer layer for the detection of polycyclic aromatic hydrocarbons (PAHs). For that purpose, the surface of gold microelectrodes were modified by an original photoiniferter activated by a thiol function to form a self-assembled monolayer (SAM) on gold substrate. This SAM was used to perform a surface-initiated controlled/living radical photopolymerization directly on the electrode surface. Thereby, an e-MIP based on ferrocenylmethyl methacrylate as redox probe and functional monomer, ethylene glycol dimethacrylate as crosslinker and BaP as template was further "grafted from" the surface by photopolymerization. The formation of the SAM and polymer layers were controlled by electrochemical impedance spectroscopy and voltammetry and the polymerization time was optimized. After characterization of the film formation by SEM and AFM, the e-MIP film was used to detect the presence of BaP in aqueous samples with a significant improvement of the limit of detection (0,19 nM) compared to carbon paste electrodes prepared with e-MIP particles (90 nM [1]).



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A novel proteomics approach using molecular imprinting

Elena Piletska, Stanislav Piletsky, Damla Ulker, Ammar Ibrahim, Sergey Piletsky

School of Chemistry, University of Leicester, LE5 1EE, UK; ep219@leicester.ac.uk

The epitopes are important targets of the protein imprinting. Much efforts were spent on the identification of the unique and diagnostically important epitopes by Alessandra Bossi, who was using the *in-silico* methods for their determination and creation of peptide libraries. Question was still remaining, which of the peptides are good targets for molecular imprinting?

A novel "snapshot" imprinting method was developed by Leicester Biotechnology group. It is an effective tool for identifying the linear surface epitopes of the individual proteins, whole cells and viruses using molecularly imprinted polymers (MIPs). The developed approach is based on self-assembly of the functional monomers and cross-linker around of the peptides possessing side chains that are good targets for complex formation. A priory, the epitopes identified using snapshot imprinting are good templates for MIP or, potentially, for antibodies generation.

During last five years a number of proteins and cell lines were characterised and many new molecular biomarkers were discovered. Among them are senescent cells, cells with radiation resistance and drug resistance. The specific epitopes are biological markers for particular cellular conditions. The MIP nanoparticles (nanoMIPs) specific for these epitopes could be labelled and used for imaging and diagnostics.

It was shown that nanoMIPs made for different domains of the individual proteins could activate or inhibit their activity, e.g., activation of acetylcholine esterase or inhibition of beta-lactamase.

The nanoparticles made for identified epitopes are shown to demonstrate specific binding which make a perfect tool for controlled drug delivery. It was also found that nanoparticles specific for intracellular and extracellular domains of EGFR show effect on cell viability and could be on its own a potential tool for cancer therapy. The in vivo biocompatibility of nanoMIPs demonstrated by our team gives a green light for Life Science applications of nanoMIPs.

This presentation is an overview of the snapshot imprinting project to date delivered by Leicester team.

Synthesis of nanoMIP Beacons for the Detection of Methamphetamine

William Goulding and Jon Ashley*

*School of Pharmaceutical and Biomolecular Sciences, Liverpool John Moores University, 3 Byrom Street, Liverpool L3 3AF, * j.ashley@ljmu.ac.uk*

The combination of molecularly imprinted and aptamers as an enhanced molecular recognition has been explored as a strategy for improving both specificity and selectivity in terms of utilising the unique interactions that both MIPs and aptamers offer. While the thermal stability and durability of MIPs help to increase the thermal stability of aptamers. Furthermore, the combination of aptamers and MIPs allows for the possibility for the development of new sensing strategies.

Our research introduces a sophisticated approach utilizing aptamers and nanoMIPs in a synergistic manner, establishing an all-in-one sensor platform (**Figure 1**). This system is uniquely designed for the detection of methamphetamine in biological matrices such as urine and blood. The sensor demonstrates an advanced capability for switchable fluorescence transduction, a co-operative binding mechanism and tunable dynamic ranges.

NanoMIP beacons showed only minimal dynamic based quenching against different concentrations of both methamphetamine aptamers and scrambled aptamer sequence control in the absence of methamphetamine while the nanoNIP beacon imprinted in the absence of methamphetamine showed significant static based quenching towards the methamphetamine aptamer. The nanoMIP beacons showed high sensitivity and selectivity when incubated with different concentrations of methamphetamine and a fixed concentration of methamphetamine aptamer achieving a LOD of 23 nM while the scrambled sequence demonstrated only minimal . The nanoMIP beacons achieved adequate recoveries in both urine diluent and blood serum.

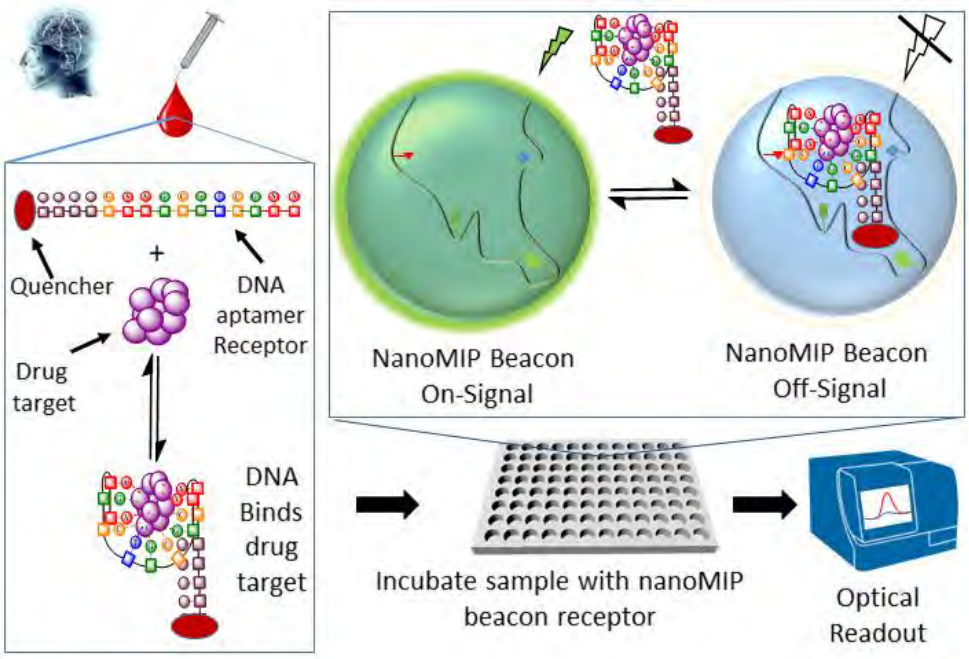

Figure 1 overview of the nanoMIP beacons for the detection of methamphetamine.

NanoMIPs Enable the Rapid and Highly Sensitive Detection of a Crucial Biomarker for Myocardial Infarction, Troponin I

Joshua Saczek[1], Oliver Jamieson[1], Ioakim Spyridopoulos[2], Francesco Canfarotta[3], Jake McClements[1], Marloes Peeters[4]

[1] Merz Court, School of Engineering, Newcastle University, NE17RU Newcastle upon Tyne, U.K.

[2] Department of Cardiology, Freeman Hospital and Newcastle University, Translational and Clinical Research Institute, NE7 7DN Newcastle upon Tyne, U.K.

[3] MIP Diagnostics Ltd., Bedford MK44 1LQ, U.K.

[4] Department of Chemical Engineering and Analytical Science, School of Engineering, University of Manchester, Manchester M20 4BX, U.K.

Jake.mcclements@newcastle.ac.uk

Myocardial infarctions (*e.g.,* heart attacks) have the highest patient mortality and morbidity of any cardiovascular disease. Typically, myocardial infarctions are diagnosed by measuring the levels of the protein biomarker troponin I within the blood. However, current testing methods require costly laboratory-based immunoassays with slow turnaround times, which is detrimental to patient outcomes and wasteful of resources. Consequently, we have developed a nanoMIP-based thermal sensor for troponin I, which demonstrates excellent sensitivity and specificity in spiked-buffered solutions and has been validated in patient samples.

NanoMIPs were synthesized using a small epitope of troponin I as a target and immobilized to low-cost screen-printed electrodes using a simple electrografting protocol (**Figure 1a**). Thermal detection was performed using a 3D-printed measurement cell (**Figure 1b**), and the nanoMIPs exhibited high sensitivity for troponin in buffered solutions with an excellent detection limit of 0.5 ng/L. This detection limit is lower than a commercial immunoassay and comparable to the most sensitive tests from the literature (**Figure 1c**). Furthermore, measurement time was only 30 min, and the sensor displayed excellent specificity against similar but unwanted proteins. The device has also been comprehensively validated using numerous patient samples, further highlighting the potential of the nanoMIP-based sensor for the rapid and low-cost diagnosis of myocardial infarction.

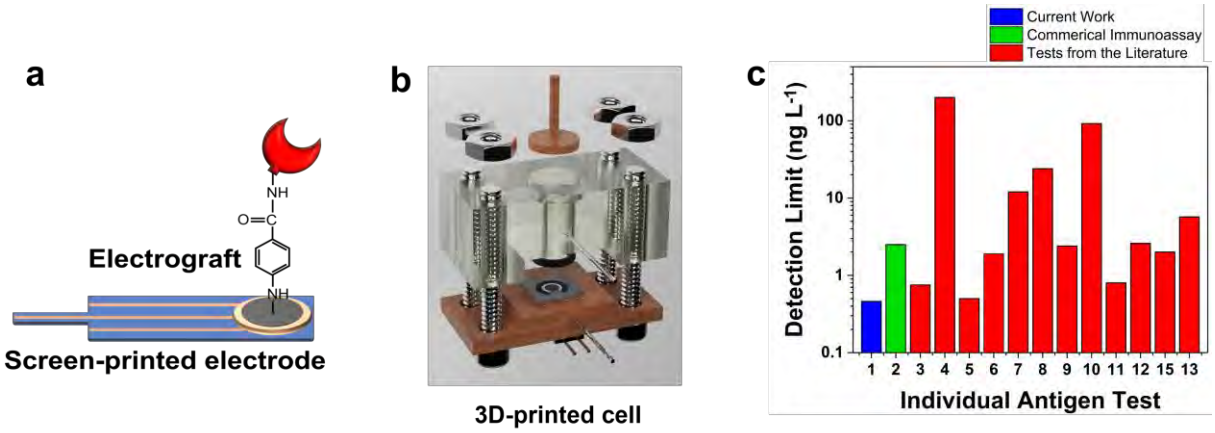

Figure 1: a) NanoMIPs are electrografted to screen-printed electrodes. **b)** The 3D-printed measurement cell utilized for thermal measurements. **c)** Detection limit values for our nanoMIP sensor (blue), a commercial lab-based immunoassay (green), and recently developed sensors from the literature (red).

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Abstracts: Short Oral Presentation

Imprinted hollow TiO_2 microspheres for selective photocatalysis

Vanessa R.A. Ferreira*, Manuel A. Azenha, Carlos M. Pereira and António F. Silva

CIQ-UP, Institute of Molecular Sciences, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

**vanessa.ferreira@fc.up.pt*

TiO_2 is recognized as an efficient photocatalyst, which, when associated with the hollow spherical form, stands out for offering greater efficiency in the absorption of UV light compared to solid TiO_2 microspheres. The crystallinity of TiO_2 is another crucial factor for the efficient generation and migration of photogenerated e^-/h^+ pairs, resulting in a greater photocatalytic efficiency. Due to the high band gap of TiO_2 (~ 3.2 eV), the photocatalytic response of these photocatalysts is limited to UV light irradiation. To overcome this problem, metal doping has been widely studied to make absorption in the visible region of the spectrum possible. Despite all efforts to develop photocatalysts with enhanced photonic activity, there is a gap in the literature regarding the lack of highly selective photocatalysts [1].

This work aimed at the introduction of selectivity into hollow TiO_2 microspheres (HTM) through the sol-gel molecular imprinting technique, reconciling improved photonic efficiency and high photocatalytic selectivity [2]. The synthesis process was optimized to obtain bilirubin-selective HTM, using SiO_2 microspheres as the sacrificial core and bilirubin as the template. Parameters such as solvent, temperature and TiO_2 precursor were studied and optimized. Furthermore, it was demonstrated that the anatase crystallinity of TiO_2 can be obtained without compromising the molecularly imprinted sites using acid pretreatment and calcination at mild temperatures (250 ºC, 18h) [3]. Ag doping has also been explored to improve the response to the visible spectrum, with the timing of doping during synthesis being crucial to the success of the molecular imprinting technique. The results indicate that selective HTM showed the expected photocatalytic activity under visible irradiation, together with a positive catalytic effect of Ag doping [4]. Furthermore, for the first time, a mixture of TiO_2 precursors, including one organically modified, was tested to obtain organically modified TiO_2 microspheres selective for bilirubin by molecular imprinting. The successful incorporation of organic groups into hollow TiO_2 and the effectiveness of molecular imprinting were demonstrated for in an organically modified titania material [5].

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https://doi.org/10.1016/j.ceja.2020.100071
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https://doi.org/10.1016/j.apcata.2022.118912
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https://doi.org/10.1016/j.apsusc.2023.158457
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https://doi.org/10.3390/ molecules27238510

Molecularly imprinted polymer (MIP) nanoparticles for targeted breast cancer therapy and controlled drug delivery

Perla Ben ghouzi,[a] Lila Louadj[b], Michele Sabbah[b], Nébéwia Griffete[a]

[a] Sorbonne Université, CNRS, PHysico-chimie des Electrolytes et Nanosystèmes InterfaciauX, PHENIX, F-75005 Paris,France.

[b]Sorbonne Université, Saint-Antoine Research Center (CRSA), INSERM, CNRS, F-75012 Paris, France.

perla.ben_ghouzi@sorbonne-universite.fr

Despite undeniable progress in the prevention, screening and treatment of breast cancer, this disease remains a major health problem. While the majority of these cancers are curable at an early stage with treatments such as surgery and/or chemotherapy-radiotherapy, the main therapeutic weapons in situations at risk of recurrence (resistance to treatment) or in metastatic situations are targeted therapies. In this context, the recent emergence of the glycoprotein Trop-2 (Trophoblast Cell Surface Antigen 2) as a promising therapeutic target has led to new therapeutic paradigms for treating patients with advanced or metastatic breast cancer. Recently, antibody-drug conjugates (ADC) have been developed and launched to the market for this purpose. However, the production of ADCs is highly complex, time consuming and costly. Thus, an alternative must be developed to provide a new approach to breast cancer treatment. Indeed, this is what we are focusing on in our project. Using a completely new approach in the field of nanomedicine, we have developed fluorescent synthetic nanoparticles with a TROP2 imprint (MIPs-TROP2), encapsulating active molecules (chemotherapies, targeted therapies) used in breast cancer treatment. The goal of the study is to use these MIPs-TROP2 nanoparticles to specifically target breast tumors overexpressing TROP2 protein and deliver the encapsulated therapeutic molecule precisely to the tumor site.

The synthesis process of the MIP relies on a double-layer technique using the solid-surface synthesis known in the literature.[1] After the formation of the first layer containing the imprint, a second layer is induced on the top in order to encapsulate SN38.[2] The size and shape of the obtained nanoparticles, approximately 200 nm, were evaluated using transmission electron microscopy and dynamic light scattering. To achieve this, first in vitro analyses using flow cytometry, NanoITC, confocal microscopy and cell viability were performed to validate the fluorescent nanoparticles imprinting and then to assess their toxicity and biocompatibility. We used four breast cancer cell models overexpressing the protein of interest (MCF7, T47D, MDAMB231 and SUM149) and one cell model not expressing the protein as a control (SUM159). The results showed specific targeting of TROP2-positive cell lines compared to the SUM159 control, confirming the affinity and accessibility of the imprint to its target. This binding specificity was confirmed by confocal microscopy in 3D cellular models. In addition, no decrease in viability was observed, confirming the cellular biocompatibility of the nanoparticles. Furthermore, ultrasensitive isothermal titration calorimetry (ITC) was used as a method for thermodynamic monitoring of non-covalent molecularly imprinted polymer bindings to evaluate the interaction with cancer cells.[3] Taken together, our results confirm that the use of molecularly imprinted polymers as an alternative to ADC against cell membrane receptors represents a promising and innovative new line of nanomedicine.

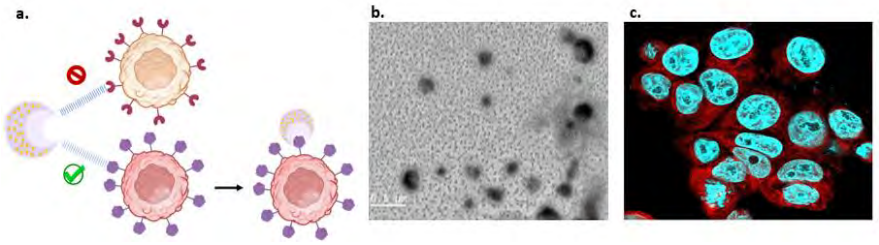

Figure: a) Schematic representation of MIP recognition on two cell lines. b) TEM image of the MIP. c) Confocal microscopy of the MIP on MCF7.

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Acknowledgments

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A glycan shield-targeting broad-spectrum antiviral nanomedicine provides potent therapeutic and prophylactic effects

Jingran Chen[1,#], Ying Li[1,#], Li Xiao[2], Zhanchen Guo[1], Jizong Li[2], Weihua Lu[1], Jin Huang[2], Bin Li[2,*] & Zhen Liu[1,*]

[1] *Nanjing University, Xianlin Campus, School of Chemistry and Chemical Engineering, State Key Laboratory of Analytical Chemistry for Life Science, 210023, China.*

[2] *Jiangsu Academy of Agricultural Sciences, Institute of Veterinary Medicine, Key Laboratory of Veterinary Biological Engineering and Technology, 210014, China.*

**zhenliu@nju.edu.cn*

Effective antiviral drugs and vaccines play determining role when confronting the ever-evolving and newly emerging fatal viruses. Although seemingly little intersection, they could be exquisitely integrated to achieve acute protection and long-term prevention against infection of various viruses. The combination of both could fulfill timely, completely and broad-spectrum virus eradication. However, due to the difficulty in the drug development, such double-punch super antiviral agent is currently lacking.

Herein, we report the rational engineering of viral glycan shield-targeting [1,2] photothermal nanomedicine for broad-spectrum, all-round and long-term inhibition of viruses (Figure 1). The synthesized antiviral nanomedicine exhibited high affinity and specificity, and could efficiently induce viral aggregation and block virus attachment. Benefiting from the photothermal effect, the synthesized nanomedicine could effectively promote viral lysis and thoroughly inhibit the infection of various viruses including pseudoviruses of SARS-CoV-2 and its major variants, LASV and authentic PDCoV virus. *In vivo* experiments further demonstrated its double benefit on rapid inflammation suppression and effective production of protective antibodies against authentic PDCoV infection. Therefore, this multifunctional nanomedicine provides an unprecedented paradigm for treating and preventing infection of various viruses, indicating a brand-new avenue for the development of potent antiviral agents.

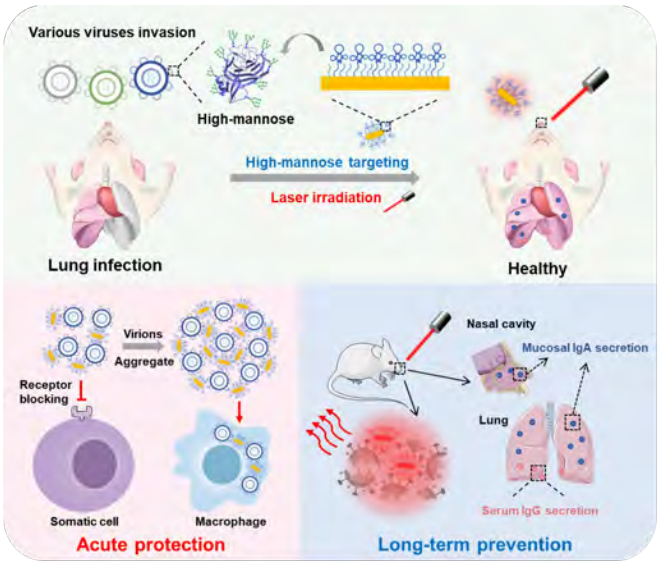

Figure 1. Hypervalent and photothermal nanomedicine for broad-spectrum, all-round and long-term virus inhibition.

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Towards a Computational Polymer Design Protocol for Biomarkers Detection: 1) Prostate-specific Antigen, Water and Cyrene interactions

C. Donaldson, H. Leese & C. Herdes*

Department of Chemical Engineering, University of Bath, Claverton Down, Bath, Somerset BA2 7AY, United Kingdom

** cehm21@bath.ac.uk*

Biomarkers are pivotal in pharmaceutical discovery, offering insights into drug mechanisms, efficacy, toxicity during development and aiding in patient group stratification. Their utility extends to disease monitoring, pre-diagnosis screening, and risk assessment. In diagnostics, they facilitate staging, therapy selection, and post-diagnosis monitoring, proving invaluable for subsequent treatments and disease tracking [1].

It is crucial to develop precise biomarker detection tests, yet it presents challenges due to biomarkers' complex structures, binding specificity, and stability. **The research project aims to establish a computational protocol for designing molecularly imprinted polymers (MIPs) capable of selectively binding specific biomarkers**. Using the prostate-specific antigen, PSA, as a case study, and molecular dynamics simulations will explore interactions between PSA's carboxyl-terminus tail epitopes, MIP components (functional monomers and crosslinkers), and solvents.

PSA is a serine protease enzyme produced by the columnar epithelium of prostatic tissue. While sensitive, it lacks specificity, meaning both benign and malignant conditions can lead to an elevation in its levels. Despite this it still retains utility as a biomarker, as its elevated levels is the most common initial laboratory abnormality, and it remains useful in determining the extent of the malignancy, progression, and monitoring treatment response [2].

The protocol simulations will identify optimal functional monomers for precise biomarker recognition and determine the ideal crosslinker quantities to enhance binding capacity and selectivity for PSA epitopes. Varying crosslinker concentrations will be investigated to establish the optimal ratio for maximising binding capacity. Additionally, the MIPs' performance will be assessed across diverse solvent environments, examining solvent-dependent effects on their capabilities. Temperature and pressure variations will also be considered to evaluate MIP stability under differing conditions comprehensively.

The selection of the solvent in MIP production is essential as it generates a homogeneous system which facilitates the complexation stage and controls the porosity of the MIP. A suitable solvent enables the development of a well-defined pore structure and a high surface area [3]. The porogenic solvent is also responsible for adequately dissolving all the agents during polymerisation while not interacting with the formed template-monomer complex. Therefore, it needs to be selected carefully [4]. Typically apolar, non-protic such as

toluene or chloroform are preferred for MIP synthesis, however, polar protic solvents or water may also be selected if hydrophobic forces are present in the complexation stage [5] .

Cyrene, a green solvent, was first developed in 2014 by Circa Group in partnership with Professor James Clark, PhD, at the University of York's Green Chemistry Centre of Excellence. Classed as a non-polar aprotic solvent with polarity parameters comparable to NMP [6], it is derived from cellulose-based biomass. It has only recently been explored as a reagent and solvent and reviewed in many studies [6-8], where it has shown potential application as a replacement for traditional polar aprotic solvents.

In this initial contribution to MIP 2024, we explore the case study of the ternary system PSA/water/Cyrene to answer the following questions:

1. How good is the Cyrene/water solvent mixture for PSA's renaturation? i.e., the spontaneous refolding of a denatured PSA into the correct tertiary structure and
2. Is there an optimal solvent mixture composition? i.e., what Cyrene/water ratio is optimal for PSA,s renaturation.

The successful implementation of this MIP design protocol could revolutionise diagnostic methodologies, enabling the rapid development of point-of-care diagnostic tools, efficient biomarker detection, and a streamlined research and development process. This protocol can create a new era of fast, customisable, cost-effective diagnostic solutions.

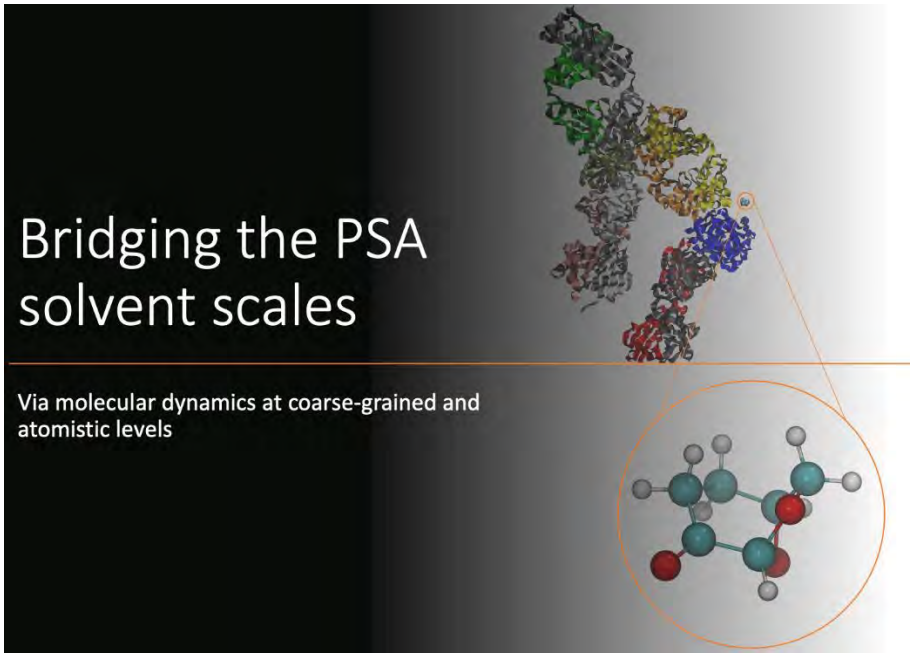

Figure 1. Crystal structure of PSA in Fab sandwich with a high affinity and a PCa selective antibody (3QUM) [9] and Cyrene molecule

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Molecularly imprinted nanoprobes and time-resolved fluorescence spectroscopy in a nanosensing device for the detection of ultralow protein concentrations

A. Marinangeli, [a] A. Quaranta, [b] L. Pancheri, [b] D. Maniglio, [b] A.M. Bossi [a]
[a] *Dept. of Biotechnology, University of Verona, Strada Le Grazie 15, 37134 Verona, Italy*
[b] *Dept. of Industrial Engineering, University of Trento, Via Sommarive 24, 38123 Trento, Italy*
alice.marinangeli@univr.it

Keywords: molecularly imprinted nanoparticles, nanosensor, fluorescent decay, time-resolved fluorescence spectroscopy

Molecularly imprinted nanoparticles (nanoMIPs) are synthetic receptors with tailor-made recognition sites prepared by a template assisted synthesis.[1] NanoMIP-based optical sensors are currently attracting significant interest as they rely on the combination of the MIP's selective capability with optical techniques that offer exquisite sensitivity, low detection limit and real-time response.[2]
In the present work, an optical nanosensor based on MIP was designed for the detection of human serum albumin (HSA) through time-resolved fluorescence spectroscopy (Fig. 1).[3] Fluorescent nanoMIPs (Fluo-nanoMIP) were synthesized using a total monomer concentration of 0.2% w/v and HSA was used as template. Fluorescence was entailed by adding the monomer fluorescein O-methacrylate in the polymeric network. Fluo-nanoMIPs were physically characterized by dynamic light scattering showing a hydrodynamic size of about 120 nm. Scanning electron microscopy and atomic force microscopy confirmed the size of the nanoparticles. Steady-state fluorescence spectroscopy was used as a classical method to study the ability of Fluo-nanoMIPs to bind HSA showing an apparent dissociation constant (K_{app}) of 30 pM. Moreover, the cross-reactivity of Fluo-nanoMIPs were tested against different proteins demonstrating high selectivity for the analyte. Then, Fluo-nanoMIP based sensor, challenged with increasing concentrations of HSA, was tested in solution through time-resolved fluorescence spectroscopy. A decrease in fluorescence lifetime decay was detected and characteristic saturation binding isotherm was observed with a K_{app} of 18 pM, a linear dynamic range of 3.0 – 83.5 pM and a limit of detection of 1.26 pM. As a proof of concept, nanosensor was shown to detect HSA spiked in wine, presenting a new potential method for monitoring allergens in beverages. Finally, with the idea of knowledge transfer, we attempted to immobilize Fluo-nanoMIP onto a surface in order to develop a portable, compact and easy-to-use device.

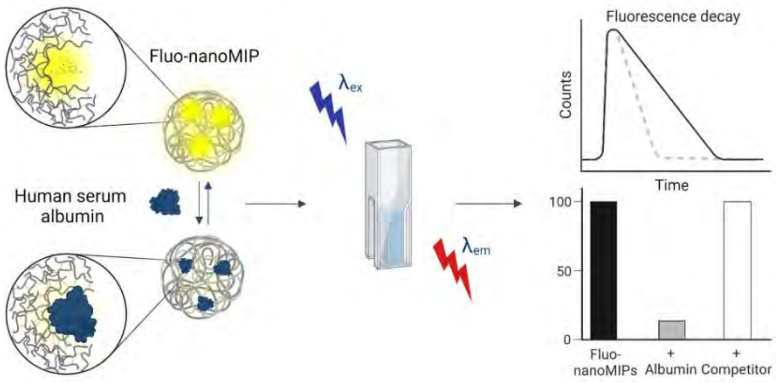

Fig. 1 Fluo-nanoMIP based optical sensor.

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Gold screen-printed electrodes coupled with molecularly imprinted conjugated polymers for ultrasensitive detection of streptomycin in milk

Margaux Frigoli[a*], Manlio Caldara[a], Jeroen Royakkers[a], Joseph W. Lowdon [a], Thomas J. Cleij [a], Hanne Diliën [a], Kasper Eersels [a], Bart van Grinsven [a].

[a] *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, the Netherlands*

*m.frigoli@maastrichtuniversity.nl

Antibiotic resistance is a global health threat, challenging traditional treatments and complicating the food safety process.[1] This study introduces an electrochemical detection method for streptomycin sulfate, utilizing gold screen-printed electrodes (Au-SPE) functionalized via electropolymerization of a custom-made naphthalene diimide-based conjugated monomer (Th_2-NDI-PIA). This modification creates specific binding sites for streptomycin, allowing a rapid detection of the antibiotic. The sensor's response to different concentrations of streptomycin was studied via Differential Pulse Voltammetry (DPV) in a wide linear range from 10^{-13} M to 10^{-9} M, with a limit of detection (LoD) of 0.190 ± 0.005 ρM (Figure 1).

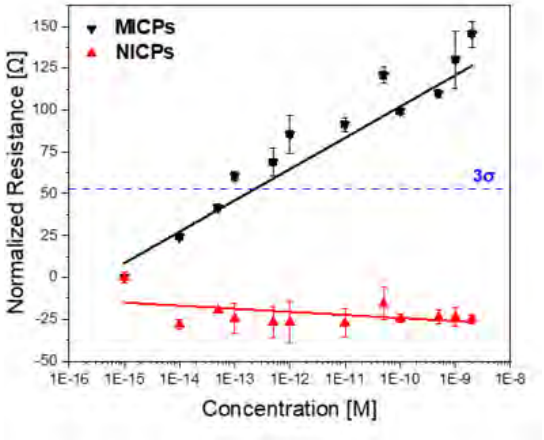

Figure 1: Dose-response curve for molecularly imprinted conjugated polymer (black line) and non-imprinted conjugated polymer (red line) after exposure to different concentrations of streptomycin.

The imprinted electrode demonstrates selectivity to other antibiotics, such as vancomycin and amoxicillin, but also to common interferents that can be found in milk such as lactose, glucose, riboflavin and bisphenol A. Successful proof-of-principle in whole cow milk highlights the sensor's efficacy in detecting antibiotic residues in food samples, offering a promising alternative for a rapid and portable detection technique.

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Supercritical CO_2-assisted metal–Biomolecular Imprinting: Rational design using Molecular Dynamics

A. I. Furtado[1,2#], V. D. B. Bonifácio[2,3], S. F. Sousa[4], R. Viveiros[1], T. Casimiro[1*]

[1]*LAQV–REQUIMTE, Chemistry department, NOVA School of Science & Technology, NOVA University of Lisbon, Caparica 2829–516, Portugal.*

[2]*iBB-Institute for Bioengineering and Biosciences and i4HB–Institute for Health and Bioeconomy, Instituto Superior Técnico, University of Lisbon, Lisboa 1049–001, Portugal.*

[3]*Bioengineering Department, Instituto Superior Técnico, University of Lisbon, Lisboa 1049–001, Portugal.*

[4]*LAQV-REQUIMTE, Biomolecular SIMulations Research Group (BioSIM), Faculty of Medicine, University of Porto, Portugal.*

[#]ai.furtado@campus.fct.unl.pt *teresa.casimiro@fct.unl.pt

The Periodic Table has an extensive collection of chemical elements, many of which have not yet been fully explored, thus presenting an opportunity for the development of novel advanced materials. Metals, allied to molecular imprinting techniques, exhibit a significant potential for biorecognition by creating selective binding sites within polymeric matrices. Metal–Molecularly Imprinted Polymers (metal–MIPs) are emerging advanced materials that take advantage of metal coordination bonds between template and metal–based monomers during the imprinting process, enhancing the molecular recognition performance, both affinity and selectivity [1]. This work focuses on the development of metal–MIPs for L–leucine (LEU) recognition, using a supercritical carbon dioxide ($scCO_2$)-assisted polymerization based on a rational design using a Molecular Dynamics (MD) model for $scCO_2$. The potential of $scCO_2$-assisted MIP synthesis for the development of high–value materials has been demonstrated [2-4]. CO_2 is an abundant, non–toxic alternative solvent, that can be easily removed after polymerization without additional energy input, being $scCO_2$ also a scalable technology [2]. The $scCO_2$ MD model was implemented using the *Amber* software to comprehend the behavior of MIP systems produced with this technology. The choice of the functional monomer(s) and the stabilization of LEU–monomer complexes in $scCO_2$ were evaluated through the binding free energies using an adapted Molecular Mechanics Poisson-Boltzmann Surface Area (MM–PBSA) method. Multiple simulations were conducted by varying functional monomers, molar ratios, cosolvents, using supercritical conditions. The best systems were validated experimentally. Further, the interactions within the template–metal monomer complexes were confirmed experimentally by comparing the metal–MIP and the non–metal MIP. The performance of the produced materials was evaluated through static binding tests using a 0.5 mg/mL LEU aqueous solution, revealing promising results: a binding capacity (*Q*) of 43 mg LEU/g of MIP, and an Imprinting Factor (*IF*) of 11, thus envisaging a great potential for bio–applications.

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Bispecific Immune Checkpoints nanoBlocker Reinvigorate Both Innate and Adaptive immunity against Triple Negative Breast Cancer

Peixin Guan, Wanting Qu, Fang Jin, Song Gao, Zhen Liu*

State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, 163 Xianlin Avenue, Nanjing 210023 P.R. China

* Email: zhenliu@nju.edu.cn

Immune checkpoints blockade (ICB) therapy has made substantial strides in cancer treatment. However, exiting platforms suffer from intricate manufacturing issues and severe immune-related adverse effects. Herein, we report bispecific molecularly imprinted nanoblocker (bsMINB) that unleashes durable antitumor immunity against triple negative breast cancer (TNBC) via innate and adaptive ICB. Using N-terminal dodecapeptide of PD-L1 and SIRPα as template epitopes, antibody-like bsMINB was prepared via the state-of-the-art imprinting strategy. [1] This multi-pronged design endowed bsMINB with high affinity for both PD-L1 on TNBC cells and SIRPα on macrophages, effectively blocking the PD-L1/PD-1 and CD47/SIRPα interactions. These disruptions significantly restored macrophage-mediated tumor phagocytosis, promoted the presentation of tumor-associated antigens on macrophages and reinvigorated T-cell-mediated tumor killing. In vivo experiments further confirmed the significantly inhibited effect of bsMINB on tumor growth, inducing durable anti-tumor response. This study not only introduces a versatile and tailored approach for multi-targeting cancer immunotherapy, but also expands the toolkit for developing antibody mimics with multiple recognition capabilities via imprinting technology for various diseases.

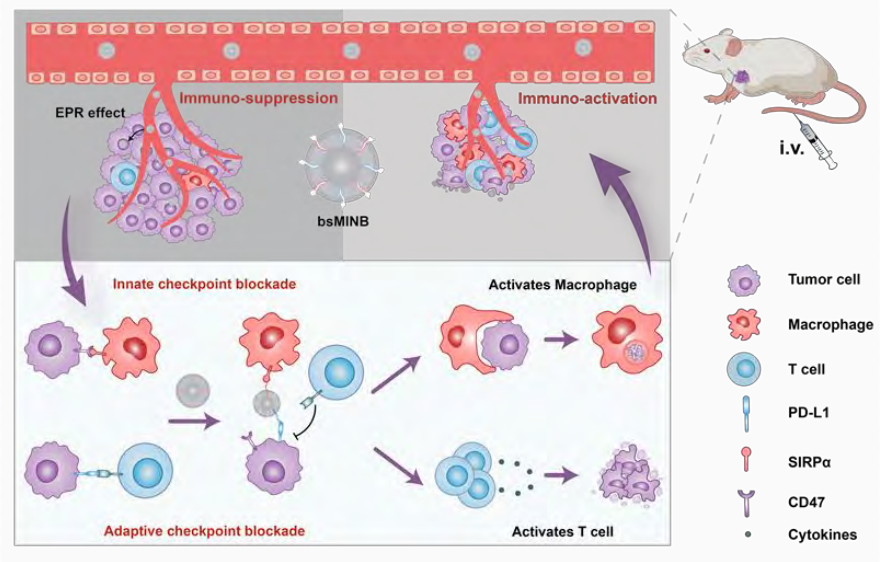

Figure 1. Schematic illustration of dual immune checkpoint blockade strategy via bispecific molecularly imprinted nanoblocker (bsMINB).

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Electropolymerized Molecularly Imprinted Polymer-modified Interdigitated Electrodes: A proof-of-concept Testing for Cystatin-C Detection

Meriem Kassar[a], Marcel Bauer[a], Matthias Franzreb[a], Gözde Kabay[a]

[a]*Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Baden-Württemberg 76344, Germany*

meriem.kassar@kit.edu

Molecularly imprinted polymers (MIPs) are highly cross-linked artificial networks specifically engineered to replicate the functionality of natural receptors, such as antibodies and enzymes. The specialized imprinted sites facilitate the selective capture and binding of specific target molecules, a phenomenon known as molecular recognition, upon reintroducing them into the system. MIPs possess distinctive features, encompassing ease of production and customization, cost-effectiveness, exceptional physical and environmental stability, durability, suitability for large-scale manufacturing, and an extended shelf life[1,2]. Consequently, significant research endeavors have been directed toward exploring various synthesis approaches for MIPs, aiming to effectively tailor them for diverse applications such as drug delivery, separation, purification, and mainly chemical or biological sensing.

Moreover, this study investigates the applicability of the electropolymerization approach for the reproducible MIP synthesis onto interdigitated electrodes (IDEs) and their adaptation for biosensing. To construct the MIP-modified IDEs (MIP-IDEs), 2,2′-bithiophene is selected as a crosslinker, whereas 2,2′-bithiophene-5-carboxylic acid and 2,2′-bithiophene derivatized with catechol are used as monomers, and Cystatin-C as the template protein. A full factorial experimental design was performed to systematically determine the optimal electropolymerization parameters. Electrochemical impedance spectroscopy (EIS) analyses and scanning electrode microscopy (SEM) imaging are used for parameter optimization (Figure 1).

First, cyclic voltammetry analysis was conducted to identify the voltage range at which the oxidation (electropolymerization) of 2,2′-bithiophene took place, establishing this range to be between 1.5–1.7 V. Subsequently, potentiostatic scans were executed to facilitate the electropolymerization of MIPs, utilizing a constant voltage that selected within the predefined range. As a result, it was determined that 1.6 V yielded a homogenous and thin MIPs layer formation on the IDE, thus entitling it as the optimum voltage for further electropolymerization steps. Several potentiostatic scans at 1.6 V are performed to optimize the MIPs formulation. The SEM images and EIS analyses revealed that the crosslinker-monomer molar ratio of 1:10 and monomer-protein molar ratios spanning from 1:100 to 1:1000 yielded consistent and reproducible MIP synthesis.

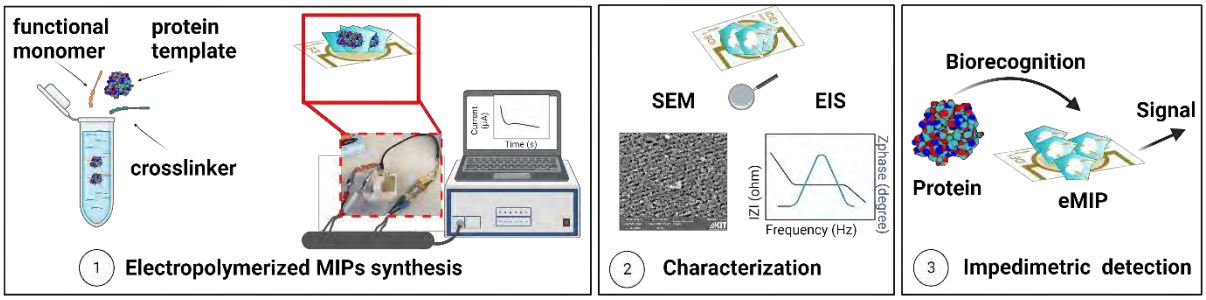

Figure 1: Summarized workflow of a systematic development of MIP-modified IDE biosensor. The figure is created with BioRender.com)

In the final stage, we evaluated the imprinting site's functionality of the electropolymerized MIPs by Cystatin-C sensing. Toward this goal, EIS analyses before and after Cystatin-C binding to the MIPs were performed. The impedance spectra shift demonstrated the electropolymerization method's suitability for producing functional MIPs specifically tailored for Cystatin-C detection. Overall, our study presents a straightforward yet reliable synthesis approach, enabling reproducible and selective MIPs production.

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NanoMIP as synthetic receptor for rabbit IgG: effect of different crosslinker amount

V.Testa, L.Anfossi, S.Cavalera, F.Di Nardo, T.Serra, C.Baggiani,

Department of Chemistry, University of Turin

v.testa@unito.it

The binding selectivity typical of molecularly imprinted polymers (MIPs) is of fundamental importance in many analytical applications, such as solid phase extraction, immunochemical assays, and sensoristics. The Solid-Phase Polymerization Synthesis (SPPS) represents an innovative approach to preparing Molecularly Imprinted nanoParticles or "nanoMIPs". SPPS technique showed its validity for different types of polar templates such as small organic molecules, peptides and proteins, nucleic acid, and whole cells.

Despite this, SPPS[1] uses a pre-polymerization formulation with a nearly fixed composition between the different components of the mixtures, typically composed of acrylic acid (AA) as a functional monomer, t-butylacrylamide (tBAM), and isopropyl acrylamide (NIPAM) respectively as moderately hydrophobic and thermoresponsive co-monomers. Regarding the cross-linker, the most used is methylene-bis-acrylamide (BIS) at 2% mol concentration[2]. In literature, it is possible to find some polymerization in which BIS is used at 16% molar concentration, or in 0% applicate in linear molecularly imprinted polymer approach[3].

Until now the effect of different amounts of crosslinker has never been reported in detail because, usually, the binding properties have been related to the interactions with the functional monomers rather than the crosslinker. Here we report the effect of different amounts of BIS ranging between 0 (non-crosslinked) - 50% mol concentrations towards binding properties of nanoMIPs imprinted with rabbit IgG.

Binding properties have been tested with equilibrium partition towards rabbit IgG and, to get the selectivity, against bovine IgG. The results show that the degree of cross-linking defines three distinct types of nanoMIPs: (i) those with a low degree of cross-linking, including nanoMIPs without cross-linker (0–05 mol%), showing a low binding affinity about $1.0 \pm 0.2 \times 10^6$ mol L^{-1}, high density of binding sites, and low selectivity; (ii) nanoMIPs with a medium degree of cross-linking (1–18 mol%), showing higher binding affinity about o $14.4 \pm 0.7 \times 10^6$ mol L^{-1}, low density of binding sites, and high selectivity; (iii) nanoMIPs with a high degree of cross-linking (32–50 mol%), characterized by non-specific nanopolymer–ligand interactions, with low binding affinity about $1.6 \pm 0.3 \times 10^6$ mol L^{-1}, high density of binding sites, and no selectivity.

In conclusion, the results are particularly relevant in the synthesis of high-affinity, high-selectivity nanoMIPs as they demonstrate that a significant gain in affinity and selectivity could be achieved with pre-polymerization mixtures containing quantities of cross-linker up to 10–20 mol%, well higher than those normally used in this technique.

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Adenosine detection using a molecularly imprinted polymer biosensor with incorporated modified thymidine monomers.

Molly I. Wild, Mark V. Sullivan, Chester Blackburn, Nicholas W. Turner*

Department of Chemistry, University of Sheffield, Dainton Building, 13 Brook Hill, Sheffield, S3 7HF, UK.

Stress is a response to stimuli which disrupt the homeostasis of a cell or organism. Adenosine is a purine nucleoside which functions as an immunomodulator and signalling molecule, with elevated levels present in tissues exposed to stress. Current methods used to determine adenosine levels within the body involve chromatography coupled with mass spectrometry, which while sensitive is time consuming and costly, highlighting the need for a quicker and more cost-effective detection method.

Six nanoMIPs were produced using solid-phase synthesis targeting adenosine: a plain nanoMIP, an acrylamide-dT nano-MIP (bearing an acrylamide-modified thymidine molecule), and a carboxy-dT nanoMIP (bearing a carboxy-modified thymidine molecule) were made using two different methods. The first involved glutaraldehyde as the linker molecule connecting the template to the solid phase, whilst the second used EDC/NHS coupling chemistry. This allowed us to alter the orientation of the template to present either the base or sugar outwards.

SPR was used to test the nanoMIP binding affinities and selectivity against adenosine, thymidine, deoxyguanosine and deoxycytidine. It was found the binding affinities of the nanoMIPs increased with use of the modified thymidine monomers, with equilibrium dissociation constants (K_D) values of the plain nanoMIP, acrylamide-dT nanoMIP and carboxy-dT nanoMIP being 221 nM, 9.35 nM, and 2.11 nM respectively for the glutaraldehyde method. The following K_D values were obtained for the EDC/NHS method: 212 nM, 5430 nM, and 111 nM for the plain nanoMIP, acrylamide-dT nanoMIP and carboxy-dT nanoMIP respectively. This illustrated the glutaraldehyde method produced more effective nanoMIPs than using EDC/NHS. This is surprisingly as it is counter-intuitive to the imagined Watson-Crick pairing.

When challenged with the other nucleosides, excellent selectivity was observed. Fetal bovine serum was used to test the capability of the nanoMIPs in complex matrixes with consistent results produced throughout.

Detection of inflammatory biomarkers using core-shell imprinted nanocomposites

Rahil Radfar[1], N. Sanda Moldovean-Cioroianu[1], Zeynep Altintas[1*]

[1]*Department of Bioinspired Materials and Biosensor Technologies, Kiel University, Kaiserstraße 2, 24143, Germany*

**za@tf.uni-kiel.de*

Interleukin-6 (IL-6), a protein from cytokine families, is mainly known as one of the biomarkers in inflammatory diseases, while it also plays other vital roles in the body, such as regulating the immune response, bone maintenance, and body temperature as well as controlling cell growth. In addition, the overexpression of IL-6 in the body can indicate different health complications [1]. Therefore, highly sensitive and specific biosensing platforms are crucially needed for the detection of IL-6. The application of molecularly imprinted polymers (MIPs) as recognition elements in biosensing has been long established [2]. However, the use of computational modeling to develop enhanced formulation in the synthesis of MIPs has recently become the center of attention in the field. Moreover, preparing multifunctional MIPs, such as inorganic-organic core-shell structures, demonstrating combined properties of core and shell materials, which broaden their applicability in different fields, has caught much attention from researchers [3].

In this study, IL-6 specific magnetic molecularly imprinted core-shell structures with fluorescent properties with a core diameter of 50 nm were synthesized through an epitope imprinting approach using both conventional and computational recipes (MMIPs, and in-situ MMIPs, respectively). The successful synthesis of both MMIPs was confirmed using various characterization tools, including light scattering methods, Fourier Transform infrared spectroscopy, fluorescent spectroscopy, contact angle measurements, scanning, transmission, and fluorescence microscopies. Furthermore, the sensing performance of both MMIPs was validated and compared in terms of affinity, sensitivity, and specificity using an electrochemical sensor. The results confirmed that the established platforms could be used for highly sensitive detection of IL-6 at sub pM range.

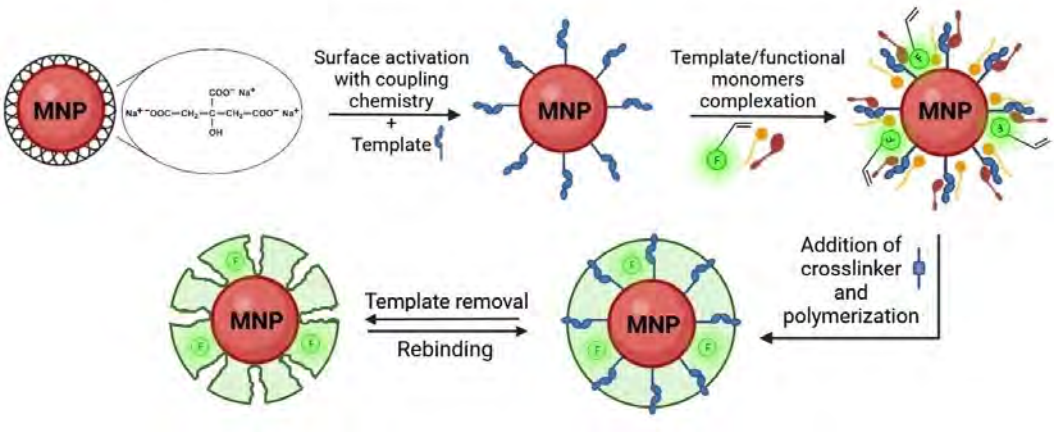

Figure 1: Schematic representation of the synthesis procedure of the core-shell imprinted nanocomposites.

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Tailored Macroscopic Geometries of Porous Molecularly Imprinted Polymers via LCD-Based 3D Printing

B. Keitel,[1,2] A. Batista,[2] S. Schimana,[1] B. Mizaikoff [1,2] & M. Dinc*,[2]

[1] *Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany.*

[2] *Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany.*

**Mehmet.Dinc@Hahn-Schickard.de*

Molecularly imprinted polymers (MIPs) with tailored macroscopic architectures expand the applications of molecular imprints. With this contribution, we present a novel concept that combines polymerization-induced phase separation in LCD-based 3D printing with non-covalent molecular imprinting technology (Fig. 1). In contrast to the ongoing trend towards miniaturization, this merging of self-assembly processes allows for reproducible and scalable fabrication of porous polymers with tailored macroscopic structures while preserving molecular recognition properties. Thus, additively manufactured MIPs promise to mimic natural recognition systems at the molecular level while being integrated as macroscopic components for the intended application, e.g., filters in piping systems.

This research aimed at the emulsion-free fabrication of hierarchical porous MIPs. To prove the concept outlined above, initial results on inherently porous lattice cubes imprinted with 17β-estradiol as a model template are presented. Batch incubation studies revealed that the 3D-printed MIPs exhibit approximately twice the binding capacity for 17β-estradiol compared to porous non-imprinted control polymers despite having a similar surface area. With some modifications, the proposed concept can be extended to various target templates, including peptides and small molecules.

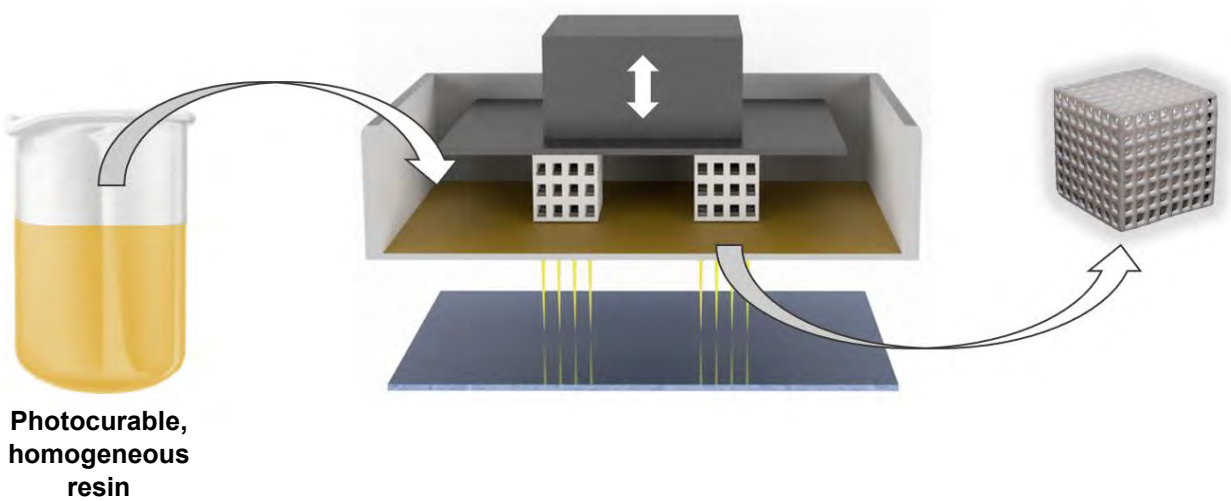

Figure 1. Fabrication process for additively manufactured molecularly imprinted polymers.

Development towards a novel screening method for nipecotic acid bioisosteres using molecular imprinted polymers (MIPs) as alternative to *in vitro* cellular uptake assays

Niels Knippenberg [a*], Joseph W. Lowdon [a], Thomas J. Cleij [a], Kasper Eersels [a], Hanne Diliën [a], Bart van Grinsven [a]

[a] *Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, The Netherlands*

[*] *niels.knippenberg@maastrichtuniversity.nl*

The GABAergic system is a prime target for the diagnosis and treatment of various CNS diseases, as disruptions in this neurotransmission system are associated with the pathogenesis of these disorders. As such, the development of medication and imaging probes addressing the GABA transporter 1 (GAT1) are highly desirable. Most current GAT1-inhibitors and radioligands are lipophilic analogues of the cyclic GABA-mimic nipecotic acid (Figure 1, left panel), but suffer from poor brain-uptake [1].

The incorporation of nipecotic acid bioisosteres is a promising strategy to improve the brain uptake of medication and imaging probes addressing GAT1. Therefore, it is important to know which isosteric replacements bind efficiently into the GAT1 binding site. In order to screen nipecotic acid bioisosteres for their affinity to GAT1 in a time- and cost-effective manner, this research aims to develop a molecular imprinted polymer (MIP) that mimics the natural binding site of GAT1 and can act as an alternative screening tool to the current radiometric and mass spectrometry cellular-based assays (Figure 1).

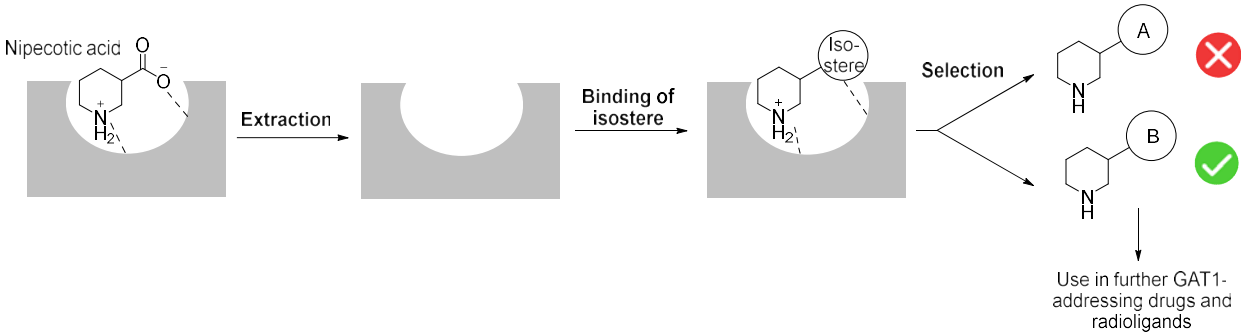

Figure 1: Schematic overview of the screening of nipecotic acid bioisosteres using MIPs. The grey sphere represents a part of the MIP with a nipecotic acid imprint; dashed lines represent potential sites for non-covalent interactions between the analyte and the MIP.

To this end, a nipecotic acid MIP was created through electropolymerization of *ortho*-phenylenediamine (oPD) by cyclic voltammetry (CV). The optimization of the generated receptor layer was achieved by varying the scan rate (50 – 250 mV/s) and number of CV cycles (5 – 12), yielding an optimized MIP with an average imprinting factor of 2.6 as analyzed by electrical impedance spectroscopy (EIS). Selectivity studies allowed for the comparison of the binding characteristics of various analogues, facilitating the determination of the major binding interactions between the MIP and substrate and finally the usability of the developed MIP as synthetic GAT1 mimic.

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Glycan Shield-Targeting Nanoparticles for Pan-coronavirus Neutralization with a Dual Thermal-effect Virucidal Mechanism

Ying Li[1,#], Jingran Chen[1,#], Li Xiao[2], Zhanchen Guo[1], Song Gao[1], Baoxuan Xie[1], Jin Huang[2], Jizong Li[2], Bin Li[2,*] & Zhen Liu[1,*]

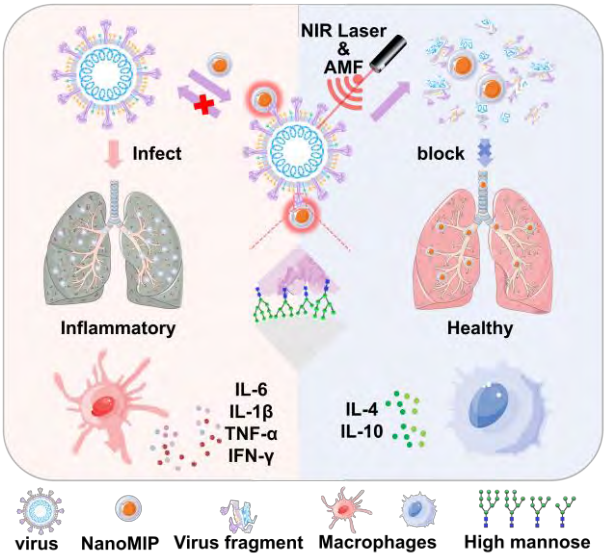
[1] *State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China*

[2] *Institute of Veterinary Medicine, Jiangsu Academy of Agricultural Sciences Academy of Agricultural Sciences, Nanjing 210014, China.*

*zhenliu@nju.edu.cn

Viral infection, especially the past SARS-CoV-2 pandemic, has posed severe threat towards global healthcare. Available antiviral drugs are virus-specific and active against a limited panel of pathogens. Hence, a lot of broad-spectrum viral nano-inhibitors have been developed, which prevent the first step of virus-cell interaction by binding some highly conserved target of viral structure. However, the reversible binding mechanism severely limits their efficacy, because the dissociated virus particles are still infectious and could continue to infect the host. Therefore, to eradicate viral infectivity, the key lies in the switch of mechanism from reversible binding to irreversible inhibition, then a broad-spectrum virucidal strategy rather than a virustatic approach is in imperative demand.

Herein, we report an unprecedented broad-spectrum virucidal strategy, breaking various virus particles into pieces via the synergistic effect of magnetocaloric and photothermal activity in glycan-shield-targeting molecularly imprinted nanoparticles (nanoMIP). The nanoMIP was prepared via integrating our unique strengths in boronate affinity-based saccharide recognition[1] as well as a novel controllable molecular imprinting and cladding technique[2]. Benefiting from the introduction of magnetocaloric Fe_3O_4 core and photothermal dye ICG, the dual thermal-effect nanoMIP was endowed with ultra-fast heating rate ever reported. The nanoMIP targeted viral glycan shields by binding the conserved high-mannose glycans of multiple viruses with high avidity, with a K_d value of 10^{-10} M. After being treated with an alternating magnetic field (AMF) and near-infrared (NIR) laser irradiation, the irreversible viral deformation was visualized by the low voltage scanning microscopy (LVSEM). Notably, a maximum 100% neutralization efficiency for seven tested SARS-CoV-2 pseudovirus variants was obtained, with IC50 values around 10^{-10} M ~ 10^{-11} M. In animal experiments, the dual thermal-effect nanoMIP sterilized PDCoV with near-complete neutralization efficiency in intranasally challenged BALB/c mice, highly effective in both therapeutic and prophylactic assays. Thus, this potently dual thermal-effect broad-spectrum virucidal strategy opens a new access to eradicating viral infectivity.



Scheme 1. Illustration of broad-spectrum virucidal strategy.

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Hybrid light emitting array for the wireless electroanalysis of mycotoxins

Tamara Moya-Cavas,[1] Leslie R. Arias-Aranda,[3] Gerardo Salinas,[3] Neso Sojic,[3] Guillermo Orellana[2]*

[1] Departments of Analytical Chemistry and [2] Organic Chemistry, Chemical Optosensors & Applied Photochemistry Group (GSOLFA), Faculty of Chemistry, Complutense University of Madrid, 28040 Madrid, Spain. [3] University of Bordeaux, CNRS, Bordeaux INP, ISM, UMR 5255, F-33607 Pessac, France.

tammoya@ucm.es

The unique features of molecularly imprinted polymers (MIPs) namely, molecular recognition, cost-effective production, versatility, stability, and reusability have led to widespread applications, including food analysis [1]. For example, over 60% of the globally consumed food contains multiple mycotoxins, posing an escalating challenge in guaranteeing food safety. Mycotoxins are hazardous secondary metabolites produced by various fungi under multiple conditions. Thus, the easy and fast analysis/sensing of such contaminants is highly required. In this work we designed a hybrid light emitting array for the wireless electroanalysis of zearalenone (ZON). This device capitalizes on the efficient molecular recognition of the mycotoxin by a tailored MIP, coupled to the emission of light from a light-emitting diode (LED) for an optical readout [2]. The hybrid polymeric-microelectronic device was designed using a MIP and gold wire as the anode and cathode of the LED, respectively. The anode was functionalized with polymerizable groups on its surface to yield a MIP nanolayer that produces an instantaneous response in the presence of the target mycotoxin. By applying an electric field, the induced redox reactions trigger the light emission when the mycotoxin binds to the MIP (or to the non-imprinted polymer, NIP, as a control). The LED electroluminescence intensity is proportional to the analyte concentration, opening up the possibility to quantify several mycotoxins in food samples (Fig.1).

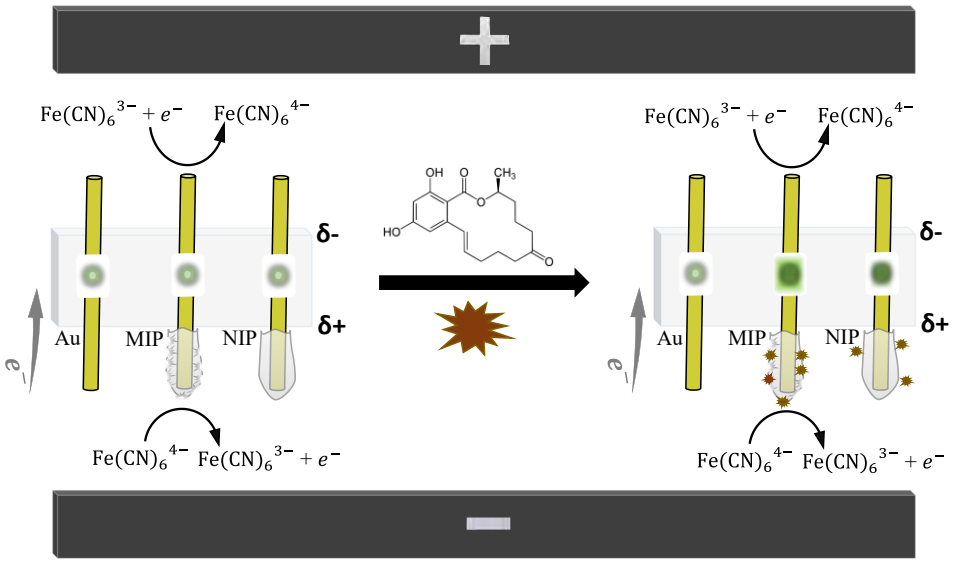

Figure 1. Illustration of a hybrid wireless light-emitting system for ZON analysis using bipolar electrochemistry, with an artistic depiction of the polymer-functionalized gold wire (MIP or NIP), chemical reactions, and electron flux.

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Surface Imprinted Polymers for the Detection of Fungal Spores

Nathalie Philippaerts[1]*, Rocio Arreguin Campos[1], Joseph W. Lowdon[1], Thomas J. Cleij[1],Hanne Diliën[1], Kasper Eersels[1], Bart van Grinsven[1]

[1]*Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, P.O. Box 616, 6200 MD Maastricht, the Netherlands*

nathalie.philippaerts@maastrichtuniversity.nl

In the Netherlands, 9688 ha of greenhouses account for a total energy consumption of 106.8 petajoules and the main portion of this total energy input goes to heating (74%) [1]. The continuous threat of fungal infection to the crop yields, demands frequent venting and heating to ensure a low relative humidity [2]. Detection and continuous monitoring of the fungal spore count in a greenhouse could be a solution to reduce the frequency of venting and heating and thereby reduce the total energy consumption. This study presents the development of a fungal spore sensor based on surface imprinted polymers, a strategy that was successfully employed for the detection of bacteria in prior research [3]. The imprints were prepared by allowing free assembly of the template spores (with sizes ranging roughly from 3-10 µm) on a pre-cured PDMS polymer, followed by extraction. Brightfield microscopy results confirm the formation of imprints and partial template extraction (Figure 1). Two read-out techniques, heat-transfer method (HTM) and impedance were used in parallel to analyze the specificity and sensitivity of the receptor layer by exposure to a wide range of increasing spore concentrations (100 – 200 000 CFU/mL in PBS). Both HTM and impedance results show an increasing effect size with increasing spore concentration. The results in this work emphasize the applicability of the sensor in monitoring spore count, ultimately contributing to more sustainable and energy-efficient greenhouse agriculture.

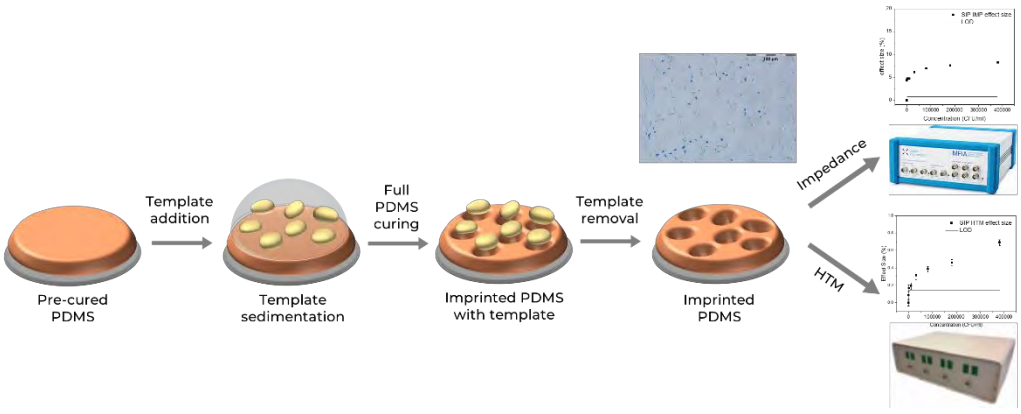

Figure 1: Schematic representation of the surface imprinting procedure, Brightfield microscopy of the extracted imprint stained with lactophenol blue and rebinding analysis results with HTM and impedance.

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MIPs for robust affinity-based capture of phosphorylated and methylated proteins

Kristin Sultan[1], Anıl Incel[1], Sudhirkumar Shinde[1], Celina Wierzbicka[1], Ignacio A. Diez[2], Maria M. Stollenwerk[1], Tina Ravnsborg[2], Magnus E. Jakobsson[1], Ole N. Jensen[2], Börje Sellergren[1*]

1 Biofilms Research Center for Biointerfaces, Department of Biomedical Sciences, Faculty of Health and Society, Malmö University, SE-21432 Malmö, Sweden,

2 Department of Biochemistry and Molecular Biology, University of Southern Denmark, DK-5230 Odense M, Denmark

** borje.sellergren@mau.se, +46 40 665 78 10*

Molecularly Imprinted Polymers (MIPs) offer an innovative platform for the targeting of protein post-translational modifications such as phosphorylation, glycosylation, and methylation [1-8]. We here present high-affinity MIPs designed for phosphorylated and methylated proteins. Our initial focus involved the Tyr-492 and Tyr-493 kinase regulatory motif within the SH2 domain of ZAP70, a pivotal player in T-cell receptor signaling, as well as the SH2 domain of Src, a proto-oncogene tyrosine-protein kinase by targeting pYEEI peptide sequences. Phospho-tyrosine (pTyr) targeting MIPs are created to specifically recognize mono- or diphosphorylated tryptic peptides, binding with low µM Kd values in aqueous media and buffers [7,9]. Secondly, we developed affinity reagents for histidine phosphorylation (pHis), enabling selective enrichment and detection of pHis peptides without the use of acidic solvents [8]. Lastly, we explored methylation-specific affinity reagents using MIP technology, creating isomer-specific MIPs for methyl histidine (meHis) and high-affinity binders for methyl lysine (meLys). These MIP-based approaches offer robust techniques for enriching phosphopeptides and methylated peptides, showing great potential for clinical applications.

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Thermal Detection of Riboflavin in Fruit Juices Using Molecularly Imprinted Polymers

G. van Wissen*, J.W. Lowdon, T.J. Cleij, H. Diliën, K. Eersels and B. van Grinsven

*g.vanwissen@maastrichtuniversity.nl

Department of Sensor Engineering, Faculty of Science and Engineering, Maastricht University, Duboisdomein 30, 6229 GT Maastricht, the Netherlands.

Abstract: Riboflavin, also called vitamin B2 is an essential part of our diet and its deficiency is widespread among different cultures [1]. This necessitates the development of an easy-to-use on-site device for its detection and quantification in a variety of foods. A promising solution that allows for direct on-site measuring are molecularly imprinted polymers (MIPs). MIPs are highly cross-linked synthetic polymeric materials, able to selectively bind specific targets [2]. A recently developed readout technology is the heat-transfer-method (HTM) based on the change of thermal resistance upon analyte binding [3]. In this research, riboflavin imprinted MIPs were prepared, synthesis and rebinding conditions optimized and the imprinted material was implemented into a thermal sensing platform (HTM). For the synthesis optimization, different templates, monomers, crosslinkers, MIP compositions, solvents and their volumes were scrutinized. The best performing MIP was based on riboflavin as template, methacrylic acid as functional monomer and ethylene diglycol dimethacrylate as crosslinker. The optimized MIP was coupled to the HTM by immobilization on an aluminium substrate. Static rebinding experiments have been performed to evaluate the performance of the sensor and an imprinting factor of 2.76 was calculated (Figure 1). The selectivity of the sensor was further investigated against compounds commonly found in fruits and structural analogues. To show real-life applicability, this sensor was used to test fruit juices on their vitamin B2 content.

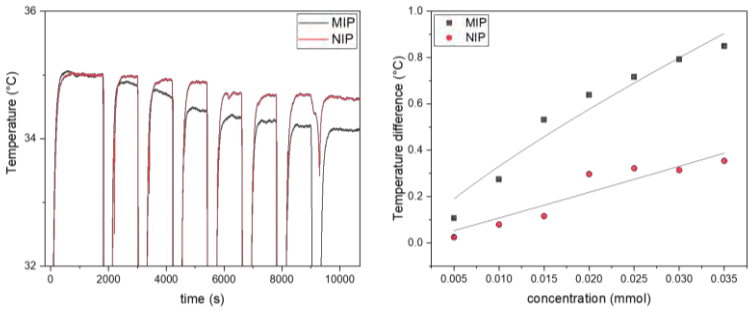

Figure 1: HTM rebinding analysis of riboflavin in MQ-water.

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MIP-based SARS-CoV-2 sensors in POCT connected to the Internet as novel strategies to address challenges in COVID-19 Diagnosis and Treatments

C. Perri[1,2*], R. Pitruzzella[2], A. Chiodi[1], R. Rovida[2], C. Minichini[3], A. Di Fraia[3], M. Starace[3], R. Fioravanti[4], S. Gioacchini[4], G. D'Agostino[1], G. Porto[1], M. Pisaturo[3], L. Zeni[2], N. Coppola[3], F. Magurano[4] and N. Cennamo[1,2]

[1] Moresense Srl, UNIMI Foundation, Viale Ortles 22/4, 20139 Milano, Italy

[2] Department of Engineering, University of Campania Luigi Vanvitelli, Via Roma 29, 81031 Aversa, Italy

[3] Department of Mental and Physical Health and Preventive Medicine, University of Campania Luigi Vanvitelli, 80138 Naples, Italy

[4] Department of Infectious Diseases, ISS, Viale Regina Elena 299 00161 Rome, Italy

**c.perri@moresense.tech*

Immediately after COVID-19 pandemic highlighted the need for portable and small-size, fast-response, inexpensive, and easy-to-use devices detecting the virus, also the capability of transmitting statistical data over the Internet, such as in this specific instance on the spread of the SARS-CoV-2 virions, has gained significant interest among the medical community. In fact, during a pandemic, these technologies can give a more accurate view of the state of emergency and improve and speed up its management.

Within the "BETTER" project funded by the Campania Region, a Point-Of-Care-Test (POCT) connected to the Internet for the Sars-CoV-2 detection was successfully developed and tested for its detection in real samples (nasopharyngeal samples). The developed POCT exploits low-cost sensor chips based on Surface Plasmon Resonance (SPR) and Molecularly Imprinted Polymers (MIPs) [1].

The project's aim was large-scale testing on about 1000 nasopharyngeal samples, positive and negative, in a Universal Transport Medium (UTM), also tested with standard Real-time PCR (Polymerase Chain Reaction) methods.
Approximately 100 positive and 800 negative nasopharyngeal samples were preliminary 1:5 diluted to reduce matrix interference and then tested via POCT. Thanks to the developed method's high sensitivity, the virus's presence can be detected even in diluted samples.

The proposed POCT sensor can detect the presence of the virus in a few minutes and transmit the outcome to a platform via the Internet, allowing automatic statistics useful for pandemic monitoring and management (all the data are available on the website: https://www.progettobetter.eu/). Moreover, this POCT also allows quantitative measurements and could represent a valid hardware and software tool for monitoring COVID-19 patients' treatment.

Further studies on different types of biological samples, e.g. saliva, are under testing, increasing the potential of such an approach in diagnostics. Finally, the proposed POCT can be applied to any other type of pathogen or analyte of interest thanks to its MIP-based high versatility and use to face new possible pandemic or emergency scenarios.

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Screen-printed electrodes coated with molecularly imprinted polymers for the detection of PFOA

Fatemeh Ahmadi Tabar [1,2]*, Patrick Wagner [1], Kasper Eersels [2], Bart van Grinsven [2]

[1] *Laboratory for Soft Matter and Biophysics, KU Leuven, 3001 Leuven, Belgium*

[2] *Sensor Engineering Department, Maastricht University, 6200 MD Maastricht, the Netherlands*

* fatemeh.ahmaditabar@kuleuven.be

Keywords: molecularly imprinted polymer, impedance spectroscopy, perfluorooctanoic acid

Perfluorooctanoic acid (PFOA) is a member of the polyfluoroalkyl substances (PFAS) and has been widely used for decades in various products. These substances have the ability to bio-accumulate and are potentially carcinogenic and neurotoxic. Therefore, a sensor that could enable highly-sensitive, rapid, and cost-effective method for monitoring PFOA is highly desirable [1]. In this study, PFOA MIPs were created by bulk free radical polymerization of acrylamide. The optimized MIPs where then immobilized on screen-printed electrodes (SPEs) and PFOA rebinding to these SPEs was analysed using electrochemical impedance spectroscopy (EIS). In Figure 1, the absolute Z values of MIP and NIP SPEs to increasing PFOA concentrations (1 nM−10 μM) in phosphate buffered saline (PBS) is presented. The data demonstrate that increasing the amount of PFOA will cause the absolute z values for MIP-SPEs to decrease. This can be explained by the fact that the target binds to the MIPs, changing the properties of the polymer. The limit of detection (LoD) for this sample was 69 pM calculated by the 3σ method. The measurements using NIP particles demonstrate that this effect is far less pronounced, which confirms the non-specific binding of the target to the polymer matrix. In summary, the sensor design makes it possible to detect PFOA via electrochemical impedance spectroscopy (EIS). This work therefore demonstrates how the coupling of MIPs with the EIS can yield a low-cost and robust sensor platform for PFOA determination.

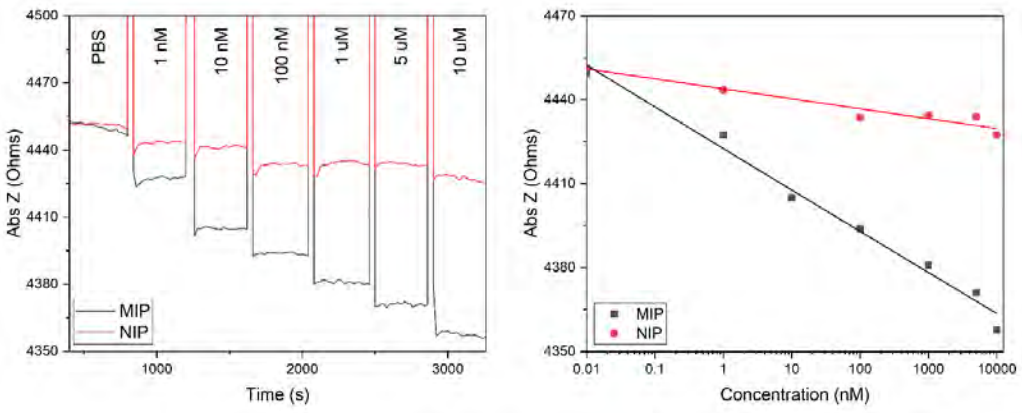

Figure 1. EIS rebinding analysis of the MIP and NIP SPEs after exposure to increasing concentrations of PFOA (1 nM–10 μM). Dose-response curves yielded from EIS measurements.

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Abstracts: Poster Presentation

Electrochemical Sensor for Atrial Natriuretic Peptide Detection based on a MIP Thin Film Receptor

Ana T. Silva, Carlos M. Pereira & José A. Ribeiro*

CIQUP/IMS, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

**jose.ribeiro@fc.up.pt*

Atrial natriuretic peptide (ANP) is a biomarker for cardiovascular diseases, in particular myocardial infarction. [1] Thereby, its rapid and accurate detection is essential for early disease diagnosis, allowing a quick response in terms of clinical treatment ultimately contributing to patients' survival. Along with this, the interaction between ANP and receptors present in cardiac cells has been very useful to develop new targeted drug delivery systems to treat ischemic heart disease, by functionalizing the surface of nanoparticles (NPs) with ANP molecules [2].

The interest in using MIPs as receptors in biosensors relies on the higher stability and low production costs that they present over natural antibodies. A simple and fast way of synthesizing MIPs is through surface electrochemical polymerization of a redox monomer, where the film thickness can be easily controlled to increase the sensitivity of the electrochemical biosensor [3, 4].

In this work, we developed an amperometric biosensor based on a MIP thin layer, prepared by electropolymerization of dopamine on the electrode surface, to quantify ANP free in solution and ANP-coated NPs (see Figure 1). Dopamine was selected due to its biocompatibility and hydrophilic nature [5]. First, the experimental conditions for biosensor construction were optimized (film thickness, template concentration and extraction procedures). Then, detection studies were performed based on calibration curves using standard solutions of ANP and ANP-coated NPs.

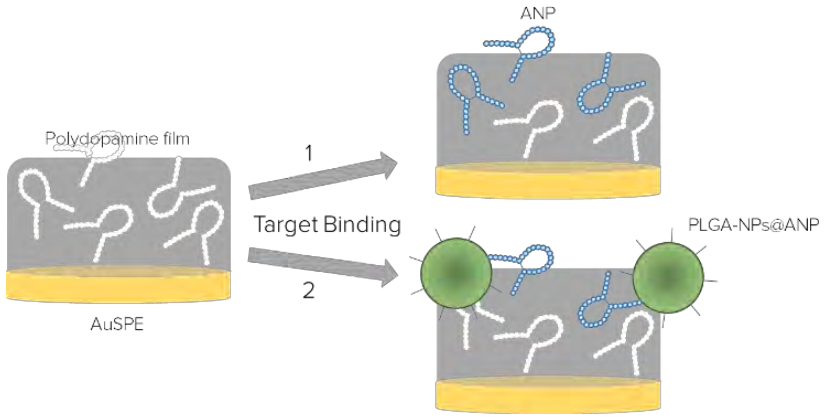

Figure 1. Schematic representation of the developed MIP sensor and ANP detection.

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P2

Enantioselective nanoMIPs toward Thyroid Hormones

V.Testa,* T.Serra, S.Cavalera, F.Di Nardo, L.Anfossi, C.Baggiani

Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, 10125 - Torino, Italy

**v.testai@unito.it*

The human thyroid hormones, thyroxine (T_4) and triiodothyronine (T_3), exist in two enantiomeric forms: Levo and Destro. The L-isomer gives the principal active effect through biological pathways while the D-isomer is a by-product of the LT_4 biosynthesis. L-thyroxine has been selected as a template to explore the potential chiral recognition capability of nanoMIPs.

This work proposes a strategy involving the Solid Phase Polymerization Synthesis (SPPS) method. Two different nanoMIPs have been synthesized where the orientation of the template covalently grafted onto the glass solid support gives the difference between the two. The "direct" – (d)nanoMIP – was prepared by LT_4 grafting onto hemisuccinated silica directly through the amino group. In this case, it is intended that ligand binding takes place near the the chiral center. The "reverse" – (r)nanoMIP – was prepared by grafting onto the glass solid support the template by the phenolic group side, in the farthest part of the molecule respect to the chiral center. To prepare this template, LT_4 was modified introducing a carboxymethoxy group on the phenolic function (L-T_4 CME). This strategy involved the protection of the chiral amino acid moiety to mask the amino group with the use of 9-borobicyclononan (9-BBN) as a protecting agent (Fig.1), avoiding the possibility of an unwanted conjugation by the amino function. 9-BBN can be quantitatively inserted on amino acids in anhydrous condition, and it is easily removable in acidic conditions.

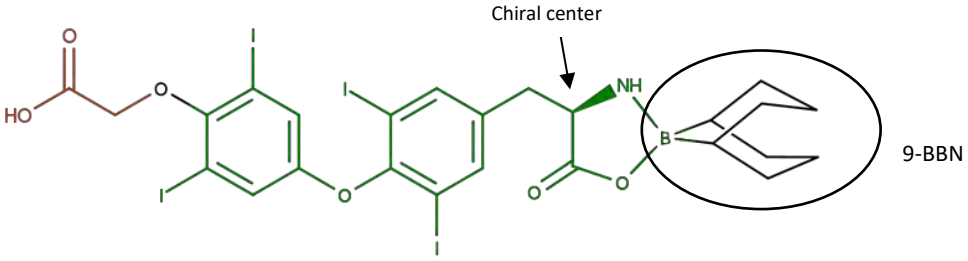


Figure 1: Molecular Structure of L-T_4CME-9-BBN

NanoMIPs were covalently linked to silica beads and batch rebinding experiments were performed with different ligands (LT_4, DT_4, LT_3, DT_3, and LT_2) to obtain the corresponding binding isotherms and, thus, evaluate binding affinity, selectivity, and enantioselectivity. Results show that (r)nanoMIP has a higher affinity for the template LT_4, with a binding constant of $1.08 \times 10^8\ M^{-1}$, which is fourfold higher than the binding constant for (d)nanoMIP. This increase in affinity could be related to the orientation of the template molecule and the availability of more functional groups to interact with the polymer. Concerning selectivity, both the nanoMIPs show a decreasing affinity for the structural analogs with fewer iodine substituents. In particular, (r)nanoMIP shows a remarkable selectivity not only towards the different thyroid hormones but also between the different enantiomeric forms of T_4. Consequently, it efficiently discriminates the L-enantiomer from the D-enantiomer and, therefore, recognizes the template with very high selectivity.

In conclusion, the imprinting against the "inverted" template confirms that to obtain enantioselectivity the chiral center must be exposed to the growing polymer, far from the covalent graft to the solid support.

P3

Grafting nanoMIPs onto Surfaces of ELISA Microplates for the Development of Biomimetic Assays

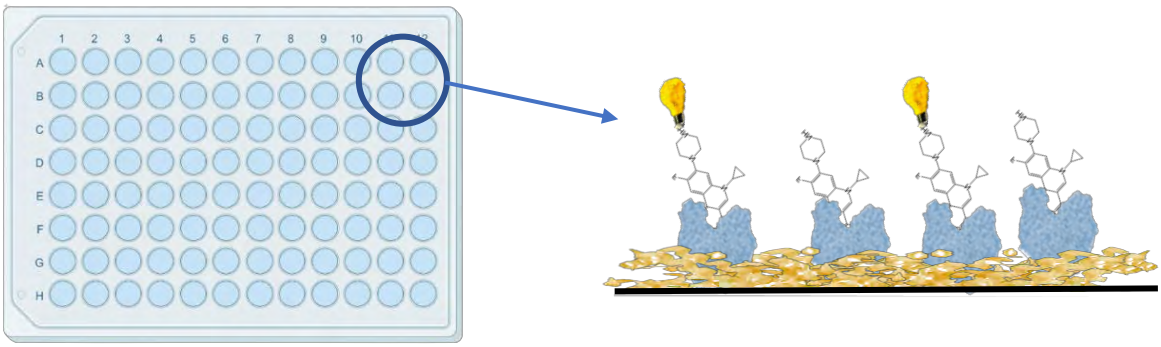
T. Serra,* S. Cavalera, F. Di Nardo, V. Testa, C. Baggiani, L. Anfossi

Laboratory of BioAnalytical Chemistry, Department of Chemistry, University of Torino, Via Giuria 7, 10125 - Torino, Italy

** thea.serra@unito.it*

Molecularly imprinted polymers (MIPs) are synthetic biomimetic materials featuring highly cross-linked structures with cavities for selective molecular recognition. The evolution of molecular imprinting technology has introduced solid-phase-synthesized nanoparticles, nanoMIPs, as an innovative approach overcoming challenges associated with traditional MIP synthesis methods. NanoMIPs have proven to be efficient artificial mimics of natural receptors and a promising alternative to antibodies in bioanalytical applications. Despite the potential of nanoMIPs the relatively new nature of this research field and the limited available literature in applying nanoMIPs to biomimetic binding assays like ELISA or LFIA still presents some technical challenges [1].

Our investigation focuses on the immobilization efficacy of nanoMIPs in combination with the binding capacity of the functionalized surface towards ciprofloxacin labeled with horseradish peroxidase (HRP).



The HRP signal simultaneously serves as an indicator of covalent grafting of nanoMIPs onto the microplate wells and the selective recognition properties towards the template molecule. This work establishes a foundation for the development of efficient and reproducible competitive pseudo-immunochemical assays. In these assays, nanoMIPs act as the recognition elements, demonstrating their potential for advanced applications in antibiotic detection and beyond.

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P4

Magnetic Molecularly Imprinted Polymers in Organic Synthesis: From Standard to Dynamic Kinetic Resolution

Huiyin LIU,[a,b] Tugrul BICAK,[a,b] Nébéwia GRIFFETE,[a] Cyril OLLIVIER[b]

[a]Sorbonne Université, CNRS, Physicochimie des Électrolytes et Nanosystèmes Interfaciaux, PHENIX, 75005 Paris, France.
[b]Sorbonne Université, CNRS, Méthodes et Applications en Chimie Organique, IPCM, 75005 Paris, France.

Huiyin.liu1995@gmail.com

Enantiomers, despite their identical chemical formulation and structure, often exhibit different biological activities or toxicology profiles *in vivo* [1]. This is why it is important to collect the enantiomer of interest from its chiral mixture. In this context, our work aims to develop an efficient method based on a stepwise conversion of enantiomers using magnetic molecularly imprinted polymers (MIPs). Indeed, MIPs are the sorbents with the ability to recognize a given molecule. Magnetic MIPs are obtained by implementing its polymerization on the surface of Fe_2O_3 nanoparticles, which allows the recycle and reuse of MIPs by using a magnet. The target enantiomer can thus be selectively adsorbed on the MIP from a racemic mixture. Thereupon, racemization of the other remaining enantiomer allows to reproduce the racemic mixture, leading to its complete conversion to the target enantiomer through the cycle of adsorption and racemization steps (Fig. 1). This multistep process, which involves the cycle of adsorption and racemization, is known as Dynamic Kinetic Resolution (DKR) [2].
Here, we try to develop these magnetic materials using different types of polymerization, different monomers, solvents and molecules to find the perfect conditions for the selective adsorption of the imprinted molecule.

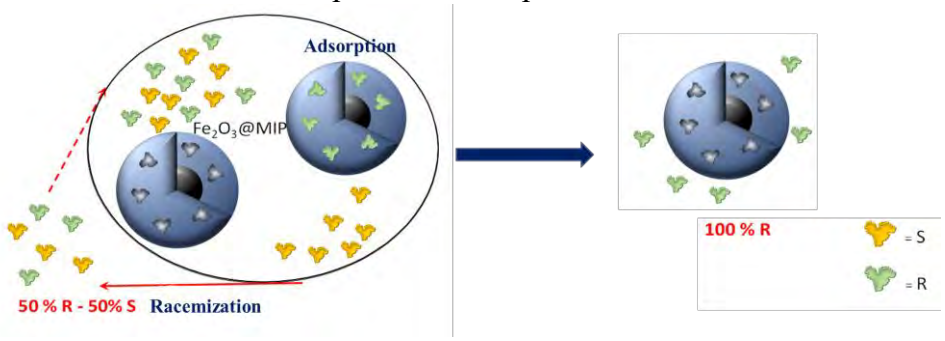

Figure 1. Dynamic Kinetic Resolution (DKR) by molecularly imprinted polymers (MIPs).

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P5

SPR Sensor based on Imprinted Nanogels for Detection of Bovine Serum Albumin in Milk

Rui Figueiredo, Manuel Azenha, Carlos M. Pereira & José A. Ribeiro*

CIQUP/IMS, Chemistry and Biochemistry Department, Faculty of Sciences, University of Porto, Rua do Campo Alegre s/n, 4169-007 Porto, Portugal

**jose.ribeiro@fc.up.pt*

Bovine serum albumin (BSA) has been used as an indicator of the health of the cow's mammary gland and milk quality [1, 2]. However, allergic reactions to this protein by consumers have been reported and some diseases, such as diabetes mellitus, membranous nephropathy and "mad cow disease", may be associated with BSA exposure [1, 2]. Therefore, it is currently important to develop new methods for BSA detection and quantification in a rapid, cost-effective, simple and highly selective manner.

Nanoscale molecular imprinting polymers (nanoMIPs) were employed in this study as a promising approach for the development of innovative synthetic receptors that can be a viable alternative to natural antibodies, offering high selectivity, stability and reduced production costs [3]. In this context, the nanoMIPs were produced using precipitation polymerization approach (in aqueous medium), demonstrating good properties in terms of size, zeta potential and polydispersity. In addition, a BSA epitope was chosen as the template molecule since there are numerous advantages to use a small epitope region for imprinting in terms of affinity, performance and/or production costs of the nanoMIPs [3].

In this work, the affinity of the synthesized receptors for BSA was evaluated by surface plasmon resonance (SPR) technique. The subsequent construction of the optical sensor for BSA detection involved the covalent immobilization of the nanogels on the gold SPR substrates. Then, the experimental conditions were optimized to enhance the sensor performance and minimize the nonspecific adsorption.

The constructed sensor exhibited promising analytical parameters, including a linear response range suitable for BSA quantification in milk samples. Preliminary studies were conducted to determine the BSA concentration in bovine milk. After sample pretreatment, the BSA concentration in milk obtained by the optical sensor was similar to that obtained by the bicinchoninic acid (BCA) reference test. The results suggested that the developed SPR sensor can potentially be a viable alternative to the colorimetric and chromatographic assays [2, 4] currently used to detect BSA in food matrices.

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Acknowledgments
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P6

Ionic Imprinted Polymers PEGDA-based for Selective Binding of Lithium Ions

V.Testa[1]*,V.Tumiatti[2], M.Tumiatti[2], M.C.Bruzzoniti[1], L.Rivoira[1], T.Serra[1], S.Cavalera[1], F.Di Nardo[1], L.Anfossi[1], F.Ibrahim[3], C.Branger[3], C.Baggiani[1]

[1] *Department of Chemistry, University of Turin - Turin, Italy*
[2] *Sea Marconi Technologies - Turin, Italy*
[3] *MAPIEM, Universitè de Toulon, 83130 - La Garde, France*

v.testa@unito.it

Recently, ionic imprinted polymers (IIPs) have attracted attention in environmental issues; since most of them have been developed as a strategy for the preconcentration, purification, recovery, and monitoring of metals in different samples[1]. Lithium is one of the most interesting alkali metals: its strategic and unique properties make it the main component of batteries, and therefore it is widely used in many fields of our life such as in the development of electric vehicles and portable electronics. Due to environmental regulation and technological transition, the demand is increasing rapidly, as a result, geological resources are expected to be depleted very soon. For these reasons, the development of new materials for the recovery and recycling of this metal is mandatory. State of the art on recycling shows some methodologies available for the recovery of lithium from the leaching solution of disassembled batteries show that most of them are based on hydro/pyrometallurgical processes which indeed are energy-intensive, expensive, time-consuming, and have actually low-rate lithium recovery[2]. An innovative ad alternative strategy could be found in using ionic imprinted polymers.

This work presents an original approach to obtain ionic imprinted polymers for highly selective binding of Li(I) from neutral media. Polymers are based on diacrylate polyethylene glycol (PEGDA 575) as a unique homobifunctional monomer which is known to form pseudo-crown ethers, in a polymer mixture, capable of coordinating alkali ions by macrocyclic effect [3]. In this way, the use and functionalization of expensive polymerizable crown ethers is avoided.

In detail two different polymerization techniques are explored to get imprinted materials: the traditional bulk polymerization (DMSO, water) and the most innovative inverse suspension (DMSO in Mineral Oil, Water in Mineral Oil). For each polymer, binding parameters are obtained through partition equilibrium of Li^+ standard solutions (0.2-30 ug/mL) followed by ion chromatographic analysis of the free fraction of Li^+. Finally, the selectivity factor towards competitive binding ions (Na^+, K^+) and the imprinting factor, as a ratio to the non-imprinted polymer (NIP), are defined. Experimental data show that bulk polymerization allows the production of IIPs able to rebind lithium with a binding capacity between 51.7 ± 3.6 µmol/g and 4.7 ± 0.5 µmol/g with a good reusability up to 6 cycles after recovery with acidic or basic eluents. These data will be compared to the ones obtained using IIPs produced by inverse suspension to better understand which material gives the best response.

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P7

Evaluation of deep eutectic solvents in the synthesis of molecularly imprinted fibers for the solid-phase microextraction of triazines in soil

Alexia Monnier, Myriam Díaz-Álvarez, Esther Turiel, Antonio Martín-Esteban*

Department of Environment & Agronomy. INIA-CSIC. Carretera de A Coruña km 7.5. 28040 Madrid, Spain

* amartin@inia.csic.es

Nowadays, molecularly imprinted polymers (MIPs) are well established and considered excellent materials for performing selective extractions. However, with the progressive implementation of the Principles of Green Chemistry, it is necessary to search greener alternatives for both the synthesis and further use of MIPs in sample preparation. Accordingly, in the present work, different deep eutectic solvents, DES, (both hydrophilic and hydrophobic), as an alternative to the conventional organic solvents (i.e. toluene), were evaluated as porogen for the synthesis of imprinted fibers (monoliths), using fused silica capillaries as molds, for solid-phase microextraction (SPME).

From this study, the polymer prepared with propazine (dummy template), methacrylic acid (monomer), ethylenglycol dimethacrylate (cross-linker) and a formic acid:L-menthol (1:1) DES (porogen) showed the best performance to selectively rebind triazines. After optimization of the different variables involved in SPME, the new imprinted fibers were successfully applied to the extraction of target analytes (desisopropylatrazine, desethylatrazine, simazine, and atrazine) from soil sample extracts, providing relative recoveries ranging from 75.7 to 120.1 %, reaching limits of detection within the range 6.2-15.7 $ng.g^{-1}$, depending upon the analyte.

Acknowledgements

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P8

Screen-printed electrodes modified by electropolymerized Molecularly Imprinted Polymers (e-MIP) to develop voltammetric sensors

Giancarla Alberti, Camilla Zanoni, Lisa Rita Magnaghi, Raffaela Biesuz
Department of Chemistry, University of Pavia, via Taramelli, 12 – 27100 Pavia (Italy)
e-mail: galberti@unipv.it

Selective cheap and rapid electrochemical sensors are developed by modifying the working electrode of screen-printed cells with a film of elecrosynthesized molecularly imprinted polypyrrole (e-MIP).

At present, electrochemical sensors are some of the most effectively used MIP-based devices and different strategies have been proposed for integrating MIPs with the sensors' surfaces.

Several studies reported on the application of electrosynthesized MIPs (e-MIPs) for developing electrochemical sensors; in fact, electropolymerization allows for highly controlled polymer growth on surfaces with a fine-tuning of the polymeric film thickness by controlling experimental conditions. Other electrochemical procedures can also be applied to enhance these e-MIPs. One of them, which is very useful, is overoxidation, performed by the electrochemical treatment of the MIP film by positive electrode potentials much higher than those required for the polymerization reaction. Overoxidation is advantageous in MIP preparation since it allows the formation of carboxyl, carbonyl, and hydroxy groups to interact by hydrogen bonds with the template molecules, promoting the formation of more selective cavities.

In this context, e-MIP-based screen-printed electrodes are proposed here for the voltammetric sensing of ascorbic acid, gallic acid and the herbicide MCPA. The polymeric film was electrodeposited on the graphite working electrode of screen-printed cells, obtaining selective and simple methods for the analyte sensing.

Chemometric tools are applied to improve the analytical performance of the electrochemical sensors, cut the cost of sensor fabrication and analysis by optimization through experimental design, reduce the dimensionality of the data, and eliminate drift effects or interference problems. Moreover, they are applied to develop multivariate models for quantitative analysis.

Dual epitope imprinted QCM sensor for selective detection of *Salmonella typhi* bacterial protein

A. Srivastava, R. Raghuwanshi[b], G. Nath[c], M. Singh[a,*]

[a]*Department of Chemistry, MMV, Banaras Hindu University, Varanasi-221005, India*
[b]*Department of Botany, MMV, Banaras Hindu University, Varanasi, 221005, India*
[c]*Department of Microbiology, IMS, Banaras Hindu University, Varanasi, 221005, India*

[*]*meenakshi@bhu.ac.in*

The selective and sensitive detection of typhoid caused by gram-negative bacterium *Salmonella typhi* is critical for early disease diagnosis and improved prognosis. A powerful smart generation of selective sensors are represented by molecularly imprinted polymers (MIPs). Recently, dual molecule imprinting has been paid widespread and increased attention. To solve the dilemma of imprinting whole biomacromolecules, epitopes have been successfully employed as templates. Here in this work, dual epitope sequences of bacterial protein *Salmonella typhi* (SipD) are selected as template molecules. Multiple monomers were chosen for imprinting - a zwitterionic monomer 2-Methacryloyloxyethyl phosphorylcholine (MPC), benzyl methacrylate (BMA) bearing aromatic group and methacrylic acid (MAA) are selected as functional monomers using molecular modeling and N, N-methylene-*bis*-acrylamide (NNMBA) is chosen as crosslinker. MoS_2-AuNPs composite was synthesized to exploit its unique covalent bonding properties. AuNPs were introduced between the adjacent layers of the transition metal dichalcogenides to enhance the charge carrier mobility. MoS_2-AuNPs decorated epitope imprinted polymer were formed in the presence of monomer, crosslinker, and template molecules. Synthesized polymer was electrodeposited on gold-coated QCM electrode *via* cyclic voltammetry (CV). Gold-coated QCM electrode was treated with PBS to extract the peptide molecules to form an imprinted matrix. Rebinding and extraction of peptides were monitored piezoelectrogravimmatrically. Extraction was verified by HPLC, SDS-PAGE and fluorescence spectroscopy. Non-imprinted polymer (NIP) matrix was also prepared without using any template molecule as a control experiment. Response of formed dual epitope imprinted polymer sensor was monitored by rebinding of standard template molecules, real samples from patients, and probable interferents.

Solid-Phase Extraction Using a Green Metal-Organic Framework MOF-808 Integrated Molecularly Imprinted Polymer for Selective Drug Adsorption from Wastewater Samples

S.L.Z. Jiokeng,[a]* A. Kotyrba,[a] A. Huber[b] & B. Mizaikoff[a,b]**

[a]*Institute of Analytical and Bioanalytical Chemistry, University of Ulm, Ulm 89081, Germany*
[b]*Hahn-Schickard, Ulm 89077, Germany*

***sherman.jiokeng-zambou@uni-ulm.de* ****boris.mizaikoff@uni-ulm.de*

This study presents an approach for the selective removal of pharmaceutical contaminants from wastewater through the integration of a green metal-organic framework (MOF-808) and a molecularly imprinted polymer (MIP) within a solid-phase extraction (SPE) system. The escalating concern over the presence of drugs (diclofenac, carbamazepine, ibuprofen and metoprolol) in water sources necessitates innovative and sustainable solutions for efficient adsorption. The fabrication of core-shell sol-gel hybrid molecularly imprinted polymer based on metal–organic framework (MOF-177) was reported in the literature using *S*-amlodipine (*S*-AML) was as template [1] (Figure 1). The MOF-808 chosen for our work, renowned for its environmentally friendly characteristics, provides a robust and versatile framework for the development of our integrated MIP. It exhibited a good maximum diclofenac adsorption capacity of 1033.1 $mg.g^{-1}$. This integration enhances the adsorption efficiency and selectivity of the SPE system, ensuring the targeted extraction of specific drug molecules from complex wastewater matrices. The MIP, designed with molecular precision, exhibits a high affinity for the target drugs, facilitating their removal with enhanced specificity. Our novel approach not only addresses environmental challenges associated with pharmaceutical residues but also contributes to the development of sustainable water treatment technologies. The utilization of green materials such as MOF-808 underscores our commitment to eco-friendly practices in addressing contemporary water quality issues. Through this presentation, we aim to elucidate the conceptual framework of our innovative solid-phase extraction method, showcasing its potential as a sustainable and effective solution for drug removal from wastewater. This research represents a significant step towards advancing environmental remediation strategies and promoting a greener and healthier future.

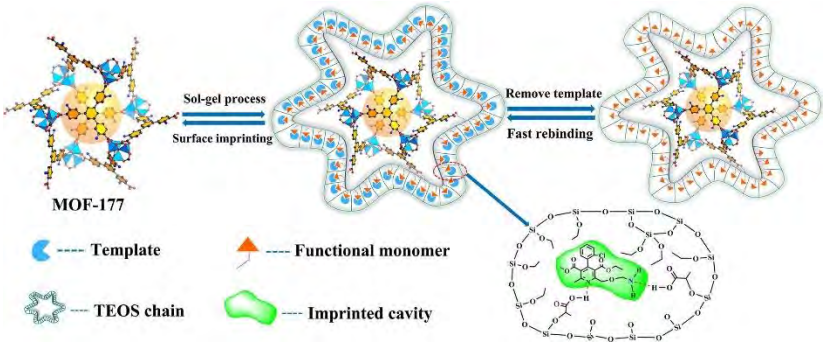

Figure 1. Fabrication of a core–shell sol–gel hybrid MIP based on MOFs.

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P11

Molecularly Imprinting polymer nanoparticles for inhibition of β-Lactamase activity

A. Ibrahim* , , E. Piletska*, G. Mukamolova[ϒ], O. Turapov[ϒ], S. Piletsky*

University of Leicester, School of Chemistry*, School of Biological Sciences[ϒ], Leicester, University Road, LE1 7RH, United Kingdom.

Antibiotic resistance is been classified by the World Health Organization (WHO) as one of the three most dangerous threats to the global health[1]. Bacteria such as (*E.coli, Klebsiella pneumoniae*, etc) cause infections and resist antibiotics by producing β-Lactamase enzymes which hydrolyse β-Lactam antibiotics and maintain bacteria`s life. In this work, Oxa β-Lactamase was purified from E.coli (BL21) (DE3) containing the resistance gene pET15bTEV plasmid and used as a target for the synthesis of molecularly imprinted polymer nanoparticles (MIPs NPs) using a solid-phase approach. Using a 96-well plate, assay for the screening of β-lactamase inhibition was assessed spectrophotometrically in a microplate reader based on the hydrolysis of nitrocefin[2] in the absence and presence of different concentrations of the synthesised MIPs NPs. β-Lactamase inhibition was assessed by measuring the difference in the absorbance between 0 to 9 minutes for each concentration of MIPs NPs.

From the results, MIPs NPs were able to inhibit 90% of β-Lactamase activity (IC50 0.11 nM) as uncompetitive inhibitor. To conclude, MIPs NPs have the potential to act as replacements or enhancers for antibiotic drugs.

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Solid phase synthesis with low molecular weight templates – challenges and approaches for imprinting of the mycotoxin deoxynivalenol (DON)

Julia Völkle [1,2,3], Sebastian Luger [3,4] Peter Lieberzeit [1], Philipp Fruhmann [3]

[1] University Vienna, Faculty for Chemistry, Department of Physical Chemistry, 1090 Vienna, Austria
[2] University of Vienna, Vienna Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria
[3] Centre of Electrochemical Surface Technology, 2700 Wiener Neustadt, Austria
[4] Vienna University of Technology, Institute of Applied Synthetic Chemistry, 1060 Vienna, Austria
julia.voelkle@cest.at

Molecularly imprinted polymer nanoparticles (nanoMIPs) derived from solid phase synthesis display a remarkably high selectivity and binding site homogeneity, largely owing to the well-defined template orientation during polymerization.[1,2] While the strengths of this synthesis method have been demonstrated for a wide range of target molecules, it requires thorough planning of the linker chemistry used for analyte immobilization. For instance, using a whole protein as the template often leads to binding site inhomogeneity. One can avoid this by using carefully designed epitopes that provide key binding motifs of the original macromolecule and are equipped with a designated anchor group.[3]

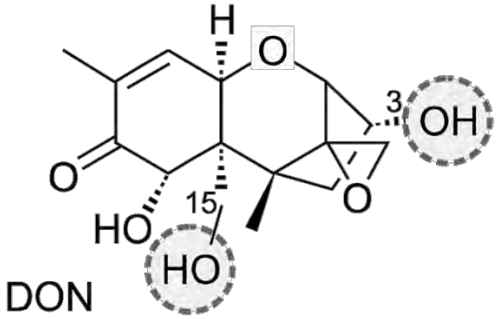

Figure 1: Structure of DON with the commonly used linkage sites (OH group in 3- and 15-position) [4]

On the other end of the molecular weight spectrum, small molecules provide only few functional groups for immobilization and specific interaction. The challenge here lies mainly in choosing the appropriate anchoring group, which defines the molecules orientation during imprinting and inevitably reduces the number of functional groups partaking in the formation of the template-monomer affinity complex.

In our work, we focus on the immobilization and subsequent imprinting of the mycotoxin deoxynivalenol (DON), shown in Figure 1. Selective immobilization was attempted via both the 3-, and 15-hydroxyl group, using acetyl protecting groups and a carbamate linkage. Further experiments will focus on the assessment of the affinity and selectivity of the resulting nanoMIPs towards the analyte molecule.

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A dust of gold to shine light on MIP

E. Iatta*, P. Lieberzeit

University of Vienna, Faculty of Chemistry, Department of Physical Chemistry, 1090 Vienna, Austria

University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria

**ester.iatta@univie.ac.at*

The project aims to develop a method suitable for characterizing the surfaces of molecularly imprinted polymer (MIP) based on the localised surface plasmon resonance (LSPR) Raman technique. To pursue this, non-spherical gold nanoparticles were chosen as the research subject [1]. It has been reported that asymmetrical AuNPs exhibit more intense plasmonic resonance effects than nano-spheres [1].

Therefore, this poster will present early results on that topic. Indeed, studies about the stability over time have been carried out on the AuNPs. In addition, our idea is to investigate the volume of the sample affected by the enhancement. The approach consists of layering different polymers and depositing the AuNPs at different depths among the layers. This kind of setup, combined with knowledge of the polymer thickness, allows us to estimate the limits of the achievable enhancement.

So far, a synthetic protocol for gold nano-triangles (AuNTs) has been optimized while deposition methods are still subject to study [2]. Although there is still room for improvement, so far we can guarantee an enhancement factor of 10^2, an evaluation of the enhancing power of AuNPs and how the deposition method affects the signal.

In conclusion, this approach will lead to an in-depth characterization of MIP in a physically independent matter. In fact, by tuning AuNPs' physical characteristics, it is possible to adjust not only the enhancing power and the Raman resolution but also target a specific bond or interaction knowing the referred band [3].

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P14

Synthesizing Molecularly Imprinted Polymer Thin Films for Sensing Carbonaceous Nanoparticles

Houra. Hadadi*, Peter. Lieberzeit

University of Vienna, Faculty of Chemistry, Department of Physical Chemistry,1090 Vienna, Austria

University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria

**houra.hadadi@univie.ac.at*

In recent decades, air pollution has become a significant environmental concern, primarily due to the excessive release of pollutants like particle matter (PM) into the atmosphere[1]. Among these pollutants, carbonaceous nanoparticles (CNPs) play a major role and are associated with adverse effects on both the environment and human health. Sensors based on molecularly imprinted polymers (MIPs) represent a promising advancement in addressing this issue. The choice of carbon as an analyte in the MIPs is well-founded due to carbon's chemical inertness and its ability to form bonds with a wide range of elements[2]. While MIP sensors are currently more commonly employed in biomedical applications, this study highlights their potential in addressing environmental challenges.

The objective of this project is to develop a sensor system capable of directly detecting PM in the liquid phase. The approach involves designing thin films of MIP and non-imprinted polymer (NIP) for carbonaceous nanoparticles using complementary synthesis strategies and in-situ polymerization. Additionally, Quartz Crystal Microbalance (QCM) is utilized to coat MIP to monitor the analyte's quantity.

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Enrichment of diclofenac and carbamazepine from wastewater using molecularly imprinted polymers

Anika Kotyrba[1], Andreas Hellmann[1], Sherman Jiokeng[1], Amelie Huber[2] and Boris Mizaikoff[1,2]
[1] Institute of Analytical and Bioanalytical Chemistry, Ulm University, 89069 Ulm, Germany
[2] Hahn-Schickard Institute for Microanalysis Systems, Sedanstrasse 14, 89077 Ulm, Germany
anika.kotyrba@uni-ulm.de

Pharmaceuticals have improved our quality of life in many aspects, allowing us to live longer, healthier and with less suffering. However, pharmaceuticals and their active metabolites released into the environment can rapidly create problems. Therefore, there is a need to monitor the concentration of these compounds and effectively remove them from wastewater to prevent their release into the environment. Hence, we developing a device combining a MIP-based solid phase extraction (SPE) with IR sensing technology. The SPE component is tailored to enrich selected target analytes from wastewater for subsequent analysis, which is essential for making concentrations below the LOD of IR techniques adressable. The target molecules in this study are diclofenac and carbamazepine. Diclofenac is an anti-inflammatory pharmaceutical with is very frequently used. Carbamazepine is an antiepileptic drug which is used to control cramp attacks. Both molecules are among the most frequently detected pharmaceuticals in aquatic environments. [1]
In this study, we have compared the performance of different stationary phases during SPE: commercial C18 columns, molecularly imprinted polymers or affinity materials. Affinity polymers are polymers whose functional groups are well suited to interact with the analyte, but without any specific imprinting.
Diclofenac can be enriched by a factor of 14 (Fig. 1).

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This work has been supported by the European Union within the framework of the EU-project "ENVIROMED", which has received funding from the European Union's horizon Europe research and innovation program under grant agreement No.101057844.

Utilizing Cyclodextrin Inclusion Complexes During Additive Manufacturing of Molecularly Imprinted Polymers for Diclofenac-Contaminated Water Samples

Amelie Huber[1,2], Anika Kotyrba[2], Sherman L.Z. Jiokeng[2], Benedikt Keitel[1,2], Boris Mizaikoff[1,2] and Mehmet Dinc[1]*

[1]Hahn-Schickard, Sedanstraße 14, 89077 Ulm, Germany.

[2]Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany.

(*corresponding mehmet.dinc@hahn-schickard.de)

Frequently used persistent drugs like diclofenac sodium salt (DCF) are contaminating aquatic environments and posing risks to aquatic life and human health, especially when entering into drinking water sources.[1] Given the low concentration of true DCF samples with only a few micrograms per liter, it is difficult to determine the exact degree of contamination, which is why amplification and pre-concentration of the analyte prior to analysis is mandatory.

In this study, monolithic inherently porous molecularly imprinted solid phase extraction substrates (MISPE substrates) were prepared and conceptually tested in the laboratory (Figure 1). The substrates were synthesized via additive manufacturing, i.e., resin photopolymerization. For selective interaction between the template molecule DCF and the MISPE substrate β-cyclodextrin was incorporated as functional monomer within an acrylate-based polymer matrix – facilitating hydrophobic interactions and hydrogen bonding.

The main objective is to develop a facile synthesis route of DCF-selective materials for the pre-concentration from aqueous samples sourced from diverse environments including sewage treatment plants. This approach showcases the potential of additive manufacturing in creating molecularly imprinted polymers for targeted water sample treatment, addressing the critical issue of persistent drug contamination.

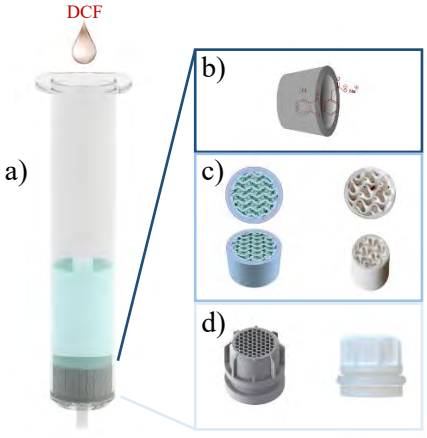

Figure 1: Depicted are the different components used within the proposed MISPE method. a) shows a loaded SPE cartridge, b) the inculusion-complex, c) the CAD model and 3D-printed substrates (which were printed with a reference resin) optimized for interaction with liquid samples, and d) the CAD model and 3D printed sample inlet.

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Keywords:
Molecularly imprinted polymers, MIPs, pre-concentration, purification, solid phase extraction, Diclofenac sodium salt, additive manufacturing, 3D printing.

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P17

Novel Materials and Methods for Thyroid Hormone Bioanalysis

Turki Alfuhayr[1*], Panagiotis Manesiotis[1]

[1]School of Chemistry and Chemical Engineering, Queens University Belfast, David Keir Building, Belfast, BT9 5AG, United Kingdom.

[*] talfuhayr01@qub.ac.uk

Thyroid hormones are essential hormones for several vital functions inside human beings including growth and development processes. The imbalance of their levels causes numerous diseases such as hyperthyroidism and hypothyroidism. As a result, they must be precisely monitored to correctly diagnose and then provide an optimal intervention. The currently used methods, immunoassay-based techniques, have been criticized, and their results are suboptimal to the clinical requirements. The present research aims to validate an alternative approach for thyroid hormone quantification in biological samples with a high degree of accuracy. The strategy of molecular imprinting polymers (MIPs) was exploited to prepare different polymers to produce a polymer that can extract the target. Upon extracting the target, liquid chromatography coupled with mass spectroscopy (LC-MS) was used to separate and quantify the components of the sample. The results confirmed that a significant interaction between the analyte target and the selected urea-based functional monomer can be obtained. This was proven by the ^{1}H-NMR titration method where the results revealed that the association constant of the complex was in the order of magnitude of 10^{3} M^{-1}. The imprinted materials showed outstanding performances in terms of capacity and affinity compared to the non-imprinted polymers. The results of LC-MS showed an accepted linearity with an adequate limit of quantification and limit of detection. The feasibility of using MIPs followed by LC-MS to selectively extract and then quantify thyroid hormones is proved in this work, and it might be a valuable tool in the evaluation of patient status.

Application of molecularly imprinted polymer nanoparticles for lung cancer cell surface proteomics

K. Magumba,[a] E. Piletska,[a] D. Jones,[b] S. Macip,[c] T. Cao[b]

University of Leicester, Department of Chemistry,[a] Department of Genetics and Genome Biology,[b] Department of Molecular Cell Biology,[c] University Road, Leicester, LE1 7RH, United Kingdom.

[a]mkm34@le.ac.uk, [a]ep219@le.ac.uk

Lung cancer is one of the most severe and common types of cancer and is responsible for about 20% of all cancer-related deaths in the UK.[1], [2] The identification and targeting of lung cancer cell surface proteins is important for drug development and clinical diagnostics. This work outlines the use of a novel 'snapshot imprinting' approach to characterise the differences between cell surface proteome of lung cancer cells, with the aim of identifying cell surface markers for diagnostic and therapeutic applications. Molecularly imprinted polymer nanoparticles (nanoMIPs) were formed in the presence of whole cells. Following trypsinolysis, protein epitopes protected by complex with nanoMIPs were eluted from the nanoparticles and analysed by LC-MS/MS. The analysis compared cell lines resistant to radiation ionisation, which include A549 and NCI-H460, with a more sensitive cell line NCI-H522. In the comparison between A549 and NCI-H522, 514 proteins were identified, and in the comparison between NCI-H460 and NCI-H522, 508 proteins were identified. However, only proteins with a fold change of ≥2 and p-value of ≤ 0.05 were considered significant. The utilisation of nanoMIPs provides a great alternative to 'classical' approaches for analysing cell surface proteins, as it eliminates the need for fractionation, affinity separation, and labelling.

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Systematic studies on surface imprinting on the micrometer scale

Chiara Luna Onorati[1,2], Peter Lieberzeit[1],

[1] University of Vienna, Faculty for Chemistry, Department of Physical Chemistry, Währinger Straße 42, 1090 Vienna, Austria
[2] University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Molecularly Imprinted Polymers (MIPs) represent a versatile technique in various applications, ranging from medical diagnosis to environmental sensing. [1] While significant progress in molecular imprinting has been made, there is still little systematic investigation of the physiochemical processes governing the synthesis of surface MIP thin films, which is necessary for gaining a comprehensive understanding and unlocking their full potential. Several factors influence the outcome of a successful MIP detector, thus a further understanding of the elaborate interplay between the structural, chemical, and mechanical properties of these thin films is the focal point of this study. To reach this aim, methodical studies on MIPs thin films were carried out, using functionalized and unfunctionalized silica microparticles as the templates. They were chosen given the relatively big size and defined spherical shape, and, additionally, they are easy to functionalize. Different polymers were investigated including the polystyrene-co-divinylbenzene and acrylate-based commercial polymers. In the first one, different mixtures of monomer-cross linkers ratios were tested. A high level of cross-linker in the polymer mixture was considered since gives a high stability to the three-dimensional polymer matrix which is translated into a retention of functional group orientation within the cavities after template removal. The structural characterization of MIPs thin films, encompassing morphology, porosity, and surface features, was featured using advanced imaging techniques, such as scanning electron microscopy (SEM) and atomic force microscopy (AFM). Chemical composition analysis was conducted using spectroscopic techniques such as Raman Microscopy, offering insights into the functional groups and bonding patterns within the thin films. Additionally, for a comprehensive understanding of the mechanical properties, including stiffness, elasticity, and adhesion forces, Peak Force Quantitative Nanomechanical Mapping (QNM) studies were undertaken. This technique provides important insights for optimizing the synthesis protocol. The optimization of the synthesis protocol to achieve well-defined and homogeneously distributed imprints on the polymer matrix is also an important aspect of this study. This involves several stages such as choosing the suitable stamp and polymer, followed by the removal and washing steps [2].
A homogenous polymer layer with particle cavities was obtained for a 50:50 polymer mixture (monomer-crosslinker). However, reducing the amount of crosslinker results less uniform polymer layer. Instead, when comparing the synthesized polymer with the commercial one, the latter shows evenly distributed silica particles and a smooth polymer layer. By elucidating the physical chemistry properties of MIPs thin films, we pave the way for their optimal utilization in advanced applications, including sensors, targeted drug delivery systems, and efficient separation technologies. In conclusion, this abstract advocates for a concerted effort to fully realize the potential of MIPs thin films, emphasizing their crucial role in functional materials.

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P20

In-situ synthesis of MIP to Detect Au Nanoparticles on QCM

M. Bagheri,*[1,2] S. Bakhshi Sichani,[3] P. Wagner,[3] P.A. Lieberzeit[1,2]
[1]*University of Vienna, Faculty of Chemistry, Department of Physical Chemistry, 1090 Vienna, Austria*
[2]*University of Vienna, Doctoral School of Chemistry (DoSChem), 1090 Vienna, Austria*
[3]*KU Leuven, Soft-Matter Physics and Biophysics Section, Department of Physics and Astronomy, 3001 Leuven, Belgium*
**Mahdieh.bagheri@univie.ac.at*

In recent years, there has been an increasing interest in gold nanoparticles (AuNPs) in the field of MIPs due to their remarkable optical, electronic, and catalytic properties. However, meager attention has been directed towards detecting Au NPs considering the large amount of their usage. This work introduces surface imprinted polymers using Au NPs with 75 diameters as the template (capped with PVP) and acrylic polymer through RAFT-assisted synthesis[1]. Synthesis involves in-situ polymerization[2] by immobilizing the 2,2'-Azobis(2-methylpropionamidine) dihydrochloride (AAPH) as photoinitiator on Quartz Crystal Microbalance (QCM) chips (168 µm thick and 13.8 mm in diameter) by using EDC/NHS coupling. Moreover, precise control of the polymerization process is crucial for applications that require consistency, specifically in sensing measurement. The height of the resulting polymer is systematically controlled by polymerization time, The polymer thickness is measured by a network analyzer and maintains a range of 10-20 nm in 3.5 hours of polymerization.

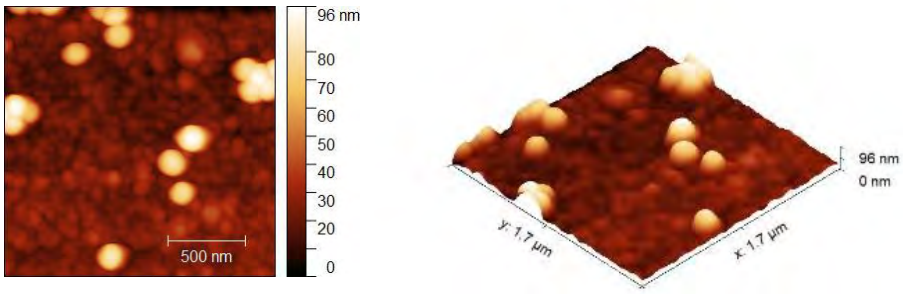

Figure 1:2D and 3D AFM images of Au NPs MIP surface after polymerization.

For better Au NP removal from the polymer, we substituted the PVP shell with 16-Mercaptohexadecanoic acid (16-MHDA) as a hydrophilic stabilizer before imprinting in the polymer. The polymer surface was scanned by AFM and SEM before and after washing/removal of Au NPs. Figure 1 reveals a good particle distribution and an even polymer surface. it also shows most of the particle surfaces are out of polymer which eases the removal step.

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P21

Soft molecularly imprinted nanoparticles coupled with simultaneous lossy mode and surface plasmon multi-resonances optical platform for femtomolar sensing of proteins

Mimimorena Seggio*[a], Francesco Arcadio [b], Laurent Noël [c,d], Domenico Del Prete [b], Olivier Soppera [c,d], Nunzio Cennamo [b], Luigi Zeni [b] & Alessandra Maria Bossi [a]

[a] *Department of Biotechnology, University of Verona, Strada Le Grazie 15, 37134 Verona, Italy.*
[b] *Department of Engineering, University of Campania "L. Vanvitelli", Via Roma 29, Aversa, Italy.*
[c] *CNRS, IS2M UMR 7361, University of Upper-Alsace, 68100 Mulhouse, France.*
[d] *Université de Strasbourg, 67000 Strasbourg, France.*

mimimorena.seggio@univr.it

A multi-resonances optical platform functionalized with soft molecularly imprinting nanoparticles (nanoMIPs), specifically entailed the selectivity towards the protein biomarker human serum transferrin (HTR), was developed [1].
The simultaneous interrogation of both lossy mode (LMR) and surface plasmon (SPR) resonances was herein exploited for the first time. Two distinct metal-oxide bilayers, i.e. TiO_2–ZrO_2 and ZrO_2–TiO_2, were used in the SPR–LMR sensing platforms.
The responses to binding of the target protein human serum transferrin (HTR) of both sensing configurations (TiO_2–ZrO_2–Au-nanoMIPs, ZrO_2–TiO_2–Au-nanoMIPs) showed femtomolar HTR detection, LODs of tens of fM and K_{Dapp} ~ 30 fM. Selectivity for HTR was demonstrated. The simultaneous resonance monitoring is advantageous for point of care determinations, in terms of measurement's redundancy, that enables the cross-control of the measure and to optimize the detection, by exploiting the individual characteristics of each resonance.

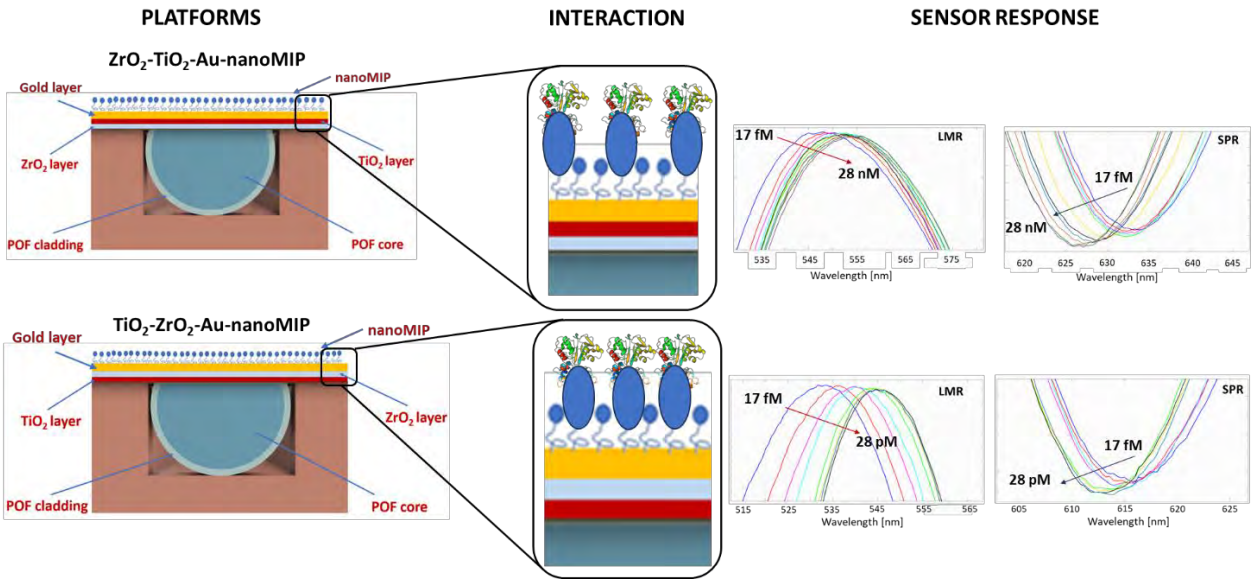

Figure 1: Scheme of LMR-SPR-nanoMIP-based platform and response to HTR protein

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P22

Molecularly imprinted polymer nanogels for the detection of the heart failure biomarker Troponin T

Grisel Palome Villezcas,[1] Noel Kalacas,[1] Alessia di Fiore,[1] Bernadette Tse Sum Bui,[1] Karsten Haupt[1,2]

[1]*Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*

[2]*Institut Universitaire de France*

Molecularly imprinted polymers (MIPs) [1] are synthetic antibodies that specifically recognize molecular targets. They are cross-linked polymers synthesized in the presence of a molecular template, which induces three-dimensional binding sites in the polymer that are complementary to the template in size, shape and chemical functionality. The aim of this work was to develop MIP nanogels against the heart failure biomarker Troponin T for diagnostic applications. MIPs against Troponin T were obtained through a rational approach starting with *in silico* epitope design. Chemically synthesized peptide epitopes were then used as templates in a solid-phase protocol for MIP synthesis [2]. Fluorescence binding assays and SPR demonstrated that the MIP recognizes and binds its target with an affinity and selectivity like a biological antibody. A protocol for the interfacing of MIP nanogels by click chemistry with optical fibre-based biosensors was then developed. These materials have great potential for applications in the clinical diagnostics of heart disease.

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P23

A MIP based sensor for highly sensitive detection of Human Chorionic Gonadotropin (hCG): Towards a reusable pregnancy test

R. Zubryte[1]*, R. Porter[2], M. Sullivan[3], A. Mattsson[1], B. Sellergren[4]

[1] Pharmista Technologies AB, *Scheelevägen 3, Lund, 223 63, Sweden,* [2]RAPIvD Ltd, *Exchange Building, Colworth Science Park, Sharnbrook, Bedfordshire. UK, MK44 1LZ,* [3] University of Sheffield*, Dainton Building, Brook Hill, Sheffield S3 7HF, Great Britan*, [4] Malmö University, Biofilms Research Center for Biointerfaces, *Per Albin Hanssons väg 35, Malmö 214 32, Sweden*

* radvile@pharmista.se

Since their introduction in the 1970s, pregnancy tests have become the most widely utilized diagnostic assays for at-home use.[1] These tests rely on the lateral flow assay (LFA) technique, a well-established method. Despite its prevalence, LFA exhibits several drawbacks, including challenges in manufacturing, suboptimal accuracy, sensitivity to adverse storing conditions, and restriction to single use.[2–4]

A key to overcoming these drawbacks is to address the labile nature of the antibody-based assay. In this context, Molecularly Imprinted Polymers (MIPs) emerge as a promising solution, offering distinct advantages marked by heightened physical and chemical stability, the ability for regeneration and repeated use, as well as a notable reduction in preparation time and cost.[5]

In the present study, we report on an imprinted polymer (MIP) – based electrochemical sensor for the recognition of Human Chronic Gonadotropin (hCG). Through dispersed-phase synthesis and epitope imprinting, we developed nanoMIPs exhibiting high affinity and selectivity for hCG. These nanoMIPs, compatible with various sensor transducer principles (e.g., QCM, SPR, EC), also showcase the sensor's repeated reusability. This offers a new building block towards future sustainable diagnostics where patients are able repeatedly track their condition using the same device.

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Molecularly imprinted polymers sensitive to S-metolachlor

D. Rapacz,* K. Smolińska-Kempisty & J. Wolska

Wroclaw University of Science and Technology, Faculty of Chemistry, wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wroclaw, Poland

**dominika.rapacz@pwr.edu.pl*

S-metolachlor is a herbicide belonging to the chloroacetanilide group, widely used to control annual grasses and small-seeded broadleaf weeds, in maize, sunflower, cotton, and soybean cultivation. [1] Compared to other herbicides from this class, S-metolachlor is more persistent in the soil and can be washed into groundwater due to its relatively good solubility in water (488 mg x L^{-1} at 20°C) and low sorption in soil particles. [1,2]

Green molecularly imprinted polymers toward S-metolachlor were synthesized by bulk polymerization with use N-isopropylacrylamide and acrylamide as functional monomers, N,N'-methylenebis(acrylamide) as a cross-linker, ammonium persulfate as an initiator, and N,N,N',N'-tetramethylethylenediamine as a co-initiator. Polymer synthesis was carried out following *sustainable chemistry*, employing water as a porous agent and at ambient temperature. Sorption of S-metolachlor from a model and real solution prepared from tap water was successfully performed. The obtained MIP showed high selectivity towards S-metolachlor contrasted to other plant protection products.

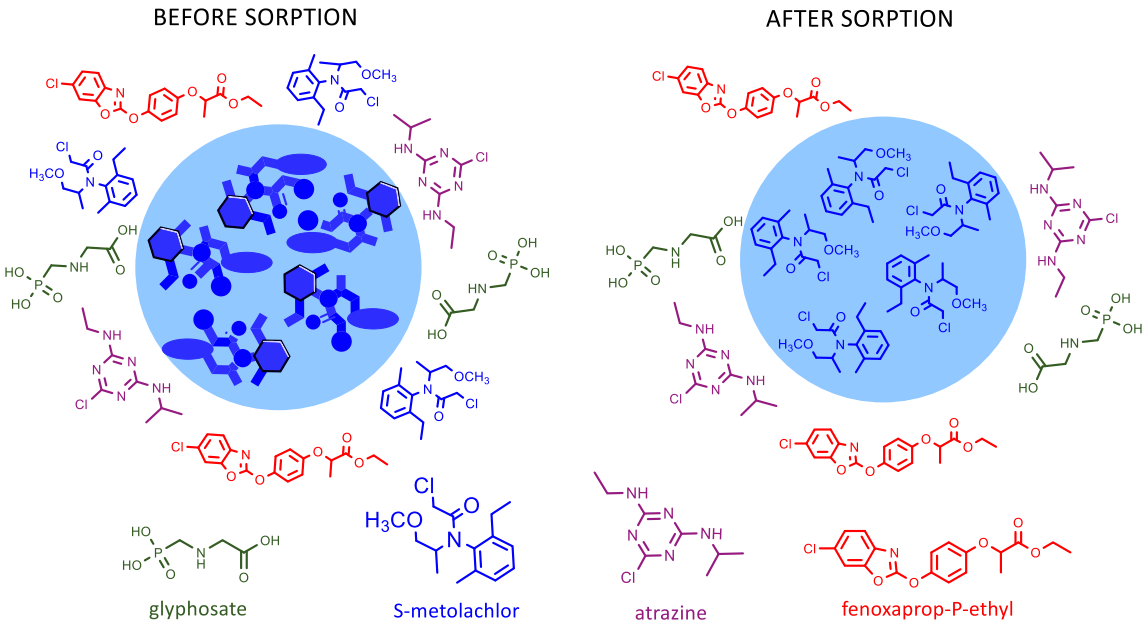

Figure 1. Graphical depiction of S-metolachlor capture by MIP.

Acknowledgments
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Rational Design of Non-Covalent Molecularly Imprinted Polymers Based on the Combination of Molecular Dynamics Simulation and Quantum Mechanics Calculation

Xue Yu[12], Zanxia Cao[1], Mengxia Yan[1], Jiawen Wu[1], Jianhui Xin[1], Junfen Wan*[2], Xuejun Cao*[2]

[1]Shandong Key Laboratory of Biophysics, Institute of Biophysics, Dezhou University, Dezhou, 253023, P.R. China

[2]State Key Laboratory of Bioreactor Engineering, Department of Bioengineering, East China University of Science and Technology, 130 Meilong Rd, Shanghai 200237, China

Corresponding author: Junfen Wan

Fax numbers: +86-21-64252960

E-mail: wanjunfen@ecust.edu.cn

Corresponding author: Xuejun Cao

Fax numbers: +86-21-64252695

E-mail: caoxj@ecust.edu.cn

Abstract

Molecular imprinting technology (MIT) is a promising method to create polymeric materials as artificial receptors. Nevertheless, only several types of molecularly imprinted polymers (MIPs) are commercially available and most of the studies on MIP$_S$ are still in the experimental stage. One of the main limitation factors was the difficulty in screening an imprinting systems, especially those for some weak functional target molecules. In this study, a novel combined approach of quantum mechanics (QM) calculation and molecular dynamics (MD) simulation was applied to screen appropriate 2,4-dichlorophenoxyacetic acid (2,4-D) imprinting system. QM calculation was carried out in Gaussian 09 software. MD simulation was performed with the Gromacs2018.8 suite of program. The results of QM calculation were well consistent with the results obtained from MD simulation. In MD simulation, to approach a more realistic representation of the "actual" prepolymerization mixture, large multiples of components were introduced in the simulation to comprehensively investigate all non-covalent interactions in imprinting. This work systematically studied the MIPs system by computer simulation and established the theoretical prediction model of MIPs' affinity and selectivity. The combined strategy of QM calculation and MD simulation provides a sound basis for the rational design of MIPs.

Keywords: Quantum mechanics; Rational design; Molecular imprinting; Molecular dynamics

P26

Double surrogated imprinting for the preparation of virus-selective particles

B. Fresco-Cala[1,2],* A. Gálvez-Vergara[2], D. Baumgarten[2] & B. Mizaikoff[2,3].

[1]*Affordable and Sustainable Sample Preparation (AS2P) research group, Departamento de Química Analítica, Instituto Químico para la Energía y el Medioambiente IQUEMA, Universidad de Córdoba, Campus de Rabanales, Edificio Marie Curie, E-14071, Córdoba, Spain.*

[2]*Institute of Analytical and Bioanalytical Chemistry, Ulm University, 89081, Ulm, Germany*

[3]*Hahn-Schickard, 89077 Ulm, Germany.*

**Beatriz.fresco@uco.es*

This work entails the development of surrogate-imprinted polymers designed for the specific detection of SARS-CoV-2. To attain this objective, an innovative dual imprinting method was employed, utilizing carboxylated-polystyrene (PS-COOH) nanoparticles and a peptide derived from the covid-virus (Figure 1). The first step consisted of the imprinting of the holes mirroring the size and shape of the target virus. For that, PS-COOH nanoparticles (~100 nm) were chosen as the template (dummy-virus particles). Thus, these PS-COOH nanoparticles were incubated with the PS-NH_2 microspheres (core particles), forming bonds through electrostatic interactions. Following this, a silica layer, utilizing tetraethyl orthosilicate (TEOS) as a monomer, was deposited onto the surface of the PS-NH_2 microspheres. Additionally, a specific covid peptide sequence, representing the most abundant/relevant protein on the target virus's surface, served as the second template and was also incorporated into the polymerization mixture. A layer of TEOS/phenyltriethoxysilane (PTES) was then generated around the PS-NH_2 microspheres. Ultimately, the PS and the covid peptide were eliminated through multiple washes, leaving behind double surrogate-imprinting sites comprising dummy particle-holes and peptide-binding cavities. Comprehensive studies were conducted on variables related to polymerization, imprinting routes, and the binding efficiency of the final double-imprinted polymers. Peptide identification and quantification were carried out using high-performance liquid chromatography with UV detection (HPLC-UV).

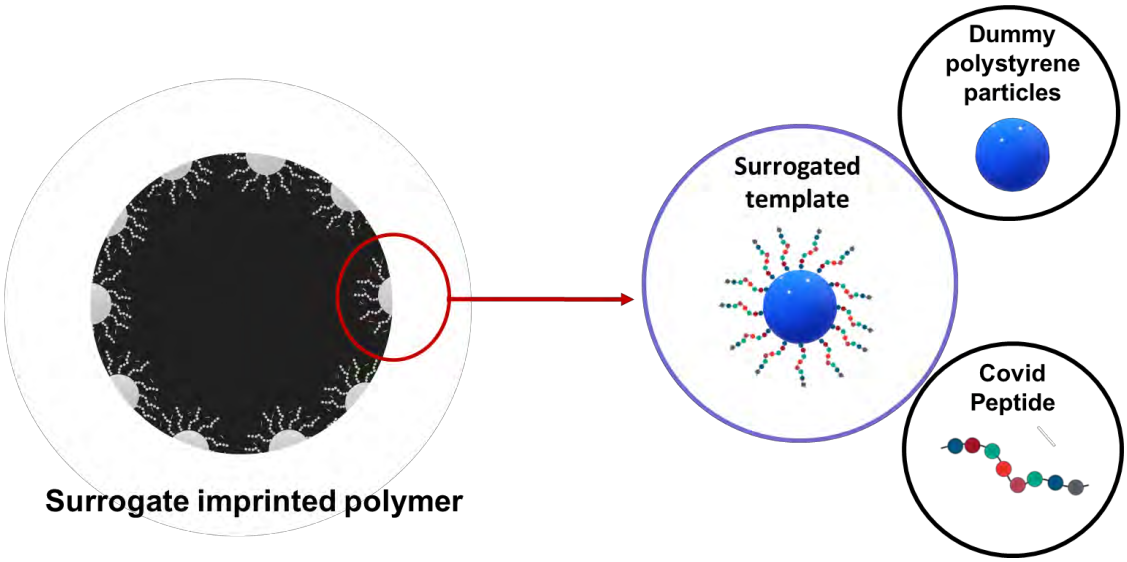

Figure 1. Graphical abstract of the dual imprinted polymers obtained and the surrogated templates used in the synthesis.

Molecularly Imprinted Nanoparticles for the Detection of Norovirus in Food

Amy Dann[a,b], Jake McClements[a] ,Pankaj Singla[b], Sloane Stoufer[c], Mark Sullivan[d], Nicholas Turner[d], Mark Geoghegan[a], Shayan Seyedin[a], Matthew Moore[c] and Marloes Peeters[b]

[a] School of Engineering, Merz Court, Claremont Road, Newcastle University, Newcastle Upon Tyne, NE1 7RU, United Kingdom

[b] Department of Chemical Engineering and Analytical Science, School of Engineering, University of Manchester, Manchester M20 4BX, United Kingdom

[c] Department of Food Science, University of Massachusetts, Amherst, MA, United States

[d] Department of Chemistry, University of Sheffield, Dainton Building, 13 Brook Hill, Sheffield, S3 7HF, United Kingdom

Norovirus is the predominant cause of foodborne illnesses globally, resulting in around 685 million cases per year[1]. However current methods used to detect norovirus in food, such as ELISA immunoassays and PCR, are costly, time intensive, and require trained personnel. Consequently, there is a strong drive for rapid and straightforward norovirus detection techniques, particularly those that could be utilised for in-field measurements of food samples. In response to this need, molecularly imprinted polymer nanoparticles (nanoMIPs) have been synthesised to act as synthetic recognition elements for norovirus. Using the solid-phase approach alongside epitope imprinting offers a fast and biosafe method of nanoMIP production whilst still enabling the detection of much larger virus-like particles.

The nanoMIPs were electrografted onto low-cost screen-printed electrodes, which enables them to be integrated into a thermal sensor. The heat transfer method (HTM) offered faster detection times (~ 15 min) than traditional methods and improved limit of detection values (6.5 pg/mL) in spiked-buffered solutions. Moreover, the nanoMIPs could effectively detect traces of norovirus in high-risk real food samples with complex matrices, as shown in **Figure 1**. A significant advantage of nanoMIPs over various biological receptors lie in their ability to accurately detect pathogens in food samples despite their diverse inhibitors and varying pH levels. Consequently, the sensor has potential for industrial applications, advancing efforts to prevent norovirus infections.

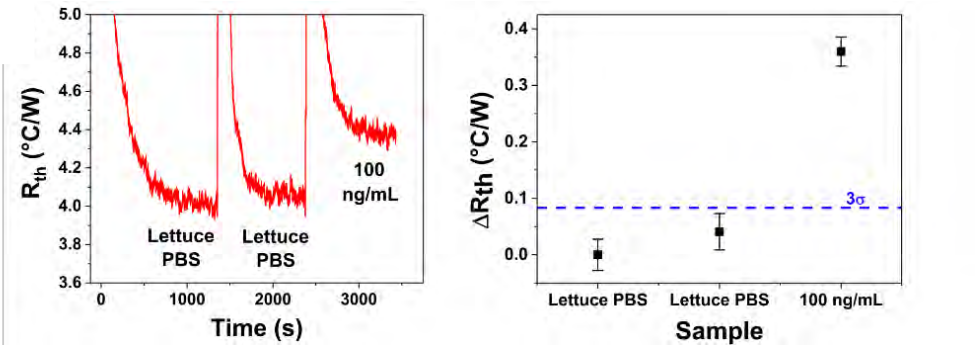

Figure 1: Thermal detection of norovirus in romaine lettuce rinse water using nanoMIPs. a) Raw thermal detection data and b) corresponding dose-response plot showing the change in thermal signal compared to a control when norovirus is added to the sensor.

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Rational Design of MIPs for Precise Discrimination of Viral and Bacterial Infections

Soumya Rajpal[a,b]*, Boris Mizaikoff [b,c], Prashant Mishra [a]

[a] Department of Biochemical Engineering and Biotechnology
Indian Institute of Technology Delhi
Hauz Khas, New Delhi 110016, India

[b] Institute of Analytical and Bioanalytical Chemistry
Ulm University
Albert-Einstein-Allee 11, 89081 Ulm, Germany

[c] Hahn-Schickard
Sedanstraße 14, 89077 Ulm, Germany

**soumya.rajpal@uni-ulm.de*

Accurate diagnosis is paramount for effective patient care and the containment of antimicrobial resistance outbreaks. Distinguishing between bacterial and viral infections remains challenging, given limited advanced diagnostic tools and overlapping symptoms. This study employs molecular imprinting techniques to develop chemically stable, cost-effective antibody analogs for precise viral-bacterial differentiation. Our approach centers on interferon-induced proteins as distinctive markers for viral infections. Utilizing epitope imprinting, we target specific biomarker regions critical for interaction. Computational calculations guide the design of MIPs by assessing monomer-epitope interactions. Introducing a novel multi-monomer simultaneous docking (MMSD) protocol efficiently maps cooperative effects, offering a theoretical alternative to labor-intensive experimental polymer optimization. Simulations unveil binding mechanics and intermediates, highlighting unique interactions that enhance MIP-peptide complementarity. *In silico*-guided MIP optimization produces high-performance receptors selectively binding to the target epitope over non-specific proteins. A proof-of-concept study demonstrates protein binding to synthetic receptors. Similar to antibodies, MIPs show promise for accurately detecting viral infections, addressing current diagnostic limitations.

Exploring the influence of the peptide length used as template on binding performance of nanoparticles produced by epitope imprinting

Ainhoa Elejaga-Jimeno[1]*, Lucía Diez-Caballero[1], Gontzal García del Caño[2], Nora Unceta[1], M. Aránzazu Goicolea[1], Ramón J. Barrio[1], Alessandra M. Bossi[4], Alberto Gómez-Caballero[1].

Department of [1]Analytical Chemistry, [2]Neurosciences, and [3]Pharmacology, University of the Basque Country UPV/EHU, 01006 Vitoria-Gasteiz (Spain)

[4]Department of Biotechnology, University of Verona, 37134 Verona (Italy)

*ainhoa.elejaga@ehu.eus

The main objective of this work is to know how the length of the peptide (used as template) influences the created epitope and the binding performance of plastic nanoparticles produced by solid phase synthesis and the epitope imprinting approach. This method imitates the selective recognition behaviour displayed by natural antibodies, which only bind to precise fragments of their target molecules, commonly denoted as epitopes. The work is focused on the C-terminal section of the cannabinoid CB1 receptor, and peptides of 6 (458-TSAEAL-472), 9 (458-STDTSAEAL-472), 12 (458-MSVSTDTSAEAL-472) and 15 (458-KVTMSVSTDTSAEAL-472) amino acids have been used as template, which match with the final section of the receptor. Anti-CB1 imprinted nanoparticles (MIN) were fabricated for each described peptide.

In order to be able to discriminate between different peptide lengths for proper imprinting, the binding event was assessed through different techniques. Anti-CB1 nanoparticles produced for 6, 9, 12 and 15 aa peptide fragments were tested using the 15 aa length peptide and the fusion recombinant GST-protein (GST-CB1$_{414-472}$) as ligands. Thermodynamic data of MIN-ligand binding for each type on material were acquired using isothermal titration calorimetry (ITC). Prior to this experiment, the size of the polymers was determined through Dynamic Light Scattering under optimal binding conditions. Non-imprinted polymers were also produced and tested as a negative control.

The results obtained indicated that the developed MIN exhibited comparable dissociation constant (K_D) values for both the 15 amino acid peptide and the recombinant protein. This consistency aligns with the principles of the epitope imprinting approach. Moreover, the determined K_D values fell within the nanomolar range, closely resembling the values typically observed with natural antibodies. These data were compared with affinity data obtained by surface plasmon resonance, using the GST-CB1$_{414-472}$ recombinant protein as target for the binding of the developed MIN. To this end, nanoparticles were immobilized onto the gold surface of the sensor via carbodiimide chemistry. The affinity values obtained from these studies were of the same order of magnitude as the ones obtained at previous ITC experiments, confirming the reproducibility of the developed materials.

P30

Influence of the cross-linker percentage on the thermoresponsive character and binding behaviour of peptide imprinted nanoparticles produced against the CB1 cannabinoid receptor

Ainhoa Elejaga-Jimeno[1], Alberto Gómez-Caballero[1*], Amaia Alday-Izaguirre[1], Miquel Saumell-Esnaola[3], Gontzal García del Caño[2], M. Aránzazu Goicolea[1], Joán Sallés[3], Ramón J. Barrio[1].

Department of [1]Analytical Chemistry, [2]Neurosciences, and [3]Pharmacology
University of the Basque Country UPV/EHU, 01006, Vitoria-Gasteiz (Spain)

*a.gomez@ehu.eus

This work intends to demonstrate how the cross-linker amount on the polymerisation mixture influences phisycochemical characteristics and the binding behaviour of plastic nanoparticles. Peptide imprinted artificial receptors were produced here against the C-terminal fraction of the CB1 cannabinoid receptor, particularly for the sequence (458-KVTMSVSTDTSAEAL-472) which comprises 15 aminoacids.

Previous works developed by our research group demonstrated that produced anti-CB1 nanoparticles presented remarkable binding behaviour in western blot experiments towards the recombinant GST-CB1$_{414-472}$ and GST-CB1$_{414-442}$ fusion proteins, as target and negative control proteins (1). Here, we wanted to go further on this research in order to know how BIS influenced the plasticity of the material, and, at the same time, how that plasticity may compromise the affinity of the binding event. Material plasticity was assessed examining the thermoresponsive character presented by nanoparticles on turbidity experiments. This was possible because the functional monomers NIPAm and TBAm are known to undergo a transition from a collapsed state (insoluble in water) to an expanded state (soluble in water) based on the temperature of the medium. This temperature-induced shift between the collapsed and expanded states is commonly referred to as the lower critical solution temperature (LCST).

Molecularly imprinted nanoparticles (MIN) produced here were synthesised by solid-phase synthesis, using constant amounts of N-isopropylacrylamide (NIPAm), N-tert-butylacrylamide (TBAm), N-(3-aminopropyl)methacrylamide (3-APMA), and acrylic acid (AA) as functional monomers, and variable quantities N,N-methylenbis(acrylamide) (BIS) as cross-linker. Physicochemical and affinity characterisation was performed by X-ray Photoelectron Spectroscopy (XPS) and batch rebinding experiments. Upon comparing the synthesised MIN and corresponding NIN, different LCST were observed, which denoted different thermoresponsivity, and, consequently, different plasticity-rigidity. Notably, high amounts of cross-linker in the composition resulted in a reduction of the lower critical solution temperature, accelerating the transition from expanded to collapsed state. Additionally, the proportion of cross-linker also influenced other aspects of the polymers, including their affinity towards the epitope. In brief, MIN synthesized using 10% of cross-linker, in comparison to the other polymers, exhibited a binding curve that most effectively fitted to the Langmuir model, which presupposes a single homogeneous binding site for each particle. The K_D and B_{max} values obtained from the fitting were 6.78×10^{-8} M and 0.23 µmol peptide/g MIN, respectively.

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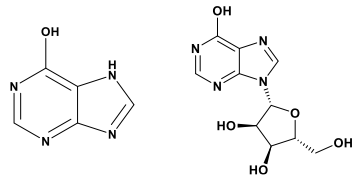
Development of Hypoxanthine Sensor Using Molecularly Imprinted Polymer

Sato Yui[1], Yoshimi Yasuo[1]*, and Aaryshree[1,2]

[1]*Department of Applied Chemistry, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo, Japan*
[2]*Innovative Global Program, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo, Japan*
yosimi@sic.shibaura-it.ac.jp*

Introduction

Adenosine triphosphate (ATP), present in both meat and fish meat, undergoes a gradual degradation, ultimately transforming into hypoxanthine (Hx) via inosine (HxR) and various intermediate products. This biochemical transition is a key indicator of the freshness of meat products. Our research aims to create an Hx sensor using Molecularly Imprinted Polymer Carbon Paste (MIP-CP) to monitor meat freshness. We have successfully established a method for creating MIP-CP electrodes [1]. The study aims to create a highly sensitive detector for Hx using Hx-specific MIP-CP (Hx-MIP-CP), which is made of graphite particles grafted with MIP and bound together using a specific oil binder. We studied the electrode responsiveness to different concentrations of Hx by analyzing their oxidative and reductive currents.



Hypoxanthine (Hx) Inosine (HxR)

Experimental Methods

First, the surface of graphite particles was modified with the N-diethyldithiocarbamate methylene group as an initiator for radical graft polymerization. Then, a pre-polymerization solution was prepared by dissolving Hx, methacrylic acid, methylenebisacrylamide, ethylene dimethacrylate, and vinyl ferrocene in dimethylsulfoxide. To this, initiator graphite was added, and the suspension was irradiated with a xenon lamp for 60 minutes for graft copolymerization. The Hx template was extracted using 3 M HCl to prepare the MIP-grafted particles. MIP-CP was obtained by mixing the MIP particles with silicone oil in a 7:3 weight ratio. The performance of the Hx-MIP-CP was evaluated by conducting cyclic voltammetry using electrodes coated with MIP-CP on screen-printed electrode chips. The Hx-MIP-CP performance was evaluated by analyzing the relationship between the oxidative or reductive currents and Hx or HxR concentration (0-420 μM).

Results and Discussion

We observed that both the reductive and oxidative currents displayed by the sensor were linearly correlated with the concentration of hypoxanthine (Hx) as shown in Fig.1. The currents observed exhibited no noticeable relationship with the concentration of inosine (HxR), thereby highlighting the sensor's specificity towards Hx. The measurement took 30 s only. Thus, the results indicate that the Hx-MIP-CP is feasible as a highly selective and rapid sensor for Hx.

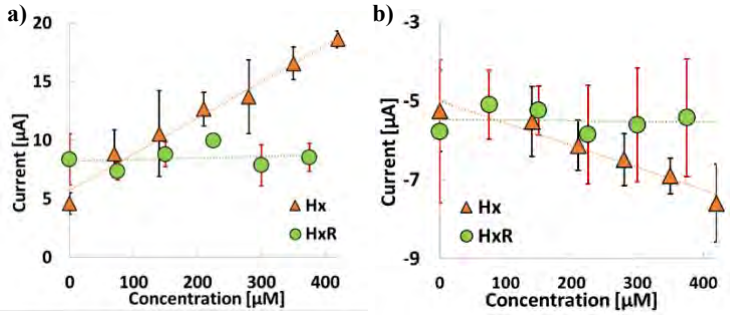


Fig.1: Effect of the Hx and HxR concentration on: a) the oxidative (+1.0 V vs Ag/AgCl) and b) the reductive currents (-0.5 V vs Ag/AgCl) .

Conclusion

We have successfully developed a hypoxanthine sensor using MIP-CP, which will measure the freshness of fish through simple procedures.

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Development of a Disposable Histamine Sensor Using Molecularly Imprinted Carbon Paste for Freshness Evaluation of Fish

Hina Sakurai[1], Aaryashree[1,2], and Yasuo Yoshimi[1]

[1]*Department of Applied Chemistry, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-kuTokyo, Japan*
[2]*Innovative Global Program, Shibaura Institute of Technology, Tokyo, Japan*

Introduction:
Histamine (Hm), a toxic compound, is produced due to an enzymatic reaction when histidine (His)-rich redfish such as tuna and mackerel or their processed products are improperly stored (e.g., left at room temperature). The rise in consumption of raw fish has increased the demand for Hm analysis. However, the conventional immunoassay method is costly, time-consuming, and technically demanding, burdening wholesalers heavily. Molecularly Imprinted Polymer grafted Carbon Paste (MIP-CP) is a feasible sensor tool due to its high selectivity, stability, and ease of production. In this study, we aimed to develop a disposable sensor using MIP-CP for Hm sensing.

Experimental Methods
The process began with fixing a radical polymerization initiator on the surface of graphite particles [1]. Next, histamine dihydrochloride, methacrylic acid, methylene bisacrylamide, and vinyl ferrocene were dissolved in a DMSO, and the initiator-fixed graphite was added to prepare a polymerization solution. This polymerization solution was irradiated with a xenon lamp for 60 min, The Hm template was extracted using acetic acid. To prepare MIP-CP, the MIP-grafted graphite and silicon oil containing ferrocene were blended in a 7:3 weight ratio. A similar procedure was used to make non-imprinted polymer (NIP)-CP, with the critical difference being the absence of Hm in the process. Cyclic voltammetry tests were conducted using electrodes coated with MIP-CPs on a disposable chip [2]. The efficiency of the HM sensor was determined by examining the correlation between the reduction current and the concentration of Hm within a measurement range of 0 to 100 ppm.

Experimental results
The cathodic current at the MIP-CP electrodes was sensitive to histamine Hm with high linearity (R^2 = 0.9633) but was insensitive His, as shown in **Fig. 1**. This sensitivity was specific to the MIP-CP electrodes, whereas the NIP-CP electrodes did not exhibit sensitivity to Hm. These findings suggest that the changes observed in the MIP-CP electrodes are due to the specific interaction between Hm and the Hm-imprinted cavities in the MIP. The dynamic range of the sensor, spanning from 0 to 100 ppm, effectively covers the range of Hm concentrations typically considered acceptable in fish. The MIP-CP electrode is a suitable option for fish freshness monitoring.

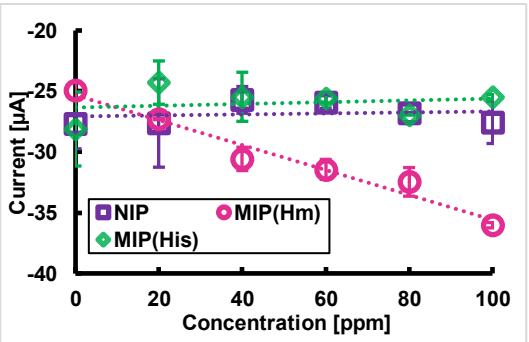

Fig.1 Comparison between Hm and His calibration curves by MIP-CP, NIP-CP

Conclusion
We successfully developed a reagentless, disposable histamine sensor using MIP-CP, which provides a rapid, reliable, and cost-effective method for histamine detection in fish.

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Development of A Disposable Inosine-Molecularly Imprinted Polymer Carbon Paste Electrodes for Freshness Evaluation of Fish

Takumi Iwasaki [1], Aaryashree [2], Yasuo Yoshimi [1]*

1) Dept. Applied Chem. and 2) Innovative Global Program, Shibaura Institute of Technology

3-7-5, Toyosu, Koto-ku, Tokyo, Japan, Email: yosimi@sic.shibaura-it.ac.jp

Introduction:

Inosine, a derivative of adenosine triphosphate found in fish meat, is a critical indicator of fish freshness, with its concentration directly indicating fish quality [1]. Though accurate, conventional analysis via high-performance liquid chromatography proves challenging for implementation at distribution centers. In this study, we have developed a carbon paste electrode that can provide real-time current values reflecting inosine concentration. To achieve this, an electron transfer substance was introduced into MIP using inosine as a template and mixed with silicon oil.

Experimental Method:

Initiator-fixed graphite particles were dispersed in a mixture of an aqueous solution of inosine and *N, N'*-dimethyl formaldehyde solution of methacrylic acid, 3-methacrylamidophenylboronic acid, *N, N'*-methylene bisacrylamide, and vinyl ferrocene. Graft radical copolymerization was allowed to occur at the surface of the particles. After the removal of the inosine template by hydrochloric acid, the MIP-grafted particles were dried in a vacuum. The particles were mixed with silicon oil containing ferrocene to obtain inosine MIP carbon paste (MIP-CP). A carbon screen printed electrode (Zensor, Taipei) with MIP-CP applied on the working electrode was filled with pH 7.4 phosphate buffer solution containing inosine of 0-112 μM. Differential pulse voltammetry was performed to evaluate current sensitivity to the inosine concentration.

Experimental Result:

The relationship between the anodic current at 0.9V and inosine concentration in the sensor coated with MIP-CP is shown in **Fig.**; MIP-CP showed a high sensitivity to inosine and a high correlation coefficient of 0.0387 A・L/mol and R^2=0.9387, respectively. The lower sensitivity to sodium inosinate of -0.0012 A・L/mol and R^2=0.4410 indicates the high selectivity of the MIP-CP.

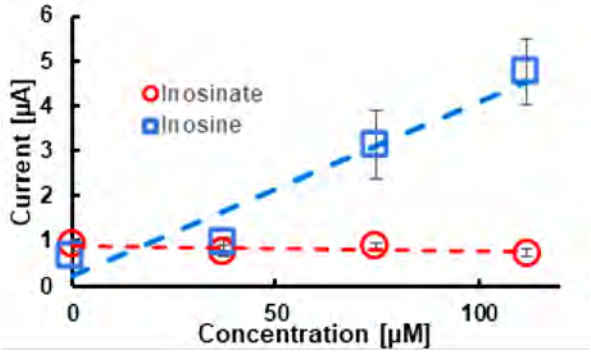

Fig. Current of intensities at 0.9 V for sensors coated with MIP-CP as functions of inosine and inosinate concentration.

Conclusion:

The inosine-templated MIP-CP is feasible for real-time and selective sensing of inosine concentration at the fish distribution sites.

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Cladded molecularly imprinted nanoparticles for fluorescence imaging of polysialic acid on tumor issues

Lingrui Huang, Song Gao, Fang Jin and Zhen Liu*

State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering, Nanjing University, 163 Xianlin Avenue, Nanjing 210023 P.R. China

* Email: zhenliu@nju.edu.cn

Abnormal glycosylation of proteins, often linked to cancer, has implications for tumor diagnosis and treatment. Polysialic acid (polySia), a unique glycan, is a linear homopolymer linked by sialic acid with α-2,8 or α-2,9 bonds. It exhibits elevated expression levels in numerous malignant human tumors and is strongly correlated with tumor progression and poor prognosis. [1] However, existing polySia-specific binding reagents face challenges in selectivity, affinity and versatility, hindering precise analysis of the glycan. Molecularly imprinted polymers (MIPs), as designable artificial antibody mimics, offer substantial potential to address these issues. Oligosialic acid imprinted nanoparticle (oSia-MIP) was previously prepared for targeting polySia. [2] While it has shown promise for neuroblastoma therapy, the synthesis procedure and recognition performance require further improvement. Herein, we proposed a streamlined and universal MIP-based strategy to create a fluorescent nanoprobe for glycans with exposed carboxyl groups. We alkylated exposed carboxyl groups of polySia to form amphiphilic templates. Then, using the reverse microemulsion-confined surface imprinting and cladding approach, [3] polysia-imprinted nanoparticle (polySia-MIP) with improved affinity and selectivity was prepared. By analyzing polySia expression in various cancers through fluorescent imaging on tumor tissues, we investigated the correlation between polySia expression levels and tumor classification or typing. This study systematically analyzed polySia expression in various cancers and presented a generic strategy for preparing glycan-MIPs through similar glycan modification. It strongly supported the potential of polySia as a diagnostic or therapeutic target, providing new insights into characteristic tumor glycans.

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P35

Molecularly-imprinted polymer synthesis for tramadol determination using venlafaxine as a dummy template

B. Fresco-Cala,* T. Mansilla-Cejas & S. Cárdenas.

Affordable and Sustainable Sample Preparation (AS_2P) research group, Departamento de Química Analítica, Instituto Químico para la Energía y el Medioambiente IQUEMA, Universidad de Córdoba, Campus de Rabanales, Edificio Marie Curie, E-14071, Córdoba, Spain.

Beatriz.fresco@uco.es

This research focuses on the synthesis of a molecularly imprinted polymer (MIP) for the selective determination of tramadol (Figure 1). Typically, the template molecule used in MIP synthesis corresponds to the target analyte. However, due to the cost and restricted availability of tramadol, venlafaxine was employed as a dummy template due to its similar structure, size, and functionality. Thus, MIPs were synthesized through photopolymerization on a cellulose paper support using methacrylic acid (MAA) as a functional monomer and ethylene glycol dimethacrylate (EDMA) as a cross-linker. To anchor covalently the polymers to the supports, the papers were previously treated firstly with benzophenone and sequentially with EDMA. The variables related to the synthesis procedure, including the monomer/cross-linker ratio, porogen type, polymerization time, and template concentration, were optimized in order to achieve the maximum rebinding capacity and therefore the highest imprinting factor (IF). SEM characterization of the MIP and its corresponding non-imprinted (NIP) was also conducted, showing a similar morphological structure. As expected, the resulting MIP exhibited selectivity towards tramadol, with an imprinting factor of 2.86. This study demonstrates a potential approach for the preparation of tramadol-selective sorbents, addressing challenges associated with the availability and cost of the target opioid.

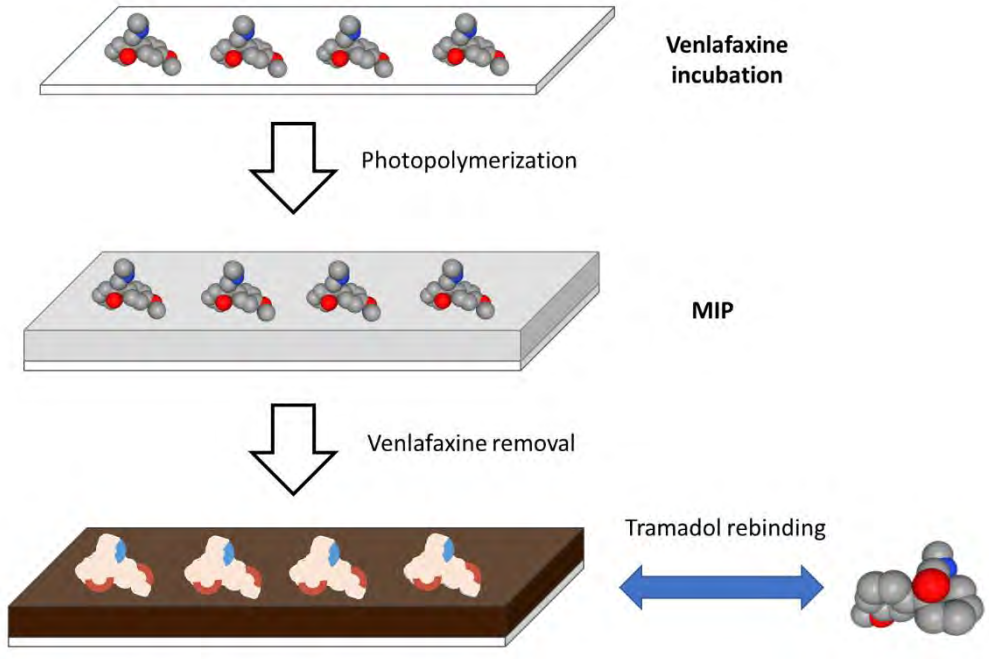

Figure 1. Schematic diagram of the molecularly imprinting process.

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Molecularly Imprinted polymers with bio-based monomers to adsorb carbamazepine from wastewater

Elettra Savigni, Laura Sisti*, Elisa Girometti, Carla Maggetti, Davide Pinelli, Dario Frascari
University of Bologna, Department of Civil, Chemical, Environmental and Materials Engineering, Bologna, Italy
laura.sisti@unibo.it

In aqueous effluents, the presence of pharmaceuticals is becoming increasingly relevant day by day. These molecules are considered contaminants of emerging concern due to their persistence and toxicity also at low concentration. Indeed, current wastewater treatment plants are not able to completely remove them. One of the most commonly found pharmaceutical globally is carbamazepine, a psychiatric drug mainly used as an anti-epileptic. [1] From this perspective, this study proposes new resin materials based on molecularly imprinted polymers (MIPs) to remove carbamazepine from wastewater. Selective polymers that remove carbamazepine are already present in literature, most of them use methacrylic acid as monomer and ethylene glycol dimethacrylate as cross-linker. [2] In this work, six polymers have been prepared using a trifunctional cross-linker, trimethylolpropane triacrylate (TRIM), and six different biobased monomers: methacrylic acid, eugenol, p-coumaric acid, 3-(2-furyl) acrylic acid, fumaric acid and ferulic acid. A trifunctional cross-linker was chosen to produce more stable and rigid materials, with a focus on a future application in adsorption columns. The monomers were chosen to study the interaction of carbamazepine and different functional groups; most of them containing an aromatic ring to promote also the π-stacking interactions.

For preparing the materials a bulk polymerization has been selected to minimize the amount of solvent involved: the reaction conditions used are 70°C for 4h and a ratio of 1:10:50 between template, monomer and cross-linker. After the polymerization the materials are milled and a washing step is conducted to remove carbamazepine: an incubation washing technique is employed using a solution of methanol and acetic acid (9:1, v:v). The polymers obtained were characterized by thermogravimetric analysis to evaluate their stability, while their adsorption capacity was measured using UV-vis and UPLC.

The absorption capacity is evaluated by spiking a real treatment plant effluent with carbamazepine to study the performances of materials considering matrix effects. For each material different concentrations of carbamazepine were tested: 1, 2, 4 and 5 mg/L and adsorption isotherms were plotted (Figure 1). The adsorption performances of MIPs obtained were compared with two industrial resins: activated carbon (NORIT) and Amberlite XAD16N. The results show that all materials are stable up to 280°C and the prepared polymers with eugenol and with p-coumaric acid exhibit at low concentrations better adsorption capabilities compared to commercial materials.

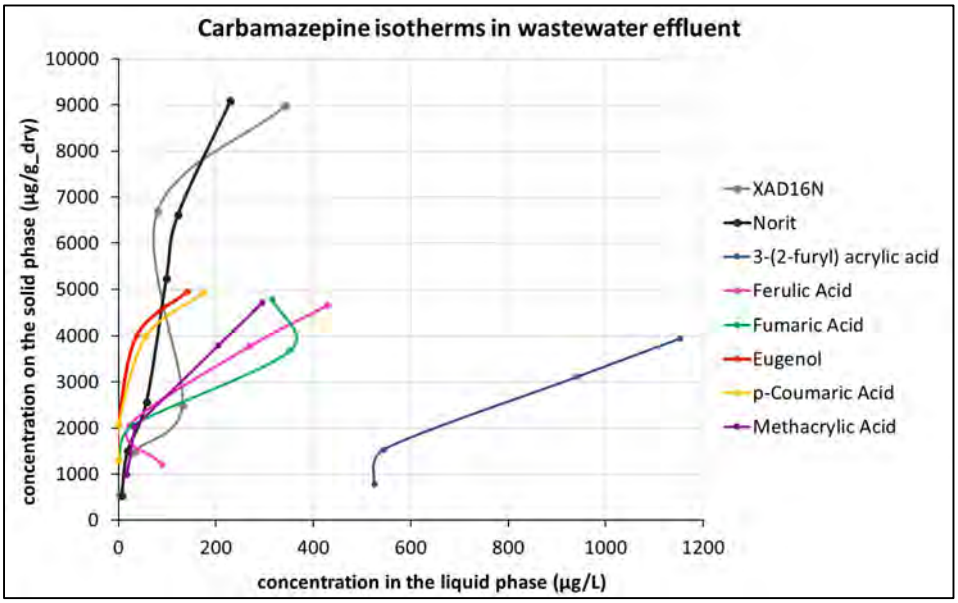

Figure 1: Adsorption isotherms performed in wastewater effluents.

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Development of a MIP-based fluorescent sensor for the detection of foodborne pathogenic bacteria

Rahil Radfar[1], Mattis Neubauer[1], Zeynep Altintas[1*]

[1]*Department of Bioinspired Materials and Biosensor Technologies, Kiel University, Kaiserstraße 2, 24143, Germany*

**za@tf.uni-kiel.de*

Campylobacter jejuni (C. *jejuni*), a pathogenic foodborne bacterium, is the primary cause of human campylobacteriosis, the most prevalent gastroenteritis disease resulting from the consumption of contaminated foods such as undercooked poultry meat, contaminated water, etc [1]. The steady increase in the *Campylobacter* infections in recent years [2] has underlined the need for the development of fast, simple, and reliable diagnostic tools to create an alternative to the conventional methods for both the food industry and clinical applications. Among different recognition elements, molecularly imprinted polymers have attracted much attention in biosensing fields [3]. In this research, fluorescent molecularly imprinted polymer nanoparticles (nanoMIP) were prepared through epitope imprinting approach via solid phase synthesis method using an immunodominant epitope of C. *jejuni*. Carbon dots (CDs) and RhodamineB dye (RhB), as fluorescent tags, were embedded in the nanoMIPs during the synthesis by conjugating the fluorophores with a functional monomer in order to develop a fluorescent sensor with the nanoMIPs as the receptor for the detection of C. *jejuni.* Fluorescent sensors were developed using three different techniques including the intensity, anisotropy, and time-resolved fluorescent spectroscopies. Successful synthesis of nanoMIPs were confirmed by dynamic light scattering, Zeta potential measurements, Fourier-transform infrared spectroscopy, and scanning electron microscopy, while the fluorescent properties of the nanoMIPs were studied by fluorescent spectroscopy. The developed sensors showed a high-detection performance in terms of sensitivity, selectivity, and specificity for measuring C. *jejuni* in a user-friendly and robust manner.

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P38

Combating the AMR Crisis: Utilizing Molecular Imprinting Technology for the Dual Detection of Antibiotics in Environmental and Food Samples.

O. Jamieson[1,2], J. Bell[3], J. Saczek[2], K. Novakovic[2], K. Rurack[3], M. Peeters[1].

1) University of Manchester, School of Engineering, Manchester, M20 4BX
2) Newcastle University, School of Engineering, Merz Court, Claremond Road, NE1 7RU, Newcastle Upon Tyne
3) Chemical and Optical Sensing Division, Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Straße 11, 12489 Berlin, Germany

The antimicrobial crisis is currently a top worldwide concern with the U.N. warning that overuse of antibiotics is on course to cause 10 million fatalities annually by 2050[1]. It has been calculated that a single resistant strain of bacteria can incur a financial cost as high as €1.6 billion[2]. One approach to tackle this problem is to monitor antibiotic contamination in the environment which leads to the selective pressure which cultivates resistant bacteria strains (Figure 1). Tetracyclines (TC) are a family of broad-spectrum antibiotics that are widely used for treatment of bacterial infections in both humans and animals and they are also commonly used as a food additive within the food industry. However, their overuse has led to a significant rise in antimicrobial resistance (AMR)[3] and bioaccumulation, leading to severe health impacts[4]. Due to their persistent nature and development of new TCs containing heavy metal groups, there is now more need than ever to revolutionise the detection of this class of antibiotic[5].

Figure 1- Depiction of antibiotic entry into the water system (red arrows) and how removal attempts are not fully efficient (amber arrow)

The work undertaken saw a dual detection system developed for the sensing of TC in aqueous and food samples. The sensor platform employed both a thermal and fluorescent read out system which act as synergistic validation increasing its practical and commercial aspects.

Molecularly Imprinted Polymers (MIPs) pose as a promising recognition element since they rival the affinity of antibodies but have the added benefits of low-cost, high robustness and versatility. The MIP developed for TC exhibited an additional 34% fluorescent quenching over that of a reference polymer, highlighting that it also possesses the required high level of specificity. It also displayed a 12x greater response against a reference polymer through thermal analysis highlighting its specificity. A second polymer imprinted for another antibiotic, levofloxacin, was also produced and displayed 9-fold specificity for its intended target. Detection of tetracycline in spiked eggs samples was carried out to show increasing response on increasing tetracycline concentrations showing that sensor function is valid even when subjected to complex sample matrices.

The work undertaken has invoked the use of a highly tailored MIP composition and custom designed printed flow cells to allow for application to both analysis techniques as well as the use of a bespoke fluorescent analysis set up. The devised sensor is the first step in a new generation of sensor platform, which will be portable and so applicable for infield testing without the need for expensive infrastructure or skilled personnel to carry out the analysis.

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Sensing Clinically Relevant Proteins through Electrochemical Detection with Electrodes Decorated with Molecularly Imprinted Polymers

Vitali Syritski*, Jekaterina Reut

*vitali.syritski@taltech.ee

Department of Materials and Environmental Technology, Tallinn University of Technology, Estonia

Proteins play essential roles in various biological processes and are often indicative of health conditions or diseases when their levels or activity are altered. By accurately detecting and quantifying proteins, healthcare professionals can diagnose illnesses, monitor disease progression, assess treatment efficacy, and make informed decisions regarding patient care. This emphasizes the significance of developing sensitive, reliable, and efficient protein detection methods, which are vital for advancing medical diagnostics and improving patient outcomes. Electrochemical sensors are especially promising in the realization of point-of-care testing (PoCT) formats, as they are portable, provide rapid response times enabling real-time monitoring, are cost-effective requiring minimal sample volume and reagents, are user-friendly, and can be miniaturized, allowing for integration into wearable devices or lab-on-a-chip systems. Most currently used biosensors and PoCT devices rely on a biological recognition element, such as an enzyme, antibody, or DNA, which is interfaced with the transducer to provide the necessary specificity for targeting analyte. However, one of the major limitations of these recognition elements is their instability in various thermal and pH conditions, leading to limited applicability and shelf-life. In addition, their production is costly, and often involves animals, a matter of concern. The use of Molecularly Imprinted Polymers (MIPs) as robust biomimetic receptors in sensing devices is an attractive approach to overcome limitations associated with biological recognition elements. However, the imprinting of proteins poses challenges due to their intrinsic properties, including large size, structural complexity, and conformational flexibility. Our group has developed a strategy for synthesizing protein-imprinted polymers (protein-MIPs) using the surface imprinting approach. This method enables the formation of binding sites directly on or near the surface of a polymer film generated by electropolymerization on the sensor transducer.

Here, we present the recent achievements of the research group in developing electrochemical sensors with MIP endowed selectivity toward clinically relevant proteins including (i) brain-derived neurotrophic factor (BDNF) as a potential neurodegenerative disorder biomarker [1], (ii) SARS-CoV-2 virus proteins NP and S1 as COVID-19 diagnostic markers [2,3]. The analytical performance of the sensors was evaluated using DPV in the presence of an external or internal redox probe. The results demonstrated the sensors' capability to detect the respective target protein in both buffer solutions and real biological samples with acceptable sensitivity at relevant concentration ranges. In essence, the electrochemical characteristics of the sensor can be easily handled by a portable potentiostat allowing on-site measurements thus holding a great potential as a PoCT platform for rapid clinical diagnostics.

This work was supported by the Estonian Research Council (grants PRG2113, PRG307).

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P40

Molecularly imprinted drug reservoir for targeted glioblastoma cell treatment: *in vitro* and *in vivo* characterization

Alexandra-Iulia Bărăian[1], Bogdan-Cezar Iacob[1*], Olga Soriță[2], Cosmin Pește[3], Alexandru Florian[4], Sergiu Șușman[5,6], Ede Bodoki[1], Ștefan Florian[4]

[1]Department of Analytical Chemistry, Faculty of Pharmacy, "Iuliu Haţieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania;
[2]Laboratory of Tumor Cell Biology and Radiobiology, Institute of Oncology "Prof Dr. Ion Chiricuță", Cluj-Napoca, Romania;
[3]Department of Anesthesiology and Surgical Propaedeutics, University of Agricultural Sciences and veterinary Medicine, Cluj-Napoca, Romania;
[4]Department of Neurosurgery, "Iuliu Haţieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania;
[5]Department of Morphological Sciences, "Iuliu Haţieganu" University of Medicine and Pharmacy, Cluj-Napoca, Romania;
[6]Department of Pathology, IMOGEN Research Centre, Cluj-Napoca, Romania
*e-mail: iacob.cezar@umfcluj.ro

Glioblastoma (GBM) is one of the most complex and aggressive central nervous system tumors, mainly because of its highly invasive properties (1), and is still considered incurable to this day (2). A complete surgical resection is virtually impossible due to the tumor's diffuse nature, so the median survival time is limited to 12-15 months despite any treatment.

Within this study, our objective was to address the existing limitations of chemotherapy in treating GBM by designing a molecularly imprinted drug reservoir. The aim was to achieve sustained release of the antitumor agent ruxolitinib (RUX) within the tumor post-resection cavity, targeting residual infiltrative cancer cells while minimizing toxic effects. Several studies have demonstrated its efficacy on GBM cell cultures, with data suggesting that RUX is an ideal candidate for GBM chemotherapy (3). However, RUX does not cross the blood-brain barrier, so its systemic administration cannot ensure effective brain concentrations (4). In pursuit of this goal, we successfully developed and characterized four distinct molecularly imprinted polymers (MIPs), one of which progressed to the *in vivo* assessment stage.

The synthesis of MIPs involved precipitation polymerization, using acrylamide, trifluoromethacrylic acid (TFMAA), methacrylic acid, and styrene as functional monomers. To assess the cytotoxic efficacy of the polymers, an *in vitro* evaluation was conducted using the Alamar Blue cell viability assay. Additionally, an *in vivo* assessment was performed using an orthotropic model in Wistar rats.

The polymer based on TFMAA (MIP 2) revealed the most favorable risk-benefit profile over the course of 96 hours. MIP 2 exhibited superior efficacy against GBM cells, while its non-imprinted counterpart showed low toxicity. Within the *in vivo* evaluation, animals treated with MIP 2 experienced a significant increase in survival time, extending from 20 to 50 days.

This study focused on the development and characterization of four distinct MIPs to create a drug reservoir for localized administration of RUX in GBM. MIP 2 emerged as the most effective, significantly extending the survival time of animals by 30 days.

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A versatile vapor-phase polymerization approach for molecularly imprinted polymers (MIPs) in optical sensing

T. Di Giulio[1], I. M. Asif[1], C. Malitesta[1], M. Corsi[2], G. Barillaro[2], E. Mazzotta[1]*.

[1] *Dipartimento di Scienze e Tecnologie Biologiche e Ambientali, Università del Salento, Lecce, Italy.*
[2] *Dipartimento di Ingegneria dell'Informazione, Università di Pisa, Pisa, Italy.*

elisabetta.mazzotta@unisalento.it

Molecularly imprinted polymers (MIPs) are artificial materials with unique molecular recognition capabilities, which are the result of their synthesis process [1]. Due to their properties, MIPs have been used for a wide variety of purposes including their function as synthetic receptors in chemical sensors [1]. However, more than 50 years after the introduction of molecular imprinting, MIP-based sensors struggle to find real-world application, probably due to the difficult adaptation of laboratory-developed protocols to industrial scale and/or the lack of versatile synthesis approaches, possibly enabling their integration with whatever transducer surface [1]. In this context, we propose an innovative and adaptable room temperature vapor-phase synthesis approach to merge the selective binding properties of MIPs with the optical features of nanostructured porous silicon ($PSiO_2$) with an aspect ratio exceeding 100, acting as an interferometer [2]. The aim is to obtain a robust, highly sensitive, and selective optical sensor for distinct target analytes, specifically the chemotherapeutic drug doxorubicin (DOXO) and the flavonoid quercetin (QU).

Pursuing the synthetic approach we recently developed for the imprinting of a macromolecule [3], we utilize pyrrole (Py) as a monomer, showcasing the broad applicability of this innovative imprinting scheme. Py serves as a functional monomer due to its vapor-phase transition at room temperature, leading to the formation of adherent polypyrrole (PPy) thin films on the surface of $PSiO_2$ after polymerization (Figure 1).

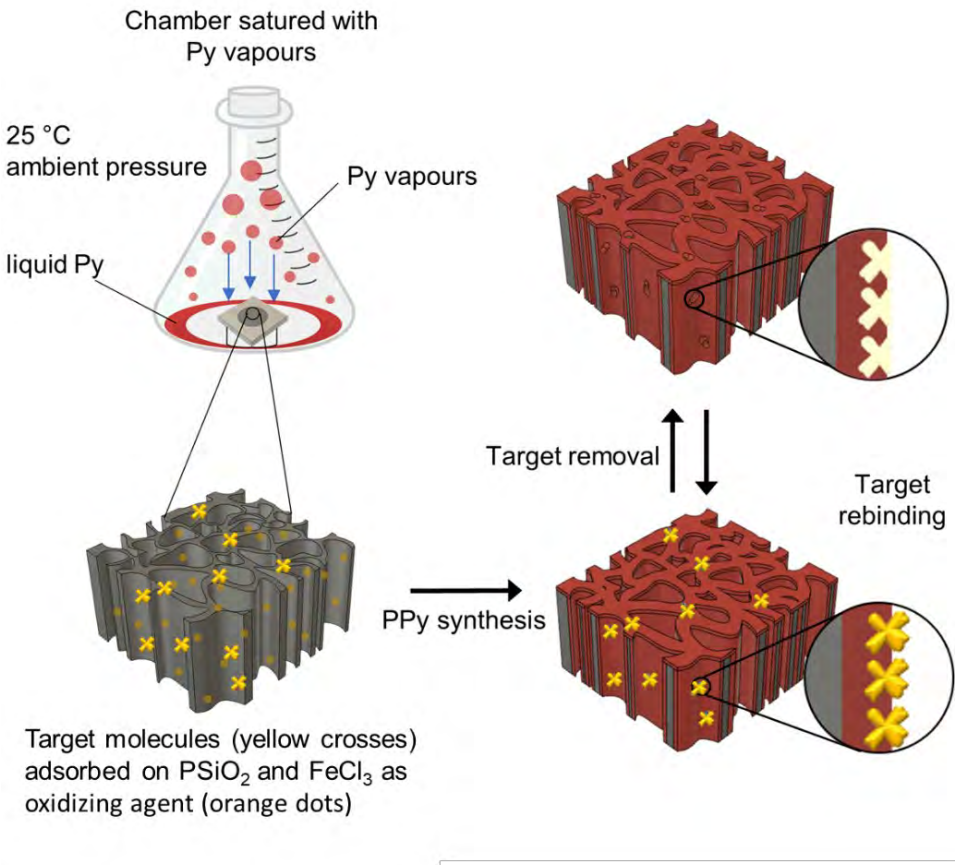

Figure 1: Schematic representation of MIPs deposition on $PSiO_2$ scaffolds by vapor-phase synthesis approach.

Before initiating MIP synthesis, the template molecule is anchored to the transducer surface. This step enhances the imprinting effect [4], creating more uniform imprinted cavities and enabling the use of only monomeric species in subsequent vapor-phase polymerization, eliminating the need to vaporize the template. Specifically, the target DOXO is anchored using a layer-by-layer approach, while QU is anchored using 1,1'-carbonyldiimidazole as a linker. Subsequent removal of the target from the polymer matrix produces imprinted cavities (Figure 1).

Preliminary detection tests conducted through UV-VIS reflectance spectroscopy demonstrate that the sensor can detect QU in aqueous solutions within a dynamic concentration range of 0.5 to 200 μM, with a satisfying reproducibility (RSD% 10.5%, n=3) exhibiting excellent selectivity against caffeic, vanillic, ferulic, gallic acid, luteolin, and rutin. Regarding DOXO, the sensor's response is linear in the concentration range of 0.1 to 10 μg/ml, achieving good reproducibility (RSD% 11.5%, n=6). The sensor also exhibits satisfactory selectivity when tested against other drugs such as paclitaxel, 5-fluorouracil, and cyclophosphamide. Furthermore, DOXO detection tests in artificial serum demonstrate the sensor's capability to operate in complex media.

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P42

Molecularly imprinted polymers in the process of gentamicin monitoring

K. Smolińska-Kempisty

Wroclaw University of Science and Technology, Faculty of Chemistry, wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wroclaw, Poland

**katarzyna.smolinska@pwr.edu.pl*

Nowadays, the problem of micropollutants present in water is raising substantial concern, worldwide. Mainly due to the fact that the pollutants may have adverse impacts on the aquatic ecosystem and human health [1]. One of the problems in removing micropollutants from water is the problem of their identification. Many harmful substances appearing in the waters create the so-called chemical cocktails. The very large variety of these compounds, often similar to each other in terms of molecular weights, makes their separation and identification very difficult, and sometimes even impossible [2].

In the presented project molecularly imprinted polymers (SMIP), capable of selective complexing gentamicin, based on smart polymers, were obtained. After changing the sorption conditions, the antibiotic absorbed by the imprinted materials were washed out by rinsing the sorbents with water at the appropriate temperature. According to green chemistry rules, the presented SMIPs were synthesized using N-isopropylacrylamide in an aqueous medium at ambient temperature.

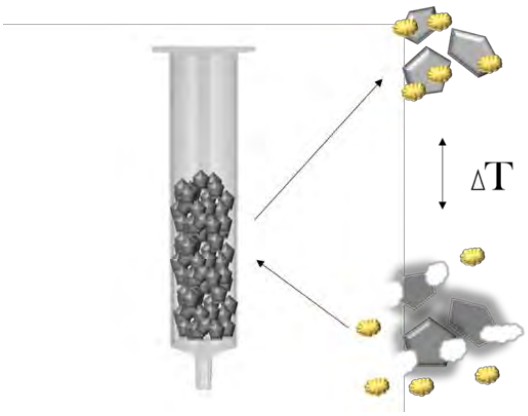

Figure 1. SPE column with SMIP toward gentamicin.

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P43

Integrated molecularly imprinted membranes for the monitoring of bisphenol A in the capacitive deionization process

J. Wolska,* K. Smolińska-Kempisty, A. Siekierka

Wroclaw University of Science and Technology, Faculty of Chemistry, Wyb. Wyspiańskiego 27, 50-370 Wroclaw, Poland

**joanna.wolska@pwr.edu.pl*

Hazardous substances, such as compounds from the group of endocrine disruptors (EDs), can be present in water in trace amounts [1]. Small micropollutants often exceed the detection threshold of commercially available measurement methods. This gives the illusion that the analyzed water sample is not contaminated. Methods used to isolate trace chemicals from a sample, such as SPE or membrane extraction, are frequently used [2,3]. However, they need to work better to thicken the selected compound. Mainly due to their low selectivity and blocking of the bed when filtering larger amounts of the sample [4]. In addition, it is necessary to use organic solvents in the analyte elution step [3,4]. Therefore, in the presented study, it was decided to find a potentially easier way to monitor the presence of one of the representatives of EDs, bisphenol A, which is found in solutions below the detection threshold. MIPs toward bisphenol A (BPA) in the shape of microspheres with an average sphere size of 40 µm were obtained by a two-step process of membrane emulsification and then suspension polymerization. The synthesized microspheres were then integrated into thin solid membranes made of poly(vinyl chloride) (PVC). The imprinted merged membranes were used in the capacitive deionization (MCDI) process to concentrate the amount of BPA in aqueous solutions. The 30-minute process allowed for a bisphenol A concentration of 63.7%. Three sorption/desorption cycles were performed. The total sorption capacity of BPA reached more than 80 mg/g. In all of these cases, a concentration of BPA was achieved of more than 60%.

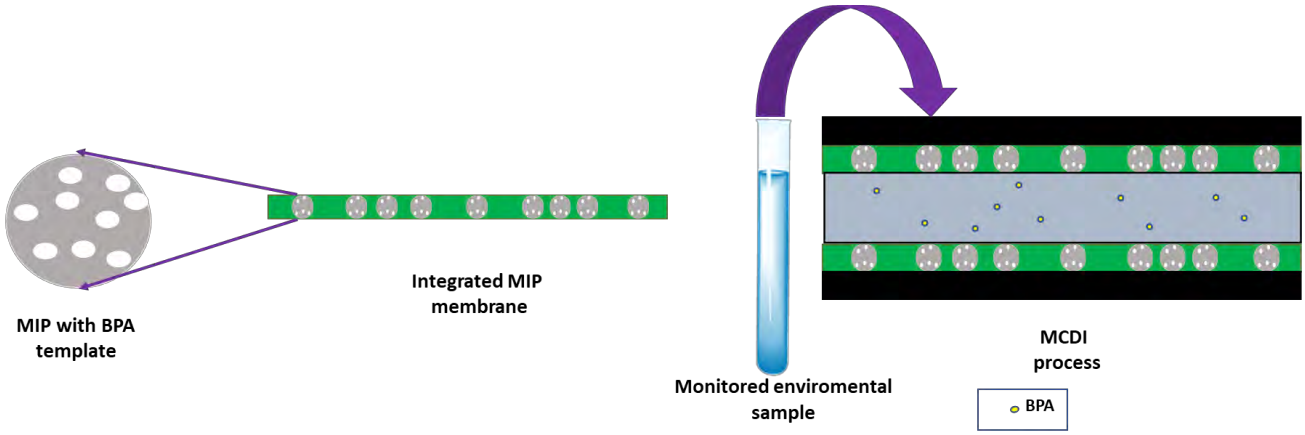

Figure 1. Graphical depiction of BPA monitoring by the integrated MIP membrane in MCDI process.

Acknowledgments

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Tailoring Drug Delivery: Ellagic Acid Imprinted Polymer Nanoparticles-Entrapped Hydrogels for Enhanced Loading and Controlled Release

Necla Yucel Ayten[1*], Gokhan Cayli[2], Pinar Cakir Hatir[3]

[1]*Yildiz Technical University, Institute of Sciences, Department of Bioengineering, Istanbul, Turkey*
[*]*necla.yucel@std.yildiz.edu.tr*
[2]*Istanbul Cerrahpasa University, Faculty of Engineering, Department of Engineering Sciences, Istanbul, Turkey*
[3]*Istinye University, Faculty of Engineering and Natural Sciences, Department of Biomedical Engineering, Istanbul, Turkey*

Oxidative stress is a critical factor in illness progression, with significant impacts from oxidants. Ellagic acid's potent antioxidant properties position it as a promising treatment for diseases by neutralizing free radicals [1]. However, its therapeutic efficacy is hindered by limited solubility and oral bioavailability [2]. Incorporating ellagic acid into hydrogels for controlled release is challenging due to its hydrophobic nature. This study addressed these issues by preparing ellagic acid imprinted polymer nanoparticles (EA-MIPNPs) [3] and integrating them into temperature-responsive cationic hydrogels (Figure 1). The EA-MIPNPs were synthesized using a template-assisted polymerization method. The stimuli-responsive hydrogel designed within the scope of the study was synthesized with a novel monomer that we developed and named Meg-Epi. Hydrogels were formed in the presence of a photoinitiator and a temperature-sensitive monomer, namely 2,2-dimethoxy-2-phenylacetophenone (DMPA) and N-isopropylacrylamide (NIPAM), respectively. Employing various characterization techniques, including FTIR, DSC, SEM, TGA, and biodegradation studies, the study demonstrated the EA-MIP hydrogel's excellent specificity for ellagic acid and its stimuli-responsive behavior. This innovative system holds promise for precision drug delivery, allowing modulation of ellagic acid release based on specific physiological or environmental cues through the integration of molecular imprinting with stimuli-responsive hydrogels.

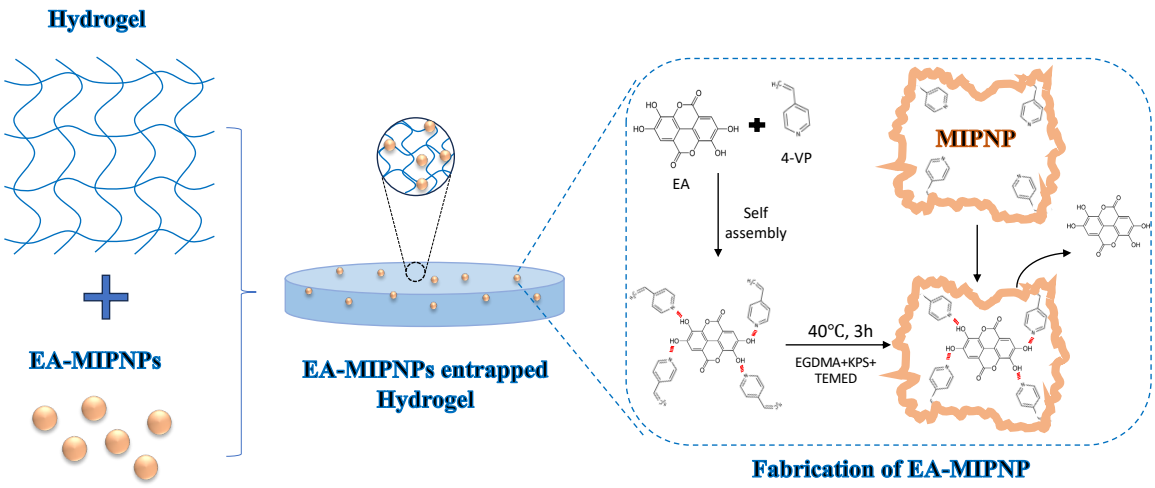

Figure 1. Schematic structure of EA-MIPNPs loaded hydrogel

Keywords: Molecularly imprinted polymer nanoparticles, hydrogel, ellagic acid

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P45

Electrochemosensor based on molecularly imprinted poly o-phenylenediamine membranes for the ultrasensitive detection of cytochrome c

Najmeh Karimian [a,*], Davide Campagnol [a], Flavio Rizzolio [a,b], Paolo Ugo [a]

[a] *Department of Molecular Sciences and Nanosystems, University Ca' Foscari of Venice, via Torino 155, 30172 Venice, Italy*

[b] *Pathology Unit, Centro di Riferimento Oncologico di Aviano (C.R.O.) IRCCS, 33081 Aviano, Italy*

[*] najmeh.karimian@unive.it

Molecularly imprinted polymers (MIPs) have found extensive application as synthetic receptors in the detection of disease biomarkers. Considering the advantages of their excellent chemical and physical stability, low-cost, ease of production, reusability, and high selectivity, MIP-based electrochemical sensors have attracted great interest in disease diagnosis and demonstrated superiority over other biosensing techniques.

Trace detection of Cytochrome c (Cyt c) is important because even small changes in its concentration can indicate abnormalities in apoptosis, providing valuable insights into various pathologies and potential disease states. A highly sensitive electrochemical sensor was developed for the detection of Cyt c based on thin molecularly imprinted poly(o-phenylenediamine) films deposited on a gold electrode by anodic electropolymerization of o-phenylenediamine in the presence of Cyt c as the template [1]. Electrochemical characterization and analytically useful signals were obtained using ferrocenecarboxylic acid (FcCOOH) as redox probe able to compete with Cyt c for the MIP cavities. So that FcCOOH voltammetric signals scale inversely with the Cyt c concentration in the sample. The sensor exhibited a low detection limit and a strong affinity for Cyt c, with a high association constant (Ka) of 5×10^{11} M^{-1}. Satisfactory analytical recovery tests performed in the presence of possible interfering proteins and in diluted human serum confirmed the selectivity of the MIP-sensor as well as its potential applicability for real samples analysis.

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Imaging of Neurotransmitter Secretion in Living Microbrain Probed by Fluorescent Molecularly Imprinted Nanoparticles

Yasuo YOSHIMI*
Dept. Appl. Chem., Shibaura Institute of Technology
3-7-5 Toyosu Koto-ku, Tokyo, 135-8548, Japan
yosimi@sic.shibaura-it.ac.jp

Analysis of the secretion of neurotransmitters in the nervous system is essential for elucidating the mechanism of the neural network in the nervous system. Thus, developing a probe that can track a specified neurotransmitter in real-time with high selectivity has been required. Molecularly imprinted polymer (MIP), a molecular recognition material obtained by polymerization with a template effect of the target molecule, may be applied to the probe. In this study, a nanoparticle of MIP including a fluorescent group (fMIP-NP) was developed as the probe of serotonin [1]. The serotonin, as the template, was immobilized on glass beads by using mixed silane couplers with different chain lengths. The template-immobilized beads were fluidized in a hybrid solution of a fluorescent monomer, a template-affinity monomer, an aminated monomer, a crosslinking monomer, and a photoinitiator of radical polymerization under UV irradiation. The colloidal fMIP-NP was collected from the surface of the beads by washing them with dimethylformamide. The dispersion medium of the colloidal fMIP-NP was replaced with physiological phosphate buffer saline. The addition of serotonin increased the fluorescent intensity and the radius of the fMIP-NP but was insensitive to L-tryptophan. A buccal mass, a cerebral ganglion, and a buccal ganglion were sampled from *Aplysia* sea snails with keeping the nervous connection. The fMIP-NP could covalently adsorb on the cerebral ganglion via poly (glycidyl methacrylate -*co*-methacrylamide). Fluorescent intensity change was not observed during the administration of Nori seaweed extraction, which has the preferred taste, or distilled water which has the unpreferred taste. The taste preference was modified by administration of distilled water immediately after giving the Nori extraction. The spike response in the fluorescence of the stained abdominal ganglion during the administration of Nori extraction after the preference modification. The result indicates that fMIP-NP is a potential probe to detect serotonin secretion concerning *Aplysia*'s learning. The imaging with fMIP-NP will reveal the neurotransmitter networks that control an animal's learning and memory.

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P48

On-Site Detection of Perfluoroalkyl Carboxylic Acids with Dual Fluorescent Molecularly Imprinted Particles Coupled to a Miniaturized Opto-Microfluidics Platform

Kornelia Gawlitza, Víctor Pérez-Padilla, Yijuan Sun, Virginia Valderrey, Jérémy Bell and Knut Rurack

Bundesanstalt für Materialforschung und prüfung (BAM), Richard-Willstätter-Str. 11, 12489 Berlin, Germany

Per- and polyfluoroalkyl substances (PFAS) represent a class of synthetic organofluorine chemicals extensively utilized in the manufacturing of various materials such as firefighting foams, adhesives, and stain- and oil-resistant coatings. In recent years, PFAS have been considered as emerging environmental contaminants, with particular focus on perfluoroalkyl carboxylic acids (PFCAs), the most prevalent type among PFAS. PFCAs are characterized by a fully fluorinated carbon backbone and a charged carboxylic acid headgroup. Notably, they have been designated as Substances of Very High Concern and added to the REACH Candidate List due to their persistence in the environment, non-biodegradability and toxicological effects.[1,2]

Conventional techniques for the analysis of PFCA, such as GC-MS, HRMS and HPLC-based methods, are laborious, not portable, costly and require skilled personnel. In contrast, fluorescence assays can be designed as easy-to-operate, portable and cost-effective methods with high sensitivity and fast response, especially when analyte binding leads to a specific increase of a probe's emission. Integration of such probes with a carrier platform and a miniaturized optofluidic device affords a promising alternative for PFCA monitoring.

Here, a novel guanidine BODIPY fluorescent indicator monomer has been synthesized, characterized, and incorporated into a molecularly imprinted polymer (MIP) for the specific detection of perfluorooctanoic acid (PFOA). The MIP layer was formed on tris(bipyridine)ruthenium(II) chloride doped silica core particles for optical internal reference and calibration-free assays. Such system allows selective and reliable detection of PFCA from surface water samples, with minimum interference by competitors, matrix effects and other factors. Integration of the assay into an opto-microfluidic setup resulted in a miniaturized and easy-to-operate detection system allowing for micromolar detection of PFOA in less than 15 minutes from surface water sample.

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Multi-functional nanocavity for specific sensing of small extracellular vesicles prepared by template polymerization using a polymerizable functional polymer

Hirobumi SUNAYAMA[1]*, Eri TAKANO[2], Toshifumi TAKEUCHI[3,4]*
[1] *Graduate School of Medicine, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
[2] *Graduate School of Engineering, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
[3] *Center for Advanced Medical Engineering Research & Development (CAMED), Kobe University, 1-5-1, Minatojima-minamimachi, chuo-ku, Kobe 650-0047 JAPAN*
[4] *Advanced Photonics and Biosensing Open Innovation Laboratory, AIST-Osaka Unverisity, 2-1 Yamadaoka, Suita, Osaka, 565-0871, JAPAN*

*Email: sunayama@penguin.kobe-u.ac.jp, takeuchi@gold.kobe-u.ac.jp

Extracellular vesicles (EVs) a nanovesicles of 30-150 nm with lipid bilayer and secreted from cells and present in body fluids such as blood, saliva, urine, and tear fluid. Its interior contains proteins, metabolites, and nucleic acids (mRNA, miRNA, DNA) derived from secretory cells, which play an important role in intercellular communication. EVs are also secreted by cancer cells and are associated with cancer metastasis, invasion, and growth. This is why EVs have attracted considerable attention in cancer-related research in recent years [1]. Therefore, various technologies for EVs detection have been reported. However, these systems are besed on conventional ELISA, thus tedious multi-step procedure or specific instruments are neccessary and sensing performances of these systems are insufficient for highly sensitive detection of EVs for early diagnosis.

Previously we have developped a facile and highly-sensitive EVs detection nano-cavity prepared by dynamic molding chemical nano-processing approach which insipred by molecular imprinting and post-imprinting modification [2]. His-tag and *N*-(2-((2-aminoethyl)disulfaneyl) ethyl)methacrylamide modified silica nanoparticle was used as a dynamic mold, and immobilized on the substrate via the interaction between His-tag and Ni-nitorilotriacetic acid (NTA). Polymer layer was fabricated by surface initiated atom transfer radical polymerization (ATRP) using 2-methacryloyloxyethyl phosphorylchline (MPC). After TCEP treatment for reduction of disulfide bond, silica nanoparticle was removed, resulting in polymer nano-cavity incorporating SH group and NTA group. In chemical nano-processing, thiol-reactive group such as maleimide derived fluorescnt dye was reacted with SH group and antibody toward antigens expressed on EVs was introduced into the cavity via His-tagged protein G, yielding EVs sensing nano-cavity. It is expected that one-step EVs detction was achieved.

In this study, multi-functional nanocavity for EVs sensing was prepared by dynamic molding approach using a polymerizable functional polymer. Polymerizable functional polymer was designed and synthesized, where amine group for interaction with template silica nanoparticles, a disulfide bond for post-polymerization modofication and a methacryl group which conneted via disulfide bond were consisted.

Silica nanoparticles were complexed with a functional polymer via electrostatic interaction and then, immobilized on the Au-coated glass substrate which Br group and carboxy group were introduced by self-assembled monolayer formation using thiol compounds. Then the polymer layer formation and in-cavity functionalization for EVs sensing were carried out by the similar manner described above. EVs sensing property of prepared functional nanocavity was investigated and the results will be disucussed in this presentation.

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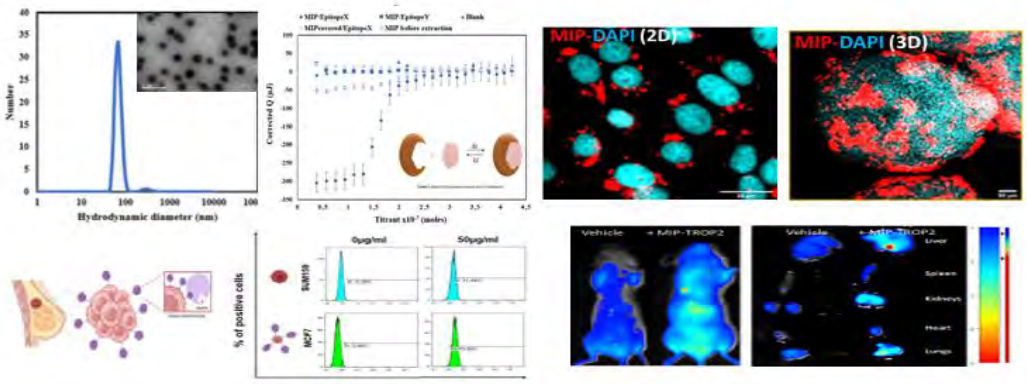
P50

TROP2-molecular imprinting polymers nanoparticles for breast cancer targeting therapy

Lila Louadj[1,2], Perla Benghouzi[1], Michèle Sabbah[2], Nébéwia Griffete[1]
[1] PHENIX, Sorbonne Université, CNRS UMR 8234 Paris, France
[2] CRSA, Sorbonne Université, UMR INSERM 938 France
Contact : lila.louadj@hotmail.fr

Despite undeniable progress in the prevention, screening and treatment of breast cancer, this disease remains a major health problem with alarming incidence and mortality rates worldwide. While the majority of these cancers are curable at an early stage with locoregional treatments such as surgery and/or chemotherapy-radiotherapy, the main therapeutic weapons in situations at risk of recurrence (resistance to treatment) or in metastatic situations are targeted therapies. In this context, the recent emergence of the glycoprotein Trop-2 (Trophoblast Cell Surface Antigen 2) as a promising therapeutic target has led to new therapeutic paradigms for treating patients with advanced or metastatic breast cancer (1). Recently, antibody-drug conjugates (ADC) have been developed and launched to the market for this purpose (2, 3). However, the production of ADCs is highly complex, time consuming and costly. Thus, an alternative must be developed to provide a new approach to breast cancer treatment. Indeed, this is what we are focusing on in our project. Using a completely new approach in the field of nanomedicine (4), we have developed fluorescent synthetic nanoparticles with a TROP2 imprint (MIPs-TROP2), encapsulating active molecules (chemotherapies, targeted therapies) used in breast cancer treatment. The goal of the study is to use these MIPs-TROP2 nanoparticles to specifically target breast tumors overexpressing TROP2 protein and deliver the encapsulated therapeutic molecule precisely to the tumor site. To achieve this, first in vitro analyses using flow cytometry, NanoITC, confocal microscopy and cell viability were performed to validate the fluorescent nanoparticles imprinting and then to assess their toxicity and biocompatibility. We used four breast cancer cell models overexpressing the protein of interest (MCF7, T47D, MDAMB231 and SUM149) and one cell model not expressing the protein as a control (SUM159). The results showed specific targeting of TROP2-positive cell lines compared to the SUM159 control, confirming the affinity and accessibility of the imprint to its target. In addition, no decrease in viability was observed, confirming the cellular biocompatibility of the nanoparticles. Second, in vivo studies were performed in a mouse model. The accumulation and biodistribution of the nanoparticles in the different organs of the animal were evaluated by imaging. Preliminary results show that MIPs-TROP2 accumulate mainly in the liver. They also accumulate slightly in the kidneys and lungs of mice.Taken together, our results confirm that the use of molecularly imprinted polymers as an alternative to ADC against cell membrane receptors represents a promising and innovative new line of nanomedicine.



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Fluorescent signaling molecularly imprinted polymer nanogels for assembly of a biotic/ abiotic sensing platform

Hirobumi SUNAYAMA[1]*, Cheubong CHEHASAN[2], Eri TAKANO[2], Toshifumi TAKEUCHI[3,4]*
[1] *Graduate School of Medicine, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
[2] *Graduate School of Engineering, Kobe University, 1-1, Rokkodai-cho, Nada-ku, Kobe 657-8501 JAPAN*
[3] *Center for Advanced Medical Engineering Research & Development (CAMED), Kobe University, 1-5-1, Minatojima-minamimachi, Chuo-ku, Kobe 650-0047 JAPAN*
[4] *Advanced Photonics and Biosensing Open Innovation Laboratory, AIST-Osaka Unverisity, 2-1 Yamadaoka, Suita, Osaka, 565-0871, JAPAN*

*Email: sunayama@penguin.kobe-u.ac.jp, takeuchi@gold.kobe-u.ac.jp

Enzyme-linked immunosorbent assay (ELISA) is a powerful tool for detecting the target molecules. Conventionaly, two or more antibodies are necessary for specific detection of target molecules, where capture antibody for capturing the target molecule on the substrate, primary antibody for binding the epitope on the target and secondary antibody which conjugated with enzymes or fluorescent dyes for readout the binding events. These multiple steps are trend to time-consuming and expensive.
In this study, secondary antibody mimic, fluorescent signaling molecularly imprinted polymer nanogels (MIP-NGs) capable of Fc domain recognition, were prepared via post-imprinting modifications (PIMs). PIMs are promissing strategy for cavity-specific functionalization of moleculaly imprinted cavities, where a functional monomer bearing modifiable parts have been used for preparing molecularly imprinted polymers (MIPs) and cahemical modification on the functional groups derived from a modifiable functional monomer was undergone for introduction of an additional functionality [1].
For preparetion of fluorscent signaling MIP-NGs, a modifiable functional monomer, 4-(2-methacrylamidoethylaminomethyl) phenylboronic acid (MAPBA) [2] was used. MAPBA. NIPAm, MPC, MBAA and Fc domain was dissolved in phosphate buffer saline, and emulcifier-free precipitation polymerization was carried out at 50 ˚C for 12 h after the addition of initiator [3]. After purification step by throught the size-exclusion chromatography and ion-exchnage chromatography, 20 nm-sized MIP-NGs was obtained. In PIMs, fluorescent dye, ATTO647N-NHS ester was reacted with MAPBA residues on the MIP-NGs, yielding fluorescent signaling MIP-NGs. The fluorescent signaling properties were investigated using a custam-made liduid handling robot equiepped with fluorescent microscope. The fluorescent intensities were changed with increasing Fc-domain concentration, indicating that Fc-domain imprinted cavity was created in the MIP-NGs and fluorescent dye, ATTO647N was successfully introduced into the imprinted cavity [4]. Then, a biotic/abiotic sandwich detection system was assembled using natural antibody and prepared fluorescent signalling MIP-NGs. Detailed characteristics of the prepared MIP-NGs and proposed sandwich detection system will be discussed in theis presentation.

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Epitope imprinted polymers for sensing bacterial proteins

Akriti Srivastava[1], Richa Raghuwanshi[2], Rajniti Prasad[3], Gopal Nath[4] , Abhay Kumar Singh[5] and Meenakshi Singh[1,*]

[1]Department of Chemistry, MMV, [2] Department of Botany, MMV

[3] Department of Paediatrics, IMS, [4] Department of Microbiology, IMS,

[4] Department of Physics, ISc,

Banaras Hindu University, Varanasi, 221005, India

meenakshi@bhu.ac.in

Epitope imprinting has made protein sensing feasible and accessible in a facile manner. Proteins have elegant 3D specifically contoured built up maintained by covalent and non-covalent binding forces, which could be easily compromised while working on them, leading to denaturation. The selective and specific imprint created on imprinted surface induces the binding of whole protein through their specific epitope(s). Self assembled monolayers (SAM) of cysteine appended epitope sequences on gold surface are subjected to polymerization prior to polymerization. The polymeric matrix is woven around the cysteine appended epitope SAMs through multiple monomers and crosslinker. On extraction of the peptide sequences, imprinted cavities are able to selectively and specifically bind targeted epitope sequences in laboratory samples as well as 'real' samples of patients. Selectivity of sensor is examined through mismatched peptide sequences, proteins and certain plasma proteins also. The sensor was able to show specific binding towards the biological samples of infected patients, even in the presence of 'matrix' and other plasma proteins. Even other peptide sequences, similar to epitope sequences only with one or two amino acid mismatches were unable to show any binding. The analytical performance of sensor was tested through selectivity, specificity, matrix effect, detection limit, quantification limit, reproducibility. Hence a diagnostic tool for bacterium causing disease is fabricated in a facile manner which will broaden the clinical access and efficient population screening can be made feasible.

Keywords: Molecularly imprinted polymer; Epitope imprinting; protein imprinting; bacterial protein.

Rational Design of MIPs for Precise Discrimination of Viral and Bacterial Infections

Soumya Rajpal[a,b]*, Boris Mizaikoff [b,c], Prashant Mishra [a]

[a] Department of Biochemical Engineering and Biotechnology
Indian Institute of Technology Delhi
Hauz Khas, New Delhi 110016, India

[b] Institute of Analytical and Bioanalytical Chemistry
Ulm University
Albert-Einstein-Allee 11, 89081 Ulm, Germany

[c] Hahn-Schickard
Sedanstraße 14, 89077 Ulm, Germany

**soumya.rajpal@uni-ulm.de*

Accurate diagnosis is paramount for effective patient care and the containment of antimicrobial resistance outbreaks. Distinguishing between bacterial and viral infections remains challenging, given limited advanced diagnostic tools and overlapping symptoms. This study employs molecular imprinting techniques to develop chemically stable, cost-effective antibody analogs for precise viral-bacterial differentiation. Our approach centers on interferon-induced proteins as distinctive markers for viral infections. Utilizing epitope imprinting, we target specific biomarker regions critical for interaction. Computational calculations guide the design of MIPs by assessing monomer-epitope interactions. Introducing a novel multi-monomer simultaneous docking (MMSD) protocol efficiently maps cooperative effects, offering a theoretical alternative to labor-intensive experimental polymer optimization. Simulations unveil binding mechanics and intermediates, highlighting unique interactions that enhance MIP-peptide complementarity. *In silico*-guided MIP optimization produces high-performance receptors selectively binding to the target epitope over non-specific proteins. A proof-of-concept study demonstrates protein binding to synthetic receptors. Similar to antibodies, MIPs show promise for accurately detecting viral infections, addressing current diagnostic limitations.

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Molecularly imprinted polymers fighting antimicrobial resistance

Sara Spada,[1] Tiffany Auroy,[1] Karsten Haupt[1,2]

[1]*Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*

[2]*Institut Universitaire de France*

Antimicrobial resistance is considered by the World Health Organization (WHO) as one of the major health challenges of our time. Gram-negative bacteria, especially the ESKAPE pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter* species) head the list of pathogens having the highest resistance indices of all bacteria threatening human health [1]. One of the main mechanisms that leads these bacteria to acquire resistance is the efflux pump system. Indeed, efflux pumps confer resistance to multiple classes of antibiotics by their ability of expelling antibiotic molecules outside the bacteria cells [2]. The aim of this work was to synthesise Molecularly Imprinted Polymer (MIP) nanogels able to target and bind an *E. coli* efflux pump and potentially affects its activity. MIPs were synthesized using a solid-phase approach with peptide epitopes of the target protein as the template [3]. They were characterized the specific binding of their target protein by fluorescence binding assays and QCM, and for their affinity for the whole bacteria cell through flow cytometry and confocal microscopy. Inhibition of the efflux pump was the demonstrated in a dedicated bioassay.

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Molecularly imprinted polymer nanogels for the detection of acute kidney injury biomarker KIM-1

Kyra Magdato,[1] Alejandra Mier,[1] Noel Angelo Kalacas,[1] Bernadette Tse Sum Bui,[1] Karsten Haupt[1,2]

[1]*Université de Technologie de Compiègne, CNRS Enzyme and Cell Engineering Laboratory, Compiègne, France.*

[2]*Institut Universitaire de France*

Acute kidney injury (AKI) is a severe condition that affects one out of 10 hospitalized patients and 50 percent of the patients entering intensive care units. Early detection of AKI is important to allow for personalized treatment of AKI avoiding evolution into chronic kidney disease, which is an important public health problem due to the requirement of hemodialysis and kidney transplant. In the present work, we aim to develop molecularly imprinted polymers (MIPs) [1] as synthetic antibodies that specifically recognize the early AKI biomarker Kidney Injury Molecule 1 (KIM-1). MIPs are cross-linked polymers synthesized in the presence of a molecular template, which induces three-dimensional binding sites in the polymer that are complementary to the template in size, shape and chemical functionality. MIPs against KIM-1 were obtained through a rational approach starting with *in silico* epitope design. Chemically synthesized peptide epitopes were then used as templates in a solid-phase protocol for MIP synthesis [2]. Fluorescence binding assays and solution NMR (STD and WaterLOGSY) demonstrated that the MIP recognizes and binds its target with an affinity and selectivity like a biological antibody [3]. Implementing a fluorescent detection scheme, we demonstrate that these synthetic antibodies have great potential for diagnostics of AKI.

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Molecularly Imprinted Polymers combined with Peptide Nucleic Acids as a Novel Hybrid Receptor for miRNA 21

Muhammed Abdel-Hamied,[1 2*] Boris Mizaikoff,[1 3*] Christine Kranz,[1*]

[1] *Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert Einstein Allee, 11, 89081, Ulm, Germany*
[2] *Chemistry Department, Faculty of Science, Cairo University, Giza, 12613, Egypt*
[3] *Hahn-Schickard, Sedanstrasse 14, 89077 Ulm, Germany*
muhammad.abdelhamied-abdeltawab@uni-ulm.de, boris.mizaikoff@uni-ulm.de, christine.kranz@uni-ulm.de

The recent advances in high-throughput profiling and cancer biomarker sensing has the potential of invaluable insights for early diagnosis and a more profound understanding of cancer etiology [1]. Among these biomarkers, microRNAs (miRNA), i.e., small non-coding RNA molecules ranging from 18 to 26 nucleotides stand out due to their pivotal role as post-transcriptional gene regulators. This underlines the importance for the development of ultrasensitive and highly specific sensing methods dedicated to detecting and quantifying miRNAs [2].

Challenges toward that goal include the small size of miRNA sequences, their low natural abundance, and the presence of various miRNAs with a high degree of sequence similarity, which pose formidable obstacles for their selective determination [3]. In response to these challenges, the use of molecularly imprinted polymers (MIPs) combined with electrochemical biosensing strategies is a potential approach. MIPs offer several advantages including stability of the molecular recognition motif and design flexibility [4]. However, achieving high specificity remains a persistent challenge, especially for measurements in complex matrices owing to non-specific binding to MIP matrices [5].

In this contribution, we discuss the feasibility of MIP-based electrochemical biosensors employing electropolymerization to customize the molecularly imprinted layer at the electrode surface tailored for the selective detection and quantification of miRNAs. In order to specifically mitigate non-specific binding, we propose the hybridization of peptide nucleic acids (PNA) to MIPs. The incorporation of PNA serves as a dual purpose, i.e., as a supportive recognition motif and to establish a specific miRNA orientation prior to the imprinting process minimizing the formation of non-specific binding sites. The characterization of these sensors and first proof-of-principle measurements will be presented.

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