periodica polytechnica

Chemical Engineering
51/2 (2007) 71–74
doi: 10.3311/pp.ch.2007-2.12
web: http://www.pp.bme.hu/ch

ABSTRACTS

Conference of MSc students – abstracts of the best contributions

Krisztina László (ed.)

Received 2007-02-07

Preparation of Ultrathin Multifunctional Coatings by Wet Colloid Chemical Routes

Nóra Ábrahám

Supervisor: Zoltán Hórvölgyi
Department of Physical Chemistry,
e-mail: zhorvolgyi@mail.bme.hu
Consultant: Lívia Naszályi
Department of Physical Chemistry,
e-mail: lnaszalyi@mail.bme.hu

The purpose of this work was to prepare ultrathin, multifunctional coatings of nanoparticles on transparent substrates. The thin films with advantageous photocatalytic and antireflective properties were prepared on glass substrates by using the Langmuir-Blodgett (LB) technique. Consecutive deposition of ZnO (6 nm diameter) and SiO_2 (40 nm diameter) particles resulted in formation of complex LB films in which the semiconductor particulate layers provided the photocatalytic activity and the silica layers (with lower refractive index) gave an increased transmittance of visible light in a broad wavelength range. The morphology, the photocatalytic and optical properties of the prepared coatings were investigated in terms of the deposition order of the uniform (ZnO or silica) layers and the composition of the films.

The morphology of the films was investigated by scanning electron microscopy (SEM). The SEM images showed that the uniform layers (both from silica and ZnO particles) are close-packed and homogeneous, and their alternative deposition resulted in complex LB films. The optical properties of the films were studied by UV-Vis spectroscopy method investigating the transmittance spectra in the wavelength range of 300-1000 nm. The coated substrates showed an improved light transmittance in a broad range of the visible light. For investigating the photocatalytic properties of the films, the coated substrates were immersed into the aqueous solution of Methyl Orange dye which was irradiated by a 400 W UV lamp. The photocatalytic activity of coatings was characterized by the degree of photodegradation of Methyl Orange which was determined after different irradiation times by using optical spectroscopic method. In the case of the most efficient photocatalytic film 90% degradation of dye was observed.

The photocatalytic capacity of the complex LB films was also investigated. It was found that the activity of the films diminished after the photodegradation experiment. The effect was attributed to the photocorrosion of the very small ZnO particles. Applying larger ZnO particles (110 nm diameter) for the film preparation, an increased photocatalytic capacity of films was observed but the light transmittance slightly weakened.

The results unambiguously show that applying particles with optimum sizes for the film preparation will result in the fabrication of multifunctional coatings which can be utilized in different applications as self-cleaning surfaces with improved light transparency in the future.

Experiments for the Construction of the Ibophyllidine Skeleton. The First Synthesis of (±)-18-hydroxy-20-epiibophyllidine.

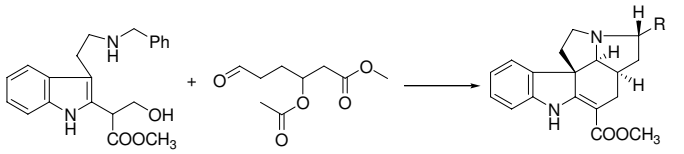
Dániel Vajk Horváth

Supervisor: György Kalaus
Department of Organic Chemistry,
e-mail: kalaus@mail.bme.hu
Consultant: Flórián Tóth
Department of Organic Chemistry

A new convergent synthesis strategy has been developed for building up the pseudoaspidospermane skeleton at the Budapest University of Technology and Economics, Department of Organic Chemistry, Research Group for Alkaloid Chemistry. In the procedure, an appropriately formed tryptamine derivate, as common starting material, was allowed to react with adequately built-up aldehydes or aldehyde-equivivalents. As a result of reactions, tetracyclic esters were obtained from which the target compound could be produced in several steps [1]. Based on this

Krisztina László
Faculty of Chemical Enginering, Budapest University of Technology and Economics, H–1521 Budapest,, Hungary

strategy, the objective was set to produce (±)-18-hydroxy-20-epiibophyllidine **(1)** [2].



The tryptamine derivate **(2)**, as the key molecule of the convergent synthesis, was allowed to react with an appropriately functionalized aldehyde **(3)**. In accordance with our expectations only one product was obtained. Debenzylation and intramolecular N-alkylation reaction with full epimerization furnished the molecule containing ibophyllidine skeleton **(4)**. Finally, by reduction of the ester **(4)** with $LiAlH_4$, we could isolate the target molecule, (±)-18-hydroxy-20-epiibophyllidine **(1)**.

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Development of Biochips for Surface Plasmon Resonance Imaging Detection of Aptamer – Ligand Interactions

Gergely Lautner

Advisor: Robert E. Gyurcsányi
Dept. of Inorganic and Analytical Chemistry
e-mail: robertgy@mail.bme.hu

Consultant: Júlia Szűcs
Dept. of Inorganic and Analytical Chemistry
e-mail: szucsj@mail.bme.hu

The exquisite selectivity of biomolecular interactions on one side provides the opportunity for measurements in complex samples without sample preparation and separation (biosensors), on the other side serves as basis for the development of biochip technology and high throughput bioanalysers.

Aptamers, which are oligonucleotides capable of binding with high selectivity and affinity given target molecules, are an emerging class of synthetic compounds for biorecognition. The combinatorial chemistry based *in-vitro* selection and targeted chemical and biochemical modifications of aptamers provides prospects for making new, more effective drugs, and bioaffinity reagents. The analytical importance of the aptamers is outlined by their synthetic origin and capability of replacing antibodies in many bioanalytical applications. Therefore, we were interested in selecting and designing novel DNA aptamers for the detection of both large (Thrombin, MT32 apple steam pitting virus coat protein), and small molecular weight (Ochratoxin A micotoxin) ligands and to investigate the feasibility of surface plasmon resonance imaging detection of DNA aptamer – ligand interactions.

To take advantage of the multiplex detection capability of the imaging surface plasmon resonance system (iSPR) we have developed and applied novel surface modification strategies based on microcontact printing and microfluidics. In case of the microcontact printing, photolithographic and laser ablation methods were used for patterning the polydimethylsiloxane (PDMS) stamps.

We have optimized the immobilization methodology of the aptamers and ligands for optimal binding performance and designed sandwich assays using different aptamers that recognize different epitopes of the thrombin molecule. The sensitivity of the aptamer-ligand assay was enhanced by synthesizing and implementing gold nanoparticle labelled aptamers. Their use resulted in ca. two orders of magnitude amplification of the analytical signal in case of thrombin detection.

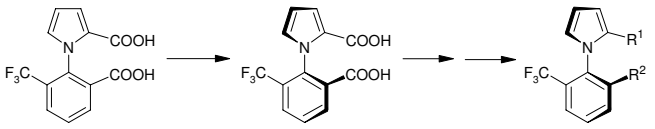
Synthesis of Optically Active 1-[(2-Trifluormethyl)phenyl]pyrrole Derivatives

Béla Mátravölgyi

Supervisor: Ferenc Faigl
Department of Organic Chemical Technology
e-mail: ffaigl@mail.bme.hu

In the last decade, detailed investigations have been carried out in our research group dealing with the regioselective mono- and dimetalation reactions of 1-arylpyrrole derivatives. In the framework of this ongoing research programme we aimed at the development of efficient methods for the synthesis of new optically active 1-[(2-trifluoromethyl)phenyl]pyrrole derivatives.

The racemic mixture of the atropisomeric 1-[(6-trifluoromethyl)-2-carboxyphenyl]pyrrole (**1**) was synthetized from 2-trilfuoromethylaniline by Paal-Knorr pyrrole synthesis followed by dilithiation and carboxylation, according to a previously published preparation method [1].



R^1: COOH, $CONR^3R^4$, $CH_2NR^3R^4$;
R^2: $COOR^5$, CH_2OH, CH_2NHR^6

The tryptamine derivate **(2)**, as the key molecule of the convergent synthesis, was allowed to react with an appropriately functionalized aldehyde **(3)**. In accordance with our expectations only one product was obtained. Debenzylation and intramolecular N-alkylation reaction with full epimerization furnished the molecule containing ibophyllidine skeleton **(4)**. Finally, by reduction of the ester **(4)** with $LiAlH_4$, we could isolate the target molecule, (±)-18-hydroxy-20-epiibophyllidine **(1)**.

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Structure-property Relationships in Polyether Polyurethane Elastomers

Imre Szőke

Supervisors: Béla Pukánszky
Kristóf Bagdi
e-mail: pukanszky@mail.bme.hu

Most artery-related aneurysms are formed as the results of some abnormality in the evolution of the artery. The wall of the arteries is weakened at certain locations leading to the burst of the aneurysm and causing bleeding. Aneurysms developing in the cerebral arteries are especially dangerous, because their bleeding is fatal for 50 % of the patients and the chances for permanent cerebral damage are large, even if they survive. Aneurysms can be treated only by operation. Recently intra-arterial techniques are used more and more often, which are less invasive then open surgery and more favourable than other techniques currently used. The newest of these methods applies polymer solutions for embolization.

The project focuses attention on the development of a linear polyurethane (PUR) elastomer, which can be used for embolization. Polyurethane elastomers with various compositions were synthesized, characterized by various techniques and their structure-property correlations were determined. The particular goal of the study was the preparation of polymers with specific end groups and the investigation of their effect on properties, especially on solubility, which is one of the most important criteria for the utilization of polymers as embolizing compounds.

According to the expectation, our results revealed that the properties of the elastomers are strongly influenced by the structure of their chains and the type of their end groups. The mechanical properties of the samples varied in a wide range with composition. The transparency of the samples differed significantly indicating the development of dissimilar supermolecular structures. Experiments carried out in dimethyl sulphoxide showed that solubility is influenced by composition and by the end groups of the macromolecules. Several samples could not be dissolved in the solvent, but swelled only, what indicated the presence of cross-links, or strong interactions among the polymer chains. The properties of the samples prepared in our laboratory were compared to a reference material, which was extensively tested in clinical experiments and proved to be appropriate for embolization. Although most of the properties of our material corresponded to those of the reference polymer, some characteristics, mainly solubility, must be improved to meet all the criteria of clinical application.

Connection between the Cell Cycle and the Circadian Clock in Mammalian Cells

Judit Zámborszky

Supervisor: Attila Csikász-Nagy
Department of Agricultural and Chemical Technology, BME
e-mail: csikasz.bme.hu

It is well-known for a long time that the rotation of Earth has big influence on everyday life of living matter from cyanobacteria to humans. Activation of many molecules depends on this endogenous daily rhythm. Cells contain another important endogenous oscillatory system: the control of cell division. Recent findings tell us that the circadian clock directly regulate *Wee1* kinase that inhibits entry into mitosis. In the ‘70s the correlation of the cell cycle and circadian systems was found, but the molecular details of the molecular background of the connection between these two oscillatory systems that set the daily behaviour in mammalian cells was discovered just in the last years [1].

Considering these results I built a model for the molecular interactions in the system. The interactions of the wiring diagram were turned into a set of differential equations by the rules of reaction kinetics. I investigated the effect of this coupling on timing of cell cycle processes with the tools of computational systems biology. I used the comprehensive model of Béla Novák & John J. Tyson [2], extended it with the regulation of the G2/M transition, and connected it with a simplified circadian rhythm module. I fitted the new parameters of the nonlinear differential equations and analysed the system by simulations. Further on I also added noise to the system and investigated the effect of stochasticity.

Variation of the coupling between these two systems shows different results. The simulations reveal that cell cycle time distribution shows quantized cycles and mode-locking is observed if the circadian influence is strong on cell cycle. Quantized cell cycle in mammalian cells was first reported by R. R. Klevecz [3], but the molecular basis of this phenomenon has never been addressed. I propose that the influence of the circadian clock induces this „mode lock” behaviour of cell cycle.

It is proven that yeasts have to reach a critical mass before cell division, but it is doubtful if mammalian cells use the same regulation. This model suggests that critical cell mass control regulation in mammalian cells depends on the circadian clock: strong forcing eliminate critical mass control of cells that grow at a rate that leads to mass doubling time close to 24 hours, while the circadian system introduces strict mass control if cells grow at slower or faster growth rates. The daily rhythm “helps” the cells to maintain their sizes if the mass doubling time is close to the period length of the circadian clock, but at the same time

causes dissimilar cell cycles and cell size when the mass doubling time is different from 24 hour. Dependence of the existence of mass control on circadian clock could explain why there are controversial results in the literature about this topic [4].

This model can be used to analyse the interactions of cell cycle blocking cancer drugs with the circadian clock and helps to get even better results with chronotherapy and find a better understanding of the hallmarks of cancer. The model is also ready to test mutational behaviour and to be used as a predictive tool for analysis of perturbations of the system, like growth factor deprivation or circadian time shifts.

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