BIOPHYSICS IN AND FOR AFRICA

Report of Contributions

https://events.saip.org.za/e/biophysics2021

Contribution ID: **2** Type: **Oral Presentation**

RADIATION ATTENUATION PROPERTIES OF NATURAL PRODUCT-BASED ADHESIVE BONDED RHIZOPHORA SPP. PARTICLEBOARDS FOR TISSUE SUBSTITUTE PHANTOM APPLICATIONS

Tuesday, 23 March 2021 10:40 (20 minutes)

The present study investigates the radiation attenuation characteristics of particleboard phantoms made from Rhizophora spp. wood using natural product-based adhesives (SPI – soy protein isolate and SPC – soy protein concentrate) and sodium hydroxide (10 wt%) with two itaconic acid polyamidoamine-epichlorohydrin resin levels (10 and 15 wt%) at three different particle size (149 – 500, 74 – 149, and ≤ 74 μm). The radiation attenuation characteristics were evaluated with photons at 16.59 – 25.26 keV and 0.662 – 1.20 MeV gamma energies using X-ray fluorescence and Ludlum configurations. The most optimum characteristics of SPI-SPC-based particleboard phantoms compared to those of water and Perspex® were achieved with fine particles (≤ 74 μm) and 15 wt% IA-PAE resin. The overall findings demonstrated that cured SPI-SPC/NaOH/Rhizophora spp. particleboards with 15 wt% IA-PAE are potential materials for development of tissue substitute phantoms that mimic the radiation characteristics of human tissue at low and high photon energies.

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Presenter: Dr SAMSON, Damilola

Session Classification: X-Ray Scattering, Spectroscopy and Radiation in Biophysics

Track Classification: Biophotonics

Contribution ID: **3** Type: **Oral Presentation**

Theoretical comparison of real-time single-particle tracking techniques

Monday, 22 March 2021 15:00 (20 minutes)

One of the main challenges in studying single biomolecules in a native or near-native environment is their constant diffusion. An approach to solving this problem is real-time single particle tracking (SPT). In this study, we used statistical calculations and dynamic simulations to compare the orbital, Knight's Tour and MINFLUX localization methods, in the context of fluorescence-based and interferometric scattering (iSCAT) approaches. While the Knight's Tour method can track the fastest diffusion, MINFLUX achieves the greatest precision. The relative success of iSCAT vs fluorescence is strongly dependent on the particle size, and the photophysical properties and density of the fluorophores.

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Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **4** Type: **Oral Presentation**

The nanoscale structure of the Octopus ink: Sepia melanin

Monday, 22 March 2021 15:20 (20 minutes)

Sepia melanin isolated from the ink sacs of Sepia officinalis, is commonly used as standard in many research activities on melanin such as photobiology and photoreactivity of skin pigments. Melanins are difficult to characterize because of their intractable chemical properties and the heterogeneity in their structural features. Melanin pigments, in fact, are composed of many different types of monomeric units that are connected through strong carbon-carbon bonds. Its high insolubility and undefined chemical entities are two obstacles in its complete characterization. The morphological characterization and particle size distribution for sepia melanin by Scanning Electron Microscopy (SEM) on surface structure and Transmission Electron Microscopy (TEM) to confirm the morphology obtained from SEM was done. Both results show that Sepia melanin is formed by many aggregates agglomerated together. These aggregates are formed also by small spherical granules with different size distributions that have been determined using image-J software. The small granule diameter obtained from different TEM and SEM micrographs were 100-200nm. EDS reveals that C and O were the most abundant in sepia melanin with concentration average concentrations of about 57% and 24% respectively. The major compositions of sepia melanin are C, O, Na, Cl, while the minor are Mg, Ca, K, S and N. From TEM micrograph at high resolution, it was possible to measure the distance between polymers layers of sepia melanin using image-J software and it was 0.323 nm = 3.23 Å.

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Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **5** Type: **Oral Presentation**

EFFICIENCY OF OBTAINING CHICKEN CHICKES FROM A DIMENSIONED AUTOMATIC BIO-PHOTOVOLTAIC INCUBATOR

Friday, 26 March 2021 16:20 (20 minutes)

Abstract

The hatching using an incubator supplied from a bio-photovoltaic system, show as an alternative both efficient and sustainable, to regulate the physical factors that take part in biological processes. This research aimed to scale a autonomous bio-photovoltaic system to provide electricity in incubator with total capacity to hatch simultaneously 100 (hundred) chicken eggs. To scale the bio-photovoltaic autonomous system to the incubator was used sizing method of autonomous photovoltaic systems, which consists in calculating the rated power of the photovoltaic generator to scale it in terms of the total energy daily. We arrived to results that the incubator has the energy needs of 806.88 Wh/d, that is enough for successful working of the system, specially in mouth of the lowest radiation, the autonomy days demand that the bio-photovoltaic system was composed of 1 (one) bank of solar cells sealed with capacity of 495,0 Ah, a solar inverter with an apparent power of 400 W, 240 W load one driver current of 20 A to the DC side and 80 m copper electric cables with a minimum cross-sectional area of 1.5 mm^2. It is concluded that bio-photovoltaic electrification of the incubator is efficient, with outbreak of 80 to 99 % of total eggs and recommended compared with the incubators powered by convectional electric net, because out of present fluctuations, is a technology that is being solidified by presenting modularity, versatility, and large clean source, out of low costs of maintenance, so this results agree with those reported in Mucomole (2013), Casvassim (2004) and Wageningen et.al.(1995) where is applied the same description but for not automatic systems, that result in increasing of energy consumption and consequently its has a less efficiency.

Keyword: Biological processes, bio-photovoltaic, hatching, physical factors, eggs outbreak.

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Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **6** Type: **Oral Presentation**

Radiological Assessment of cement particles from Obajana Factory

Tuesday, 23 March 2021 11:00 (20 minutes)

Massive building constructions result to high demand of cement production in recent time. This lead Obajana cement plant to operate at maximum capacity in Nigeria. Exposure to high level radiation for prolong period can result to acute health effects such as skin burns, cancer and cardiovascular disease. This study evaluates the natural radionuclides and radiological indices of cement particles from productions plant of Obajana Factory. Gamma ray spectroscopy was used to analyze the activity level of 226Ra, 232Th and 40K in the samples. The activity concentration of the sample ranged between (7.4719±1.9179 – 60.1351±8.5508) BqKg-1, (29.4892±1.1009 – 90.1191±6.2124) BqKg-1 and (84.8930±3.8076 – 179.3318±11.4227) Bqkg-1, with the average value 36.0011±17.5529 Bqkg-1, 49.2077±21.1908Bqkg-1, and 146.6098±45.0115 Bqkg-1 for 40K, 226Ra and 232Th respectively. The activity concentrations of 226Ra and 232Th were slightly above the corresponding world average concentration of 32 BqKg-1 for 226Ra and 45 BqKg-1 for 232Th. The high concentration might be attributed to material composition used for cement production in Obajana Cement Factory. The average values of Absorbed dose (D), Annual effective dose rate (H), Annual gonad dose equivalent (AGDE) and Excess lifetime cancer risk (ELCR) are 53.303 nGy-1, 0.065 mSv, 363.961 mSvy-1 1.928 x10-3 respectively. The absorbed dose and annual gonad dose equivalent were lower than the world standard of 60 nGy-1 and 1.0 mSv respectively, while the Annual gonad dose equivalent (AGDE) and Excess lifetime cancer risk (ELCR) were slightly above the world standard of 300 mSvy-1 and 0.29 x10-3 respectively. The average value of External and Internal hazard indices (Hex and Hin) were below world standard of unity. The radiological assessment from this research compared favorably with other related published studies and world permissible limits, therefore constitute no radiological risk.

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Session Classification: X-Ray Scattering, Spectroscopy and Radiation in Biophysics

Track Classification: Biophotonics

Contribution ID: **7** Type: **Oral Presentation**

Mining the PDB for tractable cases where X-ray crystallography combined with fragment screens can be used to systematically design protein-protein inhibitors

Wednesday, 24 March 2021 11:10 (20 minutes)

The availability of small molecules able to selectively inhibit specific protein-protein interactions (PPI) in the cell would immensely facilitate our efforts to understand and manipulate the protein-protein "interactome". In our manuscript we show how a novel approach that combines X-ray crystallography and fragment screening can be used to systematically design protein-protein inhibitors. Recent technical advances in automated data collection and interpretation of electron density maps have made it possible to combine X-ray crystallography and fragment screening in a medium throughput fashion. This approach is generally used by academia and pharma to develop molecules that target the catalytic site of enzymes. In here we demonstrate that, contrary to the accepted view, the same approach can be used to chemically probe the surfaces used by proteins to interact, and use the outcome of the screens to systematically design protein-protein inhibitors. To prove it we first ran a bioinformatics analysis of the PDB which revealed over 400 protein complexes where the individual protein crystallises in a lattice where large portions of the interacting surfaces are free from lattice contacts and accessible to fragments during soaks. Among the tractable complexes identified, we chose two cases: the Il1β-ILR and p38α-TAB1 complexes and we run a single fragment crystal screen. The output of the screens showed that fragments tend to bind in clusters highlighting the small molecules hotspots on the surface of the target protein and often the hotspots overlap with the binding sites of the interacting proteins. Finally for one of the complexes, p38α-TAB1, we carried out a chemical exploration and improved the initial binding of the fragments bringing it into the micromolar range.
We believe we have developed a new paradigm for a low-cost rapid pipeline utilizing in-crystal fragment screening to develop PPI inhibitors.

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Session Classification: Structural biology I

Track Classification: Structural biology I

Contribution ID: **8** Type: **Oral Presentation**

Structure of mycobacterial ATP synthase with the TB drug bedaquiline

Wednesday, 24 March 2021 15:40 (40 minutes)

Tuberculosis (TB), the world's leading cause of death by infectious disease, is increasingly resistant to current first line antibiotics. The bacterium Mycobacterium tuberculosis that causes TB can survive low-energy conditions, which allows infections to remain dormant and decreases their susceptibility to many antibiotics. Bedaquiline was developed in 2005 from a lead compound identified in a phenotypic screen against M. smegmatis. It can sterilize even latent infections and has become a cornerstone of treatment for multidrug-resistant and extensively drug-resistant TB. Bedaquiline targets the mycobacterial ATP synthase, an essential enzyme in the obligate aerobic Mycobacterium genus, but how it binds the intact complex is unknown. We determined structures of M. smegmatis ATP synthase with and without bedaquiline. The drug-free structure suggests how hook-like extensions from the alpha subunits prevent the enzyme from running in reverse, inhibiting ATP hydrolysis and preserving energy in hypoxic conditions. Bedaquiline binding induces large conformational changes, creating tight binding pockets at the interface of subunits a and c that explain the drug's potency as an antibiotic for TB.

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Presenter: RUBINSTEIN, John (The Hospital for Sick Children)

Session Classification: Structural biology II

Track Classification: Structural biology II

Contribution ID: **9** Type: **Oral Presentation**

Photosynthesis Underneath Stones in the Namib Desert

Thursday, 25 March 2021 10:00 (20 minutes)

In hyper-arid soil environments, photosynthetic microorganisms are largely restricted to hypolithic habitats. They occupy the ventral surfaces of translucent pebbles in desert pavements. We combined fluorometric, spectroscopic, biochemical and metagenomic approaches to investigate the light transmission properties of quartz stones in the Namib Desert, and assess the photosynthetic activity of the underlying hypolithic cyanobacterial biofilms. Quartz pebbles greatly reduced the total photon flux to the ventral surface biofilms and filtered out primarily the short wavelength portion of the solar spectrum. Chlorophylls d and f were not detected in biofilm pigment extracts; however, hypolithic cyanobacterial communities showed some other evidence of adaptation to sub-lithic conditions, like the prevalence of genes encoding Helical Carotenoid Proteins, which are associated with desiccation stress. Under water-saturated conditions, hypolithic communities showed no evidence of light stress, even when the quartz stones were exposed to full midday sunlight. This work adds to an understanding of the mechanisms behind the unique robustness of photoautotrophic organisms in extreme environments.

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Presenter: GWIZDALA, Michal (University of Pretoria)

Session Classification: Cellular biophysics

Track Classification: Cellular biophysics

Contribution ID: **10** Type: **Oral Presentation**

Phycobilisomes' secret life unravelled with single molecule spectroscopy

Monday, 22 March 2021 11:00 (20 minutes)

In many strains of cyanobacteria, phycobilisomes (PBs) absorb light and transfer excitations to the photosystems. In PBs from Synechocystis PCC6803, 396 identical pigments are bound to the protein subunits that differ in their optical properties due to various pigment-protein interactions. This tuning makes PBs efficient in transferring energy from the rods to the core and finally to the photosystems.
Recently, single molecule spectroscopy has revealed the spectroscopic dynamics of PBs. We performed our SMS measurements using physiologically relevant light intensities and discovered a novel type of photoprotective mechanism. This mechanism is light-activated and does not require interactions with other proteins. Switching between thermal energy dissipative and light-harvesting states involves a conformational change.
At the single-molecule level, we have also investigated the main cyanobacterial photoprotective mechanism, involving the orange carotenoid protein (OCP). By controlling the interaction between individual PBs and single OCPs, we revealed an intermediate state of energy quenching signifying the docking of OCP on a PB. In this intermediate state, some of the rods temporarily disconnect from the core and a hidden red state is exposed.
Not all hidden states of PBs are quenched. The isolated rods of PBs can assume two different states, both of which are possibly involved in energy transfer to the photosystems. While one of these states fits the well-established model of energy transfer in PB, the other state is characterized by red-shifted emission and most likely involved with energy transfer to photosystem I.

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Session Classification: Quantum biology

Track Classification: Molecular biophysics

Contribution ID: **11** Type: **Oral Presentation**

Investigating single-beam CARS for microscopy applications

Friday, 26 March 2021 15:00 (20 minutes)

A spectroscopic study on olive oil was performed using a novel single-beam CARS implementation in order to evaluate the setup's suitability for CARS microscopy. Using a compact setup consisting of a fs-oscillator, an all-normal dispersion photonic crystal fiber and an SLM in 4f-shaper geometry, one can successfully generate and measure SB-CARS spectra. Polarization and phase shaping the excitation source with the SLM, after temporal compression using i2PIE, allows for targeting chosen Raman transitions which is ideal for chemically specific and tag free imaging of biological samples. With our phase shaping approach, we were able to target and identify characteristic Raman transitions of fatty acids contained in olive oil. This positive result confirms that our single-beam CARS approach is suitable for CARS microscopy of biological samples.

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Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **12** Type: **Oral Presentation**

EARLY DETECTION OF BREAST CANCER WITH AN OPTICAL FOURIER DOMAIN SYSTEM USING MICROWAVE SIGNALS AS SOURCE

Tuesday, 23 March 2021 15:40 (20 minutes)

Detection of developing breast tumour in women for early treatment in recent times has yielded some results. Yet only developed tumours are detected at the stage where the only treatment method is either to remove or inhibit the growth of tumour which has its effects, possibly leading to loss of human life. Ongoing research, proposes to simulate the growth stages of tumour in human breast for early detection of tumour with an implemented Optical Fourier Domain Imaging (OFDI) system using microwave signals as source by developing breast phantoms mimicking breast composition and determining the thickness of various object sizes embedded in phantom like breast. For now, determination of the depth profile of samples and thickness measurement of sample with OFDI system is demonstrated.

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Session Classification: Biophysics and maternal health

Track Classification: Biophysics and maternal health

Contribution ID: **13** Type: **Oral Presentation**

Pheno-RNA, a method to associate genes with a specific phenotype, identifies genes linked to cellular transformation

Thursday, 25 March 2021 15:00 (20 minutes)

Cellular transformation is associated with dramatic changes in gene expression, but it is difficult to determine which regulated genes are oncogenically relevant. Here we describe Pheno-RNA, a general approach to identifying candidate genes associated with a specific phenotype. Specifically, we generate a "phenotypic series" by treating a nontransformed breast cell line with a wide variety ofmolecules that induce cellular transformation to various extents. By performing transcriptional profiling across this phenotypic series, the expression profile of every gene can be correlated with the strength of the transformed phenotype. We identify ~200 genes whose expression profiles are very highly correlated with the transformation phenotype, strongly suggesting their importance in transformation. Within biological categories linked to cancer, some genes show high correlations with the transformed phenotype, but others do not. Many genes whose expression profiles are highly correlated with transformation have never been associated with cancer, suggesting the involvement of heretofore unknown genes in cancer.

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Session Classification: Computational biology

Track Classification: Computational biology

Contribution ID: **23** Type: **Oral Presentation**

Evaluation of Temperature Gradient within Different Head Tissue Layers Exposed to Radiofrequency Radiation Emitted by GSM Transceiver Base Station Using Pennes Model of the Bio-Heat Equation

Friday, 26 March 2021 16:00 (20 minutes)

Abstract
While the spectrum growth of radiofrequency (RF) emission is likely to experience astronomical increase in the years to come, the imminent query would be whether the current spectrum management process is capable of fulfilling all future requirements. Public interest in the potential health issues relating to cellular or mobile communication transceiver base station antennas (BSA) emphasize on the importance of having an accessible and easy to understand information on electromagnetic (EM) and radiofrequency radiation (RFR) levels in the surrounding environment.
In this study, measurements of electric field and magnetic field level were made around selected transceiver base station antennas in selected South-South States Nigeria, with the aid of frequency-selective equipment (CORNET, Electrosmog meter ED78S EMF RF/LF Dual mode model).
Pennes Bio-heat equation was employed to compute the temperature gradient in biological materials due to EM exposure, which takes into account the heat exchange mechanisms such as heat conduction, blood flow, EM energy dissipation, and metabolism. Using the local operator's technical parameters, a theoretical simulation/estimation was done for comparative analysis. This perfectly agrees with other models and it also shows how RF radiation affects biological materials/tissues. It proves that the most vulnerable part of the head when exposed to RF radiation is the brain with temperature gradient of 0.087934oC/mm.

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Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **25** Type: **Oral Presentation**

Quantum plasmonic biosensing

Monday, 22 March 2021 10:00 (20 minutes)

Surface plasmon resonance (SPR) is a highly sensitive technique for monitoring changes in the optical properties of a substance in the immediate vicinity of a sensor surface, this makes it very useful in biosensing and surface science research. The most common SPR setup is the Kretschmann configuration in which surface plasmons are excited using a bulk prism and a gold-coated microscope slide. It is a key technology for the characterization of biomolecular interactions and is integrated into many stages of the drug discovery process. The characterization of these biomolecular interactions involves measuring kinetic parameters.

We constructed a two-mode sensing model which we use to measure the kinetic parameters of biomolecular interactions on an SPR setup. The model was also used to measure the precision with which we can measure the kinetic parameters. In our research we made comparisons of the precision we could measure based on the input to our model, i.e., we compared the precision when we used classical states of light versus when we used quantum states of light as input to our model.

Our model showed that using quantum states of light such as the Fock state, two-mode squeezed vacuum and two-mode squeezed displaced state improves the precision in the estimation of kinetic parameters. Quantum states of light allow us to measure the parameters more accurately in comparison to classical states of light. We used our model to study a specific binding reaction, i.e, immobilized Bovine serum albumin (BSA) interaction with anti-BSA, from which we extracted the kinetic parameters and showed the precision enhancement which quantum states bring.

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Session Classification: Quantum biology

Track Classification: Quantum biology

Contribution ID: **26** Type: **Oral Presentation**

A Systematic Integration of Empirical and Computational Studies to Biophysically Describe Recombinant Nicotinate Mononucleotide Adenylyltransferase (NaMNAT) From Klebsiella pneumonia

Monday, 22 March 2021 16:00 (20 minutes)

Nicotinate mononucleotide adenylyltransferase (NaMNAT) is an indispensable enzyme in the biosynthesis of pyridine dinucleotides. Given the vital role of NAD+ in controlling key cellular processes, NaMNAT represents an attractive target for the design of novel broad-spectrum antibiotics to treat nosocomial infections associated with MDR Klebsiella Pneumonia. This study aims to characterize the biophysical structure of NaMNAT from K. Pneumonia (KpNaMNAT) using a systematic combination of experimental and computational approaches. Overexpression and purification were carried out using hexa-histidine tags in E. coli expression system and nickel ion-immobilized metal affinity chromatography. Activity studies using NMN substrate showed KpNaMNAT to demonstrate broad pH optima of 6.5-9.5 and preference for Mg2+. Structural characterisation revealed KpNaMNAT as a monomer with predominate α-helices. ATP, NMN, and NAD+ all bind at the same site on KpNaMNAT, but do not induce any significant conformational changes, however, ATP responds to Mg2+ more than the other ligands and the protein response in the presence of Mg2+. The data and insight provided by this novel research would be useful as a molecular basis for further evaluation of the enzymes for the design of structure-based inhibitors with therapeutic potential.

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Presenter: JEJE, Olamide

Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **27** Type: **Oral Presentation**

Epolactaene-derived identification of potential inhibitors of S. mansoni Hsp60 towards anti-schistosomal drug discovery

Thursday, 25 March 2021 15:40 (20 minutes)

Human schistosomiasis has heavily plagued the destitute of various tropical and sub-tropical countries of the world, particularly in sub-Saharan Africa and South America, with devastating effects in various health and economic areas [1]. Globally, the burden of schistosomiasis has been controlled by using a single chemotherapeutic drug, Praziquantel [2]. However, the drug has recently displayed various shortcomings, including its inability to destroy juvenile schistosome worms, as well as drug resistance in response to its extensive use. This has prompted efforts concentrated on the discovery and design of new anti-schistosomal drugs [3].
In this study, in silico techniques and tools were used to elucidate the structural binding and interaction between the S. mansoni heat shock protein 60 (SmHsp60) and epolactaene-based inhibitors. The upregulation of heat shock proteins in the schistosome lifecycle is significant in overcoming the proteotoxic environment experienced within the human host. Through the creation of SmHsp60 complexes with pharmacophore-derived inhibitors with the lowest binding energies, molecular dynamic (MD) simulations were performed.
Post-MD analyses of the trajectories indicates various energetic, structural and conformational changes, as well as the identity of amino acid residues involved in the interaction with the inhibitors. Our results further showed that inhibitor 2 and inhibitor 3 exhibited enhanced inhibitory activity against SmHsp60, thus suggesting their potential as “lead compounds” in the design of new anti-schistosomal drugs.

References
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[2] Masamba, P., Adenowo, A. F., Oyinloye, B. E., & Kappo, A. P. (2016). Universal stress proteins as new targets for environmental and therapeutic interventions of Schistosomiasis. International Journal of Environmental Research and Public Health, 13(10), 972.
[3] Aruleba, R. T., Adekiya, T. A., Oyinloye, B. E., Masamba, P., Mbatha, L. S., Pretorius, A., & Kappo, A. P. (2019). PZQ Therapy: How Close are we in the Development of Effective Alternative Anti-schistosomal Drugs? Infectious Disorders - Drug Targets, 19(4), 337–349.

Keywords: Epolactaene; Hsp60; Pharmacophore; Praziquantel; schistosomiasis

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Session Classification: Computational biology

Track Classification: Computational biology

Contribution ID: **28** Type: **Oral Presentation**

Structural biology using neutrons: introduction and how to get started

Wednesday, 24 March 2021 15:00 (40 minutes)

The method of choice for obtaining detailed, high resolution structural information macromolecules is X-ray crystallography. The magnitude of X-ray scattering from the electron cloud around an atomic nucleus is related to the Z number of that element, i.e., the more electrons an atom has, the better it will scatter X-rays. Due to this it is very challenging in theory and practice to determine the position of H atoms in crystal structures. Neutron diffraction offers a highly complementary approach in that the neutrons are scattered from atomic nuclei of all elements to a similar extent. This means that in practice the nuclear density maps for C, N, H (and its isotope Deuterium, or D), and O atoms all appear to a similar extent, even at medium (˜2 Å) resolution. H atoms are very important in biology as they are involved with everything – including hydrogen bonds, protein folding, solvation, electrostatics, amino acid side chain charge state, ligand binding, and enzyme catalytic mechanisms. To profit from neutron scattering properties and to be able to "see" these H atoms, it is crucial to deuterate (i.e. replace all H with isotope D) the materials to be studied. Multiple approaches to biological deuteration will be explained as well as the growth of large protein crystals for neutron diffraction. Finally, some practical aspects of what beamlines are available, and how to get access to neutron scattering facilities will be covered.

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Session Classification: Structural biology II

Track Classification: Structural biology II

Contribution ID: **29** Type: **Oral Presentation**

Structural and functional characterization of the secreted adhesion EtpA of enterotoxigenic Escherichia coli

Wednesday, 24 March 2021 16:50 (20 minutes)

Oral presentation

Primary authors: Mr NTUI, Clifford Manyo (University of Pretoria); Prof. SCHUBERT, Wolf-Dieter (University of Pretoria)

Presenter: Mr NTUI, Clifford Manyo (University of Pretoria)

Session Classification: Structural biology II

Track Classification: Structural biology I

Contribution ID: **30** Type: **Oral Presentation**

Evolutionary cues in the physicochemical description of proteomes

Monday, 22 March 2021 16:20 (20 minutes)

With the glaring exception of highly conserved binding interfaces, protein surfaces tend to be regarded as variable regions of hydrophilic character, subjected only to soft evolutionary pressures. However, in crowded cellular conditions, electrostatic interactions between surfaces take on a critical role in modulating protein interactivity, with downstream consequences for protein stability, mobility and solubility. In this context, surface net charge density stands out as the single most important determinant of protein mobility inside the cell. Moreover, in *E. coli*, proteins organise around a moderately negative net charge density value, which ensures cytosol-wide colloidal stability: molecules keep away and remain highly mobile most of the time, but close-range interactions are allowed upon small thermal fluctuations. Our results show that, across organisms, the average value at which this Goldilocks situation is achieved varies, often depending on niche and intracellular conditions: extreme lifestyles—archaeal halophiles and endosymbiotic bacteria— can be mapped to different net charge density values. By combining net charge density with other simplistic physicochemical observables, derived from sequence data alone, we can show that the profile of different organism groups changes consistently with the taxonomical hierarchy. Thus, we propose that previously unrecognised evolutionary cues can be revealed by inexpensive physicochemical profiling, and that these have the potential to contribute complementary information to state-of-art phylogenetic inference.

Primary author: VALLINA, Eloy (Stockholm University)

Presenter: VALLINA, Eloy (Stockholm University)

Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **31** Type: **Oral Presentation**

QUALITY CONTROL ANALYSIS OF DIAGNOSTIC RADIOLOGY EQUIPMENT IN 44 NIGERIAN ARMY REFERENCE HOSPITAL KADUNA, KADUNA STATE, NIGERIA

Tuesday, 23 March 2021 11:20 (20 minutes)

In this study, quality control analysis of radiographic equipment used in the Radiology unit of 44 Nigerian
Army Reference Hospital Kaduna was carried out in order to ensure that both workers and patients were within the minimum recommended radiation exposure level. The dose rate at the operator stand,
X-ray table, corridor, change cubicle, offices, and reception were measured with survey meter (RADOS,
model, RDS-120). Generally, the result obtained indicated that both parameters assessed showed a good
level of compliance, with only digital radiography that was found to have failed Half Value Layer (HVL) test. The exposure reproducibility, kVp test, beam alignment, and HVL could not be assessed for
Mammographic equipment because of its non-availability in the QA/QC kit. Visual inspection showed that the X-ray Machines and rooms dimensions are adequate, with exception of personal monitoring badges (TLD) that were not available. The background radiation dose level was found to be safe for the patient, staff, and general public. The measured leakage radiation and entrance skin dose also showed a
very good level of compliance with both National and International regulations.
Keywords: radiographic equipment; X-ray; QA/QC kit; exposure reproducibility

Primary author: Mr MUHAMMAD NURUDDEEN ABDULKAREEM, Muhammad

Co-author: Mr ABDULKAREEM, Muhammad Nuruddeen (Federal University of Kashere)

Presenter: Mr ABDULKAREEM, Muhammad Nuruddeen (Federal University of Kashere)

Session Classification: X-Ray Scattering, Spectroscopy and Radiation in Biophysics

Track Classification: Small/Wide-angle X-ray scattering in biophysics

Contribution ID: **33** Type: **Oral Presentation**

Crystallization of membrane transport proteins in Lipidic Cubic Mesophase (LCP) aided by an engineered Green Fluorescent Protein Thermal Shift Screen (GFP-TS)

Wednesday, 24 March 2021 10:50 (20 minutes)

Membrane protein crystals grown by the *in meso* or lipidic cubic phase (LCP) method generally produce higher-resolution structures, as they have a lower solvent content (type I crystals) than those grown by traditional vapour-diffusion crystallization (type II crystals). To grow LCP crystals of membrane proteins with the synthetic lipid monoolein, the purified membrane protein solution is mixed with the molten monoolein in a weight ratio of 2:3 respectively. It can be very challenging to grow LCP crystals of membrane proteins, however, and while it is generally thought to be a fairly mild environment, the stabilities of different membrane proteins have not been extensively compared.
We engineered a Green Fluorescent Protein Thermal Shift Screen (GFP-TS) and use it to identify specific lipid for the bacteria sodium proton exchanger (NhaA) and also, a specific ligand for the plant homologue of the human CMPsialic acid/CMP exchanger (SLC35A1). The former was crystallized and the structure solved by LCP in the presence of its specific lipid while the latter in the presence of its specific ligand at 2.3 and 2.8 Å respectively. No detectable crystal was obtained in the absence of either the lipid or ligand after extensive crystallization trials. The GFP-TS method should prove useful for screening lipid additives and ligands to stabilize membrane proteins for structural determination by X-ray crystallography and single-particle Cryo-EM.

References

Nji, E., Chatzikyriakidou, Y., Landreh, M. & Drew, D. (2018). An engineered thermal-shift screen reveals specific lipid preferences of eukaryotic and prokaryotic membrane proteins. Nature Communications, 9(1), 4253.
Nji, E., Gulati, A., Qureshi, A. A., Coincon, M. & Drew, D. (2019). Structural basis for the delivery of activated sialic acid into Golgi for sialyation. Nature Structural and Molecular Biology, 26(6), 415–423.

Primary author: NJI, Emmanuel (BioStruct-Africa)

Presenter: NJI, Emmanuel (BioStruct-Africa)

Session Classification: Structural biology I

Track Classification: Structural biology I

Contribution ID: **34** Type: **Oral Presentation**

Improved quality in nonlinear optical imaging using i2PIE pulse compression

Friday, 26 March 2021 15:20 (20 minutes)

We present a novel nonlinear microscopy modality using a time domain ptychographic phase measurement technique to compress supercontinuum pulses used as excitation source, in so reducing average power while improving contrast.

Primary authors: DWAPANYIN, George Okyere (Stellenbosch University); SPANGENBERG, Dirk--Mathys (University of Stellenbosch); Prof. FEURER, Thomas (University of Bern); Dr HEIDT, Alexander (University of Bern); BOSMAN, Gurthwin (Stellenbosch University); NEETHLING, Pieter (Laser Research Institute, University of Stellenbosch); ROHWER, Erich (University of Stellenbosch)

Presenter: DWAPANYIN, George Okyere (Stellenbosch University)

Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **35** Type: **Oral Presentation**

Molecular simulations of the interaction between Schistosoma mansoni axonemal dynein intermediate chain protein and dynarrestin

Thursday, 25 March 2021 16:00 (20 minutes)

Praziquantel (PZQ) has been the drug of choice for the treatment of schistosomiasis for more than 30 years. Resistance to this drug, however, has been documented severally in recent years, hence the need for effective alternatives. This study investigated the effect of an inhibitor (dynarrestin) on the identified Schistosoma mansoni axonemal dynein intermediate protein (SmAxDynIC), a potential schistosome drug target. The protein functions in schistosome cilia and flagella beating; therefore inhibiting this protein could lead to the immobility of the worm and disrupt its developmental cycle. Molecular dynamic simulations and post-MD analyses were conducted to ascertain the various characteristics of the inhibitor and its interaction with the SmAxDynIC. This was followed by the screening for a pharmacophore of the inhibitor to discover 'lead' compounds against schistosomiasis. Concluding findings of this study indicated that dynarrestin exhibits ample inhibitory characteristics against the SmAxDynIC, as well as a very strong binding affinity for the active site of the modelled axonemal dynein protein. Three additional ligands were identified using the pharmacophore and it is suggested that these will be employed for in vivo testing on various schistosomal cell lines in future interaction studies.

Keywords: Praziquantel; Schistosomiasis; Schistosoma mansoni; dynarrestin; SmAxDynIC

Primary author: Mr PILLAY, Deshan (University of Johannesburg)

Co-authors: Dr MASAMBA, Priscilla (University of Johannesburg); Prof. KAPPO, Abidemi Paul (University of Johannesburg)

Presenter: Mr PILLAY, Deshan (University of Johannesburg)

Session Classification: Computational biology

Track Classification: Computational biology

Contribution ID: **36** Type: **Oral Presentation**

COVID-proofing Biochemistry and engaging diverse students with Crystallography Research

Tuesday, 23 March 2021 16:40 (20 minutes)

My objective is to share approaches by which I incorporate structural biology into our biochemistry curriculum at Hampton University. I will also discuss methods to engage K-12 and undergraduate students in crystallographic research and structural biology (since 2001). I will show the successes and failures involved in the process of fully integrating these pre-baccalaureate students in crystallography research. Our outreach efforts have included socioeconomically underserved students or groups underrepresented in STEM. We will present strategies for recruiting and retaining STEM students. We will present the significant barriers to our research programs. We will also discuss potential funding sources. Finally, we will present how structural science has helped COVID-proof our research and biochemistry teaching approach over the past year of remote-learning.

Primary author: ASOJO, Oluwatoyin (Hampton University)

Presenter: ASOJO, Oluwatoyin (Hampton University)

Session Classification: Development of the future of biophysics in Africa

Track Classification: Development of the future of biophysics in Africa

Contribution ID: **37** Type: **Oral Presentation**

Fighting against COVID-19: A computational biophysics approach

Monday, 22 March 2021 15:40 (20 minutes)

Previously it was reported that cell-surface Glucose Regulated Protein 78 (CS-GRP78), also termed heat shock protein A5 (HSPA5), could be a possible route for SARS-CoV-2 internalization. The binding site on the spike protein of SARS-CoV-2, which can recognize CS-GRP78, was predicted in a previous study. The spike glycoprotein of the SARS-CoV-2 bear many conserved motifs to the previously determined human coronavirus strains such as HKU1, 229E, NL63, OC43, MERS-CoV, and SARS-CoV. 2 However, we would like to emphasize that using a simple bioinformatics approach can suggest a possible role of the GRP78 in cross immunization against COVID-19. Additionally, different antiviral drugs have the potential to be SARS-CoV-2 inhibitors, thus can be used against COVID-19. These drugs are tested in silico at the beginning of the pandemic, and currently, some are approved against COVID-19.

Recent Publications
1. Ismail AM, Elfiky AA. SARS-CoV-2 spike behavior in situ: a Cryo-EM images for a better understanding of the COVID-19 pandemic. Signal Transduction and Targeted Therapy. 2020;5(1):252.
2. Ibrahim IM, Abdelmalek DH, Elshahat ME, Elfiky AA. COVID-19 spike-host cell receptor GRP78 binding site prediction. Journal of Infection. 2020;80(5):554-62.
3. Elfiky AA. SARS-CoV-2 Spike-Heat Shock Protein A5 (GRP78) recognition may be related to the immersed human coronaviruses. Frontiers in Pharmacology. 2020;11:1997.
4. Elfiky AA, Ibrahim IM, Ismail AM, Elshemey WM. A possible role for GRP78 in cross vaccination against COVID-19. Journal of Infection.
5. Elfiky AA. Natural products may interfere with SARS-CoV-2 attachment to the host cell. Journal of Biomolecular Structure and Dynamics. 2020:1-10.

Primary author: Dr ELFIKY, Abdo (Cairo University)

Presenter: Dr ELFIKY, Abdo (Cairo University)

Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **38** Type: **Oral Presentation**

The characterization and crystallization of the TBR1 T-box domain in the presence and absence of the T-box Binding Element

Monday, 22 March 2021 16:40 (20 minutes)

TBR1 is a neuron-specific transcription factor involved in multiple aspects of cortical development,and has recently emerged as a master regulator of genes implicated in Autism Spectrum Disorder (ASD).It is thus possible that aberrant molecular interactions with TBR1 could underlie the altered neuro-molecular networks observed in Autism.

Currently there is no solved structure available of the TBR1 TBOX domain. In this study, we aim to obtain crystal structures of the TBR1 T-box domain in both the presence and absence of the T-box binding element, with the hope of elucidating its DNA-binding mechanism. The structure may be solved by molecular replacement using TBX21. This will shed more light on how TBR1 regulates ASD-related genes and could explain how aberrant molecular interactions influence neurodevelopmental disorders.

Preliminary structural characterization has been made by monitoring intrinsic tryptophan fluorescence and has revealed that the protein is properly folded. The DNA-binding function has been confirmed using an electrophoretic mobility shift assay. The DNA-binding properties were quantitatively assessed using fluorescence anisotropy and revealed a dissociation constant of 320 nM. Since the TBR1 T-box has been successfully characterized, it is ready for crystal trials.

Primary author: MAYET, Riyaadh (University of the Witwatersrand)

Co-author: Dr FANUCCHI, Sylvia (University of the Witwatersrand)

Presenter: MAYET, Riyaadh (University of the Witwatersrand)

Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **39** Type: **Oral Presentation**

Applications of machine learning techniques to the description of quantum coherent excitation energy transfer within the dimer model

Monday, 22 March 2021 10:20 (20 minutes)

During photosynthesis in light-harvesting complexes, energy is transferred from antenna pigments to the reaction centre to trigger photochemical reactions. The idea of quantum coherence playing a role in photosynthesis arose from observations that excitation energy transfer (EET) processes in these complexes are efficient to an extent that exceeds explanation using only classical theory. The formalism adopted to study EET processes is the Hierarchical Equations of Motion (HEOM). However, solving these equations is computationally costly due to the adverse scaling with the number of pigments. We use a trained convolutional neural network as a representation of the HEOM where elements of reduced density matrices are translated into features for the model and corresponding excited state energies and electronic couplings are used as labels. We discuss the investigation of the spin-boson-type model where our predictions of the parameters for the Frenkel Hamiltonian are gauged by mean square error and accuracy measures.

Primary author: NAICKER, Kimara

Co-authors: Prof. PETRUCCIONE, Francesco; Prof. SINAYSKIY, Ilya

Presenter: NAICKER, Kimara

Session Classification: Quantum biology

Track Classification: Quantum biology

Contribution ID: **40** Type: **Oral Presentation**

FROM NATURE TO BIOMIMICRY TOWARDS NANOTECHNOLOGY

Friday, 26 March 2021 16:40 (30 minutes)

Primary authors: Mr NGOM, Ibrahima (University of South Africa); Dr NDIAYE, Ndeye Maty (1Laboratoire de Photonique Quantique, Energie et Nano-Fabrication, Faculté des Sciences et Techniques Université Cheikh Anta Diop de Dakar (UCAD) B.P. 5005 Dakar-Fann, Dakar, Sénégal); Dr SYLLA, Ndeye Fatou (Laboratoire de Photonique Quantique, Energie et Nano-Fabrication, Faculté des Sciences et Techniques Université Cheikh Anta Diop de Dakar (UCAD) B.P. 5005 Dakar-Fann, Dakar, Sénégal); Mrs DIENG, Sokhna (Laboratoire de Photonique Quantique, Energie et Nano-Fabrication, Faculté des Sciences et Techniques Université Cheikh Anta Diop de Dakar (UCAD) B.P. 5005 Dakar-Fann, Dakar, Sénégal); Dr NGOM, Balla Diop (Laboratoire de Photonique Quantique, Energie et Nano-Fabrication, Faculté des Sciences et Techniques Université Cheikh Anta Diop de Dakar (UCAD) B.P. 5005 Dakar-Fann, Dakar, Sénégal); Prof. MAAZA, Malik (UNESCO-UNISA Africa Chair in Nanoscience and Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa, Muckleneuk Ridge, PO Box 392, Pretoria, South Africa)

Presenter: Prof. MAAZA, Malik (UNESCO-UNISA Africa Chair in Nanoscience and Nanotechnology (U2ACN2), College of Graduate Studies, University of South Africa, Muckleneuk Ridge, PO Box 392, Pretoria, South Africa)

Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **41** Type: **Oral Presentation**

Poisson Boltzmann equation for charged palettes

Thursday, 25 March 2021 16:20 (20 minutes)

Abstract
Electrostatic interaction between parallel charged palettes can be considered as a starting point to investigate the properties of complexes biological mater like AND-protein interactions. In this work, we solve numerically the Poisson Boltzmann equation to calculate the electrostatic potential between charged palettes immerged in aqueous solution containing monovalent salt. The electrostatic field and the ionic profile are also calculated.
Key words
Poisson Boltzmann equation, ADN protein, electrostatic interaction.

Primary author: SMAIN, Fatiha (Département de physique de l'université de Tlemcen)

Presenter: SMAIN, Fatiha (Département de physique de l'université de Tlemcen)

Session Classification: Computational biology

Track Classification: Computational biology

Contribution ID: **42** Type: **Oral Presentation**

Molecular basis for the transfer of large toxin plasmids in Clostridium perfringens

Wednesday, 24 March 2021 17:10 (20 minutes)

The transfer of large toxin and antibiotic resistance genes in the pathogenic bacteria *Clostridium perfringens* is mediated by the *tcp* conjugation locus. Functional genetic analysis of the tcp locus of the paradigm plasmid pCW3 has revealed that its gene products assemble into a multi-protein complex that distantly resembles a type 4 secretion system (T4SS).

Here, I will provide a brief summary of our current understanding of the DNA system., knowledge that was built upon a combination of structural biology studies and functional microbial genetics

Primary author: TRAORE, Daouda

Presenter: TRAORE, Daouda

Session Classification: Structural biology II

Track Classification: Structural biology I

Contribution ID: **43** Type: **Oral Presentation**

Structural and un-structural biology by NMR spectroscopy

Wednesday, 24 March 2021 16:20 (30 minutes)

Nuclear Magnetic Resonance (NMR) spectroscopy is an enabling technology capable to provide information and answers to biological problems that cannot be obtained by other means. NMR studies, both in solution and in the solid-state, can inform on the structure of a macromolecule in many different environments ranging from buffered solutions to intact cells, can provide insight into dynamic processes, and allow to monitor biomolecular interactions that are key to the cellular response to environmental, developmental and growth signals.
NMR is central to the study of folding, unfolding and disordered states of proteins because of its capability to define the structures of proteins in solution and to characterize the dynamic properties that are inherent to function.
As such, we will provide some examples of recent applications of NMR spectroscopy carried out at the CERM/CIRMMP infrastructure, the Italian centre for NMR spectroscopy of Instruct-ERIC.

Primary author: Prof. PIERATTELLI, Roberta (CERM, University of Florence)

Presenter: Prof. PIERATTELLI, Roberta (CERM, University of Florence)

Session Classification: Structural biology II

Track Classification: Structural biology II

Contribution ID: **44** Type: **Oral Presentation**

Laser spectroscopy for plants monitoring and medical diagnostic and therapy

Friday, 26 March 2021 15:40 (20 minutes)

In this presentation we are considering laser induced absorption and fluorescence spectroscopy together with taser breakdown spectroscopy for plant monitoring and medical diagnostic and therapy

Primary author: Prof. WAGUE, Ahmadou (African Physical; Society)

Presenter: Prof. WAGUE, Ahmadou (African Physical; Society)

Session Classification: Biophotonics

Track Classification: Biophotonics

Contribution ID: **45** Type: **Oral Presentation**

Triggering receptor expressed on myeloid cells 1 (TREM-1) and Cerebral Malaria Pathogenesis.

Thursday, 25 March 2021 10:20 (20 minutes)

Malaria continues to be a major health problem despite various interventions to eradicate the disease. Cerebral malaria caused by Plasmodium falciparum is responsible for most malaria-associated deaths. Majority of these deaths occur in children under five years mostly from sub-Saharan Africa. Currently, there is no available information to predict who will recover from cerebral malaria, or who will die or who will convert from uncomplicated Malaria (UM) to CM. This knowledge would improve CM survival and reduce CM. The disease results from a combination of vascular and inflammatory immune system dysfunction. Triggering receptor expressed on myeloid cells 1 has been shown to potentiate inflammatory response. We therefore hypothesized that, there could be an association between inflammation and microvascular damage/repair seen in the pathogenesis of cerebral malaria. This study was a cohort study using children from 2- 12 years from five different hospitals within the greater Accra region of Ghana. Techniques used in the experiment include flow cytometry, ELISA and human magnetic luminex assay. Our preliminary study has shown that, there is an increase in soluble TREM-1 production in CM as compared to UM and that CM patients have higher damage in their endothelium (73.4%) than UM patients (25.7%). Findings from this study could be employed in the diagnosis as well as therapeutics of CM.

Primary authors: Dr LARBI, Amma (KNUST(Kwame Nkrumah University of Science and Technology)); Prof. GYAN, Ben (NMIMR); Prof. FREMPONG, Margrete (KNUST)

Presenter: Dr LARBI, Amma (KNUST(Kwame Nkrumah University of Science and Technology))

Session Classification: Cellular biophysics

Track Classification: Cellular biophysics

Contribution ID: **46** Type: **Oral Presentation**

Modelling of plasmon-enhanced fluorescence in a single light-harvesting complex near a gold nanorod

Thursday, 25 March 2021 15:20 (20 minutes)

LHCII — the main light-harvesting complex of plants and green algae — is the most abundant membrane protein on earth. Here, we investigate theoretically the effect of exciton-plasmon coupling on LHCII's fluorescence quantum yield and compare our modelling results to experimental data where plasmon-enhanced fluorescence has been reported in an LHCII–gold nanorod system. One of the models relies on the modified Gersten-Nitzan approach; the other is based on classical plexcitonics. We show that the latter is more robust and leads to more
realistic enhancement factors.

Primary author: Mr UGWUOKE, Luke (University of Pretoria)

Co-authors: Dr KYEYUNE, Farooq (University of Pretoria); Prof. MANCAL, Tomas (Charles University, Prague); Prof. KRUGER, Tjaart (University of Pretoria)

Presenter: Mr UGWUOKE, Luke (University of Pretoria)

Session Classification: Computational biology

Track Classification: Computational biology

Contribution ID: **47** Type: **Oral Presentation**

Facilities for Structural Biology at the European Synchrotron

Wednesday, 24 March 2021 10:00 (30 minutes)

The European Synchrotron Radiation Facility (ESRF) has undergone in 2018/2019 a complete replacement of its machine. This upgrade greatly improved the brightness of the X-ray source by decreasing the horizontal emittance and divergence of the storage ring. ESRF-EBS is open in normal users' operation since August 2020.
The presentation will give an overview of the Structural Biology beamlines and its ancillary technique facilities and which improvements are available with the machine upgrade. The new ID29 beamline, dedicated to synchrotron serial crystallography experiments will be presented as well an overview given on the complementary services available.

Primary author: MUELLER-DIECKMANN, Christoph

Presenter: Prof. LEONARD, Gordon (ESRF)

Session Classification: Structural biology I

Track Classification: Structural biology I

Contribution ID: **48** Type: **Oral Presentation**

Using scattering approaches to understand the behaviour of drugs during digestion of milk and infant formula

Tuesday, 23 March 2021 10:00 (40 minutes)

The development of low cost and paediatric-friendly drug formulations for highly effective but poorly water-soluble drugs is critical to the progress of new medicines in low economy settings. Milk and infant formula are potential candidate formulations for this task, but the interaction of these systems with drugs during digestion is not well understood. We have developed small angle X-ray scattering based methods to understand the nature of lipid self-assembly during digestion, while simultaneously tracking the signature diffraction peaks from the drug to understand its polymorphic behaviour and solubilization into lipid digestion products. The studies have revealed that both fat content and the chain length distribution of fatty acids generated upon digestion of the lipid components are critical to the solubilization of drug. The antimalarial drug combination, artefenomel and ferroquine has consequently been investigated in the clinical as a single dose cure for malaria, in a paediatric-friendly format enabled by the lipid components in infant formula, with the ideal composition supported by these scattering studies.

Primary authors: BOYD, Ben (Monash University); Dr SALIM, Malinda (Monash University); Dr CLULOW, Andrew (Monash University); Ms RAMIREZ, Gisela (Monash University); Dr HAWLEY, Adrian (ANSTO)

Presenter: BOYD, Ben (Monash University)

Session Classification: X-Ray Scattering, Spectroscopy and Radiation in Biophysics

Track Classification: Small/Wide-angle X-ray scattering in biophysics

Contribution ID: **49** Type: **Oral Presentation**

Promising antiviral, antimicrobial and therapeutic properties of green nanoceria

Tuesday, 23 March 2021 16:00 (20 minutes)

Aim: To demonstrate synthesis of cerium oxide nanoparticles (CeO2 NPs) by a green method using Hyphaene thebaica, and investigate their therapeutic applications. Materials & methods: Structural, vibrational and luminescent properties were established using x-ray diffraction, Fourier transformed infrared spectroscopy, Raman spectroscopy, ultraviolet absorption spectroscopy, selected area electron diffraction, electron microscopy and photolumincence spectroscopy. Therapeutic properties were established using different in vitro assays. Results: CeO2 NPs were determined to be crystalline in nature with a grain size of approximately 14 nm. They had characteristic Ce–O vibration at 481 cm-1. Photoluminescence spectra revealed broad bands at 463 and 600 nm. ζ potential was recorded as -17.2 mV. Potent antimicrobial and antiviral properties with hemocompatibility were reported. Conclusion: Biosynthesized CeO2 NPs revealed multifunctional therapeutic properties.

Primary author: MOHAMED, Hamza (iThemba LABS/UNISA)

Presenter: MOHAMED, Hamza (iThemba LABS/UNISA)

Session Classification: Biophysics and maternal health

Track Classification: Biophysics and maternal health

Contribution ID: **50** Type: **Oral Presentation**

Basis-independent coherence in avian-inspired quantum magnetic sensing

Monday, 22 March 2021 10:40 (20 minutes)

Fundamentally, molecular biological systems are quantum mechanical. Some of the big questions then is whether or not quantum effects manifest and whether these quantum effects contribute to the function of the biological systems. Studies have shown that migratory birds can orientate using the Earth's magnetic field, and there is growing traction that this ability requires some measure of non-trivial quantum effects. Here, we examine an avian-inspired magnetic sensor model based on the radical pair mechanism, combined with a collisional model of its environment. By using basis-independent quantum coherence, we are able reveal the relationship between quantum effects in the sensor with its magnetosensing performance.

Primary author: Dr LE, Thao P. (University of Nottingham)

Presenter: Dr LE, Thao P. (University of Nottingham)

Session Classification: Quantum biology

Track Classification: Quantum biology

Contribution ID: **51** Type: **Oral Presentation**

GCRF-START: Enabling Structural Biology in Africa

Tuesday, 23 March 2021 16:20 (20 minutes)

The START programme (Synchrotron Techniques for African Research and Technology) funded by the UK Science and Technology Facilities Council through the Global Challenges Research Fund has significantly stimulated African work in Structural Biology, Energy Materials and Catalysis over the last three years.

The Structural biology component funded post-docs, workshops, travel, data collection and a resource centre based at UCT that enabled any of the researchers to access facilities that they did not have in their home environment.

In spite of suffering in the wake of the pandemic the programme has been extraordinarily successful. Please visit https://start-project.org/ for details.

Among the unexpected positive achievements stemming from the pandemic was the development of an on line CCP4 workshop. This will have important long-term consequences for the development of an emerging cohort of African protein crystallographers.

Primary author: Prof. BRYAN TREVOR SEWELL, Bryan

Co-author: Prof. STURROCK, Edward (UCT)

Presenter: Prof. BRYAN TREVOR SEWELL, Bryan

Session Classification: Development of the future of biophysics in Africa

Track Classification: Development of the future of biophysics in Africa

Contribution ID: **52** Type: **Oral Presentation**

The structure of the C146A variant of the amidase from Pyrococcus horikoshii bound to glutaramide suggests the basis of amide recognition

Wednesday, 24 March 2021 10:30 (20 minutes)

The literature suggests that the dinitriles: malononitrile and fumaronitrile are substrates of the nitrilase-like enzyme from Pyrococcus abyssi. We have attempted to verify this and to visualize the bound substrates by X-ray crystallography. No nitriles that we tested are hydrolyzed by the very similar nitrilase-like enzymes from either P. abyssi or P. horikoshii. The enzymes do hydrolyse a variety of amide substrates, with propionamide being the most rapidly hydrolysed of all the substrates tested. Amide substrate docking studies on the wild-type enzyme structures reveal steric hindrance between the active site cysteine sulfhydryl moiety and the incoming amide. The steric hindrance is relieved if the cysteine is replaced by an alanine. The amide then docks in a position in which the amino group of Lys-113 and the backbone amide of Phe-147 are hydrogen bonded to the substrate carbonyl oxygen and the carboxyl oxygen of Glu-42 and the backbone carbonyl oxygen of Asn-171 hydrogen bonded to the amino group of the substrate. This location of the substrate is confirmed experimentally in the case of the well-resolved crystal structure of the C145A mutant of the enzyme from P. horikoshii. Our experiment suggests a different starting position for the hydrolysis reaction sequence than prevailing model in which the amide substrate is positioned with its amino group hydrogen bonded to the two active site glutamate (Glu-42 and Glu-120) carboxyl groups prior to the attack by the cysteine on the substrate carbonyl carbon.

Primary author: SEWELL, Bryan Trevor (University of Cape Town)

Co-author: Dr MAKUMIRE, Stanley (Aaron Klug Centre for Imaging and Analysis)

Presenter: SEWELL, Bryan Trevor (University of Cape Town)

Session Classification: Structural biology I

Track Classification: Structural biology I

Contribution ID: **53** Type: **Oral Presentation**

Fluorinated Surfactants for Membrane-Protein Extraction

Monday, 22 March 2021 17:00 (20 minutes)

Surfactants carrying either fully or partially fluorinated alkyl chains are conventionally thought to be poor solubilisers of lipids and membrane proteins because of their lipophobicity. New fluorinated surfactants of different headgroups have been developed. We show that these compounds could substitute detergents' function without much interference with membrane proteins' functionality. Their self-assembly and solubilising properties were studied by the use of isothermal titration calorimetry (ITC), dynamic light scattering (DLS), and gel electrophoresis (SDS-PAGE). Micellisation was found to be mainly driven by entropy, and the critical micellar concentration (CMC) decreased with increasing hydrocarbon chain length. Notably, some of these surfactants solubilise lipid vesicles at room temperature and extract important membrane proteins directly from *Escherichia coli* membranes. Our findings demonstrated promising, mild detergent activity for maltose-based fluorinated surfactants in membrane-protein extraction and applications compared to the lactose-based compounds.

Primary author: ONYIA, Kenechi Kanayo (University of Nigeria, Nsukka)

Co-authors: Prof. BABALOLA, Jonathan Oyebamiji; Prof. DURAND, Gregory; Prof. KELLER, Sandro

Presenter: ONYIA, Kenechi Kanayo (University of Nigeria, Nsukka)

Session Classification: Molecular biophysics

Track Classification: Molecular biophysics

Contribution ID: **54** Type: **Oral Presentation**

Structural basis for the interaction of the chaperone Cbp3 with newly synthesized cytochrome during mitochondrial respiratory chain assembly

Wednesday, 24 March 2021 11:30 (20 minutes)

Assembly of the mitochondrial respiratory chain requires the coordinated synthesis of mitochondrial and nuclear encoded subunits, redox co-factor acquisition, and correct joining of the subunits to form functional complexes. The conserved Cbp3-Cbp6 chaperone complex binds newly synthesized cytochrome and supports the ordered acquisition of the heme co-factors. Moreover, it functions as a translational activator by interacting with the mitoribosome. Cbp3 consists of two distinct domains: an N-terminal domain present in mitochondrial Cbp3 homologs and a highly conserved C-terminal domain comprising a ubiquinol-cytochrome chaperone region. Here, we solved the crystal structure of this C-terminal domain from a bacterial homolog at 1.4 Å resolution, revealing a unique all-helical fold. This structure allowed mapping of the interaction sites of yeast Cbp3 with Cbp6 and cytochrome b via site-specific photo-cross-linking. We propose that mitochondrial Cbp3 homologs carry an N-terminal extension that positions the conserved C-terminal domain at the ribosomal tunnel exit for an efficient interaction with its substrate, the newly synthesized cytochrome protein.

Primary author: Dr NDI, Mama (Umeå University)

Presenter: Dr NDI, Mama (Umeå University)

Session Classification: Structural biology I

Track Classification: Structural biology I

Contribution ID: **55** Type: **Oral Presentation**

Pre-eclampsia: Infrared Microspectroscopic novel insights

Tuesday, 23 March 2021 15:00 (40 minutes)

Pre-eclampsia (PE) is a serious hypertensive disorder with unclear etiology and lack of reliable diagnostic tests. In this study, FTIR microspectroscopy technique was implemented to identify molecular changes associated with the pathogenesis of PE in placental tissues and plasma samples from pre-eclamptic women and normotensive matched controls.

The current study shed light on the promising role that the IR microspectroscopy can play in providing better diagnosis and understanding of the pathophysiology of PE.

Presenter: Dr KAMAL, Gihan (SESAME)

Session Classification: Biophysics and maternal health

Track Classification: Biophysics and maternal health

Contribution ID: **56** Type: **Oral Presentation**

The AfLS and Bioscience in Africa

Tuesday, 23 March 2021 17:00 (20 minutes)

The African Light Source has become an urgent continental priority as a priority. This large scale science research infrastructure is the leading example of a resource hosting multi/inter/trans- disciplinary research activities. These include the medical sciences, cultural heritage sciences, geosciences, environmental sciences, energy sciences, nano-sciences, materials sciences and mineral sciences, industrial R&D, amongst others. It is expected to have an enormous impact on socioeconomic development. The Bioscience area is a particularly strong motivation. For example, already, we know the HIV drug development was guided by the idea from structural biology that structural information helps to elucidate protein function and, in particular, the mechanisms of enzymes. This understanding inspires the design of new drugs. The same idea of course applies to many other diseases. The call for the AfLS was first sounded in 2002, and it is now rather mature, with a Roadmap, driven by a fully mandated international Steering Committee. Massive gains are now made, particularly in the expansion of the User Base, the profile at the African Government and Pan African Level, and the momentum of the progress on the Roadmap. A host of projects related to the light source and run by many stakeholders all with their own branding have mushroomed in the general AfLS space. The drafting of the CDR has begun. This talk will review the past, present and future prospects, as we drive the roadmap forward, and look at the synergy between the AfLS and Bioscience in Africa.

Primary authors: Prof. CONNELL, Simon (University of Johannesburg); NORRIS, Lawrence (National Society of Black Physicists); MTINGWA, Sekazi (Massachusetts Institute of Technology & Brookhaven National Laboratory& African Laser Centre); Dr NGABONZIZA, Prosper (Max Planck Institute for Solid State Research); DOBBINS, Tabbetha (Rowan University); MITCHELL, Edward (ESRF); MASARA, Brian (SAIP); D'ALMEIDA, Thierry (CEA)

Presenter: Prof. CONNELL, Simon (University of Johannesburg)

Session Classification: Development of the future of biophysics in Africa

Track Classification: Development of the future of biophysics in Africa

Contribution ID: **57** Type: **Oral Presentation**

Elettra synchrotron-ICGEB fellowships

Wednesday, 24 March 2021 11:50 (5 minutes)

Presenter: ONESTI, Silvia (N/A)

Session Classification: Structural biology I