MacroYouth 2023

ICMPP – OPEN DOOR TO THE FUTURE SCIENTIFIC COMMUNICATIONS OF YOUNG RESEARCHERS

4th Edition

November 17, 2023 • Iasi • Romania

Marking the Romanian Researcher’s Day

ICMPP – Petru Poni Institute of Macromolecular Chemistry
Iasi | Romania | November 17, 2023
https://icmpp.ro/macroyouth2023/ index.php

Edited by
Marcela MIHAI
Marius-Mihai ZAHARIA
Sandu CIBOTARU

Cover by
Diana SCHWAB

Welcome to the ICMPP-OPEN DOOR TO THE FUTURE
Scientific Communications of Young Researchers with international participation,
MacroYouth 2023

It is a great pleasure to welcome you in Iasi, on 17.11.2023, on the occasion of the 4th Edition ICMPP-OPEN DOOR TO THE FUTURE Scientific Communications of Young Researchers with international participation, MacroYouth 2023. The scientific communications event with international participation is organized by the Petru Poni Institute of Macromolecular Chemistry - ICMPP, to mark the Romanian Researcher's Day, and offers the opportunity for the doctoral students to present the results of their studies. The scientific program gives a broad overview of the topics in organic and macromolecular chemistry and physics, and more.

Best wishes for a professionally rewarding conference!

Dr. Valeria HARABAGIU and Acad. Bogdan C. SIMIONESCU
Chairpersons of MacroYouth 2023

CHAIRPERSONS of MacroYouth 2023

Dr. Valeria HARABAGIU and Acad. Bogdan C. SIMIONESCU

ROMANIAN SCIENTIFIC BOARD

- Acad. Maria ZAHARESCU
  (Romanian Academy)
- Acad. Marius ANDRUH
  (Romanian Academy, ICOS Bucharest)
- Dr. Maria CAZACU
  (ICMPP Iasi)
- Dr. Liliana CSEH
  (ICHT Timisoara)
- Dr. Sergiu COSERI
  (ICMPP Iasi)
- Dr. Mariana Dana DAMACEANU
  (ICMPP Iasi)
- Dr. Gheorghe FUNDUEANU
  (ICMPP Iasi)
- Dr. Gabriela IONITA
  (ICF Bucharest)
- Dr. Luminita MARIN
  (ICMPP Iasi)
- Dr. Mariana PINTEALA
  (ICMPP Iasi)

ORGANIZING BOARD

Chair

- Dr. Marcela MIHAI

Program

- Dr. Petrisor SAMOILA
- Dr. Florin BUCATARIU
- Dr. Corneliu COJOCARU

Editorial

- Dr. Marius-Mihai ZAHARIA
- Dr. Sandu CIBOTARU
- Catalin BUZDUGAN – IT support

Executive

- Dr. Andra-Cristina ENACHE
- Dr. Daniela PAMFIL
- Dr. Bogdan-Constantin CONDURACHE
- Dr. Dumitru POPOVICI

Petru Poni Institute of Macromolecular Chemistry, Conference Hall		
	Friday 17.11.2023	
	https://us06web.zoom.us/j/88419502009?pwd=i0BXEV5KMcx4ScZeHQCmPlOnPAHPDH.1	
S1	9:00-9:15	Opening
	9:15-9:30	OC1 - Andreica Bianca Iustina
	9:30-9:45	OC2 - Lupu Alexandra
	9:45-10:00	OC3 - Platon Ioana Victoria
	10:00-10:15	OC4 - Cobzariu (Nacu) Isabella
	10:15-10:30	OC5 - Baltag Laurentiu
	10:30-10:45	OC6 - Bogza Cosmina-Maria
	10:45-11:00	OC7 - Trofin Ioana-Alexandra
	11:00-11:30	Coffe break
S2	11:30-11:45	OC8 - Apostol Irina
	11:45-12:00	OC9 - Neculae Alexandru-Vincentiu-Florian
	12:00-12:15	OC10 - Medrihan Maria
	12:15-12:30	OC11 - Jitaru Stefania-Claudia
	12:30-12:45	OC12 - Gavril Andra-Ionela
	12:45-13:00	OC13 - Grecu Ionela
	13:00-13:15	OC14 - Dimitriu Stefan
	13:15-14:30	Lunch break - ICMPP Library
S3	14:30-14:45	OC15 - Vrabie Rafaela-Paula
	14:45-15:00	OC16 - Visan Alexandru
	15:00-15:15	OC17 - Popa Evelyn
	15:15-15:30	OC18 - Lotos Elena-Daniela
	15:30-15:45	OC19 - Petrila Larisa-Maria
	15:45-16:00	OC20 - Bardan Marius-Vasile
	16:00-16:30	Coffe break
S4	16:30-17:15	Invited - Prof. Alice MIJA
	17:15-18:00	Invited - Prof. David HADDLETON
	18:00-18:30	Analysis, Awarding and Closing Ceremony
	18:30-::::	Dinner - ICMPP Library

Awards for Best Young Scientist Oral Presentation

- **Prize I – 500 lei**
- **Prize II – 400 lei**
- **Prize III – 300 lei**
- **Prize "Sorin I. Rosca" of Romanian Chemical Society**

The scientific communications event with international participation is organized by Petru Poni Institute of Macromolecular Chemistry - ICMPP, to mark the Romanian Researcher's Day and offers the opportunity for the doctoral students to present the results of their studies.

The scientific program includes oral presentations (15 minutes, Q & A included) and the conference language will be English.

Location:
Conference hall of ICMPP.
A small number of online presentations will be accepted.

INVITED LECTURES

Prof. David HADDLETON has been working in the area of controlled polymer synthesis for over 25 years since being employed at ICI. His PhD “Photochemistry of some organometallic ethene compounds” was under the supervision of Robin Perutz at the University of York in 1986. He spent one year at the University of Toronto as a PDRA. He joined ICI in 1988 and spent one year at the University of Southern Mississippi working with polymer liquid crystals. Moving back to the UK in 1988 he spent 5 years working on GTP and anionic polymerisation prior to moving to Warwick in 1993 and was promoted to full Professor in 1998. He has published over 500 papers and has a Google H-index >85 with over 25000 citations. He has graduated over 75 PhD students from Warwick. Current work in the group is in different aspects of developing new polymerisation methodology and using this for novel polymers for industrial applications, polymers for personal care applications, (hair and skin care) and for biomedical and nano medicinal applications (new and targeted peptide and protein conjugation). Recent work includes new conjugation strategy, glycopolymers, monomer sequence control and polymerisation in biological media. He has formed two companies; currently CSO of a transdermal drug delivery company Medherant Ltd.

Prof. Alice MIJA is a scientist with 25+ years of expertise in polymer chemistry & physico-chemistry research. She did her PhD in “Polymers & material science” at the Ecole Nationale Supérieure de Mines de Paris, Sophia-Antipolis (France). From 1992-2004 she was Researcher at Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania. Since 2004 she is Prof. at University of Nice. Her research interests lie in the design, synthesis and characterization of monomers, polymers; synthesis of materials from bioresources & wastes valorization; hybrid materials and composites; self-assembly and self-organization phenomenon in macromolecular and supramolecular polymeric systems; thermodynamics in complex reactions of anisotropic polymeric systems; phase transitions; structure/property/performance relationship


MacroYouth 2023

PROGRAM

Petru Poni Institute of Macromolecular Chemistry, Conference Hall

https://us06web.zoom.us/j/88419502009?pwd=i0BXEV5KMcx4ScZeHQCmPlOnPAHPDH.1

08^{30} – 09^{00}	**Registration of Participants**	
09^{00}– 09^{15}	**CONFERENCE OPENING** Dr. Valeria HARABAGIU and Acad. Bogdan C. SIMIONESCU **Welcome to MacroYouth 2023**	
	09^{15} – 11^{00} **Session 1** **Chairs:** Dr. Daniela AILINCAI and Dr. Bogdan CRACIUN	
09^{15}– 09^{30}	**OC1. Imino-chitosan/quaternized chitosan nanofibers designed as active food packaging** Bianca-Iustina Andreica, Irina Rosca, Luminita Marin	Page 13
09^{30}– 09^{45}	**OC2. Thermosensitive Pluronic® F127 hydrogels with self-healing ability and induced antimicrobial properties** Alexandra Lupu, Irina Roşca, Vasile-Robert Grădinaru, Maria Bercea	Page 15
09^{45}– 10^{00}	**OC3. Innovative polysaccharide-based sponges with instantaneous shape recovery and multistrain antibacterial activity for controlled release of curcumin** Ioana-Victoria Platon, Claudiu-Augustin Ghiorghita, Maria Marinela Lazar, Irina Elena Răschip, Maria Valentina Dinu	Page 17
10^{00}– 10^{15}	**OC4. Biocompatible scaffolds based on functionalized polymers for soft tissue engineering** Isabella Cobzariu (Nacu), Loredana Elena Niţă, Liliana Vereştiuc	Page 19
10^{15}– 10^{30}	**OC5. Novel proton-exchange membranes based on sulfonated poly(ether ether ketone) with potential application in fuel cells** Laurenţiu Baltag, Petrisor Samoila, Corneliu Cojocaru, Valeria Harabagiu	Page 21
10^{30}– 10^{45}	**OC6. Superabsorbent lignin-based hydrogels with potential application in ecological agriculture** Cosmina-Maria Bogza, Maria-Cristina Popescu, Carmen-Mihaela Popescu	Page 23
10^{45}– 11^{00}	**OC7. Macromolecular engineering of thiophene-containing hyperbranched architectures exhibiting electrochromic properties** Ioana-Alexandra Trofin, Radu-Dan Rusu, Catalin-Paul Constantin, Mariana-Dana Damaceanu	Page 25
11^{00}– 11^{30}	**Cofee break**	

11^{30} – 13^{15}

Session 2

Chairs: Dr. Irina POPESCU and Dr. George RUSU

11^{30}– 11^{45}	**OC8. Polysaccharide-integrated lignin esters as efficient oil adsorption materials** Irina Apostol, Narcis Anghel, Iuliana Spiridon	Page 27
11^{45}– 12^{00}	**OC9. New molecular spin probes for the study of non-covalent interactions** Alexandru Vincentiu Florian Neculae, Jean Patrick Joly, George-Alin Balan, Iulia Matei, Sylvain R. A. Marque, Gabriela Ionita	Page 29
12^{00}– 12^{15}	**OC10. Nanostructured polymer materials obtained from pickering emulsion polymerization technology** Maria Medrihan, Andrei Honciuc, Valeria Harabagiu, Oana-Iuliana Negru, Ana-Maria Solonaru, Mirela Honciuc	Page 31
12^{15}– 12^{30}	**OC11. A diphenylalanine based pentapeptide with fibrillating self-assembling properties** Stefania-Claudia Jitaru, Andrei Neamtu, Gabi Drochioiu, Laura Darie-Ion, Iuliana Stoica, Brindusa-Alina Petre, Vasile-Robert Gradinaru	Page 33
12^{30}– 12^{45}	**OC12. Versatile thin films derived from triphenylamine based-oligomers: electrosynthesis, characterization and applications** Andra Ionela Gavril, Loredana Vacareanu	Page 35
12^{45}– 13^{00}	**OC13. Manganese ferrite based materials for catalytic applications** Ionela Grecu, Petrisor Samoila, Corneliu Cojocaru, Petronela Pascariu, Valeria Harabagiu	Page 37
13^{00}– 13^{15}	**OC14. Functionalization of 5-Bromosalicylaldehyde as Mannich, Schiff-base, and nitronyl-nitroxide ligands and their complexes** Ştefan Dimitriu, Sergiu Shova, Marius Andruh	Page 39
13^{15}– 14^{30}	**Lunch break**	

14^{30} – 16^{00}

Session 3

Chairs: Dr. Oana URSACHE and Catalin-Paul CONSTANTIN

14^{30}– 14^{45}	**OC15. Synthesis and structure of new pyrrol 2(5H)-one hybrids with trifluoromethyl moiety** Rafaela Vrabie, Cristina Al-Matarneh, Mariana Pinteala	Page 41
14^{45}– 15^{00}	**OC16. Role of gallic acid containing ferrocene in enhancing electrochemical detection of capecitabine using carbon-based electrode** Alexandru Vişan, Sorina Motoc, Adelina A. Andelescu, Elisabeta I. Szerb, Florica Manea	Page 43

15^{00}– 15^{15}	**OC17. Induction of liquid crystalline properties in Pt(II) coordination complexes based on terpyridine ligands**	Page 45
	Evelyn Popa, Adelina A. Andelescu, Elisabeta I. Szerb	
15^{15}– 15^{30}	**OC18. Interaction between water-soluble chitosan and thermo-responsive poly(n-isopropylacrylamide)**	Page 47
	Elena-Daniela Lotos, Maria Karayianni, Ana-Lavinia Vasiliu, Larisa-Maria Petrila, Marcela Mihai, Stergios Pispas, Bogdan C. Simionescu	
15^{30}– 15^{45}	**OC19. Catalase/polymer composite microparticles for environmental applications**	Page 49
	Larisa-Maria Petrila, Florin Bucătariu, Marcela Mihai	
15^{45}– 16^{60}	**OC20. Bioactive molecules of saffron oil extracted from biomass, tested on danio rerio as anti-tumoral and anti-inflammatory agents**	Page 51
	Marius –Vasile Bârdan	
13^{15}– 14^{30}	**Coffe break**	
	16^{30} – 18^{30} **Session 4**	
16^{30}– 17^{15}	**INVITED LECTURE** **Sustainable design of materials for space application – 100% biobased thermosets**	
	Prof. Alice MIJA Côte d'Azur University, Nice, France	
17^{15}– 18^{00}	**INVITED LECTURE** **Polymerisation in flow – use of DOSY benchtop NMR for inline measurement of molecular weight and conversion**	
	Prof. David HADDLETON University of Warwick, Coventry, United Kingdom	
18^{00}– 18^{30}	**ANALYSIS, AWARDING AND CLOSING CEREMONY**	
18^{30}– ::::	**Gala dinner – Petru Poni Institute of Macromolecular Chemistry library**	
	Romanian Chemical Society – SChR	Page 54
	Infra Suprachem Lab - Center for Advanced Research in Supramolecular Chemistry	Page 56
	Marcela Mihai, Narcisa-Laura Marangoci	
	BioMat4CAST – Multi-Scale In Silico Laboratory for Complex and Smart Biomaterials	Page 59
	Teodora Rusu, Mariana Pinteala, Aatto Laaksonen, Tudor Vasiliu	
	AMS 2000 TRADING IMPEX SRL	Page 62
	Decorias SRL	Page 65

BOOK OF ABSTRACTS

IMINO-CHITOSAN/QUATERNIZED CHITOSAN NANOFIBERS DESIGNED AS ACTIVE FOOD PACKAGING

Bianca-Iustina Andreica*, Irina Rosca, Luminita Marin
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**andreica.bianca@icmpp.ro*

Chitosan and its quaternized derivative are two well-known biopolymers that have been exhaustively studied for various applications of contemporary interest [1]. While both biopolymers have been shown to have excellent properties, such as biodegradability, low toxicity, and antioxidant activity, quaternized chitosan has been found to possess superior properties in comparison to the pristine chitosan [2]. This makes it particularly useful in the design of active packaging materials that can help to extend the shelf life of food products, a topic not very exploited yet.

In this context, the goal of this study was the development of fiber mats containing *chitosan*, *quaternized chitosan (HTCC)*, *vanillin (V)* and *poly(ethylene oxide) (PEO)* in different ratios. The selection of each component was deliberate, aiming to achieve nanofibers that meet all the necessary criteria for materials used in food packaging [3]. The role of each component in the design of the nanofibers is depicted in Figure 1.

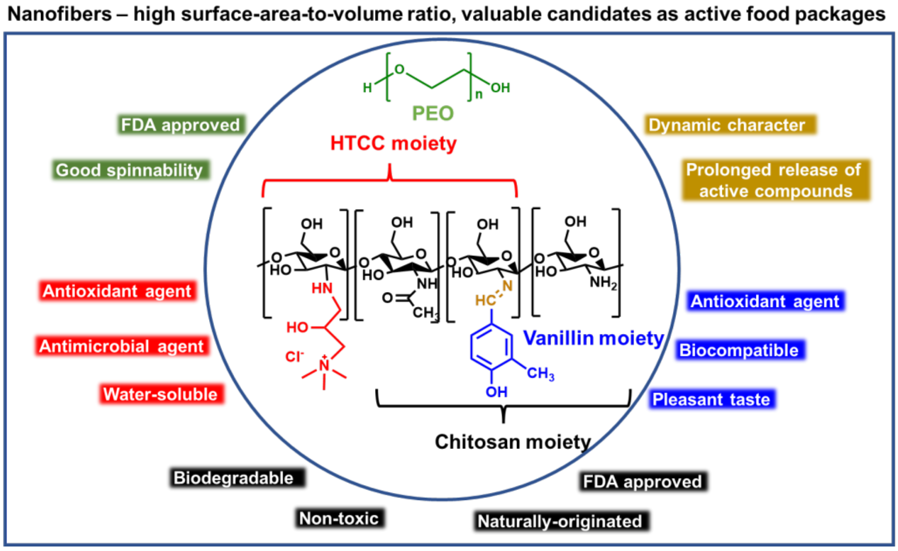


Figure 1. Rational design of the nanofibers' composition.

The structural characterization of the nanofibers by FTIR and NMR spectroscopy showed the formation of imine bonds between the amine groups of chitosan/quaternized chitosan and the formyl group of vanillin, while thermogravimetric analysis revealed a strong and stable network of H-bonds between the components, resulting in good thermal stability, suitable for food packaging applications. SEM microscopy revealed entangled continuous nanofibers, with no defects or beads, and a mean diameter of around 140 nm. The mechanical properties of the nanofibers were found to be comparable or even higher than those of other materials designed for the same application, due to the presence of quaternized chitosan, which improved the fiber mats' strength.

The evaluation of the antioxidant activity in solution and in solid state revealed high scavenging activity of the fibers, which is important for preserving food freshness for a longer time. The study also evaluated the ability of the fibers to release vanillin in food simulants media, demonstrating that the aldehyde's release is controlled by its removal from the media, and the fibers are able to rapidly absorb water while maintaining their integrity. Tested on *E. coli*, *S. aureus* and *C. albicans*, the fibers with a high content of quaternized chitosan and moderate quantity of vanillin were able to destroy up to 90% of the microbial cells. A preservation experiment assessed on raspberries as model fruits revealed that the fibers were able to extend the freshness of the fruits up to 7 days, better than the commercial packaging. The analysis of the fruits at the end of the experiment revealed that their physico-chemical and microbiological profile was improved when they were covered with the nanofibers, in comparison with blank fruits or the use of a commercial package. Moreover, the fibers completely degraded in soil in 7 weeks, complying therefore with the current trend of designing biodegradable materials.

Figure 2. Graphical representation of the nanofibers' properties, recommending them as active food packaging.

In conclusion, the rational design of choosing the above-mentioned specific components for the development of composite fiber mats met the initial expectations (Figure 2). The nanofibers showed excellent properties for food packaging applications, such as strong antioxidant and antimicrobial properties, and effectively preserved the quality of the fruits, with the added benefit of being biodegradable.

References

[1] M. Florez, E. Guerra-Rodriguez, P. Cazon, M. Vasquez, *Food Hydrocoll.* 2022, 124, 107328.
[2] B. I. Andreica, A. Anisiei, I. Rosca, A. I. Sandu, A. S. Pasca, L. Mititelu-Tartau, L. Marin, *Carbohydr. Polym.*, 2023, 302.
[3] B. I. Andreica, A. Anisiei, I. Rosca, L. Marin, *Food Packag. Shelf Life* 2023, 39, 101157.

Acknowledgment: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE2020-2717, within PNCDI III, no. PCE 2/2021 and from the project H2020-MSCA-RISE-2019, SWORD-DLV-873123.

THERMOSENSITIVE PLURONIC® F127 HYDROGELS WITH SELF-HEALING ABILITY AND INDUCED ANTIMICROBIAL PROPERTIES

Alexandra Lupu[1]*, Irina Roșca[1], Vasile-Robert Grădinaru[2], Maria Bercea[1]
[1]*Petru Poni Insitute of Macromolecular Chemistry, Iasi, Romania*
[2]*Faculty of Chemistry, "Alexandru Ioan Cuza" University, Iasi, Romania*
**lupu.alexandra@icmpp.ro*

Pluronic® F127 (PL) is a versatile amphiphilic triblock copolymer, composed of a central hydrophobic poly(propylene oxide) (PPO) block flanked by two hydrophilic poly(ethylene oxide) blocks, able to spontaneously form micelles and thermoreversible networks at increasing temperature and concentration. In sol state, PL hydrogels are easily loaded with drugs or active compounds and injected at the targeted site, acting as an efficient drug delivery system in physiological environment [1-3]. The major drawback of PL hydrogels is the lack of biological properties.

The viscoelastic properties of Pluronic F127 systems were investigated in presence of various polysaccharides: chitosan (CS), sodium alginate (Alg), gellan gum (GG), κ-carrageenan (κ-Carr) and xanthan gum (XG) [4,5]. The gelling kinetics was monitored either as a function of temperature (heating rate of 1 °C/min), or at 37 °C as a function of time. The sol–gel transition and the viscoelastic properties (G' - the elastic modulus'; G"- the viscous modulus; tan δ - the loss tangent) of different gel formulations can be controlled by the PL and polysaccharide concentration. The gelling time is an important parameter for injectable materials. Systems with the gelling time of the order of tents of minutes are preferred, so that the sol-gel transition does not take place during handling or transport to the target site.

Furthermore, we explored the possibility to induce antimicrobial properties to PL hydrogels. An antimicrobial activity was observed only in presence of chitosan [4]. Curcumin, considered an antimicrobial agent in alcoholic solution or as nanoparticles [6,7], was added to PL in sol state. A slower dynamic of the sol-gel transition was registered due to the hydrophobic interactions of curcumin with the micellar core (Figure 1).

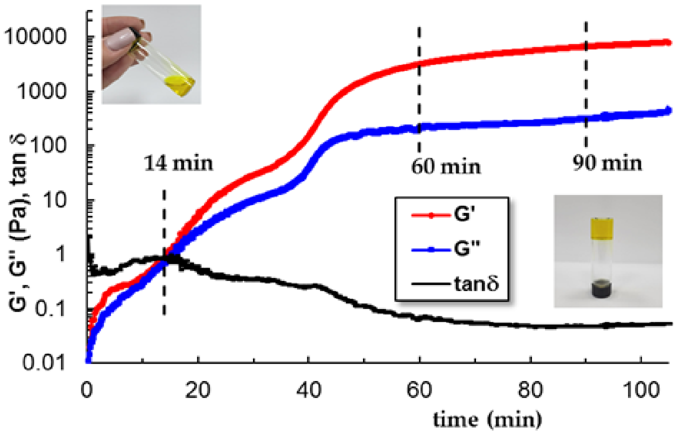


Figure 1. The viscoelastic parameters as a function of time for PL / CS / Curcumin sample [4].

One of the most important properties required for injectable hydrogels is their self-healing ability, which implies that these materials have the capacity to self-repair and autonomously recover their original structure after damage. The self-healing behavior of Pluronic F127-based gels was investigated and the effect of polysaccharide addition was evaluated (Figure 2).

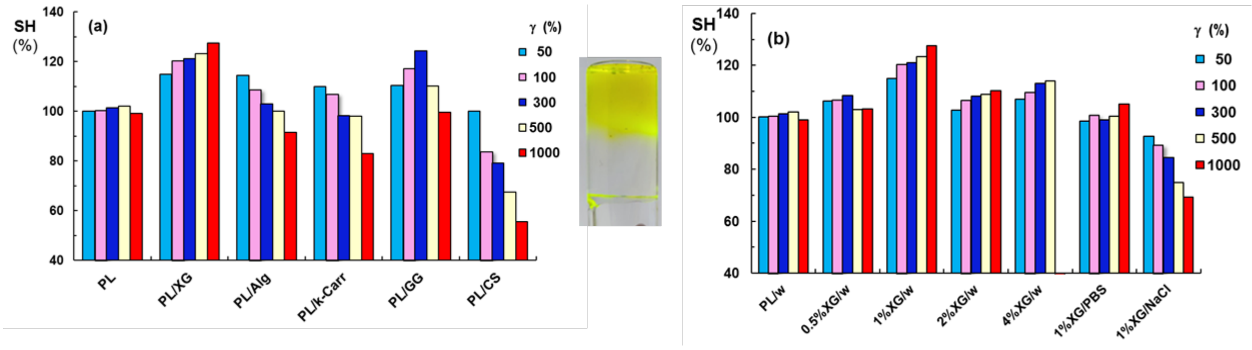


Figure 2. The influence of polysaccharide addition on the self-healing efficiency (SH) for: (a) PL and PL/polysaccharides in water and (b) PL/XG hydrogels obtained by adding various XG concentrations in water (w) or 1% XG in salted solutions (0.1M NaCl or PBS). Three step cycles were applied: γ = 1% for the steps 1 and 3 and various strain (γ) values during the step 2 [5].

The antimicrobial activity of PL/Chitosan hydrogel was considerably improved in presence of curcumin (Figure 3) [4].

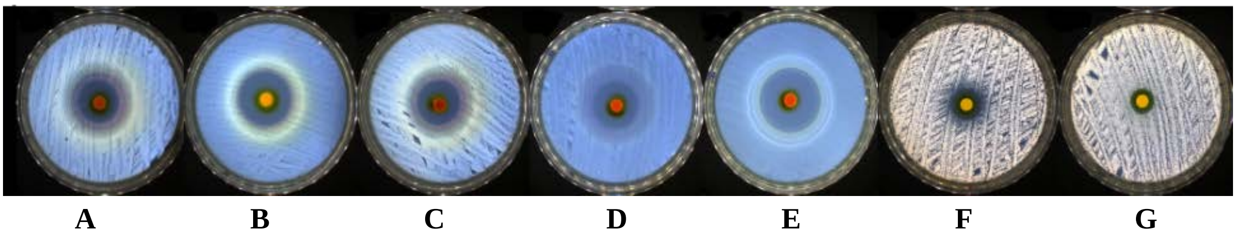


Figure 3. The antimicrobial activity of PL / CS / Curcumin gel against (A) *S. aureus*; (B) *E. coli*; (C) *E. faecalis*; (D) *P. aeruginosa*; (E) *K. pneumoniae*; (F) *C. albicans*; (G) *C. glabrata* [4].

The PL/XG hydrogels presented a porous structure with pores of 5 - 10 μm [5], shear thinning behavior, yield stress, self-healing ability and antimicrobial activity in presence of antimicrobial agents, important characteristics for injectable materials or bioinks.

References

[1] M.T Cidade, D.J. Ramos, J. Santos, H. Carrelo, N. Calero, J.P. Borges, *Materials* 2019, 12, 1083.
[2] L. Hong-Ru, C. Pei-Csang, *J. Biomed. Mater. Res. Part B Appl. Biomater*. 2013, 101B, 677-892.
[3] J. Yu, H. Qiu, S. Yin, H. Wang, Y. Li, *Molecules* 2021, 26, 3610.
[4] A. Lupu, I. Rosca, V.R. Gradinaru, M. Bercea, *Polymers* 2023, 15, 355.
[5] A. Lupu, L.M. Gradinaru, D. Rusu, M. Bercea, *Gels* 2023, 9, 719.
[6] J.K. Trigo-Gutierrez, Y. Vega-Chacón, A.B. Soares, E.G. Mima, *Int. J. Mol. Sci.* 2021, 22, 7130.
[7] Bhawana, R.K. Basniwal, H.S. Buttar, V. K. Jain, N. Jain, *J. Agric. Food Chem.* 2011, 59, 2056–2061.

Acknowledgment: The authors thank Daniela Rusu (Physics of Polymers and Polymeric Materials Laboratory, Petru Poni Institute of Macromolecular Chemistry, Iasi) for performing SEM micrographs of hydrogels.

INNOVATIVE POLYSACCHARIDE-BASED SPONGES WITH INSTANTANEOUS SHAPE RECOVERY AND MULTISTRAIN ANTIBACTERIAL ACTIVITY FOR CONTROLLED RELEASE OF CURCUMIN

Ioana-Victoria Platon*, **Claudiu-Augustin Ghiorghita, Maria Marinela Lazar,**
Irina Elena Răschip, Maria Valentina Dinu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
* *platon.ioana@icmpp.ro*

Hydrogels are tridimensional polymeric networks, physically or chemically cross-linked, that are characterized by high fluid absorption capacity [1]. In terms of water content, mechanical and viscoelastic properties, hydrogels exhibit a high degree of similarity with biological tissues, being increasingly studied for applications in medicine and pharmacy. Porous hydrogels are particularly in focus as drug encapsulation and controlled delivery systems [2,3]. Among the various techniques to obtain permanent macropores in hydrogels, cryogelation is one of the most accessible and versatile methods developed [4]. Cryogels (CG) are characterized by elasticity, ability to withstand high degrees of deformation, shape memory, rapid swelling in water, as well as high mechanical strength [5]. Polysaccharide-based cryogels are preferred for biomedical uses due to their higher resistance to the environmental conditions (pH, enzymes, and temperature), biocompatibility and biodegradability. Chitosan (CS), a cationic polymer comprised of *N*-acetyl-D-glucosamine and D-glucosamine units has drawn the attention of many scientists due to its key-features such as hemocompatibility, mucoadhesivity, antiinflammatory, antibacterial, antioxidant, and hemostatic activities [6].

In this regard, this study aimed to prepare CS hydrogels by glutaraldehyde (GA) cross-linking as novel platforms for the encapsulation of curcumin (CCM). GA is a well-known cross-linker that reacts with the amino groups of CS, forming imine bonds (Figure 1).

Figure 1. Preparation procedure of CS sponges by cryogelation and by room-temperature gelation.

Optimization of hydrogels properties was achieved by varying the CS concentration, cross-linking ratio, and gelation conditions (cryogelation *versus* room-temperature gelation). The structural, morphological, and mechanical properties of hydrogels were assessed by Fourier-transform infrared spectroscopy, scanning electron microscopy, and uniaxial compression measurements, respectively. Swelling ratio and water contact angle were also determined. In terms of *in vitro* biological properties, antimicrobial and antioxidant activities were evaluated. Furthermore, CCM *in vitro* release kinetic was studied in simulated gastrointestinal fluids.

It was found that CS concentration and cross-linking degree greatly influenced the gel-forming ability and the aspect of the gels (Figure 1). When it comes to internal morphology, all hydrogels or cryogels showed honeycomb morphology, but the porosity was strongly dependent on the composition and gelation conditions. In the uniaxial compression stress-strain measurements, the cryogels proved excellent mechanical properties and water-triggered shape recovery. They also exhibited significant antibacterial properties against both Gram-positive (*Staphylococcus aureus, Listeria monocytogenes*) and Gram-negative (*Escherichia coli, Salmonella typhimurium*) strains.

The investigation of CCM release properties indicated that its release was dependent on the gel composition and preparation strategy. The results were fitted using three different mathematical models: Higuchi, Korsmeyer–Peppas and first-order kinetic. The CCM release kinetics was best fitted by the Korsmeyer–Peppas model. Considering the values of the diffusional exponent calculated from the Korsmeyer–Peppas equation, a pseudo-Fickian diffusion-controlled mechanism was identified for the release of CCM. Moreover, the high antioxidant activity values for CCM extracted from the CS cryogels confirmed their ability to protect and preserve bioactive compounds.

References

[1] N. Micale, C. Andrea, M.S. Molonia, A. Speciale, F. Cimino, A. Saija, M. Cristani, *Molecules* 2020. 25(14), 3254.
[2] E.S. Dragan, M.V. Dinu, C.-A. Ghiorghita, *Gels* 2022, 8(4), 240.
[3] M.V. Dinu, M.M. Lazăr, C.-A. Ghiorghiță, I.E. Răschip; in Dodda J.M., Deshmukh K., Bezuidenhout D. (Eds); Multicomponent Hydrogels: Smart Materials for Biomedical Applications, Ed. Royal Society of Chemistry, 2023, p381-424.
[4] V.I. Lozinsky; in: Okay O. (Ed.), Advances in Polymer Science, Ed. Springer International Publishing, New York, 2014, pp. 1–48.
[5] A. Memic, T. Colombani, L.J. Eggermont, M. Rezaeeyazdi, J. Steingold, Z.J. Rogers, K.J. Navare, H.S. Mohammed, S.A. Bencherif, *Adv. Therap*. 2019, 2, 1800114.
[6] I.V. Platon, C.-A. Ghiorghiță, M.M. Lazăr, I.E. Răschip, M.V. Dinu, *Int. J. Mol. Sci.* 2023, 24 (5), 4452.

Acknowledgment: This work was supported by a grant from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI–UEFISCDI, project number PN–III–P1-1.1-TE-2021-1683 (TE6/2022).

BIOCOMPATIBLE SCAFFOLDS BASED ON FUNCTIONALIZED POLYMERS FOR SOFT TISSUE ENGINEERING

Isabella Nacu[1,2]*, **Loredana Elena Niţă**[1], **Liliana Vereştiuc**[2]
[1] *Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania*
[2] *Faculty of Medical Bioengineering, "Grigore T. Popa" University of Medicine and Pharmacy, Iasi, Romania*
**cobzariu.isabella@icmpp.ro*

Introduction. Wound healing is a complex and constantly evolving biological process that stimulates the immune response to repair damaged tissue. Wound dressings are designed to facilitate wound healing, promote tissue development, and facilitate the tissue regeneration without scars [1]. In the last decade, the regenerative medicine was focused on development of stimulative materials, including 3D printed matrices, in order to enhance the healing of skin wounds [2]. The 3D printing technique is using polymeric biomaterials, particularly natural polymers with high biocompatibility (gelatin, alginate, fibrin, and chitosan) or a combination of natural and synthetic polymers [3] and crosslinking processes to establish a durable and viable structure, according to the intended 3D shape. In this regard, GelMa (gelatin with methacryloyl side groups) has undergone extensive testing and characterisation due to its ability to be covalently cross-linked under UV light and to provide good cell stability and viability at low concentrations, but it has low mechanical resistance. Other modified biopolymers can be added to improve the mechanical properties of the functionalised gelatin. Therefore, the paper presents the obtaining of 3D printed scaffolds using combinations of gelatin methacrylate (GelMa), alginate methacrylate (AlgMa) and xanthan methacrylate (XGMa) and evaluate their potential as matrices for biomedical applications.

Methodology. The biopolymers (gelatin, alginate, xanthan gum) were modified using the approach outlined by Camci-Unal [4], with minor modifications of the procedure. To prepare inks, GelMa, AlgMa and XgMa were combined in varying ratios, along with a specified quantity of LAP photoinitiator, according to the Table 1. The mixtures were then homogenized, printed using a Inkredible Cellink bioprinter, and afterwards subjected to freeze-drying for further characterisation (54 °C; 0.07 mBar).

Table 1. 3D Printed Composition.

Nr.Crt	Biopolymers	Polymer Ratio	Swelling degree (%)	
			PBS	DMEM
1.	*GelMa*	*100*	*solubilization*	*solubilization*
2.	*GelMa-AlgMa$_1$*	*50:50*	*995 ± 1.30*	*1105 ± 1.24*
3.	*GelMa-AlgMa$_2$*	*25:75*	*322 ± 1.14*	*948 ± 0.61*
4.	*GelMa-XGMa$_1$*	*50:50*	*5517 ± 1.38*	*5227 ± 0.44*
5.	*GelMa-XGMa$_2$*	*25:75*	*5281 ± 0.91*	*4806 ± 0.66*

The scaffolds were characterised for their structural modifications using FT-IR analysis. Then, the scaffolds underwent to other several characterization methods to assess their morphology (stereoscopic and SEM microscopy), swelling behavior under two types of simulated physiological solutions (HBSS and DMEM), bioadhesion, *in vitro* degradability, and *in vitro* cytocompatibility.

Results and Conclusion. High swellable 3D printed hydrogels have been prepared using methacrylated biopolymers. FT-IR spectroscopy data indicate that methacrylic groups were grafted onto the biopolymeric chains (gelatin, sodium alginate and xanthan gum), and are responsible of the polymers crosslinking under UV light. SEM microscopy demonstrated the formation of 3D structures with controlled porosity suitable for growth and proliferation of cells. Alginate methacrylate (AlgMa) and xanthan methacrylate (XGMa) interacted with methacrylated gelatin to significantly enhance pore diameter and regulate the hydrogel scaffolds susceptibility to enzymatic attack under simulated physiological solutions and temperature. On each material, cytocompatibility and morphological analysis were performed and values of cells viability were over 90%. The morphological test was carried out to support the compatibility data and no changes in cells morphology were observed. The 3D printed scaffolds are non-cytotoxic and are capable to support the further development of cells, being suitable for soft tissue engineering.

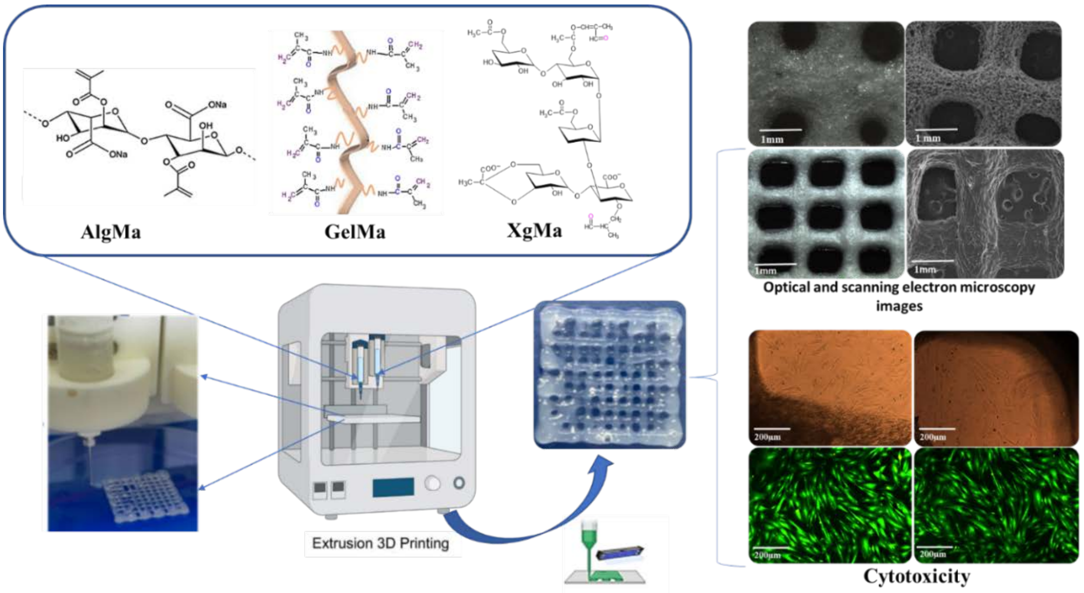


Figure 1. The printing process of the supports, their morphological structure and citotoxicity results.

References

[1] R.Z. Murray, Z.E. West, A.J. Cowin, B.L. Farrugia, *Burns & Trauma* 2019, 7, s41038-018-0139–7.
[2] K. Yu, X. Zhang, Y. Sun, Q. Gao, J. Fu, X. Cai, Y. He, *Bioact. Mater.* 2022, 11, 254–267.
[3] E.H.-P. De León, A.U. Valle-Pérez, Z.N. Khan, C.A.E. Hauser, *Curr. Opin. Biomed.* 2023, 26, 100450.
[4] G. Camci-Unal, D. Cuttica, N. Annabi, D. Demarchi, A. Khademhosseini, *Biomacromolecules* 2013, 14, 1085–1092.

Acknowledgements: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2021-3003, within PNCDI III.

NOVEL PROTON-EXCHANGE MEMBRANES BASED ON SULFONATED POLY(ETHER ETHER KETONE) WITH POTENTIAL APPLICATION IN FUEL CELLS

Laurențiu Baltag*, Petrisor Samoila, Corneliu Cojocaru, Valeria Harabagiu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**baltag.laurentiu@icmpp.ro*

Fossil fuels (coal, oil, and gas) are the primary source in global energy systems but also a big contributor to one of the main issues we are facing right now: global warming. The temperature on earth has started to grow since the pre-industrial period without showing any signs of stopping. One of the main ways to redress global warming is by reducing greenhouse gas emissions. To achieve the proposed goal, the entire global energy system will have to go through fundamental changes [1]. One sector that started to change is the transportation sector, either by replacing the internal combustion engine or fuel source.

Polymer electrolyte membrane fuel cells (PEMFC), also known as proton-exchange membrane fuel cells, along with electric cars, are the chosen alternative for replacing the internal combustion engine [2]. PEMFCs are made up of an electrolyte, a proton-exchange membrane (PEM), and electrodes, which are composed of a catalyst layer, a gas diffusion layer and a plate responsible for gas distribution and flow. The polymeric membrane and catalyst layer are the most important components with the highest contribution to fuel cell efficiency. For good performance, PEM has to balance serval properties, being a challenge to develop membranes. In this aspect, considerable research efforts were made to replace the commercially available PEM (perfluorosulfonic acid, such as Nafion) with materials that have similar or better properties. Sulfonated poly(ether ether ketone) (SPEEK) is one of the most promising materials with an attractive potential to replace Nafion and for commercialization. Introducing sulfonic acid group into the poly (ether ether ketone) backbone provides a significant proton conducting mechanism for SPEEK [3]. Furthermore, SPEEK membranes have been shown to have great chemical and thermal stability, as well as outstanding mechanical and electrical properties.

In this work, we have obtained sulfonated poly(ether ether ketone) using a simple method, involving an ultrasonic bath [4]. Obtaining high degrees of sulfonation are essential for applications such as proton exchange membranes. Thus, the degree of sulfonation (DS) of the modified polymer was determined from the ^{1}H NMR spectra (given in Figure 1), obtaining a DS = 64%. The such obtained SPEEK was further employed in the preparation of the composite membranes, along with inorganic fillers, such as TiO_2 and spinel ferrites. The inorganic compounds were used to induce high added-value to the final materials, by developing membranes with promising characteristics to be used as PEMs. Three spinel ferrites were prepared by using sol-gel auto-combustion method $ZnFe_{1.96}Pr_{0.04}O_4$, $NiFe_{1.96}Pr_{0.04}O_4$ and $Zn_{0.5}Ni_{0.5}Fe_{1.96}\text{-}Pr_{0.04}O_4$ [5]. Their magnetic properties and particle sizes are given in Table 1. In addition, the structural and morphological properties of synthesized spinel ferrites were analyzed by FTIR, XRD, VSM and TEM.

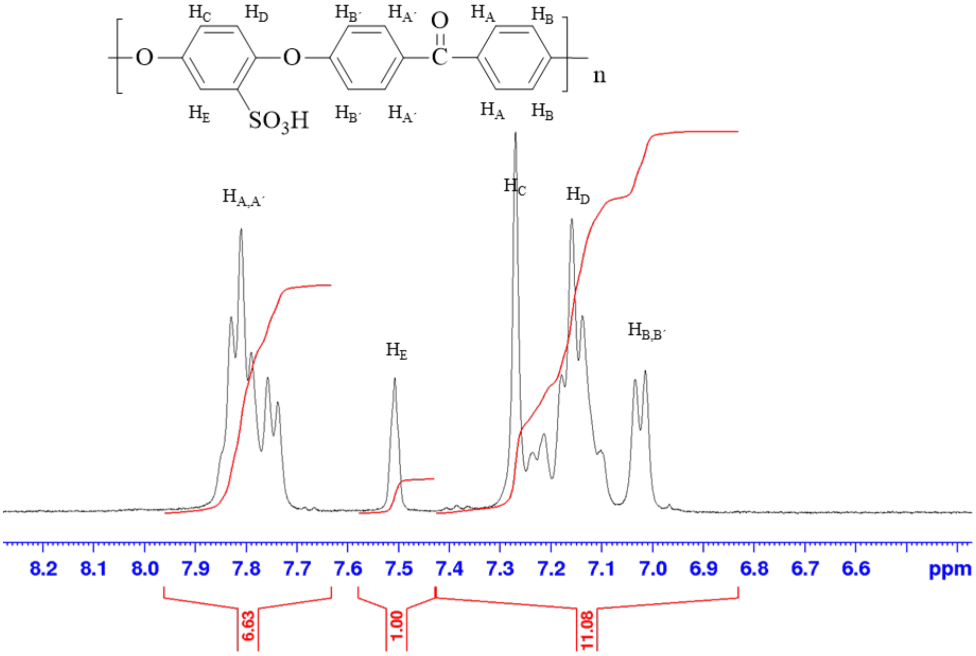


Figure 2. ^{1}H NMR spectra of sulfonated poly(ether ether ketone).

Table 1. Magnetic properties and particle size of synthesized ferrites.

Sample	Coercivity (Oe)	Intrinsic coercivity (Oe)	Remanence (emu/g)	Saturation moment (emu/g)	Nano-particle size (nm)
$ZnFe_{1.96}Pr_{0.04}O_4$	$0.55*10^{-2}$	15.01	0.01	5.35	23
$NiFe_{1.96}Pr_{0.04}O_4$	1.91	135.08	4.98	31.41	23
$Zn_{0.5}Ni_{0.5}Fe_{1.96}Pr_{0.04}O_4$	3.06	56.84	5.46	61.96	29

The final composite membranes were tested for their water-uptake properties and chemical stability, by investigating the membranes endurance in oxidative environment (Fenton reactive) and in acidic solution with pH 3 (H_2SO_4). Moreover, the membrane morphology was analyzed using SEM, and the thermal stability was determined by thermogravimetric analysis. Finally, the most important property of proton exchange membranes, which can directly affect fuel cell performance, was pursued: the proton conductivity of the wet membrane was evaluated by dielectric spectroscopy. The findings of this study suggest the use of composite membranes based on SPEEK for fuel cells.

References

[1] D. Möst, S. Schreiber, A. Herbst, M. Jakob, A. Martino, W.-R. Poganietz, The Future European Energy System: Renewable Energy, Flexibility Options And Technological Progress, Ed. Springer, New York, 2021, pp 3–7.

[2] M.M. Tellez-Cruz, J. Escorihuela, O. Solorza-Feria, V. Compañ, *Polymers (Basel)* 2021,13, 1–54.

[3] W.N.E. Wan Mohd Noral Azman, J. Jaafar, W.N.W. Salleh, A.F. Ismail, M.H.D. Othman, M.A. Rahman, F.R.M. Rasdi, *Mater. Today Energy* 2020, 17, 100427.

[4] P. Samoila, L. Baltag, C. Cojocaru, M. Ignat, V. Harabagiu, RO134943A2, 2021.

[5] S.N. Pund, P.A. Nagwade, A.V. Nagawade, S.R. Thopate, A.V. Bagade, *Mater. Today Proc.* 2022, 60, 2194–2208.

SUPERABSORBENT LIGNIN-BASED HYDROGELS WITH POTENTIAL APPLICATION IN ECOLOGICAL AGRICULTURE

Cosmina-Maria Bogza*, Maria-Cristina Popescu, Carmen-Mihaela Popescu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**bogza.cosmina@icmpp.ro*

Three-dimensional (3D) hydrophilic polymeric networks that are physically or chemically crosslinked and capable of absorbing huge volumes of water (or biological fluids) and swell are known as hydrogels. Any (semi-)flexible polymer is capable of creating hydrogels virtually in a range of physical shapes, including slabs, membranes, beads, microgels (microspheres), and nanogels (nanoparticles). Hydrogels can then be freeze- or supercritical dried to produce cryogels or aerogels, respectively [1].

Biopolymer-based hydrogels have been demonstrated to have applications in a wide range of industries, including hygiene (disposable diapers and feminine care products), agriculture (water retention and pesticide delivery), biomedicine (drug carriers, wound dressings, and tissue engineering scaffolds), pollutant adsorbents (heavy metal ions, dyes, and pesticides), biosensors, etc. Biopolymer-based hydrogels have been created using a variety of natural polymers or their salts, including sodium alginate, starch, protein, gelatin, hyaluronate, hemicelluloses, lignin, cellulose, chitin, and their derivatives [2].

In this work, physically cross-linked hydrogels composed of poly(vinylalcohol) (A), casein (C) and lignin nanoparticles were obtained (Table 1) by repeated freeze-thawing cycles (5 cycles) of aqueous solutions of these polymers.

Table 1. Experimental design.

Crt. Nr.	Solution	Mass Ratio	Lignin conc.
1	C:A	1:2	10%
2		2:1	10%
3		1:2	10%
4		1:2	5%
5		2:1	5%
6		1:1	5%
7		1:2	2%
8		2:1	2%
9		1:1	2%
10		1:2	0%
11		2:1	0%
12		1:1	0%

The molecular chain of PVA can easily form hydrogen bonds and has a good water solubility favorable for the production of hydrogels, casein possesses a number of characteristics suitable for the development of hydrogels, such as high hydrophilicity, good biocompatibility, lack of toxicity and availability of reactive sites for chemical modification, while lignin due to its large molecule can act as spacer to form large pores into the hydrogel matrix.

The obtained hydrogels showed excellent water and urea absorption capacity. When the concentration of PVA becomes higher, phase separation is favored, resulting in a lower swelling ratio. Since casein itself has a natural tendency to form a reversible gel, increasing its concentration in the mixture induces an increase of the pore sizes. This results in faster and easier penetration of water molecules into the hydrogel.[3] Further, the addition of lignin nanoparticles, leads to an even larger increase in the rate of water absorption into the hydrogel.

Hydrogels formed under optimal conditions were characterized by using FT-IR spectroscopy and X-ray diffraction in order to obtain information about structure, chemical changes and interactions occurring in the samples. Morphological aspects of the samples were evaluated by scanning electron microscopy (SEM), while the rheological studies were used to observe important viscoelastic behaviors of these materials.

Having a high-water holding capacity in their structure, the obtained cryogels have been used for agricultural applications, specifically for maintaining moisture in the soil. Therefore, the obtained cryogels were added into the soil in order to observe if they influence the germination of (pea) seeds, their lifespan and root and shoot length, and were compared to a control sample containing no hydrogels. It was observed that the hydrogels do not influence seed germination, but they increase the life span of the pea seedlings and depending on the concentration of each component into the hydrogel, the length of the shoot/rootstock differs.

The obtained hydrogels present potential to be used as materials in ecological agriculture as water retention products, when the weather conditions are not favorable, during long periods of drought for reducing the irrigation times.

Reference:

[1] X. Shen, J.L. Shamshina, P. Berton, G. Gurau, R.D. Rogers, *Green Chem.* 2016, 18(1), 53-75.
[2] R.A. Ramli, *Polym. Chem.* 2019, 10(45), 6073-6090.
[3] A. Bajpai, R. Saini, *Polym. Int.* 2005, 54(5), 796-806.

MACROMOLECULAR ENGINEERING OF THIOPHENE-CONTAINING HYPERBRANCHED ARCHITECTURES EXHIBITING ELECTROCHROMIC PROPERTIES

Ioana-Alexandra Trofin*, Radu-Dan Rusu, Catalin-Paul Constantin,
Mariana-Dana Damaceanu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**trofin.ioana@icmpp.ro*

As one of the most commercially appealing classes of conjugated polymers, conducting polymers are frequently investigated for use in modern applications, such as sensors, actuators, electrochromic devices, and smart windows, as well as for energy storage in supercapacitors, batteries, and fuel cells, or for energy harvesting in solar cells [1].

Currently, there is a significant amount of research being conducted on conjugated polymers that exhibit electrochromic properties. Thiophene-based macromolecular frameworks are extensively employed in the fabrication of optically- and/or electronically-responsive devices due to their notable characteristics, including elevated electrical conductivity, diminished oxidation potential, high stability in the oxidized state, trustworthy optical properties, thermal stability, and strong environmental durability [2,3].

When thiophene is integrated into hyperbranched (HB) architectures using well-established, accessible synthetic methods, it is possible to obtain materials with attractive electrochemical and optical properties, while also ensuring a controllable, straight-forward, industrially-desirable one-pot synthetic method.

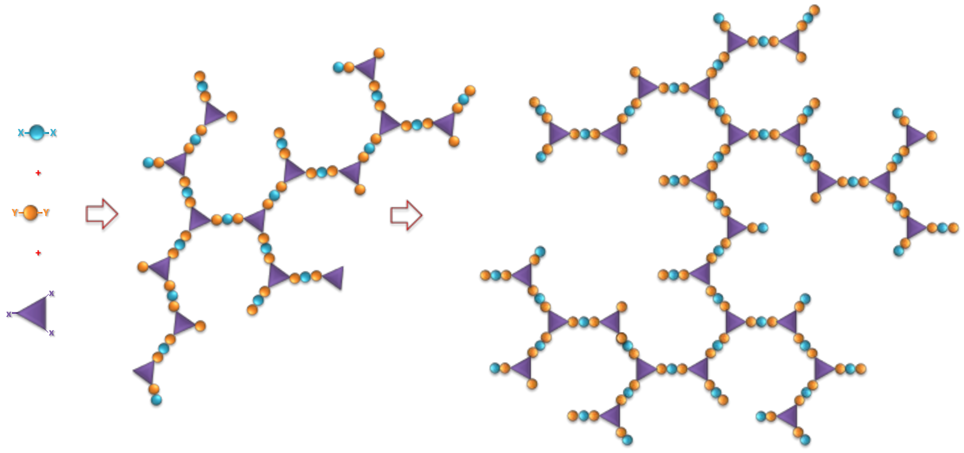


Figure 1. Synthetic strategy for HB polymers containing thiophene units.

This study focuses on the advancement of electrochromic and energy storage materials by developing HB macromolecular architectures that incorporate two other (hetero)aromatic building blocks besides the afore-mentioned thiophene, based on the synthetic strategy depicted in Figure 1. The subject matter encompasses various aspects derived from experimental design, and macromolecular engineering, with a primary emphasis on establishing reliable correlations between structural characteristics and material properties.

To examine the optical features and to evaluate the thiophene impact on UV-VIS and PL behaviour we carried out solution and solid state experiments, that showed the polymers exhibit one important absorbtion maxima, and one emission maxima (Figure 2).

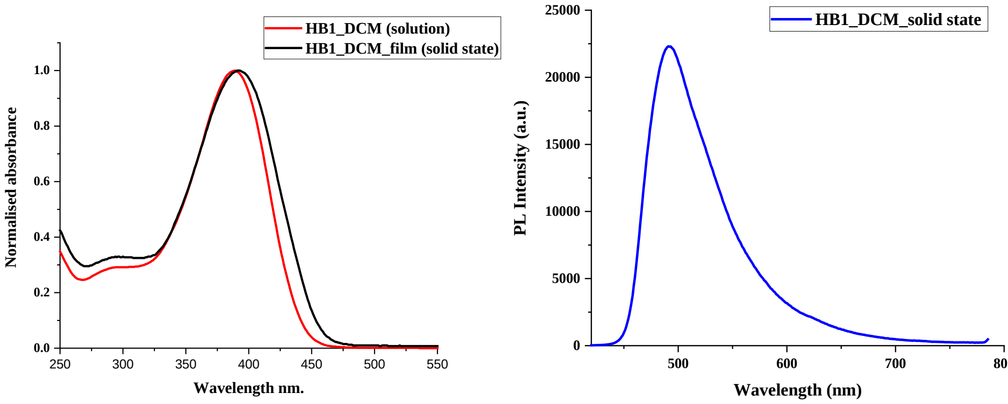


Figure 2. UV-Vis and PL spectra for HB thiophene polymer.

One notable advantage is the potential to attain customizable intrinsic microporosity based on the free volume created between polymer segments, which can enhance the efficiency of ion conduction and transfer in electrochemical devices [4]. SEM studies confirmed the ability to obtain microporos thin films from various solvents, one example is shown in Figure 3.

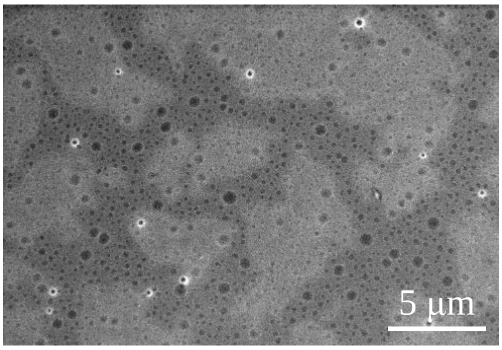


Figure 3. SEM image of HB thiophene based polymer.

Furtheron, the study was focused on the mechanism behind the electrochromic outcome and materials' response during charge and discharge cycles. Moreover, if follows the capacity to fulfill the stringent criteria for energy storage and smart window devices [1,3].

References

[1] A.P. Chiriac, C.-P. Constantin, M.D. Damaceanu, *Energies* 2023, 16, 3999.
[2] D.D. Hebert, M.A. Naley, C.C. Cunningham, D.J. Sharp, *Mater.* 2021, 14, 6146.
[3] M.D. Damaceanu, H.-D. Gilsing, B. Schulz, A. Arvinte, *RSC Adv*. 2014, 4, 52467.
[4] Y. Cai, X. Wen, Y. Wang, H. Song, Z. Li, Y. Cui, C. Li, *Sep. Purif. Technol.* 2021, 266, 118542.

Acknowledgment: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-III-P4-PCE-2021-1728 (contract number 46/2022) within PNCDI III.

POLYSACCHARIDE-INTEGRATED LIGNIN ESTERS AS EFFICIENT OIL ADSORPTION MATERIALS

Irina Apostol*, **Narcis Anghel, Iuliana Spiridon**
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**apostol.irina@icmpp.ro*

1. Introduction

Due to their widespread consumption, vegetable oils significantly contribute to water contamination. When subjected to elevated temperatures, light, or moisture, oils undergo several chemical transformations, such as oxidation, hydrolysis, and fatty acid decomposition. These can lead to the formation of harmful compounds like peroxides, aldehydes, and ketones, rendering the oils toxic [1,2]. The current research is focused on the obtaining of novel adsorptive materials derived from xanthan (XG) and lignin esters. Their adsorption capacity towards degraded sunflower oil, which underwent roasting twice at approximately 170°C was explored.

2. Experimental

LignoBoost (LB) lignin was esterified with oleic (OL) or stearic acid (ST). LB and its esters (LBOL and LBST) were incorporated into the XG matrix, resulting the adsorptive materials (XG/LB, XG/LBOL, and XG/LBST). FTIR spectroscopy, Scanning Electron Microscopy (SEM) and X-ray photoelectron spectroscopy were used to investigate the physicochemical and structural properties [3]. Kinetic and equilibrium studies were performed in order to evaluate the adsorptive properties of materials for degraded sunflower oil.

3. Results and discussion

The adsorption experiments have confirmed that all the studied materials successfully retained 50 g/g of the degraded sunflower oil (Table 1).

Table 1. Adsorption capacity values.

Material	**$^{a}q_e$ ± SD (g/g)**		
	Sunflower oil		
	1 g	**2 g**	**3 g**
XG	*56.62 ± 1.65*	*59.23 ± 1.96*	*62.45 ± 2.93*
XG/LB	*48.93 ± 4.90*	*53.56 ± 1.44*	*62.16 ± 3.96*
XG/LBOL	*43.20 ± 2.91*	*55.59 ± 2.19*	*51.95 ± 4.43*
XG/LBST	*41.56 ± 3.10*	*44.62 ± 2.74*	*50.07 ± 1.86*

[a] Data are expressed in the mean ± standard deviation (n = 3).

The adsorption process reached the equilibrium state after ~2 minutes. The amount of retained oil increased with the increment of the oil dosage from 1 to 3 g. These results showed that the concentration gradient promotes mass transfer. The kinetic analysis of adsorption demonstrated that the data aligns most favourably with the pseudo-second order (PSO) kinetic model (Figure 1). This model is suited for expressing the kinetics associated with physisorption and mass transfer/diffusion processes [4].

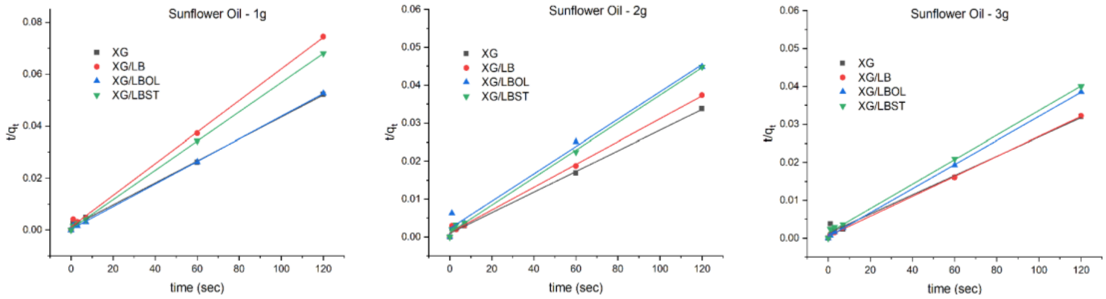


Figure 1. Experimental data fitted to PSO kinetic model

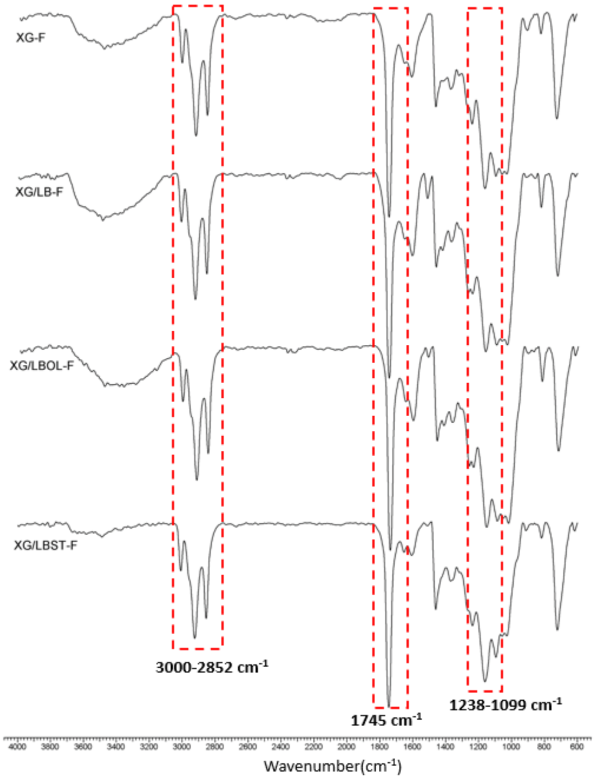


Figure 2. FTIR spectra of materials after degraded sunflower oil adsorption.

After the adsorption process, the FTIR spectra of the oil-loaded materials (Figure 2) did not indicate the formation of any novel chemical bonds between the oil molecules and the polysaccharide matrix. This certify that the adsorption process has a physical nature. Also, a slight decrease of the constant rate (k_2) value was observed with an increasing oil amount from 1 to 3 g. These results are attributed to an intense competition among oil molecules to reach the materials' pores.

When it comes to adsorption equilibrium, the interaction of altered sunflower oil with XG, XG/LB, and XG/LBST materials is best represented by the Harkin-Jura model, that explains multilayer adsorption of the adsorbate onto the heterogeneous surface of an adsorbent. The equilibrium for sunflower oil adsorption onto XG/LBOL resonates more with the Henry isotherm model that typically describes adsorption at lower concentrations.

4. Conclusions

Materials based on XG and LB esters were obtained and their adsorptive properties were evaluated. Each of the adsorbents demonstrated the capacity to retain over 50 g/g of degraded sunflower oil. Kinetic assessments fitted well with the PSO model. Based on the FTIR spectra of the oil-loaded materials, it was inferred that the adsorption mechanism predominantly operated on a physical level. When equilibrium was considered, the Henry and Harkin-Jura isotherm models satisfactorily described the adsorptive removal of degraded oil.

References

[1] D. Sha, R. Zheng, B. Wang, J. Xu, K. Shi, X. Yang, X. Ji, *React. Funct. Polym.* 2021, 165, 104975.
[2] B. Wiege, E. Fehling, B. Matthaus, M. Schmidt, *Foods.* 2020, 9(9), 1273.
[3] I. Apostol, N. Anghel, M.V. Dinu, F. Ziarelli, A. Mija, I. Spiridon, *React. Funct. Polym.* 2023, 190, 105620.
[4] W. Plazinski, W. Rudzinski, *J. Phys. Chem. C.* 2009, 113(28), 12495–12501.

NEW MOLECULAR SPIN PROBES FOR THE STUDY OF NON-COVALENT INTERACTIONS

Alexandru Vincentiu Florian Neculae[1]*, Jean Patrick Joly[2], George-Alin Balan[1], Iulia Matei[1], Sylvain R. A. Marque[2], Gabriela Ionita[1]

[1]*“Ilie Murgulescu” Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania*
[2]*Aix Marseille University, CNRS, ICR, UMR 7273, Marseille, France*
* *aniculae@icf.ro; alexandru.neculae.chimie@gmail.com*

Supramolecular systems that are built upon non-covalent interactions have numerous applications in chemistry and biology [1]. These interactions are spontaneous and reversible, involve structural units and surrounding solvent molecules, and determine the structure, dynamics and function of the system. In this study, non-covalent interactions in host–guest systems involving cyclodextrins with different cavity size (α-, β-CD) and the surfactant sodium dodecyl sulfate (SDS) are investigated by electron paramagnetic resonance (EPR) spectroscopy using a series of newly synthesised spin probes. This series includes two β-phosphorylated nitroxides (denoted **1** and **6**), two TEMPO-type radicals (**2**, **4**) and two PROXYL radicals (**3**, **5**), as shown in Figure 1. The study relies on the sensitivity of the EPR parameters of the spin probes (isotropic hyperfine coupling constants of nitrogen, a_N, and phosphorous, a_P, atoms; rotational correlation time, τ) to the local polarity, and to changes in molecular mobility. To estimate the EPR parameters, spectral simulations are performed using the WinSim [2] and EasySpin [3] programs.

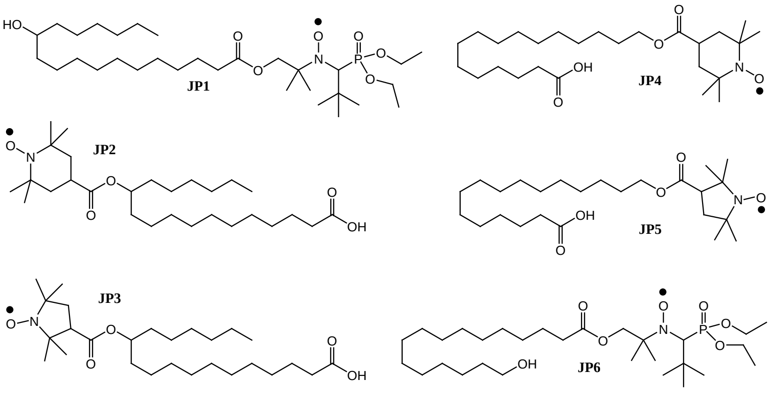


Figure 1. Structures of the spin probes used in the study.

The complexation of the **1-6** spin probes with CD cavities or with SDS micelles is accompanied by: i) a decrease in the a_N and a_P values, due to inclusion of the spin probe into a hydrophobic cavity, and ii) a broadening of spectral lines, due to slower tumbling of the complexed species. As an example, the behaviour of the TEMPO-type **2** probe upon addition of increasing concentrations of β-CD or SDS is shown in Figure 2.

Assuming a 1:1 stoichiometry, the **1-6**:CD association constants (K) were estimated from the proportions of free and complexed probe at each CD concentration [3], in the case of **1** and **6**, and from the dependence of the τ value on the CD concentration [4], in the case of **2-5**. The K values are listed in Table 1 and are in line with literature data.

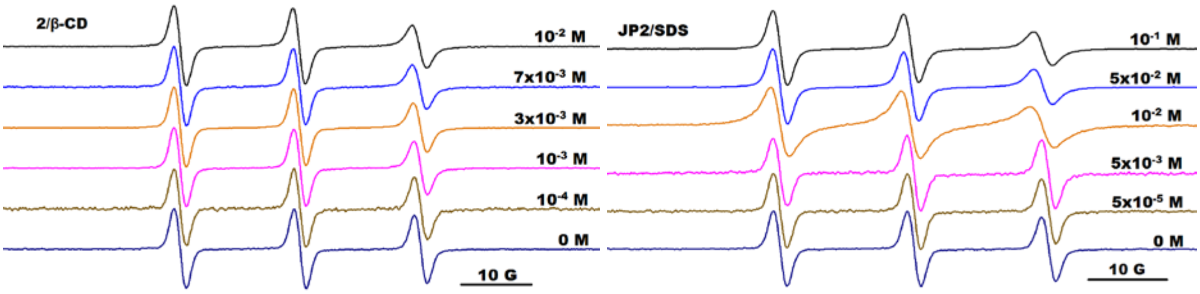


Figure 2. The EPR spectra of the TEMPO spin probe **2** in the absence and in the presence of increasing concentrations of β-CD (left) or SDS (right).

Table 1. Association constants (K, in units of M^{-1}) of spin probes **1-6** with cyclodextrins.

	1	2	3	4	5	6
α-CD	115	2752	521	242	2522	8
β-CD	123	46	139	488	519	113

The differences in EPR parameters between CD and SDS systems recommend the spin probes as good analytical reporters of solution composition. As such, competitive binding experiments were performed at constant CD concentration and increasing SDS concentration, revealing an interesting interplay of free and complexed species (Figure 3). At SDS concentrations below *cmc*, the spin probes are complexed with CDs. At SDS ~5×10^{-2} M, the spin probes are released from these complexes, as revealed by the fast motion (**2-5**) or lack of EPR signal (**1**, **6** are insoluble in water). At SDS 10^{-1} M, **1-6** become entrapped into SDS micelles formed once the CD cavities are saturated by SDS monomers. We remark the greater sensitivity of β-phosphorylated nitroxides to non-covalent interactions in CD/SDS systems as compared to TEMPO and PROXYL probes.

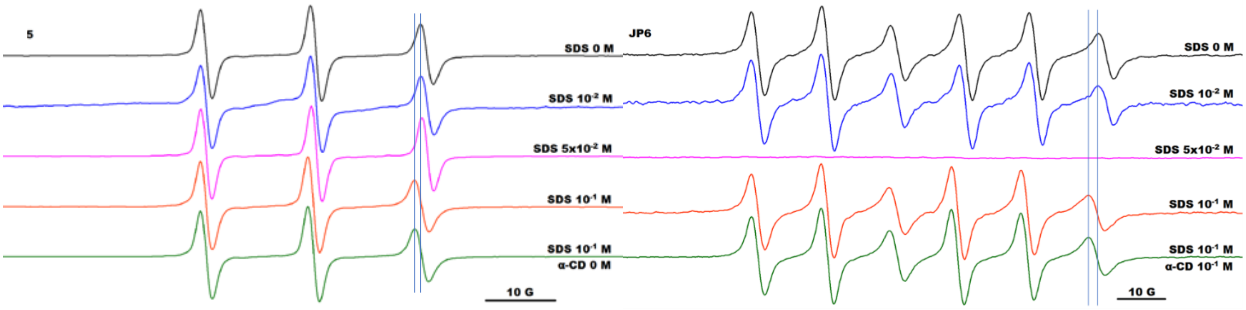


Figure 3. The EPR spectra of a PROXYL nitroxide (**5**, left) and of a β-phosphorylated nitroxide (**6**, right) at constant β-CD (10^{-2} M) and increasing SDS (10^{-5}–10^{-1} M) concentrations.

References

[1] X. Ma, Y. Zhao, *Chem. Rev.* 2015, 115, 7794-7839.
[2] D.R. Duling, *J. Magn. Reson. B* 1994, 104, 105-110.
[3] S. Stoll, A. Schweiger, *J. Magn. Reson.* 2006, 178, 42-55.
[4] A.V.F. Neculae, G. Audran, S. Bourdillon, G. Ionita, J.P. Joly, S.R.A. Marque, I. Matei, S. Mocanu, *J. Mol. Liq.* 2022, 364, 119983.
[5] G. Ionita, S. Mocanu, I. Matei, *Phys. Chem. Phys.* 2020, 22, 12154–12165.

Acknowledgment: This work was supported by the Romanian Academy within the research direction “EPR and fluorescence studies on supramolecular interactions in inhomogeneous systems” of the “Ilie Murgulescu” Institute of Physical Chemistry.

NANOSTRUCTURED POLYMER MATERIALS OBTAINED FROM PICKERING EMULSION POLYMERIZATION TECHNOLOGY

Maria Medrihan*, Andrei Honciuc, Valeria Harabagiu, Oana-Iuliana Negru, Ana-Maria Solonaru, Mirela Honciuc

Petru Poni Institute of Macromolecular Chemistry, Iași, Romania
**medrihan.maria@icmpp.ro*

Ion imprinted polymers are being currently developed for their potential use in metal ion extraction from aqueous environments [1]. As a consequence of industrial activity, the heavy metal ion contaminants that can be found in wastewater, represent a major issue to the well-being of humans, wildlife, and the ecosystem, because of their high toxicity, their persistence and susceptible carcinogenic effect [2]. However, polymer nanostructured materials have shown to be very versatile with respect to capturing and removal of metal ions from contaminated waters [3]. Among these, metal, or ion imprinted polymers (MIPs or IIPs) are being used in separation and purification sciences because of their high selectivity, good stability, simplicity, and low cost. They have been mainly used for selective removal of organic pollutants [4], preconcentration of metal ion [5], sensing and other fields [6]. IIPs are crosslinked polymers that have pores and binding sites specifically tailored for the desired ions and molecules that are negatively or positively charged. Typically, functional monomers, crosslinkers, initiators, and templates are used in a reaction mixture to create IIPs. Different methods can be used to imprint the template ions in a polymer matrix.

Similarly, to key and lock systems, IIPs are developed to recognize and remove the targeted ions from wastewaters, industrial waters, or in hydro mining of resources. Compared to polymer-based ion exchangers [7], the IIPs are very effective in identifying and specifically binding transitional metal ions, particularly heavy metals and even radioactive elements [1]. Thus, the key element of the IIPs is the template, which is the metal ion complex. Also, the interaction of the functional groups of monomers with the template is one of the most important requirements for the efficient binding and selectivity of the metal ions with the imprinted material. Better selectivity and binding capacity depend on the ratio and choice of these components, which have an impact on the final physical and chemical characteristics of IIPs [8].

Several synthesis methods are currently used for the synthesis of IIPs, whose advantages and disadvantages have been extensively reviewed [9]. Among these we mention: (i) block polymerization, whereas the end products are monoliths that need to be crushed, grounded down to micron or nano sized particles before they can be used in ion extraction and recovery, steps which are consuming additional energy, (ii) suspension emulsion polymerization that require use of surfactants and polymer pseudo-surfactants, which are not environmentally friendly and involve an extra-step for the purification of the product, (iii) precipitation polymerization implies great costs and a lot of organic solvent, harmful to the environment, and also the method provides not so well defined nano- or micron-sized polymeric particles, etc.

As we come along in the current state of the art, to address the issues already mentioned, we developed a new method for obtaining IIPs, namely Pickering Emulsion Polymerization Technology (PEmPTech). PEmPTech is a green method, water based technology that achieves great performances by obtaining macro and nanoparticles without using surfactants [10].

Pickering-type emulsions generally consist of a water-insoluble monomer, stabilizing nanoparticles, and initiators. The process consists in the emulsification of the phases (nanoparticles are dispersed in water and then the oil is added) using magnetic stirring or ultrasonication, resulting in the adsorption of nanoparticles at the water interface, followed by polymerization. In comparison to classical emulsions stabilized by molecular surfactants, Pickering emulsions have better kinetic stability because the interfacial desorption energies of nanoparticles are greater than those of molecular surfactants [11]. In addition, a whole range of nanoparticles, such as environmentally neutral silica nanoparticles, can be used to stabilize the emulsions.

In the current work, PEmPTech was used in a series of experiments in which the main goal was the extraction and the recovery of different metal ions from aqueous solutions. In this study, for the obtaining of ion imprinted polymers, we came forward with three different approaches: (i) using only the ligand, (ii) using the complex formed in situ, and (iii) using the complex synthesized previously. We further compare the extraction and recovery capacities of IIPs and non-imprinted polymers. In addition, we also test the versatility of different imprinting techniques.

References

[1] C. Branger, Meouche, W.; Margaillan, A. *React. Funct. Polym.* 2013, 73 (6), 859–875.
[2] P.E. Hande, A.B. Samui, P. S. Kulkarni, *Sci. Pollut. Res.* 2015, 22 (10), 7375–7404.
[3] J. Fu, L. Chen, J. Li, Z. Zhang, *J. Mater. Chem. A* 2015, 3 (26), 13598–13627.
[4] H. Ebrahimzadeh, E. Moazzen, M.M. Amini, O. Sadeghi, *Anal. Methods* 2012, 4 (10), 3232.
[5] C. Teodosiu, R. Wenkert, L. Tofan, C. Paduraru, *Rev. Chem. Eng.* 2014, 30 (4), 403–420.
[6] K. B. Chipasa, *Waste Manag.* 2003, 23(2),135-143.
[7] L. Wang, J. Li, J. Wang, X. Guo, X. Wang, J. Choo, L. Chen, *J. Colloid Interface Sci.* 2019, 541, 376–386.
[8] V. V. Kusumkar, M. Galamboš, E. Viglašová, M. Daňo, J. Šmelková, *Materials* 2021, 14 (5), 1083.
[9] J. P. Rao, K. E. Geckeler, *Prog. Polym. Sci.* 2011, 36 (7), 887–913.
[10] A. Honciuc, A.-M. Solonaru, M. Honciuc, *ACS Appl. Polym. Mater.* 2023, 5 (10), 8012–8022
[11] Honciuc, A., Chemistry of Functional Materials Surfaces and Interfaces: Fundamentals and Applications, 1st ed.; Ed. Elsevier: Cambridge, 2021.

Acknowledgements This work was supported by a grant of the Ministry of Research, Innovation and Digitization of Romania, CNCS/CCCDI-UEFISCDI, project number PN-III-P4-PCE-2021-0306 (Contract Nr. PCE62/2022).

A DIPHENYLALANINE BASED PENTAPEPTIDE WITH FIBRILLATING SELF-ASSEMBLING PROPERTIES

Stefania-Claudia Jitaru[1*], **Andrei Neamtu**[2,3], **Gabi Drochioiu**[1], **Laura Darie-Ion**[1],
Iuliana Stoica[4], **Brindusa-Alina Petre**[1,2], **Vasile-Robert Gradinaru**[1]
[1]*Faculty of Chemistry,"Alexandru Ioan Cuza" University, Iasi, Romania*
[2]*TRANSCEND—Regional Institute of Oncology, Iasi, Romania*
[3]*Department of Physiology,"Gr. T. Popa" University of Medicine and Pharmacy, Iasi, Romania*
[4]*Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania*
**jitaru.stefania@yahoo.com*

In the last few decades, self-assembling bioinspired molecules have gained significant interest due to their simple structure, biocompatibility and biodegradability. In response to a variety of stimuli, such as pH, temperature, or ionic strength, peptides and the related compounds can self-assemble into a variety of nanostructures of varied shapes and sizes [1].

Here, we describe the synthesis, characterisation, and capacity to form distinct fibrillar structures of a pentapeptide derived from lysozyme. The Fmoc/t-Bu solid phase peptide synthesis method was used to obtain our targeted FESNF-NH_2 peptide (where F-phenylalanine, E-glutamic acid, S-serine, N-asparagine) (Figure 1), which was further purified using reversed-phase high-performance liquid chromatography (RP-HPLC) and confirmed by matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS respectively MALDI-MS/MS) [2].

The pattern of marginal phenylalanine residues and spectroscopic characteristics of this pentapeptide were investigated by both UV-visible and fluorescence spectroscopy. Self-assembling capabilities were assessed using atomic force microscopy (AFM), aggregation index, and thioflavin T assays (ThT). The FESNF-NH_2 peptide has shown the ability to produce fibrillar structures (Figure 2) [3]. Moreover, the experimental data were in concordance with the molecular dynamics' simulation studies. The peptide capacity to generate fibrils may pave the way in the development of innovative material supports for medical and cosmetic application.

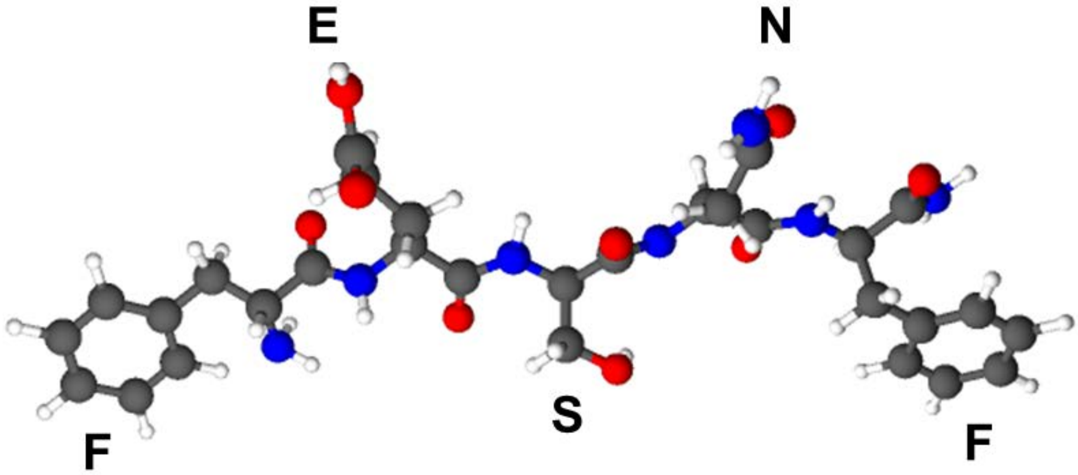


Figure 1. Molecular structure of FESNF-NH_2 pentapeptide (Balls and sticks model), where gray is carbon; blue is nitrogen; red is oxygen and white is hydrogen.

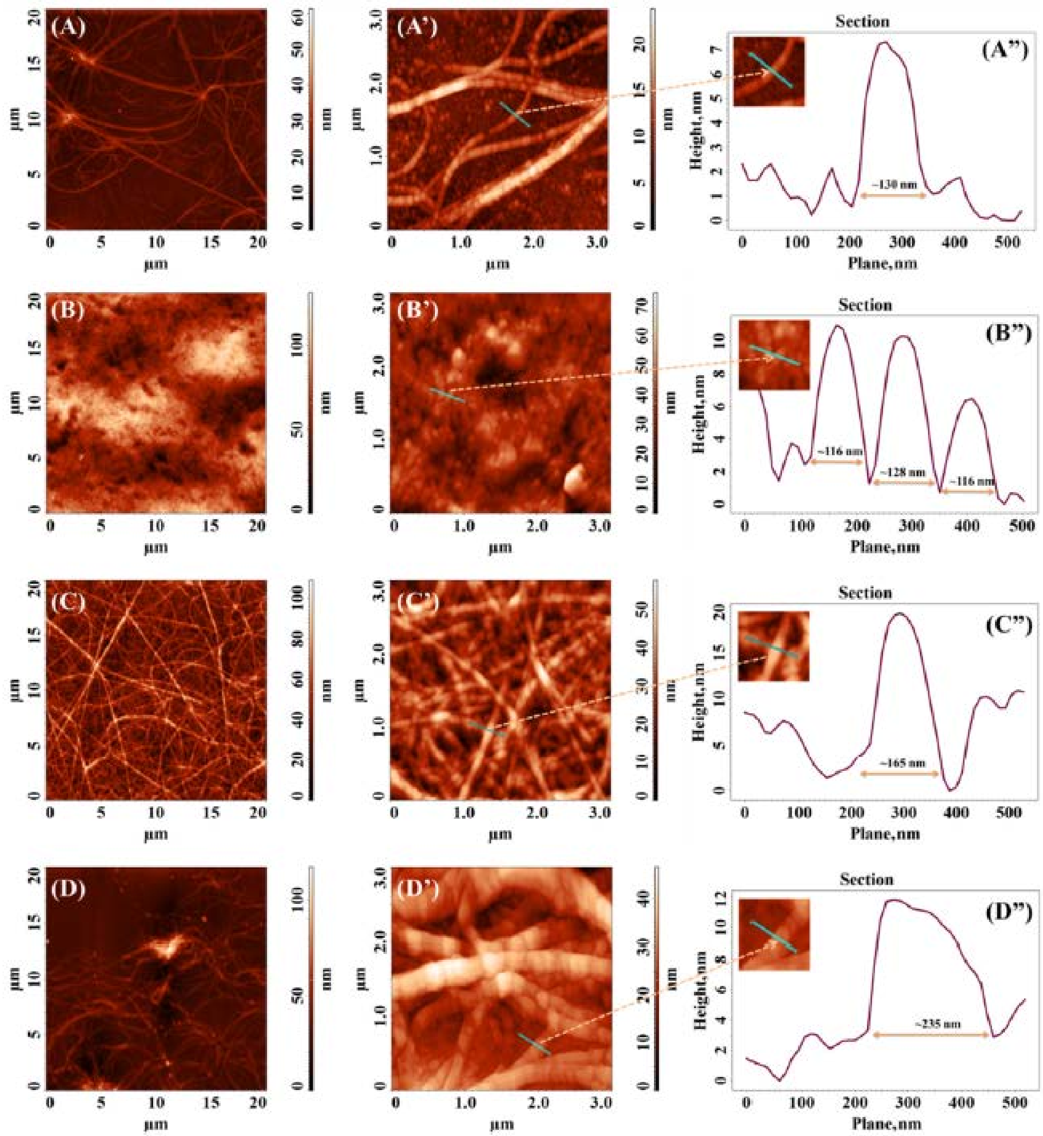


Figure 2. Two-dimensional (2D) AFM images, collected on 20x20 µm^2 and 3x3 µm^2 areas and the corresponding cross-section profiles of the samples obtained from various FESNF-NH_2 solutions (1 mg/mL) in (A, A', A") ammonium acetate 45 mM pH 5.5; (B, B', B") Tris 45 mM pH 7.4; (C, C', C") Tris 45 mM pH 8.2; (D, D', D") 4.5% methanolic solution.

References

[1] J. Yang, H.-W. An, H. Wang, *ACS Appl. Bio Mater* 2021, 4, 24-46.

[2] P.R. Hansen, A. Oddo, Fmoc Solid-Phase Peptide Synthesis. In *Peptide Antibodies*; Ed. Humana Press, New York, NY, USA, 2015, pp. 33–50.

[3] S.C. Jitaru, A. Neamtu, G. Drochioiu, L. Darie-Ion, I. Stoica, B.A. Petre, V.R. Gradinaru, *Pharmaceutics* 2023, 15(2), 371.

Acknowledgment: This work was co-funded by the European Social Fund, through Operational Programme Human Capital 2014-2020, project number POCU/993/6/13/153322, project title "Educational and training support for PhD students and young researchers in preparation for insertion into the labor market".

VERSATILE THIN FILMS DERIVED FROM TRIPHENYLAMINE BASED- OLIGOMERS: ELECTROSYNTHESIS, CHARACTERIZATION AND APPLICATIONS

Andra Ionela Gavril*, Loredana Vacareanu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**andra.gavril@icmpp.ro*

Electropolymerization is a versatile technique for the synthesis of polymeric electrode materials, involving the direct deposition of insoluble polymers onto electrode surfaces through the coupling reaction of soluble monomers. Particularly for the synthesis of conductive conjugated polymers, which are typically insoluble due to their rigid and highly conjugated network structure, electropolymerization offers a suitable method to obtain electroactive polymers onto conductive substrates, allowing precise control over their shape and dimensions, thickness and morphology of films, while circumventing issues related to processability [1].

Triphenylamine (TPA) presents an attractive option for constructing conjugated crosslinked building blocks with several beneficial properties, including a low redox potential, fast electron transfer rate, and efficient hole transport capacity. Its propeller-like structure further enables the development of cross-linked conjugated polymers based on TPA, leading to enhanced capacity and superior rate performances [2]. Moreover, TPA serves as an electrochromic chromogenic group, displaying a noticeable colour contrast between its neutral and oxidized states [3].

Taking advantage of TPA's geometric features and electrochemical activity, three oligomers with fully conjugated structures and star-shaped architectures were synthesized, incorporating TPA as both the core and peripheral units. The oligomers were synthesized by two palladium-catalysed C-C coupling reactions, the Heck and the Sonogashira reaction, and by different reaction parameters such as reaction temperature, the solvent used, and the type of catalysts, the oligomers were obtained in very good yields, over 85%. The introduction of systematic changes in the design of oligomers allows to establish relationships between their electro-optical properties with molecular structural parameters. Hence, this study provides a model for designing star-shaped oligomers capable of forming electroactive conjugated polymers with potential applications in electronic and optoelectronic devices. The presence of end-capped TPA units ensured their suitability for electropolymerization, and thus, their corresponding thin-film state polymers were prepared by the electropolymerization method using conductive ITO/glass substrates (the working electrode). The resulting films were structurally characterized by FT-IR spectroscopy confirming their proposed chemical structure and morphologically by SEM spectroscopy which revealed that the morphological features strongly depend on several factors, such as the solvent used and the electrochemical parameters, such as the number of the cyclic voltammograms performed during the deposition steps. In Figure 1 the repetitive cyclic voltammograms recorded for the deposition of one of the oligomers (PTPA-s1) are presented **(a)**, its corresponding FT-IR spectrum and **(b)** SEM image **(c)**.

During the electrochemical stability experiments which revealed that electrodeposited films have reasonable stability/reversibility over 10 cycles, all polymer films exhibited also electrochromic behaviour, manifesting colour shifts from green to dark blue, as exemplified for one of the oligomers (Figure 2). The electrochromic parameters, such as coloration efficiency (CE), and optical contrast (ΔT %), were determined for all the investigated thin films.

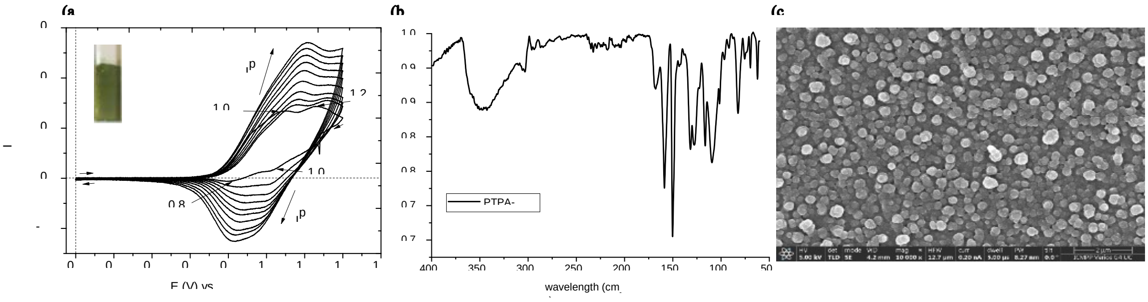


Figure 1. a) CV’s (20 cycles) for the electrodeposition of the polymer films (**PTPA-s1**) from DCE solution containing electrolyte support (TBAP, 10^{-1}M), by sweeping the potential of the ITO/glass on the positive range with 10 mVs^{-1} scan rate; b) FT-IR-ATR spectra and **b)** SEM image of **PTPA-s1** deposited film on ITO/glass.

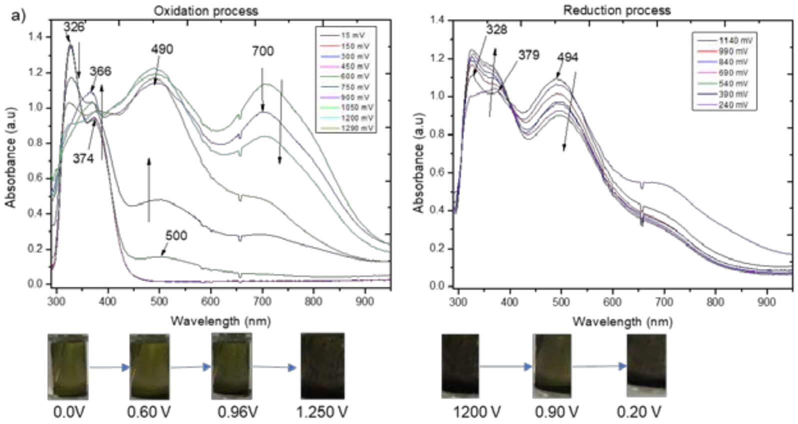


Figure 2. The in-situ spectroelectrochemical spectrum PTAP-s1 deposited on ITO/glass recorded during the oxidation and reduction processes, in ACN/TBAP (10^{-1}M) solution.

The impressive charge transfer properties observed in the electropolymerized polymer films have motivated us to employ them as sensors for detecting harmful environmental compounds such as nitroaromatic derivatives (picric acid). These sensing capabilities have shown promise, even in the initial testing phases, indicating the potential for creating a specialized device. The linear voltammetry results clearly illustrate that the potential increases exponentially with increasing concentrations of picric acid.

References

[1] Q. Zhang, H. Dong, W. Hu, *J. Mater. Chem. C* 2018, 6, 10672-10686.
[2] Q. Huang, J. Chen, X. Shao, L. Zhang, Y. Dong, W. Li, C. Zhang, Y. Ma, *J. Chem. Eng.*, 2023, 461, 141974
[3] H.J. Yen, G.-S. Liou, *Polym. Chem.* 2018, 9, 3001.

Acknowledgment: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2021-1068, within PNCDI III.

MANGANESE FERRITE BASED MATERIALS FOR CATALYTIC APPLICATIONS

Ionela Grecu*, Petrisor Samoila, Corneliu Cojocaru, Petronela Pascariu, Valeria Harabagiu
Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**grecu.ionela@icmpp.ro*

Nanostructured spinel ferrites are a unique class of mixed iron oxide-based compounds, frequently used as candidates for various catalytic applications [1]. In addition to their chemical stability, high specific surface area, narrow band gap and low production cost, these compounds have unique magnetic properties that makes them ideal for catalysis. These materials can be easily recovered by using an external magnetic field, once the catalytic experiments are completed [1-3]. Manganese-based ferrites have emerged as the most promising catalytic candidates among ferrites. On the other hand, recent works revealed that modifying the crystallite and grain size and/or producing crystallite defects in the spinel lattice, by adding low quantities of rare earth cations can enhance the catalytic performances of ferrites [2]. To encourage the integration of rare earth ions into the spinel matrix, high temperature thermal treatments are usually used [3]. The manganese ferrite is one particular case, which is unstable at sinterization at high temperatures, because manganese ions have a susceptibility to oxidize [1]. As a result, adding lanthanides cations to $MnFe_2O_4$ by raising the sinterizing temperature has a negative impact on the phase purity.

In this regard, our attention was drawn to the synthesis and investigation of the catalytic activity of manganese ferrite, with the general formula $MnFe_{1.96}RE_{0.04}O_4$ (RE = La, Gd, Er, Ce). The materials were characterized by XRD, FTIR, TEM and VSM.

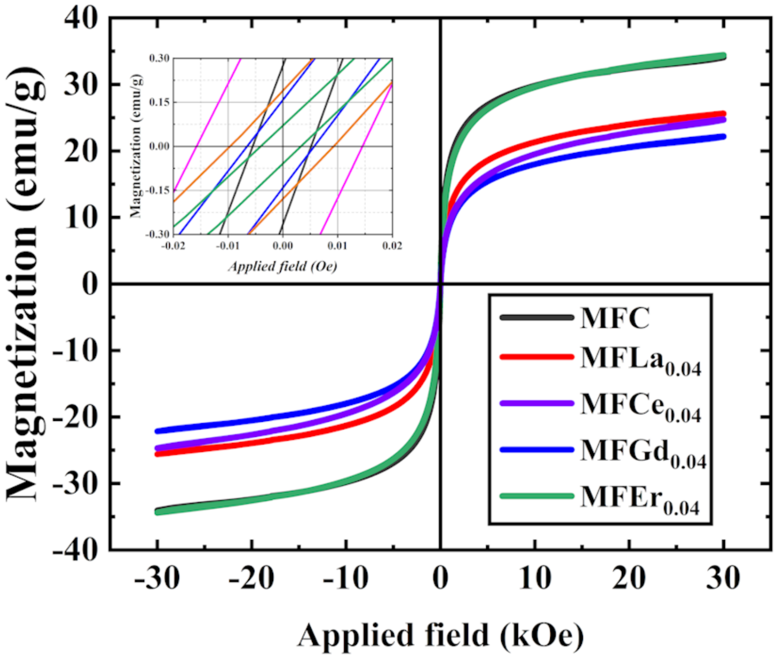


Figure 1. Representative hysteresis loops of pristine and rare-earth doped manganese ferrite, measured at room-temperature.

The magnetic properties of the synthesized materials were assessed using a vibrating sample magnetometer (VSM) at room temperature. To improve the accuracy of the results, the samples were demagnetized before. The hysteresis loops depicted in Figure 1 are specific to materials with superparamagnetic behavior, which is defined by coercivity and remanence, with values that are close to 0. These magnetic characteristics of mixed manganese ferrites are explained by the placement of metal cations between the active centers. The hysteresis allure of new materials is not altered by doping with metals from the rare earth group [4].

Table 1. Saturation magnetization (M_S), remanent magnetization (M_r) and coercivity (H_c) of new manganese ferrite-based nanoparticles.

Sample	Formulation	Ms (emu/g)	Mr (emu/g)	Hc (Oe)
MFC	$MnFe_2O_4$	33.97	0.27	4.00
$MFLa_{0.04}$	$MnFe_{1.96}La_{0.04}O_4$	25.51	0.15	4.60
$MFCe_{0.04}$	$MnFe_{1.96}Ce_{0.04}O_4$	24.60	0.18	7.09
$MFGd_{0.04}$	$MnFe_{1.96}Gd_{0.04}O_4$	22.08	0.06	2.76
$MFEr_{0.04}$	$MnFe_{1.96}Er_{0.04}O_4$	34.30	0.57	11.36

In Table 1 it can be observed that all of the samples show low values for the magnetic parameters, such as coercivity (Hc) and remanence (Mr), indicating that they are superparamagnetic materials.

The results of structural and morphological investigations are integrated with the magnetic behavior of developed ferrites. The magnetic properties are directly correlated with the variation of crystallite and particle size. As a result, the addition of rare earth elements to the ferrite matrix provides improved magnetic characteristics required for the recovery and reutilization of these materials for future (photo)catalytic applications [5].

References

[1] B.I. Kharisov, H.V.R. Dias, O.V. Kharissova, *Arab. J. Chem.* 2019, 12(7), 1234-1246.

[2] P. Samoila, C. Cojocaru, L. Sacarescu, P. Dorneanu, A.A. Domocos, A. Rotaru, *Appl. Catal. B: Environ.* 2017, 202, 21–32.

[3] A.-C. Enache, I. Grecu, P. Samoila, C. Cojocaru, V. Harabagiu, *Gels* 2023. 9(5), 358.

[4] S.-U. Rather, U. Saeed, A.A. Al-Zahrani, H.S. Bamufleh, H.A. Alhumade, A.A. Taimoor, O.M. Lemine, A.M. Ali, B. Al Zaitone, M.M. Alam, *J. Nanomater.*, 2021, 9410074

[5] P. Samoila, L. Sacarescu, L., A.I. Borhan, D. Timpu, M. Grigoras, N. Lupu, M. Zaltariov, V. Harabagiu, *J. Magn. Magn. Mater.* 2015, 378, 92-97

Acknowledgment: This work was supported by a grant from the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-III-P1-1.1-TE-2021-0030, within PNCDI III.

FUNCTIONALIZATION OF 5-BROMOSALICYLALDEHYDE AS MANNICH, SCHIFF-BASE, AND NITRONYL-NITROXIDE LIGANDS AND THEIR COMPLEXES

Ştefan Dimitriu[1,2]*, Sergiu Shova[3], Marius Andruh[1,2]
[1]*“Costin D. Nenitzescu” Institute of Organic and Supramolecular Chemistry, Bucharest, Romania*
2Faculty of Chemistry,University of Bucharest, Bucharest, Romania
[3]*Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania*
**stefan.dimitriu.02@gmail.com*

5-bromosalicylaldehyde presents two sites that can be functionalized (Figure 1) in order to design various ligands. A Mannich reaction in the ortho position relative to the hydroxyl group can be performed to build a compartmental structure [1]. Next, the formyl groups can be converted into imines, to increase the diversity of the ligands, or to nitronyl-nitroxide radicals [2], which present paramagnetic properties.

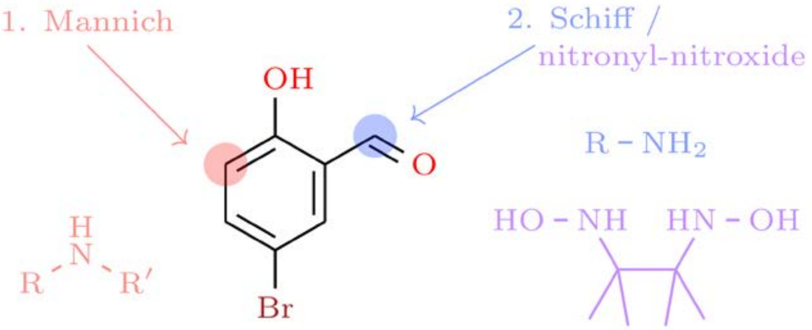


Figure 1. Functionalization of 5-bromosalicylaldehyde.

In this work, a series of Mannich bases (Figure 2) was obtained from 5-bromosalicylaldehyde, using amines bearing a different number of secondary amine groups. The products have been characterized by NMR spectroscopy.

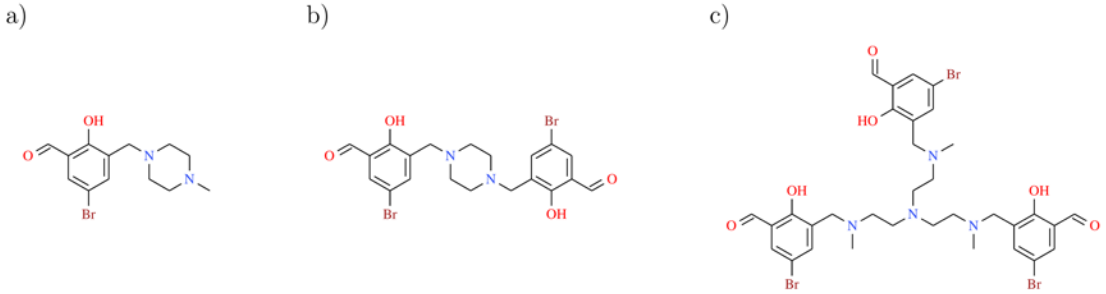


Figure 2. Mannich bases obtained starting from 5-bromosalicylaldehyde and: (a) N-methylpiperazine; (b) piperazine; (c) tris[2-(methylamino)ethyl]amine.

Complexes of a tripodal Mannich base were synthesized and their structure was resolved using single crystal X-ray diffraction measurements. Ni(II), Co(II), and Mn(II) ions entered the lower compartment of the molecule, while Cu(II) ions form a tetranuclear coordination compound (Figure 3).

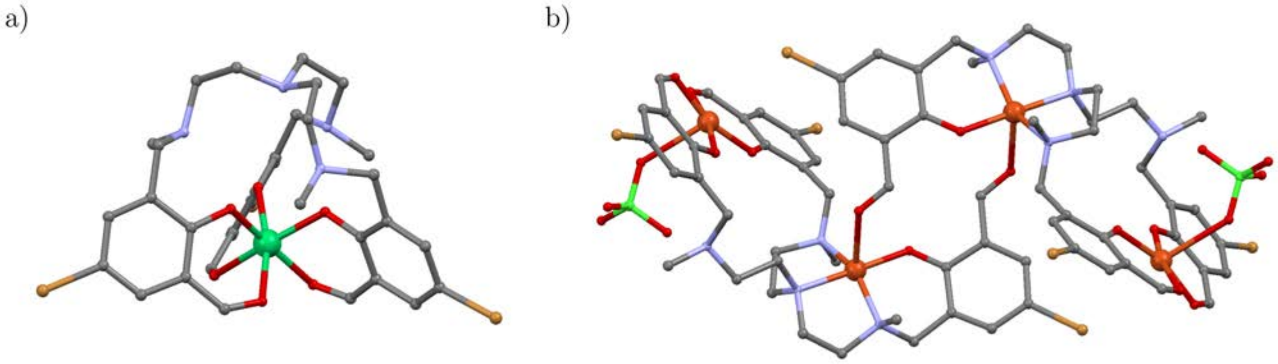


Figure 3. Coordination compounds of the tripodal Mannich base with: (a) Ni(II); (b) Cu(II).

Conversion of the formyl groups of the Mannich bases to nitronyl-nitroxide moieties led to paramagnetic ligands. A binuclear complex with Ni(II) was obtained (Figure 4), when the nitronyl-nitroxide radical was spontaniously reduced to an imino-nitroxide radical.

Lastly, Schiff bases and their corresponding complexes were obtained from the Mannich bases. Amines bearing different numbers of primary amine groups have been employed. One example is a Mannich-Schiff cage (Figure 4), where a template synthesis was involved. The Ni(II) ion, by entering the lower compartment, acts a template and brings the arms of the ligand in position for a triple Schiff condensation reaction.

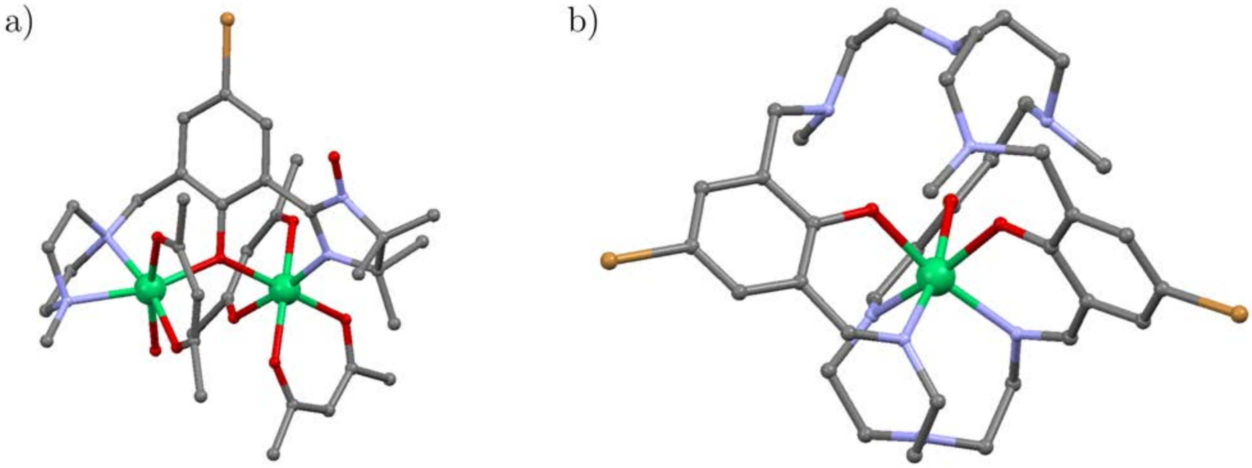


Figure 4. Ni(II) coordination compounds of: (a) the imino-nitroxide radical obtained from the simple Mannich base; (b) a Mannich-Schiff cage.

References

[1] J.D. Crane, D.E. Fenton, J.M. Latour, A.J. Smith, *J.Chem.Soc.*, *Dalton Trans.* 1991, 2979-2987.
[2] E.F. Ullman, J.H. Osiecki, D.G.B. Boocock, R. Darcy, *J.Am.Chem.Soc.* 1972, 94, 7049-7059.

Acknowledgments: S.D. is grateful to Constantin Drăghici, Mihai Răducă, Victorița Tecuceanu, Andrei Pătrașcu, Cristian Spînu and Augustin Mădălan for their help.

SYNTHESIS AND STRUCTURE OF NEW PYRROL 2(5H)-ONE HYBRIDS WITH TRIFLUOROMETHYL MOIETY

Rafaela Vrabie[1]*, **Cristina Al-Matarneh**[2], **Mariana Pinteala**[2]
[1]" Cristofor Simionescu" Faculty of Chemical Engineering and Environmental Protection "Gheorghe Asachi" Technical University of Iasi, Iasi, Romania.
[2]Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania
**rafaela-paula.vrabie@student.tuiasi.ro*

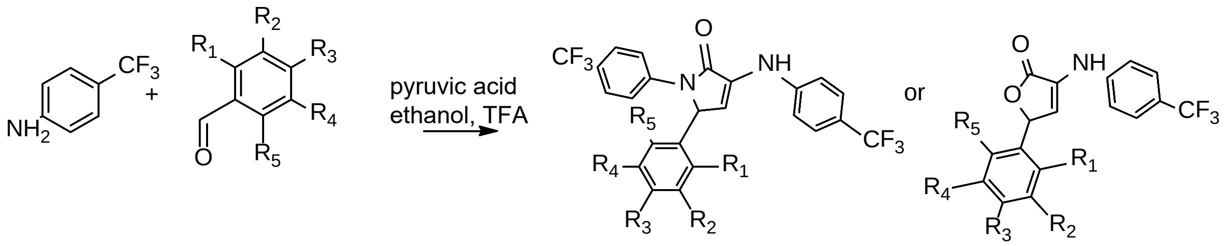
On October 13, 2020, the WHO declared antimicrobial resistance (AMR) is one of the top 10 global public health threats facing humanity and requires urgent multisectoral action in order to achieve the Sustainable Development Goals. In this context, the creation of new classes of antibacterial drugs, with lower toxicity, greater efficacy and lower production costs will be of significant importance for medical industry.

Microbial infections remain one of the top causes of mortality and the majority of nosocomial infections, posing a significant burden on the global health system, mainly due to the emergence of antimicrobial resistance (AMR). AMR is a growing health concern being described as a 'slow tsunami' capable of quickly wiping out all currently available antibiotic treatments [1]. In this context, drug discovery efforts are focused on the discovery of new antimicrobial agents endowed with chemical and mechanistic innovations in order to expand the ever-shrinking arsenal of clinically available drugs and combat AMR. Drug design is a complex process that, to some extent, still relies on lucky accidents and, despite the development of various modern techniques, there is still no general responsive approach. Although so-called more rational methods, such as *in silico* modeling, are becoming more popular, they have little effect on overall drug design efficiency. Therefore, rational design based on experimental data analysis remains one of the main screening methods for antimicrobial drug development.

One crucial component in the structure of many current antimicrobial drugs are heterocyclic rings. It is now well accepted that nitrogen presence has a positive impact on lipophilicity and promotes hydrogen bonds formation. Thus, N-heterocyclic rings are used to enhance pharmacological and pharmacokinetic properties of drugs and to lower toxicity. The presence of a heterocyclic ring, functioning as central piece, is an event that occurs commonly in many natural and synthetic drugs. Among N-heterocyclic derivatives, pyrrol-2-one-modified occur in numerous bioactive natural compounds, including pyrrocidine A, quinolactacin C, ypaoamide, holomycin, and thiolutin. Some of the biological properties of the pyrrole cycle include FPR1 antagonists, antibacterial agent, antioxidant, cytotoxic and antitumor agents or inhibitors for tyrosinase, carbonic anhydrase and also annexin A2-S100A10 protein interaction. Fluorine incorporation into biologically active molecules results in significant changes in their molecular properties (chemical, physical, and biological). Because of its stereo electronic properties, the trifluoromethyl group increases the bioactivity [2], alters the chemical, physical and biological characteristics of biologically active compounds. Due to its stereo electronic qualities, it increases a molecule's lipophilicity and enhances *in vivo* transport. At the same time, secondary metabolite formation is reduced due to the strength of the C-F bond [3].

Having all this data in mind, the goal of the current study was to synthesize novel bioactive hybrid molecules with pyrrol-2-one as a core and two active binding groups on its sides.
In order to obtain the proposed derivatives para-trifluormethyl aniline was reacted with aldehyde derivatives aromatic, or O-heterocyclic aldehyde class and pyruvic acid, in ethanol media in the presence of trifluoroacetic acid, in a catalytic amount. The library of newly synthesized compounds consists of compounds with 1H-pyrrol-2(5H)-one structure and 2-oxo-2,5-dihydrofuran derivatives.

All the compounds were obtained in good yields (between 47 and 88%), the chemical structures were verified through NMR, IR, X-Ray and Maldi-MS techniques.



Pyrrole-containing analogs are found in many natural products which are considered a potential source of physiologically active chemicals. One of the biological activities of these compounds is their antimicrobial activity. Taking into account the acute need of developing novel anti-infective drugs, the synthesized compounds are currently tested *in vitro* for their antimicrobial activity against *S. aureus* ATCC 25923, *P. aeruginosa* ATCC 27853 and *C. albicans* ATCC 10231 strains, using qualitative and quantitative assays.

S. aureus and *P. aeruginosa* infections are “still unresolved issues”, being included in the list of the most fearful opportunistic and nosocomial bacterial agents due to their multidrug resistance. Both pathogens can cause serious infections such as bloodstream infections, pneumonia, or bone and joint infections [4].

Candida spp. is now regularly detected among the top five causes of healthcare-associated bloodstream infections, their prevalence being higher than any bacterial sepsis. Among fungi, *C. albicans* is the most important species of human opportunistic fungi, causing a variety of severe mucosal and systemic infections especially in immunocompromised patients, worsened by the development of antifungal resistance. Systemic candidiasis has become a life-threatening challenge for human health and finding the treatment for it is an actual challenge [5].

References

[1] B. Garudachari, M.N. Satyanarayana, B. Thippeswamy, C.K. Shivakumar, K.N. Shivananda, G. Hegde, A.M. Isloor, *Eur J Med Chem* 2012, 54, 900–906.
[2] C.V. Maftei, E. Fodor, P.G. Jones, C.G. Daniliuc, M.H. Franz, G. Kelter, H.H. Fiebig, M. Tamm, I. Neda, *Tetrahedron* 2016, 72, 1185–1199.
[3] C. Al-Matarneh, I. Rosca, S. Shova, R. Danac, *J. Serbian Chem. Soc.* 2021, 86, 901–915.
[4] C.O. Vrancianu, I. Gheorghe, E.G. Dobre, I.C. Barbu, R.E. Cristian, M. Popa et al., *Int. J. Mol. Sci.* 2020, 21, 1–46.
[5] T. Mourer, M. El Ghalid, G. Pehau-Arnaudet, B. Kauffmann, A. Loquet, S. Brûlé, V. Cabral, C. d’Enfert, S. Bachellier-Bassi, *NPJ Biofilms Microbiomes* 2023, 9, 1–16.

ROLE OF GALLIC ACID CONTAINING FERROCENE IN ENHANCING ELECTROCHEMICAL DETECTION OF CAPECITABINE USING CARBON-BASED ELECTRODE

Alexandru Vişan[1]*, Sorina Motoc[1], Adelina A. Andelescu[1], Elisabeta I. Szerb[1], Florica Manea[2]
[1]*” Coriolan Dăgulescu” Institute of Chemistry, Romanian Academy, Timişoara, România*
[2]*Department of Applied Chemistry and Engineering of Inorganic Compounds and Environment Politehnica University of Timisoara, , Timişoara, Romania*
* *visan.alexandru@acad-icht.tm.edu.ro*

Introduction. Capecitabine (CPB), from cytostatic class of pharmaceuticals, is widely used in treatments of several forms of cancers, which make it to be present in various matrices of water, e.g., hospital effluents, wastewater treatment plants and surface water, with various concentrations related to the water matrix [1]. Electrochemical method is considered as being one of the most viable methods for CPB determination due to its well-known advantages related to simplicity, ease-to-operate, good sensitivity and time effectiveness [2, 3]. In this work, the effect of gallic acid containing ferrocene (Figure 1 - Gal_Fc) towards capecitabine oxidation and its byproducts reduction onto carbon nanotubes-carbon quantum dots paste electrode is studied in order to improve sensing performance.

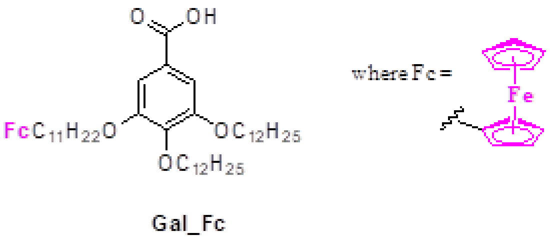


Figure 1. Molecular structure of Gal_Fc

Materials and Methods. All working paste electrodes were obtained by simple mechanical mixing of certain amount of carbon quantum dots (CQD), carbon nanotubes (CNT), gallic acid containing ferrocene precursor (Gal_Fc) and paraffin oil (oil), to assure CNT:oil = 1:1 for CNT electrode, CNT:CQD:oil = 0.8:0.2:2 for CNT-CQD electrode, and CNT:Gal_Fc:CQD: oil = 0.6:0.2:0.2:2 for CNT-Gal_Fc-CQD electrode.

Results and discussions. The electrochemical behavior of CNT, CNT-CQD, CNT-Gal_Fc-CQD were studied by cyclic voltammetry (CV), and the series recorded onto each electrode type in the presence of various CPB concentrations ranged from 1 to 5 mg·L^{-1} in 0.1 M Na_2SO_4 supporting electrolyte, are presented in Figure 2a, b. For CNT electrode no increasing the current in the presence of CPB, which informed that no CPB oxidation/ reduction onto CNT paste electrode (data not shown here). In the presence of CQD, one anodic peak is manifested at +0.13V/ SCE and corresponding cathodic one at +0.06V, both increasing at CPB concentration increasing (Figure 2a). Moreover, the presence of Gal_Fc within CNT-CQD composition modified CV shape by integration of Fe/Fe(II) redox couple at more negative potential (-0.45V/SCE) besides overlapping ferrocene/ ferrocenium redox couple with CQD oxidation/ reduction and ferrocene oxidation (+0.551 V/SCE) which is in according with the literature data [4]. All linear calibrations allowed determining the sensitivities, based on which all electroanalytical parameters of the CPB detection onto the tested electrode are determined and presented in Table 1.

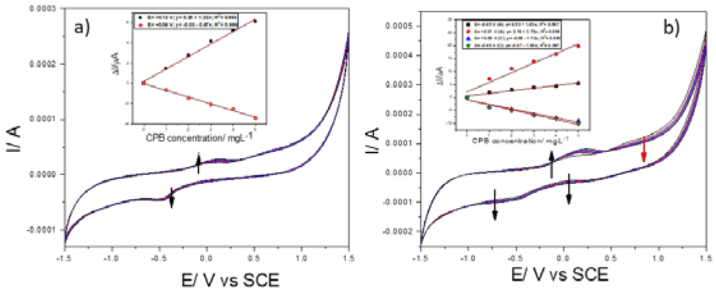


Figure 2. Cyclic voltammograms recorded in 0.1 M Na_2SO_4 supporting electrolyte (black line) at a scan rate of 0.05 $V \cdot s^{-1}$ in the presence of CPB concentrations ranged from 1 to 5 $mg \cdot L^{-1}$ (curve 2-6), within the potential range of −1.5 to +1.5 V/SCE with: (a) CNT-CQD electrode; Inset: Calibrations plots of peak current vs CPB concentrations recorded at each potential value and (b) CNT-Gal_Fc -CQD electrode; Inset: Calibrations plots of peak current vs CPB concentrations recorded at each potential value.

Table 1. The electroanalytical parameters for CPB detection obtained by CV technique.

Electrode type	Detection potential (peak type)/ V vs SCE	Sensitivity/ $\mu A/mg \cdot L^{-1}$	RSD/ %	LOD/ $mg \cdot L^{-1}$	LQ/ $mg \cdot L^{-1}$	R^2
CNT	-*	-	-	-	-	-
CNT-CQD	+0.13 (A)	1.23	0.19	0.10	0.34	0.993
	+0.06 (C)	0.67	0.41	0.16	0.54	0.995
CNT-Gal_Fc -CQD	-0.45 (A)	1.03	0.73	0.23	0.75	0.967
	+0.21 (A)	3.72	0.11	0.05	0.17	0.960
	+0.08 (C)	1.72	0.27	0.12	0.41	0.960
	-0.70 (C)	1.70	0.06	0.10	0.33	0.961

*no electrochemical signal;

It is obviously the superiority of the Gal_Fc - modified carbon electrode in CPB detection.

4. Conclusions

In this work, the significant role of gallic-acid-containing ferrocene in capecitabine detection was demonstrated using cyclic voltammetry technique. Two detection potentials corresponding for Fe/Fe(II) redox couple involving in oxidation of CPB and its byproducts reduction were manifested at the potential value of - 0.45 V/SCE. Also, within more positive anodic range, the electrocatalytic activity of carbon quantum dots was manifested and the presence of ferrocene enhanced the kinetics of oxidation and reduction processes and as consequence, detection sensitivity. The lowest limit of detection was 50 $\mu g \cdot L^{-1}$ at the potential value of +0.21 V/SCE. The electrochemical performance should be further improved through advanced voltametric and amperometric techniques, which will be optimized in the future work.

References

[1] M. Afzalia, A. Mostafavia, T. Shamspur, *Arab. J. Chem.*, 2020, 12, 6626-6638.
[2] S. Motoc, F. Manea, A. Baciu, C. Orha, A. Pop, *Int. J. Environ. Res. Public Health*, 2022, 19, 29.
[3] S. Motoc, F. Manea, A. Baciu, S. Vasilie, A. Pop, *Sci. Total Environ*, 2022, *846*, 157412.
[4] E. Popa, A.A. Andelescu, S. Ilies (b. Motoc), A. Visan, C. Cretu, F. Scarpelli, A. Crispini, F. Manea, E.I. Szerb, *Materials*, 2023, *16*, 1946.

Acknowledgment: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1958, within PNCDI III.

INDUCTION OF LIQUID CRYSTALLINE PROPERTIES IN Pt(II) COORDINATION COMPLEXES BASED ON TERPYRIDINE LIGANDS

Evelyn Popa*, Adelina A. Andelescu, Elisabeta I. Szerb
“Coriolan Dragulescu” Institute of Chemistry, Romanian Academy, Timisoara, Romania
**pevelyn@acad-icht.tm.edu.ro*

2,2':6',2"-terpyridine (*tpy*) and its 4 -substituted derivatives form metal complexes with a wide range of transition metal ions, which have potential applications in different fields as photophysics, catalysis and so on [1,2]. Platinum(II) terpyridine complexes are regarded as an important class of transition metal coordination compounds due to their spectroscopic and photophysical properties, having potential applications as chemosensors, photonic molecular switches, photocatalysis [3]. A series of ionic Pt(II) complexes with terpyridine ligands were reported to be promising candidates as luminescent supramolecular assemblies both in liquid crystalline phases and gels [4]. Highly luminescent metallomesogens (liquid crystals containing metals) are promising candidates for applications in electrooptic, more specifically in obtaining polarized emission for display devices [5,6].

On this background, herein we report a series of Pt(II) complexes based on *tpy* and a lipophilic gallate (Gal) unit as ancillary ligand, which were prepared according to a previously published procedure as described in Figure 1 [7].

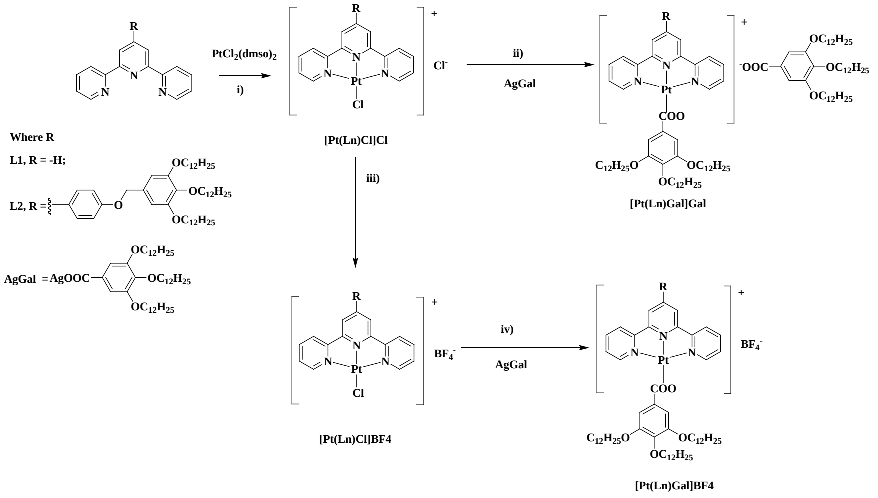


Figure 1. The synthethic pathway of Pt(II) tpy complexes with ligands L1 and L2; Reagents and conditions: i) MeOH, ΔT, 1.5 hours; ii) $CHCl_3$/MeOH 1:1, r. t., 2 hours; iii) NH_4BF_4, $CHCl_3$/MeOH 1:1, r. t., 1 hour; iv) $CHCl_3$, r. t., 2 hours.

The precursors and the final metallomesogens were characterized by spectroscopic (FT-IR and ^{1}H NMR) and analytic (elemental analysis) methods. Their liquid crystalline behaviour was assessed by polarized optical microscopy (POM) observations. Complexes lacking the lipophilic gallate unit did not possess LC behavior, having the melting temperatures >250 °C, accompanied by decomposition of the samples. The complexes containing one gallate unit [Pt(Ln)Gal]BF_4, and those containing two gallate units [Pt(Ln)Gal]Gal respectively, were found to posses low temperature LC behaviour (Table 1).

Complex [Pt(L1)Gal]Gal exhibit room temperature mesomorphism. The fan-shaped textures and presence of homeotropic zones observed on POM suggests the organization into supramolecular columnar mesophases (Figure 2).

Table 1. LC behaviour of complexes on POM.

Complex	**POM observations**
Pt(L2)Cl]Cl	Cr 131 ^{o}C Iso
Pt(L2)Cl]BF_4	Cr 140 ^{o}C Col 200 ^{o}C Dec
Pt(L1)Gal]Gal	Col 145 ^{o}C Iso
[Pt(L1)Gal]BF_4	Cr 125 ^{o}C Col_1 240 ^{o}C Col_2 >250 ^{o}C Iso
[Pt(L2)Gal]BF_4	Cr 70 ^{o}C Col_1 120 ^{o}C Col_2 251 ^{o}C Iso

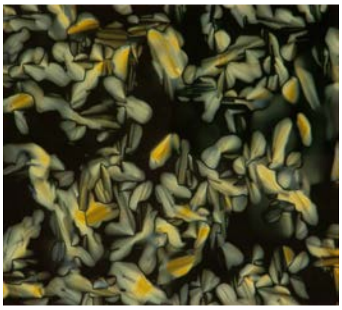


Figure 2. POM micrograph at of the texture observed at 130 ^{o}C, first cooling, magnification x50, for complex [Pt(L1)Gal]Gal.

In conclusion, the induction of liquid crystalline properties in Pt(II) coordination complexes was carried out successfully. Complex [Pt(L1)Gal]Gal presented room temperature columnar liquid crystalline properties. The study will be followed by investigation of their photophysical properties in solution and condensed states.

References

[1] C. Wei, Y. He, X. Shi, Z. Song, *Coord. Chem. Rev.* 2019, 385, 15, 1-19

[2] N.S. Saleesh Kumar, M.Z. Shafikov, A.C. Whitwood, B. Donnio, P.B. Karadakov, V.N. Kozhevnikov, D.W. Bruce, *Chem. Eur. J.* 2016, 22, 8215 – 8233.

[3] (a) F. Camerel, R. Ziessel, B. Donnio, C. Bourgogne, D. Guillon, M. Schmutz, C. Iacovita, J.P. Bucher, Angew. *Chem. Int. Ed.* 2007, 46, 2659–2662, (b) Y. Chen, C.-M. Che, W. Lu, *Chem. Commun.* 2015, 51, 5371–5374, (c) K. Li, G.S.M. Tong, Q. Wan, G. Cheng, W.-Y. Tong, W.-H. Ang, W.-L. Kwong, C.-M. Che, *Chem. Sci.* 2016, 7, 1653–1673, (d) S. Elmas, W. B., S. J. Bradley, R. Kroon, G. Laufersky, M. Andersson, T. Nann, *ACS Sustainable Chem. Eng*. 2017, 5, 11, 10206–10214

[4] C. Cuerva, M. Cano, C. Lodeiro, *Chem. Rev.* 2021, 121, 12966−13010.

[5] B. Doistaul, J.-R. Jiménez, C. Piguet, *Phys. Chem. Chem. Phys.* 2020, 22, 19903-19912

[6] A.A. Andelescu, B. Heinrich, M. A. Spirache, E. Voirin, M. La Deda, G. Di Maio, E. I. Szerb, B. Donnio, O. Costisor, *Chem. Eur. J.* 2020, 26, 4850–4860.

[7] D. Mahendiran, R.S. Kumar, V. Viswanathan, D. Velmuruganc, A.K. Rahiman, *Dalton Trans.* 2016, 45, 7794-7814.

Acknowledgment: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1958, within PNCDI III.

INTERACTION BETWEEN WATER-SOLUBLE CHITOSAN AND THERMO-RESPONSIVE POLY(N-ISOPROPYLACRYLAMIDE)

Elena-Daniela Lotos[1]*, Maria Karayianni[1], Ana-Lavinia Vasiliu[1], Larisa-Maria Petrila[1], Marcela Mihai[1], Stergios Pispas[1,2], Bogdan C. Simionescu[1]
[1]*Petru Poni Institute of Macromolecular Chemistry, Iași, Romania*
[2]*Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece*
**daniela.lotos@icmpp.ro*

Introduction: Biopolymers have gained attention in the past few decades due to their abundance and excellent biocompatibility. Chitosan is obtained from chitin, the second most widespread natural resource, by the deacetylation process [1]. Due to its antimicrobial properties, biocompatibility, biodegradability and non-toxicity, chitosan is suitable for numerous applications, such as food additives, removal of metallic ions, skincare products, drug delivery, tissue regeneration and wound healing [2,3].

Materials and methods: The aim of this study was to investigate the electrostatic interaction between water-soluble chitosan ($M_w = 162{,}000$ g/mol, CHI_{162k}) and a poly(*N*-isopropylacrylamide) ($M_w = 19{,}300$ g/mol, $PNIPAM_{19k}$) with a carboxylic end group. First, the chitosan sample was characterized using several methods: FTIR-ATR, WXRD, NMR and potentiometric titrations. Subsequently, electrostatic complexes between the two macromolecules were prepared by keeping constant the CHI_{162k} volume (4 mL) and varying that of $PNIPAM_{19k}$ (1, 2 or 4 mL), namely Complex 4/1, 4/2 and 4/4. The solution properties of the obtained complexes in regard to their mass, size and charge were studied by dynamic and electrophoretic light scattering (DLS / ELS). Moreover, the morphology of the samples was followed by STEM. Finally, the influence of solution temperature was investigated for all complexes (from room temperature up to 45 °C).

Results and discussion: In Figure 1a it is observed that the scattering intensity is increasing with increasing $PNIPAM_{19k}$ concentration. This indicates an increase of the mass of the complexes, proving that the electrostatic complexation between the two components occurred. Furthermore, the measured zeta potential values are slightly decreasing, as expected, due to the interaction with the negatively charged $PNIPAM_{19k}$. Size distributions (Figure 1b) exhibit the presence of one population of particles in the case of CHI_{162k} and two or three populations for $PNIPAM_{19k}$ and the complexes, respectively. The various observed populations most probably correspond to complexes comprising of different total numbers of chains. Additional details about the shape of the complexes can be deduced from the representative STEM micrograph obtained for Complex 4/1 shown in Figure 1c. The image shows uniform spherical shaped and dense structures at nanometric scale.

Ultimately, by taking DLS measurements at various temperatures, the thermal behavior of the prepared complexes was investigated. Figure 1d presents the corresponding size distributions for Complex 4/1 and reveals that above 35 °C only one population is present, indicating the formation of compact structures, apparently due to the increase of the hydrophobicity of the $PNIPAM_{19k}$ chains in the complexes. However, the system returns to the initial state after cooling.

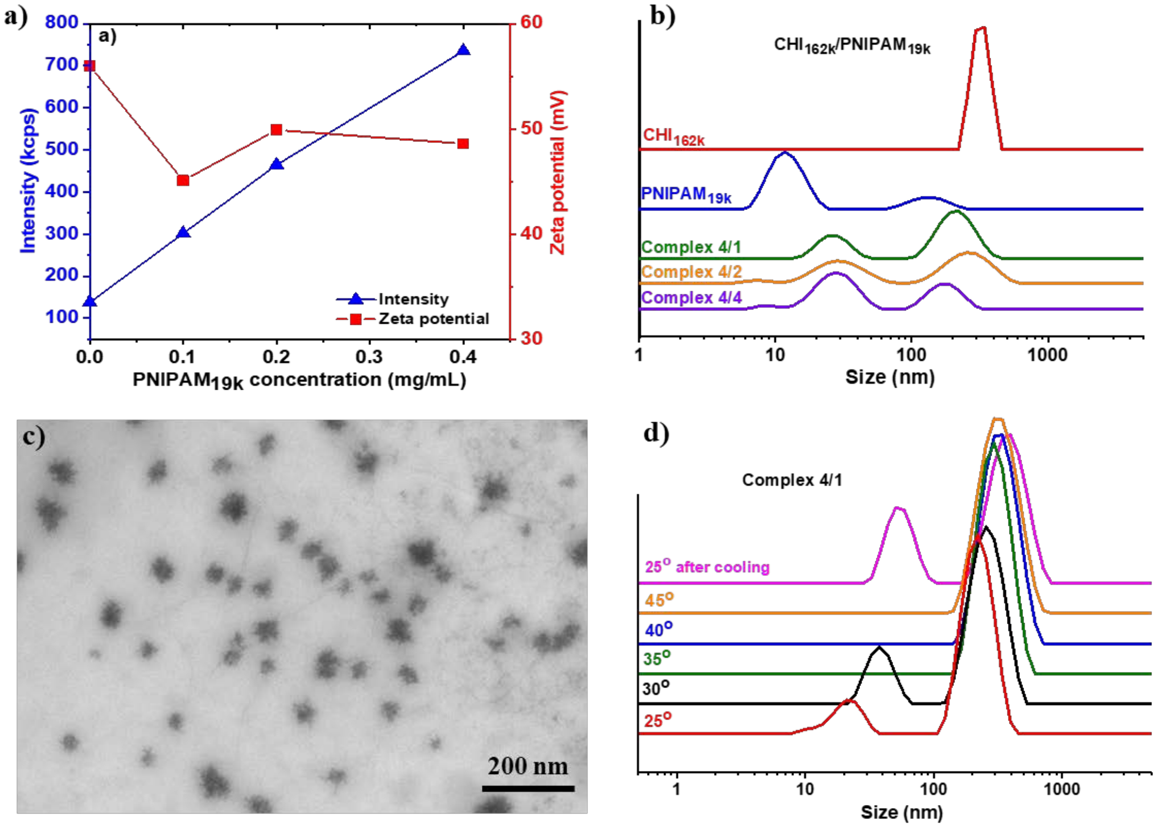


Figure 1. (a) Scattered intensity and zeta potential; (b) size distributions, for the CHI_{162k}/$PNIPAM_{19k}$ complexes; (c) STEM micrograph for Complex 4/1; (d) size distributions for Complex 4/1 at different temperatures.

Conclusions: We obtained thermo-responsive hybrid nanostructures by electrostatic interaction of a water-soluble chitosan and PNIPAM with one carboxylic functional group on its chain. The overall physicochemical characteristics of the formed complexes proved dependent on the ratio of the two macromolecular components.

References

[1] F. Hisham, M.H. Maziati Akmal, F. Ahmad, K. Ahmad, N. Samat, *Ain Shams Eng. J.* 2023, 102424.

[2] M. Karayianni, T. Sentoukas, A. Skandalis, N. Pippa, S. Pispas, *Pharmaceutics* 2023, 15, 1849.

[3] M.A.S. Abourehab, S. Pramanik, M.A. Abdelgawad, B.M. Abualsoud, A. Kadi, M.J. Ansari, A. Deepak, *Int. J. Mol. Sci.* 2022, 23, 10975.

Acknowledgment: This work was supported by the Ministry of Research, Innovation and Digitization, by project number PN-III-P4-ID-PCE-2020-1541, within PNCDI III - CCCDI-UEFISCDI, and by project number PNRR-III-C9-2022-I8-201, within the National Recovery and Resilience Plan.

CATALASE/POLYMER COMPOSITE MICROPARTICLES FOR ENVIRONMENTAL APPLICATIONS

Larisa-Maria Petrila*, Florin Bucătariu, Marcela Mihai
Petru Poni Institute of Macromolecular Chemistry, Iași, Romania
**larisa.petrila@icmpp.ro*

Introduction: The development of human society and the fast increase in the demand for resources and their consumption lead, in the last few years, to an unprecedented increase in the pollution of water, air and land. The unsustainable use of natural resources and the scanty treatment of secondary products of industry and daily life open the door to one of the most important challenges humankinds is facing – the need to develop new and efficient methods to decrease the impact of pollution. The water pollution is maybe the most important problem we have to mitigate, as water can easily be polluted by various human activities, with important issues related to health and wellbeing. Water is one of the most versatile resources on earth and can play the role of a solvent to many emerging pollutants such as dyes, metal ions, pharmaceutical compounds, pesticides and so on. In this context, efficient water treatment methods are on demand, with both classical and innovative methods being studied and optimized by the scientific community. The use of composite materials as treatment agents for the sorption and/or degradation of concerning pollutants are one of the methods of interest because of their increase potential for targeting specific pollutants [1]. Between the composite materials that can be used for water treatment, immobilized enzyme-based materials are outstanding because of their natural origin, selectivity for emerging pollutants such as dyes or endocrine disruptors, high catalytic/degradation capacity and easy recovery and reuse [2]. This study proposes a novel immobilized-enzyme composite material based on catalase and chitosan, with increased degradation capacity towards organic dyes. The fabrication methods, properties and potential applications of these composites in the degradation of a model pollutant, namely Indigo carmine, are presented. The results obtained suggest that the immobilized catalase composite microparticles can be successfully used in water treatment.

Methodology: The fabrication of immobilized-enzyme composite microparticles was achieved by the direct deposition of an enzyme/ polyelectrolyte complex formed with chitosan and catalase on Silica microparticles (SP1k type). The deposition of a stable organic shell was ensured by the chemical cross-linking of the polyelectrolyte chains employing glutaraldehyde, leading to the formation of a stable polymer/enzyme composite material (denoted SP1k/(CHI/CAT)_c). In order to compare the characteristics of the enzyme-based composite material, a control sample was fabricated by the deposition of an organic shell of chitosan on the Silica microparticles (denoted SP1k/CHI_c). The sample was fabricated and stabilized in similar conditions, but in absence of CAT. The successful fabrication of the composite materials was confirmed by ATR-Fourier-transform infrared spectroscopy and the properties of the composite samples were evaluated based on potentiometric titrations. In order to assess the potential environmental applications of the catalase-based composite materials, the degradation of Indigo carmine, as a model pollutant, was studied in different conditions. The experiments were also performed employing the control sample.

Results and conclusions

The method proposed for the fabrication of the enzyme-based composite materials lead to fabrication of composite materials with immobilized catalase by a fast and simple protocol. The immobilization of catalase was ensured by the deposition of an interpolyelectrolyte complex formed between the enzyme and chitosan, as oppositely charged polyelectrolyte, on the Silica particles. The method allowed the formation of core-shell inorganic/organic composites materials, characterized by mechanical stability and satisfactory chemical properties based on the increased and accessible number of functional groups of the organic shell. The successful immobilization of catalase on the polymeric shell was demonstrated by the potentiometric titrations (Figure 1a), which highlighted the effect of the catalase on the isoelectric point (iep) of the material. By comparing the ieps of a control sample and the CAT-based composite, we can observe that the presence of CAT, a negatively charged enzyme, shifts the iep towards the acidic region, confirming the presence of the enzyme on the material’s surface.

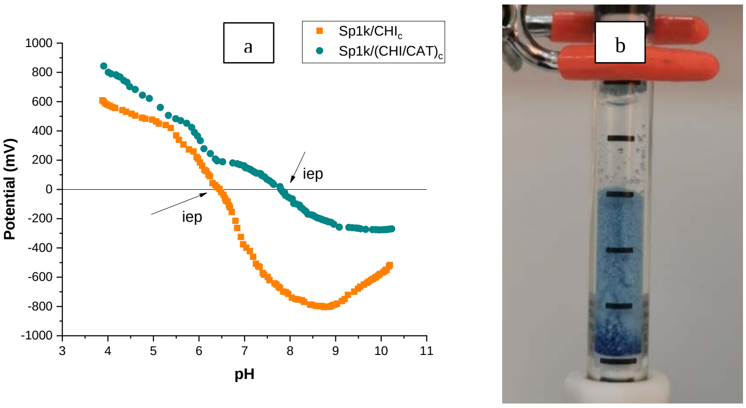


Figure 1. (a) The variation of the potential as a function of pH for the SP1k/CHI$_c$ and SP1k/(CHI/CAT)$_c$ composites; (b) interaction with Indigo Carmine in dynamic conditions.

The potential employment of these composites in water treatment was assessed by studying the sorption and degradation of Indigo carmine from a diluted aqueous solution in the presence of the SP1k/(CHI/CAT)$_c$ composite and H_2O_2 in dynamic conditions (Figure 1b). The degradation of the dye in the water sample was successfully achieved in the presence of the composite material by a combination of sorption and enzymatic degradation processes, leading to a water cleaning efficiency of more than 90%.

Conclusions

The results obtained so far suggest that the catalase-based composite materials presented can be successfully used for water treatment applications in various experimental conditions. Further studies will be focused in the optimization of the water treatment method proposed here.

References

[1] F. Bucatariu, C. Teodosiu, I. Morosanu, D. Fighir, R. Ciobanu, L.M. Petrila, M. Mihai, *Polymers* 2021, 13, 3963.
[2] L.M. Petrila, R. Grădinaru, F. Bucatariu, M. Mihai, *Chemistry* 2022, 4(4), 1312-1338.

Acknowledgement: This work was supported by the Ministry of Research, Innovation and Digitization, by project number PNRR-III-C9-2022-I8-201, within the National Recovery and Resilience Plan.

BIOACTIVE MOLECULES OF SAFFRON OIL EXTRACTED FROM BIOMASS, TESTED ON DANIO RERIO AS ANTI-TUMORAL AND ANTI-INFLAMMATORY AGENTS

Marius – Vasile Bârdan*

Department of Chemistry, Physics and Environment"Dunarea de Jos" University, Galati, Romania
**nifonmariusvasile@gmail.com*

The preparation of medicinal plants for experimental purposes is an initial step and key in achieving quality research results. It involves the extraction and determination of quality and quantity of bioactive constituents before proceeding with intentional biological testing. The main objective of this study was to evaluate various methods used in the preparation and screening of medicinal plants within our daily research. Although extracts, bioactive fractions or compounds obtained from medicinal plants are used for different purposes, the techniques involved in their production are generally the same, regardless of the biologic desired testing. The major steps included in acquiring the quality bioactive molecule are selection of a suitable solvent, extraction methods, phytochemical screening, procedures, fractionation methods and identification techniques [1].

Saffron contains iron, protein, curcumin - it is the strongest natural anti-inflammatory, antioxidant with anti-cancer and antiviral effects, volatile oils, sodium, potassium, vitamins B1 and B2, phytohormones, it is appreciated as a medicine, due to its component, and therapeutic properties, known since antiquity [2]. Its beneficial effects are still appreciated today in natural medicine such us: tonic effects on the heart and on the respiratory system, improves blood circulation, inhibits the development of cancer cells stops fat deposition in the body due to curcumin content, helps vision and prevents macular degeneration, lowers cholesterol and triglycerides in the blood, stimulates the digestive tract, helps relieve hepatic steatosis, treats burns and light wounds and helps to regenerate the skin, it has also anti-aging effects. In recent years, in Romania, interest in saffron cultivation has increased, which is why quite a few saffron crops have appeared. However, those who cultivate do not yet have solutions for processing floral residues obtained after harvesting stigmas, the only solution being their disposal as vegetable waste. In general, saffron floral residues are disposed of as waste, added to compost and therefore used as fertilisers [3] or recovered by extraction of natural textile dye [4]. Few studies on other parts of *C. sativus* flowers have been conducted. The use of saffron residues as food is less widespread and perhaps less well known. The most important compounds in saffron are crocin, picrocrocin and safranal, responsible for its color and flavor [5]. The quantities of these main compounds are used to express the quality of saffron [6]. There are some studies confirming that these main compounds could also have a significant concentration in floral residues. Nowadays, saffron petal is used as an organic agent in agricultural industries [7]. Phytochemical studies have reported the presence of flavonoids and anthocyanins in saffron petals, which have shown beneficial effects due to their bioactive potential [8, 9]. In traditional medicine, saffron petals are used as antispasmodics, stomachic, anxiolytics, antitumors and antidepressants.

Due to the phytochemical compounds in the composition and their traditional use, they can be used in various medicinal fields. The beneficial properties of saffron floral residues are due to their high flavonoid content [10-15]. They are also a rich source of kaempferol 3-O-sophoroside (K3-S) [12] and delphinidin 3,5-di-O-glucoside [13]. Anti-inflammatory effects in human endothelial cells of K3-S have been demonstrated [16] and their analgesic activity [17]. Delphinidin is a potent inhibitor of epidermal growth factor receptor [18] and angiogenesis [19]. Phytochemical analysis has shown that saffron flowers are rich in antioxidant compounds such as flavonols, flavanones, crocin [20] and crocetin. Antioxidants have been thought to be the active ingredients responsible for a variety of health-enhancing properties that have traditionally been attributed to saffron.

References

[1] A.R. Abubakar, M. Haque, *J. Pharm. Bioall. Sci.* 2020, 12, 1-10.

[2] M. Negbi, 2005, Saffron: Crocus sativus L., Harwood Academic Publishing Singh D., J. Davidson, 2015, The Magic of Saffron – For Beauty and to Heal

[3] A.R. Astarei, M. Eskandari-Torbaghan, R. Abbasi-Ali Kamar, II Int Symp. Saffron Biol. Technol. 2006, 739, 87-91.

[4] M. Bergoin, PhD Thesis, Institut National Polytechnique de Toulouse, Toulouse (2005).

[5] U. Bulbake, S. Doppalapudi, N. Kommineni, W. Khan, *Pharmaceutics* 2017, 7, 9(2), 12.

[6] A.N. Cadinoiu, C.A. Peptu; in Popa, M., Uglea, C.V. (Eds.); Polymeric nanomedicines, Ed. Bentham Science Publishers, 2013, pp. 293-316.

[7] L. Favot, S. Martin, T. Keravis, R. Andriantsitohaina, C. Lugnier, *Cardiovasc. Resc* 2003, 59, 479–487.

[8] J.A. Fernandez, Biology, biotechnology and biomedicine of saffron, Recent Research in Developmental Plant Science 127-159 (2004).

[9] S.A.H, Goli, F. Mokhtari, M. Rahimmalek, *J. Agric. Sci.* 2012, 4, 175-181.

[10] P. Goupy, M. A. Vian, F. Chemat, C. Caris-Veyrat, *Ind. Crops Prod.* 2013, 44, 496–510.

[11] A. Hosseini, B.M. Razavi, H. Hosseinzadeh, *Iran J. Basic Med. Sci.* 2018, 21, 1091- 1099.

[12] H. Hosseinzadeh, J. Behravan, M. Ramezani, K. Ajgan, *J. Med. Plants.* 2005, 3, 59-65.

[13] T. H. Kim, S. K. Ku, I. C. Lee, J.S. Bae, *Inflamm. Res.* 2012, 61, 217–224.

[14] I. Marchioni, La. Pistelli, B. Ferri, P.L. Cioni, A. Copetta, Lu. Pistelli, B. Ruffoni, *Bulg. Chem. Commun.* 2019, 51, 131-136.

[15] S. Meiers, M. Kemény, U Weyand, R. Gastpar, E. von Angerer, D. Marko, *J. Agric. Food Chem.* 2001, 49, 958-962.

[16] P. Montoro, M. Maldini, L. Luciani, C.I.G. Tuberoso, F. Congiu, C. Pizza, *J. Food Sci.* 2012, 77, 893-900.

[17] S.M. Mortazavi, M. Kamali Moghaddam, S. Safi, R. Salehi, *Prog. Color Colorants Coat*. 2012, 5, 75-84.

[18] R. Nørbæk, K. Brandt, J. K. Nielsen, , M. Ørgaard, N. Jacobsen, *Biochem. Syst. Ecol.* 2002, 30, 763–791.

[19] S. Palanichamy, S. Nagarajan, *J. Ethnopharmacol.* 1990, 29, 73-78.

[20] A. M. Sánchez, G. Jerz, J. Serrano-Díaz, G. L. Alonso, P. Winterhalter, Flavonol composition and isolation of kaempferol 3-O-sophoroside from saffron (*Crocus sativus* L.) floral bio-residues. In Gesellschaft Deutscher Chemiker. Proceeding 40. Deutscher Lebensmittelchemikertag (pp. 231). Germany: Halle. (2011).


MacroYouth 2023

ROMANIAN CHEMICAL SOCIETY
SOCIETATEA DE CHIMIE DIN ROMANIA, SChR

"Chemistry is not everything, but anything is nothing without chemistry"

SChR Objective: *"Attracting young people towards chemistry as study field and profession "*

Sections and Local Branches

21 Local branches

7 Sections

3000 Members

(including honorary and affiliated members – students and pupils)

The activity of organizing scientific meetings is continued and developed:

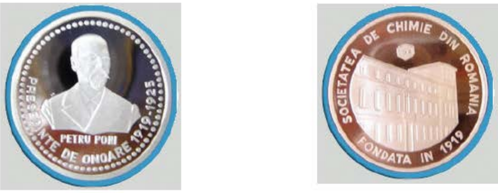
- *ICOSECS, The International Conference of the Chemical Societies of the South Eastern European Countries* is organized by regional cooperation with the chemical societies from Albania, Bulgaria, Cyprus, Greece, Macedonia, Montenegro and Serbia
- *COFrRoCA, The Franco-Romanian Colloquia of Applied Chemistry* is organized in cooperation with the universities of Bacau (Romania) and Orleans (France)
- Periodically international conferences of a high scientific level are organized in cooperation with the University Politechnica Bucharest, Ovidius University Constanta, Petru Poni Institute of Macromolecular Chemistry Iasi.

The present publications of SChR include the ***Bulletin of the Romanian Chemical Society*** (an information journal on the activity in chemistry in Romania), ***Revista de Chimie*** (a scientific journal publishing original results, with a constantly rising ISI impact factor), ***Chimia*** (a publication for undergraduates), as well as a series of publications of the local sections of SChR: *ProChimia*, *Universul Chimiei*, *ChimMax*.

The ***Bulletin of the Romanian Chemical Society*** founded in 1919, since the very beginning of SChR, aims to periodically present the life and activity of SChR, the actions of the Society for the promotion of chemistry and its position on the chemistry policy.
Among the modern numbers is the one from 2009 where one can find detailed information about the SChR history as well as about some outstanding personalities of the Romanian chemistry.

For high school students, the journal ***Chimia*** was launched in the early 2000s. It included comprehensive articles on the topics of contemporary chemistry (sometimes written by eminent students), exciting problems and experiments, curiosities and biographical notes of the great Romanian or universal chemists.

"SChR grants medals, prizes and awards as recognition of scientific and/or professional activities of the chemists, located in the country or abroad" – SChR Rules



Petru Poni – first SChR medal

...in Pre-university Education

....in Inorganic Chemistry

... in Organic Chemistry

... in Chemical Engineering

Many important figures of the chemical world are honorary members of SChR and visited Romania on various occasions. SChR signed bilateral agreement papers with several societies within Europe.

SChR - Member of EUChemS

EuChemS, the European Chemical Society, is an umbrella organisation representing national Chemical Societies and other chemistry-related organisations in Europe. EuChemS aims to nurture a platform for scientific discussion and to provide a single, unbiased European voice on key policy issues in chemistry and related fields. Contact: www.euchems.org

EuChemS
European Chemical Society

The local sections of SChR together with the universities have as an important activity to attract young people in the study of chemistry. The constant orientation to increase weight of the experimental activity is not aleatory, nor is it isolated. It comes from the tendency to fill, even partially, the gaps in experimental instruction of the undergraduate studies and it follows the recommendations of SChR. Many of the activities promoted by the local sections and the sections of the society belong to this line of action.

STC – "Sectia Tinerilor Chimisti" - the Youth Division of SChR is an active and dynamic group.

The STC SChR members were part of the initiative group that sign the formation of EYCN in 2007 in Berlin. Since then, members of STC were part of the EYCN board and in 2011-2013 chaired EYCN/

Contact: Romanian Chemical Society, Str. Gheorghe POLIZU, nr. 1-3, sector 1, BUCURESTI, ROMANIA, Phone: +4 021 402 3962; +4 021 402 3912, Email: secretargenschr@icmpp.ro

UNIUNEA EUROPEANĂ
Instrumente Structurale
2014-2020

INFRA SUPRACHEM LAB - CENTER FOR ADVANCED RESEARCH IN SUPRAMOLECULAR CHEMISTRY

Marcela Mihai, Narcisa-Laura Marangoci
Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania
**marcela.mihai@icmpp.ro*

1. General information

- *Beneficiary*: Petru Poni Institute of Macromolecular Chemistry Iasi (Institutul de Chimie Macromoleculara Petru Poni, ICMPP)
- Project co-financed by European Regional Development Fund under the Competitiveness Operational Program 2014-2020
- *Priority Axis 1* – Research, Technological Development and Innovation to Support Economic Competitiveness and Business Development
- *Investment priority 1a* – Improving research and innovation infrastructures and capacities to develop excellence in RDI and promoting centers of expertise, especially those of European interest
- *Action 1.1.3* Creating synergies with the RDI actions of the European Union's HORIZON 2020 framework program and other international RDI programs
- *Period*: 25.02.2021 – 24.06.2023.
- *MySMIS*: 108983

2. General objective

The overall objective of the Infra SupraChem Lab project is to create an advanced infrastructure that deserves the supramolecular chemistry working group SupraChem Lab, a group created within the Horizon 2020 Project WIDESPREAD 2-2014: ERA Chairs (667387) - SupraChem Lab Laboratory of Supramolecular Chemistry for Adaptive Delivery Systems ERA Chair initiative.

3. Specific objectives / Expected results

O1. Realization of the design component for the Infra SupraChem Lab project - objective already in implementation
O2. Realization of the infrastructure of the SupraChem Lab center
O3. Equipping and launching the SupraChem Lab center
O4. Dissemination and publicity
O5. Project management

The implementation of the Infra SupraChem Lab project represents the creation of an adequate structure for the activity of the SupraChem Lab group, a group formed through a Horizon 2020 ERA CHAIR project (Horizon 2020 WIDESPREAD 2-2014: ERA Chairs Project no 667387).

The SupraChem Lab project started in 2015 and with the support of EC investment of 2.5 MEuro, the foundation of a young team of researchers was laid, focused on the principles of supramolecular chemistry knowledge.

The team's research areas range from the creation of dynamic systems for targeted biomedical applications to the dynamic molecular modeling of the interaction of complex supramolecular systems. The group human resource represents a secure core for the training of new generations of specialists, able to continue and develop new fields with great applicative impact.
Over the last ten years, ICMPP's research directions have clearly evolved into interdisciplinary fields and have been adapted to global research trends, while also presenting their own original directions, based on knowledge and experience gained over time.

The implementation of the Infra SupraChem Lab project would contribute to the improvement of the existing research within ICMPP and SupraChem Lab team and to the development besides the fundamental research directions and of some applied research directions for new top products.
An important part in the development of new directions is based on a modern infrastructure, aimed at interdisciplinary research. An infrastructure based on the synthesis and complete characterization of new materials represents a real support for the development of application fields. The Infra SupraChem Lab infrastructure is a step forward to create the premises for application of the results of fundamental research obtained by the newly created group.

Infra SupraChem Lab will be set up in spaces owned by the ICMPP - in buildings currently unused, under conservation. The new center will also benefit from the arrangement of auxiliary spaces, for the storage of chemicals, glassware and laboratory materials as well as the related access ways to facilitate the access to the research infrastructure.

The structure of Infra SupraChem Lab will include the following departments:
A. **Operating department** consisting of:
A1. Chemical and biochemical synthesis laboratory
A2. Laboratory for the study of special properties and possible applications
A3. Physical and chemical characterization laboratory
The laboratories are be provided with chemical ventilation niche and specific laboratory equipment for chemical syntheses (eg: magnetic stirrers, inert gas purification installations, vacuum pumps, electric ovens, etc.), study of properties and material characterization (e.g. X-ray diffractometer for wide angles, Photo-DSC, Automatic confocal imaging system for scanning, characterization and data analysis in cell biology, Semi-automatic inverted fluorescence microscope, Diffractometer with dual X-ray source for single crystals, Motorized stereomicroscope with fluorescence with the possibility of in-depth analysis, and many others).

B. **Data processing department**
Within this department, the data will be processed and structural optimization studies will be performed.

C. **Department of projects and technology transfer**
All departments are provided with computers connected to the Internet and implicitly to the internal network of the center.

The project has as direct beneficiaries the SupraChem Lab team, the project being addressed also to other interest groups as follows:

- graduates of the universities of Iasi and not only who could join the SupraChem Lab team or could benefit from training within the newly created Center
- teachers from universities in Iasi and not only, who will be able to carry out educational activities within the center
- researchers from ICMPP or other collaborating research institutions, who will be able to perform tests or determinations on the equipment within the center
- different SMEs that will be able to benefit from technology transfer facilities of the patented results that will be obtained within the center.

PETRU PONI
INSTITUTE OF
MACROMOLECULAR
CHEMISTRY

Infra SupraChem Lab

Center for Advanced Research in Supramolecular Chemistry

BioMat4CAST
MULTI-SCALE IN SILICO LABORATORY FOR COMPLEX AND SMART BIOMATERIALS

Teodora Rusu,* Mariana Pinteala, Aatto Laaksonen, Tudor Vasiliu
Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Iasi, Romania
**teodora.rusu@bionanotech.ro*

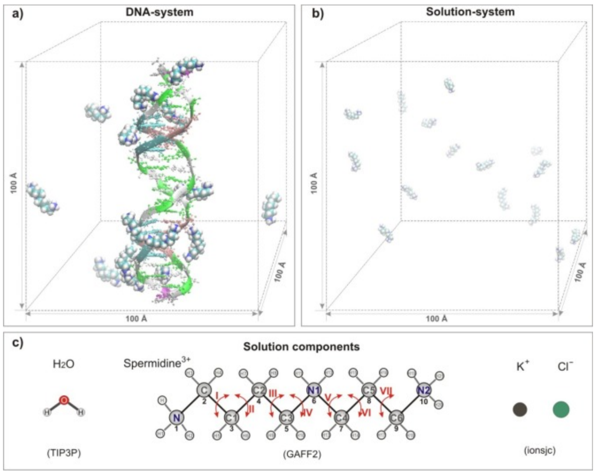
1. Introduction

The Multi-Scale In Silico Laboratory for Complex and Smart Biomaterials, BioMat4CAST, is a European research project focused on developing computational models to design and test biomaterials for various biomedical applications. The project uses advanced computational simulations to model different factors such as the material's structure, properties, and interactions with biological systems.

The strategic objective of the BioMat4CAST project is to implement a structural change within in the scientific management paradigm of “Petru Poni” Institute of Macromolecular Chemistry (ICMPP), Iasi, Romania, by setting up a competitive research group in the field of computational chemistry under the supervision of an outstanding researcher manager in the field of computational chemistry, Prof Aatto Laaksonen (Arrhenius Laboratory, Stockholm University, Sweden). The BioMat4CAST project addresses the design and development process for smart biomaterials applications in fields ranging from drug delivery systems, implantable devices, and tissue engineering to regenerative medicine and personalized medicine. The technology developed in the project has the potential to accelerate the discovery and development of new biomaterials for biomedical applications.

2. Computational Chemistry

The computational chemistry has revolutionized the way we approach research in the field of chemistry, providing a powerful tool for investigating the structures, properties, and interactions of molecules and materials without the need for extensive laboratory experimentation. As a result, many researchers believe that computational chemistry is the laboratory of the future, offering numerous advantages that traditional laboratory methods cannot provide. An example of a situation where computational chemistry has a clear advantage over traditional laboratory methods is in elucidating the interaction between different compounds, as depicted in the figure to the right, where two simulations were performed to compare how spermidine, a natural polyamine that plays an important role in DNA condensation, behaves when alone in solution or when interacting with the DNA molecule.



Understanding these types of interactions between DNA and natural molecules, i.e. how spermidine changes is conformational space, is important to better design new and improved non-viral carriers for DNA [1]. One of the significant benefits of computational chemistry is the speed and efficiency in simulating experiments. It is possible to perform extensive simulations of chemical and biological systems quickly and accurately, making it easier to identify chemical reactions and molecular interactions that might not be observable under laboratory conditions. Another significant advantage of computational chemistry is the ability to access molecular structures in unprecedented detail. By using molecular modelling and simulation techniques, researchers can observe the behaviour of molecules at the atomic level, which can provide valuable insights into the chemical and physical properties of materials and substances. The design of polymers with imposed properties involves tailoring the chemical structure of the polymer to achieve specific properties, such as mechanical strength, thermal stability, or biodegradability. This process can be achieved through various methods, including monomer selection, polymerization conditions, and post-polymerization modifications. Polymerization conditions can also be adjusted to influence the properties of the final polymer. For example, the type of initiator, solvent, and temperature used in the polymerization process can affect the molecular weight, reaction rate, and morphology of the polymer. By properly controlling these parameters, it is possible to tailor the polymer's properties to meet specific requirements. Post-polymerization modifications can also be used to adjust the properties of a polymer. These modifications can include chemical reactions, physical treatments, or the addition of other substances to alter the polymer's properties. For example, surface modification techniques can be used to improve the biocompatibility of a polymer for medical applications.

In summary, the design of polymers with imposed properties involves a combination of monomer selection, polymerization conditions, and post-polymerization modifications. By carefully tailoring these factors, it is possible to create polymers with precisely targeted properties to meet specific needs.

3. The Safe and Sustainable by Design (SSbD) European Strategy

The SSbD framework is an approach to guide the innovation process for chemicals and materials, that *“aims to:*

- *steer the innovation process towards the green and sustainable industrial transition*
- *substitute or minimise the production and use of substances of concern, in line with, and beyond existing and upcoming regulatory obligations*
- *minimise the impact on health, climate and the environment during sourcing, production, use and end-of-life of chemicals, materials and products*

The framework is composed of a ***(re-)design phase*** *and an* ***assessment phase*** *that are applied iteratively as data becomes available”* [2].

The central objective of the safe and sustainable by design strategy is to minimize the environmental and health impact of products and materials throughout their entire lifecycle, from the manufacturing stage to the end of the product's useful life.

There are several key principles of this strategy:

- Use non-toxic and sustainable raw materials for the production of products and materials wherever possible.
- Strive to minimize or eliminate hazardous substances and chemicals that can pose a threat to human health and the environment.
- Minimize waste and pollution by designing products and materials that can be easily recycled and reused.
- Design for durability and longevity to reduce the need for frequent replacement and disposal of products and materials.
- Promote sustainability throughout the entire supply chain, including responsible sourcing of raw materials, responsible manufacturing practices, and safe and sustainable disposal and recycling practices.
- Consider the entire lifecycle of the product in the design process, including the energy required to produce the material, the energy consumed during use, and the impact on the environment and human health after disposal.

By incorporating these principles into the design process, the safe and sustainable by design strategy aims to create products and materials that are safe for human health and the environment, durable, and conducive to sustainability. Thus, the BioMat4CAST project will support the ICMPP research to comply with the sustainable by design chemicals and materials principles by focusing on the aim to minimize the use of non-renewable resources, reduce waste and pollution, and promote a circular economy.

4. Conclusions

In conclusion, computational chemistry has the power to change the future of laboratory-oriented chemistry, providing researchers with powerful tools to predict, design, and develop new molecules and materials, while also reducing the cost and environmental impact of laboratory experimentation. The BioMat4CAST project is bringing the future of chemistry in ICMPP.

References

[1] S. Perepelytsya, T. Vasiliu, A. Laaksonen, L.D.V. Engelbrecht, G. Brancato, F. Mocci, *J. Mol. Liq*. 2023, 389, 122828.

[2] See documents defining the SSbD framework on: https://ec.europa.eu/info/research-and-innovation/ research-area/industrial-research-and-innovation/key-enabling-technologies/advanced-materials-and-chemicals_en

Acknowledgements

This paper is supported by European Union's Horizon Europe research and innovation programme under grant agreement No 101086667, project BioMat4CAST (BioMat4CAST - Multi-Scale In Silico Laboratory for Complex and Smart Biomaterials).

ELEVATING SCIENTIFIC RESEARCH WITH RIGAKU'S CUTTING-EDGE EQUIPMENT PORTFOLIO

AMS 2000 TRADING IMPEX SRL, Bucharest, Romania
**claudia.gavrilescu@ams.ro; www.ams.ro; 0730 711 952*

1. Introduction

AMS 2000, member of BATM Group, is one of the most reliable, experienced and well-known companies in analytical and medical solutions in Romania.

The company started operating back in 1997 as an accredited distributor for several renowned international suppliers and currently operates with three departments: Analytical Department, Medical Department, Food Industry and Environment Department.

Since 2010, the year when the Analytical Department was established within AMS 2000, the company aimed to develop as a market leader in the X-ray equipment supply segment in both academia and industry. Under the aegis of the prestigious Japanese company, Rigaku Corporation, present on the international market for more than seven decades, AMS 2000 have brought to the Romanian market scientific and industrial instruments based on X-ray technologies, as well as Raman spectroscopy technology.

Today, with hundreds of major innovations to their credit, the Rigaku group of companies are world leaders in the fields of general X-ray diffraction, thin film analysis, X-ray fluorescence spectrometry, small angle X-ray scattering, protein and small molecule X-ray crystallography, Raman spectroscopy, X-ray optics, semiconductor metrology, X-ray sources, computed tomography, nondestructive testing and thermal analysis.

The Rigaku equipment into the AMS 2000 portfolio:

X-ray technology equipment

- X-ray diffractometers (XRD) for powders and thin films
- Single crystal X-ray diffractometers for small molecules 3D structure analysis and proteins
- Wavelength dispersive X-ray fluorescence spectrometers
- X-ray microscopy systems
- X-ray residual stress measurement systems
- Micro CT (computed tomography) systems

Raman technology equipment

- Raman portable spectrometers

„At AMS 2000 Trading Impex, we are proud of our reputation built in the 13 years of collaboration with researchers in Romania, which positions us as a reliable and reliable partner in this high-level scientific community. we understood from the very beginning the challenges facing the research field and we are committed to providing the best equipment to researchers, sometimes unique at the national and global level, at the highest level of service, with on-going technical and scientific support from the manufacturer Rigaku Corporation.” mentions Claudia Gavrilescu, Sales Manager within the Analytical Department.

Supermini200
High-power benchtop sequential WDXRF spectrometer

Elemental analysis of solids, liquids, powders, alloys and thin films

As a high-power benchtop sequential wavelength dispersive X-ray fluorescence (WDXRF) spectrometer, for elemental analysis of oxygen (O) through uranium (U) in almost any material, the Supermini200 uniquely delivers low cost-of-ownership (COO) with high resolution and lower limits-of-detection (LLD).

Analyzing complex matrix materials with a wide range of light and heavy elements, from trace to high concentration levels, is this instrument's core competency. With its high powered (200 W) X-ray tube, Rigaku Supermini200 delivers high XRF sensitivity for light elements with superior spectral resolution for resolving line overlaps in complex matrices without the need for complicated mathematical peak deconvolution. Analyzing low concentration levels of light elements (F, Na, Mg, Ca, Si, Al, and P) is easy.

SmartLab 9kW
Automated multipurpose X-ray diffractometer

SmartLab 9kW: Whether you are working with thin films, nanomaterials, powders, or liquids the SmartLab will give you the XRD functionality to make the measurements you want to make when you want to make them. Coupling a computer-controlled alignment system with a fully automated optical system, and the User Guidance functionality within the SmartLab Studio II software, makes it easy to switch between hardware modes, ensuring that your hardware complexity is never holding back your research.

Rigaku

XtaLAB Synergy-ED
Fully integrated electron diffractometer

XtaLAB Synergy-ED: XtaLAB Synergy-ED is a new and fully integrated electron diffractometer, creating a seamless workflow from data collection to structure determination of three-dimensional molecular structures. The XtaLAB Synergy-ED combines core technologies from the two companies: Rigaku's high-speed, high-sensitivity detector (HyPix-ED), and instrument control and single crystal analysis software platform (CrysAlisPro ED), and JEOL's expertise in generation and control of stable electron beams.

XtaLAB Synergy-S
Combining the ultrabright microfocus PhotonJet X-ray source technologies and innovative HyPix detectors

XtaLAB Synergy-S: Using a combination of leading-edge components and user-inspired software tied together through a highly parallelized architecture, the XtaLAB Synergy-S produces fast, accurate data in an intelligent fashion. In the latest generation of Rigaku's XtaLAB Synergy systems, the combination of the latest ultrabright microfocus PhotonJet X-ray source technologies and innovative HyPix detectors allows us to lower the barrier for absolute structure determination.

CT Lab HX
Compact X-ray microtomography

CT Lab HX: Rigaku CT Lab HX is a benchtop micro CT (computed tomography) scanner. The adjustable SOD (source-to-object distance) and SDD (source-to-detector distance) make this benchtop micro CT scanner flexible. It covers from 2.1 um voxel resolution in the high-resolution mode and 200 mm FOV (field of view) in the large FOV mode. The CT Lab HX is equipped with a 130 kV - 39 W high power X-ray source. The X-ray source settings and X-ray filters are adjustable to optimize the X-ray energy to various sample materials and sizes.

If you would like to find out more about the projects implemented using Rigaku equipment distributed by AMS 2000 Trading Impex, please reach out to us.

AMS 2000
Analytical & Medical Solutions For All Laboratories

Scan to have a brief
story of Rigaku

DECORIAS SRL, Rediu, Romania

**office@decorias.ro; www.decorias.ro; www.reactivi.ro*

1. Introducere

Furnizor pe plan național de aparatură și echipamente de laborator, consumabile, reactivi pentru analiză și cercetare în chimie, biochimie, microbiologie, standarde și materiale de referință, scheme de intercomparare. Suntem ingineri chimiști, experți, pasionați de chimie, cu aproximativ 20 de ani vechime în dotarea laboratoarelor din universități, instituții de cercetare și laboratoare de analiză chimică, fizică și microbilogică din industria alimentară, a mediului, farmaceutică, petrochimică, feroase, neferoase etc. Oferim toată gama de produse necesare în desfășurarea activității de laborator de la consumabile, sticlărie și reactivi, la echipamente dedicate aplicațiilor. Produsele furnizate de noi sunt de înaltă calitate, respectă standardele internaționale ISO 9001, ISO/IEC 17025, ISO 17034 și ISO 1043, produse de firmele de top din domeniu. Compania noastră este Certificată ISO 9001:2015 și deține autorizații speciale de comercializare emise de organismele statului roman.

2. Ne plac provocările!

Dacă nu reușiți să identificați un furnizor sau producător de reactivi necesari în desfășurarea proiectului dumneavoastră, contactați-ne pentru a ne transmite lista dumneavoastră. Avem reputația de a-i ”*scoate și din piatra seacă*”. În parteneriat cu producători mondiali, oferim reactivi chimici de laborator cu utilizare specială, reactivi chimici *custom made*, de puritate înaltă, pentru diferite aplicații de laborator. Reactivii sunt însoțiți la livrare de Certificate de Analiză, Fișe de Securitate și MSDS-uri. Deținem autorizații de comercializare emise de instituțiile statului român, pentru comercializarea reactivilor controlați sau cu regim special. Furnizăm reactivi chimici de laborator, de puritate înaltă, puritate analitică sau tehnică folosită în industria chimică sau în laboratoarele de cercetare și analiză. În gama noastră se regăsesc solvenți, reactivi pentru cromatografie, reactivi HPLC, standarde analitice, materiale de referință, etc. Oferim produse de nișă și reactivi controlați, utilizați în laboratoare de analize specifice în toxicologie și criminalistică. Reactivi acreditați ISO/IEC.

3. Control extern

Furnizăm scheme de intercomparare/control extern organizate de parteneri internaționali acreditați ISO 17043. Matrici: apă potabilă, apă reziduală, produse lactate, produse alimentare, furaje, analize clinice, aer, contaminare sol, băuturi alcoolice și sucuri, bere, cosmetice, jucării, medicamente de abuz, toxicologie, radiochimie, lubrifianți, textile, țesut animal, etc.

În portofoliul nostru găsiți o gamă largă de materiale de referință și standarde analitice, cum ar fi:

- tulpini de referință pentru microbiologie;
- standarde analitice și materiale de referință obținute prin sinteză și purificarea substanțelor naturale;
- standarde și materiale de referință pentru analiza chimică a alimentelor și a mediului;

- standarde pentru pesticide;

- standarde pentru industria farmaceutică;
- standarde ICP/ICP-MS, AA, IC, HLPC;
- reziduuri veterinare etc.

Valorile noastre fundamentale se reflectă în tot ceea ce facem. Fiecare ne amintește să rămânem fideli cu noi înșine, să modelăm caracterul echipei noastre în timp ce oferim cele mai bune soluții pentru clienții noștri. Învățăm unii de la alții, ne aliniem, împărtășim cunoștințe, oferim și primim feedback obiectiv. Comunicarea ne ajută să creștem ca echipa și stabilește baza pentru a lucra împreună în mod constructiv și respectuos, pentru a obține soluții inovatoare și pentru a îndeplini solicitările clienților noștri.

4. Suntem prezenți și în Sistemul Electronic de Achiziții Publice (S.E.A.P)

Produsele ofertate, pot fi achiziționate prin intermediul catalogului nostru din SEAP. Departamentul de achiziții al instituțiilor publice, poate solicita publicarea anumitor produse ofertate sau pot achiziționa direct produse deja publicate în catalog.


MacroYouth 2023


PETRU PONI