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SEKCE DOKTORSKÝCH STUDENTŮ

POSTEROVÁ STŘEDOŠKOLSKÁ SEKCE

Validace komerčně dostupných T-DNA inzerčních mutantů *Arabidopsis thaliana*

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Vzhledem k současnému vývoji vědy a snaze vytvořit nové generace odolných odrůd plodin byla na základě časové náročnosti přípravy mutantní rostliny založena instituce NASC (Nottingham Arabidopsis Stock Centre). Jelikož tato instituce produkuje rozsáhlé množství mutantních linií modelového organismu huseníčku rolního (*Arabidopsis thaliana)*, je vždy výrazně doporučováno ověření správnosti dané linie před započetím výzkumného procesu. Cílem této práce bylo ověření přítomnosti mutace u celkem 10 vybraných genů HSP, za účelem sestavení kolekce mutantních linií rostlin využitelné pro následující výzkum role proteinů HSP v regulaci klíčení semen. Genotypování bylo provedeno na základě polymerázové řetězové reakce (PCR) a následné agarosové elektroforézy. Každá mutace byla ověřena ve dvou PCR reakcích s využitím tří specifických primerů. Bylo zjištěno, že 6 linií skutečně neslo danou mutaci, avšak zbylé 4 nebyly v daném genu mutantní, přestože mutace byla deklarovaná dodavatelem semenného materiálu. Z výsledků vyplývá, že ověření správnosti požadované mutace je vzhledem k poměrně výrazné chybovosti nutné u všech komerčně dostupných T-DNA inzerčních linií *A. thaliana* a musí předcházet všem následným výzkumným experimentům.

Studium reakčních procesů v rámci sanační metody ISCO

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Kontaminace podzemních vod je významným environmentálním problémem současnosti. Mezi celosvětově nejčastěji se vyskytující kontaminanty patří chlorované etheny. K jejich odstranění z podzemních vod se používá řada sanačních metod. Mezi inovativní metody patří in situ chemická oxidace (ISCO) s využitím peroxodisíranu (PDS) aktivovaného pomocí Fe(II) chelatovaného kyselinou citronovou.
Hlavním cílem této práce bylo v laboratorním měřítku otestovat účinnost této metody pro odstranění trichlorethenu (TCE) jakožto významného zástupce chlorovaných ethenů. Mezi dalšími cíli bylo testování vlivu počátečního molárního poměru PDS/Fe(II) na účinnost jak odstranění TCE, tak využití PDS. Závěrem byly kriticky vyhodnoceny nedostatky experimentálního designu a navrhnuta vylepšení pro navazující výzkumné práce.
Experimenty probíhaly v navrženém reaktoru PRSOR. K dosažení cílů bylo dále využito head-space plynové chromatografie a kapilární elektroforézy.

Klíčová slova: *dekontaminace podzemních vod; trichlorethen; in situ chemická oxidace; peroxodisíran; síranový radikál*

Vývoj voltametrické metody stanovení léčiva atomoxetinu

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Atomoxetin (ATX, (3R)-N-methyl-3-(2-methylphenoxy)-3-phenyl-propan-1-amine) působí jako účinná látka v léčivech, která se využívají pro tlumení symptomů hyperkinetické poruchy známé jako ADHD (Attention Deficit Hyperactivity Disorder). Nejčastěji používanou metodou jeho stanovení v biologických i farmaceutických vzorcích je vysokoúčinná kapalinová chromatografie ve spojení s různými detektory.

Předmětem této práce byl vývoj voltametrické metody stanovení ATX na borem dopované diamantové elektrodě. Nejprve bylo studováno jeho voltametrické chování a bylo zjištěno, že poskytuje jeden oxidační signál, jehož potenciál i výška jsou závislé na pH elektrolytu. Následně byly testovány parametry diferenční pulzní voltametrie a postupy aktivace povrchu pracovní elektrody. Poté byla vyvinutá metoda s velmi dobrými výsledky aplikována při analýze modelových roztoků. Analýza reálných vzorků bude následovat.

Mým osobním cílem je také zpopularizovat voltametrické metody jako celek a připomenout světu jejich neodmyslitelné výhody, na které pomýšlel i sám laureát Nobelovy ceny za chemii, Jaroslav Heyrovský. Toto může být zrealizováno i prezentací získaných výsledků na studentské konferenci.

Klíčová slova: *atomoxetin, stanovení, voltametrie, borem dopovaná diamantová elektroda*

SEKCE BAKALÁŘSKÝCH A MAGISTERSKÝCH STUDENTŮ

Produkcia polyesterov pomocou extrémofilných baktérií

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Medzi popredné spoločenské témy súčasnosti patrí ochrana životného prostredia. Jednou z viacerých príčin, ktorou človek prispieva k zhoršovaniu podmienok života na Zemi je nadmerná spotreba plastov. Väčšina z bežne používaných plastov je vyrobená petrochemickou cestou, ktorá ponúka nízke výrobné náklady. Ich nevýhodou je neschopnosť biologicky sa odbúravať, čo spôsobuje akumuláciu plastového odpadu na skládkach a v oceánoch. Povedomie o enviromentálnej záťaži vedie k celosvetovej snahe vyvíjať materiály s podobnými vlastnosťami, ktoré by boli biologicky rozložiteľné. Vďaka svojej biodegradabilite a vlastnostiam pútajú veľkú pozornosť aj polyhydroxyalkanoáty radiace sa do triedy lineárnych polyesterov. Sú syntetizované mikroorganizmami vo forme intracelulárnych iklúzií ako zásoba uhlíka a energie. Prekážkou komerčnej výroby sú však ich vysoké výrobné náklady a nízke výnosy. Výsledná cena produktu závisí najmä od výberu vhodného mikrobiálneho kmeňa, substrátu a podmienok kultivácie. Pri výrobe PHA vykazuje veľké riziko mikrobiálna kontaminácia, ktorá by mohla ohroziť proces výroby. Z tohto dôvodu je pri výrobe kladený dôraz na sterilitu, ktorá zvyšuje náklady.

Z biotechnologického hľadiska sú stále viac a viac zaujímavejšie termofilné baktérie, ktoré dokážu prežívať a prosperovať pri teplotách, ktoré sú pre väčšinu organizmov neprijateľné. Zvýšenou teplotou fermentácie sa znižuje riziko kontaminácie a tak aj náklady spojené so sterilizáciou. Vyššia kultivačná teplota tiež znižuje nároky na chladenie procesu. Štúdia bola preto zameraná na tri termofilné bakteriálne kmene, ktorých schopnosť akumulácie PHA doposiaľ nebola preskúmaná. Bakteriálne kmene *Thermomonas hydrothermalis* (DSM 14834), *Schlegelella thermodepolymerans* (DSM 15344) a *Schlegelella aquatica* (LMG 23380) boli vystavené niekoľkým kultivačním podmienkam s cieľom pozorovať biosyntetickú schopnost PHA. Bola pozorovaná schopnosť využitia rôznych zdrojov uhlíku, optimálna teplota rastu a schopnosť tvorby kopolymérov. Vďaka sľubným výsledkom bol kmeň *Schlegelella thermodepolymerans* kultivovaný v laboratórnom bioreaktore a taktiež bol sledovaný vplyv kyslíka na rast a produkciu PHA.

Kľúčové slová: *polyhydroxyalkanoáty, polyhydroxybutyrát, termofilné baktérie, Schlegelella aquatica, Schlegelella thermodepolymerans, Thermomonas hydrothermalis*

Využití metabolomiky pro charakterizaci hlavních změn révy vinné v rámci vegetačního cyklu, a při různých způsobech kultivace

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Vinná réva (*Vitis vinifera*) je historicky jednou z nejdéle kultivovaných rostlin. Díky produkci hroznů patří mezi celosvětově ekonomicky významné plodiny. V kulinářství nebo v tradiční medicíně se však také využívají i ostatní části této rostliny, například listy (balkánská kuchyně). Chemické složení vinné biomasy je silně ovlivňováno vnějšími faktory, jako je lokalita pěstování, zemědělské agropraktiky, odrůda, vegetační období nebo přírodní podmínky. Rozdíly v chemickém složení lze také pozorovat v jednotlivých částech rostliny (stonek/list). Tato práce se zabývá studiem metabolomu rostliny révy vinné za využití pokročilých nástrojů moderní analytické chemie – ultra-vysokoúčinné kapalinové chromatografie ve spojení s vysokorozlišovací hmotnostní spektrometrií (U-HPLC-HRMS/MS). Metabolomickému fingerprintingu byl podroben biomateriál z rostliny vinné révy (listy a stonky). Celkem bylo analyzováno cca 520 vzorků reprezentujících čtyři různé odrůdy odebrané ze dvou českých vinic. Odběr vzorků probíhal ve všech čtyřech ročních obdobích, díky čemuž mohl být prozkoumán celý vegetační cyklus rostliny. Cílem této studie bylo demonstrovat potenciál metody metabolomického fingerprintingu pomocí U-HPLC-HRMS/MS, která by sloužila jako nástroj pro autentizaci listů/stonků révy vinné.

Klíčová slova: *Vitis vinifera, listy, stonky, autenticita, ultra-vysokoúčinná kapalinová chromatografie ve spojení s vysokorozlišovací hmotnostní spektrometrií*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Visible-light photoinitiators for cationic and free-radical photopolymerization studied by indirect EPR techniques

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Recently, the development and use of photopolymerization processes, both cationic (CP) and free-radical photopolymerization (FRP), has greatly increased due to the advantages afforded by light-induced polymerization compared to traditional thermal polymerization methods. However, the oxygen inhibition in the free radical polymerization (FRP) and frequent utilization of harmful UV light signify major limitations. Therefore, it is necessary to establish new photoinitiating systems (PIS) or photoinitiators (PI), which will match to the near UV or visible light emission. In this contribution, we focused on detailed study of visible-light active two component photoinitiating systems, consisting of various photoinitiators and photosensitizers (PS), by indirect EPR techniques (spin-trapping or spin-scavenging) [1-4]. We successfully identify reactive paramagnetic species generated upon visible-light irradiation and we confirmed the effective generation of reactive oxygen species (e.g. superoxide radical anion) in the visible-light exposed systems containing photosensitizers and molecular oxygen. the mechanism of FRP was also affirmed by generated

reactive carbon-centered radicals, as corresponding spin-adduct, upon visible-light exposure of photosensitizers in combination with iodonium salts (electron acceptor) or amines (electron donor) under inert atmosphere. Furthermore, photosensitizers (e.g. *chlorophyllin* or *pyropheophorbide-a*) have a promising utilization in photodynamic therapy (PDT) in the destruction of tumors (in summary oncological and also multiple non-oncological diseases) by produced reactive oxygen species (ROS).

Acknowledgement: This work was supported by the Scientific Grant Agency of the Slovak Republic (VEGA Project 1/0026/18).

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Use of Poly(3-hydroxybutyrate) as Polymer Base for Drug Delivery Systems

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One of the most discussed applications of polyhydroxyalkanoates (PHA) is their use in medicine as scaffolds, drug carrier systems, and wound dressings, made by solution casting, electrospinning, or thermoplastic extrusion. Often, the porosity was found as an essential attribute of specimens used for pharmaceutical and medical applications. the PHA porous materials offer unique properties such as biocompatibility, bioactivity, non-cytotoxicity, and biodegradability. This contribution is focused on the study of the release of active substances from porous structures based on poly(3-hydroxybutyrate) (PHB) films. PHB is a semicrystalline biopolyester with the ability to degrade in vivo and in vitro without toxic substances.

The porous scaffolds were formed from PHB by electrospinning. This work confirmed that the morphology of PHB scaffold is possible to varied by the PHB concentration and solvents used for electrospinning. Scanning electron microscopy revealed the formation of different morphologies, including porous, filamentous/beaded, and fibre structure films. As the model drug for incorporation into PHB meshes was used Levofloxacin, which possess with a high antibacterial efficiency against gram-positive and gram-negative bacteria. Its entrapment efficiency was found to be dependent on the viscosity of the PHB solution used for electrospinning, its incorporation in meshes was confirmed by Fourier-transform infrared spectroscopy and UV-VIS spectroscopy. the effect of the morphology of the films on the Levofloxacin release profile was screened in vitro in phosphate-buffered saline solution. the antimicrobial efficiency of all tested samples was confirmed by agar diffusion testing.

Acknowledgement: This work was funded through the Internal Brno University of Technology project FCH-S-20-6316.

Keywords: *polyhydroxyalkanoates, scaffolds, electrospinning, antimicrobial activity, morphology*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Analýza G-kvadruplexů v genomech lidských parazitických červů

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Onemocnění způsobená parazitickými červy jsou velmi rozšířená u lidí v rozvojových zemích. Podle WHO je parazity celosvětově infikováno přibližně 2 miliardy lidí. Etiologickými činiteli parazitických infekcí jsou zejména parazité kmene *Nematoda* (hlístice) a *Platyhelminthes* (ploštěnci) vyvolávající reakce imunitního systému, podvýživu a chudokrevnost, které jsou primární příčinou onemocnění. Vzrůstající rezistence parazitů na lidská anthelmintika je urychlována jejich nadužíváním, špatnou prevencí a kontrolou infekce. Terapeutický potenciál malých molekulových ligandů vázajících G-kvadruplexy (G4s) byl demonstrován například při stabilizaci G4 struktur, anebo eliminaci patogenů rezistentních na léky. G4s jsou typem sekundární struktury nukleových kyselin tvořené v oblastech bohatých na guanin se schopností regulovat proces genové exprese, opravy poškozené DNA, nebo transkripce a translace v onkogenech. K identifikaci a porovnání potenciálních sekvencí tvořících G-kvadruplex (PQS) v jaderných a mitochondriálních genomech šesti zástupců kmene *Platyhelminthes* a čtyř zástupců kmene *Nematoda* (které by mohly ukázat vhodná cílová místa pro navázání G4 ligandů sloužící k predikci nových míst účinků léčiv a pomoci při vývoji efektivnějších léčiv) byl požit webový nástroj G4Hunter. Byla potvrzena nenáhodná distribuce PQS v genomu a mtDNA analyzovaných organismů. Nejvíce G4 bylo lokalizováno v těsné blízkosti genů, což naznačuje jejich roli v genové regulaci. Zajímavé je, že v méně infekčních zástupcích, jak z kmene *Platyhelminthes*, tak z kmene *Nematoda* bylo nalezeno více PQS, naproti tomu více infekční zástupci vykazovali nižší frekvenci PQS a nižší celkový obsah guaninu a cytosinu.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Neural networks and their use in study of quantum-chemical systems

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Computational chemistry has become an integral part of many workplaces in recent years, offering the opportunity to obtain information about systems without the use of expensive measuring techniques. Despite advances in computational technology, quantum-chemical methods are still time-consuming or, in the case of faster methods, inaccurate. Neural networks are a potentially effective tool for solving this issue. Assuming we have a sufficient number of molecular geometries and their corresponding energies, the neural network should be able to learn these relationships between the molecular geometry and its energy. Therefore, such a network can be used for fast and accurate energy prediction, which can then be advantageously used, e.g. in molecular dynamics including chemical reactions.

In this contribution we selected 20 basic proteinogenic amino acids as a dataset. the database for the amino acid model was created by molecular dynamics in XTB 6.2.2 [1]. All conformations from the simulation trajectory were used in the database. From the obtained molecular-dynamic trajectories, we created 4 databases, three of which contained selected separate amino acids (alanine, histidine and aspartic acid) and the fourth includes all 20 amino

acids. for training models we used SchNet software package [2]. Models trained on individual molecules have achieved high accuracy exceeding the level of chemical accuracy. It can be assumed that these models could be successfully used together with molecular dynamics to rapidly obtain relatively accurate quantum-chemical information and monitor their evolution over time. The optimal strategy is represented by models learned on the database of 20 amino acids. These should describe the dynamics of the individual amino acids with sufficient accuracy. However, such a model is likely to insufficiently map the interaction between amino acids. Therefore, for use in proteins, it would be necessary to expand the database to include amino acid dimers. However, they already consist of more than 20 atoms, which requires significantly higher learning time.

Keywords: *neural network, machine learning, SchNet, aminoacids*

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Efekt povrchové modifikace škrobových plniv pomocí polydimethylsiloxanu na proces plnění tvrdých želatinových tobolek

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Jedním z klíčových faktorů, které ovlivňují proces plnění tvrdých želatinových tobolek, jsou sypné vlastnosti plněného prášku. Ty se odráží nejen v požadovaných atributech kvality finálního produktu, jako je např. plněná hmotnost nebo hmotnostní proměnlivost, ale také v efektivnosti a bezproblémovém provedení samotné jednotkové operace. Jelikož jsou sypné vlastnosti ovlivněny charakterem použitého materiálu i procesními podmínkami, je nutné věnovat studiu sypných vlastností značnou pozornost a při jejich optimalizaci brát v úvahu oba tyto aspekty.

Cílem práce bylo studium a optimalizace třísložkové směsi (kukuřičný škrob, aktivní farmaceutická substance (API), dimetikon), která je průmyslovým partnerem používána pro plnění tvrdých želatinových tobolek pomocí plnícího disku. Na základě provedených měření byla stanovena závislost tokových vlastností směsí na zvolené formulační strategii (postupu přípravy) a charakteru použitého škrobu. Za tímto účelem byly v rámci provedené studie hodnoceny dva nativní (Merizet 141, Uni-Pure FL) a dva předželované škroby

(Lycatab C, Starcap 3001), které se lišily svými fyzikálně-chemickými vlastnostmi.

Při studiu tokových vlastností se nejprve stanovily hodnoty Carrova kompresibilitního indexu (CI). Dále byl pro analýzu využit práškový reometr Freeman FT4. Vybrané směsi byly následně charakterizovány i pomocí skenovacího elektronového mikroskopu (SEM) s využitím detektoru sekundárně odražených elektronů (SE).

Z výsledků provedených testů bylo zjištěno, že na sypné vlastnosti směsí má největší vliv charakter použitého škrobu. Směsi připravené z částečně předželovaných škrobů vykazovaly obecně lepší tokovost než směsi připravené ze škrobů nativních. Nativní škroby jsou dle provedených měření na rozdíl od předželovaných škrobů klasifikovány jako kohezní a mají tedy tendenci k soudržnosti vlivem přítomnosti nevazebných interakcí mezi částicemi. To má obecně za následek jejich horší sypné vlastnosti.

Dále bylo patrné, že jednotlivé typy škrobů reagují na modifikace odlišným způsobem. To je především způsobeno charakterem částic škrobu. Částice použitých předželovaných škrobů jsou velké, členité a mají nerovnoměrný povrch. Dimetikon tak není distribuován na povrchu, nýbrž se dostává do nerovností. V důsledku toho nevykazovaly modifikace originálního postupu přípravy v případě předželovaných škrobů výrazný efekt. Naopak v případě nativních škrobů, kdy jsou částice méně členité a mají hladký povrch, zůstává dimetikon přítomen na jejich povrchu a vytváří kapalinové můstky mezi částicemi škrobu. Dochází tak ke vzniku aglomerátů. Použitý způsob modifikace má následně dopad na distribuci dimetikonu a charakter vzniklých aglomerátů odrážející se ve výsledné sypné vlastnosti finální směsi. Ke vzniku aglomerátů pravděpodobně přispívá i vlhkost ve vzorcích jednotlivých škrobů.

Manufacturing of personalised medicines by impregnation of mesoporous silica tablets

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Current drug manufacture methods are based on large scale production with few dosage strength variations. A new manufacturing method is needed to reach the patient-specific requirements for personalized medicine. the main idea of personalized medicine is that drugs are tailored to the individual patient using patient-specific information. Different ways of producing personalized medication are currently investigated, for example 3D print or drop-on-demand (DoD) technique.
This work aimed to explore the effect and possible use of placebo tablets with silica particles to meet the patient-specific requirements for personalized medicine. the placebo tablets containing mesoporous silica were prepared to meet the manufacturing criteria such as hardness and friability. the tablets were filled layer-by-layer with a precise dose of API by drop-on-demand (DoD) technique, which is a liquid dosing system with validated precision. It was found that the number of layers affects the dissolution profile of the tablet. Thus, different dissolution profiles can be achieved. Overall, this method shows the potential to be used in personalized medicine, where various doses and specific dissolution profiles are needed to fit the patient's requirements.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Evolučné inžinierstvo PHA produkujúcich baktérií

Halomonas Halophila
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Práca sa zaoberá evolučným inžinierstvom PHA produkujúcich baktérií, princípom produkcie PHA a riešením nevýhod tejto výroby, ale taktiež aj využitím týchto biopolymérov. Jej cieľom bola najmä produkcia polyhydroxyalkanoátov baktériou Halomonas halophila so ziskom čo najvyššieho obsahu 3-hydroxyvalerátu (3HV) vo vzniknutom kopolymére poly(3HB-co-3HV), ktorý sa v týchto baktériách tvorí intracelulárne. Ten bol dosiahnutý pridaním kyseliny valérovej ako prekurzoru 3HV pre bakteriálne bunky. Kultivačné podmienky boli optimalizované, pretože kyselina valérová má zároveň inhibičný efekt na rast buniek. Bolo zistené, že vyššie koncentrácie ako 3 g/l nevedú k produkcii dostatočnej koncentrácie PHA. Pri veľmi nízkych koncentráciách kyseliny valérovej 0,1 g/l a 0,5 g/l bol obsah 3HV v PHA nízky. Vyhovujúca koncentrácia tohto prekurzoru, pri ktorej bunky vykazujú dostatočnú produkciu PHA, je 3 g/l. Taktiež bolo zistené, že kyselina by mala byť pridaná až po 24 hodinách kultivácie v minerálnom produkčnom médiu. Bunky sú už takmer v stacionárnej fáze a inhibičný efekt kyseliny má na nich menší vplyv, čo navýši množstvo utilizovaných PHA.

V práci sú aj porovnávané pôvodné kmene baktérie Halomonas halophila s kmeňmi, ktoré boli adaptované na kyselinu valérovú predstavujúcu stresový faktor pre baktérie. Nárast kolónií bol pozorovaný pri nižších koncentráciách kyseliny 1 g/l, 2 g/l (okrem riedenia kultúry 10-1) a 3 g/l. Koncentrácie kyseliny 5 g/l a 7g/l boli pre baktérie inhibujúce. Bol potvrdený predpoklad, že u adaptovaných kmeňov baktérií dochádza k lepšej utilizácii kyseliny valérovej a väčšej inkorporácie do kopolyméru, ako u pôvodných kmeňov (bolo zistené, že vyšší obsah 3HV v kopolymére bol dosiahnutý u adaptovaných kmeňov). Z výsledkov práce vyplýva, že u adaptovaného kmeňa označeného ako B bol obsah 3HV v kopolymére 20,24 mol. %. U pôvodných kmeňov bol pri použití rovnakej koncentrácie kyseliny zistený obsah 3HV v kopolymére len 6,74 mol. %. Práca dokazuje, že evolučné inžinierstvo je nástroj, ktorý má potenciál pre zlepšenie produkčných vlastností H. halophila, a to nielen vzmysle navýšenia výťažku, ale tiež vylepšenia materiálových vlastností pripravených materiálov. Vyšší obsah 3HV v kopolymére by zmenil jeho výsledné vlastnosti a zabezpečil tak lepšie využitie v niektorých priemyselných procesoch a odvetviach. PHA ako prírodné polyestery by mohli nahradiť konvenčné plasty. Nepredstavovali by tak hrozbu pre životné prostredie a boli by rozkladané neenzymaticky alebo enzymaticky pomocou extracelulárnych enzýmov mikroorganizmov

Kľúčové slová: *Evolučné inžinierstvo, adaptácia, polyhydroxyalkanoáty, Halomonas halophila, kopolymér poly(3-hydroxybutyrát-co-3-hydroxyvalerát), kyselina valérová.*

Sledovanie poškodenia miechy potkana pomocou magnetickej rezonancie metódou DTI

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Poranenie miechy môže spôsobiť vážne poruchy pohybového aparátu ako dočasné alebo permanentné ochrnutie. Je preto dôležité čo najpresnejšie charakterizovať rozsah vzniknutého poškodenia a zvoliť adekvátnu terapiu. Zobrazovanie tenzora difúzie pomocou magnetickej rezonancie (DTI) je metóda, ktorá umožňuje skúmať vláknité štruktúry ateda je často využívaná pri charakterizácii poškodenia bielej hmoty v centrálnej nervovej sústave. Cieľom tejto štúdie bolo zhodnotiť vplyv aplikovanej terapie na báze aktívneho alginátu na modely kontúzneho poškodenia miechy ex vivo.

Na DTI analýzu boli použité izolované miechy z dvoch skupín zvierat po kontúznom poškodení a následnou aplikovanou liečbou (N=7), alebo aplikáciou fyziologického roztoku (N=6) a izolované miechy zo skupiny sham operovaných zvierat (N=6). MR dáta z difúzne vážených obrazov boli spracované v programe DSI Studio, kde bol vypočítaný tenzor difúzie a na zobrazenie traktov bol použitý deterministický fiber tracking algoritmus.

Poškodenie miechy sme kvantifikovali pomocou štyroch základných parametrov difúzie: frakčná anizotropia (FA), axiálna difúzivita (AD), radiálna difúzivita (RD) a priemerná difúzivita (MD). Parametre sme vyhodnocovali na úrovni celej miechy, na úrovni rezu a na úrovni regiónu v oblasti dorzálneho traktu.

Rozdiel medzi liečenou a neliečenou skupinou bol pri vyhodnocovaní na úrovni celej miechy aj v jej jednotlivých rezoch výrazný pri hodnotách FA. Pri parametroch AD a MD sme pozorovali vplyv aplikovanej terapie taktiež na úrovni rezu. Výsledky z oblasti dorzálneho miechového traktu korelovali s kvantifikáciou na úrovni rezu.

Metódu DTI sme použili pri štúdii kontúzneho poškodenia miechy potkana. Sledovali sme vplyv aplikovaného liečiva na stav poškodenia, pričom sme použili 3 prístupy kvantifikácie. Konkrétne kvantifikáciu na úrovni celej miechy, na úrovni rezu a kvantifikáciu v rezoch z oblasti dorzálneho traktu. Vo všetkých 3 prípadoch bol signifikantný rozdiel medzi zdravou a poškodenou miechou vo všetkých sledovaných parametroch. Rozdiel medzi liečenou a neliečenou skupinou bol významný najmä pri parametri FA.

Metóda DTI poskytuje cenné informácie o samotnom poškodení a je užitočná aj pri sledovaní progresu počas medikamentóznej terapie. Pomocou takýchto meraní môžeme vyhodnotiť účinnosť zvolenej terapie.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Interakcia hormónov a liečiv s pôdnou organickou hmotou

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Do životného prostredia sa neustále dostávajú rozličné chemické látky, čoho následkom môže byť ohrozenie človeka a aj ekosystému. Medzi tieto látky sa v súčasnosti zaraďujú liečivá a hormóny. Táto práca sa zameriava na problematiku výskytu hormónov a liečiv v pôde a ich interakciu s pôdnou organickou hmotou.
Určité typy liekov v ľudskom organizme nepodliehajú úplnej metabolizácii a môžu byť vylúčené v aktívnej forme. Čistiarne odpadových vôd nie sú dostatočne účinné v eliminácii týchto látok, dôsledkom čoho vstupujú do životného prostredia. Odpadová voda kontaminuje pôdu a jej presakovaním taktiež dochádza ku kontaminácii podzemných vôd. Zdrojom kontaminácie pôdy je tiež používanie odpadovej vody na zavlažovanie polí v krajinách, ktoré trpia nedostatkom vody.
Hormóny sú produktmi endokrinného systému organizmu u ľudí a zvierat, zároveň môžu byť konzumované vo forme liekov. Veľké riziko pre životné prostredie predstavujú najmä steroidné estrogénne hormóny. Rovnako ako v prípade liekov je hlavným spôsobom kontaminácie životného prostredia nedostatočná eliminácia týchto látok z odpadových vôd. Výsledkom je že sa ocitajú v pôde, podzemnej, povrchovej a tiež aj v pitnej vode.

Pre bližšie preskúmanie tejto problematiky bol zvolený Ibuprofén. Vykonané boli dva experimenty, u ktorých bola pozorovaná sorpcia a desorpcia tohto liečiva na jeden typ pôdy s určitými vlastnosťami. Zámerom bolo zaznamenať zmeny v koncentráciách Ibuprofénu, ktoré nastali po uskutočnení týchto procesov.
Konkrétne množstvo Ibuprofénu bolo vypočítané z dát získaných kvapalinovou chromatografiou shmotnostne spektrometrickou detekciou. Naviazanie Ibuprofénu bolo dokázané infračervenou spektrometriou s Fourrierovou transformáciou.

Ošetření nápojů pomocí pulzního elektrického pole

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Tato práce si klade za cíl představit novou perspektivní non-termální metodu ošetření potravin – pulzní elektrické pole. Je věnována stručnému vysvětlení základních principů, na kterých je tato metoda a její účinnost založena. Popisuje jednotlivé konstrukční komponenty systému PEF pro ošetření potravin. Dále je zaměřena na možné aplikace pulzního elektrického pole v oblasti potravinářství a blíže popisuje dosažených výsledků použití této metody při pasteraci, extrakci, sušení a zmrazování. V práci jsou rovněž shrnuty účinky této metody na nutričně hodnotné a biologicky aktivní látky, stejně jako na procesní kontaminanty a mikroorganismy. Vzhledem k zaměření na ošetření nápojů, je v ní rozebrána i aplikace v nápojovém průmyslu.
V experimentální části práce je studován účinek ošetření pulzním elektrickým polem na suspenzi *Saccharomyces cerevisiae*. Je posuzován vliv nastavení hlavních parametrů ošetření (intenzita elektrického pole a frekvence pulzů) na redukci počtu mikroorganismů. Dosavadní výsledky prokazují, že vyšší účinnosti je dosaženo při nastavení vyšší frekvence pulzů a rovněž i vyšší intenzity elektrického pole.

Optimalizácia SPME v spojení s GC-MS/MS na stanovenie cypermetrínu v chemických postrekoch

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Cypermetrín je insekticíd nachádzajúci sa v produktoch určených na plošné poľnohospodárske, ale aj domáce účely. Kontrola kvality týchto produktov je veľmi dôležitá v krajinách s rozvinutým poľnohospodárskym priemyslom, nakoľko v posledných rokoch neustále rastie obchod s nelegálnymi a falošnými prípravkami, ktoré neobsahujú danú aktívnu látku alebo jej požadovanú koncentráciu. Tento nelegálny obchod môže predstavovať aj možné riziko pre ľudské zdravie a životné prostredie, keďže nie je známe reálne zloženie výrobkov. Problémom ich analýzy je však vysoká koncetrácia pesticídu (cypermetrínu), ktorá sa v týchto produktoch nachádza. To spôsobuje komplikácie pri ich analýze pomocou plynovej chromatografie v spojení s tandemovou hmotnostnou spektroskopiou (GC- MS/MS). Pred analýzou chemických postrekov je potrebné zriedenie vzoriek, čo spôsobuje značné chyby meraní.
Cieľom práce je vývoj jednoduchej, rýchlej a šetrnej metódy na stanovenie vysokej koncentrácie cypermetrínu v chemických po-

strekoch. Bola optimalizovaná automatizovaná metóda, pri ktorej chyba analýzy bola minimalizovaná vďaka odstráneniu opakovaného kroku zrieďovania. Na extrakciu cypermetrínu z chemických postrekov sa využila mikroextrakcia na tuhej fáze (SPME) v headspace (HS) móde a na následnú analýzu GC-MS/MS metóda. Bolo zistené, že optimálne parametre analýzy sú: teplota pece 250 oC a teplota dávkovača 200 oC. Pri optimalizácií SPME sa študovali rôzne parametre, ako typ vlákna, teplota a čas extrakcie. Vhodné vlákno pre izoláciu cypermetrínu pomocou SPME je polydimetylsiloxán, použité pri extrakčnej teplote 30 oC po dobu extrakcie 30 min. Zistilo sa, že optimálny čas desorpcie je 5 min. Vyvinutá metóda GC-MS/MS v spojení s HS-SPME bola následne aplikovaná na analýzu reálnej vzorky chemického postreku sobsahom cypermetrínu 4 900 mg L-1. Výsledky ukázali, že daná metóda je vhodná na stanovenie cypermetrínu v týchto produktoch.

Kľúčové slová: *cypermetrín, chemické postreky, SPME, GC-MS/MS*

Príprava a magnetické vlastnosti železnatých komplexov s pyridyl-benzimidazolovými ligandami

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Táto práca sa v prvom kroku zameriava na prípravu aromatických N-donorových ligandov, ktoré boli ďalej použité na syntézu dvojjadrových železnatých komplexov. Prekurzorom použitým pri syntéze ligandov L3 (1,5-bis(2-(pyridín-2-yl)-1H- -benzimidazol-1-yl) pentán) a L4 (1,5-bis(2-(pyridín- 2-yl)-1H-benzimidazol-1-yl)hexán) bol pybzim (2-(pyridín-2-yl)-1H-benzimidazol). Štruktúra nových ligandov bola potvrdená pomocou NMR spektroskopie a monokryštálovej RTG difrakčnej analýzy. Tieto ligandy sa líšia dĺžkou alifatického reťazca, ktorý spája dva pyridín-benzimidazolové fragmetny cez dusík, ktorý je situovaný na benzimidazolovom kruhu. Následne sa pripravili koordinačné zlúčeniny [Fe2(L4)3](BF4)4 a [Fe2(L4)3](ClO4)4. Magnetické merania uskutočnené pomocou MPMS SQUID magnetometra sa interpretovali ako závislosť produktovej funkcie χT od termodynamickej teploty. Výsledky merania odhalili neúplný graduálny spin crossover v prípade komplexu [Fe2(L4)3](BF4)4. . V prípade druhého komplexu [Fe2(L4)3](ClO4)4 absentuje fáza plató pre nízko aj vysokospinový stav, teda spin crossover nebol preukázaný. Elementárna analýza železnatých

komplexov nebola možná, preto presná štruktúra nie je známa. Predpokladané uvedené štruktúry vychádzajú z pomeru použitých ligandov a železnatých solí. To mohlo byť dôvodom zlého určenia mólovej hmotnosti vprípade komplexu [Fe(L4)2](ClO4) a následne nesprávny prepočet hodnôt magnetického momentu na hodnoty produktovej funkcie v závislosti od teploty a neprítomnosť spin crossoveru.

Kľúčové slová: *magnetické vlastnosti; spin crossover; železnaté komplexy*

SEKCE DOKTORSKÝCH STUDENTŮ

Lipidomic Analysis as a Tool for a Comprehensive Description of Atherosclerotic Plaques

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Atherosclerosis is a chronic inflammatory disease that causes lipids accumulation and the formation of fibrotic plaques in the walls of medium and large arteries. In this way, lipids are involved in the development of coronary heart disease and ischemic stroke, which belong among dominating causes of death in Western civilization. Considering the composition of the atherosclerotic plaque, lipidomic analysis was selected as a suitable tool for its study.
To characterize lipid profile in an atherosclerotic plaque in a longitudinal direction, relevant strategy had to be implemented. In the first phase, the sample preparation of the atherosclerotic plaques (obtained in cooperation with Military University Hospital, Prague) was optimized. Then, a pilot experiment confirmed the different lipids composition in different parts of the plaque. the key experiment was a lipidomic analysis of the atherosclerotic plaque cuts, which revealed different distribution of lipids depending on the progression of stenosis and also between proximal and distal

parts. Increased levels of oxidized free fatty acids and, conversely, a reduced content of plasmalogens were observed in the most affected parts of the plaque. In addition, a targeted screening of oxidized lipids was performed, and 46 oxidized lipids in total were detected in samples. MALDI-MS imaging was also used to describe the atherosclerotic plaque's composition (in collaboration with Laboratory of Molecular Structure Characterization, Academy of Sciences of the Czech Republic). This challenging technique enabled to visualize the spatial distribution of compounds in a sample thus complemented information needed for atherosclerosis pathology study.

Keywords: *atherosclerosis, lipidomics, mass spectrometry*

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Characterization of selected non-traditional cereals for development of enriched cereal products

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Cereals are one of the major food sources in human diet and the beginning of their cultivation is dated thousand years ago. Currently, the interest of the human population in a healthy nutrition and lifestyle is growing. This trend leads to increased interest in traditional cereals and also in less traditional pseudo-cereals, such as quinoa, which is also classified as a so-called superfood. for these reasons, this study was focused on the characterization of active substances and biological effects of selected non-traditional cereals.

In the study, 8 samples of non-traditional cereals were selected, namely amaranth, sorghum, millet, kamut, buckwheat, quinoa, Job's tears and teff. Amaranth, millet and buckwheat were also analysed in the form of flakes. Teff was analysed only in the form of flakes. Sorghum and quinoa were analysed also in their coloured variations. Basic substances of selected cereals such as proteins, lipids or carbohydrates were characterized. Active compounds such as antioxidants, phenolic compounds, gluten or β-glucans were also determined. These substances were mainly analysed by spectrophotometric methods. for the determination of gluten content RIDASCREEN® Gliadin competitive assay kit was used. Mixed-linkage β-glucan assay kit was used for determination of β-glucans content. for potential application, selected cereals were tested for cytotoxicity on human cells. Determination of cytotoxicity was performed by MTT assay using human keratinocytes HaCaT and human Caucasian colon adenocarcinoma $CaCO^{-2}$.

The results show that some of these non-traditional cereals could gain more attention in the future through their health benefits compared to traditional cereals. It would be interesting to combine them with other active substances that could support immunity or digestion. the best results were obtained for quinoa, amaranth and buckwheat.

Keywords: *cereals, pseudo-cereals, active substances, antioxidants, gluten, β-glucans*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Development of an analytical method for the determination of phytocannabinoids and their bioavailability in rat blood plasma

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Phytocannabinoids are bioactive compounds occurring in Cannabis sativa L. Currently,non-psychotropic cannabidiol (CBD) has been intensively studied due to its presumed beneficial effects on the human organism (e.g. antioxidant, analgesic, and anti-inflammatory effects, etc.). CBD is sold mainly as a component of various food supplements, the most common are 'CBD oils'. However, under certain conditions, the consumption of CBD-based products carries some risks, which might be associated with the purity of the CBD (which strongly depends on the way of its isolation). To our experience, in many cases, a number of other naturally occurring phytocannabinoids are found in CBD oils, including psychotropic Δ^9-tetrahydrocannabinol (Δ^9-THC). In addition to the need to perform a purity check, the question arises regarding the bioavailability of CBD as it is an important aspect for the evaluation of its effect. for this purpose not only the parent compound but also its metabolites.

The aim of the work was to develop, optimize and validate an analytical animal method for the determination of phytocannabinoids and their biotransformation products (metabolites) in blood plasma of experimental that were administered in oil and CBD formulations differing in respective carriers. Using this method, the bioavailability of CBD as a function of time was subsequently investigated. At intervals of 2, 4, and 6 hours after intake of the preparations, blood plasma was collected for analysis by ultra-high performance liquid chromatography coupled with tandem mass spectrometry (UHPLC-MS/MS). Only CBD was detected in the samples at the level of quantification. In most cases, CBD concentration reached the apex after two hours, however, when using the oil carrier. CBD (reference) maximum concentration was reached after the four hours after administration. It should be noted that significant variability was observed within the animals' cohort.

Keywords: *phytocannabinoids, UHPLC-MS / MS, plasma*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Preparation of Mg-Al-Ti Bulk Materials Via Powder Metallurgy

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Bulk materials based on the Mg–Al–Ti system were prepared using traditional methods of powder metallurgy, as well as using the sprak plasma sintering (SPS) method. the microstructure of the material, elemental and phase composition was examined. Subsequently, Vickers hardness and flexural strength were measured, and fractographic observation of the fracture surface was performed. It was found that the aluminum was completely dissolved during sintering and subsequent heat treatment, but the titanium particles remained almost intact in the material and worked as a particulate reinforcement. X–ray diffraction spectroscopy detected multiple phases, such as magnesium phase β, magnesium–aluminum solid solution, pure titanium, and titanium nitride. Titanium nitride could be formed because of the reaction of titanium and the nitrogen atmosphere used during sintering. Materials prepared by methods of conventional powder metallurgy showed increased porosity compared to materials prepared by the SPS, resulting in lower hardness and flexural strength. This phenomenon could be caused by Kirkendall effect, where aluminum diffused into magnesium faster than magnesium into aluminum. the hardness increased with increasing the amount of aluminum and titanium and with the amount of magnesium phase β. Fractographic observation of the fracture surface showed, that titanium particles held firmly in the matrix even after formation of crack, which in some cases passed through the titanium particle itself. This fact might suggest that a diffuse connection between the reinforcement and the matrix may have occurred after the sintering process.

Keywords: *magnesium alloys, aluminium, titanium, spark plasma sintering, hardness, flexural strength*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Fixation of the Lead in Alkali Activated Materials Based on Different Types of Ashes

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The aim of this work was to prepare alkali-activated matrices of sufficient strength based mainly on ash, to reveal the method of fixation of lead in these matrices and to determine the impact of added lead on mechanical properties. the matrices consisted mainly of ash with a mixture of blast furnace slag and sodium water glass as an activator. Five different ashes were used – four of them were from fluidized bed coal combustion and one from pulverized coal combustion. After 28 days, the strengths of the samples were measured to reveal an impact of lead doping. To determine the structure, images, element maps and elemental spectra were taken using a scanning electron microscope with energy dispersive spectroscopy, the samples were analysed on an infrared spectrometer with Fourier transform, X-ray diffraction analysis and electron spectroscopy for chemical analysis were also used. Individual measurements show that lead is accumulated in the form of hydroxide. the impact of lead doping on strength of the matrix was different for individual samples.

Keywords: *alkali activated materials, inhibition, lead, fly ashes*

Bioaccessibility of Metals in Urban Aerosol

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Atmospheric pollution is an increasing cause of concern for human health. Atmospheric particulate matter (PM) is known as the source of several health effects (cardiovascular and respiratory diseases including lung cancer, neurodevelopmental and neurodegenerative diseases). Metals are of particulate interest for the assessment of PM toxicity because of the fact that they are capable generation reactive oxygen species (ROS). ROS induce oxidative stress leading to inflammatory responses and DNA damage.

Large attention should be paid the particle size. Particles in the range of 2.5-10 μm are in most cases deposited in the pharyngeal and tracheal region. In the adoral area, they can be swallowed, thus reacting also in the gastrointestinal tract. Particles less than 1 μm can reach the alveolar lung regions and interact with lung fluids.

Bioaccessibility testing is becoming an increasingly popular exposure assessment method, due to its simplicity and cost effectiveness. In this contribution, the soluble metal fraction extracted with simulated lung fluids (SLFs) is used as an estimation of metal bioaccessible fraction. Metal bioaccessibility is defined as the total metal fraction that is soluble in the target organ (lungs

for respiratory bioaccessibility). the most commonly used SLFs are water and Gamble solution. Gamble solution is representative of the interstitial fluid in the deep lung. As addition of this fluid was on Institute of Analytical Chemistry, Czech Academy of Science developed new SLF called Simulated Alveoli Fluid (SAF), which attempts to simulate extraction in alveoli.
The aim of this contribution is to assess the bioaccessibility of potentially toxic metals (i. e. Fe, Mn, Zn, Ni, Cu, Cd, Co, Pb, V, Cr) associated with urban aerosol collected on nitrocellulose filters in Brno (Veveří street). To measure the total concentration of metals, a portion of the filters were decomposed in concentrated nitric acid using microwave decomposition. Total metal concentrations were measured using ICP-MS. the bioaccessibility was determined after the incubation of samples in three solutions that mimic chemical conditions in the lungs (deionized water, Gamble solution and SAF) for 24 hours at 37 °C. the differences in metal bioaccessibility in different aerosol size fraction were evaluated by sampling two different PM size fraction: $PM_{2.5}$ and PM_1.

Keywords: *metals, bioaccessibility, aerosol, simulated lung fluid*

Aminoclay as Drug Carrier

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This study aimed to prepare new drug delivery system with use of aminoclay complexes to enhance the drug release and improve bioavailability of selected drugs. Aminoclay is a relatively new material that belongs to organically modified clays. It is a magnesium phylosilicate that contains 3-aminopropyl groups. the clay material thus modified is characterised by relatively good chemical and mechanical stability, showing no signs of toxicity even at higher concentration. Thanks to easy preparation, and thermal and mechanical stability of inorganic matrix and external amino groups is aminoclay a material with great potential for many applications. By binding the drug to the aminoclay matrix it is expected to improve properties such as solubility, stability, release, bioavailability, biodegradation, etc.
For model samples was used a selection of the bioactive substances: curcumin, diclofenac, ibuprofen, merocyanin and tocopherol. for verification of binding drugs were used methods of FTIR (Fourier Transformation Infrared Spectroscopy) and EA (Elemental Analysis). Furthermore, the content of the bound bioactive substances to the aminoclay matrix was investigated using UPLC (Ultra Performance Liquid Chromatography). What is essential for therapeutic use of bioactive substances is their value of cytotoxicity. for this

study MTT test for evaluation of cytotoxicity was used.
The main motivation of this study was to create new complexes with improved characteristics that would replace existing forms of substances used in pharmaceutical and biomedical applications.

Keywords: *aminoclay, carrier, drug*

Preparation and Characterization of Functionalized Wound Dressings

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This work is focused on preparation and characterization of bioactive hydrogels and nanofiber wound dressings functionalized by active compound in the form of antibiotic drug: ampicillin. Nanofiber dressings were constituted from poly(3-hydroxybutyrate) and hydrogel dressings were created using alginate and chitosan. Prepared wound dressings were tested for possible cytotoxic effects on human cells, antimicrobial activity and the rate of gradual releasing of the incorporated substance into model environments. Nanofibers were assembled by electrospinning and force spinning techniques. Morphology of the prepared nanofibers was confirmed by SEM. Dressings were characterized for gradual release using spectrophotometric methods. Antimicrobial activity against gram-positive and gram-negative strains of microorganisms was also evaluated. the results showed good antimicrobial efficacy of functionalized materials.
Because of the potential application for local skin treatments the cytotoxicity of the prepared materials was tested. Safety of the dressings was determined by MTT assay using human keratinocytes (HaCaT). the majority of the prepared materials has been

proved to be non-cytotoxic, and, thus, safe for topical applications in human subjects. Prepared nanofiber and hydrogel dressings with antimicrobial effect showed promising results for the local treatment of open wounds, such as skin ulcers.

Keywords: *wound dressings, ampicillin, poly(3-hydroxybutyrate), chitosan, alginate, antimicrobial activity, cytotoxicity*

Acknowledgments
This work was supported by the project Nr. FCH-S-20-6316 of the Faculty of Chemistry, Brno University of Technology

High Throughput Platform for Identification And Characterization Of Electrogenic Bacteria.

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Electrogenic and electron accepting capability of some bacteria strains, are important phenomena which promises advances in the fields of electronically stimulated biotechnological production of valuable chemicals, wastewater treatment, bioremediation, desalination, energy production, novel materials discovery and whole-cell biosensing. Significant boost towards this direction can be achieved with application of high throughput methods known from other biological disciplines. However there is currently a lack of standard and reliable hardware which would enable the same approach in the field of electrogenic bacteria.
Thus we present a platform based on standard Microplate set-up with 24 or 96 single chamber air-cathode Microbial Fuel Cells (MFCs) with integrated reference electrode inside each chamber. All electrodes are individually addressable. the device enables the direct and parallel comparative analysis of microbes from different sources or under different conditions such as electrode potential, pH and growth medium.

Determination of micro-bioplastics in solid matrix

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Mankind try to replace oil-based plastics by so-called biodegradable bioplastics to minimize plastic pollution. These bioplastics requires specific conditions for biodegradation, which are usually not met in nature. This could lead to formation of microplastic debris „Micro-bioplastics“. There are plenty of analytical methods for determination of conventional microplastic presence or concentration in aquatic systems, the less of studies focus on analysis in soils due complexity of this matrix and there is lack of methods for determination of micro-bioplastics. the most difficult, time consuming and dangerous for analyte are soil sample pre-treatment and preconcentration or extraction of bioplastics. That's why we have developed direct analytical method using evolved gas analysis (EGA, combination of thermal degradation and mass spectrometry) for determination of micro-bioplastics, which does not require any of these sample preparation techniques. We present data on use this method for determination of micro-bioplastics in Siberian and Czech soils, the standard Lufa soil and in sewage sludge. Application of this method was already successfully demonstrated for determination oil-based microplastics. In this work, as a model bioplastic was used polyhydroxybutyrate (PHB) and polylactic acid (PLA). We demonstrate a fast, robust, and easy EGA method for determination of PHB and PLA micro-bioplastics in soil and other solid matrix with possible differentiation of anthropogenic PHB from natural PHB. In addition, this method could be helpful for verification and precising of biodegradation tests and contamination evaluation of soil after applying micro-bioplastic polluted compost.

Acknowledgement
The financial support of projects FCH-S-20-6446 of Ministry of Education, Youth and Sports are acknowledged.

Keywords: *Micro-bioplastics, microplastics, evolved gas analysis, soil, sewage sludge*

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Study of Cholesterol's Effect on the Properties of Catanionic Vesicular Systems

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This work is focused on the study of properties associated with the effect of cholesterol levels on the stability of vesicular systems based on the ion pair amphiphile hexadecyltrimethylammonium-dodecylsulphate (HTMA-DS) at laboratory temperature. the HTMA-DS catanionic system was doped with dioctadecyldimethylammonium chloride in a 9:1 M ratio and cholesterol in the amount of 0, 3, 13, 23, 33, 43, 53, 63 and 73 mol.% was added. In this system, the size distributions were studied using the dynamic light-scattering technique and the zeta potential was determined. These standard techniques were supplemented by fluorescence spectroscopy technique. Specifically, generalized polarization (GP) was measured using a Laurdan probe. This probe is sensitive to fluidity and membrane hydration at a particular temperature. Due to low stability and high opalescence of samples, spectral techniques were used only for the samples with cholesterol content above 23 mol.%. the results from fluorescence spectroscopy point to a change in the amount of hydration water in the membrane, the largest amount of which is present in the samples with 43 and 53 mol.% cholesterol. Using the light-scattering technique, the short-term stability of prepared vesicular systems was also observed over the first 36 days. Obtained results confirmed that the most stable systems are those containing 43 or 53 mol.% of cholesterol. This work was supported by the Czech Science Foundation, project No. 19-14024J (GACR), and Ministry of Science and Technology, Taiwan, project No. MOST108-2923-E006-MY3.

Keywords: *Catanionic vesicles, Ion pair amphiphile, Dynamic Light Scattering, Zeta potential, Generalized Polarization, Laurdan, Hydration water.*

Characterization of Hydrogels with Amphiphilic Structures

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Nowadays there is an increasing demand for hydrogels with modifiable properties, which would find application especially in health care, pharmacy, or common consumer industry. Inspiration for hydrogel structures can be found in extracellular matrix, which has the character of a hydrocolloid and which is often simulated by hydrogels. It also has a relatively complex composition and some components „only" regulate biochemical processes, while others co-create or influence its properties. Understanding the physicochemical properties of the extracellular matrix is very complex and yet not well described. Hydrogels in this work are trying to use the knowledge gained from the proper functioning of a living organism and then transfer it to the developed hydrogels.
This work deals with the study of preparation and properties, especially rheology, of hydrogels, whose internal structure is modified and controlled by addition of suitable amphiphiles. the specific material solution of this work is based on simple hydrogel matrices, which were prepared from agarose and gelatin. In the frame of this contribution the formation of internal structures was caused by the addition of lecithin. the addition of amphiphilic

substance affects the viscoelastic moduli, the values at the cross over point as well as the relaxation properties.

Keywords: *amphiphile, hydrogel, rheology*

Study of simple electrolytes for magnesium batteries

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The study is focused on electrolytes for magnesium batteries. In contrast to electrolytes published in recent scientific articles, which were mostly prepared from either hazardous or expensive substances, the electrolytes in this work were composed of affordable solvents and chemicals, which can be handled at normal laboratory conditions. Specifically, solutions of dimethylsulfoxide and tetrahydrofurane with magnesium chloride, nitrilotriacetic acid, aluminium chloride, and disodium ethylenediaminetetraacetic acid, were examined. the ability of electrolyte to oxidize and deposit magnesium was characterized using cyclic voltammetry. More information about the kinetics of electrochemical reactions in terms of polarization resistance was obtained by electrochemical impedance spectroscopy. EIS was also used to reveal formation of oxide layer on electrode and its homogeneity. Magnesium electrodes from electrochemical measurements were finally examined by scanning electron microscopy with energy-dispersive X-ray spectroscopy. Based on the SEM pictures and EDS data, the effect of humidity and atmospheric oxygen on magnesium electrode corrosion during electrochemical cycling was discussed.

Keywords: *magnesium batteries, electrolyte, cyclic voltammetry, electrochemical impedance spectroscopy (EIS).*

Humid Air Cooling by Shell and Tube Heat Exchangers

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The processes of cooling by shell and tube heat exchangers for subsequent application in processes of removal of gaseous air contaminants via liquid absorber is the major topic of this work. the aim of the work is to verify both the theoretical computational relations and the theoretical convenience of silicon carbide as a better heat transfer surface material compared with traditional borosilicate glass material characterized by two orders of magnitude worse thermal conductivity. Heat transfer on semi-operating shell and tube heat exchangers with baffles and glass or silicon carbide heat exchange surface is examined by cooling the humid air by 50% propylene glycol in tubes having an inlet temperature just above 0 °C.

Coolant flow can be regulated in many steps, but only laminar flow rates are available. Unfortunately, the coolant inlet temperature cannot be precisely regulated, just only precisely measured (as outlet temperature). Three-way flow of coolant is used, so speed of coolant is three-times higher in tubes. Relative air humidity, temperature and flow of air is measured.

Local air heat transfer coefficient is low due to low ventilator pow-

er, low temperature, and low humidity. the effect of coolant and heat transfer surface on transferred heat is almost negligible. the efficiency of exchangers is very high (91–94 % with carbide and 88–89 % with glass). the trend of a slight increase in efficiency is observed with increasing flow of both fluids. Flow turbulization is the reason. the three-way flow of coolant may also negatively affect the efficiency, it will be verified with a higher heat transfer coefficient condition.

The theoretical model using the *j* factor, the correction factors for the baffles, and the correction for air humidity condensation have proven to be appropriate under the examined conditions. the trend of overestimating the model at higher flow rates, especially air, was shown. This trend will be examined with a higher heat transfer coefficient condition. the result is also affected by the inaccuracy of the calculation of the mean temperature difference, especially for carbide heat exchanger, caused by failure to use most of the heat exchanger potential. the results also evaluate the heat loss through the shell and the heat exchanged in addition by air humidity condensation.

After the experiments with an increased local air heat transfer coefficient, the experiments with coolant temperature below 0 °C will probably follow and heat exchange affected by icing would be observed. the air temperature profile will be computer modeled and verified by measuring the temperature close to the middle of the carbide exchanger. Then, cooling of air will be situated in front of the separation of gaseous impurities from gas into liquid using a scrubber, more effective at lower temperatures. Separation of some pollutants could also take place by condensation in the exchanger at very low temperatures, or high pressures.

Keywords: *shell and tube heat exchanger, heat transfer, cooling, humidity condensation*

Spectroscopic Study of Human Blood Plasma for Early Detection of Hepatocellular Carcinoma

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The spectroscopic analysis of biofluids, mainly blood plasma and serum, is starting to attract attention in clinical diagnostics as a more time- and cost-efficient alternative to standard procedures. It is non-invasive, requires almost no sample preparation and the collected spectra contain complex information about the analysed sample. In the presented research, the techniques of Fourier-transform infrared spectroscopy, Raman spectroscopy and electronic circular dichroism were used to study blood plasma samples of patients with hepatocellular carcinoma (HCC) and liver cirrhosis.

Hepatocellular carcinoma ranks among the cancer types with the highest incidence and mortality. the main precondition for developing HCC, liver cirrhosis, is well recognized, yet the currently employed screening methods do not achieve sufficient sensitivity to early stages of the disease. the early diagnosis is, however, essential for the success of available treatment methods. Therefore,

identification of novel biomarkers, which would allow for early detection using a simple blood test, would be a big step forward in HCC diagnostics, possibly even reducing its high mortality.
The aim of this work was to develop the procedure for the diagnosis of HCC from blood plasma samples, based on spectroscopic analysis and multivariate statistical evaluation of the collected spectra. the most significant spectral differences allowing for the classification of the samples were assigned to proteins and possible alterations of their conformation associated with the disease. A combination of principal component analysis and linear discriminant analysis was able to distinguish between the blood plasma of patients with HCC and patients with cirrhosis with an overall accuracy of 90%, misclassifying only 3 out of 33 samples. So far, the results show high potential of the spectroscopic analysis of blood plasma to become an innovative method for early diagnostics of HCC.

This work has been supported by Ministry of Health of the Czech Republic, grant nr. NV19-08-00525 and Specific University Research MSMT (21-SVV/2020).

Keywords: *vibrational spectroscopy, electronic circular dichroism, blood plasma, hepatocellular carcinoma, cirrhosis*

The Influence of Alkaline Activator Type on the Carbonatation Process of the Alkali-activated Blast Furnace Slag

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Carbonatation represents one of the potential degradation mechanisms of the construction materials. the negative impact of the carbonatation are mainly accompanied by the decrease of the pH of the pore solution under the certain value (9–10) and the formation of reaction products (various types of carbonates or bicarbonates). the progress of the carbonatation is significantly dependent on the experimental conditions like the partial pressure of CO_2 or the humidity. the various types of alkaline activators (sodium hydroxide, sodium carbonate and sodium water glass) in 6 % Na_2O dosages were used in this study for the preparation of the alkali-activated blast furnace slag samples for further carbonatation testing when exposed to various environments – exterior, interior, CO_2 chamber and water. the progress of carbonatation was evaluated with a meaning of carbonatation depth determination using the phenolphthalein technique and optical analysis method. the impact of the carbonatation on the mechanical properties was assessed by the compressive and flexural strength measure-

ments. No rapid deterioration of the mechanical properties was observed in case of the sodium hydroxide alkaline activation process. However, a noticeable changes were found for the sodium water glass activated systems especially in terms of exterior and interior storage.

Keywords: Alkali-activated blast furnace slag, carbonatation, carbonatation depth, degradation

Characterization of Bacterial Strains Obtained in Evolutionary Engineering

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Evolutionary engineering is a valuable tool for improving properties of microorganisms on phenotype level without a need of a deeper knowledge of genetic characteristics. the bacteria's cell generation time is 0.5 hour, compared to the humans 20 years. It is therefore advisable to study evolutionary engineering on bacteria, as in a relatively short time we can see chances in the phenotype. the application of stress factors under laboratory conditions leads to an unexpected augmentation of bacteria performance in the stressful environment. the criterion chosen in this work to evaluate the success of an adaptation to a specific stress was the amount of polyhydroxyalkanoates (PHAs) generated by wild and adapted strains, moreover, the activities of selected were analyzed to get insight into stress adaptation mechanisms.

Two bacterial strains, *Cupriavidus necator* H16 (CCM 3726) and *Halomonas halophila* (CCM 3662), were chosen for the evolutionary experiments. There strains are producers of PHAs which are biopolyesters stored in cells as energy storage materials by various microorganisms. It is a fully biodegradable and biocompatible family of polymers with interesting physicochemical properties. Copper cation (Cu^{2+}) and sodium chloride (NaCl) were chosen

as the selective pressure for *C. necator* H16; acetic acid (AA) and levulinic acid (LA) for *H. halophila*. the adapted strains were analyzed in regular intervals during long-time evolutionary experiments. A growth potential of the bacteria, together with a yield of PHAs from the biomass by the means of gas chromatography with flame ionization detector (GC-FID) and polymer physicochemical properties (molecular masses and polydispersities) by the means of size exclusion chromatography with multi-angle light scattering (SEC-MALS) were determined. the adapted strains were also exposed to selected stress factors and the amount of viable cells was evaluated by spectral flow cytometry (FC). Metabolic characterization was provided by a determination of specific enzyme activities of enzymes involved in selected cycles. Biomass and PHA production of both wild and adapted *H. halophila* strains cultivated in lignocelluloses hydrolysates were determined. the successful adaptation of adapted strain *H. halophila* to LA in the LA environment was confirmed. This strain was able to produced almost 70% more PHAs than the wild-type strain of this bacteria in the LA environment from the lignocelluloses waste. It was also concluded that *C. necator* H16 successfully adapted to Cu^{2+}.

Keywords: *Evolutionary engineering, polyhydroxyalkanoates, selective pressure, adaptation, bacteria.*

Assessment of potential heavy metal pollution of road dust in arid urban area

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In urbanized areas, heavy metal contamination represents a major issue in terms of environmental quality and health risks related to chronic exposition. Traffic routes are one of major sources of heavy metals in dust, which can be easily transported into environment through wind or rainfall. the main constituents of road dust are industrial ashes, seasonal products of chemical treatment of road surfaces and abrasive emissions from roads and vehicles. Up to 75% of road dust consists of particles smaller than 50 μm. These dust particles adsorb higher contents of heavy metals due to their high specific surface and are most readily transported into surrounding environment. Road dust samples discussed in scope of this study originate from roads in Ulaanbaatar, Mongolia as a city with high degree of air pollution originating from extensive coal burning and industry. After sampling, drying and sieving, the samples were processed into three grain size fractions (<45 μm, 45–63 μm, 63–125 μm). Aqua regia leachates of the samples were obtained using microwave digestion system and analysed using inductively coupled plasma mass spectrometry (ICP-MS) to

obtain content of As, Cd, Cr, Cu, Ni, and Pb. Initial results after analysis of the grain size fraction 45–63 μm do not indicate significant elevation in obtained heavy metal contents compared to published data on road dust in other parts of the world. Obtained contents are utilized for visualization of content profile changes between city centre and adjacent environs. the second part of this study focuses on statistics and correlation between individual heavy metals for further differentiation of heavy metal mobility between individual grain size fractions.

Keywords: *environmental chemistry, inductively coupled plasma, mass spectrometry, road dust, Mongolia, urban pollution, air pollution*

Surface Treatment of Cementitious Systems by Silicates

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The efficiency of the silicate-based surface treatment agents, other words sealers, has been widely investigated over the past decades. the surface treatment utilization protects the cementitious system against the penetration of undesirable substances. Another purpose of sealers application is to reduce the risk of deterioration of cement structures that leads to increasing their durability. Nevertheless, understanding of the several aspects concerning the silicate-based sealers is not entirely clear. This study deals with the action mechanism of selected silicates such as potassium, sodium, lithium silicates and colloidal silica with the cementitious surface. Effectiveness of used sealers in terms of water absorption, hydration mechanism, same as the effect on the microstructure of the cement substrate was studied and evaluated with the contribution of following techniques – rheometry, mercury porosimetry, isothermal calorimetry, Xray diffractometry and scanning electron microscopy. Silicatebased treatment agents were assessed on two sets of specimens; fresh cement pastes (at the age of 1 hour) and on the hydrated ones (24 hrs.), respectively.

As result, certain effectiveness of the used sealers was verified. Film-forming sealers have shown higher effectiveness in

case of their usage on the hydrated cementitious surfaces (24 hrs.). Thus, the dependence of sealers efficiency on the substrate hydration progress was confirmed.

Keywords: *Concrete sealers, treatment agents, calcium silicate hydrate, microstructure*

Study of the influence of water coefficient on porosity and mechanical properties of high-performance concrete

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Constant pressure on concrete preparation with the best possible properties is important for both economic and environmental reasons. Choosing the ideal concrete preparation process, concrete with better properties can be prepared from the same raw materials and thus save building material. One of the important parameters in the preparation is the water coefficient, which has a direct effect on the porosity of concrete. In case of more mixing water than necessary for cement hydration is added to the mixture, pores weaken the macrostructure of the concrete after drying. In the case of a low water coefficient, even a material with a sufficient flow limit for processing may have too high viscosity resulting in insufficient degassing and a residual air pores in the concrete which weaken it. the aim of this work is to monitor the influence of water coefficient on mechanical properties and porosity of high-performance concrete and to find the ideal water coefficient to reduce macroporosity.

Keywords: *porosity, concrete*

Microwave-Assisted Preparation of Organo-Lead Halide Perovskite structures for electronics

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Organo-lead halide perovskites are promising materials for the development of solar cells, solid-state lasers, light emitting diodes (LEDs), photodetectors, etc. Perovskites can easily be deposited from their precursor solutions into a thin film by solution-based processes [1]. Nevertheless, the prepared films possess defects which cause non-radiative recombination, current-voltage hysteresis and rapid degradation due to the low stability of the resulting devices [1].The efficiency of the functional devices descends dramatically when amorphous materials are implemented instead of highly crystalline ones. Therefore, it is challenging to optimize and up-scale the production of large-sized single crystals of perovskite materials. Here, we describe a novel and original approach to MAPbBr3, FAPbBr3, MAPbI2 and FAPbI2 lead halide perovskite single crystals preparation which consists in applying microwave radiation during the crystallization [1]. the facile microwave assisted method of preparation is highly reproducible, fully automated and in addition, it can be applied for various different perovskite

structures. Simultaneously, this eco-friendly method is expected to be easily up-scalable because of its versatility and low energy consumption. We believe that this method will make preparation of single crystals, nanosystems, 2D systems and the final functional devices fabrication (like solar cells, LEDs, photodetectors, i. e.) more convenient and efficient.

The work was supported by the FCH-S-20-6340

[1] Jan Jancik, Anna Jancik Prochazkova, Markus Clark Scharber, Alexander Kovalenko, Jiří Másilko, Niyazi Serdar Sariciftci, Martin Weiter, and Jozef Krajcovic, Crystal Growth & Design 2020 20 (3), 1388 – 1393, DOI: 10.1021/acs.cgd.9b01670

Keywords: *microwave, organo-lead halide perovskite, single crystal*

Relaxation Behaviour of Hydrogel Materials Using Classical Rheology Methods

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Proposed paper investigates relaxation behaviour of hydrogel materials using classical rheology methods as a part of the complex rheological characterization of these systems. Specifically, creep and recovery tests as well as three interval thixotropy tests were studied in this paper.
Extensive optimization of these tests was carried out in order to find ideal measurement settings, which for creep tests consist in proper values of applied stress, temperature and duration of loading and relaxation step. the essential variables for three interval thixotropy tests are frequency of oscillation, temperature and applied strain as well as duration for each step. the optimization procedure was performed using 1 wt. % physically crosslinked agarose hydrogel and the tuned tests were applied besides other different concentrations of agarose hydrogel also to hyaluronic acid based hydrogels formed due to interactions between negatively charged polyelectrolyte groups with positively charged surfactants and to polyvinyl alcohol gels chemically crosslinked via borax. These samples were selected to cover a variety of hydrogels with mutually different crosslinking principle.
Both experiments confirmed, the agarose gel proved to have the best ability to recover after deformation of all studied samples. Moreover, increasing agarose concentration and decrease in duration of deformation step led to better sample regeneration. on the other hand, the hyaluronic acid based hydrogel reported the worst relaxation properties. Although these results were comparable from both experiments, the percentage structural regeneration from each test was different. Hence, the complex relaxation characteristics cannot be defined using one of the mentioned tests alone and both the creep and the three interval thixotropy tests are highly beneficial in case of study of hydrogel materials' relaxation behaviour.
Obtained results from this paper may lead to more precise description of deformation and relaxation characteristics, which are frequently occurring during treatment as well as application of hydrogel materials.

Keywords: *Rheology, creep tests, three interval thixotropy tests, hydrogels*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Simple multi-analyte LC-MS method for the determination of food additives in soft drinks and alcoholic beverages

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Usage of food additives in the food industry is a common manufacturing practice. Due to potential negative biological effects in some population groups suffering from specific health disorders, toxicological evaluations are done for each substance to be used as a food additive. To ensure the safety of the consumer, every additive has its own maximum level limits for various commodities. for the confirmation of the compliance with these limits, reliable and fast analytical methods are being developed. for this purpose, a rapid LC-MS method was developed for the simultaneous determination of different classes of synthetic food additives. the method is capable of nine food colourants, seven sweeteners, two preservatives, and two purine alkaloids determination. Ultra-high performance liquid chromatography with the reverse phase column separation was coupled to mass spectrometry with a single quadrupole mass analyzer. the developed method was applied to the analysis of 76 beverages, including 14 soft drinks, 19 energy drinks, 23 liquors, 14 spirits, and 6 ciders. In addition, the concentrations quantified conformed to the limits prescribed by the EU (Regulation [EC] No. 1333/2008). the designed method is fast and allows parallel determination of substances with different physico-chemical parameters.

Keywords: *food additives, liquid chromatography, mass spectrometry, beverages*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Preparation of metakaolin with high whiteness

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The term kaolin is used to describe white clays whose main mineral is kaolinite Al2Si2O5(OH)4. Kaolinite is formed by the decomposition of various of feldspars and therefore is usually doped with other minerals (quartz, sulphur, feldspars, micas and iron and titanium oxides). the quality of the clays and over all kaolin is measured in function of iron content, because this element gives the red-brown colour to this type of minerals.

This paper summarizes the various possibilities of kaolin bleaching by firing. Kaolin of 20 grams dosage was fired at 1 100 °C for 2 hours. Several types of reducing agents (spar, specially ground quartz (SGQ), alumina and a mixture of graphite and sodium chloride) were used during firing with a goal to reduce the present iron 3+ to less colouring state of Fe2+ thus increase the whiteness of kaolin. It was found that the best effect on increasing the whiteness of kaolin has the firing of the raw material itself. Reducing agents were added in weight rations of 1, 3 and 5 % and have been able to partially increase the whiteness in some cases, but this is an increase of units of percent.

Subsequently, the reduction mixture was selected and used for firing in a sintering furnace. the whiteness of kaolin obtained in sintering furnace was not sufficient. the low efficiency of the sintering furnace was mainly due to unsuitable furnace setting.

Keywords: *bleaching clay, kaolin, sintering furnace, reducing agent*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Thermophilic Bacterium *Schlegelella thermodepolymerans* DSM 15344 as a Producer of Polyhydroxyalkanoates

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Thermophilic microorganisms grow and thrive even at temperatures that are inhibitory or even lethal to most microorganisms. for a long time, thermophiles have been considered a unique source of thermostable substances, especially enzymes. However, in the last few years, thermophilic microorganisms have also been considered as production cultures for other substances, e.g. polyhydroxyalkanoates. Higher culture temperatures make it possible to achieve a higher reaction rate, a higher solubility of most chemicals or a reduction in the sterility requirements of the process.

Polyhydroxyalkanoates (PHAs) are biodegradable and biocompatible polyesters that are produced and accumulated by bacteria as intracellular granules. These biopolymers have similar properties to some synthetic plastics but are not harmful to the environment. for that reason, they could be a suitable alternative. Unfortunately, their production cost is still high. Therefore, approaches are being sought to produce PHAs cheaper. One of the possibilities is

the use of the aforementioned thermophilic microorganisms.

One of the representatives of thermophilic microorganisms is the gram-negative bacterium *Schlegelella thermodepolymerans* DSM 15344. This strain was isolated from activated sludge and is unique in its ability to degrade a copolymer containing 3-hydroxybutyrate and 3-mercaptopropionate. the process of PHA degradation was described. Therefore, we began to investigate its biotechnological potential. Our bioinformatic analysis of available draft genomes revealed, that *S. thermodepolymerans* possess *phbCAB* operon and, therefore, might be a producer of PHAs. Production conditions were tested at various temperatures, carbon substrates and precursors suitable for the synthesis of polymers with modified properties. *S. thermodepolymerans* is able to utilize xylose very well, surprisningly, it even prefers xylose over other saccharides and harbors unique operon containing genes encoding for enzymes involved in xylose metabolism. Since xylose is present in numerous lignocellulosic materials, we cultured the bacterium also on model hydrolysates and we also evaluated its sensitivity to microbial inhibitors present in lignocellulose hydrolysates. According to our results, *S. thermodepolymerans* appears to be a very promising producer of PHAs.

Funding: This study was supported by Brno University of Technology intra-university junior project FCH/FEKT-J-20-6399.

Keywords: *Schlegelella thermodepolymerans, thermophiles, polyhydroxyalkanoates, biopolymers*

Development of a method for simultaneous determination of various esters of MCPD and glycidol in palm fat by supercritical fluid chromatography

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Fatty acid esters of 2- and 3- monochloropropanediol (2- and 3-MCPD) together with glycidyl fatty acids esters belong to a group of process-induced chemical contaminants, formed in high temperature environments mainly during industrial food processing. They most commonly occur in refined vegetable oils, especially in palm fat. Most potent precursors of MCPD esters are partial esters of glycerol, such as diacylglycerols (DAG). the other major variable is a chlorine source; which was mainly considered to be naturally present inorganic chlorine. However, recent studies, including that by Nestlé Research Centre, indicate the possibility of certain lipophilic organochlorine substances to participate in MCPDs formation.

With regards to the documented toxicity of free MCPD and glycidol, which are effectively released by enzymatic hydrolysis in gastrointestinal tract, and considering the occurrence of these

contaminants in food supply, the Directorate-General for Health and Food Safety (DG SANTE) proposed in 2019 maximum limits for several food commodities. Hence, the requirements for adequate analytical methods and better elucidation of their formation pathways are constantly increasing.

The aim of this study was to develop and optimise a method enabling a rapid, simultaneous determination of various intact esters of MCPD and glycidol in palm fat, with the use of supercritical fluid chromatography coupled with mass spectrometry (SFC-MS) and the possibility to use ion mobility (IM) to separate 2- and 3-isomers of MCPD esters was tested too. Contrary to a routine GC-MS method which determines total MCPD esters after hydrolysis, this way, the pattern of individual species can be characterized.

The SFC-MS method effectively separates and detects 9 esters of MCPD and 7 esters of glycidol in concentration range between 0,1 and 12,5 mg/kg. However, additional modifications are required to meet the recovery and repeatability at 125 µg/kg required by legislation. Separation of the 2- and 3-MCPD isomers by IM has not yet been achieved under the conditions tested so far. As a part of this presentation, critical comparison of SFC-MS and reversed phase LC-MS, the alternative analytical strategy, will be provided.

Keywords: *palm fat, 3-MCPD esters, glycidyl esters, SFC-MS, ion mobility*

Tuning Solid State Polymorph Emission of Sterically Hindered Push-Pull Substituted Stilbenes

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Organic luminophors exhibiting far red or near infrared (FR/NIR 650–900 nm) emission are highly interesting in the fields of bio-imaging and organic light emitting diodes (OLEDs) fabrication. the low photoluminescence quantum yields (PLQY) of these low band-gap compounds makes useful emitters scarce. A molecule of structure DPA-DPS-DCV (DPA = diphenylamino, DPS = 2,5-diphenyl-stylbene, DCV = dicyanovinylene) is presented. the shifts of absorption and fluorescence maxima in solvents of varying polarity is bathochromic, as is expected in DPA-stilbene-EWG based molecules (EWG = electron withdrawing group). the molecule forms various crystal polymorphs of emission differing in both wavelength and PLQY. First shows moderate monomer-like red emission (5 %, 672 nm), while the second one exhibits more intense and red-shifted (32 %, 733 nm) emission ascribed to the excimer fluorescence. Investigation into tuning these polymorphs brought about a third polymorph with hypsochormic shift (610 nm). the possibility of transition between these polymorphs is studied.

Keywords: *Solid state emission, infrared emission, crystal polymorphs, emission tuning*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Monitoring of Pharmaceuticals in Scottish Rivers Using Passive Sampling Devices

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Constantly increasing consumption of pharmaceuticals along with the low capacity of wastewater treatment plants for the effective elimination of these compounds from water is inevitably leading to the emissions of pharmaceuticals into the environment. the presence of such compounds in waters can have various adverse effects on non-target organisms.
Grab sampling technique is usually used for the evaluation of pharmaceutical presence in the water. Although this technique is the easiest and simplest to do it comes with a few shortcomings. It brings only information about pharmaceuticals concentrations at the time of sampling. If the grab sampling frequency is not sufficient it is hard to make any assumptions about the average concentrations of pharmaceuticals in the given area. Average concentrations can be under- or over-estimated by grab sampling. the alternative to the grab sampling is to use passive sampling devices that are placed into the sampled medium (e. g. river) for the extended period of time in which they are continuously sampling.

In our work, we used the combination of passive sampling along with grab sampling technique to evaluate the pharmaceutical contamination of two Scottish rivers, river Dee, and river Thurso. Selected target compounds were: ibuprofen, diclofenac, trimethoprim, clarithromycin, fluoxetine, carbamazepine, paracetamol, and 17α-ethynylestradiol. for passive sampling, POCIS (polar organic chemical integrative sampler) was constructed and calibrated in the laboratory before the field deployment. Grab water samples were processed by the solid-phase extraction and analyzed along with the extracted samples from POCIS by the LC-MS/MS technique. Both sampling techniques proved the presence of pharmaceuticals in river Thurso and Dee. Concentrations were in the units of ng/L with ibuprofen and diclofenac be the most abundant compounds. the overall frequency of the detection of pharmaceuticals was higher when using POCIS.
This work was financially supported by the project FCH-S-20-6446.

Keywords: *POCIS, pharmaceuticals*

Numerical Simulation of Heterogenous Catalytic Reactions

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The catalytic hydrogenation of liquid nitrobenzene is one of the most important chemical processes in the synthesis of aniline, which is a very important compound in the plastics industry. This process, usually occurring in slurry or gas lift reactors, can be generally described as a gas-liquid-solid system, in which a liquid phase acts as a continuous phase, in which reacting gas and catalyst particles are dispersed. Even though this technology is established, the process is usually only studied experimentally, which makes it difficult to study internal phenomena in the reactor. the use of numerical simulations in this area is not very widespread and usually, the simulations only focus on the reaction kinetics and the effects of hydrodynamics are often neglected.

In this work a custom 3D numerical model describing a multiphase reacting flow, which coupled the continuum flow with the Lagrangian discrete particle method, was implemented into Ansys Fluent software. the model was used to investigate the catalytic hydrogenation of liquid nitrobenzene in an injection site of a gas lift reactor. As the complete reaction mechanism is very complicated, a simplified version was used. In the first step, nitrobenzene reacts with hydrogen gas, which produces aniline and water. Then, aniline can react with hydrogen to produce cyclohexylamine, which is a side product. To obtain a good quality of the product, it is necessary to maintain the temperature of the mixture in a defined range as for higher temperatures, the side reaction will overtake the main reaction. the results obtained from simulations can help with identifying the effects of the flow on the particle catalysts distribution, heat transport and in result, on the overall reaction mechanism. the presented model can be used to improve the design of existing reactors and increase the production and the quality of the product.

Keywords: *multiphase flow, particle tracking, heterogenous catalysis, Ansys Fluent*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Wet Pre-treatment Methods in Macroelements Recovery from Fly Ash Combined with Acid Leaching

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Fly ash (FA), as a mass-produced secondary material (coal combustion product) since the middle of the last century, reached up to 30–40 % to be recycled and reused. One of the most auspicious applications of FA in the following decades possibly appears to be a raw material base – the source of macro- and microelements.
This paper summarizes wet types of FA pre-treating techniques to obtain the maximum leachability of macro- elements, such as Al, Fe and Ti in the process of acid leaching. FA pre-treatment or chemical activation is the single key to increase the efficiency of separated elements.
In this research, the wet experiment was based on FA pre-leaching in hydrochloric acid solution (1–5 wt. %). Both high-temperature (HTFA) and fluidized-bed fly and bottom ash (FFA. FBA) were the aims of the study. In the case of FBA and FFA, this reaction led to lower the total alkaline content, esp. reactive calcium oxide, as a result of flue gas desulphurization. the lower free lime content brings a positive effect, while the leachability of Al and Fe increased 2–4 times. Secondary, the grain surface after deposition in HCl solution changed by the meaning of the creation of new pores, as observed via SEM. Based on experimental data, taking into account the economic ratio and the increase in performance, the use of dilute (1 wt. %) HCl in a molar excess of 30 % to free CaO with a deposition time of 10–30 min at room temperature and constant stirring appears to be the most suitable conditions. on the other hand, in the case of HTFA samples which contain only a small amount of total alkaline content, it is much more advantageous to use more concentrated solutions so that the glass-covered surface of the particles is disturbed and the extraction medium can penetrate the resulting defects and dissolve selected elements.
To conclude, it can be evaluated that the extraction efficiency in the case of FFA and FBA increased 2–4 times, thus achieving a total leachability of up to 85 % of iron and more than 50 % of aluminum in a single-phase extraction into sulfuric acid at room temperature. In the two-stage extraction, the leachability reached up to 95 % Fe and 92 % Al.

Keywords: *fly ash, fly ash utilization, macroelements recovery, acid leaching*

OECT as a Device for Material Characterization: the Role of Parasitic Series Resistance

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The organic electrochemical transistor (OECT) is finding increasing application in the field of bioelectronics and material characterization. Due to the relatively wide range of applications, the requirements for this device are diverse. Some applications require fast response, while others require high sensitivity and therefore a low signal-to-noise ratio. In the case of sensing applications, mainly high sensitivity is required. the sensitivity of the device can be characterized by the transconductance value, which is calculated from the transfer characteristics. the transfer characteristics are measured as the dependence of the output current on the applied voltage at the gate electrode. Based on the obtained values of the transconductance and the parameters of the active OECT channel, also other parameters related to the used semiconducting material can be determined. Those parameters are used to benchmark organic semiconductor materials. This is based on the dependence of transconductance on channel length, width and thickness (*Wd*/*L*). However, when this dependence is plot for short-channel OECT (large ratio of *Wd*/*L*) the dependence decline from the expected linearity with increasing *Wd*/*L* ratio. That means some other parameters are involved, e.g. contact resistance or series resistance. In order to study the effect of contact and series resistance, the OECTs with different channel length and thickness (with different ratio of *Wd*/*L*) were prepared. the poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) was used as the active channel material. From the transfer characteristics the peak transconductance value was calculated for each OECT, then the corrected transconductance value were calculated based on Antoniadis and Chou model. These corrected values could largely describe the observed deviation from the expected linearity. the results suggests that the serial resistance is the main factor worsening the sensitivity of the studied OECT devices.

Keywords: *OECT, PEDOT:PSS, conductivity, contact resistance, series resistance, transconductance, organic semiconductor*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Visualization of a Ge Structure Using Fluorescent Nanoparticles

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This contribution describes the visualization of the hydrogel structure using the fluorescence lifetime imaging microscopy (FLIM) and subsequent modifications using other software. This method, in conjunction with fluorescent nanoparticles, allows to visualize the exact structure of hydrogels. It is also possible to define the pore size. Only the average value of pore size was mentioned in the articles published so far, but this often does not correspond to the actual structure of hydrogels.

The work is focused on the imaging of selected hydrogels using FLIM analysis and subsequent modification in the specialized software. the simplest way is to use nanoparticles with a specific diameter, where one FLIM image is created for each particle size. Thanks to the z-scan and the selected program, there is possible to convert these images into a 3D structure. Unfortunately, it is not possible to measure exactly the pore size by this measurement, so it has no informative value, but only allows visualization of the actual structure of the hydrogel. for a more accurate analysis, nanoparticles of different sizes and colours were selected, which could be used in one experiment at a time. It could be possible to track sites of varying pore sizes within a single experiment thanks to them.

Aqueous solution of agarose was chosen as the physically crosslinked type of hydrogel and fluorescent-labeled gold nanoparticles with diameters ranging from 10 to 100 nm were used as fluorescent probes.

Keywords: *fluorescence microscopy, nanoparticles, hydrogel, FLIM, 3D image, structure*

Plasticized poly(3-hydroxybutyrate)/poly(D,L-lactide) blends filled with tricalcium phosphate for FDM 3D printing and their biological properties

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Additive manufacturing or 3D printing is a production technology capable of producing nearly any desired shape including complex porous structures. Thanks to this, it is often exploited for the manufacturing of scaffolds for tissue engineering, a modern approach of regenerative medicine. In this work, we have successfully prepared plasticized poly(3-hydroxybutyrate)/polylactide 70/30 blends modified with bioceramic tricalcium phosphate (13 wt%) and used them for Fused Deposition Modeling 3D printing. Two commercial plasticizers, Citroflex B6 (*n*-Butyryl tri-*n*-hexyl citrate) and Syncroflex 3114 (oligomeric adipate ester), in the amount of 12 wt% were used. the materials were firstly subjected to printing parameters optimization, afterwards printability, thermal and mechanical testing and as well as series of biological tests *in vitro* were conducted. Citroflex plasticizer was proven to be effective in enhancing the processability and mechanical properties of studied biopolymer blend, however the biocompatibility of samples with this citrate-based plasticizer was rather poor. on the other hand, Syncroflex materials showed better warping properties than commercial grade PLA filament and moreover the results of biological tests revealed its potential to be used for stem cell-seeded scaffolds for regenerative medicine of bones.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Monitoring of Gadolinium Anomaly in Soil, Grapevine and Wine Samples from the Czech Republic

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Rare earth elements (REEs) naturally occur in all components of the environment but may become environmental pollutants in the future. the reason is their widespread application in medicine, agriculture and industry currently. Mining of REEs is also increasing due to the significant interest in their use in modern technologies. A particularly monitored element is gadolinium and its anthropogenic concentrations in environmental components. Gadolinium of anthropogenic origin is observed mainly in surface and waste water and in soil. It can be bioaccumulated in plants and animals through increasing the concentration of anthropogenic gadolinium in soil and water. Water-soluble REEs and REEs released from the soil enter the human body through the food chain. REEs can accumulate in the human body and subsequently cause serious health issues. for these reasons, it is appropriate to monitor the concentrations of anthropogenic gadolinium in agricultural plants and crops.

The aim of this work was to monitor the presence of gadolinium anomaly in samples from vineyards (soil, leaves and berries

of grapevine, wine) in the Czech Republic (Bohemia and Moravia). the ICP-MS method was used to determine REEs (Ce, Dy, Er, Eu, Gd, Ho, La, Lu, Nd, Pr, Sm, Tb, Tm, Y, Yb) concentrations in samples. A positive gadolinium anomaly was confirmed for the analysed samples indicating the presence of anthropogenic gadolinium in soil, grapevines and wine. the average value of the gadolinium anomaly was 1.75 for soil samples, which is slightly higher compared to the threshold value of 1.5 reported in literature. By comparing the results with the available data in literature, it was determined that the values of gadolinium anomaly found in the soil are lower than the values for surface waters and sediment found in the East Bohemian region.

Keywords: *gadolinium anomaly, rare earth elements (REEs), Czech Republic, soil, grapevine, wine, ICP-MS*

Olive Oil Authenticity: Detection of Soft-Deodorized Oils in Extra-Virgin Olive Oils Using Metabolomic Approach

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Extra-virgin olive oil represents a popular food commodity not only due to its sensory quality but also for its health-promoting effects. However, high-price with continuously increasing demand for high-quality olive oil makes it vulnerable for economically motivated fraudulent practices. This study has been focused on extra-virgin olive oil adulteration with soft-deodorized olive oils, which is recently one of the most serious olive oil authenticity issues.

Metabolomic fingerprinting (non-target screening) has been chosen as a promising strategy to discriminate between samples of extra-virgin olive oils and soft-deodorized olive oils and their mixtures. Polar (methanol-water) extracts of olive oils were investigated using ultra-high performance liquid chromatography coupled to high-resolution mass spectrometry (UHPLC-QTOF-HRMS) and subsequent chemometric evaluation of generated data was performed to construct classification models and identify marker compounds. the results showed, that deodorization process, although performed under 'soft' conditions compared to 'classic' high temperature deodorization, induced some oxidation, and ten tentatively identified markers were mainly oxidized fatty acid derivatives.

To lower the detection limits and to investigate the possibility to target these markers with low-resolution instruments in control laboratories, all the samples were analyzed also by UHPLC-QqQ-MS/MS. Two compounds, methyl ricinoleate and unspecified oxidized derivative of oleic acid, were selected as the best markers enabling recognition of undeclared soft-deodorized olive oil addition.

Keywords: *extra-virgin olive oils, authenticity, soft-deodorization, metabolomic fingerprinting, UHPLC-HRMS*

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Assessment of air pollution in the Czech Republic by emerging chlorinated contaminants

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Polychlorinated naphthalenes (PCNs), polychlorinated biphenyls (PCBs) and short-chain chlorinated paraffins (SCCPs) are listed as persistent organic pollutants (POPs) on the Stockholm convention. They can be found in various environmental compartments, including atmosphere. Air pollution might be a significant source of human exposure to these contaminants. SCCPs are suspected of having adverse effects on human health and are classified as possibly carcinogenic to humans. PCBs and PCNs are suspected of being hepatotoxic and several of the congeners exhibit dioxin-like toxicity. PCBs are considered probable human carcinogens. the aim of this study was (i) to implement the analytical procedure for the simultaneous isolation of SCCPs, 11 congeners of PCNs and 8 congeners of PCBs from filters of high volume samplers used for air sampling and (ii) to apply the newly validated method within the pilot study assessing the air pollution in two regions of the Czech Republic, the locality Litvínov (area polluted by industry) and the locality České Budějovice (reference area). Extraction of target compounds was carried out in the Soxhlet apparatus (hexane: dichlormethane, 1:1, *v*/*v*) and followed by purification on

the silica column (analytes eluted by hexane:dichlormethane, 3:1, *v*/*v*). PCNs and PCBs were then analyzed simultaneously by gas chromatography – tandem mass spectrometry in electron ionisation (GC-EI-MS/MS) and CPs were analyzed by gas chromatography – high-resolution mass spectrometry in negative chemical ionization (GC-NCI-HRMS). Limits of quantification (LOQs) were determined as 10 pg/filter (SCCPs), 0,005–0,05 pg/filter (individual PCNs) and 0,01 pg/filter (PCBs). Firstly the method was validated for both SCCPs and PCNs, recoveries determined from spiked samples ranged from 86 % to 102 % (SCCPs) and from 79 % to 120 % (PCNs). Repeatabilities were 9 % and 5–16 % for SCCPs and PCNs, respectively. Within the pilot survey, the successfully validated analytical procedure was applied to a set of 50 samples of high-volume air sampling filters collected from two localities of the Czech Republic (České Budějovice, Litvínov) at various seasons. Comparing the concentrations of aromatic pollutants air in České Budějovice was more contaminated by more than 60 % than in Litvínov. the average concentration in the air of České Budějovice was 0,013 pg/m³ for sum of detected PCNs (tri-penta congeners) and 2 pg/m³ for the sum of all indicator PCBs. However, opposite trends were found in SCCPs, in which twice as high concentrations were measured in the air from Litvínov, compared to the air from České Budějovice. the average concentration of SCCPs in the Litvínov was 119 pg/m³.

Keywords: *persistent organic pollutants, gas chromatography, ambient air*

Contamination of Urban Soils by Cd: An Example of a Coal Mining City (Shariin Gol, Mongolia)

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Cadmium is considered worldwide as one of the most common and at the same time the most dangerous pollutants from the group of heavy metals. the most common ways in which Cd can enter the environment anthropogenically include mining, coal burning, smelting or transport. Therefore, especially coal mining cities can be severely contaminated and need special attention. the aim of this study was to evaluate the pollution of urban soils (0–10 cm) by Cd in an important coal mining Mongolian city Shariin Gol using the Single Pollution Index (PI) and the Dutch Soil Guidelines target value for Cd as a background. PI values ranged from 1.10 to 2.38 with an average value of 1.82, which represents low pollution. Although the pollution of topsoil in Shariin Gol is low, it locally achieves moderate pollution (PI value is between 2 and 3). Due to the fact that mining heaps around the city have higher Cd contents (PI > 2.0), it can be expected that due to wind and water erosion there will be continuous contamination of urban soils by transport of cadmium-contaminated material in future years, which can be further increased by active and intensive mining activities and transport. Based on the results, it can be concluded that although there is a theoretically very significant risk of pollution by Cd, the real pollution of the topsoil by this element is currently low and therefore does not pose a risk to human health and local ecosystems.

Keywords: *urban soils, heavy metals, mining, coal, Single Pollution Index*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Fast Centrifugal Partitioning Chromatography (FCPC) – Innovative Method for Separation of Biologically Active Compounds from *Cannabis*

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Plants of the genus *Cannabis sativa* L. are unique producers of phytocannabinoids and many other bioactive compounds. In the recent decade, products based on non-psychotropic phytocannabinoid, cannabidiol (CBD), have become very popular as they are believed to provide several health benefits (e.g. antioxidant, anti-inflammatory, and analgetic effects). However, the isolation of pure CBD, free of psychotropic Δ^9-tetrahydrocannabinol (Δ^9-THC), and its precursor Δ^9-tetrahydrocannabinolic acid (Δ^9-THCA-A) which are always present, in at least small amounts, in *Cannabis* plants together with many other phytocannabinoids, is not an easy task.
In this study, we investigated the potential of Fast Centrifugal Partitioning Chromatography (FCPC), a hydrostatic version of countercurrent chromatography, to separate CBD and its precursor, cannabidiolic acid (CBDA) from other common components of hemp extract obtained by supercritical fluid extraction.

In the first phase, we experimentally determined partition coefficients (K_D) and calculated separation factors (α) for 17 phytocannabinoids in altogether 46 model immiscible solvent mixtures, UHPLC-HRMS technique was used for the analysis of individual phases. the following solvent systems were identified as the most suitable: (i) heptane:ethyl acetate:ethanol:water (3:1:3:1, *v:v:v:v*) and (ii) hexane:ethyl acetate:methanol:water (9:1:9:1, *v:v:v:v*). Both systems enabled the separation of CBD/CBDA from Δ^9-THC-like compounds and differ in their separation efficiency within individual groups of substances, which may be further of interest, depending on the specific application.

Keywords: *Fast Centrifugal Partitioning Chromatography, bioactive compounds, phytocannabinoids, UHPLC-HRMS*

The Influence of Non-canonical Structures on the P53 Isoforms Binding to DNA

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Protein p53 is one of the most studied tumor suppressor protein. It plays important roles in regulating basic biological processes including cell cycle, apoptosis, senescence and metabolism. the human p53 gene contains alternative promoters and thank to alternative splicing could be expressed in several isoforms. P53 protein function is realized by binding to specific DNA response elements (RE) and transactivation of target genes. Here we present results of p53alpha, p53beta and p53gamma isoforms interaction with DNA studied by yeast isogenic system for in vivo transactivation studies. We used a panel of Saccharomyces cerevisiae haploid isogenic strains differing in p53 target site propensity to form different local DNA secondary structures located upstream of the luciferase reporter gene. the strains were prepared by the replacement of the ICORE cassette with the sequence of interest, following the Delitto Perfetto approach. Yeast isogenic strains differing in the p53 target site (with different propensity to form cruciform structure) were transformed for the expression of p53 isoform proteins. Our results show that transactivation is in vivo correlated better with the relative propensity of a RE to form cruciform structure that to its theoretically expected DNA binding affinity. These results point to the fact that structural features of DNA are an important determinant of DNA-binding and transactivation function.

Keywords: *yeast isogenic system, transactivation activity, p53 protein, G-quadruplex*

Novel method for isolation of PHB from bacterial biomass

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Polyhydroxybutyrate (PHB) serves as an alternative to conventional plastics for a variety of applications. To find large-scale use, its production must be profitable, sustainable and environmentally friendly, while meeting challenging quality demands. We have developed an isolation method employing salts of fatty acids that is more economical and greener than comparable methods with other surfactants. Concentrated *Cupriavidus necator* biomass suspension is digested using small amount of sodium salts of fatty acids. After the reaction, the polymer is separated by centrifugation. the method offers several advantages over other surfactant-based methods. Other surfactants are produced from petrochemical or primary agricultural raw materials by complex multi-step processes. the sodium salts of fatty acids, on the other hand, can be obtained by a one-step reaction using a secondary feedstock (waste cooking oil). After use of other surfactants, hard-to-manage wastewater is obtained. In our method, the wastewater can be processed via simple precipitation with small amount of acid to reduce content of organic carbon, which simplifies wastewater treatment. the precipitate contains mainly fatty acids and other biomolecules and was found to be readily metabolized by the PHB-producing bacteria. Therefore, it can be utilized in the process as co-substrate for biomass production. Furthermore, this method provides high quality PHB (purity 96%, M_w = 389 000) in high yields (99%). We used the polymer for a real-world application (3D printing) to demonstrate its applicability for material development.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Effects of microplastics to aquatic environment

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Plastics with their pervasive distribution are gradually becoming a global threat to the environment. Plastic items undergo slow degradation and fragmentation to smaller particles called microplastics. This is done by various factors in the environment such as sunshine, abrasion, interaction with living organisms. Microplastics can be defined as solid synthetic particles or polymer matrices with regular or irregular shape and with a size in the range of 1 μm to 5 mm. These particles are insoluble in water.
Waste water treatment plants and applications of sewage sludge are main entrance pathways of microplastics into the ecosystem. Also, the transmission of particles from their original storage (landfill, construction zone) to the environment occurs by the action of wind. Microplastics are transported different ways after entering the ecosystem. Transport routes can be divided into aquatic, terrestrial and atmospheric. Thus, the invasion of microplastic particles occurs across all ecosystems at different trophic levels.
Ecotoxicological studies of microplastics are focused to two types of compounds – to polymers and their additives and then to chemical compounds sorbed on plastic particles from the environment (metals, PCB). These compounds can be toxic, mutagenic or endocrine disruptors. Some of these compounds may be released again either in the environment or in bodies of living organisms. These days, we deal with influence of PHB microparticles to aquatic organism *Daphnia magna* via acute and reproductive ecotoxicity tests.

Keywords: *microplastics, ecotoxicity tests, PHB*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

New possibilities in the analysis of modified trichothecenes type A in oats: immunoaffinity purification and enzymatic hydrolysis

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In the recent years, growing attention has been paid to modified / 'masked' mycotoxins, i.e. mycotoxin conjugates which are formed during (i) plant detoxification processes, or (ii) specific food technologies. In addition to glycosides of the most well-known trichothecene deoxynivalenol (DON), the presence of mono- / oligoglycosides of other trichothecenes, e.g. HT-2 / T-2 toxins (HT-2 / T-2), has also been published so far. the presence of these modified mycotoxins in a human diet has become an issue of health concern, which is underlined also by Scientific opinion issued by European Food Safety Authority in 2017. Whereas analytical standards for mycotoxin glycosides (except DON-3-glucoside) are not available, effective strategies for their isolation and detection are of major importance. In our study, we focused on the quantification of free and modified HT-2 and T-2 in oat samples for which these contaminants are characteristic. Both direct analysis of free HT-2 / T-2, as well as indirect analysis of HT-2 after the enzymatic hydrolysis, were utilized (the glucosidase from *Aspergillus niger* used in our work was shown to effectively cleave the glycosidic bond in HT-2 glycosides only). Altogether, 52 oat samples were processed by using our previously developed purification and pre-concentration based on the immunoaffinity chromatography cross-reacting with the HT-2 / T-2 glycosides (*Prusova et al., 2019*). the enzymatic hydrolysis was performed for the aliquot of the pre-concentrated extract. Analytical determination of both free mycotoxins, as well as their modified forms (both before and after hydrolysis), was realized by ultra-high performance liquid chromatography coupled to high resolution tandem mass spectrometry (U-HPLC-HRMS/MS). Free T-2 was quantified in all 52 samples and its monoglucoside was present in 43 samples. In the case of HT-2, free form as well as its monoglucoside was present in 48 samples, and HT-2-diglucoside was detected in 29 samples. the percentage of HT-2 originally present in the form of glycosides from the total HT-2 content ranged from 0.1% to 56%.

Keywords: *U-HPLC-HRMS/MS, modified mycotoxins, oats, immunoaffinity columns, enzymatic method*

Acknowledgements: This work was supported by the Ministry of Education, Youth and Sports (project No 8E18B045) and by Specific university research (grant No A2_FPBT_2020_061).

Reference: Prusova, N. et al. New possibilities in effective isolation of modified type A trichothecenes: survey of suitability of commercially available immunoaffinity columns. 9th International Symposium on Recent Advances in Food Analysis; Prague, Czech Republic; 5.–8. 11. 2019.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Study of the Influence of Selected Compounds on Stability of Beer Foam

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Beer foam as an important aspect in evaluating the beer quality is one of the qualitative parameter during beer consumption. Czech consumers prefer thick, creamy and long lasting beer foam. Beer contains various amounts of constituents that may positively or negatively influence the beer foam stability. Whereas proteins, iso-α-acids, phenolic compounds, some metal ions and polysaccharides increase formation and the stability of beer foam, e.g., lipids have the opposite effect. In this research, the relation between selected parameters (proteins, phenolic substances and bitter substances) and the beer foam stability was studied in various types of Czech beer (lager beers, lager beers originated from microbreweries and lager beers with different original gravity) and comparison of eventual differences within studied groups of Czech beer. the beer foam stability was determined by the NIBEM-T method, total protein content (PC) was determined using Hartree-Lowry method, total phenolic content (TPC) was determined according to the Folin-Ciocalteu's method. Bitter substances were determined by standard European Brewery Convention method (EBC 9.8) as bitterness of beer. Differences between tested groups of beer were evaluated by ANOVA with $\alpha = 0.005$. Within the groups of Czech beers, no statistically significant differences were found in the stability of beer foam determined by the NIBEM method ($p = 0.3150$). A statistically significant difference was observed in total protein content between lager beers with different original gravity and other two groups of lager beers ($p = 0.0004$). All three studied groups differed statistically in total phenolic content and bitterness ($p < 0.0001$). Correlation analysis of chemical composition factors with the beer foam stability was performed. the results showed weak positive correlation between total protein content ($r = 0.40$) and beer foam stability (NIBEM 30) and very similar trend was observed for total phenolic content ($r = 0.34$). Bitterness reported slightly stronger positive correlation ($r = 0.46$). the results of this study did not indicate significant influence of the selected parameters on the stability of beer foam.

Keywords: *beer foam stability, proteins, phenolic substances, bitter substances*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Analysis of the Mixing Process Performance in Mixtures for Direct Tablet Compression Using Segregation Test

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In solid dosage forms manufacturing, segregation (driven by particle size, shape or density differences in used materials) and content uniformity are an issue, especially in formulations with very low active ingredient (API) content (usually less than 5 %). Maintaining homogeneity throughout the process steps ranging from mixing to direct tablet compression is a great challenge in the pharmaceutical industry. Particularly in low dosed mixtures even a slight API segregation can cause tablets to fail meeting the required specification. Therefore, enhancement of mixing process strategy, such as alternating mixing, component addition and sieving steps, are being adopted in the industrial practice.
The aim of this work was to use a standardized segregation test for describing the development of homogeneity in low API content blends. for each batch of tested API two mixtures having the same composition were prepared – the first by simple mixing and the second by multi-step procedure including sieving. Afterwards, they were subjected to the segregation test, based on the observation of segregation in a cylindrical tube, in which the material flowed. Samples were collected during the test and their API concentrations were determined using the HPLC analysis. Segregation profiles were then put together using measured values in order to compare the segregation tendencies and to eventually justify the use of the more complicated and time demanding preparation process.
Segregation observed after the multi-step preparation for one tested batch of API was almost four times less distinct than the segregation after simple mixing. In this particular case the preparation procedure with sieving is crucial for the blend uniformity. However, tested API has various particle size and morphology throughout different batches and suppliers. Thus, investigation of these variants could point out some candidates for potential process simplification.

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Keywords: *segregation, content uniformity, mixing process*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

The authenticity of Poppy Seeds: How to Detect the Undeclared Hydrothermal Treatment?

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The adulteration of quality food poppy seeds by cheap waste seeds from pharmaceutical varieties has become a frequent practice in recent years. the pharmaceutical varieties of *Papaver somniferum* L. are characterized by high opium alkaloids content in poppy straw and, consequently, the poppy seeds surface is often fairly contaminated during latex collection. for that reason, such seeds cannot be used for human consumption, moreover, their sensorial quality is rather poor. In any case, the high content of opium alkaloids and their pattern may indicate fraud as the food poppy varieties registered in the Czech Republic never exceed the national legislative maximum limit of 25 mg/kg of morphine alkaloids in seeds. However, counterfeiters have found a way how to reduce the amount of opium alkaloids on the seeds surface. They use a process dedicated to poppy seeds "stabilization" during which are seeds exposed to high temperature and hot steam. the process is mentioned in the European Commission Recommendation 2014/662 / EU on good practices to prevent and to reduce the presence of opium alkaloids in poppy seeds and poppy seed products. Although significant seeds decontamination occurs in this way, the use of this process has to be declared on the label, which is not often the case.

This study is devoted to methods suitable for distinguishing thermostabilized poppy seeds from untreated seeds. the first method chosen was a metabolomic analysis using ultra-performance liquid chromatography with high-resolution tandem mass spectrometric detection (U-HPLC–HRMS/MS). A chemometric model capable of distinguishing thermostabilized seeds from untreated seeds and correctly classifying 100 % of samples was created. Furthermore, characteristic markers were identified. In addition, it was possible to distinguish mixtures of thermostabilized and untreated seeds mixed in different ratios. As a cheap and rapid alternative, a new method based on the Fourier-transform infrared spectroscopy (FTIR) was developed for the measurement of lipase activity in seeds. While the growing signal of the carboxylic group of successively released free fatty acid can be observed in native seed (34–163 % after 24 hours), thermostabilized samples showed no change in acid value. It was further observed, that neither the variety nor the years of harvest had a significant effect on the lipase activity. However, the possible effect of the origin of seeds was observed.

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STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Inorganic Thermal insulation material for masonry elements

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With the increasing focus on energy balance of buildings and simplifying of the building construction process, hollow clay bricks with cavities filled with thermal insulating material, are finding increasing popularity in the recent years. However, all of the commercially available products use either organic insulators or a combination of inorganic material with an organic binder for this purpose. In this work, foam glass was used as an insulating filler for hollow clay bricks as a more environmentally friendly substitute of common insulators with the aim to increase longevity, recyclability and fire resistance compared to the commercially available filled masonry blocks.

Foam glass was prepared from waste packaging glass and limestone via powder sintering method. Influence of foaming agent content, water content, glass cullet particle size, foaming temperature and holding time on bulk density, pore size and morphology of foam glass samples was investigated. Possibilities of using foam glass to produce purely inorganic filled hollow clay bricks without any additional binders, by direct foaming of glass in the cavity of the brick, were investigated. Different approaches to manufacturing thermal insulating masonry blocks by foaming of glass inside fired hollow bricks were investigated. Lastly, we successfully prepared hollow bricks filled with foam glass by direct foaming of glass in the cavity of an unfired brick using firing regime similar to that of typical masonry ceramics. Prepared foam glass showed good adhesion to the ceramic body and low bulk density.

Keywords: *Thermal insulating materials, foam glass, masonry elements*

Mixotrophic growth and increased salinity – possible tools for increasing the PHB production in cyanobacteria?

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Polyhydroxyalkanoates (PHA) are microbial biopolymers which occur in the cell as intracellular granules and serve as a carbon and energy source. PHA have comparable physicochemical properties as some petrochemical plastics, furthermore, they are completely biodegradable. Nevertheless, PHA production is financially demanding. To reduce the price many waste products are used as input material for heterotrophic bacteria. To promote PHA production frequently it is necessary to apply some stress factors – temperature, salt, lack of nutrients, etc. the most important heterotrophic PHA producers are *Cupriavidus necator* H16 and *Halomonas halophila*.

Cyanobacteria are ecologically important prokaryotic gram-negative organisms capable of oxygenic photosynthesis. They also synthesize many secondary metabolites such as glycogen, carotenoids, but importantly also the PHA. the PHA production by cyanobacteria is time demanding and not effective enough, but the big advantage is the fact they do not require any organic substrate because cyanobacteria can fix CO_2. for PHA cyanobacterial production only the water, some minerals, light and CO_2 are required. In this work, we employed cyanobacterial strains *Synechocystis* PCC 6803 and *Synechocystis* CCALA 192. In our study firstly we investigated the effect of NaCl in media on PHA production. Secondly, we looked into mixotrophic growth of cyanobacteria with several compounds such as acetate, propionate, glucose or their combinations. We tested the ability to produce PHB and copolymers. In the third case, we investigated the viability of PHA poor and rich cultures exposed to various stress factors to investigate the involvement of PHA in the stress response of cyanobacteria.

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Keywords: *cyanobacteria, PHA, heterotrophic, salinity*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

An isolation of a protein from a wheat bran

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The wheat bran is an outer layer of a wheat kernel and a by-product of flour production. Annual worldwide production of the wheat bran is about 150 million tons, but only about 60 % of this amount is utilized, especially for food supplementation. Wheat bran is rich in dietary fiber, minerals, vitamins or phenolic compounds, which could be prevention of many diseases (colon cancer, cardiovascular diseases). Proteins are also valuable component of the wheat bran (about 16 wt. %). They positively influence dough properties and bread quality, which is the reason why their extraction could be profitable.

The model experiment of protein extraction from wheat bran was held in five steps. First, wheat bran proteins were released from the matrix by water (1:20), which pH was adjusted to 11 by 1M NaOH, and shaken for 30 min (100 rpm). Then the suspension was centrifuged (8000 rcf, 15 min) and the supernatant was collected. the value of the pH of the supernatant was adjusted to 4 by 1M H_2SO_4. the solution was shaken to support the precipitation of proteins and then centrifuged again. Finally, sedimented material was lyophilized, weight and amount of proteins in the material was verify by Hartree-Lowry method.

Optimalization steps of extraction were divided into 3 categories: a pre-treatment of the wheat bran, a modification of the extraction process and a modification of the precipitation. Every step was implemented to the model extraction individually. the defatting (1:3 hexane, 30, 45 and 60 °C) and the grounding of wheat brans were parts of the pre-treatment. Different extraction times (1, 2, 3 h), the temperature (30, 45 and 60 °C), the ratio of bran and extract water (1:15, 1:30) and repeated extraction (2´, 3´) are the optimalization steps of the extraction process. the modification of the temperature (-4, 4 °C) and the pH (3, 5) was the optimalization of the precipitation of proteins. After evaluation of individual steps, a combination of several steps was also realized.

With the combination of optimalization steps 81,4 ± 0,7 mg/g of material was gained and it contains over 90 % of pure proteins. the most of it was proved as digestible during the GIT simulation experiment. the most abundant amino acids are arginine and glutamic acid. According to total amino acid content, the extracted material could be considered a potential vegan food supplement.

Keywords: *Wheat bran, protein, protein extraction.*

Utilization of recycled brick waste for growing the agricultural plants

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Brick recyclate, as same as brick, excel with very high porosity. for this reason this work deals with possible implementation of plant growth aids (fertilizers) on the inside surface of such highly porous material. This work studies possibilities of preparation of brick recyclate with the content of components supporting plant growth and what is maximum amount of supporting substances, that later will be released back into surrounding enviroment (soil), is possible to incorporate into the brick recyclate. Brick recyclate is a material that can bind water in the soil and nourish cultivated plants at the same time. Brick recyclate was saturated with commercial NPK fertilizer and laboratory prepared fertilizer based on NPK. Such prepared brick recyclate was used for growth experiment on agricultural plants (tomatoes, corn). Prepared brick recyclate was subjected to x-ray diffraction, thermogravimetry and differential thermal analysis, scanning electron microscopy and energy dispersive spectroscopy analysis. Amount of available plant nutrients have been determined by ultraviolet-visible spectroscopy and inductively coupled plasma optical emission spectrometry. Subsequently, the growth course, germination and yields of selected crops were monitored. It was verified that the material based on recycled brick enriched with nutrients improves the distribution of nutrients in the soil and positively affects the germination, growth and yields of tested crops.

Klíčová slova: *brick production, brick recyclate, sorption capatity, soil, fertilizer, nutrients for plants, agricultural plants*

Characterization of SiO_2 Nanofluid by High Resolution Ultrasonic Spectroscopy

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Lately, interesting properties of nanoparticles have attracted the attention of many researchers. Silicon dioxide, also called silica nanoparticles, is inorganic material widely used in biomedical fields, especially due to their biocompatibility, stability, high surface area, controllable shape, size and surface charge. High-Resolution Ultrasonic Spectroscopy is a novel non-invasive, non-destructive real-time method for characterization of molecular and micro-structural transformation in solutions or dispersions. the advantage of this technique is that the sample does not need to be transparent because the ultrasonic waves propagate through most materials. As the ultrasound wave propagate through the sample, it evaluates intermolecular forces in the sample by repetitive compression and decompression during propagation in the sample. As the sound wave causes compression and decompression of the sample, it loses part of energy. This energy loss causes lowering of sound wave amplitude. It gives the information about structural changes, ligand binding to macromolecules, association and other chemical changes of the sample. In

this work, LUDOX® colloidal silica (TM-40, HS-40, SM) water suspension of different particle size (22, 12, 7 nm) and concentration range (0–30, resp. 40 wt%) was studied by High-Resolution Ultrasonic Spectroscopy and DSA 5000 M Density and Sound Velocity Meter. Also, their interactions with representative proteins were investigated. the effect of temperature, 25 and 37 °C, on nanoparticles properties was studied.

Keywords: *Silicon dioxide, LUDOX®, High-Resolution Ultrasonic Spectroscopy, density*

Determination of biogenic amines in Swiss and Dutch type cheeses

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HPLC is well-established technique in the analysis of food biogenic amines, usually performed for qualitative analysis. This project presents an elaboration of several Edam and Emmental type cheeses to quantify biogenic amines that are typical in the dairy products and an evaluation of suitability of this technique to detect adulteration of dairy products. Compounds representing main biogenic amines of the dairy products were investigated: 2-phenylethylamine, cadaverine, histamine, putrescine, spermidine, spermine, tryptamine, tyramine. Amongst analyzed cheese were found significant differences in the content of cadaverine, histamine, putrescine, and tyramine. the sample from German manufacturer showed an increase of cadaverine and putrescine by a factor of 8 and 10 respectively, yet the lowest total content of biogenic amines. the Edam samples review uncovered comparable content of cadaverine, 2-phenylethylamine, spermine and spermidine from all the polish producers. Significant differences were found within all the samples, which endorses the possibility to establish an adulteration pursuit model.

Keywords: *Biogenic Amines, second keyword: Cheese*

Study of Liposomes Membrane Properties by Fluorescence Spectroscopy

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Liposomes are biocompatible and biodegradable vesicles composed from lipids with size range from nm to μm. They are considered as a safe drug delivery system for hydrophobic or hydrophilic drugs. Hydrophobic drugs are stored in the liposomes membrane (hydrocarbons tails) and hydrophilic in the cavity of vesicles (water). Leakage of encapsulated or incorporated drugs from liposomes is influenced by membrane properties. To prevent this leakage, it is important to understand membrane fluidity (viscosity) and its phase behaviour. It is also necessary to found out how some components of phospholipid bilayer influence these properties. Fluorescence spectroscopy is a very useful and sensitive tool for this problematic. Laurdan is an amphiphilic probe located in the outer part of the membrane and it reacts to the fluidity of the membrane. Anisotropy of Diphenylhexatriene examines the microviscosity of the inner part of the bilayer. Both probes carry complex information about membrane properties.

Keywords: *Liposomes, Dynamic Light Scattering, Electrophoretic Light Scattering, Fluorescence Spectroscopy, Laurdan, Diphenylhexatriene.*

Contamination of Vegetable Oils by Mineral Oils and Polycyclic Aromatic Hydrocarbons: A Czech Market Survey

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Mineral oils are a crude oil fraction consisting of a complex mixture of saturated hydrocarbons (MOSH) and aromatic hydrocarbons (MOAH). MOSH might pose as tumour promoters and MOAH may be mutagenic to humans, and it is therefore important to monitor their occurrence in food.

In this study, a method for the determination of MOSH/MOAH in vegetable oils using comprehensive gas chromatography coupled with time-of-flight mass spectrometry (GCxGC-TOFMS) was developed. A solid phase extraction technique with a silver modified (0.3 % *w*/*w*) silica gel as a stationary phase and a mixture of hexane:dichloromethane (3:1, *v*/*v*) as a mobile phase was used for the isolation of MOSH/MOAH from vegetable oil samples. the instrumental analysis was carried out employing 6890N GC system (Agilent Technologies, USA) coupled with Pegasus 4D (LECO Corporation, USA).

The method was validated on a sunflower oil on three different concentration levels (n=6 for each level; 25, 100 and 250 mg/kg) spiked by mineral oil standard mixture (Type A and B for EN 14039 and ISO 16703, Sigma-Aldrich, USA). the quantification was performed using a standard addition method. the mean recoveries varied from 84 to 92 % and the repeatabilities (expressed as relative standard deviations, RSDs) varied from 7 to 19 %.

The MOSH/MOAH were determined in vegetable oils from the Czech market (n=29; rapeseed oils, n=10; sunflower oils, n=10; olive oils, n=7; blended oils, n=2). the concentrations ranged from <10 to 88 mg/kg (MOSH, which were determined above limit of quantification (LOQ) of 10 mg/kg in 10 out of 29 oils) and <0.7 to 1.9 mg/kg (MOAH, which were determined above LOQ of 0.7 mg/kg in 7 out of 29 oils). the rapeseed oils were the most frequently contaminated (6 out of 10 contained either MOSH or MOAH above LOQs). Another contaminants determined in the vegetable oils were 12 polycyclic aromatic hydrocarbons (PAHs), which are produced by pyrosynthesis from organic matter and some of them are carcinogenic. They were isolated from the lipids by gel permeation chromatography (GPC) using Bio Beads S-X3 (Bio-Rad Laboratories, USA) as a stationary phase and chloroform as a mobile phase. An ultra-high performance liquid chromatography with fluorescence detection (1290 Infinity II, Agilent Technologies, USA) was employed for the PAHs analysis. the concentrations ranged from 4 to 36 µg/kg (sum of 12 PAHs; all oils contained at least 9 out of 12 monitored PAHs above their LOQs). There was no observed correlation between MOSH/MOAH and PAHs contamination levels.

Acknowledgement: Grant of Specific university research No A1_FPBT_2020_002, METROFOOD-CZ (MEYS Grant No: LM2018100) are greatly acknowledged.

The Effect of Freezing Rate on Properties of PVA Hydrogels Prepared by Cyclic Freezing/Thawing

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Hydrogels are hydrophilic, three-dimensional networks that can absorb large amount of water or biological fluids, and thus have the potential to be used as prime candidates for biosensors, drug delivery systems, and carriers or matrices for cells in tissue engineering. Optical, mechanical, and transport properties of hydrogels are crucial for their potential applications. One of the widely used polymers for preparation of hydrogels for biomedical applications is polyvinyl alcohol (PVA). PVA hydrogels can be formed via physical crosslinking (e.g. by cyclic freezing/thawing of aqueous PVA solutions) or with a chemical cross linker (e.g. glutaraldehyd). Physically crosslinked PVA hydrogels are more suitable candidates for biomedical applications because they do not contain residues of potentially hazardous substances (e.g. crosslinkers and others). Properties of a physically crosslinked PVA hydrogel can be influenced by the concentration of PVA and by the temperature of freezing that defines the freezing rate.
This work therefore focuses on the study of changes in the optical and mechanical properties caused by the modification of

the preparation process of PVA hydrogels. the microstructure was also observed and the connection between the change in optical and mechanical properties and the change in structure were evaluated. Hydrogels in this work were prepared via cyclic freezing/thawing under different cryogenic conditions (liquid nitrogen, two different laboratory freezers and ice bath) and with different concentrations of polyvinyl alcohol (2.5 to 15 wt. %).
Rheology was the main technique to study the mechanical properties of the hydrogels. Optical properties were studied only visually because of the insufficient transparency of some samples. the microstructure of selected samples was observed by scanning electron microscopy after freeze-drying. Results showed that the concentration of polyvinyl alcohol in the hydrogel partially changes the properties of the resulting hydrogel. However, the rate of freezing has the major effect on the properties.

Keywords: *hydrogel, polyvinyl alcohol, rheology, scanning electron microscopy*

The Effect of Substitution and Aromatic Ring Condensation on the Optical Properties of Alloxazine: a Theoretical Study

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Alloxazine and its derivatives have been the subject of a large amount of studies, due to their wide presence in living organisms as flavoproteins and coenzymes. Furthermore, these molecules have been shown as promising in the field of bioelectronics. This is due to their compatibility with biosystems, and their easily tunable optical properties. In this contribution, a theoretical study of Alloxazine, its tautomeric form isoAlloxazine and 16 derivatives has been carried out using the density functional theory. Absorption bands of the molecules were computed using the time-dependent density functional theory. the derivatives ranged from alloxazine substituted with simple electron-donating or accepting groups, to different heterocyclic systems and a large fused aromatic system. Based on the mutual comparison of the computed results, the differences in absorption spectra of Alloxazines and their isomers have been explained. Furthermore, the theoretical ability to change the absorption wavelengths by up to 300 nm has been demonstrated in the case of Alloxazine substituted with heterocycles.

Keywords: *Alloxazine, flavin, absorption properties, computational chemistry, density functional theory*

Occurrence of chlorinated paraffins in human blood serum and problems of their quantification

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Short chain chlorinated paraffins (SCCPs) and medium chain chlorinated paraffins (MCCPs) are a group of several thousand compounds of similar chemical structure. SCCPs have been classified as persistent organic pollutants. Dietary intake is considered to be the main source of exposure to SCCPs and MCCPs but another road of exposure could be inhalation. SCCPs and MCCPs have been identified in fish, vegetable oil, seeds and ither food commodities.

The aim of the study was to validate the method for the determination of SCCPs and MCCPs in human blood serum. the triple liquid-liquid extraction procedure employing extraction mixture n-hexan:diethylether (9:1, v/v) followed by purification on the SPE florisil column was applied. Final identification/quantitation of SCCPs and MCCPs were performed using gas chromatography coupled with high resolution mass spectrometry operated in negative chemical ionization.

The method validation was performed at 3 concentration levels 3000, 15000 and 35000 ng/g lipid weight (lw). Recoveries of SCCPs and MCCPs ranged from 98 to 130 % and from 80 to 113 %, respectively. Repeatabilities of both groups of CPs were in the range 8–20%. the successfully validated analytical method was used for analysis of 274 human blood serum samples collected in two sampling periods (142 samples in spring and 132 samples in autumn) in three regions of the Czech Republic (Prague, Ostrava and České Budějovice.). These samples were obtained from police officers participating in the project „Healthy Aging in Industrial Environment“. Concentrations of SCCPs in the serum samples in both the 1st round and the 2nd round range between <100–3019 ng/g lw (median 464 ng/g lw) and <100–2748 ng/g lw (median 120 ng/g lw), respectively.

The quantification of MCCPs in some human serum samples was a challenging task. In 38 serum samples collected within the 1st sampling period an amount of MCCPs was below limit of quantification. for 41 serum samples the response of MCCPs was out of a calibration curve and thus could not be quantified. Just in 63 serum samples the concentration of MCCPs could be calculated. These samples were divided into two groups based on the chlorine content and the results of samples from group 1 were several times higher than in 2nd group. This problem with MCCPs specific congener identification and quantitation could be caused by different congeners C_{16} and C_{17} profile in samples and standards. the solution would be the application of well characterizes standards which are unfortunately not currently commercially available.

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Can high-resolution mass spectrometry (HRMS) –based metabolomics be used for a varietal classification of wines?

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Wine is one of the most popular alcoholic beverages in many countries worldwide. However, due to its great financial value and relatively large amount produced, it is also one of the most common commodities which are subject to fraud and mislabelling. Several wine attributes can be adulterated including geographic origin, harvest year, variety from which it was prepared etc. Therefore, in the last few years, there has been growing interest in developing analytical methods for wine authentication. While analytical methods for the identification of wine by geographical origin exist and are implemented in official control, a sufficiently reliable strategy for authentication of wine variety is still missing.
Considering the complexity of wine matrix, metabolomic fingerprinting in combination with sample direct injection (without prior extraction), was selected as a suitable tool to address this challenging task. As an analytical platform, U-HPLC-Q-Orbitrap instrument (Q-Exactive Plus) was used. In total, 61 authentic samples

of three different wine varieties (obtained in cooperation with German Federal Institute for Risk Assessment, Berlin) were analyzed within our study. the generated data, after automated data mining and alignment, were processed by principal component analysis (PCA) and then by partial least squares discriminant analysis (PLS-DA). Statistically significant variables important for the grape variety classification were chosen according to their VIP (variable importance in projection) score. the resulting statistical models were validated and assessed according to their R2 (cum) and Q2 (cum) parameters. the most promising model enabled successful classification of 96 % of wine samples. In addition, tentative identification of the variable with highest VIP score (3-O-Caffeoylquinic acid, $C_{16}H_{18}O_9$, also possible: 4-O-, 5-O-) was performed. Our results indicate that the metabolic fingerprinting of wine samples might be used as an effective tool for variety authentication.

Keywords: *wine, authentication, metabolomics, mass spectrometry*

Acknowledgement: This work was supported by specific university research (MSMT No 21-SVV/2020) and METROFOOD-CZ research infrastructure project (MEYS Grant No: LM2018100) including access to its facilities.

Utilization of Mica Separated from Washed Kaolin

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This paper aims to laboratory test the possibilities of utilization mica separate, which arises during the process of floating kaolin as a by-product together with sand, which is not widely used today. Mica and sand are then separated by flotation or vibration. the mica separate thus formed was subjected to analysis. XRD and heating microscopy methods were used for analysis. XRD analysis detected multiple phases, such as quartz, kaolinite, muscovite and couple of feldspar (orthoclase, albite). Subsequently, experiments with mica separation as a filler in composites based on epoxy resins were set up and performed. Furthermore, the separate was tested as a part of plasters and visual building elements. Last but not least, the separate was mixed into the ceramic, which was then subjected to firing in the selected mode and XRD analysis was also performed on fired samples with ceramic. This paper provides a comprehensive overview of the above-mentioned possibilities of using mica separation, which is based on a sufficient amount of experimental data.

Keywords: *mica, muscovite, floating kaolin, mica separate, ceramic, composites, plasters*

Antidepressants and Anxiolytics in the Environment

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Antidepressant and anxiolytics are groups of psychoactive pharmaceuticals that represent a serious environmental risk when released to the water streams. Increased consumption of antidepressants and anxiolytics leads to the potential effect on non-target organisms such as changes in food and reproductive behaviour, socialisation or boldness. These changes can lead to reduced survival chances in aquatic organisms as well as some birds or mammals.

Growing consumption of these pharmaceuticals is a world-wide problem since effects on non-target animal were observed all around the world – in fresh and marine water. In the Czech Republic, antidepressants rank high on the list of most commonly prescribed drugs and in our environment behaviour-changing concentrations of anxiolytics were already detected. Our wastewater treatment plants (WWTP) are not constructed to effectively remove these substances from waster. Small streams and its organisms are more endangered because there is not so much dilution in the effluent from the WWTP. Also, small villages tend to use alternative wastewater management systems and – for example – root zone wastewater treatment plants seem to have no removal

efficiency. So far, there are only a limited number of economically meaningful solutions to eliminate antidepressants from water.

Keywords: *Antidepressants, Anxiolytics, Advanced Oxidation Processes, Psychoactive pharmaceuticals*

Use of a pilot scrubber separation device for specific pollutant in the air

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Industrial gas cleaning, also called scrubber, is a basic chemical engineering issue that aims to capture gaseous components from a mixture of gases. Various physicochemical processes and biological processes are part of this issue, and one of these processes is absorption. If we talk about the process in which chemical reactions take place, we are talking about chemisorption. In general, we can separate any gaseous substance in a scrubber. This work is mainly focused on industrial waste gases. These are mainly carbon dioxide and ammonia gases. the choice of these two gases is due to current worldwide research, which proves that they are one of the most difficult gases for the atmosphere, so this work deals mainly with the problem of these gases. the economics of the operation of such a separation device also play an extremely important role, which is why our device is designed to be able to operate even in smaller companies. the goal is to find a scrubber separation device that will have perfect efficiency at the lowest possible acquisition cost. All this can be achieved with the right combination of separation liquids and a suitable design of the entire scrubbber device.

Keywords: *gas scrubber, liquid, gas, carbon dioxide, sodium hydroxide, absorption, chemisorption, ammonia,*

Police Officer Exposure to Polycyclic Aromatic Hydrocarbons in Three Locations of the Czech Republic

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental contaminants which are formed during incomplete combustion of organic matter. the carcinogenic potential of some metabolites created in exposed organisms during metabolic processes can pose a risk to human health. the major metabolites excreted into urine are monohydroxylated PAHs (OH-PAHs) which are typically considered as biomarkers of human exposure. the aim of this study was to analyse 11 OH-PAHs in urine samples using ultra-high performance liquid chromatography coupled with tandem mass spectrometry (UHPLC-MS/MS). the urine samples were collected from Czech police officers within the HAIE project (Healthy Aging in Industrial Environment) in 2 sampling periods (*spring*, less air polluted season and *autumn*, more air polluted season). A total of 277 urine samples were collected from police officers in 3 different cities of the Czech Republic (Ceske Budejovice, Prague and Ostrava). the most abundant analytes in all measured samples were naphthalene-2-ol and phenanthrene-1-ol. the analytes chrysene-6-ol and benzo[*a*]pyren-3-ol were not detected in any samples. In the 1st sampling round (*spring*) the median concentration of sum 9 OH-PAHs in the urine samples decreased in the order of: Ostrava > Ceske Budejovice > Prague (5.84 > 5.14 > 4.43 μg/g creatinine). In the 2nd sampling round (*autumn*) the median concentration of sum 9 OH-PAHs in the urine samples decreased in the order of: Ostrava > Prague > Ceske Budejovice (7.37 > 6.05 > 5.22 μg/g creatinine). In both sampling periods the highest concentrations of the 9 OH-PAHs were found in urine samples from Ostrava. In all studied locations the concentrations measured in urine samples collected in the spring were lower compared to the concentrations measured in urine samples collected in the autumn. However, a statistically significant difference (α=0.05) in the concentrations between sampling periods was observed only for samples from Ostrava. Within the HAIE project the analysis of 24 PAHs in the air from personal air samples was also performed. No significant correlation was found between concentration of PAHs in the air and their metabolites (OH-PAHs) in urine from exposed police officers. the authors would like to thank the Institute of Experimental Medicine AS CR in Prague and the University of Ostrava for providing the samples.

Keywords: *ultra-high performance liquid chromatography with tandem mass spectrometry, monohydroxylated PAHs, urine*

Utilization of Grape Seed Lignin in Polyhydroxyalkanoate Blends

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Lignin is one of the most widespread biopolymers in the world. It is a complex polyphenol compound with a branched three-dimensional structure. This structure is formed by aromatic monolignols derived from hydroxycinnamyl alcohol. Nowadays, lignin is mostly obtained as a by-product in the pulp and paper industry. Lignin is most often used as a waste fuel. Laboratory lignin can be isolated by various technics, including the most common methods such as Kraft, sulfite, soda or organosolv process. the fundamental effect on lignin properties has the presence of sulfur in the structure. Sulfur compounds arise through Kraft and sulfite processes. Lignin obtained from the sulfite process is soluble in water, Kraft lignin only in alkaline solutions. the main advantage of organosolv and soda lignin is that they are sulfur-free. However, both are insoluble in water.

Lignin due to its bio-origin, aliphatic-aromatic composition and high abundancy possess theoretically a wide range of applications. Attention is mostly focused on the copolymerization and blending of lignin with various kinds of polymers, such as polyurethanes, phenol-formaldehyde and epoxy resins, polyesters and others.

In our research, we used lignin isolated from grape seeds that are waste products in the wine industry. Lignin was isolated by soda process and showed a high antioxidant activity thanks to its phenolic structure. Our work summarizes the effect of lignin addition on the properties of polyhydroxyalkanoate films. Principally, grape seeds lignin was mixed with crystalline poly(3-hydroxybutyrate) and amorphous polyhydroxyalkanoate via solution casting. the PHA/lignin films showed improved mechanical, thermal and gas barrier properties. the further advantage of these films was high antioxidant efficiency. All prepared samples proved their compostability comparable with a paper standard. Moreover, the obtained biomass after composting enhanced the plant growing.

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Keywords: *lignin, grape seeds, polyhydroxyalkanoates, films, composting, physico-mechanical properties*

STUDENTSKÁ KONFERENCE: CHEMIE JE ŽIVOT

Transport Properties of Biopolymeric Hydrogels

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This work is focused on study of transport properties of biopolymer-based hydrogel systems. Studied hydrogels are based on interaction between biopolymer-like polyelectrolytes with oppositely charged surfactant ions. Mixing polyelectrolytes with oppositely charged surfactants can lead into creation micelle-like nano-containers. These nano-containers are able of binding hydrophobic compounds such as pharmaceutically active substances. the aim of this work is to determine ability of these hydrogels to absorb and release substances. Hydrogels were prepared as combination of sodium form of hyaluronan and positive charged surfactant Septonex (carbethoxypendecinium bromide). Next type of hydrogel was based on combination of modified dextran (diethylaminoethyl-dextran hydrochloride) with positive charge and oppositely charged sodium dodecyl sulfate as surfactant. As a diffusion probes in hydrogel systems Atto 488 and Nile red were used. Two different ways of diffusion were studied. the first way of study was the release of dyestuff from hydrogels based on dextran and hyaluronan into different solutions. the second way of study was the incorporation of dye from solution into these hydrogels. the diffusion of dyes was monitored in time. Transport of dyes into structure of hydrogels or release from hydrogels was characterized by diffusion coefficients and structural parameters of hydrogels.

Keywords: *diffusion, polyelectrolyte, hydrogel, dye, surfactant*

Preparation of Mg-Ti Based Bulk Materials via Powder Metalurgy

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The aim of this thesis is preparation and characterization of bulk magnesium–Titanium based materials. In the first theoretical part properties of base materials and the complexity of preparation alloy from these metals is discussed. Second part is focused on powder metallurgy and its applicability on Mg–Ti system. In another part particle composites are described.
The experimental part of this thesis was the preparation of bulk Mg–Ti materials from metal powders. for sample preparation conventional methods of powder metallurgy and spark plasma sintering was employed. Furthermore a characterisation of these materials was done. Microstructure was observed. Present phases were found using X-ray diffraction analysis. Amounts of these phases were determined using a scanning electron microscope with energy–dispersive spectrometry and using X-ray fluorescence. Furthermore hardness was measured and bending test with evaluation was done. Significant difference in results of sample preparation using conventional methods of powder metallurgy and spark plasma sintering was observed.


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