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**9. ŠTUDENTSKA KONFERENÇA  
MEDNARODNE PODIPLOMSKE ŠOLE  
JOŽEFA STEFANA IN 11. DNEVA MLADIH  
RAZISKOVALCEV (KONFERENCA KMBO)**

**Zbornik**

***9<sup>th</sup> JOŽEF STEFAN INTERNATIONAL  
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CONFERENCE AND 11<sup>th</sup> YOUNG RESEARCHERS'  
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***Proceedings***

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Martin Topole, Timotej Turk Dermastia, Matic Bergant, Andrea Jurov

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## Beseda predsednika MPŠ: Akad. prof. dr. Vito Turk

Mednarodna podiplomska šola Jožefa Stefana – MPŠ se je že uveljavila tako doma kot tudi v tujini. V vsem tem času je več kot uspešno opravljala svoje poslanstvo, kar kažejo kvalitetna doktorska in magistrska dela. To je rezultat uspešnega sodelovanja podiplomskih študentov in njihovih mentorjev. Potrebno je na prvem mestu omeniti Institut »Jožef Stefan«, ki največ doprinaša k uspešnemu delu te šole z odlično opremo, vključno s Centri odličnosti in širokim programom ter kvalitetnimi mentorji.



Vključitev in sodelovanje Nacionalnega inštituta za biologijo – NIB in Inštituta za kovinske materiale in tehnologije – IMT je še razširilo naše potenciale in prispevalo k še večji interdisciplinarnosti, kar dokazuje zadnja razširitev na aktualno problematiko senzorskih tehnologij, ki poleg že uveljavljenih treh smeri kaže na naše stalno spremljanje razvoja znanosti in inovativnosti v svetu. Danes je postala beseda »odličnost« izjemno popularna v svetu, zlasti na področju znanosti. Pri različnih razpisih, še zlasti Horizon 2020, so uspešni le tisti projekti, ki dobijo oceno odlično ali celo izvrstno. Osnovne raziskave s takimi ocenami naj bi vodile s svojimi prelomnimi dosežki do novih inovacij in proizvodov, od katerih je odvisna ekonomska rast in moč države. Zato pa je potrebno veliko naporov in finančnih vlaganj vlad, ki razumejo pomen znanosti in raziskav za razvoj celotne družbe. Pred kratkim sta predsednik Max-Planckove zveze institutov dr. Martin Stratmann in predsednik francoskega CNRS dr. Alain Fuchs poudarila pomen odličnih osnovnih raziskav ter inovacij, ki bodo kreirale raziskovalce, sposobne ustvarjanja novih idej. To počno razviti, ekonomsko šibkejša država pa bi se morale potruditi, da za priključitev k ekonomsko uspešnim državam ustvarjajo pogoje s primernim financiranjem in infrastrukturo. Le tako bodo te države lahko uspešno vzpostavile sodelovanje z industrijo ter razvijale produktivne partnerske odnose. Za Slovenijo velja, da bi morala njena vlada vlagati vsaj 1 % BDP, če želi kolikor toliko nadoknaditi že zamujeno. Trenutno vlagamo le 0,36 % BDP, kar nas uvršča na dno Evrope. Zmotno je mnenje, da bomo le s sredstvi EU in Horizon 2020 dosegli zaželeno cilje. Ker že govorimo o odličnosti, smo pri projektih ERC v odličnosti prav na dnu EU. Glede na navedeno nas ne sme presenečati, da smo priče begu možganov in ne kroženju, kot to želijo nekateri prikazovati.

Kljub vsemu naša MPŠ vlaga velike napore za doseganje več kot solidnih, v nekaterih primerih tudi odličnih rezultatov v sicer neprijaznih pogojih na področju raziskovalne in visokošolske dejavnosti. Dejstvo je, da se vpisujejo na področja delovanja naše šole praviloma odlični mladi podiplomci, ki s svojim znanjem, zagnanostjo in dosežki segajo v sam vrh kvalitetnih mladih raziskovalcev. Njihova kvaliteta raziskav se kaže z objavami v mednarodno uglednih in v nekaterih primerih vrhunskih revijah. Seveda teh uspehov ne bi

bilo brez odličnih mentorjev in somentorjev, ki so prejeli za svoje delo vrsto domačih ter mednarodnih priznanj. Naj omenim še izjemno vzdušje in kolegialne odnose, ki vladajo med podiplomci in njihovimi mentorji. Vse to omogoča tudi uspešno vpetost v mednarodne povezave tako v evropskem kot tudi v globalnem prostoru. S svojim delovanjem MPŠ prispeva k hitrejšemu prehodu iz vsesplošne krize v družbo znanja. Letošnja predstavitev raziskovalnih dosežkov naših podiplomcev je ponoven dokaz vaše uspešnosti, ki je posledica trdega dela in talenta. Vse to vam omogoča, ob pomoči mentorjev ter bližnjih sodelavcev, da se boste razvili v kreativne raziskovalce, na katere bomo ponosni. S svojim znanjem boste lahko doprinašali k boljši prihodnosti, kot vam jo ponuja sedanjost. Vso pravico imate, da se uspešno spopadate z izzivi v domačem okolju, ne pa da iščete izpolnitve svojih ambicij in eksistenčnih možnosti z odhodom v tujino.

Ob koncu bi še enkrat ponovil, kar sem že večkrat izjavil, da je »znanje vrednota, ki omogoča narodu ekonomski razvoj in obstoj«. Mladi člani Evropske akademije (YAE) pa so v odprtem pismu leta 2015 izjavili, ob opozorilu na podfinanciranje osnovnih raziskav, kar ima hude posledice za mnoge južnoevropske države, kamor sodi nedvomno tudi Slovenija, da so »osnovne raziskave v ospredju moderne kulture in nam pomagajo razumeti, kdo smo«. Pri nas tega odgovorni očitno ne razumejo, kajti če bi razumeli, bi delali drugače! Mladi vrhunski raziskovalci so pogoj za uspešen gospodarski in vsesplošen razvoj in so srce družbe znanja. Očitno so za to spoznanje potrebne globoke družbene spremembe, ki pa jih do sedaj še nismo dočakali. Vendar bodimo še naprej optimisti.

## Beseda dekanje MPŠ: Prof. dr. Milena Horvat



Raziskovalno-izobraževalni proces v intenzivnem in inovativnem raziskovalnem okolju ključno prispeva h krepitvi razvojnega potenciala znanosti in visokih tehnologij v družbi. Prav to je vodilo izobraževalnega procesa na Mednarodni podiplomski šoli Jožefa Stefana (MPŠ), ki prepleta temeljno raziskovanje s podiplomskim izobraževanjem in tehnološkim razvojem. V dobrih 12 letih delovanja beležimo številne uspehe takega delovanja na področjih nanotehnologij, informacijsko-komunikacijskih tehnologij in ekotehnologij. K temu šola v novem študijskem letu 2016/2017 dodaja še področje senzorskih tehnologij, ki bistveno dopolnjuje že obstoječe programe in ustvarja nove možnosti za povezovanje na področju medsektorskega sodelovanja. Senzorji namreč pomagajo prepoznavati določene pogoje v okolju in nanje ciljno reagirajo, zato njihova uporaba sega na skoraj vsa področja človekovih dejavnosti, kot na primer preskrbo z zdravo in varno hrano, kmetijstvo, zdravstvo, okoljevarstvo, energetiko itd. Ob vse večjih ekonomskih in okoljskih zahtevah postajajo senzorske tehnologije bistveni sestavni del vseh “pametnih” izdelkov in s tem obetavna priložnost za industrijo. Njihova proizvodnja terja hitro napredujoče visoke tehnologije, zato je to področje tudi znanstveni izziv.

Slogan letošnje konference “Skupaj na poti do uspeha – pridruži se nam tudi ti” kaže na optimizem, ki ga nova generacija študentov izseva. Ta optimizem je prepleten z odpiranjem vrat, ki omogoča povezovanje študentov že v času študija. To pa je predpogoj za snovanje bodočega in odprtega sodelovanja.

Tako so študenti MPŠ podali predlog, da se najprej povežeta dve tradicionalni konferenci: Študentska konferenca MPŠ in Dan mladih raziskovalcev kemije, biokemije, materialov in okolja (KMBO) na Institutu “Jožef Stefan” (IJS). K temu pa so pritegnili tudi študente

zunaj IJS in MPŠ, kar je vsekakor uspeh organizatorjev konference in celotnega Študentskega sveta MPŠ, ki so konferenco promovirali na različne načine.

Izmenjava znanj in izkušenj med študenti in raziskovalci krepi in bogati raziskovalno delo, ki je po naravi večinoma interdisciplinarno. Letošnja konferenca nadaljuje s prakso prejšnjega leta, da je potrebno o znanosti govoriti na način, ki je razumljiv kar se da širokemu spektru ljudi. Take veščine so prirojene le redkim, zato je program konference posvečen tudi pridobivanju veščin javnega nastopanja.

V Sloveniji je vloga javnosti v znanstveni sferi pogosto zanemarjena, čeprav Evropa prepoznava, da je ta segment ključen pri prenosu znanja v prakso, zato je to zapisano tudi v strateških ciljih, kar se odraža v zahtevah tematskih razpisov Obzorja 2020. Tudi MPŠ prepoznava pomen komunikacije širši javnosti kot sestavni del izobraževalnega procesa, zato bo tovrstne dejavnosti še naprej podpirala.

V sodelovanju s partnerskimi raziskovalnimi institucijami in industrijo želimo na MPŠ ustvariti pogoje, ob katerih študentje lahko ustvarjajo odlično mednarodno primerljivo znanost, hkrati pa razvijajo svoje kreativne in poslovne sposobnosti, s čimer bodo prispevali tudi k zagotavljanju pogojev za uspešen razvoj poslovnih modelov in posledično k vidnim rezultatom v družbi. K temu vsekakor sodi tudi povezovanje programov MPŠ z ostalimi slovenskimi in tujimi univerzami, saj želimo študentom nuditi najboljše znanje in spretnosti, ki jih bodo v prihodnje rabili na svoji karierni poti.

Vsem udeležencem študentske konference želim uspešno delo, ki bo ostalo v spominu kot kreativno in prijetno druženje.



## **Beseda predstavnice gospodarstva: dr. Jožica Rejec**



Predstavitev rezultatov raziskav na letni študentski konferenci Mednarodne podiplomske šole Jožefa Stefana in v zborniku daje celovit pregled dosežkov študentov in raziskovalnih področij šole. Čestitke študentom in mentorjem.

Bilo je veliko vložnega dela, odkritih do sedaj neznanih pojavov, vplivov in nakazanih možnih rešitev in nadaljnjih raziskav. Običajno je pot od drobnih odkritij do dodane vrednosti v gospodarstvu, ki edino osnovno dodano vrednost ustvarja in omogoča nadaljnja raziskovanja, dolga. Potrebni je še veliko raziskovanja, različnih faz industrializacije, prilagoditev tržnim zahtevam in možnostim. Druga možnost uporabe rezultatov raziskav je razjasnitev dogajanj v realiziranih produktih, ki omogočijo večjo zanesljivost, robustnost, uporabo cenejših materialov, izboljšanje karakteristik in tako povečajo dodano vrednost in konkurenčnost.

Bralci zbornika, mentorji in mladi ustvarjalci, bodimo povezovalni in ambiciozni ter omogočimo kakšni od napisanih idej realizacijo v praksi slovenskega gospodarstva.

## **Direktor Inštituta Jožef Stefan: Prof. dr. Jadran Lenarčič**

Z velikim veseljem spremljam vsakoletno srečanje mladih s področij kemije, biokemije, materialov in okolja. Na vsak dosežek gledam z velikim spoštovanjem in ponosom, še posebej glede na vse težje razmere, ki jih imajo mlajše generacije raziskovalcev v Sloveniji. Kljub temu pa so rezultati, ki jih vidimo konferenci, na zelo visokem nivoju. Naš inštitut še posebej odlikujejo mednarodne povezave ter povezave z gospodarstvom in prav te so ključ h kakovostnemu raziskovanju in omogočajo dodatno financiranje raziskav, ki jih sicer nebi mogli izvajati. Tovrstna srečanja imajo velik pomen. Podpiram jih predvsem zato, ker lahko na njih prihaja do izmenjav, do novih zamisli in načrtov. Temu se predvsem mladi nebi smeli nikoli odreči.

## **SKUPAJ NA POTI DO USPEHA – PRIDRUŽI SE NAM TUDI TI!**

### **Študentski svet MPŠ**

Letošnja študentska konferenca ponovno prinaša nekaj novega. Tokrat smo dve konferenci združili v eno samo. V skupno konferenco smo tako povezali študentsko konferenco Mednarodne podiplomske šole Jožefa Stefana (MPŠ) in Dan mladih raziskovalcev oziroma konferenco KMBO (kemija, materiali, biokemija in okolje). Združitev konferenc je posledično s seboj prinesla tudi potrebo po združitvi organizacije. MPŠ konferenco običajno organizira študentski svet, medtem ko se nosilci te funkcije pri konferenci KMBO menjajo. Letos je bil za organizacijo odgovoren Odsek za znanosti o okolju (O2). Obe konferenci sta prvenstveno namenjeni mladim raziskovalcem oziroma podiplomskim študentom (magistrskim in doktorskim) z namenom, da predstavijo svoje delo v obliki posterja in kratke predstavitve. Predlog za združitev smo utemeljili na podlagi izkušenj iz prejšnjih let, saj sta bili konferenci namenjeni istim študentom in sta potekali v zelo kratkem časovnem razmaku. Veliko študentov se je tako udeležilo le ene izmed konferenc. Odbor za konferenco KMBO, sestavljen iz predstavnikov vodij različnih odsekov, ki zajemajo področja kemije, biokemije, materialov in okolja, ter dekanja Mednarodne podiplomske šole prof. dr. Milena Horvat, so se s predlogom strinjali in začeli smo z organizacijo.

Večina stare ekipe se je poslovila, saj obveznosti s pisanjem doktorske disertacije zahtevajo preveč časa. Iskanje novih članov je vedno težavno, saj so študenti precej obremenjeni z raziskovalnim delom in običajno zavračajo vsakršno dodatno aktivnost, ki je izven okvira njihovega raziskovanja. Tu so nam bili v veliko pomoč mentorji, ki so predlagali po njihovem mnenju najbolj primerne kandidate. Od stare ekipe sta tako ostali le lanska predsednica Majda Pavlin, ki je prav tako v zaključni fazi doktorskega študija, in Anja Pecman, študentka drugega letnika smeri Nanoznanosti in nanotehnologije na Nacionalnem inštitutu za biologijo (NIB). Novi člani so večinoma študenti prvega letnika: Andrea Jurov – Senzorske tehnologije, Martin Topole – Nanoznanosti in nanotehnologije, David Levovnik – Ekotehnologije, Matic Bergant – Ekotehnologije in Timotej Turk Dermastia – Ekotehnologije. Blaž Škrlj in Jan Kralj sta magistrski in doktorski študent Informacijskih in komunikacijskih tehnologij (IKT), Tjaša Gornik pa je v drugem letniku smeri Ekotehnologije in se je z delom na Inštitutu »Jožef Stefan« (IJS) in MPŠ že deloma spoznala.



Sveže ideje, samoiniciativnost in entuziazem so tisto, kar vodi ekipo naprej. Organizacija konference je vedno velik zalogaj, ampak ob dobri ekipi, ki je pripravljena prispevati h končnemu cilju, je to lažje dosegljivo. Letos smo dali nekoliko več poudarka tudi na samo prepoznavnost konference. Vse to se nam je obrestovalo in prejeli smo kar 69 prispevkov. K temu je zagotovo prispevalo tudi dejstvo, da sta dve konferenci združeni v eno, poleg tega pa ni bilo več potrebno napisati prispevka v daljši obliki, ampak samo kratek povzetek na eni strani. Prejeli smo 51 prispevkov študentov, ki so vpisani na MPŠ, in 18 prispevkov študentov, ki so vpisani na podiplomske programe Univerze v Ljubljani oziroma na univerze v tujini. V organizacijo smo vključili društvo Mlada akademija (bivše Društvo mladih raziskovalcev Slovenije), ki nam je pomagalo pri pripravi okrogle mize. Poleg tega smo k sodelovanju ponovno povabili Društvo Satena, ki je tudi letos podelilo nagrado za najboljši »pitch« po mnenju novinarjev. Pozitivno so se odzvala različna podjetja, ki so nas podprla finančno (podjetje Scan, VWR in Primatron), in ostali, ki so prispevali promocijski material (Sanolabor, Chemass in Kemomed) in vstopnice za različne dogodke (Cankarjev dom in Mestno gledališče ljubljansko, MGL). Ekipa Videlectures, ki deluje v okviru IJS, pa nam je ponudila pomoč pri snemanju »elevator pitchev«. Pri iskanju sponzorjev so pomagali tako sodelavci z Odseka za znanosti o okolju kot tudi tajništvo MPŠ. Prof. dr. Zvonka Jeran (Odsek za znanosti o okolju, O2) in prof. dr. Saša Novak Krmpotič (Odsek za nanostrukturne materiale, K7) pa sta nam ves čas stali ob strani s svojimi predlogi, komentarji in bili v pomoč tudi pri izvedbi dogodka.

Namen konference ni samo v predstavitvi raziskovalnih del mladih raziskovalcev oziroma podiplomskih študentov, ampak tudi medsebojno povezovanje, izmenjava idej, predlogov in kritik ter sklepanje novih poznanstev tako med študenti kot tudi s profesorji, podjetji in zunanjimi obiskovalci, ki jih tematika zanima. Interdisciplinarnost v znanosti je vedno bolj pogojena s sodelovanjem različnih strok, saj ni več dovolj, da raziskovalci oziroma strokovnjaki prihajajo samo iz določenega področja. Zato je potrebno že v času

doktorskega študija gojiti miselnost, da moramo med seboj sodelovati in se povezovati, saj bomo le tako dosegli, da bodo naši rezultati, produkti in ideje celostno podkrepjeni. Po drugi strani pa se zavedamo, da je znanost še vedno preveč za zaprtimi vrati in širša javnost premalo pozna naše raziskovalne dosežke. Že lani smo se odločili, da je potrebno nekoliko več truda vložiti v veščine, ki zajemajo predstavitev naših del na poljuden, razumljiv, predvsem pa zanimiv način, ki je blizu tako znanstvenim sodelavcem kot tudi širšemu občinstvu. Tudi letos smo povabili štiri različne novinarje, ki se s tematiko znanosti srečujejo pri vsakdanjem delu; novinarke oddaje Ugriznimo v znanost Renato Dacinger, Anjo Čuček in Natašo Čuček Ivanuš ter voditeljico na VAL-u 202 Majo Ratej. Poleg tega, da znajo kritično presoditi, kaj je pri poročanju raziskovalnega dela bistveno in hkrati zanimivo za poslušalce, poznajo tudi veščine javnega nastopanja in načine, kako se tovrstna vsebina podaja. Vse študente smo razdelili v štiri skupine glede na tematiko, s katero se ukvarjajo. Namen delavnice je bil pridobiti osnovna znanja, kako predstaviti raziskovalno delo poljudno, zanimivo in hkrati dovolj strokovno v kratkem časovnem intervalu. Zaradi velikega števila prispevkov smo prosili profesorje, da so po svoji presoji določili študente, ki bi bili primerni za »elevator pitch«. Tako smo dobili 40 kandidatov, ki so imeli na konferenci predstavitev, ostali pa so se predstavili s posterjem. Pripravljalne delavnice za kratko predstavitev, ki smo jo naslovili podobno kot lani »3 minute za moje doktorsko delo«, so bile odprte vsem sodelujočim, tudi tistim, ki kasneje na konferenci niso sodelovali. Program konference je bil sestavljen iz dveh ločenih delov, prvi dan smo imeli predstavitev »elevator pitchev«, drugi dan pa smo se usmerili v »Karierne poti« posameznikov in podjetij. »Elevator pitchi« so bili ocenjeni s strani ekipe novinarjev: Luka Hvalc – Val 202, Lea Udovč – STA, Slavko Jerič – RTV-SLO, Ana Slavec – Metina lista in društvo Mlada akademija ter članica Satene, dr. Kristina Žagar., na koncu dneva pa smo razglasili tri zmagovalce po mnenju novinarjev, Roka Kocena, Mišela Cevzarja in Tjašo Parkelj, ki so prejeli nagrado Društva Satena.

Usposabljanje za mladega raziskovalca, bodisi preko agencije ARRS, Ad future ali iz kakšnih drugih sredstev, je časovno omejeno. Zavedamo se, da po končanem študiju le malo doktorandov ostane na fakultetah, institutih in ostalih raziskovalnih institucijah. Poleg tega za samo napredovanje potrebujejo usposabljanje v tujini. To jim daje upanje, da se v matični instituciji zaposlijo po vrnitvi, po drugi strani pa odpira paleto dodatnih možnosti. Kot že omenjeno, se večina študentov po zaključenem doktoratu usmeri v industrijo, različna mala podjetja, oziroma iščejo druge opcije, ki jim omogočajo razvoj lastnih potencialov in uresničitev želja. Da bi pokrili kar največ različnih opcij, smo v goste povabili dr. Matjaža Humarja, dobitnika nagrade »Direktorjevega sklada v letu 2016«, ki mu je omogočila postavitev lastnega laboratorija na IJS, potem vodjo razvoja v podjetju Gorenje, d.d. dr.

Boštjana Pečnika, ki je tako, kot dr. Humar, doktoriral na MPŠ, svoje delo pa nadaljuje v industriji, in dr. Klemna Zupančiča, ustanovitelja »spin-off« podjetja Biosistemika, ki izhaja iz NIB-a. Kot posebnega govorca smo povabili dr. Petra Wostnerja iz Vlade Republike Slovenije za razvoj in evropsko kohezijsko politiko, Sektor za koordinacijo pametne specializacije. Pametna specializacija je postala pomemben del raziskovalne dejavnosti in gospodarstva ter posledično sodelovanja obeh segmentov. Doktorski študenti naravoslovja premalo vemo o tem in namen tega predavanja je bil predstavitev strategije pametne specializacije.

Konferenco smo nadaljevali s panelno razpravo, ki smo jo organizirali v sodelovanju z dr. Ano Slavec, predstavnico društva Mlada akademija. Dr. Tomaž Rijavec se je pridružil kot drugi moderator razprave, razpravljavci pa so bili dr. Urška Kristan, dr. Tea Romih, dr. Eva Menart, dr. Ana Gantar in dr. Matic Lozinšek. Študentom so predstavili kam jih je vodila pot po doktoratu, kako so bili že med samim doktorskim študijem vpeti v različne projekte, kakšni so njihovi cilji v prihodnosti, ter kako so jim pri vsem skupaj pomagali mentorji.

V sklepnem delu smo podelili štiri nagrade za najboljše prispevke po mnenju strokovne komisije profesorjev (prof. dr. Boris Žemva, prof. dr. Sonja Lojen, prof. dr. Borut Smodiš, prof. dr. Veronika Stoka, doc. dr. Tomaž Klobučar in doc. dr. Andreja Benčan Golob). Komisija je opravila pomembno delo, saj pregled velikega števila posterjev in »elevator pitchev« zahteva kar nekaj časa. Zmagovalci študentske konference so bili tako Aleksander Matavž, Rok Kocen, Mišel Cevzar in Špela Alič. Odločili smo se, da podelimo nagrado tudi za poster, ki ni sodeloval pri »pitchih« (nagrado je prejela Doris Potočnik) in nagrado publike. Tudi občinstvo je izbralo Roka Kocena in Mišela Cevzarja. Miha Mrzlikar pa je prejel nagrado za najboljši poster s področja hrane, ki jo podarja ISO-FOOD. S tem se je uradni del končal.

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## **Ekotehnologija (Ecotechnology)**

## Mercury in cement production process

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Mercury (Hg) is a metallic element, known for its toxicity, volatility, persistence and bioaccumulation. Its compounds are emitted in the atmosphere from different anthropogenic and natural sources, where they are dispersed and consequently transported to different environmental compartments. It is estimated that in 2010 cement industry contributed approximately 10% to the global emission inventory [1], listing it as a priority for emission control at the Minamata Convention on Mercury [2]. In cement production, Hg is introduced predominantly with raw materials [3] (60%), and fuels (40%). Mercury from raw materials vaporizes at temperatures between 200-700°C and is released into the kiln gases in the preheater section. In the rotary kiln, high temperature environment vaporizes Hg from fuels which enters the gas as elemental mercury (Hg<sup>0</sup>). Some of the Hg is absorbed by the suspended solids which are captured by electrostatic precipitators or baghouses, which in return can be recycled back to the pyro-process. If the cement plant utilizes a bypass stack, all of the Hg will be emitted from the stack under steady-state conditions. [4] These steady-stack conditions can be difficult to achieve in a short time, which in return affects strategies to control mercury stack emissions.

Mercury removal technologies include careful selection of input materials and fuels, raw material cleaning, removal by sorbent injection upstream of existing air pollution control devices, and enhanced Hg removal by oxidation. Raw material cleaning does not appear to be feasible solution due to the large amount of raw materials used to produce cement. On the other hand, powered activated carbon (PAC) injection systems are well known commercial air pollution control systems, used for a variety of organic compounds and heavy metals. Many parameters influence the adsorption of mercury on PAC: Hg speciation and concentrations, physical and chemical properties of carbon, gas temperature and composition, mercury-carbon contact time, etc. In this Hg removal technology, it competes with a variety of gases for the adsorption sites on the activated carbon, and there are some indications that the high moisture levels in the flue gas will suppress the capture of Hg by activated carbon. Oxidation pre-treatment systems may convert elemental mercury to oxidized mercury upstream of wet scrubber systems and also upstream of conventional particulate matter control devices, with efficiency approaching 85%.

This work will be focused on further research needed to provide the best sorbent with effective Hg capture at a low cost. In the same time, lab-scale tests will help in evaluation of activated carbon as a promising tool in Hg removal.

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## Physically-based HPGe gamma detector absolute efficiency determination

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$k_0$  instrumental neutron activation analysis ( $k_0$ -INAA) requires high-purity Germanium (HPGe) gamma detectors, with their absolute full-energy peak efficiency (FEPE) known for as large an energy range as possible. The standard procedure for determining the FEPE is by using reference point gamma sources with known absolute activities, which yield the FEPE at a few discrete energies. Afterwards, polynomials are fitted to different energy regions of the efficiency data, with care taken to minimize the polynomial's discontinuities at region boundaries. Due to the choice in number and degree of polynomials and their energy regions, this is a subjective approximation, inaccurate in regions where few data points are available, especially outside the region between the smallest and largest calibration energy.

We improve this by simulating a simplified HPGe detector and gamma source, using the Geant4 simulation toolkit. It performs a full physical Monte-Carlo simulation of the passage of particles through matter, yielding a simulated energy-efficiency function. This function has the desired general shape, but is inaccurate due to simplifications in the geometrical and physical models used for the simulation. We correct this by fitting the simulated efficiency curve to experimental data, analogously to how we fitted polynomials in the standard calibration procedure, but with fewer degrees of freedom. This gives a more accurate and less subjective model of efficiency than possible from a simple polynomial fit. Because we use a reasonably accurate physical model for the prediction, we also have greater confidence in the determined efficiency outside the extremal calibration energies.

Our method thus extends the energy range of HPGe calibration, and enables a better trade-off between the number of calibration sources used, and the accuracy of the determined FEPE. The latter is particularly useful for energy regions where few or no such sources are even available.

## Simulating environmental photodegradation of sertraline in aqueous environment

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Sertraline is an antidepressant that acts as a selective serotonin reuptake inhibitor. It is among the world's most popular antidepressants [1]. It is present in the environment at concentrations of ng/L in water and ng/g in fish tissue and river sediment. Its metabolite norsertraline has also been found at a similar concentration range [2]. Its main sources in the environment are human excretion, inappropriate disposal and the pharmaceutical industry [3]. Research results up to now suggest photodegradation as the main degradation route in environmental waters [4]. Our interest was its degradation kinetics and chemical changes when exposed to sunlight during direct or indirect photodegradation. In the former the compound degrades due to absorption of solar photons, while the latter is the result of reactions with other reactive species present in the water, which work as either sensitizers or radical scavengers [5]. We observed the behaviour of sertraline dissolved in MilliQ water at different pH values and with several compounds added to simulate conditions [6] in the aqueous environment: NaNO<sub>3</sub>, 2-propanol, NaHCO<sub>3</sub>, NaH<sub>2</sub>PO<sub>4</sub> and Na<sub>2</sub>HPO<sub>4</sub>, rose bengal, anthraquinonen-2-sulfat and riboflavin. The solutions were irradiated with a medium pressure mercury lamp. The samples were then analysed with gas or liquid chromatography coupled with mass spectrometry, depending on the concentration range of the sertraline spike (µg/L or mg/L). The samples with lower concentrations were also preconcentrated with solid phase extraction beforehand. The degradation kinetic was pseudo-first order, with the degradation constant in the range of 10<sup>-2</sup> - 10<sup>-5</sup> min<sup>-1</sup>. We also observed structural changes of sertraline. The proposed transformation products identified up to date are norsertraline, sertraline imine, and two hydroxylated analogues.

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## Maternal diet and lifestyle, levels of selected elements and fatty acid composition in maternal milk from two different areas in Slovenia

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According to the literature, maternal diet and living environment can affect levels of elements and fatty acid (FA) composition and their stable isotopes in human milk. The content of  $\omega$ -6 and  $\omega$ -3 polyunsaturated fatty acids (PUFAs), could be related to the optimal growth and development of the baby. Higher intake of seafood could increase the content of  $\omega$ -3 PUFAs, but it should be taken into account, that fish also contain Hg compounds acting as neurotoxicants. Therefore, the evaluation of fish intake in context of potential risks and potential benefits should be done.

Since the FA composition is correlated with the diet, the analysis of stable isotope ratio ( $^{13}\text{C}/^{12}\text{C}$ , expresses as  $\delta^{13}\text{C}$ ) could be used for tracking dietary habits. Variation in isotopic composition of carbon ( $^{13}\text{C}/^{12}\text{C}$ ) occurs due to differences in fixation pathways which are correlated with environmental and physiological conditions.

To investigate the relationship, information obtained from questionnaires' and analytical data on milk samples (4-6 weeks after delivery) of 74 delivering women (20-38 years) and their newborns from area of Koper and area of Murska Sobota from HBM in Slovenia (2007-2014) were used.

Levels of selected toxic and potentially toxic elements were analysed using an Inductively-coupled plasma mass spectrometry (ICP-MS) for As, Cd, Cu, Mn, Pb, Se and Zn for milk samples and cold vapour atomic-absorption spectrometry (CVAAS) for Hg in milk. Identification and quantification of FAs in maternal milk were performed by in-situ trans-esterification method (FAMEs). The characterization of FAMEs were performed by gas chromatography with FID detector (GC-FID), equipped with a capillary column (Omegawax 320), while  $\delta^{13}\text{C}_{\text{FA}}$  were determined using Isoprime GV GC-C-IRMS system, using a capillary column DB-1MS.

Associations between those areas and a) predictors obtained through questionnaires and b) levels of selected elements, FA composition and stable isotopes of individual FA in maternal milk samples were tested using univariate and multiple linear regression.

Levels of selected elements did not represent any health risk for the mother-child pairs. Levels of As and Hg in milk were statistically higher in the coastal than in the inland area, so were the levels of saturated and monounsaturated FA. Whereas PUFAs,  $\omega$ -3,  $\omega$ -6 levels were lower in the coastal than in the inland area, despite higher intake of fresh sea food observed in the coast. The ratio  $\omega$ -6/ $\omega$ -3 levels did not differ significantly among the studied areas.

## Use of micro-IBA to study of fuel and impurities species migration and retention in fusion reactors

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Due to increased needs for electricity new energy sources are sought for. Nuclear fusion is one of them. Under the proper conditions the light element nuclei react and convert mass in to energy. To obtain suitable conditions for nuclear fusion light element plasma is heated to  $10^7$  K inside the magnetic confinement devices, mainly in tokamak or stelerator configurations.

One of the most critical issues in the construction of a thermonuclear reactor based on magnetic confinement in the tokamak configuration is the inner wall of the reactor. The inner wall is directly in contact with hot plasma. During the operation of a fusion device, the wall is subjected to a combination of neutron and charged particle bombardment, large and uneven thermal loads, photon irradiation and neutral hydrogen exposure. This leads to erosion, deposition, adsorption of hydrogen and material lattice damage. The processes at the surface of the material or in its bulk lead to accumulation of fusion fuel (mainly hydrogen isotopes) in the vessel walls.

Ion beam analytical (IBA) methods provide an non-destructive tool to perform post mortem analysis of sample materials exposed in experimental thermonuclear reactors. With focused ion beams, we are able to investigate process on micrometer level or in some special cases on sub-micrometer level [1]. Thickness of eroded or deposited layers are determinate with Rutherford back scattering spectroscopy (RBS). The concentration of impurities for elements with  $Z > 10$  is determinate with particle induced x-ray emission (PIXE). While for lighter we employ nuclear reaction analysis (NRA). Mainly the  $D(^3\text{He},p)^4\text{He}$  for detection of trapped deuterium [2].

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## Outdoor radon as a tracer for planetary boundary layer mixing

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Radon gas ( $^{222}\text{Rn}$ ) is an excellent natural tracer for processes in different environmental compartments, such as geophysical processes in the Earth's crust, cave air ventilation and transport of air masses in the atmosphere. The usefulness of  $^{222}\text{Rn}$  as an atmospheric tracer is mainly the result of its properties. It appears in nature from  $\alpha$ -transformation of radium ( $^{226}\text{Ra}$ ) which is present in most rocks and soils. Radon's only significant atmospheric sink is radioactive transformation, and its half-life of 3.82 days is long enough in comparison to atmospheric turbulent time scales, but sufficiently short on the time scales of larger atmospheric processes to constrain concentrations in troposphere to 1–3 orders of magnitude below the surface values. Atmospheric  $^{222}\text{Rn}$  represents an alternative, recently used method for the assessment of atmospheric conditions, more precisely, the stability of the planetary boundary layer (PBL), which plays an important role in the magnitude and time evolution of atmospheric pollution. The aim of the study is to investigate a temporal variability of the outdoor  $^{222}\text{Rn}$  concentration with respect to the PBL evolution on the diurnal time scale.

Outdoor  $^{222}\text{Rn}$  has been measured at two places, the first one located in the Ljubljana basin and the second one in the Vipava valley, characterised by different geogenic radon potential due to different lithology of the surface rocks and sediments, sea and lake sediments and flysch, respectively. Both locations are also influenced by different microclimate, e.g. strong Bora wind in the Vipava valley. Continuous  $^{222}\text{Rn}$  monitoring has been carried out by an AlphaGuard monitor (lower limit of detection  $< 2 \text{ Bq m}^{-3}$ ). The device was set up above the ground at the height of 1.5 m and 4 m in Ljubljana and Ajdovščina, respectively.

Outdoor  $^{222}\text{Rn}$  activity concentration ranges:  $1.9\text{--}83 \text{ Bq m}^{-3}$  in Ljubljana and  $1.7\text{--}55 \text{ Bq m}^{-3}$  in Ajdovščina, respectively. The concentration shows a clear diurnal pattern with a maximum in the morning and a minimum in the afternoon at both locations (Fig. 1). It is the result of mixing processes within the PBL, influencing the dilution of radon concentration during the day and increase of concentration at night due to the formation of a surface thermal inversion. The well-marked 24 h pattern of radon activity concentration occurred under well-mixed conditions at both locations. The lowest outdoor radon activity concentration was observed with the north wind (Bora wind) in Ajdovščina and with the north-eastern wind in Ljubljana.

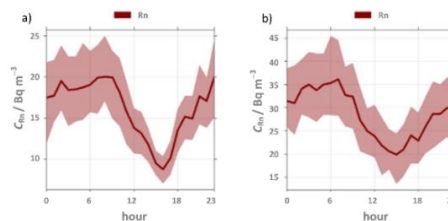


Fig. 1. Average diurnal variation of outdoor radon concentration (mean and 95 % confidence interval in the mean) for a) Ajdovščina, b) Ljubljana.

## Photodegradation of bisphenols F, S and Z in aqueous solution

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Bisphenols (BPs) are used as monomers for the production of polycarbonate (PC), epoxy resins, unsaturated polyester, and polysulfone resins. Among all reported BPs, bisphenol A (4-[2-(4-hydroxyphenyl)propan-2-yl]phenol, BPA) is the most abundant. BPA is classified as a xenobiotic and is harmful to human health due to its endocrine disrupting activity. Several BPA analogs have been produced as a replacement for BPA in various applications<sup>1</sup>. Many BPA analogs, as well as their derivatives, have been found in humans and in the environment, particularly 4-[(4-hydroxyphenyl)-methyl]phenol (bisphenol F, BPF) and 4-(4-hydroxyphenyl)sulfonylphenol (bisphenol S, BPS). They have the potential to exert similar toxic effects because of their structural similarity to BPA and it is important to study their occurrence and cycling in the environment<sup>2</sup>.

Recent studies have reported the photochemical degradation of BPs<sup>3</sup>. In this study, the photodegradation and kinetic profile of BPF, BPS and 4-[1-(4-hydroxyphenyl)cyclohexyl]phenol (bisphenol Z, BPZ) in aqueous solutions using monochromatic UV light ( $\lambda_{\max} = 254\text{nm}$ ) with an intensity of  $8.91 \times 10^{-7}$  Einstein/s and an initial BP concentration of 200 ng/L in milliQ-water is reported. Three different experiments were carried out in an immersion reactor: (UV only and UV/ $\beta$ -cyclodextrin) and photolysis by UV/ $\text{H}_2\text{O}_2$ / $\text{Fe}^{2+}$  (Fenton's reagent).  $\beta$ -cyclodextrin ( $\beta$ -CD, 1:1 molar ratio) was selected since it forms an inclusion complex with BPs and allows interactions with hydroxyl groups, which can increase photooxidation. The Fenton's reagent enhances photodegradation by generating hydroxyl radicals. For the photo-Fenton setup, [Fe (II)] and  $\text{H}_2\text{O}_2$  were added in the reaction mixture in a 1:4 and respectively 10:1 molar ratio to the BPs. The BPs were exposed to UV radiation in time intervals of 10 min to 2 h, which were determined in preliminary experiments.

The analytical method involved solid phase extraction (SPE) of the aqueous aliquot, followed by derivatization with N,O-bis(trimethylsilyl)trifluoroacetamide (BSTFA) and analysis by GC/MSD. All calibration curves showed good linearity ( $R^2 > 0.99$  for 0.14—228.57 ng/L) and LODs were 0.27 ng/L (BPF), 0.3 ng/L (BPS) and 0.07 ng/L (BPZ). Half-lives for the BPF, BPS and BPZ were the shortest when photo-Fenton was applied, followed by  $\beta$ -CD addition and direct photolysis. The enhanced photodegradation in the presence of the Fenton's reagent is likely caused by an increase in indirect photolysis due to generation of free hydroxyl radicals<sup>4,5</sup>.

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## Determining sources of CO<sub>2</sub> in Pisani rov (Postojna cave) using carbon isotopes (<sup>12</sup>C, <sup>13</sup>C and <sup>14</sup>C)

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Karstic caves can represent subterranean reservoirs of CO<sub>2</sub>, which can originate from different sources. Certain environmental conditions can cause transport of cave CO<sub>2</sub> to the open atmosphere. In order to investigate local carbon cycle it is important to determine the sources of cave CO<sub>2</sub> and mechanisms causing accumulation and ventilation of this gas. Beside its importance for the carbon balance assessment, which is one of the important global topics due to the global increase of CO<sub>2</sub> in the atmosphere, is this topic also important from the technical point of view in relation to the determination of soil or ecosystem CO<sub>2</sub> fluxes in karstic areas. Influence of cave ventilation on CO<sub>2</sub> flux measurements and its interpretations should be taken into account at such areas.

Measurements and sampling of soil and cave air were performed in the last hall of Pisani rov and soil above it. Pisani rov is a dead end passage of the Postojna cave system and is closed for the tourist. CO<sub>2</sub> concentration and stable isotopic composition were measured twice a month from October 2014 to September 2015. In addition two samplings for  $\Delta^{14}\text{C}$  in soil CO<sub>2</sub> were performed in winter 2015 (with and without snow cover) and three samplings for  $\Delta^{14}\text{C}$  in cave air (two in winter at the same day as soil air sampling and one in late summer 2015).

Our results suggest that CO<sub>2</sub> represents a mixture between atmospheric CO<sub>2</sub> and CO<sub>2</sub> coming from decomposition of soil organic matter. It indicates that the CO<sub>2</sub> concentration is not directly related to the rate of soil respiration, but it is mostly controlled by the ventilation. Sources such as CO<sub>2</sub> from deep geological origin, decomposition of organic matter in cave sediment and CO<sub>2</sub> coming from tourists or cave animals were found to be not important. Further, results suggest that sources contributing to cave CO<sub>2</sub> (beside atmospheric CO<sub>2</sub>) are decomposition of organic matter at depths where outside low temperatures do not limit the decomposition of organic matter and CO<sub>2</sub> coming to the cave dissolved in percolating water.

The main parameter affecting cave ventilation is the difference in temperatures between outside and cave air. Since the temperature in the cave is relatively constant the main driver is the change of the outside temperature. Two ventilation regimes in the cave can be observed, the summer regime when CO<sub>2</sub> is accumulating and winter regime when cave ventilates. Exceptions to this pattern happened during the winter when temperatures are below 0°C with the snow cover above the cave. At this occasion the rise of CO<sub>2</sub> concentrations in the cave was observed, which indicates that possible exits for cave air, enabling ventilation were closed accumulating of CO<sub>2</sub> in the cave.

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## Comparison of Arugula (*Eruca sativa* Mill.) and Escarole (*Cichorium endivia* L.) Interactions with Foliar- and Root-Applied Platinum Nanoparticles

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Atmospheric deposition of anthropogenic nanoparticle (NP) emissions (e.g. from automobiles and industrial operations) onto edible plant surfaces is a threat to food safety in urban areas. Nanoparticle internalization and translocation from roots to leaves has been investigated, but less is known about leaf to root translocation and leaf-NP interactions. In this study, two widely cultivated and consumed plant species with large leaves and differing foliar surface free energy (SFE; wettability): arugula (*Eruca sativa* Mill.; low SFE) and escarole (*Cichorium endivia* L.; high SFE), were exposed to Pt NPs dispersed in ultrapure water through roots (one application of 1 mg Pt NPs in 20 mL water) or leaves (5 day exposure to 2 µL droplets [5, 50, or 500 mg/L] applied per 0.5 cm<sup>2</sup> abaxial and adaxial leaf surfaces) upon reaching the 5-leaf growth stage. Platinum was ideal for this study because of its low environmental abundance (2.7 ppb) [1], resistance to dissolution, and direct connection to anthropogenic activity (e.g. catalytic converters) [2]. Throughout the exposure period, SFE of foliar-exposed leaves was evaluated by solving a variation of Young's equation based on contact angle measurements from ultrapure water, glycerol, and diiodomethane [3]. Analysis of foliar Pt NP adsorption patterns by scanning electron microscopy showed that Pt NPs appeared in larger amounts and in a more aggregated/agglomerated state on arugula leaves, consistent with the fact that at low SFE, liquid droplets are less likely to spread out and drip off or down the leaf. Platinum quantification of washed roots and leaves with inductively coupled plasma-mass spectrometry also revealed statistically higher leaf Pt concentrations for arugula, and statistically higher root Pt concentrations for escarole at all exposures. Uptake and translocation of Pt NPs from leaves to roots was statistically significant for both plants at a concentration of 500 mg/L ( $p < 0.05$ ). Since Pt is resistant to dissolution [2], the presence of Pt in unexposed plant segments was interpreted as having been in NP form. The results highlight the relevance of foliar SFE in discussions of NP retention by (edible) leaves and demonstrate the possibility for NP uptake and translocation from leaves to roots.

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## Determination of fluorine in vegetation - oxygen bomb combustion vs. alkali metal carbonate fusion

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Fluorine (F) is one of several trace elements receiving much attention owing to its possible harmful effects on health and environment. Small amounts of fluoride have proven benefits for dental health, while continuous exposure to high intakes can result in severe adverse effects in humans (and animals), which include development of dental fluorosis in children or skeletal fluorosis in both, children and adults.

Fluoride emissions represent a threat to vegetation and subsequently entire food chain in many parts of the world. Monitoring of human and environmental load with F is therefore of crucial importance in order to avoid negative impacts of fluoride emissions.

The content of F in samples is determined with fluoride ion selective electrode (F-ISE). Because this electrode measures concentrations of free fluoride ions (F<sup>-</sup>), samples containing bound F must be decomposed first in order to assure release of F from inorganic and organic compounds and formation of F<sup>-</sup>. The most important methods for decomposition of combustible material are alkali metal carbonate fusion and oxygen bomb combustion.

Alkali metal carbonate fusion has been proven to be effective for a variety types of samples, but has one big disadvantage - time of decomposition. For this reason, oxygen bomb combustion has been introduced in our laboratory. This method is widely used for sample decomposition, but there are only few articles from older studies where it has been used for decomposition of samples for subsequent determination of F and those studies do not include analysis of certified reference material (CRM) as a part of a quality assurance system.

The aim of this study was to compare the contents of F determined with F-ISE in CRM (NIST-2695) and some other vegetation samples (spruce needles, green tea and camomile) after total decomposition with oxygen bomb combustion and alkali metal carbonate fusion. The objectives were: (1) check the accuracy of both decomposition methods using CRM, (2) check if CRM's matrix (timothy grass) is representative for other vegetation sample types.

## Stable isotope and elemental characterization of Slovenian milk

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Because of recent development in food labelling and declaration regulations combined with increased consumer awareness towards correctly declared food products, there exists a demand for more sophisticated instrumentation and more appropriate analytical methods which are able to offer better qualitative and quantitative results. Thus stable isotope composition and elemental analysis are becoming an important tool for guaranteeing the unadulterated status, quality and geographical origin of milk and dairy products.

Our work utilises stable isotopes ratios of light elements ( $^{13}\text{C}/^{12}\text{C}$ ,  $^{15}\text{N}/^{14}\text{N}$ ,  $^{18}\text{O}/^{16}\text{O}$ ,  $^{34}\text{S}/^{32}\text{S}$ ) and elemental composition to verify and determine the origin of milk samples available on the Slovenian market. One of the most important tasks of this assignment was to create, implement, update and maintain a database of authentic Slovenian milk samples, which can be used as a tool for classification and verification of Slovenian samples based on regional provenance and to differentiate Slovenian milk from those produce in other European countries. First database includes isotope values of oxygen ( $\delta^{18}\text{O}$ ) in milk, the isotopic composition of carbon, nitrogen and sulphur in casein ( $\delta^{13}\text{C}$ ,  $\delta^{15}\text{N}$  and  $\delta^{34}\text{S}$ ) and the elemental composition of authentic raw milk samples collected two times per year (in summer and winter) during 2012-2014 covering different geographical regions (Alpine, Dinaric, Pannonian, Mediterranean) in Slovenia.

Linear Discriminant Analysis (LDA) was applied to the obtained data set for differentiation of Slovenian milk from the milk produced in other EU countries (Austria, Croatia, Germany, Italy). The best differentiation was observed when summer Slovenian milk from 2013 and 2014 were utilised. A projection of the Function 1 and Function 2 principal components represents 91.6% of total variance, where the former accounts for 71.5% of the variance and the later 20.1%. The most important parameters that contributed in F1 distinctiveness are  $\delta^{18}\text{O}$ , Sr, K, Ca, while F2 is most characterized by  $\delta^{13}\text{C}$  in casein, Zn, Br and  $\delta^{18}\text{O}$ . Furthermore, eleven milk samples, were classified and confirmed to be labelled correctly as "Slovenian milk". Our results showed LDA classification as an effective discrimination and verification tool for confirming correct declaration and provide clear information about geographical origin and authenticity. Information available through our study should be used to increase the transparency of milk and dairy products supply chain. This research represents a part of the ERA Chair ISO-FOOD for isotope techniques in food quality, safety and traceability.

## Mercury isotope fractionation in the Idrija mining region, Slovenia

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Idrija mercury mine is world second largest with 500 years history, and total production of 144.800 tons of mercury, which represents over 13% of the entire world production. During that time, 107.700 tons of commercial mercury have been sold and 37.100 tons of mercury was lost into the environment, which is after 20 years of mine closure still persistent in local environment. Mercury (Hg) is present in two main forms as cinnabar ore (70%) and as native Hg<sup>0</sup> (30%). Nowadays, the main sources of Hg in Idrija are: still active mine ventilation shafts, evaporation of Hg from the heavily polluted surroundings of the former smelting plant, mineralized rock dumps of primary or partially exploited ore, outcrops of the ore deposit, and ore residues treated in various ways. Novel methodologies and approaches developed and used based on identification of mercury isotope fractionation caused by different processes and sources of Hg during formation of Idrija mine in Triassic. This will enable identification of mercury isotope ratios (IR) characteristic for different environmental Hg sources and reconstruction of Hg mass balance in wider Idrija environment, and will significantly contribute to assess dynamics and transformations of mercury between former mining and smelting operations and local environment.

The objective of this research was to study Hg isotopic compositions and evaluate Hg isotopic fractionation of different ores from the mercury mine, processed (retorted) ore, native elemental Hg<sup>0(L)</sup> present in the mine and appeared in near-by Idrija river, and elemental Hg<sup>0</sup>, produced in Idrija smelting plant. Analysis has been done on Cold Vapour Generator system (CVG) coupled with MC-ICP-MS (*Nu plasma II*, Nu instruments Ltd, UK). Initial measurements showed huge difference in  $\delta^{202}\text{Hg}$  values were obtained for elemental Hg<sup>0</sup>, from  $-4.06 \pm 0.19$  ‰ in produced mercury to  $-0.74 \pm 0.12$  ‰ in the native mercury from the mine, whereas the native mercury from the Idrija river presented  $\delta^{202}\text{Hg}$  value of  $-0.35 \pm 0.15$  ‰. Soil core samples from different locations in the mining district were analysed and presented  $\delta^{202}\text{Hg}$  values from  $-1.11$  to  $0.26$  ‰ (2SD = 0.20 ‰). Hg isotope fingerprints in core samples close to the smelting plant show a big difference in comparison with other cores. The results, which give new information about Hg sources in Idrija mining region, will be presented.

## Metallothionein polymorphisms and trace elements in Slovenian mother-child pairs (CROME-LIFE+ and HEALS study)

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Methallothioneins (MT) are metal(oids) binding proteins characterised by low molecular weight (6-7 kDa), high cysteine content (~30%) and high metal affinity [1]. They have several roles in physiological system, especially in metal(loid)s homeostasis and detoxification and cellular oxidative stress protection [1,2]. Human methallothioneins are coded by at least 11 functionally active genes that are located on chromosome 16 and single nucleotide polymorphisms (SNPs) in these genes, could modify proteins functions [3,4].

In present study the data from 178 non-occupationally exposed Slovenian mother-child pairs (mothers: mean age = 38.6 years; child: 7-8 years, 50% females, 2016) was used to estimate possible associations between genotypes of various selected SNPs in *MT* genes (*MT1a*, *MT1b*, *MT1e*, *MT1f*, *MT1g*, *MT1x*; *MT2a*; *MT3*; *MT4*) and trace elements (Hg, As, Pb, Cd, Zn, Cu, Mn, Se).

DNA was extracted from venous blood and used for SNP genotyping by pre-designed TaqMan® assays (Applied Biosystems, USA) and quantitative real time PCR (qPCR), while the concentrations of trace elements were determined in blood and urine samples using an inductive-coupled plasma mass spectrometry (ICP-MS). Obtained significant associations between genotypes and trace elements were further tested by multiple linear regression models for possible confounders (age, gender, body mass index, education, current or past smoking, food consumption, essential element status etc.).

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## Optimization of headspace sampling using Solid-Phase Microextraction (SPME) for analysis of apple aroma compounds

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Solid-Phase Microextraction (SPME) is a simple and efficient solventless sample preparation method, and it is ideally suited for coupling with mass spectrometry (MS). In our study, a dynamic headspace solid-phase microextraction methodology was developed for gas chromatography-mass spectrometry (GC-MS) and gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS) analysis of various aroma compounds in apple distillate samples, for a compound identification and stable isotope analysis that can be used to differentiate between nature and synthetic aroma compounds.

The factors affecting the SPME process, such as fibre coating, sample volume, extraction and desorption time and temperature, were optimised. The effect of these variables on the extraction of active apple aroma compounds and also terpene compounds of commercial apple distillate was studied. The sample vial volume was fixed at 10 ml. Two commercially available SPME fibres (100 µm PDMS and 50/30 µm DVB/CAR/PDMS) differing in the solvent phase coating were tested and compared in this study. The DVB/CAR/PDMS fibre was efficient for all of active aroma compounds under study. On the other hand, relatively low extraction efficiency for terpene compounds was found for both types of fibre. Thus, the DVB/CAR/PDMS 50 µm coated fibre was chosen for further studies. The effect of sample volume (100 µl, 500 µl, 1000 µl and 5000 µl) on absorptivity response and equilibrium was investigated. Sample volume of 1000 µl apple distillate sample in 10 ml vial was chosen. A larger sample volume is preferred for better detection of terpene compounds. Temperature and time are the most important factors that affect the equilibrium of the volatile compounds in the sample vial. Three different temperatures (30°C, 45°C, 60°C) with combination of different exposure times of the fibre to the apple distillate sample headspace for 5, 10, 15, 20, 40, 60, 80 and 100 min was measured using GC-MSD detector response peak area. The results showed that most of desirable compounds with exception of terpene reached their adsorption capacity after 20 min at 30°C. To provide sufficient terpene components extraction, either higher temperature of 60°C with 20 min of extraction, or 30°C with longer extraction time (80 min) is needed. Finally, the desorption parameters – injection port temperature and desorption time, were optimized for the analytes involved. Time of 60 seconds and temperature of 250°C in the injection port of GC-MSD was carefully chosen. Under optimised and consistent conditions, highly consistent results from SPME were obtained.

An optimised methodology is based on DVB/CAR/PDMS coated fibre, headspace sampling mode with sample volume of 1000 µl apple distillate sample in 10 ml vial. A good optimal condition performs the SPME analysis using an adsorption time of 20 min for active aroma compounds and 80 min for terpene compounds at 30°C and desorption time of 60 s at 250°C. In our further research, a developed optimised methodology, will be used for determination of carbon isotopic composition of active aroma and terpene compounds from distillate samples of Slovenian apples. Research is implemented in the framework of Smart Specialization Program: Food for Future.

## Apolipoprotein E genotypes in relation with Hg (MeHg) concentrations in pregnant females

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Apolipoprotein E (apo E, gene *APOE*) is a lipid binding plasma glycoprotein with central roles in lipid and neuronal metabolism. Some researchers point on its metal-binding and antioxidative properties. It has three major isoforms apo E2, apo E3, and apo E4 encoded by alleles  $\epsilon 2$ ,  $\epsilon 3$  and  $\epsilon 4$  respectively. A large number of studies estimated, that isoform  $\epsilon 4$  allele could be associated with various age related disadvantages (cardiovascular diseases, Alzheimer's disease, ect). Individuals with  $\epsilon 4$  variant are also supposed to be more susceptible to metal toxicity, including methyl mercury (MeHg,  $\text{CH}_3\text{Hg}^+$ ). On the other hand, it is believed that apo E is a global activator of innate immune function and its association with higher concentrations of cholesterol, vitamin D and calcium can be beneficial early in life.

The purpose of present work was to estimate relations between *APOE* polymorphisms and concentrations of mercury in pregnant females chronically exposed to low or moderate amounts of Hg through seafood consumption during pregnancy.

We used samples and metal concentration data set of Croatian pregnant females (n=222, aged 19-44y, sampling in 3<sup>rd</sup> trimester) and their newborns (n=176): total Hg and MeHg in maternal hair, urine, milk, peripheral and cord blood. *APOE* was genotyped in archived maternal leukocytes DNA extracts by hydrolysis probes (TaqMan) pre-designed SNP assay for rs429358 and rs7412. Statistics: STATA. EU projects: PHIME, HEALS.

Mothers were divided in *APOE*  $\epsilon 4$  carriers (genotypes  $\epsilon 3/\epsilon 4$  and  $\epsilon 4/\epsilon 4$ ) and  $\epsilon 4$  non-carriers (genotypes  $\epsilon 3/\epsilon 3$ ,  $\epsilon 3/\epsilon 2$  and  $\epsilon 2/\epsilon 2$ ). Among them, we identified 17% of  $\epsilon 4$  carriers. They had significantly higher geometrical means of mercury in: i) blood ( $p=0.0165$ ;  $\epsilon 4$  carriers 2.6 ng/g vs.  $\epsilon 4$  non-carriers 2.0 ng/g), ii) hair Hg ( $p=0.0107$ ;  $\epsilon 4$  carriers 740 ng/g vs.  $\epsilon 4$  non-carriers 475 ng/g), and iii) cord blood ( $p=0.0128$ ;  $\epsilon 4$  carriers 4.0 ng/g vs.  $\epsilon 4$  non-carriers 2.7 ng/g). After taking into account the influence of possible cofounders like seafood consumption, parity, age, body mass index and smoking the observed higher concentrations of mercury in *APOE*  $\epsilon 4$  carriers were no longer significant. Limitations of the study were: too small number of *APOE*  $\epsilon 4$  carriers, low levels of potentially toxic elements and incomplete status of dental amalgams. According to that the positive associations between *APOE* and mercury should be reconsidered on larger population with wider ranges of metal exposure and nutritional status.

## Culturing the diatom *Pseudo-nitzschia* from the Gulf of Trieste for the purpose of transmission electron microscopy and determination of genetic and toxic traits

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*Pseudo-nitzschia* is a large genus of marine pelagic diatoms. Several species of this genus are responsible for harmful algal blooms (HABs) due to the production of the toxin domoic acid, which can cause amnesic shellfish poisoning (ASP). They are recognized as a potential threat to human health and environmental perturbations. The advancements in culturing, identification with molecular techniques, and toxicological analysis, has helped towards an increased understanding of the genus phylogeny and toxic species within it. However, the identification of *Pseudo-nitzschia* species remains a challenge because they are morphologically similar, and advanced methods need to be applied. Fast and reliable techniques such as RNA microarrays and others based on a genomics approach, are a promising way to identify species more quickly and efficiently without the need of culturing. They could be beneficial for routine monitoring of toxic algae, especially when they would enable the precise determination of the algal taxonomic composition. Here I present preliminary work in the investigated locality of Gulf of Trieste. Axenic cultures of *Pseudo-nitzschia* have been established in L1 medium. Species were morphologically and genetically identified, using transmission electron microscopy (TEM) and analysis of nuclear-encoded ribosomal deoxyribonucleic acid regions, namely the ITS1/5.8S/ITS2 region and the large ribosomal subunit (LSU) region, respectively. So far two potentially toxic species, *P. multistriata* and *P. caliantha* have been identified with relatively large confidence, based on a limited number of neutral genetic markers. Sampling is still underway on a monthly basis and so the culture bank is increasing. Besides the species identification we want to detect the seasonal pattern of distinct populations. Domoic acid production will be measured in the future to confirm or deny the toxicity of the strains. This work is going to extend our knowledge of the phytoplankton community in the Gulf of Trieste and provide an understanding of whether a threat of harmful *Pseudo-nitzschia* blooms exists in the Slovenian Sea. Because of heavy maritime traffic and changing environmental conditions in the Gulf of Trieste, a danger of introduced species exists as well. We hope to advance this work with the development of microprobes for *in-situ* sensing of HABs from the *Pseudo-nitzschia* genus in cooperation with foreign researchers.

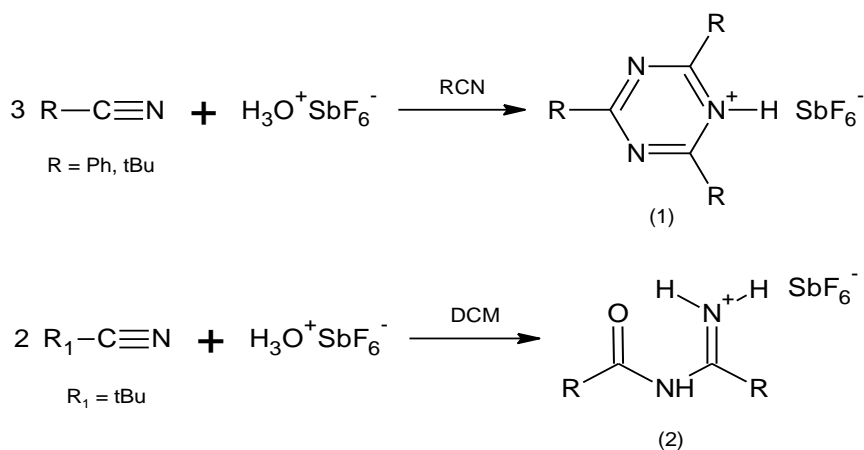
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**H<sub>3</sub>O<sup>+</sup>SbF<sub>6</sub><sup>-</sup> as a reagent in cyclotrimerization of nitriles****Žiga Zupanek<sup>1,2</sup>, Gašper Tavčar<sup>1,2</sup>**<sup>1</sup>*Jožef Stefan Institute, Department of Inorganic Chemistry and Technology, 1000 Ljubljana, Slovenia*<sup>2</sup>*Jožef Stefan International Postgraduate School, 1000 Ljubljana, Slovenia*

Cyclotrimerization of nitriles requires high temperatures and extreme pressures,<sup>[1]</sup> however use of catalysts greatly diminishes the need for extreme conditions. Most commonly used catalysts are SmI<sub>2</sub>/amine,<sup>[2]</sup> trifluoromethanesulfonic acid (TfOH)<sup>[3]</sup> and other Lewis acids.<sup>[4,5]</sup> While reaction conditions and yields are well documented, the mechanism of conversion is still relatively poorly investigated.<sup>[3,6]</sup>

Focus of our research was the use of strong Lewis acids MF<sub>5</sub> (M = As, Sb, Nb, Ta) and their products with different nitriles (R–CN). The system was investigated and reactive species were identified as well as different products. One of the obtained results was 2,4,6-trisubstituted-1,3,5-triazinium cation (1) which is a product of aforementioned cyclotrimerization. In order for reaction to proceed acidic proton (H<sup>+</sup>) is required in combination with weakly coordinating MF<sub>6</sub><sup>-</sup> moiety. Further optimization yielded easy-to-handle solid reagent H<sub>3</sub>O<sup>+</sup>MF<sub>6</sub><sup>-</sup> (M = As, Sb, Nb, Ta), which was found to produce equal results. Reaction takes place with liquid nitrile in inert conditions at room temperature, where nitrile also acts as a solvent. In addition, co-product competing to the process of 1,3,5-triazine formation was also prepared. Dissolution of 2,2-dimethylpropanenitrile (tBuCN) and H<sub>3</sub>O<sup>+</sup>SbF<sub>6</sub><sup>-</sup> in dichloromethane (DCM) yielded scarcely soluble 1-[(2,2-dimethylpropanoyl)amino]-2,2-dimethylpropaniminium cation (2) which is a dimer of two starting nitriles and corresponding anion. Our results will further elucidate the process of acidic activation of nitriles and formation of 2,4,6-trisubstituted-1,3,5-triazines.



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## Relationship between microbial communities and mercury species in the seawater of the Central Adriatic Sea

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Microbial processes in seawater and sediments can convert inorganic mercury into toxic methylmercury (MeHg). The objective of our research is to identify relationship between microbial abundance and mercury species in the Adriatic seawater. Samplings were performed aboard the research vessel Bios Dva from February 2014 to December 2015 in the Central Adriatic Sea. Research was constrained to five sampling stations in transect from the coastal Kastela Bay to the open sea island of Vis. Seawater was sampled for the determination of total mercury (THg), dissolved gaseous mercury (DGM), methylmercury (MeHg) and microbial species in Adriatic coastal and open waters. Plankton samples for the determination of THg and MeHg was collected using vertical towing nets.

The highest THg concentrations in seawater (4.58-27.8 pmol/L) are found in the Kastela Bay, which was affected by previous contamination from chlor-alkali factory. THg values are the lowest in the pristine environment of the island of Vis (0.69-5.48 pmol/L). DGM always shows lower values in the pristine environment (0.11-1.23 pmol/L) than in contaminated coastal stations (0.16-1.75 pmol/L). MeHg concentrations range from 0.05-0.17 pmol/L for all stations, with the highest values found in the Kastela Bay. The average percentage of THg present as MeHg is low (2.23%) indicating deficiency of mercury methylation or high MeHg demethylation rates. Mercury fractions (THg, DGM and MeHg) are significantly correlated with the total bacterial abundance, number of picoeukaryotes, and the number of cyanobacteria from the genus *Prochlorococcus* (Spearman Rank Order Correlation,  $P < 0.01$ ). In addition, THg and DGM are correlated with the number of cyanobacteria from the genus *Synechococcus* (Spearman Rank Order Correlation,  $P < 0.001$ ). These correlations indicate association of mercury species with the smallest members of the marine microbial community, and possible mercury transformations in the water column by the autotrophic picoplankton.

The highest average THg concentrations in plankton are found in the Kastela Bay (1.69 and 0.91 nmol/g dry weight for 53 and 200  $\mu\text{m}$  fraction, respectively), while the lowest values are found at the Split Channel station (0.29 and 0.27 nmol/g dry weight for 53 and 200  $\mu\text{m}$  fraction, respectively). The MeHg concentration are significantly higher ( $t$ -test,  $P < 0.001$ ) in the 200  $\mu\text{m}$  fraction, compared to 53  $\mu\text{m}$  fraction (on average 59.4 and 22.6 pmol/g dry weight, respectively). These results show biodilution effect of THg concentrations in plankton, which is best observed in the Kastela Bay. On the contrary, MeHg bioaccumulation along trophic levels is demonstrated through significantly higher MeHg concentrations and MeHg percentage in 200  $\mu\text{m}$  fraction, compared to 53  $\mu\text{m}$  fraction.

**Informacijske in komunikacijske tehnologije (Information  
and Communication Technologies)**

## Fall detection watch for independent living of the elderly

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The developed world is facing the problem of aging population. Better living conditions, improvements in food production, and advances in medicine have drastically increased living expectancy. On the other hand, natality is falling. This results in an upside-down demographic pyramid, and, as a consequence, an imbalance between the number of elderly that require some form of care or assistance and people who can assist them. Introduction of ICT technologies is promising to provide better care for the elderly and to prolong their independent living, at the same time reducing the burden of the carers and the health system.

We propose a state-of-the-art solution on a wristwatch that monitors user's actions and automatically calls for help in case of detected danger. The solution proposed currently supports three different standalone android watches (commercial products) that have in-built GSM, GPS, and accelerometer. Optionally, two models also have a heart rate sensor that can increase the depth of information provided by the watch. One of the watches is also water resistant and can be charged by magnet charger – which is important; majority of elderly have bad eyesight and it is hard for them to charge the device over a standard microUSB without using glasses.

The main feature of the watch is an automatic fall detection algorithm that detects falls and other dangerous situations (example: car crash). The algorithm monitors accelerations and detects fall like motion when fall occurs. Because watch is usually worn on wrist, there can be many fall-like motions during different activities. To prevent false alarms, a 20s period after the perceived fall is also monitored. If there is no substantial motion afterwards, the system interprets this as a fall and calls for help. The rationale behind this implementation is that if the user can move after the fall, he can press one button to call for help manually.

To detect other potentially dangerous situations, the watch also monitors general daily activities of the user and compares them to the last 10 days. This allows the system to detect unusual situations. For example, if the user is usually going for 2 hours walk after lunch each day and then one day he is sleeping whole day in bed, the watch will detect this and alert the carers that something unusual is happening.

People suffering from dementia sometimes leave home for a walk and get lost, perhaps ending up several kilometres away from their home and have no memory on how to get back. Thus, the watch also offers the ability to get the user's location in case of such emergency. Due to privacy concerns, the user or his legal representative have to agree with this and location can only be retrieved in case of emergency.

The watch is managed through a web portal that has the access to all watch information. Most of the watch functions can be managed remotely, such as changing phone numbers in case of emergency (carer or a call center), modifying the thresholds for fall detection algorithm, or setting reminders and notifications. To preserve the user's privacy, the portal distinguishes between multiple roles, i.e. informal or formal carer, administrator, etc. Each user (the elderly) can then be assigned a carer (either formal or informal) and only that carer can then access his information. Additional scheduling tools are also available for formal carers in order to ease the management of home visits.

## Fitts' Law for Human-Human Collaborative Reaching Task

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There is an ongoing trend in robotics for the robots to be placed outside their protective cages to work alongside humans. Furthermore, the robots and humans should work together, achieving better performance and ergonomics. In the field of neuromechanics, several studies [1][2][3] investigated human collaboration while executing a physically interactive task. In a study of Ganesh, G. *et al.* [1], multiple pairs of subjects were connected through a pair of haptic robots in an arm reaching task. The subject pairs participating in this study were unaware of the “algorithm” that governed the haptic feedback interface they felt. In other words, the participants were unaware that they were being coupled between each other. This study demonstrated that physical interaction between the partners results in an improved performance of both partners. However, they did not address how the interaction affects partners that are sensomotorically aware of each other and physically coupled by a rigid object. In our study we address this question by having subjects aware of their interaction with the other partner. Subject pairs (10 male participants) were coupled with a metal rod which had a cylinder perpendicular to the middle of the rod as shown in Fig. 1. The goal of the subject pair was to hit an appearing target on the screen with the cylinder as fast as possible. Subjects were also instructed not to talk to each other in order to focus their attention on visual perception and haptic feedback. Analysis of the data acquired by our experiment shows that the reaching motion of the subject pairs can be sufficiently described by a well-known speed-accuracy trade off model, i.e. Fitts' law [4] which was primarily used for the single hand reaching tasks. Specifically, the time needed to hit a target for a human pair follows the same principles as found in a single-person reaching tasks. For our future work, we aim to exploit our experimental findings to improve the control algorithms for robots in a human-robot cooperative setups. This will increase efficiency in a human-robot cooperative scenario and potentially enable the human partner to improve his/hers task performance skills.

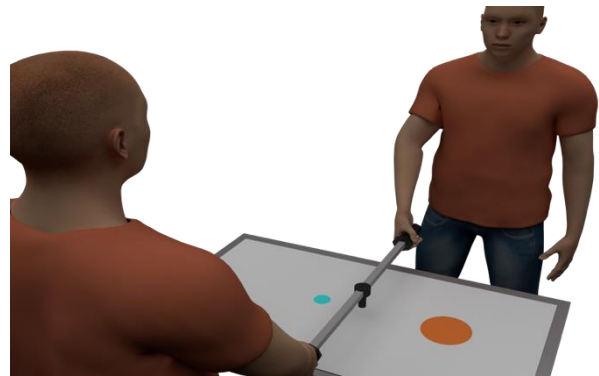


Figure 1: Experimental setup.

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## Ankle Exoskeleton with a Quasi-Passive Clutch

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Due to recent technology advancements and increased component availability, exoskeleton research is now a hot topic. Numerous exoskeletons already exist [1]. Among these, passive exoskeletons offer some advantages over active solutions, e.g., lower weight (no big motors or batteries). They use springs to store energy passively instead of using motors and batteries to actively input power into human joints.

Our work focuses on research of an exoskeleton that will assist the user in a quasi-passive way that uses motors only to change the state of the device (e.g. to close a clutch). In this case, by utilizing an elastic element in parallel with the human calf with a clutch [2], so that the device can assist the calf muscles and reduce their efforts, thus reducing the human flat terrain walking effort.



Figure 2: The 2<sup>nd</sup> prototype.

Our first prototype [3] utilized a completely mechanical clutch (inspired by the device in [2]). We tested it in a quantitative cross-over study comprised of 4 young individuals under laboratory conditions. The users showed a reduced walking effort if the spring of correct stiffness was used and if the clutch operated smoothly with a correct timing. By measuring the oxygen consumption, an effort reduction of 10% was observed in the best case, compared to normal walking. Still, we found several areas of improvement like timing issues and non-smooth clutch operation which all reduce the devices effectiveness. Both problems were improved in the second prototype (shown in Fig 1) where a small servo motor was added to the clutch to help (dis-)engage the spring. The timing is dictated by a heel-down switch activation. The second prototype was tested in qualitative crossover study [4] comprised of 7 people. Each user used the exoskeleton for a time period under different conditions and expressed his observations in a qualitative oriented questionnaire. Its results positively graded the exoskeletons operation and showed that most user did seem to feel an effort reduction.

One way to improve the current design (2<sup>nd</sup>) is by weight reduction. Its current weight is around 1.2 kg which stems mainly from the stainless steel frame. Its comfort is also not yet high enough which was pointed out in the questionnaire. Both problems also mask the feeling of effort reduction on the user. These remarks, including findings from both studies and the development experience gained, will serve as a basis for the development of an improved third version of the quasi-passive ankle exoskeleton.

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## Arm-exoskeleton control based on muscular manipulability

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Robots that collaborate with humans have been around for a while and are gaining in popularity in the recent years. An example of such robots are exoskeletons, which encase the human body and provide assistance to human motion [1].

Most of the current control methods focus on rehabilitation or power-augmentation, be it for medical, industrial or military use. In rehabilitation, the goal of the exoskeleton is to simply perform repetitive motion, replacing the work of a physiotherapist. In case of power-augmentation the exoskeleton robot needs to either help with the motion of the impaired or augment the capabilities of the able-bodied humans. This power augmentation is usually uniform and it doesn't take into account the configuration of the human limb.

We propose a control method based on human muscular force manipulability. In robotics, force manipulability describes how the end-effector position and orientation can change in a given configuration of the robot [3]. This manipulability measure is presented by an ellipsoid, whose major axis represents the direction in which the robot can exert the highest force. We humans however don't have electric motors in our limbs, they are instead driven by muscles which wrap around the joint and are attached to the bone. Contracting the muscles creates a torque on the joint and consequentially a movement of the limb. Taking into account the Hill's muscle model [4], which treats the muscle as a spring-damper system we then expand the force manipulability measure. This muscular force manipulability measure now describes how arm muscle forces relate to forces exerted by the hand in a given configuration of the human arm. This is then incorporated in an exoskeleton control method so that the exoskeleton provides more assistance in low manipulability direction in which the human can't exert high forces, compared to the high manipulability direction in which the human is naturally stronger. This method effectively reduces the effort when the human performs tasks in the directions of low manipulability.

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## POS tagger and lemmatizer evaluation: A TextFlows open science approach

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Part of speech (POS) tagging (assigning the word class to a word) and lemmatization (converting the word to its base form) are core techniques used in natural language processing (NLP) and text mining. Therefore the performance of POS taggers and lemmatizers is important and can have a significant impact on the success of NLP and text mining tasks where these operations are used. Over the years, many POS tagging and lemmatization algorithms have been developed, which are publicly available in open source natural language processing libraries. Open source libraries provide the researchers with accessible NLP tools, but further work on evaluating these tools is still needed, since there is insufficient documentation on the comparison of different POS tagging and lemmatization tools in terms of their effectiveness.

For our research we conducted an experimental evaluation of several publicly available open source POS taggers and lemmatizers on a number of annotated evaluation corpora. Several POS taggers were evaluated and the influence of various factors, such as training corpus length, training corpus genre and the use of pretrained models has been tested. Results have shown non-linear dependence between the size of the training set and the accuracy of the POS taggers, domain-specificity of POS taggers and that the use of pretrained models is not always appropriate. In lemmatizer evaluation, we have shown that preprocessing steps, such as conversion of text to lowercase, have a significant influence on the performance of some lemmatizers. In extrinsic evaluation, where the performance of the tool is measured indirectly (in the context of a larger text mining task), we tested the POS taggers' influence on the lemmatization and gender classification tasks, while lemmatizers and stemmers were evaluated through text categorization.

The experiments were conducted in the TextFlows platform, which is a cloud-based web application for composition, execution and sharing of interactive text mining workflows. The POS tagger and lemmatizer implementations in this online platform enable transparent and reproducible results, reusability of the workflow components for new tasks and provide precomposed workflows for algorithm comparison and evaluation, enabling future algorithms to be tested in the same environment.

## Statistical Generalization of Robot Movement in Autoencoder Latent Space

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Robots have started to emerge in different environments, like for example in households and medical care. In such environments they cannot be preprogrammed for all possible tasks. One solution is to equip the robots with the ability to learn, so they can adapt their behaviour to ever changing environments. One of the learning approaches is imitation learning, where a robot is given human demonstrations of the desired task execution. Typically using several demonstrations trajectories, the robot can extract suitable parameters to generate movement commands for its own motion. We used imitation learning to teach a robot to accurately throw a ball. In this case the robot is given a set of example throws and information where the ball has landed. The landing positions are used as task parameters. For every new target position, the robot should compute a new arm movement that is similar to the example movements and results in the ball hitting the target. Robot movement trajectories are described in joint coordinates. In our work we applied deep autoencoders to learn a representation of robot movements in latent coordinates. Latent spaces are useful because they provide a representation of robot movement in a lower dimensional space. An autoencoder is a neural networks made of an encoder and decoder part. The encoder part takes as input a configuration on the robot trajectory in joint space. The data are encoded through layers of the encoder network, where each layer has less neurons than the previous one. From the latent space the decoder network can transform latent space coordinates back to the original joint space. An autoencoder is usually trained using backpropagation.

In our research, we applied a deep autoencoder to lower the dimensionality of robot joint space. Statistical learning is applied to latent space representations to compute an optimal trajectory to throw a ball at a given target. In the first step, the example trajectories are transformed to their latent space representations and encoded with dynamic motion primitives (DMP). For every new throw, new DMP parameters in latent space are then computed with Gaussian Process Regression (GPR) or Locally Weighted Regression (LWR). From the computed DMP parameters, the trajectory that can be executed by a robot can be computed using the decoder part of the autoencoder.

The proposed method was evaluated in simulation of a three degrees of freedom planar robot, throwing a ball at target located at different horizontal and vertical positions. Generalization of robotic throws was performed using LWR and GPR. We compared the performance of statistical learning in the original robot joint space and in latent space. Statistical learning in the original joint space was in comparison with learning in latent space computationally slower, but with higher accuracy. The best accuracy was achieved with GPR in joint space.

## Using text mining techniques to maintain translation memories

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In this paper, we explore the use of text mining techniques for translation memory maintenance. Language service providers often have large databases of translations, called translation memories, which have been in use for a long time leading to a slow population of the translation memory with other domains (i.e. adding financial content to a technical domain translation memory). To our best knowledge, no tools exist that would effectively separate the content of a translation memory according to different domains. Having the ability to extract individual domains from low-quality translation memories could mean a significant benefit to language service providers looking to utilize modern translation methods, such as machine translation and automated terminology management. In the first stage, we used OntoGen, a semi-automatic ontology building tool, to separate the segments in the translation memory according to domains. In the second stage, we wanted to test whether we could use OntoGen's topic keywords as shortcuts for building classification models— the reason for this being that manual annotation is costly and time consuming. If the topics extracted with OntoGen are accurate enough, then we could potentially skip the manual annotation phase of text classification, thereby significantly speeding up the process. We successfully managed to build an ontology of the translation memory, but the boundaries between some topics were relatively vague. One reason for this is that we had to deal with sentences – as opposed to larger blocks of text – which are difficult to classify. Nevertheless, the results of the ontology creation were promising with manual evaluation showing that around 4 in 5 strings were assigned a correct label. The results of the second stage were less clear - the accuracy did significantly improve compared to the majority class classifier, but did not reach levels where it would be deemed useful in a professional language service provider environment.

**Nanoznanosti in nanotehnologije (Nanosciences and  
Nanotechnologies)**

## Potential new *Dickeya* sp. causing soft rot of *Phalaenopsis* orchids and bacteriophage biocontrol options

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Bacterial soft rots represent a serious limitation to the production of ornamental and others horticultural plants world-wide e.g. potatoes, tomatoes and orchids. There are currently no effective chemical agents for the soft rot disease, and this results in significant economic losses. The aim of our study was to isolate and characterize bacteria causing soft rot of orchids (*Phalaenopsis* sp.) and to investigate bacteriophages as biocontrol agents for their management.

Bacteria isolated from diseased tissues of *Phalaenopsis* orchids from a commercial production site were identified as *Dickeya* spp. based on morphological characteristics, partial sequencing of 16S rDNA, *fliC* and *dnaX* along with selected biochemical tests. However, none of the performed tests was able to resolve classification to a species level. Therefore, genomes of two representative *Dickeya* spp. isolates were sequenced using Ion Torrent technology, which has resulted in two draft genomes. As part of a comparative genomic study of genus *Dickeya*, average nucleotide analysis (ANI) and multilocus sequence analysis (MLSA) on six housekeeping genes were performed, placing the newly sequenced *Dickeya* isolates along with strains MK7 and NCCPB 3274 (isolated from water and an ornamental plant, respectively) as a new species within the *Dickeya* genus. To confirm the observed taxonomic and phylogenetic position of the putative new *Dickeya* sp. the phenotypic analysis was performed. The vast majority of the previously determined *Dickeya* virulence genes could be found in the core genome of the potential new species. Furthermore, some novel genes and genetic were identified including secondary metabolite biosynthesis pathways. Aggressiveness of the bacteria was tested phenotypically on the model plants, Belgian chicory and potato tubers, exhibiting extreme maceration potential of the new *Dickeya* isolates. Beside, inoculation of the viable potato plants was performed, showing the bacteria ability to survive and spread through the plant tissue. On the other hand, possible approaches for the *Dickeya* biocontrol were studied. Bacteriophages effective against new *Dickeya* strains were isolated from the diseased orchids and sewage water. Three different groups of bacteriophages were identified, each from different Caudovirales family. All bacteriophages were lytic and specific for the genus *Dickeya*, therefore represented suitable candidates for phage biocontrol. Furthermore, host range profile confirmed differences among bacterial isolates in the potential new *Dickeya* sp., indicating high in-species phenotypic diversity.

## In-situ observations of the growth of the gold nanoparticles

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Gold nanoparticles are versatile material, which is among many others applications also used in experimental cancer treatment where gold nanoparticle's photothermal effect [1] is employed. For that reason gold nanoparticle's nucleation processes and chemical reaction kinetics need to be well understood in-situ in liquid at the elevated temperature conditions [2]. In our experiment 1.5 mM water solution of gold(III) chloride trihydrate (chloroauric acid) as source of gold was used. The experiment was performed using Jeol JEM 2100 transmission electron microscope (TEM) operated at 200 kV combined with the liquid cell. The sample was observed at an electron dose of  $10^8$  Gy/s. Firstly the sample was observed for several minutes at the room temperature (25 °C), proving the solution is stable at these conditions. After that the sample was heated to 50 °C. After 30 s 5-10 nm sized nanoparticles (NPs) started to appear. The NPs grew for a period of 2.5 min and at this point reached the final size of 30-60 nm. After that gold monomers grow around NPs for further 3 min. In the final the stage: NPs particles did coalesce in a larger individual clusters. Selective electron diffracting analysis proved the face centered cubic crystal structure. We are suggesting that the formation of gold nanoparticles is a 4-step process. First step is the formation of seed particles, which could be explained by partial reduction of the gold precursors. This is followed by the growth of the golden hydroxide around the seed particle. In the third and fourth step all the remaining gold is reduced, which results in the inside-out growth and coalescence of the NPs.

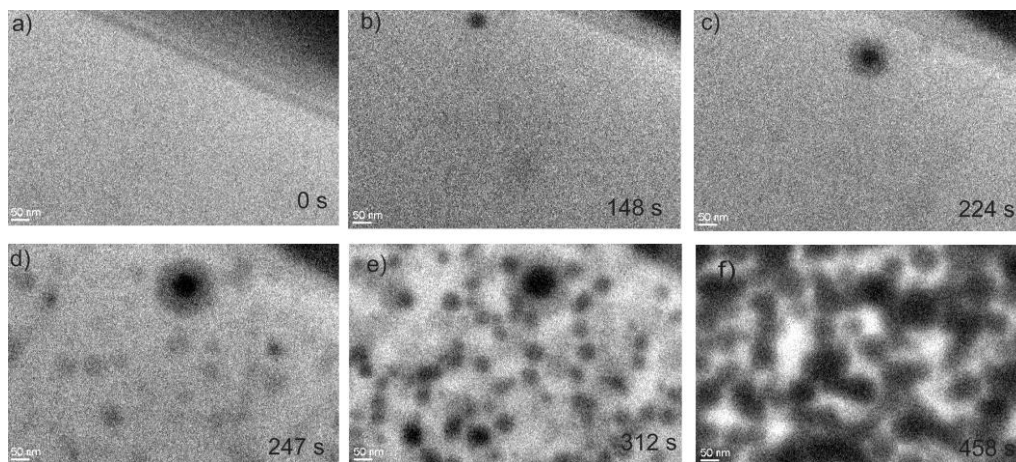


Fig. 1. Nucleation and growth process of Au nanoparticles from  $\text{HAuCl}_4$  water solution during the heating to 50 °C. a) The solution before heating was applied, b) first seed particles appear, c) around seed particles golden hydroxide grew, d) new seed particle appear, e), new nanoparticle continue to grow f) seed particles coalesce in the larger particles

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## Novel approaches for detection and quantification of genetically modified organisms (GMOs)

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Quantification of genetically modified organisms (GMOs) in food and feed products is often required for their labelling or tolerance thresholds. Today the golden standard for testing of specific nucleic-acid sequences derived from genetically modified organisms (GMOs) is real-time quantitative PCR (qPCR). However, with the increasing number of GMOs, qPCR is becoming barely time and cost-effective. Furthermore, qPCR can be limited by its sensitivity to the inhibitors that can be frequently co-extracted with the nucleic acids from complex matrices and by a significant bias when the target is present at low concentrations in a background of high levels of non-target nucleic acids.

To tackle this issues, four droplet digital PCR (ddPCR) multiplex assays, two quantifying 12 in EU authorised GM maize lines [1] and two quantifying 11 in EU authorised GM soybean lines [2], have been developed. Enabling direct quantification of 12 maize and 11 soybean lines in just four reactions. Performance was assessed for the critical parameters, including limits of detection and quantification, trueness, repeatability, and robustness. Trueness was determined on a number of proficiency programme and real-life samples. Moreover, potentially significant improvement in cost efficiency was demonstrated.

With the increased use of authorized genetically modified organisms (GMOs), especially in feed products, the possibility of intentional or unintentional presence of unauthorized or unknown GMOs (UGMOs) is also on the rise. Thus, a novel GW technology coupled with NGS called amplification of linear-enriched fragments (ALF) [3], has been developed. The approach was tested on a complex sample, containing four GMOs of different concentrations, allowing the identification of GMOs even when present in a low concentration. ALF eliminates drawbacks, such as random start of DNA amplification and semi-nested PCR, of previous GW strategies. NGS is ideally suited for sequencing all amplified fragments in a mixture. Furthermore, a first outline of an automated, web-based analysis pipeline for identification of UGMOs containing known screening elements has been developed. To prove the power of the designed pipeline to identify UGMOs, a complete sequence of one GMO in the sample was unknown, mimicking a UGMO. All four GMOs in the sample were identified, thus proving the detection of UGMO.

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## Glucosamine prevents cell mediated cytotoxicity of natural killer cell line NK-92

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Natural killer (NK) cells are a subset of cytotoxic lymphocytes of the innate immune system, which have important role in early defense against transformed and virus-infected cells. After recognition of an appropriate target cell, an immunological synapse is formed between the NK cell and the recognized target cell, followed by clustering the cytotoxic granules around the microtubule-organizing center (MTOC). The main components of cytotoxic granules, perforin and the granzymes, are then released from the NK cells, resulting in apoptosis of the target cell.

Glucosamine is a component of natural polysaccharide mixtures. It is used extensively for the management of pain in osteoarthritis, but was observed to affect different cellular processes. For example, it has long been known that glucosamine affects NK cells activity, but the mechanism of action is still unknown. In order to analyze the cytotoxic process, we investigated the NK-92 cell line that possesses strong cytotoxic activity against the K562 cell line. We analyzed cytotoxicity of direct co-culture of NK-92 and K562 cells by flow cytometry, using two labelling dyes, DiOC<sub>18</sub> to distinguish cells, and propidium iodide to detect dead cells. For activation of NK-92 cells we used different concentrations of interleukin 2 (IL-2). We showed that high concentration of IL-2 in the cell's growth media transiently increase the ERK phosphorylation. ERK phosphorylation was accompanied by polarization of granules with perforin towards the immunological synapse. In order to study the impact of glucosamine on migration of granules, NK-92 cells were pre-treated with different concentrations of glucosamine. A dose-dependent decrease in cytotoxicity of NK-92 towards K562 cells was observed. Moreover, localization of perforin migration showed that addition of glucosamine to the medium induced redirected traffic of granules, disabling cytotoxicity towards the target cells. In addition, glucosamine was found to change dynamics of ERK phosphorylation.

## Synthesis of SrTiO<sub>3</sub> Particles: Tailoring the Shape, Size and Crystal Growth Orientation

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Control of the size, shape and crystal growth orientation of multifunctional materials is of high interest, because these characteristics influence the material's electrical, magnetic and optical properties. SrTiO<sub>3</sub> particles were identified as good photo catalyst. SrTiO<sub>3</sub> particles could be also used as a substrate for epitaxial growth of other perovskites. In recent years, a number of synthesis techniques have been developed to fabricate SrTiO<sub>3</sub> crystals (e.g. molten salt synthesis, hydrothermal synthesis, sol-gel method, co-precipitation) [1]. SrTiO<sub>3</sub> is widely known ABO<sub>3</sub>-type perovskite. Synthesis of anisotropically shaped SrTiO<sub>3</sub> particles is still a great challenge, because these particles tend to grow in cube- or sphere-like rather than in anisotropic shape due to the high symmetry of their crystal structure. Different approaches to control the shape and size of ABO<sub>3</sub> – type perovskites were reported [2], including topochemical conversion [3], [4]. Desired template for the preparation of anisotropic SrTiO<sub>3</sub> particles should exhibit anisotropic shape and possesses perovskite units with corner-sharing [TiO<sub>6</sub>]<sup>8-</sup> octahedra. For our study the plate shape and cubic crystal structure are preferable. More possibilities on the selection of the template exists, however we decided to use Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> platelets as template particles since it can be easily synthesized in the shape of plate by molten salt method. In this research the topochemical conversion was performed under hydrothermal conditions. To the best of our knowledge, the hydrothermal growth of SrTiO<sub>3</sub> on the Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> plates and their complete conversion in to SrTiO<sub>3</sub> has not been reported yet. Reaction parameters (e.g. temperature, time, reactant concentration, NaOH concentration and Sr/Ti ratio) were studied and different morphology of SrTiO<sub>3</sub> particles was observed. Different mechanism pathways based on the selection of reaction parameters will be discussed.

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## Colloidal stabilisation of barium hexaferrite nanoplatelets in different media

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Barium ferrite, BaFe<sub>12</sub>O<sub>19</sub>, is a hexagonal ferrite, which is distinguished from other ferrites by a large magnetocrystalline anisotropy and high intrinsic coercivity. Recently there has been an increasing interest for biomedical applications of hexaferrite nanoparticles, for instance in hyperthermia<sup>1,2</sup>. For such application, a material has to be colloidally stable in a given media. Stabilizing molecules that can provide steric repulsive forces, electrostatic repulsive forces or both can provide for long-term stability. Different molecules have been used in water-based ferrofluids, including small molecules (citric acid - CA), polymers (polyethyleneglycol), polysaccharides (dextran), polypeptides, and surfactants (cetyl trimethylammonium bromide).

In our research, we aim to modify the nanoplatelets surface to ensure their colloidal stability and biocompatibility. Here we studied barium hexaferrite nanoplatelets substituted with Sc<sup>3+</sup>, which were synthesized using hydrothermal synthesis<sup>3</sup>. The nanoplatelets were coated with silica. Namely, silica coating provides reactive –OH surface groups, that can be used for further functionalization. CA was adsorbed on the hydrothermally synthesised nanoplatelets. In a subsequent reaction, particles were coated with silica using a modified Stöber process<sup>4</sup>. The silica coated nanoplatelets were further grafted with dextran that was previously reacted with (3-Glycidyloxypropyl)trimethoxysilane (GLYMO-dextran). The efficiency of the colloidal stabilisation was tested in different media such as deionised water (dH<sub>2</sub>O), phosphate buffer (PBS) and fetal bovine serum (FBS). The colloidal stability of the nanoplatelets in dH<sub>2</sub>O was achieved after the adsorption of CA. The nanoplatelets remained stable in dH<sub>2</sub>O for long periods of time and through all the following coating procedures. However, a long-term colloidal stability in PBS was only achieved after grafting nanoplatelets with GLYMO-dextran, which provided steric repulsive forces. When nanoplatelets grafted with GLYMO-dextran were introduced into FBS the suspension remained stable for up to 5 days. This represents a substantial progress in the colloidal stabilization of highly magnetic nanoplatelets and a step further to their possible application in biomedicine.

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## Lipid droplets are sources of pro-tumourigenic eicosanoid lipid mediators in breast cancer cells

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Most eukaryotic cells contain lipid droplets (LDs), triacylglycerol (TAG)-rich organelles surrounded by a phospholipid monolayer with embedded LD-associated proteins. Aggressive cancer cells scavenge extracellular unsaturated fatty acids (FAs) and esterify them into TAGs in LDs. The stored FAs are released from TAGs through lipolysis, mediated by cytosolic lipases, including adipose triglyceride lipase (ATGL). The released FAs provide building blocks for membrane synthesis and fuel for mitochondrial energy production, but may also trigger signalling pathways. Recently, ATGL-mediated LD lipolysis was shown to provide precursors for the synthesis of lipid signalling molecules in activated human mast cells. However, it is not clear whether LD-provided FAs may also serve as precursors for lipid mediator synthesis in other cells, including cancer.

We have recently found that the extracellular enzyme secreted PLA<sub>2</sub> (sPLA<sub>2</sub>) releases unsaturated FAs, including arachidonic acid (AA), from the plasma membrane of breast cancer cells and induces the formation of cytosolic LDs enriched with polyunsaturated FAs (PUFAs). Previous studies have shown that AA released by sPLA<sub>2</sub> may be used for the synthesis of eicosanoids, such as prostaglandin E<sub>2</sub> (PGE<sub>2</sub>), which promotes inflammation and cancer cell proliferation. We hypothesized that sPLA<sub>2</sub>-induced LDs enriched with PUFAs are a source of AA for PGE<sub>2</sub> synthesis in breast cancer cells. We first confirmed that sPLA<sub>2</sub> stimulates PGE<sub>2</sub> release from breast cancer cells in parallel with the induction of LD formation. To find out if LD lipolysis is important for the ability of sPLA<sub>2</sub> to induce PGE<sub>2</sub> production we suppressed ATGL expression by siRNA silencing. ATGL depletion led to a significant inhibition of PGE<sub>2</sub> release in sPLA<sub>2</sub>-treated cells, confirming that ATGL-mediated LD breakdown provides AA for PGE<sub>2</sub> synthesis in breast cancer cells. In summary, we identify LDs as novel sources for eicosanoid production and propose that targeting LD lipolysis provides new opportunities for fighting cancer.

## Cathepsin C is critical for the release of other cathepsins from lysosomes in leucyl-leucine methyl ester-triggered apoptosis

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Lysosomal detergents are lipophilic bases, which remain captured in acidic vesicles and can induce lysosomal membrane permeabilization (LMP). LMP is a point-of-no-return, followed by cell death, usually mediated by cathepsins. L-Leucyl-leucine methyl ester (LLOMe) is synthetic lysosomotropic detergent, which showed extremely good results in preventing the graft-versus-host disease in vivo by successfully eliminating immune cells of the donor. The mechanism of compound action is dependent on the transferase activity of cathepsin C, which leads to the formation of LeuLeu oligomers with membranolytic potential, leading to lysosomal leakage, release of cathepsins into the cytosol and triggering of cell death. However, the exact mechanism of action and interconnection between different cathepsins were never clarified.

Using several different cell lines containing different levels of individual cathepsins we have shown that incubation of cells with LLOMe leads to a very early increase in lysosomal pH, indicative of LMP, followed by release of cathepsins into the cytosol and subsequent cell death. Both the increase in lysosomal pH and cell death could be prevented by the cathepsin C selective inhibitor GlyPheDMK. In contrast, the broad spectrum cathepsin inhibitor E64d, efficiently prevented cell death, but only partially lysosomal pH increase. According to the results we can speculate that cathepsin C is required for the exit of lysosomal proteins, including the cathepsins, into the cytosol, where the latter then trigger cell death in the next step. This mechanism was confirmed using primary cells double deficient for cathepsins B and L, and cells deficient for the major cytosolic inhibitor of cathepsins stefin B. The different sensitivity of cells to LLOMe is a combination of the levels of different cathepsins, stefin B, as well as other apoptotic proteins, including Bcl2 homologs.

## 3D printing biomaterials for regenerative medicine

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There have been many advances in the field of 3D printing or additive manufacturing in the last years, and particularly 3D printing living organs is a hot topic. While directly printing living organ is not (yet) possible, researchers in the field of tissue engineering are using biocompatible materials to print 3D structures also known as scaffolds. These scaffolds are used together with stem cells and placed into a bioreactor or in a patient, where the organ or tissue can grow. Materials for such applications have to be biocompatible, biodegradable and provide appropriate conditions to house cells. On top of that, the material should be 'printable'.

We have been working with gellan gum composites that showed promising results as a scaffold material<sup>1</sup>. Gellan gum samples are made by pouring hot polymer solution into a mould, where the solution cools down and gels into a hydrogel. Rheological studies of gellan gum<sup>2</sup> showed how we can tailor gelation by changing the amount of Ca<sup>2+</sup> ions. Addition of Ca<sup>2+</sup> ions will increase temperature of gelation as well as increase the visco(ela)sticity of the initial solution. Ca<sup>2+</sup> ions can be added in the form of CaCl<sub>2</sub> or by dissolution of bioactive glass (BAG) particles in the gellan gum solution.

A specific type of 3D printing technique called 'fused deposition modelling' (FDM) was chosen as the most appropriate. This technique works by adding layer by layer of material that is usually in a form of a filament. Since gellan gum could not be made into a filament, we had to modify the printer to print it. The idea was to keep the suspension of gellan gum hot in a syringe, which would then cool down as it exits from the syringe needle (see Figure 1). By adjusting temperature in the syringe, changing the amount of Ca<sup>2+</sup> ions, adding forced cooling at the nozzle, etc. we can drastically improve printing capabilities.

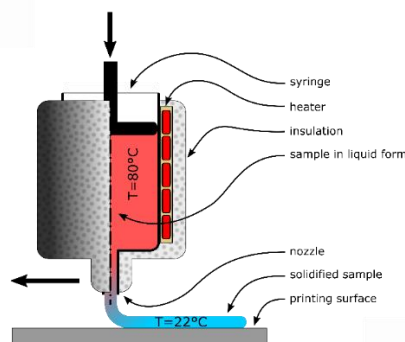


Figure 3: Heated syringe as a modification of a 3D printer's nozzle

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## Tungsten-based composite for extreme environments in fusion reactor

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In last decades we see global climate changes, such as rise of temperature due to excessive emissions of greenhouse gases. One of the main objectives of the developed world is to change from oil, coal or gas to renewable 'clean' energy. Nuclear fusion presents a possible way to produce clean and safe energy for the future. The main task in Eurofusion project is future research reactor called ITER, followed by the construction of the first demonstration fusion power plant DEMO. The walls of the reaction chamber will be exposed to extreme high heat flows and erosion by hot plasma, especially in the lower part, called the divertor. High thermal loads of 10-20 MW/m<sup>2</sup>, presents a problem for the materials from which it will be made of.

Tungsten, a candidate material for future fusion power plants, is inherently brittle at moderate temperatures that can be improved by reinforcement with small oxide or carbide particles. It has been shown that the grain growth and recrystallization at high temperatures can be suppressed by incorporation of Y<sub>2</sub>O<sub>3</sub>, La<sub>2</sub>O<sub>3</sub>, TiC, ZrC or HfC. However, none of these composites proved good solution. In our laboratory we proposed incorporation of tungsten dicarbide inclusions as an alternative.

We proposed that the carbide inclusion can be formed during sintering by high-temperature reaction of W-matrix with a precursor, such as graphene, organic source of carbon or WC. Spark plasma sintering (SPS, 1900°C, 5 min) was used to densify the powder mixtures.

The results confirm that all the used precursors reacted to form W-W<sub>2</sub>C composites. WC nanoparticles appeared the most convenient precursor for W<sub>2</sub>C. Based on the thorough microstructural analysis we found that samples with low concentration of carbon form unwanted oxide phase, while at concentration above 5 vol. % of WC all the oxide phase has reacted with carbon precursor to volatile species. Instead, due to the carbon deficiency in WC, W<sub>2</sub>C secondary phase form at the tungsten grain boundaries.

The results also suggest that presence of small W<sub>2</sub>C grains enhance densification of tungsten, inhibit the growth of tungsten grains at high temperature up to at least 1300 °C and significantly improve mechanical properties of the material.

The work will present the main characteristics of W- W<sub>2</sub>C composites prepared by SPS, i.e. relevant microstructural characteristics of the composites in comparison with tungsten, their mechanical properties.



## Lipid droplets are antioxidant organelles that protect cancer cells from nutrient stress

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Breast cancer is one of the most common causes of cancer death in women worldwide. Despite extensive research and attempts to develop appropriate and effective therapies, many tumors are still characterized by a poor prognosis and high mortality. Cancer cells scavenge unsaturated fatty acids (FAs) from their environment in order to cope with nutrient and oxidative stress, but the mechanisms of FA uptake and use are poorly understood. The human group X secreted phospholipase A<sub>2</sub> (sPLA<sub>2</sub>-X) is a lipolytic enzyme that acts on the plasma membrane of cancer cells, releasing unsaturated FAs, which are esterified into triacylglycerols and stored in cytosolic lipid droplets (LDs). LDs are dynamic organelles, present in most eukaryotic cells, that regulate the uptake, storage and use of lipids according to cellular needs. The main aim of this study was to test the hypothesis that LDs are important regulators of stress in cancer cells. We thus treated highly aggressive MDA-MB-231 breast cancer cells with sPLA<sub>2</sub>-X and different unsaturated FAs and examined the role of LDs in supporting cell survival during metabolic stress caused by nutrient deprivation or FA excess. We found that sPLA<sub>2</sub>-X and low micromolar concentrations of unsaturated FAs, including ω-3 and ω-6 polyunsaturated FAs (PUFAs), stimulate LD formation, reduce starvation-induced oxidative stress and prevent cell death induced by nutrient deprivation. On the contrary, we found that high micromolar concentrations of PUFAs, but not oleic acid, display lipotoxicity and induce oxidative stress-dependent apoptosis in breast cancer cells. sPLA<sub>2</sub>-X reduces oxidative stress and lipotoxicity by increasing the amount of LDs enriched with PUFAs. Furthermore, suppressing LD breakdown by depletion of adipose triglyceride lipase (ATGL) in cells treated with PUFAs reduced oxidative stress and lipotoxicity, suggesting that storing PUFAs in LDs is protective for the cell. Indeed, blocking PUFA incorporation into LDs by inhibiting diacylglycerol acyltransferase 1 (DGAT-1) increased PUFA lipotoxicity. Our results clearly show a dual – pro-survival and cytotoxic – effect of unsaturated FAs in breast cancer cells and identify LDs as key regulators of both processes. Therefore, LDs are antioxidant and pro-survival organelles that protect cancer cells against stress and are attractive targets for novel therapeutic interventions.

## Serine protease homologue from the venom of the nose-horned viper, a promising new anticoagulant lead molecule

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Most frequently used anticoagulant therapies, based on aspirin, heparin and warfarin, may induce severe complications. To overcome these limitations, new anticoagulants from natural sources have been intensively searched for. We report here the purification and characterization of a glycoprotein from the venom of the European most venomous snake, the nose-horned viper (*Vipera a. ammodytes*), which significantly prolonged the activated partial thromboplastin time (aPTT) in human plasma, which indicates perturbations in the intrinsic pathway of blood coagulation. Amino acid sequence of this monomeric N-glycosylated protein of 34 kDa revealed it as a serine protease possessing two mutations in its catalytic triad that renders it enzymatically inactive. Hence the name *Vipera a. ammodytes* serine protease homolog 1 or *VaaSPH-1*.

Detailed analysis of the mechanism of blood coagulation by *VaaSPH-1* exposed that the molecule inhibits the activity of tenase (comprised of blood coagulation factors VIIa, VIIIa, IXa and X) and prothrombinase (comprised of blood coagulation factors Va, Xa and II) complexes, the former with IC<sub>50</sub> of 142 nM and the latter with IC<sub>50</sub> of 134 nM. We demonstrated that the inhibition of the formation of complexes is due to the binding of *VaaSPH-1* to all above mentioned blood coagulation factors (either zymogen or active forms), except to FVIIIa. *VaaSPH-1*, which is a basic protein, was also found to bind specifically to negatively charged phospholipids, phosphatidylinositol and phosphatidylserine, the latter being crucial for constitution of previously described coagulation complexes on cellular membranes. We predict that *VaaSPH-1*'s major anticoagulant action is due to binding to FIX/FIXa. This is suggested by its marked effect on aPTT and additionally supported by the highest substrate recognition regions homology between *VaaSPH-1* and FXIa, which is FIX activator in the intrinsic blood coagulation pathway. Three-dimensional structure comparison of FVII, FIX, FX, FII and their respective activated forms suggested two areas on their surfaces, in the proximity of their active sites, where *VaaSPH-1* binds. Such proposal was supported also experimentally as FIXa, complexed to *VaaSPH-1*, retained its enzymatic activity towards chromogenic peptide substrates.

As a potent non-enzymatic and coagulation factor active-site independent inhibitor of blood coagulation process, *VaaSPH-1* is unique and therefore very interesting for further characterization to design, based on its structure, a novel family of selective coagulation factor IXa inhibitors of therapeutic relevance for anticoagulant therapy.

## Making sintered zirconia ceramics machinable

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Advanced ceramic materials based on zirconia are very suitable for different structural applications owing to its high strength and toughness. Machining of sintered zirconia ceramics is limited to diamond tools that is expensive, time consuming and limited to simple geometrical complexities. Electrical discharge machining (EDM) can overcome the limitations of machining with diamond tools, however, it can only be performed on electro-conductive ceramics (ECC) exhibiting sufficient conductivity. This is usually achieved by incorporation of electro-conductive (EC) phase into the insulative ceramic matrix.

Up to now zirconia-based ECC containing various EC phases, such as, TiC, TiCN, WC, ZrB<sub>2</sub>, TiN, carbon nanotubes (CNT) and/or graphene, have been prepared by mixing of commercial powders, their consolidation and sintering. Attaining homogeneous microstructures, however, is a challenge yet to be overcome. In case the particle size of both EC and ceramic matrix phase is in the same range, the electrical conductivity required for EDM is attained at high content of EC phase (>30 vol. %), which can be detrimental for mechanical properties as a result of microstructural inhomogeneities. On the other hand, when the particles of EC phase are in the nanoscale range and/or nonpolar (as CNT and graphene are), they are prone to agglomeration and are difficult to homogeneously disperse in aqueous suspensions.

Here several alternative, novel processing approaches, based on aqueous colloidal processing combined with rapid consolidation in the Spark plasma sintering furnace, will be presented, providing homogenous, highly electro-conducting, EDM machinable zirconia ceramic composites.

## Inkjet printing thin-film electronic devices from solution-based inks

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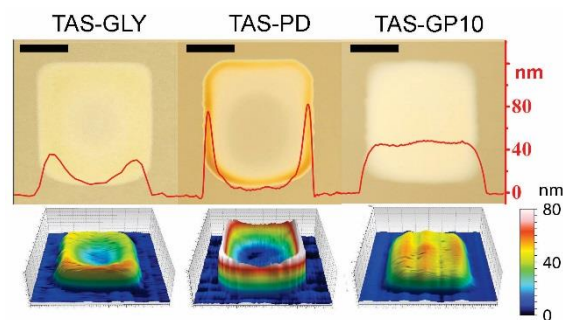
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Due to their unique characteristics, direct-writing techniques have a large potential in the production of modern, large-area electronic devices. Inkjet printing offers several attractive features, including additive deposition, direct patterning with micrometre resolution, and easy pattern modifications. Yet, a high complexity of the printing process—extending from the jetting concerns to the issues connected with the morphology of dried deposit—has impaired the fabrication of electronic devices using inkjet printing.

We report on the inkjet printing of functional metal-oxide structures for applications in transparent electronics. The structures with the thickness in nanometre range are deposited from solution-based inks, which consist of metal oxide precursors dissolved in a suitable solvent. The printed structures commonly dry in a way that the ring-like deposit forms; the phenomenon known as “coffee stain” effect. [1] A standard approach to improve the uniformity of dried deposits is by combining a solvent and a co-solvent with different boiling points and surface tensions. Consequently, these solvents evaporate with different rates, which leads to variations in the solvent composition in the drying feature. Moreover, the composition variations can lead to the changes in the physical properties, and thus produce a rich variety of complex phenomena observed when the printed features are drying.

We highlight the influence of the ink's solvent composition, wetting of the substrate, and drying temperature on the morphology of wet and dried structures. These parameters appear to be interrelated in the drying process; well-defined structures with the flat thickness profile can be printed only when all three parameters are optimized. We demonstrate such optimization for inkjet printing of transparent thin-film capacitors composed of tantalum oxide-based dielectric and indium-zinc oxide electrodes. The capacitors were uniform and showed good electrical and optical properties.



**Figure 1.** Optical images and profilometry micrographs of inkjet-printed tantalum oxide-based dielectric structures after drying and annealing. TAS-GLY and TAS-PD inks clearly produce coffee stain effect after drying, whereas the optimized ink TAS-GP10 produces uniform structures. Scale bars = 250  $\mu\text{m}$ .

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## Phylogenomic analysis of RNA viruses in invertebrates

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More than 350 different human pathogens and most of the etiological agents of emerging diseases are RNA viruses. The WHO has released a list of current emerging diseases likely to cause major epidemics: Crimean Congo haemorrhagic fever, Ebola virus disease, Marburg, Lassa fever, MERS, SARS, coronavirus diseases, Nipah and Rift Valley fever. One of the most apparent reasons for the weak development of broadly acting antiviral compounds is the lack of knowledge on the distribution and diversity of the pathogen. Until now, arthropods were believed to be at the centre of RNA viral diversity. Such a view may be misleading since a number of invertebrate lineages have not yet been screened for RNA viruses. Some of these lineages are the oldest insect lineages (Collembola, Diplura, Zygentoma, Monocondylia), Lophotrochozoa (Eumetazoa; Bilateria) and the oldest metazoan lineages (Cnidaria, Ctenophora, Porifera).

The main focus of our research was to screen the above mentioned lineages for the presence of new RNA viruses and endogenized viral elements and to characterize their genomic architecture. Our aim was to infer the differences between the distribution of RNA viruses in these lineages and in arthropods, which could clarify the pattern of evolution of RNA viruses in invertebrates. We have found more than **200 dsRNA, ss(+)-RNA and ss(-)-RNA** viruses in Lophotrochozoa and oldest hexapod lineages and **35 endogenized RNA viral elements**. These novel viruses belong to 17 clades: Birna, Partiti-Picobirna, Reo, Toti, Picorna, Hepe, Flavi, Narna, Noda, Toga, Tombus, Luteo-Sobemo, Nege, Mononega, Bunya, Orthomyxo and Qinvirus. We have found a new clade of Negevirus. The majority of endogenized viral elements belong to the order Mononegavirales. The pattern of distribution is similar to arthropods which indicates that diversity of RNA viruses is typical for all invertebrates and is not limited to the arthropods. Our future research will be on the analysis of diversity of RNA viruses in the phyla that are not well analysed yet, e.g. in Cnidaria, Ctenophora and Porifera.

## Local structural studies of Sr-buffered Si surface prepared with pulsed laser deposition

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A successful integration of functional oxides with silicon could lead to the design of a wide variety of novel electronic devices with sensing, logic and energy-harvesting capabilities. However, the silicon surface is highly reactive, and needs to be passivated by an appropriate buffer layer that is chemically stable as well as structurally compatible with the overgrown oxide layer. A buffer layer based on  $\frac{1}{2}$  monolayer (ML) of Sr on Si(001) has been shown to fulfil both requirements [1,2]. While this surface has been conventionally prepared by Molecular Beam Epitaxy (MBE), one of the most promising techniques for overcoming its numerous shortcomings is Pulsed Laser Deposition (PLD). Plenty of studies for MBE-derived surfaces can be found in the literature, but to the best of our knowledge, there have been no local structural studies of such a surface when prepared by PLD. Nevertheless, a local study of the buffer layer structure is needed to assure a highly-ordered surface, required for a successful integration of oxide materials.

In this contribution, the results of Scanning Tunneling Microscopy (STM) analysis of  $\frac{1}{2}$  ML of Sr/Si(001) surfaces prepared by PLD will be presented. The samples were prepared following a procedure previously developed by our group [3], and transferred using an ultra-high vacuum suitcase, in order to ensure an adsorbate free surface necessary for the STM measurements. Large-scale STM images confirm the  $(2\times 1)$  reconstructed Sr/Si(001) surface detected by *in-situ* reflective high-energy electron diffraction measurements. This reconstruction covers the surface area entirely, and exhibits two equivalent  $90^\circ$ -rotated domains on the neighbouring terraces. High resolution images reveal chain-like structures running along the  $[011]$  and  $[0\bar{1}1]$  directions with a lateral distance of 0.78. Apart from the well-ordered chains, an abundance of various defects can be distinguished. However, the quality of the surface is still comparable to the MBE prepared surfaces. This study represents the first local structural analysis of a PLD prepared Sr-buffered Si surface and confirms that PLD can be used for the preparation of a high quality buffer layer necessary for achieving epitaxial growth of complex oxides on silicon using this technique.

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## Precipitation of harmful $\sigma$ -phase in 1.4462 duplex stainless steel grade at high temperatures

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Duplex stainless steel grade 1.4462 with ferrite/austenite microstructure has excellent corrosion properties. The material can be used for components that service in aggressive corrosive environments. It is resistant to pitting and crevice corrosion, stress corrosion cracking in chloride-bearing and hydrogen sulfide containing environments and resistant to corrosion fatigue. Among this, it also has high mechanical strength, shows super plastic behavior and good weldability. Attention has to be given to processes that occur at elevated temperatures during annealing or hot working. Additionally proper cooling procedure has to be considered. As duplex stainless steels contain high amount of alloying elements such as Cr, Ni and Mo, harmful intermetallic phase precipitation can occur, namely the  $\sigma$ -phase. Chromium rich brittle tetragonal  $\sigma$ -phase highly influences the material properties, especially toughness and corrosion resistance.

The effect of temperature on the intermetallic phase precipitation in duplex stainless steel grade 1.4462 was investigated. The attention was given to intermetallic phase precipitation in the 800 to 950 °C range. Specimens were firstly solution annealed at 1080 °C for 30 min and water quenched. Then they were isothermally annealed at different temperatures from 800 to 950 °C with increment of 50 °C. Temperatures were chosen according to thermodynamic calculations by Thermo-Calc software and monitored by using thermocouple measurements on the specimens. The kinetics of intermetallic phase precipitation was investigated by annealing the specimens at chosen temperatures for 1 min, 10 min, 100 min, 1000 min and 10000 min.

The specimens were investigated by light optical microscopy, hardness measurements and ferritoscope measurements.

The ratio between ferrite and austenite during annealing was determined. The amount of precipitated intermetallic phases was investigated.

## Design and development of novel titania nanotubes based photo(electro)catalytic reactor

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A new highly-efficient photo(electro)catalytic reactor for water and air purification was designed and assembled based on photoelectrocatalytic technology to completely degrade organic pollutants without any hazardous oxidants. The active part of the reactor consists of nanosized titanium dioxide, which is illuminated with UV light, hence generating electrons and holes that take part in the oxidation and reduction reactions at the semiconductor's surface. Since titania nanotubes film is grown by anodic oxidation process it is consequently firmly attached to different forms and shapes of metal titanium and cannot be washed away during the treatment. In our work we studied the most important parameters of anodic oxidation and annealing procedure that determine the morphology, length, and crystal structure of polycrystalline TiO<sub>2</sub> nanotubes. We found out that the optimum length of titania nanotubes is between 15 to 20 μm which enables effective capture of the incident UV illumination and control of electron-hole recombination time. The efficiency of thus processed active photocatalytic parts was measured via degradation studies of caffeine and phenol. These active photocatalytic anodes were later assembled into a large-volume reactor (1.5 l) and positioned next to metal cathodes and UV light sources in such a way to achieve a uniform illumination of the photocatalyst. Currently, this large-volume reactor is tested to degrade organic compounds present in real waste waters from textile, pharmaceutical and paper production industries.



## 1-D and 2-D Ni-based nanomaterials for formaldehyde electrochemical sensing devices

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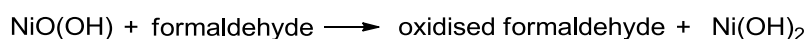
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In this study we used KOH-modified Ni electrodes (films and nanowires) for the electro-oxidation of formaldehyde (HCHO), which are promising to be used as effective electrochemical receptor element. Ni "films" were deposited on Au substrates by the electro-deposition from acidic and neutral NiSO<sub>4</sub>-based solutions with subsequent modification in 1 M KOH. From the SEM results we found out that pH of Ni<sup>2+</sup> solution affects the morphology of the deposited films. Under acidic conditions homogeneous Ni film was formed, but under neutral conditions porous Ni film was deposited. Ni nanowires (200 nm diameter, ~1 μm length) were prepared with template-assisted electrodeposition into alumina templates. After the electro-deposition of the nanowires, the template was removed in 10 M solution of NaOH in order to get free standing wires.

The modification step with KOH is very important for the further investigations of HCHO oxidation, because NiO(OH)/Ni(OH)<sub>2</sub> redox couple exhibits high catalytic activity towards HCHO. The electro-catalytic activity of modified Ni nanowires and Ni films (Ni-OOH) for formaldehyde detection in alkaline media was investigated via a series of electrochemical measurements. The potential range for modification in KOH has to be chosen in the region where oxygen does not form (the maximum potential 0.6V), because molecular oxygen can be adsorbed on the electrode and inhibits further oxidation of HCHO [1].

Experimental results show that the 2D and 1D Ni-based electrode (nanowires and films) displays a remarked electro-catalytic activity for the oxidation of HCHO and exhibit a linear relationship in a concentration range from 1 mM to 0.5 M. An oxidation peak was obtained at potentials around 0.5 V vs. Ag/AgCl for concentrations 1 mM – 0.1 M and around 0.8 V vs. Ag/AgCl for concentrations above 0.1 M. Results showed that the reaction of the electro-oxidation most probably proceeds by a chemical reaction with NiO(OH) as shown on Scheme 1 [2]. The experimental data further reveal that Ni nanowires exhibits a higher sensitivity (approximately 7x higher) compared to the homogeneous and porous Ni electrode, because the slope of the curve current signals vs. concentrations reached higher value. The detection limit was 0.1 mM for Ni nanowires, 0.4 mM for porous Ni film and 0.5 mM for homogeneous Ni film. It was concluded from results that Ni nanowires exhibit a higher catalytic activity due to the more surface active sites and connected higher amounts of adsorbed –OOH groups on the surface that promote the electron transfer between receptor elements and HCHO molecules. These advantages of Ni nanowires make them promising for providing a low cost and simple method in real samples.



*Scheme 1: Formaldehyde oxidation on modified Ni electrodes*

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## **Naravoslovne znanosti (Natural Sciences)**

## Cellular model of amyotrophic lateral sclerosis

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Amyotrophic lateral sclerosis (ALS) is a fatal neurodegenerative disease with a signature pathology of dying motor neurons, leading to muscle wasting, paralysis and death. In most cases, the affected neurons harbor cytoplasmic inclusions predominantly consisting of TDP-43 protein. TDP-43 is a member of hnRNP protein family and is involved in multiple steps of RNA processing. In healthy cells, the majority of TDP-43 is localized to the nucleus, with a small cytoplasmic fraction. In pathological conditions, however, TDP-43 is mislocalized into the cytoplasmic aggregates, where it is cleaved, phosphorylated and tagged for degradation. About 5-10 % of the cases are of genetic origin and for all of the others, the etiology is unknown. Despite extensive studies of numerous groups into ALS mechanisms, the lack of appropriate models is slowing the development of new pharmaceuticals targeting the disease. To this end, we developed a cellular model reproducing certain features of ALS pathology *in vitro*. Following transfection into neuron-like SH-SY5Y cells, fluorescently tagged TDP-43 amino-terminal fragments assemble into the cytoplasmic inclusions and sequester the endogenously expressed TDP-43 protein into the aggregates. These aggregates interfere with normal cellular activities, like nuclear-cytoplasmic transport and protein degradation, finally resulting in the death of the cell. The conditions in the cell therefore closely resemble the pathological conditions in the affected neurons of ALS patients. With this model we can now test new hypothesis associated with ALS and try reversing the pathology using different drugs. Our cellular model of ALS is thus bringing us a step closer to finding the cure for this horrifying disease.

## Alternative activated carbon and the removal of radioactive micropollutants from environmental water

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Activated carbon is one of the most common adsorbent involved in water treatment due to its high specific surface area and high degree of surface reactivity. It is widely used as one of the first steps in drinking water preparation and in the removal process of industrial pollutants. But, the price of commercially available activated carbon is rather high and not always easily affordable. The synthesis and characterization of activated carbons obtained from lignocellulosic precursors is therefore a topic widely studied by a number of researchers worldwide. The group of Faculty of Technical Sciences at University in Novi Sad on the Department of Environmental Engineering joined this community by conducting the research with the aim to find the appropriate and cheap raw material from agricultural, industrial or vegetable (lignocellulosic) wastes, reduce the cost of production by changing the synthesis of alternative activated carbon, characterize newly developed material and test its efficiency on different types of pollutants. The alternative activated carbons derived from apricot (*Prunus armeniaca*), plum (*Prunus domestica* L.) and cherry/sour cherry (*Prunus avium/Prunus cerasus*) kernels were produced by thermo-chemical activation using phosphorous acid. The materials were already tested on wastewater polluted by heavy metals [1] and pharmaceuticals. The results were encouraging and the study was extended to radioactive inorganic micropollutants. Environmental water obtained in the vicinity of former uranium mine at Žirovski Vrh was the first analysed sample due to its rather high content of radionuclides which can be easily analysed by accredited screening method for determination of gross alpha and beta activity. The testing procedure is rather simple: 100 mg of activated carbon is added to 50 ml of the sample in Erlenmeyer flasks. For increased performance of adsorption pH was adjusted to 6 to set slightly acidic matrix and also to be near neutral value. After 30 min of shaking, solution was separated from activated carbon and prepared for liquid scintillation counting. Results show feasibility of alternative activated carbons usage comparing with commercial one. The ability of the alternative activated carbons for removal of radioactive emitters in low concentrations will be tested also on the regular tap waters with the content of alpha emitters close to the recommended range of 0.1 Bq/L. Additional kinetic and other studies will be performed as well. After this study, new technique can be developed for simple and economic removal of radioactive micropollutants on a large scale.

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## Distribution of Macroinvertebrate Assemblages and its Differential Structure Along Longitudinal Profile of the Sava River

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The Sava River has a course more than 900km long. It flows through four states and all its hydromorphological characteristics vary greatly longitudinally. The river has many tributaries, and its basin is under various anthropogenic pressures. All these features lead us to expect interesting differences in the macroinvertebrate communities along the Sava River. Accordingly, the aim of the study was to determine the distribution of macroinvertebrate assemblages and its differential structure along the longitudinal profile of the Sava River. GLOBAQUA survey on the Sava was carried out in September 2015 at 14 sampling sites along the whole Sava watercourse, from the Sava Dolinka River (Ljubljana) to its confluence into the Danube River (Belgrade). Macroinvertebrate community was sampled at all sites following the multihabitat sampling procedure (10 subsamples at each locality, from all available habitats in respect to their ratio at site). During investigation a total of 348 macroinvertebrate taxa were recorded. Aquatic insects were found to be the dominant group in the community with 46,82% (Diptera 30%, Ephemeroptera 6,84%, Trichoptera 6,48%, Coleoptera 1,44%, Plecoptera 0,80%, Odonata 0,73%, Heteroptera 0,42%, and others). Subdominant groups with significant share in the community were Oligochaeta (21,52%), Mollusca (20,47%), and Crustacea (10,28%). For observing changes in the community structure along the course we have chosen the following groups: Diptera, Insecta without Diptera, Mollusca, Crustacea, and Oligochaeta, according to their presence in the river course. A gradual decrease of total number of taxa (N), as well as abundance of insects (without Diptera) was noticed in downstream direction along the course. Oligochaeta share was relatively constant at all sites, in spite of expecting lower abundances at upper stretches, where rocky bottom is present. Crustacea and Mollusca were groups that have increasing abundance downstream, which was in accordance with mollusks preferring river bed with more sediment. Diptera were abundant along the course, but with highest abundance in most upstream sites. Among Diptera, Chironomidae were the most numerous. Nevertheless, there was a difference between upper and lower stretches regarding taxa dominance: the most dominant genera in the upper stretch were *Microspectra* sp., *Synorthocladius* sp., and *Tanytarsus* sp., while in lower stretches the most dominant species were *Microchironomus tener* and *Polydillum nubeculosum*. Further research is needed to explain the recorded community structure, to determine the extent of anthropogenic impact on the current state of communities, and/or impact on available habitats and hydromorphological conditions at investigated localities.

## **Aquatic Macroinvertebrate Assemblages in Assessment of Ecological Status - Sutjeska National Park Case Study**

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The aim of this study was to assess the ecological status of the River Sutjeska and its tributaries, based on macroinvertebrate assemblages. Alongside fish and algae, in assessment of ecological status of watercourses, macroinvertebrates are the most commonly used group of organisms. This group is characterized by high diversity, relatively long life, and low mobility. Also, these assemblages are constituted of numerous taxa with different tolerance to pollution and other pressures as hydromorphological degradation. These traits make the group favorable bioindicators. Biological and environmental value of watercourses can be assessed with use of biological indices. Nowadays, the Sutjeska basin is under low anthropogenic influence, and the main area of the basin is within borders of the Sutjeska National park. Since Sutjeska tributaries provide high amount of water, especially in spring, there is intention for building small hydropower plants on some of these watercourses. Constructing and putting them into operation would pose a real threat to the biodiversity of the area. For the ecological status of the watercourses assessment following indices were used: Total number of taxa, Diversity Index (H'), Saprobic Index (SI), Biological Monitoring Working Party (BMWP) and Average Score Per Taxon (ASPT). Samples from 10 watercourses (16 localities) were taken using standard benthological hand-net (multihabitat sampling procedure) in summer of 2015. During the investigation, a total of 119 taxa, from 16 main macroinvertebrate groups were recorded. The most diverse and abundant groups were insects belonging to orders Ephemeroptera, Plecoptera, Trichoptera and Diptera. According all indices at the majority of localities water quality was excellent (I class), with following indices values (min-max): Number of taxa (22-54), Diversity (2,28-2,93), Saprobic index (1,22- 1,76), BMWP score (104-164), and ASPT (6,12-7,5). Only two localities at two small tributaries had good to moderate water quality (II-III class), which is due to its location where moderate anthropogenic pressure is present. Significant part of the assemblages are organisms that have xeno and oligo-saprobic valence. Construction of power-plants within borders of a national park is illegitimate. Also, the potential harm of such facilities threatens the recorded diversity and undisputable ecological value of the area, which makes it undesirable.

## Tritium levels in Cameroon water samples and coconuts

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Coconut is an important nutrition source for most people under the tropical and subtropical belt all over the World. The fruit becomes very popular also in so called western cultures because of its richness of vitamins, minerals and bioactive compounds that are essential for better health.

The paper of Narayan [1] attracted the attention with the thesis that the coconut fruit pre-concentrates the tritium in respect to tritium concentration in environmental water such as irrigation water and precipitation. In order to ascertain if that theory is valid in general or if it is valid only under specific conditions like the types of coconuts, soil or tritium background, quite similar investigation was initiated in Cameroon, nicknamed also “Africa in miniature” due to its large ecological diversity. For this purpose, three regions with different landscape and climate specificity were selected where coconuts are generally cultivated namely Edea area and towns of Makenene and Limbe. The local water sources used also for irrigation coconut trees were sampled as well, the stream flowing inside the Limbe botanic garden and two wells situated in Edea and Makenene, respectively.

Tritium concentrations in environmental water samples and values of Tissue Free Water Tritium (TFWT) and Organically Bound Tritium (OBT) for coconuts for three different Cameroonians will be presented, evaluated and compared with results for Indian coconuts. The correlations between tritium concentrations in water and coconuts will be checked as well.

These measurements are the first of its kind in Cameroon and as such they also play the role of a zero point values for the regions at very early industrial stage.

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## Characterisation of L1 ORF1p in mammalian cells

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In the evolution of the human genome an important role was played by mobile elements – DNA sequences that are able to “jump” to different sites in the genome. Depending on the target sites of their integration they can cause approximately 65 different diseases, mostly cancers. Mobile elements constitute about 45 % of human genome and are divided into three groups: DNA transposons, LTR (long terminal repeats) retrotransposons and non-LTR retrotransposons. DNA transposons are cut from their original site in genome and transferred to the new target site by the enzyme called transposase that is encoded in their sequence. On the other hand, retrotransposons move to new target sites by “copy paste” mechanism that is enabled by RNA intermediate. RNA transcript of retrotransposons is reverse transcribed to cDNA which is inserted to the target site. About 17 % of human genome is constituted of the sole autonomous non-LTR retrotransposon in human genome - LINE-1. LINE-1 is a 6kb long DNA sequence with two open reading frames that encode for L1 ORF1p and L1 ORF2p. These two proteins are also used by other, non-autonomous retrotransposons. The latter is a 150 kDa protein with an endonuclease and reverse transcriptase activity. L1 ORF1p has a size of 40 kDa, the role of this protein is still largely unknown. L1 ORF1p is known to have RNA binding activity but the library of target RNA molecules has not been determined so far. The goal of our work is to characterise the protein in mammalian cells and define target RNA molecules of L1 ORF1p in order to better understand the role of this protein in the cell and during mobility of different groups of retrotransposons. In order to do so we established inducible HEK 293T, HeLa and SH-SY5Y cell lines expressing L1 ORF1p by the FlpIn system. We also used 2012Ep and NT-2 cells which express high levels of endogenous L1 ORF1p. Cells were characterised by immunolocalization using custom made anti-L1 ORF1p antibodies. Protein was detected in clusters formed mostly in the cytoplasm. Furthermore, we successfully immunoprecipitated protein constructs containing either GFP or Flag tag, which allowed us to proceed with the iClip experiment. iClip experiment enables us to detect protein-RNA interactions *in vivo* and therefore determine target RNA molecules of L1 ORF1p in chosen mammalian cell lines.



## Trace elements in riparian soils in several localities in Slovenia

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Riparian soils and vegetation are under intense pressure from various anthropogenic sources and heavy metal pollution seriously contributing to multiple stress conditions. In order to determinate the extent of pollution in the riparian zone of the Sava River, bioavailability of heavy metals in soils and metal uptake by *Salix alba* L. were measured. The study area covered about 200 km of the Sava River stretch, through Slovenia, and included 5 sampling sites (Mojstrana, Radovljica, Litija, Vrhovo and Čatež).

To estimate heavy metal content and potential ecological risk on riparian soil, total and bioavailable concentrations of cadmium (Cd), chromium (Cr), copper (Cu), nickel (Ni), and zinc (Zn) were analysed and the Risk Assessment Code (RAC) was calculated. RAC revealed that Cr, Cu, and Ni come under the no risk category (<1%) and Zn comes under the low risk category (<10%) for the environment at all the sampling sites. According to RAC, bioavailable concentrations of Cd indicated high risk (30-50%) for the environment in Mojstrana and Radovljica sites, and medium risk (<30%) for the environment in Litija, Vrhovo, and Čatež sites.

In order to assess whether *Salix alba* is suitable for remediation of polluted riparian soil, concentration, transfer, and accumulation of heavy metals from soil to roots and leaves in terms of the Biological Concentration Factor (BCF) and the Translocation Factor (TF) were evaluated. The study indicates that Cr and Ni accumulated by the willow trees were largely retained in roots (TF<1), whereas Cd, Cu, and Zn were accumulated in leaves, as the TF value was found to be >1 at the most sampling sites. Our results of BCFs and TFs showed that *Salix alba* trees limit mobility of Cr and Ni since TF is <1, which makes this species potentially suitable for phytostabilisation of chromium and nickel. BCF and TF for cadmium, copper, and zinc indicates willows potential for phytoextraction of these trace elements.

## Pigment stability for solar absorber coatings

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Coal, oil, natural gas and nuclear energy provided 85.9 % of total global primary energy supply in year 2014<sup>1</sup>. These energents are causing harm to the environment through climate change, air and water pollution, soil contamination and radioactive releases, not to mention that their reserves are limited.

The solution to this problem is the replacement of fossil fuels with solar energy. For comparison, total global energy consumption in year 2012 was  $5,792 \times 10^{20}$  joules<sup>2</sup>. Solar radiation, which hits earth surface gives the same amount of energy in less than two hours<sup>3</sup>. Technology to convert solar energy are concentrating solar power plants (CSP), which efficiently convert solar energy to thermal energy and then via steam turbine to electric energy<sup>4</sup>.

Important parts of CSP plant are solar absorbers, which absorb and convert solar energy into heat. Spectrally selective coatings are used on solar absorbers for maximum absorption of the solar spectrum, minimal heat loss because of low thermal radiation and protection of absorber material. Optimal absorber temperature for highest efficiency of CSP plant should not exceed 1383 K<sup>5</sup>.

This paper presents a study of high temperature effects in combination with addition of different elements on commercial black spinel pigment used for the preparation of high solar absorptivity coatings for concentrated solar power plants. As the CSP absorbers and coatings are exposed on the field to atmospheric conditions, the pigments were exposed to different elevated temperatures between 700 and 1100°C in air. Furthermore, metallic powders were added to the pigment in order to study diffusion effects of metallic atoms at high temperature. The samples were ground with the pestle and mortar, pressed into tablets and heated. The samples were exposed to high temperature for 24 hours and after regrounding. Structural and optical properties of modified pigments particles were studied using TEM, XRD, IR and UV/VIS/NIR spectroscopy. Presented results disclose gain in optical properties, as the formation of new phases (Mn and Mo rich) dramatically increases solar absorptance values.

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## Identification of biotechnologically important genetic networks and the design of new generation industrial yeast strains

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Most heritable traits are polygenic, including the accumulation of neutral lipids exploited in biofuel industry. Besides bioethanol, where *Saccharomyces cerevisiae* is the major producing organism, yeast strains are also promising as producers of biodiesel. *S. cerevisiae* represents a good model organism to study polygenic traits because it can reproduce sexually and because the molecular and genetic engineering tools are well developed. To identify genetic loci responsible for high triacylglycerol (TAG) content in an industrial *S. cerevisiae* strain, we used extreme quantitative trait loci (X-QTL) mapping method [1]. This method enables detection of all genetic loci even with small effects on a given trait. By crossing an industrial strain with high TAG content with a reference laboratory strain, we generated a progeny in which the genetic material from the parental strains is combined. On the basis of fluorescent staining of TAG and flow cytometry sorting we selected two subpopulations of these segregants, an average one and one with extremely high TAG levels. We genotyped both segregant pools as a whole using tiling microarrays and whole-genome sequencing. Within the discovered QTLs, we identified candidate causative genes using a novel custom-made bioinformatics algorithm. In the next step, potential genetic interactions between the causal genes and possibilities to further increase the resolution of the causative genetic elements have been studied by iterations of back-crossing the segregants with the highest TAG content to both parental strains. Finally, to test whether the identified candidates are indeed the causative genes, alleles have been swapped between the strains using CRISPR-Cas9 system. TAG content will be determined in the resulting strains. Such approach enables identification of biotechnologically important genetic networks and strain design towards industrial processes for production of chemicals based on microbial fermentation.

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## A DFT Study of the Bonding of Silanol Molecules to Oxidized Aluminum Surfaces

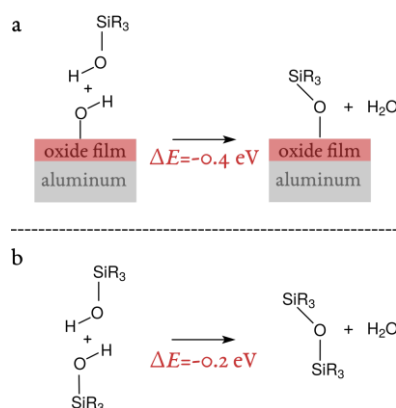
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One of the most promising novel corrosion resistant coatings, used for the protection of aluminum and its alloys, are hybrid sol-gel coatings, which combine the properties of organic and inorganic materials. Novel coatings are needed because traditional high-performance chromate conversion coatings are toxic and cancerogenic. One of the precursors for the synthesis of hybrid sol-gel coatings are silanol molecules and it is assumed that they react with the surface primarily via a condensation mechanism, as shown in figure 1a [1,2]. To shed some new light on the atomistic mechanism of bonding, the interactions of a simple silanol molecule (methylsilanetriol) with a model of the oxidized aluminum surface at the solid/vacuum interface, were studied within the framework of Density Functional Theory (DFT) utilizing periodic boundary conditions and the PBE exchange-correlation functional. The condensation reaction between two methylsilanetriols in the gas-phase (Figure 1b) was compared to the condensation reaction between the molecule and the oxidized surface (Figure 1a). According to the calculations both reaction energies are exothermic. The reaction of the molecule with the surface is by about 0.2 eV more exothermic, indicating that the bond between the molecule and the surface is slightly stronger than the bond between the silanol molecules themselves. Our calculations thus show that the currently proposed silanol–surface bonding mechanism is physically sound.



**Figure 1.** a) Reaction scheme and the calculated reaction energy ( $\Delta E$ ) of a silanol molecule bonding to the surface via the proposed condensation mechanism. b) Reaction scheme and the calculated  $\Delta E$  of the dimerization reaction between two silanol molecules.

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## Modelling of Water radiolysis in the Liquid Cell Electron Microscopy

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Liquid cell electron microscopy is used to study liquid samples with the TEM electron beam. With this technique it is possible to visualize and study different phenomena such as nanoparticle growth and decomposition, catalysis, biological materials etc. [1] However, an electron beam can have an effect on the matter in the observed area. Many of the water radiolysis products are radicals which are especially strong oxidizers or reducers. In that manner we cannot freely observe the system without affecting it. The control of conditions is therefore critical for accurate observations with liquid cell electron microscopy. One of the solutions is modelling of water radiolysis to determinate a net oxidizing/reduction effect on the nanoparticles. [2] Modelling of water radiolysis is also important in the area of nuclear chemistry to predict corrosion effects in the nuclear plants.

We collected primary radiation yields and rate constants from nuclear chemistry to determinate the composition of electron radiated water at different operating conditions (radiation dose rate, temperature, initial composition of observed system). A sensitivity analysis is performed to identify the important reactions and also to simplify the system.

We will use this data to explain the experimental observations of metal nanoparticle etching and growth. In this way we can predict and minimize the observation effects for other materials. Furthermore, we could also study the electron radiolysis effect on nanoscale and locally manipulate material using radiation chemistry.

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## The interaction of carbon nanomaterials with serum proteins and cholinesterases

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In recent years, nanomaterial (NM) production has been rising and NM application in biology and medicine has been developing quickly. Biomedical applications of NM (as drug carriers or platforms for tissue growth) are dependent on the interaction of NM with biomolecules. Upon entering a biological system, most materials are immediately coated by a layer of proteins. This is especially relevant for NM, which have a large surface-to-volume ratio and can therefore bind many proteins relative to their volume. This layer of proteins is called a protein “corona” and represents what the organism actually “sees” when encountering a NM, rather than the original NM surface. Proteins that compose the corona govern the destiny of the NM in the body, therefore knowing the composition of the NM protein corona is very important for predicting the possibility of the use of a NM in biomedical purposes. Carbon-based NM are among the most sorbent ones. Furthermore, it has been shown that carbon-based NM can adsorb physiologically important enzymes such as acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) to their surface, alter their tertiary structure and inhibit their enzymatic activity. In our study we have coated carbon-based NM of different shape and surface properties (amorphous carbon black - CB, graphene oxide - GO and multi-walled carbon nanotubes - MWCNT) with either bovine serum albumin or human serum and studied their influence on the structure and function of the isolated electric eel AChE, isolated horse serum BChE and intrinsic human serum BChE. The effect of the coated NM on the activity of enzymes was assayed using the modified Ellman assay. Carbon-based nanoparticles, pre-coated with albumin, had a considerably lower ability to adsorb and therefore to inhibit the activity of AChE and BChE. This effect was less prominent with GO, which, though it bound the highest amount and diversity of serum proteins, bound less serum albumin than the other two studied NMs. When mixed with human serum, GO, unlike CB and MWCNT, reduced the activity of the intrinsic BChE, which we assume is also the consequence of its weaker affinity towards serum albumin. The analysis of the composition of the human serum protein corona of the studied NM, showed that the corona is enriched in apolipoproteins and complement factors. The complement system represents an important part of the immune and inflammatory response towards foreign substances such as NM and can play an important role in the formation of allergies. The binding of lipoproteins E, A-I and B-100 facilitates the translocation of NM through the blood-brain barrier. Thus, the apolipoproteins in the corona of the investigated NM could be either beneficial – for example for targeted drug delivery to the brain – or harmful, when the translocation of the environment-present NM to the brain would be uncontrolled.

## Diversity of a Devastated Landscape

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The Borska River is situated in Eastern Serbia. This river is under significant anthropogenic pressure. The greatest threat to the environment in the area is pollution from the Bor mining complex (the largest copper mining and smelting facility in Serbia and one of the largest on the Balkans; not only recent, but historical pollution took place in the area, since exploitation of the Bor deposit started in 1887). The aim of our study was to investigate the status of the Borska River and six tributaries (all together 10 sites) using aquatic macroinvertebrates, based on the material collected in 2015-2016. Macroinvertebrates are commonly used as indicator in ecological status assessment of different water bodies in Europe due to known biology for the majority of species, low mobility, easy collection and availability of historical data.

Despite the high environmental pressure, many species managed to thrive in the tributaries of the Borska River. A total of 107 taxa were recorded belonging to 16 taxa groups. The most numerous groups were Ephemeroptera, Trichoptera and Plecoptera. Generally, larvae of these groups of insects are stress sensitive, prefer clean waters with high O<sub>2</sub> concentration and low organic pollution. Beside, species belonging to Amphipoda, Decapoda (Crustacea), Coleoptera, Diptera, Odonata (Insecta), Gastropoda (Mollusca) and Oligochaeta (Annelida) were also found to be important in respect to taxa richness and/or population densities. Highest diversity of taxa was found in the Brestovacka River (46 taxa), while the lowest was recorded in the Suva reka stream (10 taxa). The most abundant species was found to be *Baetis rhodani* (Picket 1843) recorded with significant population density on all sites. Site on the Kalinik River stands out with high number of *Gammarus* sp. individuals (1500). Among others, we underline finding of *Helicopsyche bacescui*, a rare protected caddisfly with a restricted distribution area (detected in Džanov potok Stream and in the Grčava Stream). Ecological status assessment of investigated streams was determined using several indices (Saprobic, Shannon Diversity, BMWP and ASPT). Results have shown good or high status of all examined water bodies except for the Borska River (poor ecological status). Our results point that, despite high level of anthropogenic pressure, the small size water bodies in the area are still in good ecological status. In contrary, the Borska River is significantly devastated and there is an obvious need to design and implement mitigation measures. Due to high anthropogenic pressure, the water bodies in the region should be regularly monitored with higher frequency and larger number of monitoring sites in compare to other areas, in order to effectively establish operational and surveillance monitoring networks.

## Evasin-displaying lactic acid bacteria bind different chemokines and could be used for therapy of inflammatory bowel disease

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Chemokines, small chemoattractant cytokines, are key signals in the intestinal immune system. They play an important role in the recruitment and activation of immune cells in mucosa, which is a fundamental event in the pathogenesis of both forms of inflammatory bowel disease (IBD), Crohn's disease and ulcerative colitis. The development of chemokine binding proteins as potential therapeutic agents in IBD is therefore of great interest.

Recombinant lactic acid bacteria (LAB) were engineered to bind different families (CC and CXC) of chemokines by displaying chemokine binding proteins (CKBPs) evasins-1, -3 and -4 on their surface. We used CKBPs produced by the salivary gland of the brown tick *Rhipicephalus sanguineus*, named evasins. Evasins are small proteins, which have the ability to bind and neutralize chemokines of different families (CC and CXC) and inhibit the chemokine-mediated recruitment of leukocytes. Evasin genes were cloned into a lactococcal surface display vector and over-expressed in *L. lactis* NZ9000 and NZ9000 $\Delta$ htrA in fusion with secretion signal and surface anchor. Expression of evasin fusion proteins was confirmed by Western blot and the surface localization was indirectly confirmed with flow cytometry and whole cell ELISA. Functionality of evasins on the bacterial surface was confirmed via the ability to remove chemokines from the solution with ELISA and Luminex multiplexing system assays. Using different evasins-displaying bacteria we have demonstrated the binding from 15% to 90% of 11 different chemokines. The binding was largely dependent on bacterial concentration. The evasin fusion protein-containing growth medium of *L. lactis* was used for heterologous coating of non-recombinant bacterial cells of *Lactobacillus salivarius* ATCC 11741 and its ability to bind chemokines was also confirmed. Evasin- displaying *L. lactis* NZ9000 $\Delta$ htrA cells had superior chemokine binding ability. Evasin-3-displaying *L. lactis* removed 88.0% of IL-1 $\beta$ -induced CXCL8 from the supernatant of Caco-2 epithelial cells. It also prevented secretion of CXCL8 from Caco-2 cells in a time dependent manner when added before induction with IL-1 $\beta$ . Evasin-displaying LAB have the ability to bind multiple chemokines simultaneously and exert synergistic activity. This innovative treatment approach therefore has the potential for mucosal therapy of IBD and will be tested in an animal model.



## Design and shaping of inorganic supports for enzyme immobilization

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Green chemistry is a rapidly growing field which addresses the increasing demand for sustainable production of chemicals.[1] Biocatalysts are a viable alternative in the manufacture of pharmaceutical and other fine chemicals, but the long-term operational stability and difficult recovery and re-use of enzymes limit their widespread industrial application. Those disadvantages can be overcome by immobilization. [2]

Although polymeric carriers are used predominantly, inorganic carriers offer several advantages such as higher stability against pressure, pH, temperature and solvents. Among the inorganic materials several materials have been used as catalyst supports for different applications[2]. Alumina and titania are a versatile material, as it is highly insoluble and non-toxic, but also inert and relatively low in cost[3]. Immobilization on this material is mostly tested in the powder form, hindering the industrial acceptance. In this study we will shape these mesoporous titania and alumina into uniform microspheres using droplet coagulation. The challenge is to obtain microspheres with sufficient mechanical stability and retaining enough surface reactivity for further functionalization [2]. The next step is the functionalization of the surface of the beads with an epoxy amino group to covalently immobilize the enzyme, sucrose phosphorylase. Experiments using silanisation with ethoxysilanes were initiated to this end [6].

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## The coexistence of electrocaloric and magnetocaloric effects in $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$ ceramics

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Solid-state refrigeration technology represents a promising alternative for the replacement of low energy efficient and ecologically harmful conventional vapor-compression refrigeration systems. Most current activity in cooling research is looking at one of the caloric effects – electrocaloric (EC), magnetocaloric (MC) or mechanocaloric – where the material's entropy changes under the application of external stimuli – electric, magnetic or mechanical (stress).<sup>1</sup> In bulk ceramic materials the caloric effect is currently not large enough for commercial use. One idea how to overcome this problem is to prepare a multicaloric material where two or more single caloric effects coexist in one material in which the application of both stimuli can enhance the total, multicaloric effect. Even more, different caloric modes can be applied in different temperature regions extending the operating temperature range of the cooling device. The coexistence of the MC and EC effects had been theoretically proposed five years ago<sup>2</sup> followed by experimental confirmations.<sup>3,4</sup> It is very challenging to prepare efficient multicaloric materials and the search for them is not finished yet. In this work we experimentally prove that the  $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$  (PFN) exhibits both MC and EC effects and is therefore the multicaloric material.

For the preparation of the PFN the homogenized, stoichiometric powder mixture was mechanochemically activated in a high-energy planetary mill for 30 h at 300 rpm and milled in an attrition mill for 4 h at 800 rpm. The powder compacts were isostatically pressed and sintered in an oxygen atmosphere at 1273 K for 2 h. This method yielded PFN ceramics with a theoretical density of 96 % and uniform microstructure with average grain size of 2.3  $\mu\text{m}$ . The dielectric permittivity and dielectric losses at room temperature and 10 kHz were measured with a HP 4284A precision LCR Meter and were 3580 and 0.038, respectively. For the indirect EC measurements, the polarization vs. electric field hysteresis loops were measured by an Aixact TF analyser 2000. At room temperature the EC temperature change was 0.81 K at 80 kV/cm. The maximum EC temperature change of 1.29 K was obtained at 80 kV/cm and 373 K. The magnetization vs. temperature at different magnetic fields was measured using a Superconducting Quantum Interference Device. The maximum MC temperature change of 0.16 K was obtained at 50 kOe and 2 K.

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**Informacijske in komunikacijske tehnologije – magistrski študenti (Information and Communication Technologies – masters students)**

## Comparison of cooperative and non-cooperative radio localization algorithms

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Localization has become an important research field in last decade, due to the potential services or products that can be offered knowing the costumer location. While the localization for outdoor users is efficiently solved using GPS, the node localizations indoors is currently not solved yet mainly due to harsh radio propagation environment, which results in high number of anchor nodes (nodes with known location). In order to decrease the required number of anchor nodes in a network, a set of algorithms have been developed, which by cooperation among agents (nodes with unknown location), and anchor to agents cooperation efficiently solve this problem. These set of algorithms are known as cooperative localization algorithms.

In this paper, we review state of the art cooperative localization algorithms, select the most efficient one and compare its performance with a non-cooperative one in terms of mean square error comparing estimated location and actual location of the agents. The selected algorithm is a convex relaxation algorithm [1], which set forth a convex underestimator of maximum likelihood cost function. The algorithm then minimizes this convex underestimator applying standard minimization approach for convex problems. The fully distributed algorithm, with a simple implementation at each node has been evaluated.

The algorithm evaluation has been performed by Matlab simulations. Four anchors are placed at the corners of rectangular area. The agents have been randomly and uniformly distributed within the area. The Gaussian noise has been added to the ranging information. The estimated locations have been compared to the non-cooperative algorithm, which applies the multilateration approach to estimate agent locations, relaying only on ranging to anchor nodes.

The simulation results show, the mean square error of the location using cooperative localization is considerably smaller compared to non-cooperative approach. Furthermore, by increasing the number of agents the mean square error of non-cooperative approach is constant, while the mean square error using cooperative localization is decreasing by increased number of agents. Additional agent to agent ranging information improves the localization precision. The impact of number of agents and ranging error on the localization error will be given and discussed on the poster. The preliminary simulation results reveal that cooperative localization improves the location accuracy of nodes.

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## **Analysis on medical and health – related data about adult obesity using supervised and unsupervised learning**

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Obesity is a growing problem in most developed countries and it is responsible for a significant degree of morbidity and mortality. Overweight and obesity are linked to more deaths worldwide than underweight, and globally there are more people who are obese than underweight. Prevention is better than cure and easier. However, there are many ways to overcome this problem and be healthy. First comes the recognition that there is a problem and the person's willingness to change.

This research focuses on an analysis using medical and health – related data concerning the problem of adult obesity from a project from the department of Computer Systems at Jožef Stefan Institute, in particular applying data mining algorithms on this kind of data and analyzing the obtained results. The project is a program for obese adults who are trying to lose weight in a healthy way with the help from qualified medical specialists. This program was active all across Slovenia, in many cities and it dates from the middle of 2016, so the data is relatively new and it has not been explored and analyzed previously. After data exploration, summary and statistics, based on all collected data an adequate feature extraction is selected and the relevant features are derived.

In order to get the most out of the data, two machine learning techniques – supervised and unsupervised learning are used. Classification is selected as a supervised learning method and adequate labeling of the data is introduced. Several classification algorithms (J48, RandomForest, LogitBoost, FilteredClassifier, ClassificationViaRegression, and Bagging) are applied and evaluated with 10 – fold cross validation, then the obtained results are compared. The end results show that it is possible to predict the outcome from the program. As an unsupervised method clustering is chosen, with the goal of identifying groups of participants that exhibit similar behavior in terms of the results from the programs. For this purpose, the k-medoids clustering algorithm known as *PAM* (Partitioning Around Medoids) is applied and the visualization method *t* – distributed stochastic neighborhood embedding (*t* – SNE) is used to represent the detected clusters. The results gained from this research give a representative of how the level of expertise of the trainer - based on their education, profession and years of experience, and the quality of the program provided by the medical centers contribute to the participant's success in losing weight.

## Towards automated background knowledge construction for semantic rule learning

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Biological systems are among the most complex, not fully understood phenomena studied in modern science. In the last years, machine learning (ML) methods proved to be invaluable for discovery of new knowledge in diverse fields like proteomics, genomics and disease biomarker discovery, and can contribute greatly to precision medicine, an emerging field where treatment strategies leverage detailed genomic and proteomic information obtained using modern ML approaches.

Our contribution to this field consists of a pipeline, combining different methodologies for semantically analyzing biological data. One of the main problems when using ML methods that exploit domain knowledge, such as semantic subgroup discovery, is background knowledge construction (BKC). Usually, a domain expert helps the ML expert in gathering (and potentially also encoding) background knowledge related to the problem at hand. This process can be very time consuming and error-prone, if no existing appropriate databases exist. We propose a new method, which can to some extent automate the BKC process. While our approach is theoretically applicable to any domain, our initial experiments were done on biomedical data, consisting of genes and proteins related to a selected disease (e.g., cancer).

The proposed approach consists of three main steps. In the first step, an initial background knowledge graph is constructed using the knowledge base of the Biomine platform [1], i.e. a database joining more than eight different bio-related databases. Subsets of input terms are used to construct subgraphs, which are then merged into the final graph. The nodes of the obtained graph are terms provided at the beginning of the process, while the edges are significant connections found by the Biomine platform. The obtained graph is fully annotated with information on: species, type of connection, type of node, description and other connections added in the incremental graph construction. In the next step, the background knowledge graph is pruned using node ranking obtained by using a personalized PageRank approach [2]. As a result, the last step of our approach consisting of semantic subgroup discovery [3] proved to be more efficient and more effective.

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## Tree Methods for Hierarchical Multivariate Regression

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Machine learning develops algorithms that learn from data. Many real-life problems concern the prediction of a numeric variable by using a model, therefore the task of regression is widely addressed in the data mining community. There are also many real-life problems that concern the prediction of multiple continuous variables, hence raising attention to the task of multivariate regression. A recent effort is made by the research community to develop methods for directly addressing the multivariate regression task [1]. This work advances the task of multivariate regression by introducing the concept of learning hierarchical multivariate regression models.

Many real-life objects tend to exist within organizational structures. For example, in evaluating the status of Parkinson's disease patients, typically the unified Parkinson's disease rating scale, i.e., movement impairment scores are used. These scores can then be organized into a hierarchical structure by aggregating together groups of scores according to the anatomy of the body. The introduced hierarchical structure can be exploited to obtain better predictive models. The individual scores in the hierarchy follow the hierarchy constraint: the score that belongs to a given hierarchy node automatically belongs to all its supervariables. If an example has multiple continuous outputs in a hierarchy that we want to predict, then the task is called hierarchical multivariate regression (HMVR).

The predictive models that we consider in order to build a model for hierarchical multivariate regression are called predictive clustering trees (PCTs) [2]. They are an approach for different types of outputs and can efficiently construct models valid for the output structure as a whole, i.e., construct a single model valid for all of the target variables. One major reason why we consider PCTs beside their good predictive performance is their interpretability since the model is a tree. This representation is easily understood by people from different backgrounds and expertise. The predictive clustering framework is proposed for implementation of the suggested solution for the HMVR task. This effectively means that a definition for the variance and distance function of the model is proposed. The model also allows the possibility to define the hierarchy aggregation function based on the task at hand. Hence, PCTs for HMVR will exploit the additional information of such hierarchical organisation of the outputs. The performance of the proposed method is evaluated on a case study consisting of 713 Parkinson's disease patients described with imaging data and UPDRS scores.

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## Data-driven modeling of nonlinear dynamic systems

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Many applications in a variety of domains consider data-driven modeling of systems that change over time. Nonlinear black-box models are considered to achieve highly accurate reconstruction, and often prediction, of an observed system's behavior. Here we investigate this conjecture by employing standard machine learning methods to the task of data-driven modeling of nonlinear dynamic systems.

For the task of modeling, we use standard methods for regression. Moreover, to simulate the behavior of the learned model's output, we consider two different methods for numerical prediction: one-step ahead simulation and full simulation. The former relates to using the true values of the system variables at a given time point for calculating the system's response at the subsequent time point. On the other hand, full simulation uses the predicted value of a variable at each time step when predicting its value at the next one.

In this work we pose two research questions:

- Which modeling method yields best predictive performance?
- With which simulation method can we obtain more accurate predictions?

To adequately investigate these questions, the experimental analysis considers eight experiments combining the choices for the two simulation methods. We use linear regression, regression tree, model tree and k-nearest neighbors as learning methods. The learned models are then used to produce both one-step ahead predictions and full simulations.

As proof of principle, we experiment with reconstructing a well-known benchmark in the domain of system identification, i.e., a cascaded water tanks system. The system is a cyclic fluid-control system which consists of two cascaded water tanks with free outlets fed by a pump. The input signal to the system is the voltage applied to the pump, which transports the water to the upper of the two tanks. The task is to model the response of the lower tank.

From the empirical evaluation, we can conclude that model trees, regardless of the simulation method, yield the best predictive performance as compared to the models learned with the other three methods. Regarding the methods of simulation, the one-step ahead simulation has slightly better performance than the full simulation method. However, note that for performing one-step ahead simulation, we are constrained by the available measured data, that is, we cannot simulate/make predictions beyond the time-period of the available measured data. On the other hand, when performing full simulation, even when measured data is only available for learning the models, the simulation can run well beyond the time-period captured in the training data. This feature in particular is in line with our plans for future work, which include investigating the performance of these black-box modeling approaches when compared to different methods for automated modeling of dynamic systems. Finally, we also plan to apply these modeling methods to other nonlinear dynamic systems.



**Nanoznanosti in nanotehnologije – magistrski študenti  
(Nanosciences and Nanotechnologies – masters students)**

## Colorimetric assay for TiO<sub>2</sub> nanoparticles detection in complex matrices as food samples

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Titanium dioxide (TiO<sub>2</sub>) nanoparticles are used in food industry as colorants and antimicrobial agents. They can be found mainly in confectionary products as chewing gums, powder food as baby formulas and in food contact materials like plastic and frying pans [1-3]. However, due to their small size, they can present potential danger. They can penetrate through cell membranes, create ROS - reactive oxygen species, adsorb biomolecules etc. [4].

The detection and characterization of nanoparticles in food samples is challenging due to the presence of other molecules in samples as well as due to their small size and quantities [5]. Colorimetric method represents an easy and quick assay for determining the presence of nanoparticles [6] without the use of any other aggressive and hazardous chemical.

The goal of this work was to adapt an established colorimetric assay from the literature [6] for the specific detection of TiO<sub>2</sub> nanoparticles (Figure 1). In this system nanoparticles act as a catalyst for the electron transfer reaction between sodium borohydride (reducer) and methylene blue (oxidizer). Monitoring the colour change enables an estimation of catalyst presence, in this case TiO<sub>2</sub>.

During the process, TiO<sub>2</sub> nanoparticles were found to be less active than silver nanoparticles [6], while their activity depended on buffering agent ageing (HEPES). In the right conditions, this assay represents a potential method for TiO<sub>2</sub> nanoparticle detection in complex matrices as food samples.



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Figure 1: Scheme of purpose of this work.

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## Thickness-dependent structural and microstructural properties of self-poled BiFeO<sub>3</sub> thick films

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The self-poling effect, i.e., a built-in polarization in as-sintered samples created without external application of the electric field, has been often reported in ferroelectrics. While the effect is detrimental for memory devices, it can be an advantage for non-switching polar materials, such as piezo-actuators. Many factors can influence the magnitude and direction of the built-in polarization, one of them is also strain gradient. Due to large strain gradients, a significant self-poling effect can be expected in epitaxial thin films (with strain gradients  $10^5$ – $10^6$  m<sup>-1</sup>), relative to bulk ceramics (strain gradients 0.1–1 m<sup>-1</sup>)<sup>1</sup>. In contrast, self-poling effects and strain gradients have rarely been investigated in thick films.

Recently, a self-poling effect was discovered in ~20 μm thick films of multiferroic bismuth ferrite – BiFeO<sub>3</sub> (BFO). A strong self-poling effect occurred during cooling of the film through its ferroelectric-to-paraelectric phase transition at T<sub>C</sub> ~ 820 °C. The presence of a compressive strain gradient across the film thickness was experimentally confirmed and suggested to be responsible for the self-poling effect of BFO films. These self-poled films exhibited a microstructure with randomly oriented columnar grains<sup>2</sup>.

The aim of our work was to investigate the influence of film thickness on the structure and microstructure of self-poled BFO thick films. In addition, the self-poling effect was evaluated by measuring the direct piezoelectric response of as-sintered films with different thicknesses.

We prepared BFO thick films with different thicknesses ranging from 5 μm to 50 μm by screen-printing a Bi<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub> mixture on a Pt-electroded alumina substrate. The films were sintered for 4 hours at 780 °C and post-annealed at 850 °C. Using scanning electron microscopy, we analysed the density, thickness and phase composition of the thick films. Electron backscatter diffraction mapping was used to determine the grain size and morphology while piezo force microscopy was used for investigating the domain morphology inside the grains. In addition, room-temperature X-ray diffraction analysis (XRD) was used to determine the lattice parameters and the degree of domain orientation in BFO films with different thicknesses. According to XRD analysis, the perovskite BFO peak positions change as the thickness of the BFO film is varied; the thinner is the film, the more the peaks are shifted to higher 2θ values, which implies a decrease in the out-of-plane BFO unit-cell parameter. In the presentation the crystal structure and microstructure of self-poled BFO films with different thicknesses will be shown and its correlation discussed.

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**Naravoslovne znanosti – magistrski študenti (Natural  
Sciences – masters students)**

## Analysis of Neonicotinoid Pesticides in Honey

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Neonicotinoids are a group of pesticides that are similar in structure to the nicotine molecule. This group includes the compounds acetamiprid, clothianidin, dinotefuran, flonicamid, imidacloprid, nitenpyram, thiacloprid, and thiamethoxam. They are systemic insecticides, meaning that they are sufficiently soluble in water so that they can be absorbed by a plant and move around in its tissues. They are used to provide in-plant protection from insects for a period during plant establishment. Neonicotinoids may be used in various forms: as seed dressings, foliar sprays, granules, and soil drenches. Although originally considered safe in the environment, their use has been linked to honey-bee colony collapses. Research has shown that very small amounts can have large effects on the bees and residues can be transferred to honey and other bee products. The use of neonicotinoids has now been limited or prohibited. In 2011, Slovenia adopted a decree that prohibits the use of plant protection products containing the active substances clothianidin, imidacloprid and thiamethoxam, for the treatment of seeds of maize, sugar beet and oilseed rape [1]. The main reason for the prohibition was the collapse of 2500 bee colonies in Prekmurje, which was linked to the use of clothianidin on seed corn. On the 1<sup>st</sup> of December 2013 the European Commission banned the use of imidacloprid, clothianidin and thiamethoxam on crops attractive to bees [2]. An EFSA neonicotinoid review is due to be finalised in the second half of 2017.

Honey is a very complex, highly viscous sample with a high sugar content. In addition, the neonicotinoid residues are expected to be present in very low concentrations (<100 ng/g). For successful analysis of honey samples, sample clean-up and concentration of the analytes are necessary. In this study, we compared two different extraction techniques (Solid Phase Extraction and QuEChERS) and two different analysers (HPLC-UV and HPLC-MS/MS) in terms of extraction efficiency, matrix removal, repeatability, limit of detection (LOD), and limit of quantification (LOQ). Once validated, we will apply the method to the analysis of a large number of Slovenian honey samples from different geographic regions and farming regimes in order to monitor the effectiveness of the ban.

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## Distribution of Po-210 in the fish tissues from the Gulf of Trieste (Northern Adriatic Sea)

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Radionuclides from the U-238 decay chain such as Ra-226, Pb-210 and Po-210 are ubiquitous components of the natural radiation, and are thus found in most abiotic and biotic materials leading to direct and indirect human radiation exposures. In the marine environment Po-210 is largely produced from the decay of Pb-210 deposited from the atmosphere. Moreover, natural levels of these radionuclides in aquatic ecosystems may be increased by industrial waste releases. Several studies have demonstrated that the natural alpha emitting radionuclide Po-210 is accumulated to exceptionally high levels in tissues of a variety of marine organisms, well above the levels of the parent radionuclide Pb-210, due to its higher affinity for organic matter (1, 2). Due to its short half-life of 138.4 days, Po-210 as a pure alpha emitter, is one of the radionuclides with the highest radiotoxicity and one of the important sources of the internal dose received by humans from alpha emitters. Marine and freshwater organisms (including algae, bacteria) metabolise Po-210 and can accumulate it into cellular components mostly associated with S-containing proteins.

This study is dealing with accumulation and distribution of Po-210 in various fish tissues of four species (*Lisa aurata*, *Sparus aurata*, *Dicentrarchus labrax* and *Pagellus erythrinus*) collected in the Gulf of Trieste (Northern Adriatic Sea). After collection, each fish was dissected in subsamples of muscle, liver, kidney, gonad, stomach, *pyloric caeca*, intestine, spleen and gills. Each subsample was transferred to a glass beaker, weighted, lyophilised and weighted again to determine the dry to wet ratio. After drying the Po-209 tracer was added to the same beaker and then the sample was digested using HNO<sub>3</sub> and H<sub>2</sub>O<sub>2</sub>. For the gills samples, only HF and HClO<sub>4</sub> were added for digestion. After dissolution a spontaneous deposition of polonium radioisotopes on silver disc was carried out before alpha-particle spectrometric measurement. The results obtained showed that the Po-210 levels (distribution) in fish tissues were as follows: liver > kidney > *caeca* > stomach > intestine > spleen > gonad > gills > muscle. Together with fish samples, Po-210 was determined in locally and timely related samples of seawater, sea sediments, and meso(zoo)plankton. Data obtained were compared to levels found at other Adriatic and Mediterranean areas (1, 2).

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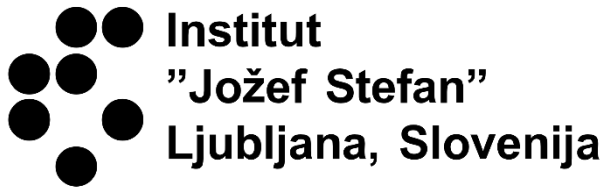
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