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**CNB 2022**

## **17<sup>th</sup> NATIONAL CONFERENCE OF BIOPHYSICS WITH INTERNATIONAL PARTICIPATION**

23-25 September 2022

Târgu Mureș, Romania

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**BOOK OF ABSTRACTS**

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# **BIONANOTECHNOLOGY, BIOSENSORS, BIOCOMPATIBILITY AND BIOMATERIALS**

## MALIGNANT DNA DETECTION BASED ON THE ADSORPTION AFFINITY TO SILVER NANOPARTICLES

Stefania D. Iancu<sup>1</sup>, Vlad Moisoiu<sup>1</sup>, Adrian Bogdan Tigu<sup>2</sup>, Alexandra Maria Chiriac<sup>1</sup>, Luca David<sup>3</sup>, Alexandru Stefan Chis<sup>1</sup>, Georgiana Ion<sup>1</sup>, Zoltán Bálint<sup>1</sup>, Ciprian Tomuleasa<sup>2</sup>, Nicolae Leopold<sup>1</sup>

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**Background:** The global cytosine hypomethylation is a recurrent epigenetic modification in cancer, which also modifies the physico-chemical properties of DNA, including its adsorption affinity to metallic surfaces. In our study, we show that the adsorption rate of genomic DNA (gDNA) onto silver nanoparticles (AgNPs) depends on the global 5-methyl cytosine (5mC) level, a feature that could discriminate between cancer and normal DNA. **Material and methods:** gDNA was extracted from the following immortalized human cell lines: HaCaT (immortalized keratinocytes), SK-HEP-1 (hepatocellular carcinoma), MDA-MB-231 (breast cancer), A549 (lung cancer), TF-1 (erythroleukemia) and HCT116 (colon cancer). The cytosine methylation level was assessed by ELISA, confirming that gDNA from non-cancerous cell lines is hypermethylated (global 5mC levels of 0.91% for HaCaT) compared with gDNA from cancer cells (5mC levels 0.42% for SK-HEP-1, 0.3% for A549, 0.29% for MDA-MB-231, 0.17% for TF-1 and 0.16% for HCT116). Surface-enhanced Raman spectroscopy (SERS) enabled the direct monitoring of adsorbed gDNA, whereas fluorescence emission enabled the tracking unadsorbed (i.e. free) gDNA by labelling with SybrGreen nucleic acid stain. **Results:** SERS and fluorescence spectroscopy showed that the adsorption of gDNA to the metal surface increases with higher 5mC level. In regard to SERS, the relative 5mC concentration of gDNA adsorbed onto AgNPs was determined based on the intensity of the SERS band characteristic to cytosine ring stretching at 790 cm<sup>-1</sup>. A significant positive correlation of the SERS band at 790 cm<sup>-1</sup> with the level of 5mC in the cell lines was found (R<sub>Pearson</sub>=0.94, p=0.005). Independent of SERS measurements, we determined the amount of free (i.e. unadsorbed) gDNA to the silver surface by fluorescence spectroscopy. The results of the fluorescence spectroscopy showed an exponential relation between the proportion of adsorbed gDNA (A) and the nanoparticle to gDNA ration (r) of the form:  $A=A_0\exp(-kr)$ . The exponential decay decreased with higher 5mC level, from k=5.85 for HCT (0.16% 5mC) to k=2.95 for SK-HEP-1 (0.42% 5mC) and k=1.28 for HaCaT (0.91% 5mC). This result emphasizes that the amount of unadsorbed gDNA is negatively correlated with the 5mC level. **Conclusions:** Both optical methods showed a higher adsorption rate of non-cancerous gDNA, as compared to malignant gDNA, which we linked to the higher degree of cytosine methylation of non-cancerous gDNA. Thus, the dependence of gDNA adsorption affinity on the global 5mC levels opens new avenues for the development of nanoparticle based biosensors for cancer detection.

**Keywords:** cancer, DNA, nanoparticles

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## TOXICOLOGICAL EVALUATION OF NANOPARTICLES ON CELL CULTURE

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**Background:** Epithelial and pulmonary cells may change their behaviour when interacting with nanomaterials. Such changes could be relevant for the development of new technologies and for the management of graphene-based particles regarding health and safety. **Material and methods:** MTT assay was used for evaluating the cell viability status and for finding the optimal concentration for the further experiments. Oxidative changes were evaluated by measuring the enzymatic and non-enzymatic antioxidants, such as catalase activity, superoxide dismutase activity and glutathione concentration. **Results:** Following the light microscopy evaluation of cells after exposure to nanoparticles, their morphology may appear to be affected, and biochemical investigations could demonstrate significant intracellular oxidative stress. However, an increased sensitivity of cells to a particular type of nanoparticles could be easily observed. **Conclusions:** *Summa summarum*, nanoparticles may have an aggressive or toxic effect on human cell cultures.

**Keywords:** cell culture, nanoparticles, oxidative stress, optical microscopy



## LT4 QUANTIFICATION USING BIOMOLECULAR INTERACTIONS AND NANOMATERIALS

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**Background:** Levothyroxine (LT4) is the artificial form of the thyroid hormone thyroxine (T4) used as a medicine in a variety of thyroid disorders, such as hypothyroidism. Many biomolecules, but also medication, such as LT4, are transported by serum albumin (BSA). Since there are many factors that can influence the transport of LT4 in the blood, new detection methods are needed as simple and reliable tools for monitoring the effect of LT4 administration, which are currently mainly achieved through clinical observations. **Material and methods:** Monitoring the interaction of LT4 with albumin [1] was studied using UV-Vis, fluorescence, and infrared spectroscopic measurements. Fluorescence quenching and electrochemistry were used as complementary analytical methods for LT4 detection. **Results:** Spectroscopic studies highlight the presence of conformational changes in the structure of serum albumin under the action of denaturing factors. These changes lead to increased structural stability of the protein complexed with LT4 and a prolonged storage time of LT4 in blood plasma. In addition, the BSA-LT4 interaction can be used for the development of spectroscopic biosensors which can detect LT4 down to 230 nM. To improve the sensitivity, electrochemical sensors based on nanoparticles were also implemented. Carbon nanotubes [2] and bimetallic nanoparticles on graphene oxide sheets [3] were used to develop free-label sensors for LT4 with detection limits between 30 nM and 6 pM. **Conclusions:** UV-Vis, fluorescence and infrared spectroscopic measurements were used to characterize, compare, and optimize the biomolecular interactions between albumin and LT4. The most suitable method for the analytical detection of LT4 at pM level was based on nanoparticle-based electrochemical sensors.

**Keywords:** levothyroxine, biomolecular interactions, spectroscopy, biosensors, nanomaterials

## FOLATE FUNCTIONALIZED SILICA NANOPARTICLES CELLULAR UPTAKE - LOCALIZATION AND QUANTIFICATION IN 3D RECONSTRUCTIONS

Luminita Claudia Miclea<sup>1</sup>, Mona Mihailescu<sup>2</sup>, Nicolae Tarbă<sup>3</sup>, Ana-Maria Brezoiu<sup>4</sup>, Ana Maria Sandu<sup>5</sup>, Raul-Augustin Mitran<sup>6</sup>, Daniela Berger<sup>4</sup>, Cristian Matei<sup>4</sup>, Mihaela G. Moiescu<sup>1</sup>, Tudor Savopol<sup>1</sup>

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**Background:** Nano scaled therapeutics and diagnostics based on drug delivery systems led to a new research domain, nanotheranostics, which holds great promise for anti-tumoral advanced medical treatments. Present in vitro study examined the impact on cellular metabolism of unlabeled mesoporous silica nanoparticles (MSNs) functionalized with folate and loaded with cytotoxic Irinotecan (Iri). Targeting folate receptors, the MSNs played the role of "trojan horse" in cancer cells in delivering Iri. **Material and methods:** Two modules from CytovivaR device were used: enhanced dark field microscopy (eDFM) with fluorescence imaging and hyperspectral microscopy (HSM). Caco-2 and NIH3T3 cells were grown for 24h, then incubated with MSNs for additional 24h or 48h. Further on, their metabolic viability was assessed using colorimetric formazan-based assay (MTS). For HSM, cells were used fixed and unlabeled. For eDFM cells were stained for cytoskeletal actin with AlexaFluor488 Phalloidin and for nucleus with DAPI. Acquired Z-stacks of fluorescence and dark field images were subject to CytovivaR plugins and MATLAB based lab-made scripts. Therefore, we extracted pixel based spectral profiles, made cellular 3D reconstructions and quantified MSNs intracellular distribution in digitally segmented nucleus and cytoplasm compartments. **Results:** For all incubation times, folate proved to be a successful enhancer for Iri cytotoxicity, which was more evident for Caco-2 cells than NIH3T3. The differences in response between the cell lines mirror the MSNs intracellular penetration, higher for cancer cells, which are known to have an elevated expression of folate receptors. The digital processing of microscopic images showed that folate successfully increased the intracellular MSNs presence and favored their localization in the proximity of nucleus. **Conclusions:** The eDFM

and HSM combination allowed to assess quantitatively the MSNs cellular uptake. Dedicated innovative MATLAB routines were developed for 3D reconstructions to reveal their intracellular localization. **Acknowledgments** : This work was supported by projects PN-III-P2-2.1-PED2019 (contract no. 525PED/2020) and Project No. P\_36\_611, MySMIS code 107066.

**Keywords:** mesoporous silica nanoparticles, cellular 3D reconstruction, nanoparticle intracellular localization, enhanced dark field microscopy, hyperspectral imaging

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## NANOSCALE BIOPHYSICAL PROPERTIES OF SINGLE VIRUS PARTICLES

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**Background:** The advancement of novel perimental tools has led to the establishment and development of single-molecule biophysics, a field that permits access to the mechanistic detail of biological molecules. The use of single-molecule biophysical techniques in exploring viruses provides insight into their properties. Here we review our recent investigations into the nanoscale biophysical properties of the enveloped ssRNA virus SARS-CoV-2 and its variants, and the life cycle of the dsDNA bacteriophage T7. **Material and methods:** We used AFM, TIRF phase contrast microscopy to image and mechanically manipulate individual virions and bacterial host cells. **Results:** Unfixed SARS-CoV-2 showed a dynamic surface brush due to the rapid spike motion. Virions were compliant and able to recover from extreme mechanical stress. The global virion structure was temperature resistant but gradually lost spikes. Alpha and delta variants had significantly smaller radii than the wild type. T7 virions attached reversibly to the E.coli membrane through two-dimensional diffusion. Stable anchoring was achieved by spatially isotropic binding. T7 infection led to the launch of an irreversible program in the host in three steps: a) bacterial surface roughening; b) membrane blebs formation; c) host cell was lysis followed by the release of phage progeny. Partial DNA ejection from T7 could be evoked in vitro by photothermal excitation. **Conclusions:** The dynamics and the mechanics of SARS-CoV-2 affect its stability and interactions. It is the most compliant virus investigated so far and possesses a remarkable mechanical resilience. The variants have an increased specific surface that likely contributes to their greater infectivity. The T7 phage virions apparently find their receptors on the E.coli surface by diffusion-driven rolling. The partial DNA ejection revealed that genome release is mechanically controlled to prevent premature delivery of host-lysis genes.

**Keywords:** Atomic force microscopy, optical tweezers, single-molecule mechanics, total internal reflection fluorescence

# **(BIO-)SPECTROSCOPIC TECHNIQUES**

## SERS LIQUID BIOPSY FOR MEDICAL DIAGNOSIS

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**Background:** Surface-enhanced Raman scattering (SERS), coupled with machine learning algorithms is emerging as a novel strategy for biofluid analysis. We aim to provide here an overview on the molecular information derived from serum, urine and saliva SERS analysis, and to highlight the potential of small, portable Raman instruments operated in clinical environment, in performing SERS liquid biopsy for classification of patient and control samples.

**Material and methods:** In SERS, only molecules that adsorb to the surface of nano-substrates contribute to the spectroscopic signal. The adsorption to the metal surface occurs competitively, thus from the complex biofluid matrix, purine metabolites, occupy most of the available adsorption sites, due to their high affinity for the metal surface. Further, we showed that the number of adsorption sites for anionic analytes can be increased by supplementing the colloidal solution with cations such as Mg<sup>2+</sup>, leading thus to higher SERS intensities. In contrast, iodine, due to its high surface affinity, replaces anionic purine metabolites on the surface, and facilitates the adsorption of proteins. **Results:** The SERS spectra of (deproteinized) serum, urine and saliva show striking similarities. Beside purine metabolites, SERS bands of ergothioneine and resonance Raman bands of carotenoids were identified in serum samples, and SERS bands of creatinine in urine samples. We analyzed the SERS spectra of serum samples from 53 patients with gastrointestinal tumors and 25 control subjects. For sample classification, we used a quadratic discriminant analysis, PCA-QDA, and cross-validation, yielding a classification accuracy of 77%. In another study, we analyzed urine samples from prostate cancer patients and control subjects, formed by patients with benign prostate pathology. The classification was performed with external validation (the classification model was developed without the samples from the validation data set) the classification accuracy being around 80%, for the used algorithms: kNN, Naïve Bayes, Random Forest, Support Vector Machine and Logistic Regression. Lastly, saliva probes were analyzed by SERS for the classification of samples from patients with Sjögren syndrome and controls. The cross-validated PCA-LDA analysis of the SERS spectra yielded a total accuracy of 94%. **Conclusions:** Concluding, SERS liquid biopsy shows potential for the development of medical screening methods. Miniaturization of Raman instruments is a key aspect in the translation of Raman methods in clinical settings. However, there is a need for standardization of the experimental parameters. In this regard, we obtained best results on urine biofluid, by using the green and red laser line and silver nanoparticles as SERS substrate.

**Keywords:** surface-enhanced Raman scattering, liquid biopsy, machine learning, purine metabolites

# **MODELING, BIOMOLECULAR SIMULATIONS AND COMPUTATIONAL BIOPHYSICS**

## COMPUTATIONAL ASSESSMENT OF THE HUMAN HEALTH EFFECTS OF THE STEREOISOMERS OF DIFENOCONAZOLE

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**Background:** Difenoconazole (DFC) is a triazole fungicide widely used in the management of agricultural crops. It contains two chiral centres and has four stereoisomers: (2R,4R)-, (2R,4S)-, (2S,4R)- and (2S,4S)-difenoconazole. The marketed product contains a mixture of all stereoisomers. Residues of difenoconazole have been identified in many vegetables, fruits and even in drinking water. **Material and methods:** A computational approach has been used to predict the absorption, distribution, metabolism, excretion and toxicity (ADMET) profiles and to evaluate the human health effects of the DFC stereoisomer. **Results:** Several toxicological endpoints have been identified for all the DFC stereoisomers: inhibition of the human cytochromes, hepatotoxicity, mutagenicity, moderate potential to produce endocrine disrupting effects, skin sensitization potential, high affinity for the plasma proteins. Few distinguishing results have been obtained for the (2S,4S)-difenoconazole as it showed reasonable probabilities to produce both cardiotoxicity and carcinogenicity, and to negatively affect numerous nuclear receptors. **Conclusions:** The outcomes of this study emphasize the possible stereoselective effects of DFC on the human health. Taking into account that chiral compounds used in agricultural practice represent more than 30%, their stereo selectivity should be considered in the safety assessment and regulatory decisions.

**Keywords:** difenoconazole, stereospecificity, ADMET properties

## MULTICELLULAR SELF-ORGANIZATION IN BIOPRINTED MODELS OF THE TUMOR MICROENVIRONMENT

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**Background:** Cancer progression is influenced by the tumor microenvironment (TME). Next to cancer cells, the TME includes tumor-associated fibroblasts, immune cells, mesenchymal stem cells, and vascular cells. Bioprinted cells, however, remodel the adjacent extracellular matrix, and take advantage of their motility to establish firm bonds with other cells and/or biomaterials. **Material and methods:** We studied structure formation in bioprinted models of the TME. We used extrusion-based bioprinters to build models of the TME. SK-BR-3 breast cancer cells dispersed in a hydrogel droplet were wrapped by rings of the same hydrogel loaded with tumor associated fibroblasts and peripheral blood mononuclear cells harvested from breast cancer patients. The tissue constructs were cultured for two weeks and cryosectioned for histological evaluation. To investigate the interactions responsible for the observed phenomena, we built lattice models of the bioprinted constructs and simulated their evolution using Metropolis Monte Carlo methods. **Results:** Hoechst staining demonstrated that the cells remained viable and remodeled the hydrogel. Hematoxylin and eosin staining of histological sections indicated that cells proliferated and formed heterotypic aggregates of cancer cells and peritumoral cells. The computational model represented the biological system, at single-cell resolution, in terms of 4 types of particles: tumor cells, peritumoral cells, volume elements of the hydrogel, and volume elements of the cell culture medium. Based on the differential adhesion hypothesis, computer simulations reproduced most features of the experimentally observed structure formation, but did not account for the superficial localization of the aggregates. Depending on model parameters, peritumoral cells enveloped or infiltrated cancer cell aggregates, as expected from TAFs and immune cells, respectively. **Conclusions:** Our tissue constructs allowed for refining the co-culture conditions of 3 cell types present in the TME. Future studies will also consider incorporating vascular structures. Furthermore, the computational model will be extended to describe the self-organization of all the cell types of the bioprinted constructs.

**Keywords:** breast cancer, tissue engineering, computational model

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## THEORETICAL STUDY OF LIGHT-INDUCED CROSSLINKING REACTION BETWEEN PYRIMIDINE DNA BASES AND AROMATIC AMINO ACIDS

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**Background: Abstract** : Phenomenon called DNA-protein crosslinking (DPC), when covalent bond is formed between different fragments of DNA bases and protein side chains, is on the one hand considered extremely harmful process, as they can effectively block gene transcription and DNA replication, but on the other hand is the base of chromatin immunoprecipitation (ChIP) technique, which is a powerful tool to investigate the difference between the native-chromatin and that of cross-linked with proteins (XChIP). Using a one-step DNA-protein cross-linking reagent such as formaldehyde does not always lead to successful binding of the protein to DNA [1,2]. For this propose, the ultraviolet light induced DNA-protein crosslinking could be an appropriate solution since it can be used to selectively bind the proteins to DNA based on the specific interaction between amino acids and DNA bases at the level of electronic excited states. [3]. Considering the benzene-uracil and phenol-uracil complexes as model systems, the light induced DPC reaction between the aromatic amino acids and pyrimidine-type building blocks of DNA was investigated at quantum mechanics level using the density functional theory (DFT) method. Accordingly, the low-lying electronic excited states, their relaxation pathways and reaction energetics were computed. Based on these results, different relaxation pathways for electronically excited states have been identified. These can either lead to the initial dimer-type geometric configuration or to dimerization between the aromatic rings of the uracil-benzene complex. The energetic conditions necessary for the occurrence of the resulting pathways have been discussed. It was also shown that the presence of different conical intersection points on the potential energy hypersurface between the aromatic fragments can basically influence the formation of new covalent bonds and implicitly the formation of the crosslinking between the proteins and DNA chains [4].

**References:** [1.] Nowak DE, Tian B, Brasier AR. (2005) Two-Step Cross-linking method for Identification of NF- $\kappa$ B Gene Network by Chromatin Immunoprecipitation. *Biotechniques*, 39:715–725. [2.] Bosisio D, Marazzi I, Agresti A, Shimizu N, Bianchi ME, Natoli G. (2006) A hyper-dynamic equilibrium between promoter-bound and nucleoplasmic dimers controls NF- $\kappa$ B-dependent gene activity. *EMBO J.*, 25:798–810. [3.] Stützer A, Welp LM, Raabe M, Sachsenberg T, Kappert C, Wulf A, et al. (2020). Analysis of Protein-DNA Interactions in Chromatin by UV Induced Cross-Linking and Mass Spectrometry. *Nat. Commun.* 11:5250. [4] Bende A, Farcaş A-A, Toşa V (2022) Theoretical study of light-induced crosslinking reaction between pyrimidine DNA bases and aromatic amino acids. *Front. Bioeng. Biotechnol.*, 9:806415. **Material and methods:** - **Results:** - **Conclusions:** -

**Keywords:** DNA-Protein crosslinking, DFT, Conical Intersection, uracil, phenylalanine

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## BIOPHYSICS OF INTELLIGENCE

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**Background:** Intelligence is the result of biophysical processes in the network of neurons in our brain. To model the computations underpinning intelligence, artificial neural networks (ANNs) are often used. While ANNs took inspiration from biological neuronal networks, a salient difference is that they abstract away all the details, typically considering a neuron to be summation followed by a nonlinearity and synapses just a weight. Biophysically detailed neuronal models can be simulated, but they are not used to solve tasks. **Material and methods:** I will present methods showing that networks with neuronal and synaptic models of intermediate complexity can be trained with backpropagation, which allows them to learn tasks in artificial intelligence settings. **Results:** I will show that such networks can have computational benefits over standard ANNs. But, most importantly, I will show that given the same tasks, networks with more complex components can learn to solve them differently than ANNs. In one example, I will compare experimental results on mice which learned to detect changes in input images, to two models trained on the same task: an ANN and a network with more realistic synapses. While both models learned the task, the more realistic network reproduces salient aspects of the neuronal recordings as well as the type of errors the animal makes. More interestingly, it also reacts similarly when surprising stimuli are introduced. **Conclusions:** While the example I provided shows the standard ANNs are sometimes too simple to capture salient elements of computations, it remains an open question to what level of resolution we need to simulate

biological neural networks to comprehensively describe its computations.

**Keywords:** Neural networks, Computation, Synapse

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## HOW DO PIONEER TRANSCRIPTION FACTORS UNRAVEL GENOMIC DNA ?

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**Background:** Gene regulation and cellular transitions require large structural rearrangements in the genome to facilitate accessibility to DNA. The genomic DNA is wrapped in chromatin, a dynamic structure of arrays of repetitive units with variable size and compactness. Its fundamental unit, the nucleosome, wraps 145-147 DNA basepairs around an octamer of four histone proteins. The histones have a structured core and unstructured terminal tails acting like moving antennas between DNA segments. Chemical modifications of the tails define whether chromatin is open and active or closed and inactive. Among modulators of chromatin dynamics, pioneer transcription factors induce cellular transitions by binding to both accessible DNA and closed, inactive regions of chromatin. How pioneer factors facilitate chromatin opening is not known. We discovered the structural basis of the interaction between Oct4, a pioneer regulator and inducer of stem cell pluripotency and the nucleosome at atomic resolution. First, from >25  $\mu$ s of atomistic molecular dynamics simulations of free nucleosomes, we revealed how the mobility of histone tails regulates the transient opening of genomic nucleosomes bound by Oct4. The opening depended on DNA sequence and was facilitated by the unbinding of the tails from the DNA. Then, we validated experimentally the positions of the Oct4 binding sites and built models of these nucleosome with Oct4 bound. From >50  $\mu$ s of simulations, we found that Oct4 requires intrinsic nucleosome flexibility to bind. Moreover, depending on the binding site location, Oct4 either stabilizes partly open nucleosome conformations or induces a large opening of the nucleosome. The extent of Oct4's impact depends on the mobility of histone tails, and the motion of its own DNA binding subdomains. Our findings provide an unprecedented view of pioneer transcription factors in action on complete, genomic nucleosomes and have implications for understanding chromatin dynamics during cellular transitions. **Material and methods:** - **Results:** - **Conclusions:** -

**Keywords:** pioneer transcription factor, nucleosome dynamics, chromatin dynamics, cell fate transitions, molecular dynamics simulations

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## COMPUTER SIMULATIONS OF THE INTERACTION OF DNA AND DENDRIMERS WITH PROTEIN PORES: EXAMPLES AND THEORETICAL MODELS

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**Background:** Molecules pass through membrane pores one at a time, and therefore this process is to be fundamentally understood at the single-molecule level. In my talk, I will present computer simulation results obtained by my research team that showcase several examples of pore transport. Examples will include protein translocation through mitochondrial pores, DNA ejection from bacteriophage viruses, and dendrimer transport in the context of single-pore current measurements. **Material and methods:** On the methodological side, two techniques developed for these simulations will be showcased. One uses molecular-dynamics derived parameters to scale up the dynamics on the micrometer-microsecond scale via the Kirchhoff theory for elastic rods. The other allows for the enhanced calculation of long-time kinetics in complex systems and is based on the Wiener stochastic path integral formalism: assigning weights to Langevin trajectories of artificially biased dynamics allows for the calculation of time correlation functions for the unbiased system of interest via re-weighting. **Results:** Our computational results are compared to and suggest models for single-molecule experiments (force spectroscopy and single channel ionic current recordings) as well as for bulk measurements in cryo-electron microscopy. **Conclusions:** The analysis of the models point to the need to further develop enhanced sampling methods for long time and large scale simulations

**Keywords:** statistical mechanics, molecular dynamics, elastic continuum



# **OTHER METHODS AND TECHNIQUES IN BIOPHYSICS**

## STUDY ON THE LINK BETWEEN HUMAN PAPILLOMA VIRUS INFECTION AND THE PRESENCE OF SOME VIRUSES, PARASITES, MYCOSES, NOSODES AND SKIN DISORDERS

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**Background:** Human papilloma virus (HPV) is a DNA virus that belongs to the Papillomaviridae family and it usually manifests as skin or genital mucosal lesions, although it can occur in another mucosa as well. The purinergic system has an important role in the physiopathology of inflammations, tumors, surgical complications and other organ diseases such as kidney, heart, when ATP becomes extracellular and is broken down into extracellular adenosine (Ado) by enzymes. ATP induces the attraction and recruitment of antigen presenting cells and induces pro-inflammatory responses (citokines, interleukines, reactive oxygen species) while Ado acts in immunosuppression, limiting the proliferation and activation of effector T cells. The aim is to study the appearance of viruses, parasites, mycoses, nosodes, skin pathologies in HPV positive patients, to be used in the development of a Romanian cervical cancer patients management plan, in the context of the project entitled "Program of prevention, early screening, diagnosis and early treatment of cervical cancer – Romania Center Region", POCU/826/4/9/138603, code project SMIS 138603, which started in November 2020 in Targu Mures, until December 2023. **Material and methods:** In our study in 2022 June we determined in Mures county for 35 patients infected with HPV and 15 patients without HPV using the MORA-bioresonance device invented by Franz Morell their infections with other viruses, parasites, mycoses, nosodes and skin disorders. Mora Bioresonance identifies 8 types of viruses, 20 types of parasites, 21 types of mycoses and 11 types of skin disorders. The numerical results are obtained by Excel and Graphpad programme, in order to identify the statistically significant (pResults: Patients with HPV infection were aged in 30-79 years and patients without HPV infection were aged in 16-63 years old. Of the 35 patients with HPV infection 30 patient has Epstein-Barr infection (85.71%), 2 patients had coxsackie virus (5.71%) and the others 3 patients had the different types of herpes viruses (8.57%). Of the 35 patients with HPV infection 2 patients had all kind of viruses (5.71%). In case of parasites infection 14 patient had echinococcus (40%) and other 14 patient giardia lamblia (40%) and from these patients 5 had both parasites infections. In case of mycoses from 35 patients only 1 had all types of candida infection. The more frequency skin disorders are initial form of melanomsarcoma (11 patient, 31.42%), melanoma (7 patients, 20%), and basiloma (4 patient, 11.42%). (p=0.0336) from viruses and Echinococcus with Giardia lamblia infection (p=0.0395) from parasites. **Conclusions:** The most common skin diseases, e.g warts are caused by HPV. Among those infected with the human papilloma virus (HPV), there is not only one virus infection in their body, but also mixed infection. In addition to medical treatment, we recommend a dietary consultant for these patients which consist in 5 steps: hydration, deworming-detoxification of the body, digestive system cleansing, cellular nutrition and immune protection.

**Keywords:** bioresonance, parasites, nosodes, human papilloma virus, skin disorders

# **(BIO-)PHYSICAL TECHNIQUES APPLIED IN PHYSIOLOGY, MEDICINE AND THERAPY**

## BIOFABRICATION OF BREAST CANCER MODELS USING EXTRUSION BIOPRINTING

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**Background:** The tumor microenvironment (TME) includes a diversity of cell types, which secrete soluble factors along with a specific extracellular matrix. A growing body of evidence suggests that the interaction between the tumor and its microenvironment plays a critical role in cancer development and its resistance to therapy. Model tissues that replicate the composition and structure of the native TME have attracted much interest because they might reveal novel therapeutic targets. **Material and methods:** In this work, we employed three-dimensional (3D) bioprinting of tissue constructs that recapitulate several features of the TME. The tumor was represented by a cancer cell-laden hydrogel droplet, whereas its milieu was modeled by hydrogel tori loaded with tumor associated fibroblasts and peripheral blood mononuclear cells, in equal proportions. The tumor model comprised SK-BR-3 breast cancer cells, whereas the peritumoral cells came from female patients with breast cancer. Both compartments contained one million cells/mL. The model tissues were built using two different types of extrusion-based bioprinters INKREDIBLE and BIO X. The G-code instructions for the two bioprinters were generated using original Python scripts. **Results:** The TME model tissues were bioprinted into 24 well plates. Histological cryosections prepared after two weeks of in vitro culture demonstrated that the co-culture conditions established in this study ensured cell growth and proliferation. Then, the tumor models were implanted subcutaneously in CD1 Nu/Nu immunosuppressed mice. After 28 weeks in vivo, the constructs became vascularized and grew about 4-5 times in diameter. Histopathological evaluation revealed that the excised tumors increased in cell density and complexity. Moreover, the microarchitecture of the excised construct was akin to a native TME. **Conclusions:** Our work presents a robust methodology for building cancer models of complex geometry and composition. They might serve fundamental research, enabling one to decipher cell-cell and cell-stroma interactions, as well as applicative research, paving the way towards personalized therapy.

**Keywords:** extrusion bioprinting, breast cancer models, tumor microenvironment,, in vivo evolution

## UNDERSTANDING THE BASIC MECHANISMS OF BLOOD-BRAIN BARRIER REACTIVITY TO LOW-ENERGY ACCELERATED PROTONS

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**Background:** The most common treatment for cerebral cancer is represented by a combination between chemotherapy and radiotherapy, although the chemotherapy is very limited due to the strict permeability control of the BBB. The exposure of cerebral cells to ionizing radiation comes with a lot of side effects. In particular, the brain microvascular endothelial cells can undergo endothelial activation, dysfunction, reactive oxygen species formation, BBB permeability elevation. Thus, the main objective of our study is to understand how proton beams affects the brain microvascular endothelial cells functionality. **Material and methods:** Mouse brain microvascular cell line bEnd.3 was used as an in vitro model for BBB. One beam line of a TR19 cyclotron was adapted for in vitro radiobiology experiments. Cell cultures were exposed to proton irradiation (< 10 MeV, doses range of 0-10 Gy, dose rate of 1 Gy/min). The cytotoxic (clonogenic and MTT assays), genotoxic (micronuclei and g- H2AX assays) and functional (purinergic signaling pathway and wound healing assay) effects were analyzed. **Results:** An inhibition (~90%) of the cellular proliferation and a strong increase of micronuclei number doses over 5 Gy were observed. DNA repair capacity was significantly diminished by the increased values of the dose (~100%) and the linear energy transfer - LET (~20%). At intermediate doses and high LET values the cell relative migration rate was diminished (~25%). In the case of the ATP-dependent purinergic signaling pathway non-linear influences have been observed and a more complex analysis of the specific parameters is necessary. **Conclusions:** Radiation

dose and LET non-linearly modulate the cells responses. These preliminary data suggest that proton beams in the range of Bragg peak diminishes the recovery capacity of brain microvascular endothelial cells with respect to the dose and LET. The results emphasize the necessity to gather more information about how the cell respond in this type of irradiation.

**Keywords:** calcium imaging, blood-brain barrier, ionizing radiation

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## THE 'ELECTRIC' SIGNATURE OF A PROARRHYTHMOGENIC DRUG

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**Background:** Any drug, either commercial or newly-developed, should be tested for its proarrhythmogenic risk, in order to be approved by the international drug authorities. The Comprehensive in vitro Proarrhythmia Assay (CiPA) is an European initiative to evaluate the proarrhythmogenic capacity of drugs. Briefly, this approach is based on the 'electric' signature of a drug by integrating patch-clamp recordings of cardiac ion channels with *in-silico* models of human cardiomyocytes' electrical activity. The aim of our study was to test the proarrhythmogenic risk of different drugs using the CiPA approach. **Material and methods:** We performed patch-clamp recordings on human cardiac channels, e.g. hERG1, hNav1.5, hKir2.1, hKv7.1+hMinK, stably or transiently transfected into HEK293T cells, or on human cardiomyocytes. We recorded voltage-gated Na<sup>+</sup> currents, L-type Ca<sup>2+</sup> currents, transient outward K<sup>+</sup> currents through hERG channels, delayed rectifier K<sup>+</sup> currents and "funny" hyperpolarization-activated currents, and we also computed the proarrhythmogenic risk predictors. **Results:** We tested a 12 drugs CiPA panel with low, intermediate, and high proarrhythmogenic risk. We modified the hERG blocking and unblocking rates for cisapride, quinidine, terfenadine, bepridil, sotalol, domperidone in line with our data and we evaluated the effectiveness of multiple proarrhythmogenic risk predictors based on action potential and intracellular calcium dynamics. We also demonstrated that cloroquine and hydroxychloroquine, belong to the intermediate proarrhythmogenic risk group. **Conclusions:** In conclusion, we analyzed the electric 'signature' of several drugs to assess their proarrhythmogenic risk. Currently, we extended our study on two newly FDA-approved antiepileptic drugs, e.g. cenobamate and fenfluramine. Future studies will analyze their interaction with the blood brain barrier.

**Keywords:** proarrhythmogenic risk, drug safety, patch-clamp, human induced pluripotent stem cell-derived cardio

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## USING LOW ENERGY ACCELERATED PROTON BEAMS FOR IN VITRO RADIOBIOLOGY RESEARCH AT IFIN-HH

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**Background:** The specific energy deposition of accelerated ion beams along the path across the matter (the Bragg peak curve) makes the ion beams very attractive tools for biomedical application. In the last decade, the high-power laser driven ionizing beams are considered to have a very high potential to be used in biological and medical applications, the very high available dose rate being an important advantage. For this reason, the availability of facilities for in vitro studies focused on basic research regarding the details of accelerated ions interactions with living matter is of high importance. **Material and methods:** In the last couples of years at IFIN-HH two new setups allowing exposure of biological cells cultures to accelerated protons have been developed using a tandem accelerator (3 MV Tandetron) and a 19 MeV cyclotron (TR 19). Adapted cell cultures holders and appropriate dosimetry protocols (based on a Markus ionizing chamber, Gafchromic films, CR 39 plastic detectors and silicon detectors) have been implemented to allow reproducible experimental exposures of biological samples. **Results:** A dose range of 0.5 - 10 Gy (dose rate of ~1Gy/min) is available at both of the setups for energies of 2-3 MeV (3 MV Tandetron) and 3-11 MeV (TR 19 cyclotron). The 3 MV Tandetron setup benefits of a control of exposure duration in the range of ms-seconds allowing to cover dose rate range of 5 cGy/s-500 Gy/s being suitable for high vs low dose rate irradiation conditions comparison oriented experiments. Research project probing the cell survival, ROS production, apoptosis induction and cell cycle modulation by exposure of tumoral or normal cells to proton beams at these setups are already in work and will be presented in brief. **Conclusions:** Low energy (2-11 MeV) accelerated proton beams are available at IFIN-HH for in vitro radiobiology experiments.

**Keywords:** radiobiology, accelerated particles, hadrontherapy

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## BIONICS - STRONGLY CONNECTED TO BIOPHYSICS

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**Background:** This presentation has both a pedagogical and a methodological character emphasizing the strong connection between Bionics and Biophysics. It is known that the initial goal of Bionics was the transfer of solutions experimented by the living matter to the techniques in order to realize cheaper, highly efficient and ecological technologies and devices. In the meantime, the application area of Bionics was successfully extended to other domains: agriculture, sports, entertainment and, especially, medicine. Some outstanding examples of surprising biological solution transfer to medicine are briefly presented. From these examples one can deduce that the sophisticated applications of Bionics are strongly stimulated by the advances in Biophysics as it is also synthesized by the author in his next book to be published this year in Bucharest University Press. **Material and methods:** -

**Results: - Conclusions:** References Popescu A. I. Bionics, Biological Systems and Optimal Design Principle, Acta Biotheoretica, 46, 299-310, 1998 Popescu A. I., The Principle of Optimal Design as a Legitimacy of Bionics, Proceedings of the Romanian Academy, Series A, 4, 15-18, 2003 Raicu V., Popescu A. I., Integrated Molecular and Cellular Biophysics, Springer, 2008 Wallace G. G., Moulton S. E., Kapsa R. M. I., Higgins M. J. Organic Bionics, Wiley-VCH, First Edition, 2012 Popescu A. I., Biophysics. Current Status and Future Trends, Publishing House of the Romanian Academy, 2016 Chilom C. G., Popescu A. I., High Performances of Biosystems, Bionics and beyond Bionics, Annual Scientific Conference. Faculty of Physics, University of Bucharest, June 18, 2021 Chilom C. G., Popescu A. I., Bionics: Some Outstanding Applications in Medicine, Annual Scientific Conference. Faculty of Physics, University of Bucharest, June 24, 2022 Popescu A. I., Tratat de Bionică. Perspectivă Generală cu Explicații Biofizice, pp. 300, Editura Universității din București, 2022 (under print)

**Keywords:** Bionics, Biophysics, Artificial Enzymes, Bacteriorhodopsin, Retina Prosthesis

# **MEMBRANE AND CELLULAR BIOPHYSICS**

## ORDER CHANGES OF LIPIDS IN MEMBRANES EXPOSED TO ELECTROPERMEABILIZATION PULSES

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**Background:** During electropermeabilization (EP) the cell membrane permeability is increased by exposure of cells to well characterized electric pulses. The molecular basis of this phenomenon is yet to be fully comprehended. Here, we evaluated the packing changes of lipids in membranes bilayer when exposed to electropermeabilization pulses by measuring the kinetics of generalized polarization (GP) parameter. The fluorescence was measured in real time and simultaneously to electric pulses application. **Material and methods:** Cuvette-adapted electrodes were built having a geometry that was ensuring a highly homogenous electric field and allowing excitation/emission light beams to pass. Laurdan-labelled NIH3T3 cells (murine embryonic fibroblasts) were used. GP was measured before, during and after application of various EP pulses as number or amplitudes. Isotonic buffers with various electric conductivities were used. ROS production induced by EP pulses was also evaluated using a DCFH-DA based method. **Results:** A pair of flat electrodes with 6 mm gap in-between, having a rectangular window of 2×6 mm on one of the electrodes, was used to apply the EP pulses. A highly homogenous electric field was obtained as shown by simulations in COMSOL. In high conductivity buffers there was a thermal effect of pulses which produced a negative deflection of GP. As expected, the GP deflection was proportional to the number of applied pulses and strongly depending on the buffer conductivity. In conditions in which no thermal effect appeared, EP pulses produced a positive deflection of GP. This deflection has been associated to the production of ROS and lipid peroxidation induced by EP. **Conclusions:** To do fluorescence and temperature measurements before, during and after EP of cells in suspension, an original experimental system was produced. A correlation between GP kinetics and the unpacking of membrane lipids triggered by EP was demonstrated. This work was partially funded by UEFISCDI project PN-III-P2-2.1-PED-2021-0451, contract no. 596PED/2022

**Keywords:** electropermeabilization, fluorescence, generalized polarization, ROS

## PROTON IRRADIATION PROMOTES MORPHOLOGICAL AND FUNCTIONAL CHANGES IN HEPG2 CELLS

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**Background:** The use of proton therapy for treatment of various cancers has showed the need to contribute to a better understanding of the cellular mechanisms involved. The aim of this study was to study the effects generated by the protons in hepatocarcinoma cells. **Material and methods:** We used to irradiate HepG2 human hepatocarcinoma cells a 3 MV Tandetron<sup>TM</sup> accelerator (existing facility in IFIN-HH), at doses between 0 - 3 Gy and a dose rate of 1 Gy/min. We investigated the morphological and functional changes in the cells at different time points post irradiation. **Results:** The influence of radiation on cell long-term replication was investigated using colony formation assay. Changes induced by protons at the mitochondrial level were shown by increased ROS and ATP levels as well as a decrease in the mitochondrial membrane potential. Furthermore, the cell cycle, caspase 3/7 activity and senescence induction were investigated at 24h post irradiation. Finally, we analyzed by microscopy the morphological and ultrastructural changes at the membrane level and the nucleus of the irradiated cells. **Conclusions:** Our study showed that protons can induce morphological and functional changes in hepatocarcinoma cells.

**Keywords:** hepatocarcinoma, proton radiation, reactive oxygen species, apoptosis, cell cycle arrest



# POSTERS

## SERS LIQUID BIOPSY IN BREAST CANCER. WHAT CAN WE LEARN FROM SERS ON SERUM AND URINE?

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**Introduction:** Surface-enhanced Raman scattering (SERS) is a spectroscopic method that has a high level of accessibility in biofluid analysis. This study presents the applicability of label-free SERS liquid biopsy on serum and urine samples from breast cancer patients (BC) and controls (CTRL) in order to analyse the metabolic informations of the SERS spectra and to compare the classification performance of five different machine learning (ML) algorithms applied to the SERS data. **Discussions:** The SERS spectra of serum and urine samples show high similarities, both being dominated by purine metabolite SERS bands (uric acid, hypoxanthine and xanthine). Further, to classify the BC and CTRL patients we implement the ML algorithms and found similar classification accuracies in the range of 61-89%, regardless the ML model implied. LDA performed the best classification accuracy for serum spectra (83%), while DT show the best performance for urine spectra (89%). Moreover, we show that the misclassified serum and urine samples in the LDA model are not a ML miscalculation, but they have a different metabolic profile compared to the mean SERS spectrum of the group they belong. **Conclusions:** This research highlights that SERS liquid biopsy of serum and urine provides similar classification performance, regardless of the classifier used. However, urine analysis has the advantage of being non-invasive and does not require deproteinization. Finally, our study highlights the potential of SERS spectroscopy for medical screening.

**Keywords:** spectroscopy, SERS, cancer

## SPECTRAL DIFFERENCES OF SALMON OIL AGING DETERMINED BY HYPERSPECTRAL IMAGING

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**Introduction:** The main objective of this study was to determine the spectral changes of salmon oil kept at 2 different temperatures over 4-week storage. The differences were determined both optically, using enhanced dark field microscopy, as well as by means of hyperspectral imaging. Salmon oil is rich in omega-3 fatty acids, which have been shown to have beneficial effects on the body's health by reducing the risk of heart disease, improving brain health, and reducing inflammatory processes. **Discussions:** Optically, we observed a crystallization of the sample stored at 4°C, while the RT storage did not alter the optical constitution of the sample. We obtained 3 significant peaks with spectrophotometry at 473 nm, 566 nm and 588 nm for RT, respectively. These peaks were shifted to 473 nm, 568 nm and 591 nm for the 4°C sample after 4 weeks of storage. Further, we found that the latter presented a 2-fold increase in the number of pixels in the spectral range of 560-600 nm as compared to the sample kept at RT for both solid and liquid form. Thus, showing a change in the composition of the sample stored at 4°C. **Conclusions:** We demonstrated the possibility of using hyperspectral imaging for the quality control of salmon oil kept at different temperatures. Thus, we provided a proof for this method to be used as a reference to identify environmental driven changes in fish oil composition.

**Keywords:** hyperspectral imaging, hyperspectral imaging, salmon oil, salmon oil, quality control, quality control, spectral analysis, spectral analysis

## SYBRGREEN FLUORESCENCE CAN DETECT LOW CONCENTRATIONS OF DOUBLE-STRANDED DNA AT DIFFERENT CA<sup>2+</sup> AND CL<sup>-</sup> CONCENTRATIONS

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**Introduction:** The main objective of the present study was to determine the pH and ionic strength where the double-stranded DNA (dsDNA) is stable using the fluorescence of SybrGreen bound to dsDNA. Thus, we aimed to

determine SybrGreen spectral changes of bound dsDNA in a ng/ $\mu$ L concentration range. It was shown earlier that, even at very low concentrations of dsDNA, the fluorescence of the SybrGreen dye is increasing yielding a sensitivity less than 10 pg/mL dsDNA. This makes SybrGreen suitable for detection of dsDNA with molecular precision in the analysis of the enzymatic digestion of DNA and other chromosomal studies. Moreover, the cut-off for the SybrGreen and dsDNA concentration were determined with various methods. In these studies, a pH range between 3 and 9 for the stability of dsDNA has been reported. Whereas, outside of this range the DNA denaturation process was initiated. **Discussions:** We obtained a large pH range of 3 to 12 where the dsDNA was stably bound to the fluorescent marker, with a maximum fluorescence intensity at pH 7. Further, we found that the addition of  $\text{Ca}^{2+}$  to the solution followed a competitive behaviour between the  $\text{Ca}^{2+}$  and the SybrGreen, thus the fluorescence signal was exponentially changing with the concentration of  $\text{Ca}(\text{NO}_3)_2$ . Since the dsDNA has a high affinity for  $\text{Ca}^{2+}$ , the SybrGreen binding affinity was substantially reduced. Whereas, in the case of addition of NaCl, a linear dependence between the  $\text{Cl}^-$  concentration and the fluorescence of SybrGreen was observed. **Conclusions:** We have shown the possibility to use SybrGreen fluorescence as a reporter for very low concentrations of double-stranded DNA under specified pH and ionic strengths. This opens the way for a cheap, simple and reliable method to detect the presence of dsDNA.

**Keywords:** double stranded DNA, Sybr Green, fluorescence spectroscopy, low range detection

## HYPERSPECTRAL ANALYSIS OF ACACIA HONEY

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**Introduction:** Honey is a complete food from nutritional point of view. Moreover, it has antioxidant, anti-inflammatory and antibacterial properties. We aimed to investigate the fingerprint of pure acacia honey, with hyperspectral and optical microscopy techniques to detect the specific pollen features from its composition. **Discussions:** From the analysis of the phase-contrast, polarization and dark field images of the 5 individual lots of acacia honey, we concluded that the pollen form was similar over the samples, with some size differences between the individual lots. The honey sold by the bio-stores contained more pollen particles, but with smaller sizes as compared to the ones from the supermarket. The spectral signature of the acacia honey, obtained by HSI, confirmed two main characteristic peaks around 420 nm and 900 nm, like the UV-Vis absorption spectroscopy results reported previously in the literature. The microscopy images together with the quantification of the HSI spectral information identifies the acacia pollen in the honey. **Conclusions:** Hyperspectral and microscopy imaging proved to be useful in the qualitative analysis of acacia honey. We obtained homogeneous pollen particle distribution over the samples, with characteristic differences for the five vendors. The combination of these techniques provides a possibility to identify the acacia honey, thus it could be used as a quality control in the food safety control chain.

**Keywords:** acacia honey, hyperspectral analysis, quality control, pollen features

## SPONTANEOUS AND INDUCED ADSORPTION OF AMINO ACIDS MONITORED BY CHEMICAL INTERFACE DAMPING OF SURFACE PLASMON RESONANCE AT SINGLE NANOPARTICLE LEVEL

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**Introduction:** Radiative and nonradiative mechanisms cause the decay of excited plasmons in metallic nanoparticles. Chemical interface damping (CID) is a decay process of coherent electron oscillations, based on electron scattering at the nanoparticle surface into available adsorbate energy levels. **Discussions:** The SPR band shifts significantly ( $p=0.05$ ) from 538.2-530.1 nm when leucine is added to the AgNPs. When  $\text{Ca}^{2+}$  is added, an additional significant red shift (530.1-551.8 nm) is observed ( $p=0.008$ ), as well as a widening of the SPR band ( $p=0.05$ ), indicating a CID effect. Finally, we found that in the presence of leucine,  $\text{Cl}^-$  had no effect on the SPR band. When phenylalanine is added to AgNPs, the SPR band shift from 544.2 to 560.5 nm ( $p=0.002$ ) with no hwhm variation. A further shift of the SPR band (577 nm) is detected at the addition of  $\text{Ca}^{2+}$ , as well as a widening of the SPR band. Similarly, in the presence of phenylalanine,  $\text{Cl}^-$  had no effect on the SPR band. Cysteine

adsorption causes a significant red shift (537.7-550.5 nm) as well as a widening of the SPR band. The adsorption of cysteine to the Ag surface was shown to be unaffected by  $\text{Ca}^{2+}$  or  $\text{Cl}^-$ , with no changes in the SPR band.

**Conclusions:** Our results show that the spontaneous adsorption of cysteine to AgNPs leads to a CID effect, whereas in case of leucine and phenylalanine adions are required for the adsorption of these amino acids to AgNPs and give rise to CID.

**Keywords:** chemical interface damping, SPR band, silver nanoparticles, amino acids

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## ASSESSMENT OF RAMAN ENHANCEMENT OF WATER SOLUBLE ANALOGUE OF BETA-CAROTENE BY METAL NANOPARTICLES

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**Introduction:** Carotenoid level variations were reported as important SERS liquid biopsy markers in various pathologies. However, the carotenoid characteristic bands were interpreted either as a result of a resonance Raman (RR) or as a surface-enhanced Raman scattering (SERS) effect. Our study represents a systematic approach for assessing the nature of the beta-carotene signal in the presence of metallic nanoparticles (NPs) and in the presence of albumin and purine metabolites. **Discussions:** The bands at 1003, 1153 and 1518  $\text{cm}^{-1}$  were used as carotenoids markers. Both, in resonance and out of resonance excitation regime, lead to the enhancement of the water soluble analogue of beta-carotene Raman vibrations in the presence of metallic nanostructures. When using AgNPs with an excitation wavelength at 532 nm that fits both the resonance condition of beta-carotene and the surface plasmon resonance (SPR) of AgNPs, the Raman bands of beta-carotene were enhanced. When exciting only the SPR of AuNPs using a 633 nm laser line, a lower enhancement of beta-carotene bands was observed. In the presence of BSA no beta-carotene SERS bands were detected, probably as a result of the protein corona formed around AgNPs. The addition of purine metabolites leads to a decrease in the intensity of the beta-carotene signal. However, when  $\text{Ca}^{2+}$  is used as adion, an enhancement of both purine metabolites and beta-carotene bands was observed. **Conclusions:** Concluding, the enhancement of the beta-carotene bands at 1003, 1153 and 1518  $\text{cm}^{-1}$  is a result of the SERS effect in the presence of metallic nanoparticles. However, the beta-carotene is displaced from the surface of AgNPs, partially by purine metabolites, and completely by albumin, leading to a decrease, or even total disappearance of the SERS signal of beta-carotene in serum matrix.

**Keywords:** carotenoids, surface-enhanced Raman scattering, Raman scattering

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## NIR-797 LOADED POLY (LACTIC-CO-GLYCOLIC ACID) NANOPARTICLES FOR IN VITRO FLUORESCENCE IMAGING

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**Introduction:** In 2020 global melanoma skin cancer mortality raised up to 57000 cases, melanoma being responsible for most skin cancer deaths. With proper detection, melanoma mortality rate could decrease significantly ergo, scientists have been exploring non-invasive ways through nanotechnology. Due to the property of most biological tissues to have relatively low light absorption in the near-infrared (NIR) spectral region, researches in biomedical applications developed nano-sized agents with NIR emission used for the detection of malignant cells. **Discussions:** Dynamic light scattering (DLS) measurements revealed an average hydrodynamic diameter for the newly fabricated NIR797@PLGA NPs of  $259.5 \pm 1.1$  nm, with a PDI of  $0.15 \pm 0.01$ , size that was also confirmed by scanning electron microscopy (SEM) imaging. Zeta-potential measurements,  $-20.0 \pm 1.0$  mV, provides us with the first indication regarding the good stability of the NIR fluorescent NPs. After the encapsulation of the NIR-797-isothiocyanate dye, the emission peak of NIR797@PLGA NPs was detected at 810 nm, with a loading efficiency of  $30.84 \pm 2.86\%$ . Furthermore, the viability and *in vitro* cellular uptake of the free NIR-797-isothiocyanate and NIR797@PLGA NPs were analyzed in melanoma cells, i.e., B16-F10 cell line. The WST-1 assay proved that the NIR797@PLGA NPs present no significant toxicity, while their good cellular uptake has been confirmed by confocal fluorescence imaging. **Conclusions:** To conclude, due to the good dye loading efficiency, size and stability, the NIR797@PLGA NPs can serve as efficient contrast agents for fluorescence cell imaging.

**Keywords:** PLGA nanoparticles, NIR fluorescence, melanoma skin cancer, confocal fluorescence imaging

## IN SILICO MODELING OF THE ADHESION OF ANTIMICROBIAL PEPTIDES TO BACTERIAL AND MAMMALIAN MEMBRANES

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**Introduction:** Wound healing is considered a dynamic and complex process, which involves a series of events that include cell migration, inflammation, angiogenesis, collagen synthesis and deposition, and re-epithelialization. Thus, an accurate assessment, appropriate diagnosis and optimal wound dressing are essential to ensure proper healing [NICE, 2016]. In recent years, a growing interest towards the use, of short (below 50aa) antimicrobial peptides (AMPs) was seen. AMPs are part of the host innate defense mechanisms of many eukaryotic organisms, most of which are amphipathic and cationic peptides (with a net charge ranging from +2 and +7), many with activity against multi-drug resistant bacteria [Boparai and Sharma, 2020]. **Discussions:** Here we present preliminary results on the adhesion properties of a few histidine modulated arginine- and tryptophan-based designed short AMPs [Bacalum et al., 2017] (RW-AMP). They will be used in the design of smart wound patches functionalized with these specific AMPs. We applied *in silico* molecular modeling to test the adhesion of each peptide against both bacterial and mammalian membrane models (DOPC+DOPG 85:15, and DOPC, respectively). **Conclusions:** Our results indicate more stable binding of RW-AMPs to bacterial membranes, and a 20% stronger adhesion of RW-AMPs to the bacterial membrane model versus the mammalian membrane model. Moreover, the RW-AMPs position themselves closer to the PG groups of the bacterial membrane model, which, in turn, leads to increased interaction with the DOPC headgroups in the presence of PGs. *Acknowledgements* : We would like to thank the financial contribution from UEFISCDI grant PN-III-P2-2.1-PED-2021-3342.

**Keywords:** antimicrobial peptides, potential of mean force, molecular dynamics

## THE IMPACT OF NOISE ON ANATOMICALLY CORRECT 3D MODELS OBTAINED FROM CT IMAGES

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**Introduction:** Our objective was to assess the impact of noise in medical imaging upon anatomically correct 3D printed models. The presence of noise on Computed Tomography (CT) images can seriously impact the 3D printing of these models. There is a growing number of 3D printed models used for learning, surgery planning, implants, and patient education. It was shown that these physical models outperform other didactic methods in terms of general information retention and spatial awareness. We aimed to create a 3D printed model of the fifth

lumbar vertebra (L5) and analyzed the effect of noise and filtering on the result. **Discussions:** We obtained 4 individual 3D printed models of the L5 vertebra and assessed the impact of imaging noise upon them using as readouts the visual factor, segmentation time (OD-37 min, SD10-54 min, SD20-53 min, and MF-32 min, respectively), and the number of artifacts (OD-182, SD10-176, SD20-44, and MF-52, respectively). We compared the parameters of the models at different processing stages by computing the Hausdorff distance between different landmark points on the original CT (OD) and the CT of the printed model (PM) and surface roughness maps of the models. As a quality control, we prepared an image fusion of the original dataset and the CT scan of the printed models. **Conclusions:** We confirmed that noise present in CT volumetric datasets had a significant impact on the 3D models by adding irregular structures on the surface of the models, where the most pronounced ones were spike-like structures on the z-axes. We identified a tolerance of the quality of the 3D model for a slight quantity of noise (Gaussian noise with SD10). We conclude that the realization of 3D models, using volumetric data acquired by CT is accessible and fast. It provides satisfactory results and correct anatomical models that can be used for academic purposes, surgical planning, or patient education.

**Keywords:** computed tomography, 3D printing, vertebra, noise, 3D models

## A TUG-OF-WAR BETWEEN ELECTRIC FORCES: THE NANOPORE-TWEEZING METHOD APPLIED IN MOLECULAR SENSING

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**Introduction:** To detect in real time and with high efficiency the pathogenic agents is vital for survival, as we experienced in COVID-19 pandemic. Nucleic acid or viral proteins, besides the specific symptoms, are the telltales of the pathogenic contamination in fundamental and clinical or forensic science, epidemiology, and biotechnology applications. **Discussions:** We use the  $\alpha$ -HL biosensor to detect nucleobases from short amino acid-functionalized, peptide-nucleic acids (PNA). We analysed the differences in relative changes of the open nanopore current following fragments capture to the averaged blocked substrate and we observed differences for each type of polynucleobase molecule. **Conclusions:** Our findings demonstrate that  $\alpha$ -HL sensitivity at the most constricted region provides the specificity needed in single-molecule investigative systems. **Acknowledgements.** This work was supported by grants PN-III-P1-1.1-TE-2019-0037, PN-III-P4-ID-PCE-2020-0011.

**Keywords:** nanopore, molecular sensing, DNA detection

## A COMPUTATIONAL STUDY REGARDING THE ANTI-INFLAMMATORY EFFECT OF CHITOOLOGOSACCHARIDES USED IN WOUND HEALING PROCESS

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**Introduction:** Chitooligosaccharides (COs) are oligomers containing N-acetyl-D-glucosamine and/or D-glucosamine units. Literature data reveal that COs containing up to 10 monomeric units are water soluble molecules and reveal numerous biological activities and low toxicological profiles. **Discussions:** The main molecular targets involved in wound healing and that are predicted are galectins and selectins for the totally and partially acetylated COs, and the fibroblast growing factors for COs containing totally deacetylated units. The molecular docking outcomes reveal that COs containing from 2 to 8 monomeric units are able to interact with the MD-2 protein, the interactions being stronger for the COs containing 6 and 8 monomeric units. The interaction energies between the Cos and MD-2 protein increase with the increasing molecular weight and with decreasing deacetylation degree, and are also reliant on acetylation pattern. **Conclusions:** In our opinion, mixtures of COs with distinct properties should be considered suitable candidates as adjuvants in developing scaffolds for the wound healing process. Our results conclude that chitooligosaccharides containing 2 to 8 monomeric units can bind to the active site of MD-2 protein, stronger interactions being revealed by those containing 6 and 8 monomeric units.

**Keywords:** chitooligosaccharides, myeloid differentiation factor 2 (MD-2), inflammatory process, molecular docking

## ADAPTABILITY TO DIFFERENT ENVIRONMENTAL CONDITIONS OF BACTERIA ISOLATED FROM COPPER TAILING IN MOLDOVA NOUĂ AREA

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**Introduction:** Mining activities, although essential to industrial activities, infrastructure and economic development can have a negative impact on the environment and on society as well. Air, soil and water within mining areas are widely contaminated, therefore in such places, there is a strong need for remediation. Bioremediation using microorganisms is one promising method that can be used for the treatment of contaminated sites. **Discussions:** Three of the bacterial strains isolated from tailing were able to grow and survive at high copper concentrations (up until 400 mg/L). Moreover, all three bacterial strains were well adapted to the environmental conditions tested, surviving at all NaCl concentrations and all pH values tested. **Conclusions:** This study revealed that copper-resistant bacteria isolated from copper tailing near the Moldova Nouă area were able to thrive in harsh environmental conditions, meaning there is a great potential in using these strains for bioremediation of copper mining polluted areas.

**Keywords:** bioremediation, microorganisms, copper mining, tailing

## STUDY ABOUT THE RELATIONSHIP BETWEEN INFECTIONS AND FOOD INTOLERANCE

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**Introduction:** Food intolerance is a non-immunological disease and may occur in response to pharmacological effects of food or food components upon our body. Food intolerance should not be confused with food allergy which is typically mediated by IgE antibodies, whereas food intolerance is mediated by IgG class of antibodies. It is believed to be caused by increased gut permeability, and it is involved in a variety of other disorders. **Aim:** To study the relationship between food intolerance and infections, to be used in the development of a Romanian cervical cancer patients management plan, in the context of the project entitled "Program of prevention, early screening, diagnosis and early treatment of cervical cancer – Romania Center Region", POCU/826/4/9/138603, code project SMIS 138603, which started in November 2020 in Targu Mures, until December 2023. **Discussions:** From 1.128 patients, 1.110 (98,4%) had different types of food intolerance. There were statistically significance correlations (pConclusions: The connections between food intolerance and infection was proved and starting from this we recommend introducing food intolerance testing at adults at cancer risk, for a primary and secondary preventive medical intervention protocols.

**Keywords:** bioresonance, food intolerance, HPV infection, cancer risk, herpes virus

## THE STANDPOINT OF MEDICAL PHYSICIST IN MULTIDISCIPLINARY APPROACH OF TREATING CANCER

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**Introduction:** In a cancer therapy setting, a multidisciplinary approach is related to a tumor board, in which a number of experts in different specialties review and discuss the medical condition and treatment options of a patient. In radiation therapy, medical physicists develop and implement procedures for dosimetry and treatment

planning, for treatment delivery, verification, radiation safety. Therefore, their scientific and practical training should include an extensive understanding of the clinical aspects of radiobiology and cancer. We all agree that the role of medical physicists expanded along with technological discoveries in radiotherapy, however, according to some authors, their clinical role decreased even more since the modern techniques like IMRT and IGRT are used. In numerous countries, including Romania, the focus of the medical physicists is centered on developing technical skills, rather than overall knowledge. We aimed to review the critical role of medical physicists in cancer treatment.

**Discussions:** Even though the first task of medical physicists in radiotherapy is to figure the isodose curves to provide maximum tumour coverage, in accordance with the constraints to healthy tissues, there are some details that depend on their personal view. Treatment planning systems have some built-in limitation related to the restriction of the algorithms that model interaction with the body and requires a deep knowledge for evaluating the limitations of the various dose delivery methods, to obtain optimal beam configuration. **Conclusions:** We consider that there is a need for further research on how tumor boards should be best structured and conducted, and that the participation of medical physicists in such meetings is highly recommended.

**Keywords:** medical physicist, multidisciplinary, cancer treatment, radiotherapy, tumor board

## ASSESSMENT OF THE ENVIRONMENTAL TOXICITY OF CHITOLIGOSACCHARIDES. A COMPUTATIONAL APPROACH

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**Introduction:** Chitin is an abundant polymer in nature being found in the exoskeleton of crustacean and insects and containing mainly N-acetyl-D-glucosamine (GlcNAc) units. Chitosan is obtained by chemical or enzymatic deacetylation of chitin, contains both N-acetyl-D-glucosamine and D-glucosamine (GlcN) units and reveal numerous medical applications. Chitooligosaccharides (COs) are oligomers resulting from the degradation of chitin or chitosan and those containing up to 10 monomeric units are water soluble molecules. **Discussions:** The outcomes of this study reveal low toxicity of the investigated COs against honey bee, *Tetrahymena pyriformis*, Fathead minnow, *Daphnia magna*. The degree of toxicity usually increases with decreasing molecular weight and with increasing deacetylation degree and is reliant on the deacetylation pattern. **Conclusions:** Taking into account the outcomes of this study the chitooligosaccharides covered in this work pose only little or no environmental hazard.

**Keywords:** chitooligosaccharides, toxicity, computational study

## ESTIMATION OF THE EFFECTS OF TRITICONAZOLE ON SOIL ENZYMATIC ACTIVITY

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**Introduction:** Triticonazole (TTZ) is a triazole fungicide used as seed treatment for the control of common soil and seed diseases, legumes and fruit tree diseases. This study assesses the effects of TTZ on the activities of soil dehydrogenases (DHA), ureases (UA) and phosphatases (PhA) and on the soil microorganisms. TTZ has two enantiomers: (R)-TTZ and (S)-TTZ. **Discussions:** DHA and PhA decrease and UA increases in the first 14 days, every of these activities needs at least 21 days to recover. The molecular docking reveals small differences in the interactions energies of the enantiomers of TTZ with soil enzymes. In the case of microorganisms, the TTZ application conducts to a decrease of the entire population, the decrease being more accentuated for the maximum dose of TTZ. **Conclusions:** The effects of the seeds treatment with TTZ against the soil enzymes are not dose dependents. Both (R)-TTZ and (S)-TTZ are not able to bind to the active site of *Bacillus pasteurii* urease. In the experimental conditions, TTZ did not affect the soil microbial community. Further assessments are needed to highlight the long-term effect of the fungicide on microorganisms. Acknowledgement: This research was funded by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI-UEFISCDI, project number PN-III-P1-1.1-PD-2019-0255, within PNCDI III.

**Keywords:** soil enzymes, microorganisms, human health



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## ESTIMATION OF AQUATIC TOXICITY OF TRIAZOLE FUNGICIDES

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**Introduction:** Literature data reveal triazole fungicides used for the treatment of fungal diseases in various crops can reach the aquatic environment and could affect the organisms living in this environment. **Discussions:** Among the studied fungicides, metconazole was highly toxic, tebuconazole and tetraconazole being moderately toxic, while the other three fungicides were slightly toxic against duckweed. In addition, computational data were obtained for an extended set of fungicides and the outcomes emphasize moderate toxicological effects of these fungicides against numerous aquatic organisms (fish, crustaceans, aquatic invertebrates, algae), epoxiconazole and difenoconazole emphasizing the highest toxicity. **Conclusions:** An adequate management of the triazole fungicides in agricultural practices allows to mitigate their effects on the organisms living in aqueous environment and contributes to development of a sustainable agriculture.

**Keywords:** triazole fungicides, aquatic toxicity, duckweed growth inhibition assay

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## CHARACTERIZATION OF SURFACE AND GROUNDWATER SAMPLES POTENTIALLY CONTAMINATED WITH MINING POLLUTANTS FROM MOLDOVA NOUĂ AREA, CARAȘ-SEVERIN COUNTY, ROMANIA

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**Introduction:** The abandoned mining dumps generated by the former copper mining activities from Moldova Nouă area represent a potential pollution threat to both human health and the environment. **Discussions:** Most of the physicochemical parameters were within normal ranges for both surface water and groundwater samples. While none of the groundwater samples exceeded the maximum acceptable concentration (MAC) for all analyzed heavy metals, the surface water samples exceeded the MAC values for Cu, Fe, Hg and Mn. None of the tested samples showed ecotoxic effects to duckweed, although some samples showed a slight reduction of green frond number. It was observed that Mn and Fe affected the number of green fronds after exposure to the surface water samples. **Conclusions:** The analyzed samples were not highly polluted with heavy metals, the physicochemical parameters being in the normal ranges. This is also highlighted by the duckweed growth inhibition assay, none of the tested samples showing ecotoxicity.

**Keywords:** surface water, groundwater, mining, pollution

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## MULTI ANGLE LIGHT SCATTERING (MALS) ENABLES THE IDENTIFICATION OF THE MONOMERIC FRACTION FOR A KEY PROTEIN OF BACTERIAL FLAGELLUM

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**Introduction:** The flagellum is a supramolecular assembly. For flagella construction on the cell surface, the flagellar type III secretion system (fT3SS) transports building blocks from the cytoplasm to the distal end of the growing flagellar structure. One of the key components of fT3SS is trans-membrane protein FlhA, which coordinates the protein export with the flagellar assembly process by an unknown mechanism. In order to be able to describe the respective mechanism, the determination of the FlhA structure is essential. For this purpose, the recombinant protein was purified in dodecyl maltoside (DM) detergent, then by employing the SEC-MALS technique, the monomeric fraction of the protein was identified in order to be subsequently used for structural studies. **Discussions:** The SEC-MALS profile of purified recombinant FlhA in 2 CMC DM displays a succession of 3 principal peaks represented by: oligomeric FlhA (peak 1), monomeric FlhA (peak 2), and impurities (peak 3), with

corresponding M.W. of protein content (in kDa) of 181, 75 and respectively 2. The SDS-PAGE confirms the biochemical purity of monomeric FlhA, with only one visible band. **Conclusions:** The monomeric fraction of recombinant FlhA was identified by SEC-MALS, in order to be used for structural studies. Acknowledgments: This work was carried out through the Nucleu Programme, supported by MCID, project no. PN 19 35 02 01 and by direct funding from OIST, Japan.

**Keywords:** SEC-MALS, membrane protein, protein aggregation

## INNOVATIVE PERIODIC NANOSTRUCTURES FOR SERS DETECTION OF BIOMOLECULES

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**Introduction:** Surface-enhanced Raman scattering (SERS) is a non-invasive spectroscopic technique which provides a huge amplification of the Raman signal of analytes in the close proximity of metallic nanostructures. SERS enables detecting and resolving the chemical signature of single molecules by concentrating the light down to molecular scale. The use of nanoimprint lithography (NIL) facilitates the implementation of large arrays of reproducible nanostructures for SERS detection of biomolecules at unimolecular level. **Discussions:** The CV detection was done on nanopillars-based substrates metalized with Au thicknesses in the range 25 nm–200 nm. A detection limit (LOD) of  $\mu\text{M}$  was reached for Au films of 50 and 200 nm. When using Ag nanotrenches with thicknesses of 10 nm–100 nm, a LOD of 10 pM has been attained and an enhancement factor of 107 has been calculated [1]. When a complex biomolecule such as nodularin has been detected on the nanotrenches-based SERS substrates, a LOD of 1 mM was found for the nanotrenches covered with 25 nm Ag. **Conclusions:** In conclusion, we fabricated flexible Ag and Au substrates-based on nanotrenches and nanopillars using NIL. We demonstrated their performances as promising SERS nanoplatforms for ultrasensitive detection of CV and nodularin. We intend to improve their LOD by Ag and Au tuning and to develop new SERS nanosensors for point-of-care testing. Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI-UEFISCDI, project number PN-III-P2-2.1-PED-2021-1998, within PNCDI III. References: [1] A. Colnita et al., Spectrochim. Acta A Mol. Biomol. Spectrosc. 276(2022)121232.

**Keywords:** SERS, NIL, nodularin, crystal violet

## HIGH-PERFORMANCE 3D FLEXIBLE PLATFORMS FOR MOLECULAR TRACE-LEVEL SENSING

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**Introduction:** Surface enhanced Raman spectroscopy (SERS) is one of the most versatile and powerful analytical techniques for the ultra low level detection of complex molecules due to the coupling of Raman scattering of a molecular system with the localized plasmon resonance of silver nanostructures. **Discussions:** Our main results reveal the SERS signal enhancement was induced by a threefold synergy: i) Ag deposition on flexible polymeric substrates; ii) the effect of the increasing thickness of nanostructured Ag films and iii) the patterning of polymeric substrates with periodical nanotrenches. The Ag nanotrenches based substrates exhibited a dramatically increased SERS signal compared to the plain Ag film. An enhancement factors up to  $10^7$  was determined for the nanotrenches covered with 25 nm Ag. **Conclusions:** This particular substrate showed a considerably lower SERS limit of detection, down to 10 pM, an improved homogeneity and a more reproducible signal. Acknowledgements: This work was carried out through the Nucleu Programme, supported by MCID, Project No. PN19350201. [1] A. Colnita et al., Spectrochim. Acta A Mol. Biomol. Spectrosc. 276 (2022) 121232

**Keywords:** Nanoimprint lithography, Surface-enhanced Raman scattering, Nanotrenches, Silver film thickness, Crystal violet

## IN SILICO MODELING OF THE DYNAMICS AND ENERGETICS OF GLYCINE DIPEPTIDES INTERACTING WITH MEMBRANE BILAYERS

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**Introduction:** Antimicrobial peptides can be used in medical applications due to their (i) antibiotic activities against bacteria, fungi and viruses, (ii) cytotoxic activity on cancer cells, and (iii) anti-inflammatory and immunomodulatory activities. In spite of their relatively short sequences, designing AMPs with high specificity is not straightforward. One of the main issues is understanding the dynamics and energetics of their interactions with the cell membranes. **Discussions:** Equilibrium dynamics simulations are used to assess the di-peptide's adhesion times/rates to the membrane bilayer, as well as the conformational sampling of the di-peptide's while interacting with it. Non-equilibrium simulations reveal the potential of mean force profile along the normal to the membrane surface, indicating the energetics of the Glycine di-peptide interacting with the membrane bilayer. **Conclusions:** Our results indicate that the simplest peptide (Gly-Gly) reveals a non-trivial interaction with a membrane bilayer model due to its changes in backbone orientation. Furthermore, the long simulations (possible due to the small system size) allowed us to determine accurately the conformational sampling and membrane adhesion energy profile. **Acknowledgements:** This work was carried out through the Nucleu Programme, supported by MCID, Project No. PN 19 35 02 01.

**Keywords:** Antimicrobial peptides, Molecular dynamics, Glycine DiPeptides

## THERMAL INDUCED STRUCTURAL CHANGES IN INNOVATIVE BIO-BASED POLYAMIDES

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**Introduction:** Bio-based polyamides help to maintain environmental quality by minimizing environmental damage during their use and are manufactured from renewable sources characterized by easy removal from the environment, health safety, energy efficiency, and reduced pollution. Polyamides (PAs) have been widely researched for decades and are an important class of polymers used in engineering. PAs are among the most important synthetic polymers produced in huge quantities for high-performance industrial thermoplastics. From this perspective, the development of polyamides from renewable resources is becoming an extremely important area in macromolecular chemistry and in today's industry. Environmentally friendly additive polyamides can be produced using conventional manufacturing, but with bio-based alternatives to conventional chemicals and coming from recycling or prepared from 100% bio-based monomers. **Discussions:** A full Raman analysis of specific groups was investigated on pure polyamides exposed to different heat treatments to analyze the influence of environmental conditions. Furthermore, the thermal protocol for the samples obtained by injection moulding, was adapted (the samples underwent a thermal treatment at 80 and 145 °C, respectively) in order to investigate the influence of the molecular chain, which can generate specific Raman fingerprint, respectively SEM topography of the surfaces after the thermal treatment. **Conclusions:** The surface of nanocomposites of bio - PA1010 was evaluated from SEM images. At the 80°C thermal treatment, the surface had no alterations. The thermal treatments below 80°C did not affect the structure which indicates the safe use of these materials for automotive industry. **Acknowledgment:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-III-P2-2.1-PED-2021-0795, within PNCDI III.

**Keywords:** bio-based polyamides, raman spectroscopy, scanning electron microscopy, thermal treatment

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## THERMODYNAMIC ASPECTS OF ETHYLENIMINE AND ETHYLENE GLYCOL POLYMERS

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**Introduction:** Polyethylenimine (PEI) and polyethylene glycol (PEG) are two polymers with a similar structure. Both structures contain ethylene groups (CH<sub>2</sub>CH<sub>2</sub>), separating the ether (O), respectively secondary amine (NH) groups. **Discussions:** The results show that the stability of the linear polymers decreases with their degree of polymerization, with the increasing of their chain length and is less influenced by the ramification range in the case of branched PEI. **Conclusions:** The values of internal energy equal the values enthalpy and the values of Gibbs free energy for the molecules studied. **Bibliography:** Roxana-Diana Pasca, Titus Adrian Beu, "Some Aspects of Thermodynamic Properties of Ethylenimine and Ethylene Glycol Linear Polymers", Studia Universitatis Babeş-Bolyai, Physica, 2019, 1, 83-90.

**Keywords:** thermodynamics, functions of state, biopolymers, PEI, PEG

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## SINGLE-CELL OPTO-ELECTRIC MANIPULATION FOR CHARACTERIZATION AND SEPARATION OF RETINAL PIGMENT EPITHELIAL CELLS

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**Introduction:** The characterization and sorting techniques based on single-cell optical and electrical micro-manipulation have become famous for a wide range of applications. We are working on the development of a technique using optical tweezers (OT) and dielectrophoresis (DEP) to characterize and separate retinal pigment epithelial (RPE) cells. **Discussions:** The cell membranes remain intact up to 1000V/cm (AC) in the PI assay. The cell doubling times under RTCA were increasing with the increase of the DEP voltages. Several EVs were recorded on single cells of different sizes from different passages of the BPEI-1 and Caco-2 lines. Different domains and distribution of EVs were obtained: BPEI-1 (3.9-5.4V), Caco-2 (2.5-4.0V). EVs were inversely varying with respect to the cell sizes. This observation relies on the size dependency of the Clausius-Mossotti factor which influences the DEP behavior of the cells. **Conclusions:** Based on these results, the DEP-OT technique showed to be a reliable method for contact-less and label-free characterization and separation of cells at a single cell level. **Acknowledgments:** European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 861423.UEFISCDI project PN-III-P2-2.1-PED-2021-0451, contract no. 596PED/2022.

**Keywords:** Dielectrophoresis, Optical tweezers, Retinal Pigment Epithelial cells, Opto-electric fingerprint, Escape voltages

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## THE RELATIONSHIP OF BODY MASS INDEX ON THE RADIATION DOSE RECEIVED DURING COMPUTED TOMOGRAPHIC IMAGING OF THE ABDOMEN AND PELVIS

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**Introduction:** The severity of the effects of ionizing radiation depends on the type of radiation, the intensity of radiation but also the duration of exposure. The anatomical and physiological characteristics of the patients have a great influence. We aimed to determine the relationship between body mass index (BMI) and the effective dose obtained from computed tomography (CT) performed for the abdomen and pelvis. After collecting the results, we want to find ways to adapt the CT exposure protocols according to BMI. **Discussions:** 79% of patients had a BMI greater than 24.9, which is considered the upper limit of normal. The average BMI was 31.3 kg / m<sup>2</sup>. The

estimated mean dose for the abdomen-pelvis patient was approximately 13.7 mSv (SD  $\pm$  11.0); for the abdomen 9.8 mSv (SD  $\pm$  9.37 and for the pelvis the dose was 7.4 mSv (SD  $\pm$  7.11). The effective dose increased with increasing BMI (p Conclusions: In general, the estimated dose from CT scans for the abdomen and pelvis was similar to those in the literature. Increased BMI significantly increases the effective dose received from CT scans of the abdomen and pelvis.

**Keywords:** CT scans, BMI, abdomen, ionizing radiation

## FLUOROMETER ADAPTED SYSTEM FOR STUDYING THE EFFECT OF ANESTHETIC GASES ON LIPID VESICLES

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**Introduction:** The mode of action of local anesthesia is quite well described while the general anesthesia is far from being fully understood. Despite their use for centuries in surgical medicine, the effects on cells of inhaled anesthetic agents need further studies. For this reason, a system has been developed for the study, by fluorometric methods, of anesthetic gases effects on the properties of membranes. **Discussions:** The system proved to be sealed and allowed the measurement of GP and r under controlled gas pressure (Nitrogen and Xenon). A less sharp phase transition of DMPC liposomes under Xenon was observed when compared to Air or Nitrogen. **Conclusions:** These results prove that the system is functional and in accordance with the requirements of a study on gases effects (at least on lipid vesicles), especially in terms of leakage and adaptability to the fluorometer. The system was originally developed for the study of lipid vesicles, but it also can be used for any fluorescence study on living cells under controlled gas atmosphere.

**Keywords:** Anesthetic Agent, Xenon, Generalized Polarization, Anisotropy, 3D Printing

## 3D PRINTING CAPABILITY IN PRODUCING SPECIALIZED DEVICES FOR BIOPHYSICS RESEARCH

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**Introduction:** In the last 10 years, 3D printing, and other CNC-based methods have improved considerably, and the price of such devices has become affordable even for the regular population. Given the considerable need for specialized adapters or systems in research, this presentation aims to highlight the usefulness of 3D printing in producing custom-based items for research. **Discussions:** The system for comet assay improved the sample per run yield from 10 to 300 samples (each sample containing various numbers of cells) for different experimental categories. The device for dielectrophoresis integrated the electric connections and allowed microscopic images acquisition simultaneously with the application of DEP field. The cells distribution within the optical field was changing depending on the DEP frequency. **Conclusions:** Both devices worked accordingly with the intended design and use case. The optimization steps to increase their reliability were easily implemented. Our devices prove that the 3D printing is an asset in today's research laboratory by producing customized items at considerably lower costs. Acknowledgment: This work was partially funded by UEFISCDI project PN-III-P2-2.1-PED-2021-0451, contract no. 596PED/2022

**Keywords:** 3D printing, filament printers, comet assay, dielectrophoresis

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## FEATURING BY IMMUNOHISTOCHEMISTRY CELL SPHEROIDS CONSTRUCTED AS 3D TUMOR MODELS FOR GLIOBLASTOMA

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**Introduction:** Glioblastoma is a highly aggressive primary brain tumor with less than 25% survival at 2 years of patients under treatment. Extensive studies are needed to fully understand the glioblastoma physiopathology and for developing new specific therapeutics. 3D cultures as spheroids are personalizing the tumor model with architectural features which expose the glioblastoma cells to conditions close to those existing in vivo. The aims of present study were: i/to customize the preparatory procedure of glioblastoma spheroids for immunohistochemistry evaluation and ii/to characterize these tumor models by specific immune assays. **Discussions:** Almost 90% of the spheroids were CyclinD1 positive, marker for high proliferation rate. ARID 1A mutation was positive in 95% of samples and was correlated statistically significant with IDH1 negativity ( $p=0.011$ ). ARID 1A is a chromatin-remodeling complex that regulates gene accessibility. The IDH1 mutations in glioblastoma reduce tumor progression and give them a less aggressive phenotype. The expression of anti-apoptotic Bcl-2 proteins was correlated to the areas of necrosis and apoptosis as revealed by hematoxylin&eosin staining. U87-MG spheroids were diagnosed as highly aggressive wildtype glioblastoma. **Conclusions:** U87-MG spheroids were well mimicking the tumoral features of in vivo glioblastoma. Spheroids preparation for immunohistochemistry evaluation was more elaborate than in the case of tissues, but achievable with common items.

**Keywords:** spheroids, immunohistochemistry, glioblastoma

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## STUDY ON THE VARIATION OF SOME PHYSIOLOGICAL PARAMETERS OF THE BLOOD UNDER THE ACTION OF ULTRASOUNDS

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**Introduction:** We aimed to study the effects of ultrasound on elements in the blood in patients with onset of low back pain. The ultrasounds were applied continuously or pulse-mode. **Discussions:** Studying the evolution of the parameter of the number of red blood cells in group L1, we obtained a statistically significant variation at five days of treatment and extremely statistically significant at 10 days after treatment. The decrease in red blood cell count is statistically significant in group L2, five days after treatment and at the end of treatment. One month after the end of the ultrasound treatment, the number of red blood cells was the same for all groups. In addition, due to exposure to ultrasound, it was found that the local temperature increased. A faster increase in temperature was observed in group L1 to which continuous ultrasound was applied. **Conclusions:** If the recovery treatment uses ultrasound, a reduction in the number of red blood cells is observed during treatment. This reduction shows that ultrasound treatment, although applied locally, intensifies metabolism.

**Keywords:** continuous ultrasound, pulse-mode ultrasound, red blood cells

## SILVER SPECIES TRANSFORMATION IN BIOLOGICAL ENVIRONMENT

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**Introduction:** Silver is a promising candidate to prevent the bacterial infections, and as a consequence it is a preferred bactericidal material used in biomaterials. However, during synthesis and after interaction with organisms, silver compounds can be converted to silver nanoparticles (AgNPS), silver chloride (AgCl) or to other species. The aim of the present study is to understand the relationship between the presence of silver in biomaterials and the formation of AgNPs and AgCl after immersion in a biological fluid. **Discussions:** After immersion in SBF beside apatite formation the AgNPs and AgCl was evidenced. Major changes after immersion in DMEM are highlighted in the case of samples with a high concentration of silver, by the appearance of specific reflections of AgCl. Important changes related to the presence of the apatite layer, after immersion in MHB, are noted for the samples with a low concentration of silver, the signals due to the formation of the AgCl compound becoming evident only for the sample with the highest value of the silver concentration. **Conclusions:** The obtained results show that the silver-containing glass samples behave differently in contact with diverse solutions (SBF, DMEM and MHB) used in biological assays. However, a small amount of NaCl can induce the appearance of AgCl. **Acknowledgements:** This work was supported by a grant of Ministry of Research and Innovation, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1138, within PNCDI III.

**Keywords:** silver, silver phosphate, antibacterial activity, cell viability

## STUDIES ON CHANGES IN CRYSTAL TRANSPARENCY UNDER THE ACTION OF IONIZING RADIATION

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**Introduction:** The radiation-induced biological effects of irradiation doses received by personnel professionally exposed to ionizing radiation in angiography laboratories (interventional radiology) is a topic of great interest, taking into account the risks of irradiation and its consequences on the health status of people exposed to ionizing radiation over a long period of time. **Discussions:** Dosimetric monitoring was carried out individually over a period of three years, evaluating doses to the upper limbs, dose to the lens of the eye and outside the lens of the eye and inside the radiation protection equipment. **Conclusions:** The final evaluation was carried out by a correlative study between the dose values obtained and the ophthalmological paraclinical analyses specific to persons occupationally exposed to ionizing radiation.

**Keywords:** ionizing radiation, lens, interventional radiology

## PARTICULARITY OF BIPHOTONIC ABSCESS IN THE PATHOLOGY OF THE OSTEOARTICULAR SYSTEM

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**Introduction:** X-rays are electromagnetic radiation in the category of ionizing radiation. In medical diagnosis, the degree of absorption of this type of radiation depends on the density of the exposed tissue, so we can talk about a physical parameter to evaluate the density. Osteoporosis is a chronic disease of the bone system and consists of a dynamic balance between osteoblasts and osteoclasts. Physiologically, bone through metabolic processes

maintains a continuous balance between osteo formation and osteo resorption. **Discussions:** The mathematical analysis and mathematical algorithms specific to this type of quantitative analysis are complex and involve (Silva, 2014): Fourier transform matrix and run length analysis. **Conclusions:** The peculiarity of the DEXA examination that uses types of waves according to the degree of penetration, one with low penetration and another with high penetration, can expand in this way through a specific algorithm a two-dimensional assessment to a three-dimensional one.

**Keywords:** bone mineral density, X-ray, bone system, DEXA

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## NUTRITION APPLICATIONS ON THE HUMAN PSYCHE

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**Introduction:** The interaction between what we eat, how we eat and when we eat, and how this affects our biochemistry, is a powerful and interdependent one. The biochemistry of the body is responsible for the proper functioning of our mind and our emotional balance. The purpose of this study was to check the mental changes due to nutrition of diet based on whole plant foods (ABAVI) **Discussions:** Patients had a positive feed-back with significant emotional and behavioral changes: for people with anger and nervousness crises, nerve episodes decreased by 92%. Patients with generalized anxieties opened up a lot, increased their circle of friends, wandered more much by nature and have hobbies they feared at first. Some patients with depression, managed to overcome the depressive episode, and those who were treated with antidepressants, managed to reduce the dose (40%) and others to complete the treatment (45%), without trace of withdrawal. The cases of attempted suicide have completely decreased. **Conclusions:** The study confirmed the hypothesis that whole plant nutrition has a positive impact on the psyche. Proper physical habits promote mental superiority. The formation of character is prevented by inappropriate treatment of the digestive system. Today, analyzing the recurrent feed used by the population, following this study, we can sincerely ask ourselves whether we still have the safety of the answer to the question: "Who am I? "

**Keywords:** nutrition, psychiatric disorders, food memory, additives, digestive - neuronal information

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## ASSESSMENT OF THE IMPACT OF POLYSTYRENE NANOPARTICLES ON STEVIA REBAUDIANA PLANTS GROWN IN VITRO

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**Introduction:** Polystyrene nanoplastics (NPs) are emerging pollutants of global importance. The aim of this work is the determination of toxicity level of polystyrene NPs for *Stevia Rebaudiana* plant, as well the development of a rapid methodology, based on Vis-NIR and Raman hyperspectral imaging (HSI) for the direct detection and quantification of NP accumulation in plant tissue. **Discussions:** The NPs stimulated photosynthesis at low concentration (< 10 mg/L). However, at 100 mg/L concentration a clear suppression in photosynthesis was observed. The root morphology and plant length are adversely affected by NPs and, with almost complete inhibition at doses of 250 mg/L of polystyrene NPs. *Stevia rebaudiana* phytochemicals were quantified using HPLC. The concentrations of chlorophyll A and B, lutein, zeaxanthin, and beta-carotene showed the same trend upon exposure to increased polystyrene NP levels. Their concentrations increased up to the 250 mg/L NPs dose, more exactly, the concentration of all the investigated analytes increased twofold, compared to controls. HSI provides beside the optical image of micro-objects a spectral (Vis-NIR extinction or Raman), in each pixel of the map, at a limit of 0.5  $\mu\text{m}$  spatial resolution. The impact of NPs on the plant length and root as well as plant weight can be assigned to a stress response of the plant. **Conclusions:** The major economic impact of the developed methodology for imaging lies in its applicability for screening food matrices at large scale, in order to detect contaminations such as polystyrene NPs, ensuring thus an important tool for food safety and security.

**Keywords:** nanoplastic, *Stevia Rebaudiana*, dark field microscopy, hyperspectral imaging

## NEGATIVE IMPACT OF STATINS ON OLIGODENDROCYTES IN VITRO

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**Introduction:** Statins have been taken into consideration as a treatment option for multiple sclerosis because of their wide range of anti-inflammatory and immunomodulatory effects. When statins are applied to oligodendrocytes (OLN), contradictory results have been described. This cell line being predominantly affected in multiple sclerosis. In this study we focus on the in vitro effects produced by simvastatin (SV) on the morphology of oligodendrocytes at cellular membrane level. **Discussions:** After a 24 h of incubation period with the statin compound, we observed that it disturbs the formation process of our cells, leading to less branched cells. **Conclusions:** We conclude that simvastatin treatment has detrimental effects on oligodendrocytes growth process, and membrane morphology which could inhibit long-term healing of lesions caused by multiple sclerosis.

**Keywords:** AFM, oligodendrocytes, simvastatin, cell membrane

## INTERACTION OF AN TRYPTOPHAN- AND ARGININE-RICH ANTIMICROBIAL PEPTIDE WITH E. COLI OUTER MEMBRANE - A MOLECULAR SIMULATION APPROACH

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**Introduction:** The outer membrane (OM) of Gram-negative bacteria is an asymmetric bilayer, with the outer leaflet consisting exclusively of lipopolysaccharide molecules and the lower leaflet made up of phospholipids. Antimicrobial peptides (AMPs) are generally small cationic and amphipathic molecules. The mechanisms by which AMPs permeate the OM of Gram-negative bacteria are not well understood at the moment. A short, 9 amino acid peptide, rich in Trp and Arg (P6-HRWWRWRR-NH<sub>2</sub>), was used in molecular dynamics (MD) simulations to investigate the interaction between AMPs and the structures of two *E. coli* membrane models. **Discussions:** In both MD simulations at least one P6 peptide has been inserted in the gap formed in the LPS layer by the OmpF porin, but at different levels. The P6 peptide mainly formed hydrogen bonds with the phosphate groups of Hep I and Hep II (L-glycero-D-manno-heptose) residues of K12 and R1 inner core. Binding energy minima was stronger for the K12 core system at -13.99 kcal/mol and -10.4 kcal/mol for the R1 core system. **Conclusions:** The analysis of the two simulations revealed the P6 peptide binding mode to the two types of LPS molecules, facilitated by the gap formed in the LPS layer which allowed access to the LPS binding site, LPS-porin interface and OmpF structure.

**Keywords:** Lipopolysaccharide, Antimicrobial peptides (AMPs), Gram-negative outer membrane (OM), OmpF,

## Molecular dynamics

## A BIOINFORMATICS ANALYSIS OF NATURAL COMPOUNDS FROM ACONITUM SPECIES

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**Introduction:** *Aconitum* species were used in traditional medicine for the treatment of inflammation, pain, fever reduction and infections. At the same time, plant extracts were used as poisons and sedatives. The beneficial effect of natural compounds from *Aconitum* species were proved both experimentally and using in silico methods. Here we used specific bioinformatics methods to derive the drug-likeness, the pharmacokinetic and pharmacodynamic profiles of twelve selected compounds from *Aconitum* species. **Discussions:** The analyzed compounds (aconitine and eleven other aconitine derivatives) present drug-like features according to Lipinski's rule of five with none up to two violations of the rule. The compounds do not appear mutagenic or cardiotoxic (with two exceptions), but most of the compounds (eight) appear hepatotoxic. Their predicted molecular targets are variable, including the serotonin transporter, the neuronal acetylcholine receptor subunit alpha, beta-glucocerebrosidase, HERG or muscarinic acetylcholine receptor M3. **Conclusions:** The predictions performed here help to understand the mechanism of action in the case of twelve compounds isolated from *Aconitum* species by predicting their pharmacokinetic profiles, their toxicity potential and by identifying their molecular targets. **Acknowledgment:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, projects number PN-III-P2-2.1-PED-2021-2866 and PN-III-P4-ID-PCE-2020-0620.PCE-2020-2269

**Keywords:** pharmacokinetics, pharmacodynamics, *Aconitum* species, aconitine, bioinformatics

## MOLECULAR DOCKING OF TWO CURCUMIN DERIVATIVES AT BETA-SECRETASE AND AMYLOID FIBRILS

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**Introduction:** Alzheimer disease is a neurodegenerative disease whose prevalence is constantly increasing. The treatment consists of acetylcholinesterase inhibitors or glutamate (NMDA) receptors antagonists. Current research is focused on the identification of effective therapeutic agents with reduced side effects, that can change disease progression by modulating its physio-pathological pathways. Such agents could be natural compounds like curcumin that was shown to modulate various Alzheimer disease targets, as well as to destabilize amyloid fibrils. Here we investigated the interaction of two curcumin derivatives with beta-secretase (BACE1) and amyloid fibrils using molecular docking methods. **Discussions:** The analyzed compounds presented drug-like features and favorable pharmacokinetic properties. The compounds did not present hepatotoxicity. Targets prediction has revealed BACE1 (an enzyme involved in the generation of beta amyloid) and beta amyloid A4 protein (constituent of amyloid fibrils) as common targets of both compounds. The molecular docking of compounds to BACE1 and to an amyloid fibril has revealed favorable interactions, confirming the ability of compounds to bind to these targets. **Conclusions:** The curcumin derivatives analyzed here should present beneficial effects on amyloid beta production by inhibiting BACE1 and should have the ability to model existing amyloid fibrils by attaching and destabilizing them. Future work will involve the usage of molecular dynamics methods to prove these interactions. **Acknowledgment:** This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, projects number PN-III-P2-2.1-PED-2021-2866 and PN-III-P2-2.1-PED-2019-1471.PCE-2020-2269

**Keywords:** molecular docking, beta-secretase, amyloid fibril, curcumin derivatives, bioinformatics

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