# 「Macromolecular Research」목차

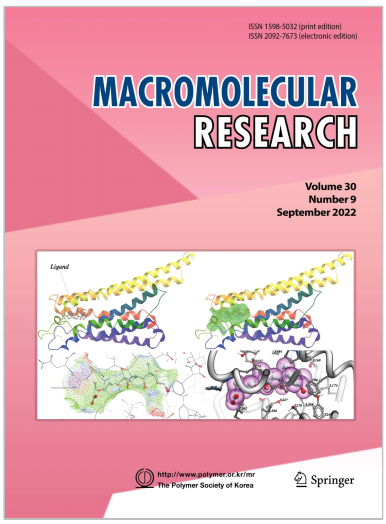
정기간행영문지_ 30권 9호 · 2022년 9월

## COVER PAPER

### Chemometric Study, Homology Modeling of G Protein-Coupled Bile Acids Receptor (GPBAR_HUMAN) of Type-2 Diabetes Mellitus, Virtual Screening Evaluation, Drug-Likeness and ADME Prediction for Newly Designed Compounds

Shola Elijah Adeniji*, Abduljelil Ajala, David Ebuka Arthur, Mustapha Abdullahi, and Omole Isaac Areguamen

Vol. 30, No. 9, pp 659-676 (2022) | SEP 25, 2022 | DOI 10.1007/s13233-022-0071-3




Chemometric validation of the reported experimental activities of nicotinamide and carboxamide analogues against diabetes were determined *via* quantitative structure-activity relationship (QSAR) model using ATS1p, AATSC1m, nHother and RDF80p descriptors. Meanwhile, GPBAR_HUMAN with a UniProtKB code (Q8TDU6) for G protein-coupled bile acid was known as a potential drug target in human TGR5 of Type 2 diabetes mellitus (T2DM) whose crystal structure wasn't found in the Protein Data Bank. With the aid of in-Silico approach *via* homology modeling helps to build a 3D protein (target) model with the availability of GPBAR_HUMAN sequence data. The swiss-Model online workspace was used to model the GPBAR_HUMAN receptor using the Cryo-EM structure of the INT-777-bound GPBAR-Gs complex with PDB code (7CFN) as a potential template. The built receptor was evaluated, validated, and used as a target protein for molecular docking simulation of some potent nicotinamide and carboxamide series. The virtual screening studies *via* molecular docking revealed the binding pockets, binding modes and poses of the GPBAR_HUMAN receptor with some prominent anti-diabetic agents. Analysis of these interactions led to computational design *via* a structure-based approach of new potent anti-diabetic compounds with significant binding scores and better interactions with the GPBAR_HUMAN receptor. Validation of the designed compounds *via* Drug-likeness and ADME prediction confirmed that these compounds are orally bioavailable with a good lipophilicity index for lipid environments and show zero violation to the drug assessment rules in order to be considered as drug candidates. Therefore, *in-vitro* and an *in-vivo* test to transform these findings into potent therapeutics are strongly recommended.

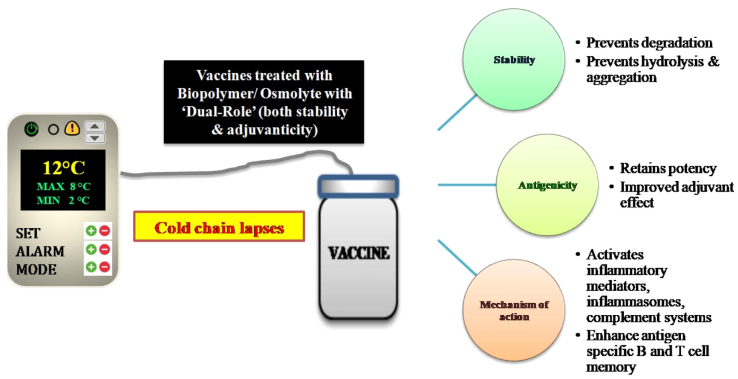
## REVIEW

### Biopolymers and Osmolytes - A Focus towards the Prospects of Stability and Adjuvanticity of Vaccines

Krubha Athirathinam, Selvasudha Nandakumar, and Ruckmani Kandasamy*

*Macromol. Res.*, **30**, 599 (2022)

Dual-role of biopolymers and osmolytes in vaccine formulation.



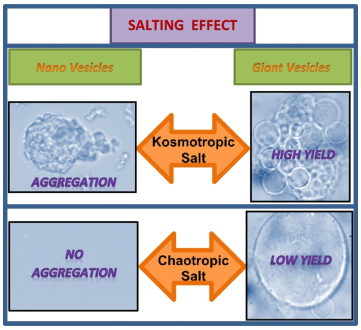
## COMMUNICATION

### Study of Salting Effect of Inorganic Salts on Nano- and Giant Polymersomes

Obed Andres Solis-Gonzalez*,
Christopher Chi Wai Tse,
Patrick J. Smith,
and J. Patrick A. Fairclough

*Macromol. Res.*, **30**, 609 (2022)

Salting effect has been studied on nano- and giant-polymersomes. Studies indicate that kosmotropic salts promote both nanovesicle aggregation and abundant giant unilamellar vesicle (GUV) formation, whereas chaotropic salts have a poor or not impact in both systems. Nanovesicle aggregation produces gel-like structures which may be used as scaffolds for tissue engineering and the efficiency of kosmotropes in GUV formation may be incorporated in GUV methodologies.



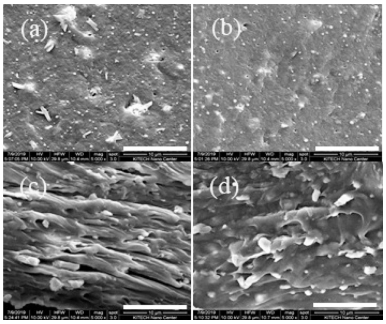

## ARTICLES

### Influence of Surface Treatment of $CaSO_4$ on the Drawability and Physical Properties of the PBAT/PLA/$CaSO_4$ Composite Sheet

Young Jun Kong, Je Sung Youm,
Tae Woong Kong, Yang Il Huh,
and Jeong Cheol Kim*

*Macromol. Res.*, **30**, 615 (2022)

A composite film was fabricated using an inorganic additive $CaSO_4$ and the biodegradable polymers, poly(butylene adipate-*co*-terephthalate) (PBAT) and poly(lactic acid) (PLA). The surface-treated $CaSO_4$ with stearic acid showed improved dispersion in the matrix polymer and improved strength and elongation of the PBAT/$CaSO_4$ composite. The drawability, mechanical property, and gas barrier property of the PBAT/PLA/$CaSO_4$ composite sheets were increased by $CaSO_4$ surface treatment.

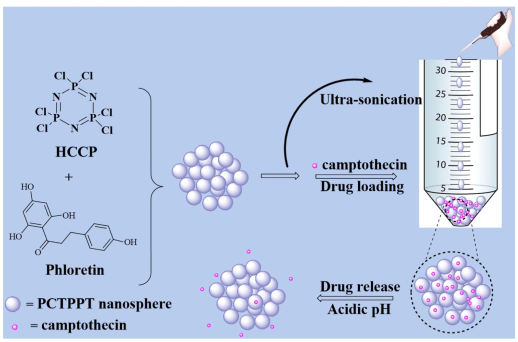



### Cross-Linked Poly(cyclotriphosphazene-*co*-phloretin) Microspheres and Their Application for Controlled Drug Delivery

Sahid Mehmood, Haojie Yu*,
Li Wang, Md Alim Uddin,
Bilal Ul Amin, Fazal Haq,
Shah Fahad, and Muhammad Haroon

*Macromol. Res.*, **30**, 623 (2022)

Cross-linked poly(cyclotriphosphazene-*co*-phloretin) microspheres are prepared *via* polymerization-induced self-assembly. The microspheres are size-controlled and thermally stable. Anti-cancer model drug (CPT) is successfully encapsulated and its controlled release is studied in different pH media.

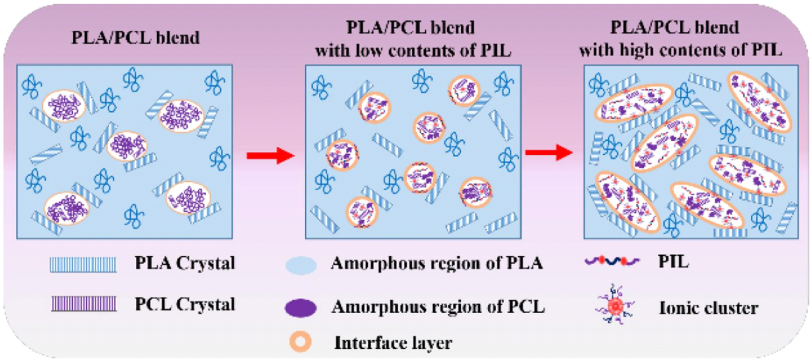


## Polymerized Ionic Liquid for the Regulation of Phase Structure of PLA/PCL Blends

Yiyang Zhou, Qiuyue Meng, Ping Wang*, Haibing Wei, Pei Xu, and Yunsheng Ding*

*Macromol. Res.*, **30**, 631 (2022)

Polymerized ionic liquid containing block structure (PIL) has been used as regulator for the phase structure of poly(lactide) (PLA)/poly(ε-caprolactone) (PCL) blends. The phase structure, crystallization, rheology behavior and mechanical properties of PLA/PCL and PLA/PCL/PIL blends were systematically investigated. PIL could be located in PCL phase or at the PLA/PCL interface, enhancing the interaction between polymer components. The crystallization ability of PLA and PCL was simultaneously enhanced with the addition of PIL, since the plasticization effect of ionic moiety and PEO segments in PIL as well as the nucleation effect of PIL-formed ionic cluster. When PIL content was 0.5 wt%, the PLA/PCL/0.5PIL blend system exhibited much better mechanical properties than additive-free PLA/PCL blend. But as PIL contents increased, the significantly change in viscosity ratio between PLA and PCL would lead to obviously change in phase structure of PLA/PCL blend, thus the mechanical properties of the blends would be degraded.

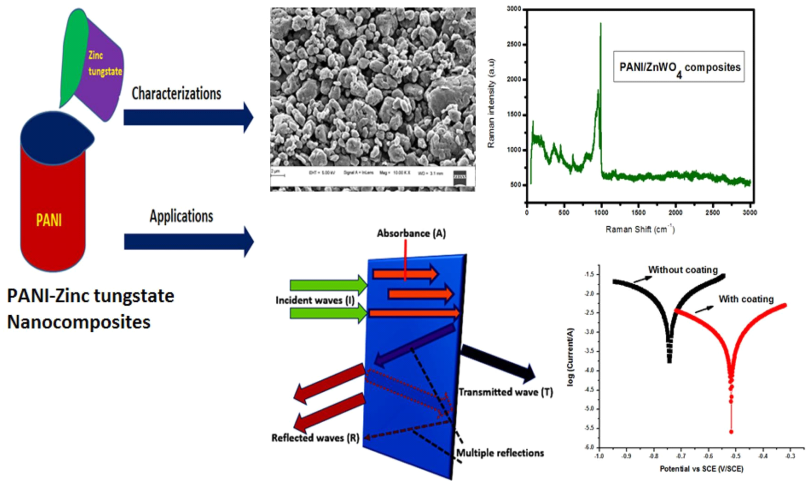



## Corrosion-Resistant Polyaniline-Coated Zinc Tungstate Nanocomposites with Enhanced Electric Properties for Electromagnetic Shielding Applications

Abdul Kadar C. H, Muhammad Faisal*, N. Maruthi*, Narasimha Raghavendra*, B. P. Prasanna, and S. R. Manohara

*Macromol. Res.*, **30**, 638 (2022)

Polyaniline-zinc tungstate nanocomposites have been synthesized by *in-situ* oxidative polymerization method. Modified composite structure with compatible synergy leads to effective modification of the electrical properties. Tunable electrical conductivity with modified dielectric attributes enables acceptable microwave shielding performance in the broad microwave X-band. The composites have shown effective EMI shielding efficiency and corrosion inhibition characteristics.

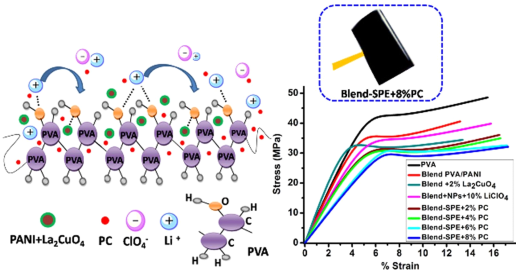


## Characterization of Opto-Electrical, Electrochemical and Mechanical Behaviors of Flexible PVA/(PANI +$La_2CuO_4$)/$LiClO_4$-PC Polymer Blend Electrolyte Films

Murad Q. A. Al-Gunaid*, Shashikala B. S., Gayitri H. M., Khaled Alkanad, Nabil Al-Zaqri, Ahmed Boshaala, and Fares H. Al-Ostoot*

*Macromol. Res.*, **30**, 650 (2022)

A new series of flexible nanocomposite-solid polymer electrolyte (SPEs) in the form of poly(vinyl alcohol) (PVA) impregnated by core-shells polyaniline (PANI)-$La_2CuO_4$ (20:2 wt%) of nanofillers, 10 wt% $LiClO_4$ as electrolyte and various amount 2, 4, 6, and 8 wt% of propylene carbonate, PC as plasticizer *via* solvent intercalation method. The obtained plasticized PVA-SPEs films were evaluated for their microstructural and morphological behaviors *via* X-ray diffraction (XRD), scanning electron microscope (SEM), and Fourier transform infrared (FTIR) spectroscopy, respectively. The surface morphology of plasticized PVA-SPEs films illustrated the finer dispersion of inclusion fillers in the PVA matrix with increasing the dosage of PC content. Optical findings exhibited higher absorbance of PVA SPE in the visible region compared with pure PVA; in addition, the band-gap energy was reduced to 2.68 eV for PVA-SPE containing 8 wt% PC. The current-voltage characteristics showed a slight deviation for all PVA-SPE films denoting to non-ohmic behavior. Besides, the maximum ac-conductivity was found at 40.3 × $10^{-5}$ S/cm for PVA-SPE film containing 8 wt% PC with enhanced their specific capacitance by two folds compared with pure PVA.

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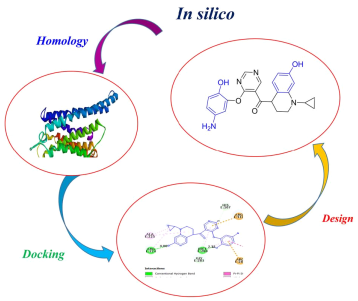
Shola Elijah Adeniji*, Abduljelil Ajala, David Ebuka Arthur, Mustapha Abdullahi, and Omole Isaac Areguamen

*Macromol. Res.*, **30**, 659 (2022)

**Cover Paper**

Chemometric validation of the reported experimental activities of nicotinamide and carboxamide analogues against diabetes were determined *via* quantitative structure-activity relationship (QSAR) model using ATS1p, AATSC1m, nHother and RDF80p descriptors. Meanwhile, GPBAR_HUMAN with a UniProtKB code (Q8TDU6) for G protein-coupled bile acid was known as a potential drug target in human TGR5 of Type 2 diabetes mellitus (T2DM) whose crystal structure wasn't found in the Protein Data Bank. With the aid of in-Silico approach *via* homology modeling helps to build a 3D protein (target) model with the availability of GPBAR_HUMAN sequence data. The swiss-Model online workspace was used to model the GPBAR_HUMAN receptor using the Cryo-EM structure of the INT-777-bound GPBAR-Gs complex with PDB code (7CFN) as a potential template. The built receptor was evaluated, validated, and used as a target protein for molecular docking simulation of some potent nicotinamide and carboxamide series. The virtual screening studies *via* molecular docking revealed the binding pockets, binding modes and poses of the GPBAR_HUMAN receptor with some prominent anti-diabetic agents. Analysis of these interactions led to computational design *via* a structure-based approach of new potent anti-diabetic compounds with significant binding scores and better interactions with the GPBAR_HUMAN receptor. Validation of the designed compounds *via* Drug-likeness and ADME prediction confirmed that these compounds are orally bioavailable with a good lipophilicity index for lipid environments and show zero violation to the drug assessment rules in order to be considered as drug candidates. Therefore, *in-vitro* and an *in-vivo* test to transform these findings into potent therapeutics are strongly recommended.

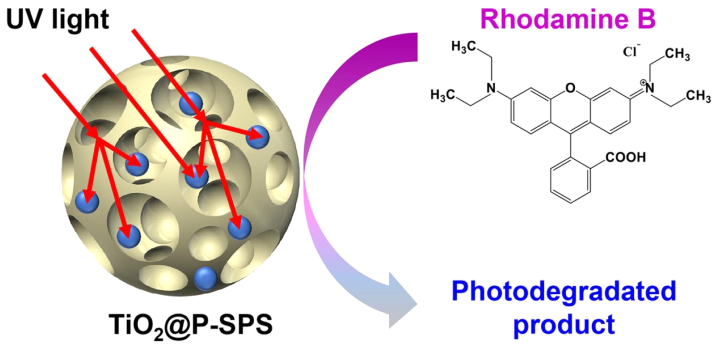


## Enhanced Photocatalytic Activity of $TiO_2$ Nanoparticles Immobilized on Porous-Sulfonated Polystyrene Microspheres through Multiple Scattering Process

Maulida Zakia and Seong Il Yoo*

*Macromol. Res.*, **30**, 677 (2022)

Nanocomposites consisting of porous-sulfonated polystyrene (P-SPS) microspheres and $TiO_2$ nanoparticles have been prepared in a solution state. In the colloidal nanocomposites, the $TiO_2$ nanoparticles can be photo-excited not only by incident light, but also by the scattered light from P-SPS microspheres, resulting in the improved photocatalytic performance of $TiO_2$ nanoparticles.



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정기간행영문지_ 30권 10호 · 2022년 10월

## COVER PAPER

### *In vitro* Therapeutic Effects of Folate Receptor-Targeted Delivery of Anti-Atherogenic Nanodrug on Macrophage Foam Cells

Yeong Jun Song, Sung Yun Jung, and Kyeongsoon Park*

Vol. 30, No. 10, pp 703-706 (2022) | OCT 25, 2022 | DOI 10.1007/s13233-022-0082-0


Folate receptors (FRs)-targetable nanodrugs were developed to specifically deliver the anti-atherogenic drug lobeglitazone into macrophage foam cells with high expression of FRs. The FRs-targetable nanodrugs significantly decreased the formation of foam cells by inhibiting the accumulation of lipid droplets in macrophage foam cells.

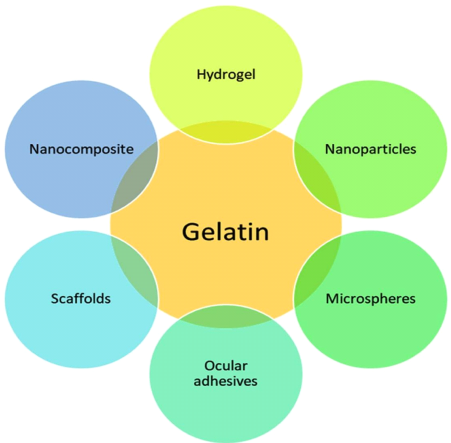
## REVIEW

### Recent Trends in Drug Delivery and Emerging Biomedical Applications of Gelatin for Ophthalmic Indications

Dhwani Rana, Sagar Salave,
Garima Rawat, and Derajram Benival*

*Macromol. Res.*, **30**, 687 (2022)

Gelatin serves as a versatile peptide-based biopolymer for delivering therapeutically active agents to the ocular surface. The present review aims to deliver the physicochemical aspects of gelatin, its conventional use, and primarily the applications of this biopolymer in ophthalmic drug delivery as well as tissue engineering.



## COMMUNICATIONS

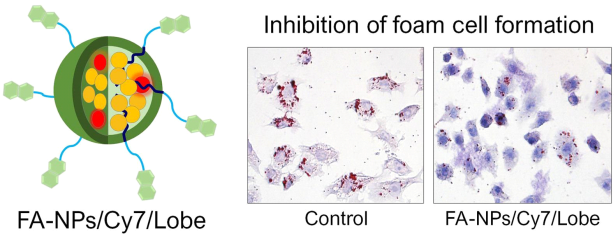
### *In vitro* Therapeutic Effects of Folate Receptor-Targeted Delivery of Anti-Atherogenic Nanodrug on Macrophage Foam Cells

Yeong Jun Song, Sung Yun Jung, and Kyeongsoon Park*

*Macromol. Res.*, **30**, 703 (2022)

**Cover Paper**

Folate receptors (FRs) are overexpressed on activated macrophages in inflammatory diseases. In this regard, the FRs-targeting strategy is a good option for the diagnosis and treatment of macrophage-mediated diseases. Here, we developed FRs-targeted nanomaterials that specifically deliver the anti-atherogenic drug lobeglitazone into macrophage foam cells *via* a strong binding affinity to FRs. The prepared FRs-targetable nanodrug is nontoxic to macrophage foam cells and efficiently delivers lobeglitazone into macrophage foam cells *via* the FRs-mediated endocytosis. Consequently, the FRs-targetable nanodrug significantly decreases the formation of foam cells by inhibiting the accumulation of lipid droplets in macrophage foam cells.

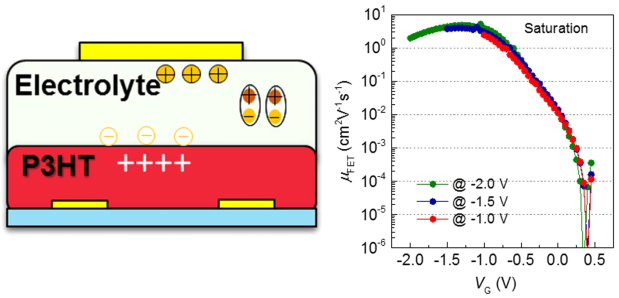



### Influence of Gate Voltage Operation on Effective Mobility of Electrolyte-Gated Organic Transistors

Vivian Nketia-Yawson, Benjamin Nketia-Yawson*, and Jea Woong Jo*

*Macromol. Res.*, **30**, 707 (2022)

The influence of gate voltage operation on the effective mobility of electrolyte-gated organic transistors (EGOTs) using poly(3-hexylthiophene) (P3HT) semiconductor and electrolyte dielectric operating at different driving voltages is reported.



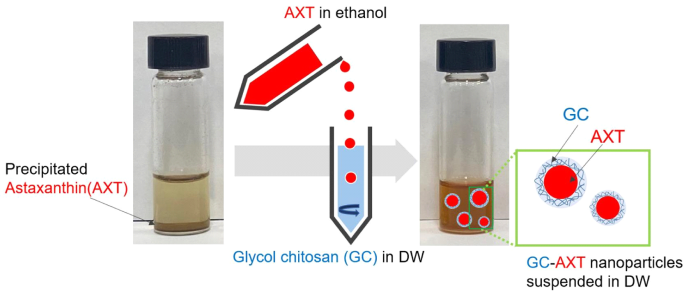

## ARTICLES

### Glycol Chitosan-Astaxanthin Nanoparticles: Water Dispersion, Antioxidant Activity, and Improved Cell Migration

Jin Kim, Chun Sung Kim, Sook-Young Lee, and Chang-Moon Lee*

*Macromol. Res.*, **30**, 712 (2022)

Glycol chitosan-decorated astaxanthin (GC-AXT) nanoparticles prepared by ionic interaction were well suspended in distilled water (DW) without any precipitation. Lipopolysaccharide-induced nitric oxide production and prostaglandin E2 (PGE2) secretion in RAW 264.7 cells were inhibited by treatment of GC-AXT nanoparticles. Migration and proliferation of L929 cells were improved effectively after treatment of GC-AXT nanoparticles. Considering these results, GC-AXT nanoparticles can broaden the bioavailability of AXT and can be used for cell and tissue regeneration.

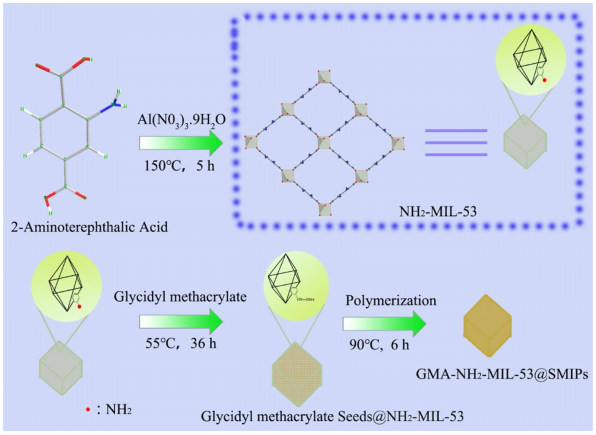


## Surface Molecularly Imprinted Polymers Based on $NH_2$-MIL-53 for Selective Extraction Ochratoxin A in Real Sample

Xing Zhang, Juan He*, Huige Wang, Pengfei Xu, Mingyu Wang, Yuanyuan Li, Jing Chen, and Lijun He

*Macromol. Res.*, **30**, 719 (2022)

In this work, the metal organic framework, $NH_2$-MIL-53, was prepared by hydrothermal method. Then the amino groups exposed on the surface of $NH_2$-MIL-53 reacted with the epoxy groups in glycidyl methacrylate to provide double bonds for subsequent synthesis. Afterwards, the surface molecularly imprinted polymers were synthesized with GMA-$NH_2$-MIL-53 as carrier and naringenin as alternative template of Ochratoxin A.

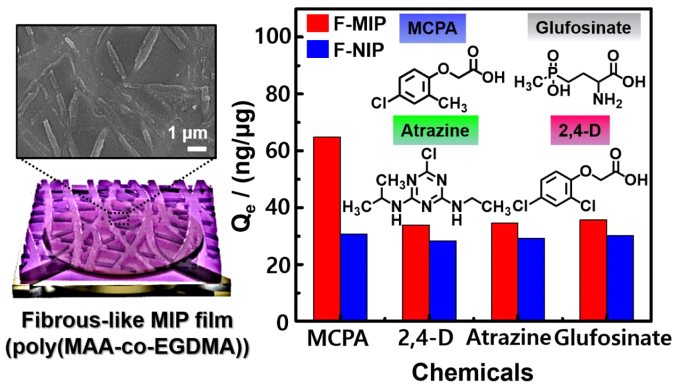



## Fabrication and Sensing Properties of Fibrous-Like Chlorophenoxy Herbicide-Imprinted Polymeric Matrix *via* Microcontact Printing

Beom Min Si, Jin Chul Yang, Deepshikha Hazarika, Je Wook Byeon, Gyu Bi Lee, and Jinyoung Park*

*Macromol. Res.*, **30**, 731 (2022)

A novel strategy for the fabrication of fibrous-like molecularly imprinted polymer (MIP) film-based QCM sensors for detecting methyl-4-chlorophenoxyacetic acid (MCPA) herbicide is demonstrated. The MCPA-imprinted poly(methacrylic acid-*co*-ethylene glycol dimethacrylate) matrix films are photopolymerized. To determine MCPA detection, the sensitivity and selectivity of MIP and nonimprinted polymer films are evaluated.

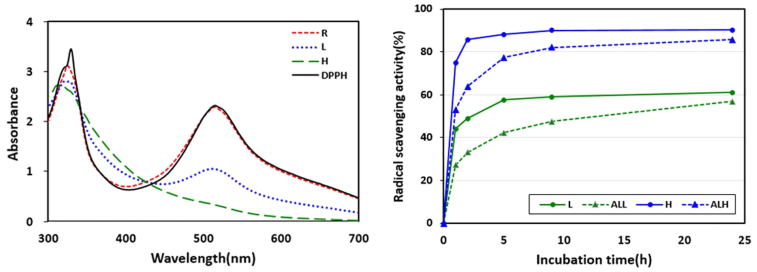



## Antioxidant and Physical Properties of Dual-Networked Contact Lenses Containing Quercetin Using Chitosan and Alginate

Hyo Jeong Kim, Ki Hong Kim, Yoon Soo Han, Young-Jin Kim, and Hyun Mee Lee*

*Macromol. Res.*, **30**, 737 (2022)

All contact lenses containing quercetin have antioxidant properties, and the higher the quercetin content, the greater the radical scavenging rate. When a contact lens containing quercetin was formed into a dual network using natural polysaccharides such as alginate and chitosan, quercetin inside the contact lens was slowly released and antioxidant activity continued for more than 24 hours.

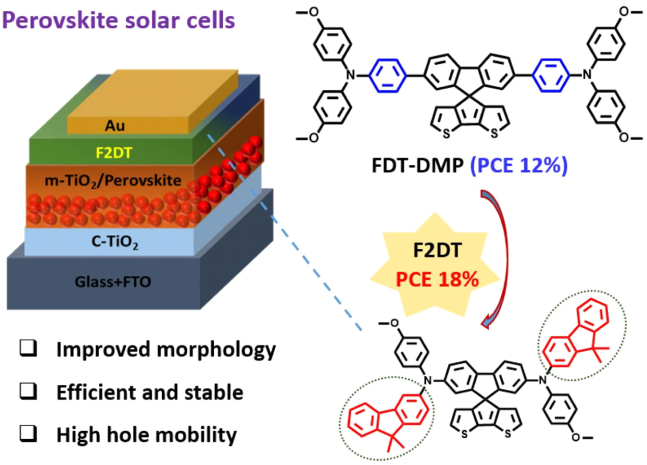


## Facile and Stable Fluorene Based Organic Hole Transporting Materials for Efficient Perovskite Solar Cells

Rajalapati Durga Gayathri, Thavamani Gokulnath, Ho-Yeol Park, Zhiqing Xie, Sung-Ho Jin*, Seung Choul Han and Jae Wook Lee*

*Macromol. Res.*, **30**, 745 (2022)

Fluorene terminal groups on fluorine-dithiophene (FDT)-based organic hole transporting materials resulted in efficient and stable perovskite solar cells. F2DT with fluorene teminal groups formed uniform and dense HTL film compared to compound without fluorene terminal group FDT-DMP. F2DT displayed higher power conversion efficiency of 18% with enhanced hole mobilities and stability over FDT-DMP.




NOTE

## Superoxide-Responsive Cargo Release of Mesoporous Silica Nanocontainers with Thioketal Linker

Jeonghun Lee and Chulhee Kim*

*Macromol. Res.*, **30**, 751 (2022)

To develop nanocontainers with a capability of superoxide-responsive cargo release, a thioketal moiety is utilized for the conjugation of gatekeeper on the surface of mesoporous silica nanocontainers. The surface gatekeepers connected by thioketal linker sufficiently block the cargo release from the mesopore of the nanocontainers without any external stimuli. In the presence of superoxide, the guest cargo is released by cleavage of thioketal linker and removal of surface gatekeepers.