

Joint Workshop IC - Ivodent Academy (Albania)

Report of Contributions

Contribution ID: 1

Type: **not specified**

Discussion and Conclusions

Tuesday, 26 September 2023 16:40 (5 minutes)

Speakers: Dr. Cinzia Giannini (IC-CNR) and Dr Altin Mele (Director Ivodent Academy)

Contribution ID: 2

Type: **not specified**

Welcome and intro IC-CNR & Ivodent Academy (Albania)

Tuesday, 26 September 2023 14:00 (15 minutes)

Presenters: Dr GIANNINI, Cinzia (Director IC-CNR); Prof. MELE, Altin (Ivodent Academy)

Session Classification: Session

Contribution ID: 3

Type: **not specified**

Rationally designed peptide conjugates in Alzheimer Disease: implications for diagnosis and therapy

Tuesday, 26 September 2023 14:15 (15 minutes)

Alzheimer Disease (AD) is a central neurodegenerative disorder characterized by behavioral disturbance and progressive cognitive impairment. It is the major cause of dementia affecting prevalently elderly individuals worldwide. The molecular pathways underlying AD onset implicates an abnormal turnover of the A β monomer undergoing an aggregation process to generate oligomers and protofibrils. A β oligomers are the most toxic substances for neurons, according to the amyloid cascade hypothesis. Unfortunately, there are challenges in diagnosing the early signs of the disease especially at the molecular level. Abnormal cognitive and behavioral clinical symptoms often indicate the accumulation of pathological markers in the brain. Therefore, early diagnosis and timely analysis of the condition are crucial for assessing the severity of the disease and providing appropriated treatment. Sensing molecules can be used to detect A β biomarker and then assists early AD diagnosis. Among these, peptides may represent an opportunity for theragnostic intervention.

Peptide-based epitopes with covalently attached other moieties able to explicate additional or complementary functions, including BBB permeation, metal chelation or aggregates disassembling, targeted imaging, and treatment, hold a promising potential for applications in AD.

In our laboratory, we have been synthesizing a variety of small peptides bio-conjugates differing by the peptide epitope or the conjugated scaffold. A range of molecular details, together with measured biological effects, have been listed with these systems, all of them accounting for the observed neuroprotection against the toxic insult induced by A β oligomerization in primary cortical neurons. In this brief communication an overview of the design principles of the peptide conjugates, their neuroprotective activity, and their capability in detecting A β peptide in solution are described in terms of potential use of these compounds as theragnostic agents and for the targeted drug delivery.

Presenter: Dr PAPPALARDO, Giuseppe (CNR-IC)

Session Classification: Session

Contribution ID: 8

Type: **not specified**

Surface energy determination of solid materials by contact angle measurement

Tuesday, 26 September 2023 15:00 (15 minutes)

The method of contact angle (CA; deg) is usually employed for the determination of surface free energy (SFE; mJ/m²) of solids and liquids (ST; mN/m). The CA method is one of the methods used in tensiometry, a non-invasive and rapid analytical approach capable of determining the surface energy properties of natural and artificial systems. The main aim of our work is the evaluation of the tensiometric variations of a raw extract of *Juniperus Communis* (REJ), extracted using liquid near-critical CO₂ as solvent in Soxhlet mode, and this extract after the demoterpenization process (DMT) performed by freezing out its monoterpene's fraction. The changes in surface properties of DMT were correlated to the modification of its chemical composition analysed by gaschromatography. In order to reach our objective, six solids test (st) having different tensiometric properties were used and in each case the CA variation with the time at st/DMT and st/REJ interfaces were measured.

Out of the six st lanolin alcohol can be considered as the reference solid test for the tensiometric evaluation of the process of demoterpenization of the extract of *Juniperus Communis*. The increase of the concentration of β -Cariophyllene and Cadinene causes the increase of CAs measured at the interface between lanolin alcohol and the extract of *Juniperus Communis* after the process of demoterpenization. The increase of Beta-Kariofilen and Kadinene concentration appear to be the main cause of the increase of polarity of the extract. This demonstrates that GC data and CA are linked to each other for that compounds that are more representative in the extract of *Juniperus Communis* (>20%). The GC data are in accord with CAs for compounds having highest concentration in DMT and REJ.

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Presenter: Dr ANDONI, Mariza (Ivodent Academy)

Session Classification: Session

Contribution ID: 16

Type: **not specified**

Simultaneous Thermal Analysis of high pressure impregnated PMMA for dental applications

Tuesday, 26 September 2023 14:30 (15 minutes)

Permanent or temporary dental prosthesis are prepared by milling PolyMethylMetaAcrylat (PMMA) commercial discs to support patients in after mouth surgery. Impregnation of PMMA with anti inflammatory/microbial compounds derived from plant extracts such as clove oil, could improve the healing process of these patients. Impregnation of PMMA is done under different pressures and densities, as well as different times of impregnation using near critical liquid CO₂.

In this study, dental PMMA is impregnated with essential clove oil using as solvent liquid carbon dioxide in which the oil is well soluble. Liquid CO₂ is known to diffuse well inside the PMMA matrix [1], transporting the clove oil inside PMMA as well.

The impregnation of the commercially available clove oil in the PMMA matrix disc was carried out in an high pressure vessel described elsewhere [2], where a known amount of clove oil, CO₂ and PMMA has been placed. CO₂ of 4.9 purity, PMMA disc Telio CAD LT B1 98.5-20 mm of manufacturer Ivoclar Digital and clove oil obtained by steam distillation of producer Argital where used. They were left inside the autoclave for 14 hours, in room temperature and pressure 64 bar. Afterwards CO₂ was released for 1 hour and samples were taken in 2 depths of PMMA disc (5 and 8mm) in order to analyse them for their content of clove oil compounds using simultaneous Thermal Analysis. The analysis is carried out in STA 449 F5 Jupiter of manufacturer Netzsch GB device in which thermogravimetric (TG) and differential scanning calorimetry (DSC) analysis are performed simultaneously.

Presenter: Dr LICA, Jeta (Ivodont Academy)

Session Classification: Session

Contribution ID: 18

Type: **not specified**

An integrative structural biophysics approach to study the interactions between ATP and neurotrophins

Tuesday, 26 September 2023 14:45 (15 minutes)

The talk will present the application of an integrative structural biology approach to the field of neurotrophins. The prototype of the neurotrophin family, Nerve Growth Factor (NGF), is essential for the development and maintenance of neurons and is crucial in immune and endocrine systems and in the pain pathway. NGF precursor, proNGF, whose pro-peptide is an intrinsically unstructured domain (IUD), is endowed with different biological properties. The binding to TrkA, p75NTR and sortilin receptors activates the NGF/proNGF signaling pathways. Much is known about NGF in neuronal physiology. However few reports described essential endogenous ligands as modulators of NGF biology.

Recently, the binding of ATP to NGF was identified. To determine the molecular elements of this binding, we used integrative structural biology with solution NMR and a set of complementary biophysical and computational methodologies, to unveil for the first time the binding cartography of ATP to NGF [1] and proNGF [2].

The used methodologies will be briefly presented, as well as the scientific results. Our results prove that ATP is responsible of a modulating quinary interaction with NGF, and that ATP binding induces a change in the conformation and/or dynamics of proNGF, predominantly in the IUD pro-peptide. These results, thus, pinpoint ATP as a likely molecular modulator of NGF and proNGF signalling, in health and disease states, and help providing an explanation for the neurotrophins' biology in neurodegenerative conditions.

Presenter: Dr PAOLETTI, Francesca (CNR-IC)

Session Classification: Session

Contribution ID: 21

Type: **not specified**

High pressure extraction of materials by near critical liquid solvents

Tuesday, 26 September 2023 15:40 (15 minutes)

The critical point of a substance represents the highest combination of temperature and pressure at which the separation between the gaseous and liquid phases remains continuous. Beyond this critical point, a state known as a supercritical fluid emerges, unifying the gaseous and liquid states and displaying properties that fall between those of gases and liquids. These distinct characteristics include reduced viscosity, diminished surface tension, enhanced diffusivity, and heightened compressibility. These attributes render supercritical fluids as effective solvents and eco-friendly alternatives to traditional organic solvents. It is crucial to note that these property shifts do not occur at a scale change at the critical point, instead, they exhibit a continuous variation in response to alterations in temperature and pressure (T/P). Making so the near-critical under conditions of liquid-vapor equilibrium substances, such as CO₂, NH₃, HCF₂Cl, or combinations like CO₂ and EtOH, to serve as extraction solvents in processes similar to Soxhlet extraction. This approach offers notable advantages, including enhanced safety of operation conditions, decreased energy requirements for compression and decompression, as well as heating and cooling of the liquid. Extraction times using Soxhlet-like extraction with near-critical substances typically range between 2 to 12 hours, and fractionation of the extract can be achieved by collecting the extract overtime to separate different groups of components.

Utilizing two commonly used herbs rich in bioactive compounds, such as Sage (*Salvia officinalis* L) and Lavander (*Lavandula angustifolia*) we conducted an extraction with near-critical liquid CO₂ under liquid-vapor equilibrium. The temperature gradient of the autoclave was between 285 K to 313 K and the pressure inside the vessel was in the range of 60-64 bar. The entire extraction process duration was 6 hours, with 20 minutes of Soxhlet cycles each.

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Presenter: Dr GJURGJAJ, Lorenci (Ivodent Academy)

Session Classification: Session

Contribution ID: 22

Type: **not specified**

Integrative Approaches in Structural Biology

Tuesday, 26 September 2023 15:55 (15 minutes)

With recent technological and computational advances, structural biology has begun to address increasingly difficult questions, including complex biochemical pathways and transient interactions between macromolecules. For many years our research group has been focused on the study of the structural characteristics of different classes of proteins. In this workshop, an example of a synergistic approach chosen from my previous research will be described and it will be shown how the joint use of in silico, solution and solid state techniques is crucial to clarify the catalytic mechanism of an enzyme that exploits the flexibility structure of its substrate.

Considering the context of this workshop, among the proteins studied by our research group, two in particular will be mentioned for their relevance in the control of the inflammatory response of the dental pulp: the first class is represented by the peroxisome proliferator-activated receptors (PPARs), a class of nuclear receptors primarily involved in metabolic homeostasis but also possessing other functions including maintaining the vitality of teeth after the removal of pathogens in dental tissues; the second protein that will be mentioned is β -catenin, which is active in several phases of dental development and whose signaling pathway seems to be involved in the regulation of the onset of periapical periodontitis.

Presenter: Dr MONTANARI, Roberta (CNR-IC)

Session Classification: Session

Contribution ID: 23

Type: **not specified**

Surface characterization of porous materials by N₂ adsorption/desorption in example of clays

Tuesday, 26 September 2023 16:10 (15 minutes)

Nitrogen adsorption isotherm measurement on porous materials at constant temperature 77 K and pressure ranging from 0.1 to 1000 mbar is the commonly used technique for the determination of their specific surface area and pore size distribution. Evaluation of specific surface area is done using the BET model and adsorption measurement in the pressure range 50-300 mbar, while the pore size distribution is estimated using the Kelvin equation in the capillary condensation pressure range, considered to happen between 400 to 1000 mbar.

This technique is used here aiming the changes of those surface parameters of natural Prrenjas clay samples when treated with sulphuric acid of different concentrations.

Prrenjas clay is a natural clay mineral from the southeast Albania of mainly montmorillonite type and high iron content. Its treatment with sulfuric acid in four different concentrations from 1.843 M up to 11.142 M, is shown to strongly influence its chemical composition, structure, specific surface area and pore volume. The acid treatment causes the leaching of almost all the metal ions present and the destruction of the crystalline structure of the clay. The Prrenjas clay is used in decoloring of edible oils in Albania. Further uses in biomedical field as carriers in drug delivery or antibacterial agent for the montmorillonites are known as well.

Presenter: Prof. MELE, Altin (Ivodont Academy)

Session Classification: Session

Contribution ID: 24

Type: **not specified**

Technologies, materials and clinical application of 3D printing

Tuesday, 26 September 2023 15:25 (15 minutes)

Since 2017 at IC - CNR started new research line to study the clinical use of image processing, reverse engineering and 3D printing for the introduction of innovative medical devices (MD) in pathways.

To this, an operative workshop for design and realization of personalized MD was designed and implemented. The first type of 3D printed MD was patient specific orthopaedic cast to be used for children requiring immobilisations. A second activity was devoted to the production of 3D models from NMR and CT images. The clinical value of the proposed devices has been verified.

Both activities have a twofold objective: (a) introduce new medical devices in the clinical pathways based on innovative techniques and (b) design production process compliant with the current European Medical Devices (MD) regulation (17/745) and on the basis of the up-to-date technical reference for 3D printing in medicine.

To this an operative workflow for the production of the personalized 3D printed medical devices has been produced.

Moreover, the project led to a specific spin off and to the launch of a Research Unit located both into the Santobono Pausilipon paediatric Hospital in Naples.

Presenter: Dr CLEMENTE, Fabrizio (CNR-IC)

Session Classification: Session