Conference on Genomics, Proteomics and Metabolomics:

All in the Bioinformatics

(CGPMB-2019)

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Conference on Genomics, Proteomics and Metabolomics:

All in the Bioinformatics

(CGPMB-2019)

27-28 July, 2019, UMFOLOZI HOTEL CASINO AND CONVENTION CENTER, EMPANGENI, KWAZULU-NATAL

Sponsored by



Organized by

Prof Khajamohiddin Syed

Assisted by Mr M L Ngwenya

Department of Biochemistry and Microbiology University of Zululand, KwaDlangezwa 3886 KwaZulu-Natal, South Africa

Website: https://cpgmb.weebly.com/

PREFACE BY THE ORGANIZERS

This conference is intended to educate young researchers, especially postgraduate students, on the latest developments and techniques available in genomics, proteomics and metabolomics as part of bioinformatics including biochemistry, microbiology and biotechnology. The main purpose of this conference is to give young researchers a chance to share their work, develop presentation skills and network with other researchers. Thus, at this conference young researchers (honors, masters, doctoral and postdoctoral students) will be given a chance to act as speakers, apart from selected plenary speakers. The plenary speakers and a panel of judges will interact with students to make suggestions on improving their skills. All the presentations and talk videos will be uploaded on the conference website and certificates will be issued to the speakers and plenary speakers to enable them to incorporate this attribute in their curricula vitae.

We are very grateful to the National Research Foundation (Grant numbers: 120053, 115032 and 114159), South Africa and the University of Zululand (C686) for supporting this initiative as part of the 4th Industrial Revolution and skills development in young researchers. We believe "Today's Students are Tomorrow's Scientists".



Prof Khajamohiddin Syed



Mr M L Ngwenya



WELCOME MESSAGE

Dear Delegates

It is great pleasure to welcome you to the CGPMB-2019 conference hosted by the Department of Biochemistry and Microbiology in the Faculty of Science and Agriculture in the University of Zululand. The delegates will not only from South Africa but form different parts of the world. As much as the conference bring together international and multidisciplinary scientists to share knowledge and latest in bioinformatics covering techniques different research fields including genomics, proteomics and metabolomics, it is more commendable that its main aim is to benefit the young scientists by providing various skills required in research. Such intergenerational dialogue inspires the



young generation to focus and excel in the development of their academic carrier because of the confidence sought in such conferences. I would like applaud Prof Syed in this initiative.

Wishing you all a great conference!

Prof N W Kunene

Dean, Faculty of Science and Agriculture

CGPMB- 2019: PROGRAM

Presentations loading on computer	Nomfundo Nzuza & Tiara Padayachee
Reception & Registration	Presentations loading on computer
Morning speakers assistants	Day 1: Zinhle Edith Chiliza & Fanele Cabangile Mnguni Day 2: Martin Naicker & Busisiwe Minenhle Xaba
Afternoon speakers assistants	Day 1: Ntokozo Minenhle Zondo & Nokwanda Samantha Ngcobo Day 2: Lungile Zethembiso Vuyiswa Dube & Felecity Kgotlelelo Mashile
Judges: Conference and Gala dinner best looking male and female - will be revealed during the gala dinner. Interviewers: Nsikelelo Allison Malinga (for female) & Fikile Thubelihle (for male). Camera: Nomfundo Nzuza & Tiara Padayachee. Gala dinner security: Makhosazana Jabulile Khumalo & Martin Naicker.	
Conference Video	Tammy Mzimela Photo Studio

PROGRAM

Day 1: 27 July, 2019		
08h00-08h30	Registration and arrival Tea & Snack	
08h30-08h45	Over-view on CGPMB-2019 by K Syed	
08h45-09h00	Welcoming by Prof G F De Wet	
09h00-09h15	Group photo	
Session 1: chaired by Prof K Syed & Mr ML Ngwenya		
09h15-09h40	Biomolecular Modeling: Methods and Applications by Dominik Gront	
09h40-10h05	Plant-Microbe Interactions and Plant Pathogen Biology – Progress at UNISA by Khayalethu Ntushelo	
10h05-10h30	Molecular Elucidation of the Dual Functional Properties of a Truncated <i>Arabidopsis Pentatricopeptide</i> Repeat Protein by Tshegofatso Dikobe	
10h30-11h00	TEA BREAK	
Session 2: chaired by Drs N Abbai & S Saheed		
11h00-11h25	Potential Diagnostic Application of Proteomics for Personalized Medicine: Human Hair as a Substrate by Henry Ademola Adeola	

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11h25-11h40	Bipolar Limbic Expression of Auto-Immune Thyroid Targets: Thyroglobulin and Thyroid-Stimulating Hormone Receptor by Meleshni Naicker
11h40-11h55	Next Generation Sequencing Application on the Pharmacokinetics and Pharmacodynamics of Tricyclic Antidepressant, in Patients with Major Depression Disorder by Teboho Mooko
11h55-12h10	Development of a novel biochemical assay for the identification of promiscuous inhibitors by Nomfundo Praise Ntombela
12h10-13h00	LUNCH
	Session 3: chaired by Drs S Fuku & T Dikobe
13h00-13h25	Insight into the structure of <i>Phycobilisome</i> from <i>Gracilaria chilensis</i> by José Martínez Oyanedel
13h25-13h50	Computational Methods for Drug Design and Discovery by Ndumiso Nhlakanipho Mhlongo
13h50-14h05	Exploring the impact of H5N1 neuraminidase (H274Y) mutation on Peramivir: A bio-computational study from a molecular perspective by Ndumiso Mpilo Buthelezi
14h05-14h30	<i>In silico</i> analysis of Cytochrome P450 Monooxygenase CYP139 Family role in the genus Mycobacterium by Puleng Rosinah Syed
14h30-14h45	Cytochrome P450 Monooxygenase Proteome Analysis between the Genera <i>Streptomyces</i> and <i>Mycobacterium</i> by Louisa Senate Moshoeshoe
14h45-15h00	<i>In silico</i> analysis of cytochrome P450 monooxygenase proteome in the fungal class <i>Tremellomycetes</i> by Olufunmilayo Olukemi Akapo
15h00-15h30	TEA BREAK
Sess	ion 4: chaired by Drs Matsobane G. Tlou & DT Zhou
15h30-15h55	Plant Metabolites in the Management of Type 2 Diabetes: Enzyme kinetics and <i>in silico</i> Consideration by Sabiu Saheed
15h55-16h20	Caught Between "Big Three" and Neglected Tropical Disease: Cryptosporidiosis by Thandeka Khoza
16h20-16h35	Phylogenetic Characterization, Diversity and Antibacterial Activity of Bioactive Compounds Produced by Novel Endophytic Fungi Isolated from <i>Sceletium tortuosum L.</i> (Kougoed) by Madira Coutlyne Manganyi

16h35-16h50	Tracking the Environmental Dissemination of Carbapenem- Resistant <i>Klebsiella pneumoniae</i> using Whole Genome
	Sequencing by Mutshiene Deogratias Ekwanzala
16h50-17h05	Application of Next Generation Sequencing and Metagenomics in Deciphering the Respiratory and Enteric Virome by Ayodeji Emmanuel Ogunbayo
17h05-17h20	Diversity and Structure of the Endophytic Seed Mycobiome of Four Legumes using Illumina Sequencing by Gilmore Taenzaniswa Pambuka
	Day 2: 28 July, 2019
08h00-08h30	Registration and arrival Tea & Snack
Session	1: chaired by Prof VSR Rajasekhar & Dr HA Adeola
08h30-08h55	Theory and Practice on Making Phylogenetic Trees by Wanping Chen
08h55-09h20	The Burden of Bacterial Vaginosis in Women from Durban by Nathlee Samantha Abbai
09h20-09h35	Genetic Diversity of <i>Gardnerella vaginalis</i> in Pregnant Women Diagnosed with Intermediate and Positive Bacterial Vaginosis by Silondiwe Philiswa Nzimande
09h35-09h50	Diagnostic Evaluation of a DNA Probe Assay for the Detection of Bacterial Vaginosis, Trichomonas vaginalis and Candida spp. in a Population of Pregnant Women in South Africa by Fazana Dessai
09h50-10h30	TEA BREAK
Session	2: chaired by Drs MC Manganyi & NN Mhlongo
10h30-10h55	Development of State-of-the-art Genomics and Bioinformatics Training Curricula for Health Professionals and Biomedical Researchers in LMICs by Danai Tavonga Zhou
10h55-11h20	Identification of Secondary Metabolites Using Various Analytical Methods by VSR Rajasekhar Pullabhotla
11h20-11h35	Catalytic Oxidation of Cyclohexane Using Metal Supported Catalysts and Ozone at Ambient Temperature and Pressure Conditions by Siphumelele Thandokwazi Mkhondwane
11h35-11h50	Catalytic Oxyfunctionalisation of 1,2-dichlorobenzene using Mn Loaded Catalysts by Nomthandazo Mkhize

11h50-12h05	Improvement of Thermal Properties of Carboxylesterases by Protein Domain Shuffling by Matsobane Godfrey Tlou
12h05-12h20	Evaluation of Cytochrome P450 Gene Expression in
	Zebrafish (Danio rerio) Liver Treated with Oleanoic acid by
	Sandile Fuku
12h20-13h20	LUNCH
Session 3	chaired by Dr MS Mthembu & Mr M L Ngwenya.
Session title: Tr	ricks of the Trade: A message from young academics to
	postgraduates
13h20-13h40	Nontuthuko Rosemary Ntuli
13h40-14h00	Vuyokazi Nongogo
14h00-14h20	Nathlee Samantha Abbai
14h20-15h00	Open discussion
15h00-15h30	TEA BREAK
	TEA BREAK Break for getting ready for Gala dinner
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B (17h30-18h00 18h00-18h10 18h10-18h20 18h20-18h30	 Break for getting ready for Gala dinner Break for getting ready for Gala dinner Gala dinner session chair: Prof K Syed Arrival drink & interaction Prof AK Basson, HOD, Department of Biochemistry and Microbiology, University of Zululand Dr MS Mthembu, Department of Biochemistry and Microbiology, University of Zululand Prof NW Kunene, Dean, Faculty of Science and Agriculture, University of Zululand Awards and certificates by Prof NW Kunene 18h40-18h50 Vote

IMPORTANT NOTES:

1. Kindly prepare your presentation such that it can be completed 3 minutes before your allocated time. Please respect other speaker's time. 2. Please make sure you load your presentation before session starts. 3. There will be presents for best looking male and female, during the gala dinner. There will be posing and short interview just like our celebrities attending the meetings. Let's have some taste in life like fashion and fun.

CGPMB-2019: ABSTRACTS & SPEAKERS' BIOGRAPHIES Biomolecular Modeling: Methods and Applications

Dominik Gront

Faculty of Chemistry, University of Warsaw, Warsaw, Poland Email: dgront@chem.uw.edu.pl

Molecular modeling is often considered as a complement to experimental

methods in life sciences as it allows investigating molecular systems at atomistic level, starting from the universal laws of physics. Structure, properties and function of biological systems may be also studied with bioinformatics, which to the contrary is based on evolutionary relationships. In this talk I will briefly present basic concepts of these two very different approaches, with particular attention on their abilities and limitations.

In the second part, I will introduce methods developed in my group: Rosetta,

BioShell and multiscale coarse grained approaches. I will illustrate this part with a few recent examples: protein-peptide docking, small molecule docking, ab-initio protein structure prediction and bioinformatics analyses.

Speaker Biography

Dr Dominik Gront gained his M.Sc degree in Chemistry in 2001 and PhD diploma in 2006, both theses defended with honours at the Faculty of Chemistry, University of Warsaw, Poland. In 2007 he won the Award of Polish Prime Minister for the Outstanding Ph.D. Thesis. After his doctoral studies he worked as postdoctoral researcher at the University of Virginia, Charlottesville (2007-2008) and University of Washington, Seattle (2008-2010). In 2010 he returned to the University of Warsaw as an assistant professor. He defended his habilitation thesis in 2016.

Dr Gront, the head of Biomacromolecule Modelling group, advances methods for multiscale simulations of biomacromolecular structure and



dynamics. He develops novel theoretical approaches and scientific software packages for biomodeling: BioShell and Rosetta. Since 2012 he is a member of Rosetta Commons - an organisation of more than 60 laboratories working on protein modelling and design.

Plant-Microbe Interactions and Plant Pathogen Biology – Progress at UNISA

<u>Khayalethu Ntushelo¹</u>, Sarah Oluwatobi Otun¹, Lesiba Klaas Ledwaba three^{1,2}, Lerato Bame Tsalaemang Matsaunyane²

1 Department of Agriculture and Animal Health, University of South Africa, Gauteng, South Africa

2 Vegetable and Ornamental Plants, Agricultural Research Council, Gauteng, South Africa

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The ever-increasing demand for food requires that crops are able to withstand disease pressure, utilize beneficial microbes to maximize productivity. Plant molecular mechanisms for disease resistance are an important subject of study so that basic knowledge for breeding and plant genetic modification can be generated. A multi-disciplinary approach which includes plant gene expression profiling, proteomics and metabolomics was embarked upon to answer such questions as: What properties does a plant need to cope with disease pressure? What mechanisms are involved in plant-microbe beneficial associations? This work utilized high-end instruments and novel information was generated to add to the body of knowledge. Biology of plant pathogens was also studied and resulted in the sequencing of partial transcriptomes of *Sclerotinia sclerotiorum* and *Fusarium oxysporum*.

Speaker Biography

Khaya Ntushelo obtained a BSc degree at the University of the Western Cape and an MSc at the University of Stellenbosch. Khaya further completed a PhD degree at the University of Florida in the United States in 2010. His research interests lie in the area of molecular biology, specifically the molecular basis of plant-microbe interactions. Khaya is an active researcher with over 20 publications in local and international journals and he has collaborations with various universities and research



institutions. He has trained nine MSc and two PhD students. Furthermore, he has supervised three postdoctoral researchers. Presently his research focusses on genetic and biochemical responses of tomato plants infected with soft rot bacteria and he continues to study the biology of plant pathogens. Khaya is an Associate Professor in the Department of Agriculture and Animal Health at Unisa. He has been a Unisa staff member since January 2012.

Molecular Elucidation of the Dual Functional Properties of a Truncated Arabidopsis Pentatricopeptide Repeat Protein

<u>Tshegofatso Bridget Dikobe¹</u>, DT Kawadza², O. Ruzvidzo¹

¹ Department of Botany, North-West University, North West Province, South Africa

² Department of Microbiology, North-West University, North West Province, South Africa

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Pentatricopeptide repeat (PPR) proteins forms one of the largest family in plants and found to be involved in various molecular and physiological functions. This protein was identified to have two putative catalytic domains adenylate cyclase (AC) and kinase, which were hypothesized to work in synergy during downstream cell signaling. Despite the identification of several kinases and ACs, no study to date has ever reported the presence of a plant molecule possessing both functions. This study focused on finding out if the putative twin catalytic domains AtPPR protein possess any possible dual catalytic function and whether such a function has any form of a cross-talking between two inherent activities with respect to increased resistance or tolerance to stress factors. To understand the exact physiological and biological roles of ACs and kinases in higher plants, a search motif derived from experimentally tested guanylate cyclases (GCs) was used to retrieve a number of Arabidopsis thaliana candidates including a pentatricopeptide repeat protein (AT1G62590; AtPPR-AC/K) with two annotated catalytic domains; the AC and kinase. To elucidate its possible functionality a bioinformatic query of this twin domain protein, followed by its cloning, recombinant expression, complementation testing using mutant E. coli cyaA, endogenous assaying, affinity purification, functional in vitro AC and kinase activities were carried out. Findings of this study established this novel protein as the first *bona fide* bi-functional soluble adenylate cyclase (sAC) plant molecule, possessing both the AC and kinase activities thus becoming the first ever higher plant protein to possess dual functional property. Furthermore, this study has proven that the AtPPR is essentially involved in critical plant biological processes such as growth, development and response to environmental stress factors. AtPPR derived functions can be potentially used for the improvement of agronomically important crops.

Speaker Biography

Dr Dikobe obtained her M.Sc. (2014) and PhD (2017) in Plant biotechnology from the North West University, South Africa. Currently she is a lecturer in the department of Botany at North West University. In addition, she supervises and co-supervises a number of postgraduate students at the same institution. Her research interests focuses on the investigation of plant stress research systems and molecular mechanisms that are applied by plants when exposed to various stresses. These include pathways that are involved in stress and pathogen related responses and broadly categorized under the following points: a) Deciphering and understanding of the molecular mechanisms of signal transduction at both the cell membranes and intracellular



matrix, b) Characterization of the biochemical and biological roles of protein/ gene and exploring the analogy between other systems. She specializes in plant proteomics and bioinformatics research through the application of molecular biology, biotechnology and biochemistry. In addition, she participates in the field of science as a reviewer of journal articles, published her work in highly reputable journals such as biomolecules, methods in molecular biology etc. She has affiliated as a member with various professional bodies.

Potential Diagnostic Application of Proteomics for Personalized Medicine:

Human Hair as a Substrate

Henry Ademola Adeola, Nandipha Mehlala, Nonhlanhla P. Khumalo

Hair and Skin Research Laboratory, Division of Dermatology-Department of Medicine, University of Cape Town, Western Cape Province, South Africa

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It is well established that the greatest components of the human hair are proteins (e.g. keratins and keratin-associated proteins). Therefore, it would be highly beneficial to provide in-depth understanding of the physiological proteome differences in human hair types; which can serve as a baseline for identification of non-invasive biomarkers for various diseases. Unfortunately, there has been a few technical limitations in the global identification of the complete protein complements in human hair samples. In addition, there is a dearth of knowledge on the physiological differences in the proteomic profiles of hair samples from men of different ethnicities. This study aims to characterize the physiological hair proteome of various ethnicities and geometrically classified hair within a South African cohort.

Label-free, shotgun proteomics analysis was carried out on various geometrically and ethnically classified hair types from a heterogeneous Western Cape population. Using various proteomics bioinformatics pipelines, we have identified ca. 450 protein groups (FDR=0.01) in the South African hair proteome. Various classes of proteins were identified, including keratins, keratin-associated proteins, histone proteins and desmosomes, *inter alia*. Functional pathway analysis revealed enrichment for skin, epidermal and tissue development as well as intermediate filament organization for biological processes. Findings in this study justify the notion that medical research urgently needs to refocus on objective human hair classification systems rather than racially-based one. In addition, the established physiological hair proteome could potentially serve as a foundation for individualized disease biomarker identification.

Speaker Biography

Dr Henry Ademola Adeola is a Senior Lecturer/ Senior Research Officer in molecular oral biology and pathology with teaching and Research experience in Japan, South Africa and Nigeria; both at the undergraduate and postgraduate level. He is also an associate fellow in oral pathology and biology of several postgraduate medical boards. He has been a visiting academic research scholar to several world class Universities. His areas of research interest include,



molecular pathoepidemiology of cancers and fibrotic diseases, clinical cancer proteomics, omics-based approaches to diagnosis and dental/medical education. Dr Henry Adeola holds a PhD in Cancer Genomics and Proteomics and has won several prestigious awards. He worked as the Project Manager of the Cancer Research Initiative (CRI) of the Faculty of Health Sciences, University of Cape Town, South Africa providing leadership for the cancer PhD programs at UCT. He is currently a Senior Lecturer and Senior Research Officer at the Hair and skin Research (HSR) laboratory of the Division of Dermatology at UCT. He is also a Principal Investigator (PI), Managing scientist and Group Leader for the Proteomics, Pathology and Molecular Imaging (PPMI)/Analytical Group at the HSR. He has several publications in high impact peer-reviewed journal and books.

Bipolar Limbic Expression of Auto-Immune Thyroid Targets: Thyroglobulin and Thyroid-Stimulating Hormone Receptor

Meleshni Naicker¹, Nathlee Abbai¹, Strinivasen Naidoo²

¹ School of Clinical Medicine Research Laboratory, Nelson R Mandela School of Medicine, University of KwaZulu-Natal, Durban, South Africa

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The associations between thyroid auto-immunity and neuro-psychiatric disorders are well-documented. However, there exists limited literature specifically linking auto-immune thyroid disease (AITD) to bipolar disorder (BD). Thus, we investigated the likely association between Hashimoto's disease (the most common cause of auto-immune hypo-thyroidism) and BD through the extra-thyroidal localisation of thyroid-stimulating hormone receptor (TSH-R) and thyroglobulin (TG) in limbic regions of normal and bipolar human adult brain. Further, we hypothesised that changes in thyroid expression in bipolar limbic cortex may contribute to mood dysregulation associated with BD. Immuno-chemistry and in-situ PCR were used to localise TSH-R/TG within the amygdala, cingulate gyrus and frontal cortex of normal (n=5) and bipolar (n=5) brains. Reverse-transcriptase qPCR provided fold-change differences in TSH-R gene expression. The results demonstrated reduced thyroid protein expression in bipolar limbic regions; these novel results correlate with other neuro-imaging reports that describe reduced cortico-limbic tissue volumes and neuro-physiological activity during BD. We also demonstrated TG-like proteins exclusive to bipolar amygdala neurons, and which relates to previous neuroimaging studies of amygdala hyperactivity and enhanced emotional sensitivity in BD. Indeed, reduced TSH-R/TG in limbic regions may predispose to, or bear relevance in the pathophysiology of mood dysregulation and symptoms of BD. Further, we attribute mood dysregulation in BD to limbic-derived TSH-R, which probably provides potential targets for thyroid auto-immune factors during Hashimoto's disease. Consequently, this may lead to inactivated and/or damaged neurons. The neuro-pathology of diminished neuronal functioning or neuronal atrophy suggests a novel neuro-degeneration mechanism in BD.

Speaker Biography

Dr Naicker has completed her M.Sc. in Medical Sciences (Medical Microbiology) and a Ph.D. in Health Sciences from the Nelson R Mandela School of Medicine, University of KwaZulu-Natal, Durban, South Africa. Currently, she is a postdoctoral fellow at the School of Clinical Medicine Research Laboratory at the University of KwaZulu-Natal. In addition, she is a co-supervisor/mentor for postgraduate research students at the same institute. Dr Naicker is also a tutor to undergraduate medical students at the Nelson R Mandela School of Medicine, University of KwaZulu-Natal.



Next Generation Sequencing Application on the Pharmacokinetics and Pharmacodynamics of Tricyclic Antidepressant, in Patients with Major Depression Disorder

Teboho Mooko, P.N. Mwangi, MM Nyaga

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Major depressive disorder (MDD) is a global problem with an increasing prevalence in the sub-Saharan Africa. The current treatment used for this disorder involves antidepressants such as, tricyclic antidepressants, selective serotonin reuptake inhibitors, and noradrenaline reuptake inhibitors. The main objectives of these treatments are to maintain remission and maintain the therapeutic effect over time. However, these goals are not achieved in the majority of MDD patients due to altered molecular mechanisms involved in poor response to these therapies. The study aims to understand the genetic variations in drug response with the use of Next Generation Sequencing technology and relating them to therapeutic and subtherapeutic effects. The study will focus on screening for mutations, particularly Single Nucleotide Polymorphisms and deletions; amplification of DNA regions encoding proteins that plays a prominent role in mechanisms involved in drug metabolism (genetic alterations of Cytochrome P2D6 and P2C19), serotoninergic receptor druginteraction (5-hydroxytryptamine receptor 2A); and some molecular aspects of neuroplasticity such as, Polymorphisms in the Brain-Derived Neurotrophic Factor gene (Val. Allele carriers). In this study, the development of CLC Genomics Workbench 11unique pipeline will be attempted, as well as protein modeling of mutated enzymes. In addition, Therapeutic drug monitoring will be performed to compare and measure therapeutic

response on patients with mutations and those without mutations.

Speaker Biography

Mr. T. Mooko is currently an NRF intern in the Next Generation Sequencing (NGS) Unit, Department of Virology, University of the Free State, under the mentorship of Dr Martin Nyaga. He holds a BSc. Degree in Human Molecular Biology, Bachelor of



Medical Science Honours (Pharmacology) and a Master of Medical Science in Pharmacology (Cum Laude) at the University of the Free State. He obtained the Dean's medal for being the best student in the Faculty of Health Sciences for his MSc.

His Master's research was on Alzheimer's Disease and cannabinoids (THC and CBD) isolated from local *Cannabis Sativa* L. plant, as a potential for a better treatment of Alzheimer's disease. Mr. T. Mooko was privileged to visit the School of Natural Product Studies at Jadavpur University, Kolkata, India, where he obtained experience in biofilm studies, heavy metal analysis of drug formulations, and animal method development for studying neurodegenerative diseases such as, Alzheimer's disease. He was also honored to present his research findings at local and international conferences such as, the 18th International Congress of International Society for Ethnopharmacology, Bangladeshi, Dhaka, and obtained the best presenter award. For his PhD studies, He has interest in exploring the Pharmacogenetics (using NGS), and Pharmacokinetics profiles of Tricyclic antidepressants in patients with Major Depressive Disorder.

Development of a Novel Biochemical Assay for the Identification of Promiscuous Inhibitors

Nomfundo Praise Ntombela, Thandeka Khoza, Raymond Hewer

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Promiscuous compounds, specifically aggregate-based inhibitors that result in false positives in biochemical activity assays present a serious and increasing interference to early-stage drug discovery processes. Although under-used, a number of purpose-specific assays have been developed to enable the identification of promiscuous inhibitors. To advance these efforts, this study aimed to develop and optimise a novel thermal shift assay to concurrently identify both true and promiscuous inhibitors. In particular, stem bromelain selected as the model protein for this study was successively isolated from the bromelain mixture through molecular exclusion chromatography and shown to be enzymatically active in the titrimetric assay (gelatin digesting unit/gm enzyme of 2024.36 - 2085.5). In the thermal shift assay, bromelain yielded a melting temperature of ~75-76 °C which then shifted by 9 °C in the presence of a true inhibitor E64. The protein was aggregated in the presence of the known promiscuous inhibitor, Congo Red, however, the addition of detergent (0.004% sodium dodecyl sulfate) effectively restored the protein to the original melting temperature. As a proof of concept, this study showed that in addition to identifying true inhibitors, the detergent-based thermal shift assay can be successfully employed to identify promiscuous inhibitors.

Speaker Biography

Nomfundo Ntombela is a PhD candidate with research interests in early drug discovery and vaccine development. Her Masters project focused on promiscuous compounds that lead to false positives in early drug discovery, where she set out to develop purpose-specific assays for the identification of such compounds.



Insight into the Structure of Phycobilisome from Gracilaria chilensis

Jose Antonio Martínez-Oyanedel

Laboratorio de Biofísica Molecular, Departamento de Bioquímica y Biología Molecular, Facultad de Ciencias Biológicas, Universidad de Concepción, Chile

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Phycobilisomes are organized in a central core and rods radiating from it. Components of phycobilisomes in Gracilaria chilensis are Phycobiliproteins (PBPs): Phycoerythrin (PE), and Phycocyanin (PC) in the rods, Allophycocyanin (APC) is found in the core, and linker proteins (L) present along the whole system. PBPs are chromophorylated proteins that share a general architecture. They are organized as heterodimers ($\alpha\beta$), which assembly themselves into trimers or hexamers. The subunits of PBPs are mono or multi chromophorylated with linear tetrapyrrols covalently bound to cysteine residues. Efficient energy transfer is achieved through a combination of position and geometry of the chromophores and the protein environment.

We solved the crystal structure of Phycoerythrin from merohedral twinning crystals that diffracted at 2.2 Å resolution at the ESFR synchrotron, the structure of Phycocyanin from monoclinic crystals that diffracted at 2.0 Å at the IMCA-CAT Synchrotron and the structure of Allophycocyanin from Crystals diffracted at Soleil Synchrotron up to 2.3 Å resolution. All PBPs share a general architecture: they are formed by a basic $\alpha\beta$ heterodimer, which has been shown to oligomerize to ($\alpha\beta$) trimers (allophycocyanin) or ($\alpha\beta$) hexamers (phycocyanin and phycoerythrin), acquiring a ring structure. Besides PBPs, they include linker proteins responsible of the assembly and stabilization of the whole complex, and the fine-tuning of the energy transfer steps between chromophores. Also the complex R-Phycoerythrin-gamma 33 subunit was built using complementary methodologies cryo-electromicroscopy and X-ray diffraction method The γ 33 subunit, in addition to having a structural role in the stabilization of the hexameric complex, has a role as intermediary in the transfer of energy through the phycoerythrin hexamer.

The crystal structures have allowed us to predict preferential light pathways across the Phycobilisomes, to understand the light transfer process in the light harvesting for photosynthesis, essential for algae and cyanobacteria. Efficient energy transfer is achieved through a combination of the position, geometry and spectroscopic properties of chromophores, and the protein environment in which they are placed. Other biophysic tools have allowed to contribute to produce a structural and functional model of the Phycobilisomes from *Gracilaria chilensis*.

Speaker Biography

Jose Antonio Martinez-Oyanedel, Biochemist, PhD in chemistry, post-doctoral in structural biochemistry, has been involved in structural analysis of proteins to establish the structurefunction relationship. Has been involved in the development of protein crystallography in Chile, is author of several crystal structure deposited in the Protein Data Bank and publications on structural biology. Since 1991 is associate professor in the Departamento de Bioquimica y Biologia Molecular from Universidad de



Concepción. In the last time the research has been direct to build a molecular model of the phycobilisome from Gracilaria chilensis, using molecular biology, crystallographic, bioinformatics, spectroscopic and proteomic approaches, solving the structure of the principal proteins that are presents in this macromolecular structure to understand the light transfer process in the light harvesting for photosynthesis, essential for algae and cyanobacteria.

Also the deep knowledge of these systems has allowed applying the use of these proteins in the antibody labelling and the design of solar cells.

Computational Methods for Drug Design and Discovery

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Drug design is an extensive, time-consuming, and expensive multidisciplinary endeavour. The availability and application of low-cost and rapid computational tools is a leading topic in medicinal chemistry. Computational methods including ligand docking, homology modeling, pharmacophore modeling, quantitative structure-activity relationships, high-throughput ligand database screening and toxicity prediction, have played a major role in the discovery and development of potent inhibitors. This talk discusses successful applications of these widely explored methods in drug discovery and development.

Speaker Biography

I obtained a BSc Medical Science (2008) and Biochemistry Honours (2010) degrees from the University of Zululand. A Master of Medical Science (Pharmaceutical Chemistry) (2014) and PhD (Pharmaceutical Chemistry) (2016) were obtained from the University of KwaZulu-Natal. After my PhD, I took a Postdoctoral Researcher position (2016) at the University of KwaZulu-Natal. Currently, I am a Senior Lecturer and Researcher (since 2017) in the School of Laboratory Medicine and Medical Sciences, Medical Biochemistry Department, University



of KwaZulu-Natal. My research group focuses on the molecular modelling of Mycobacterium tuberculosis drug targets, design and development of inhibitors against tuberculosis.

Exploring the Impact of H5N1 Neuraminidase (H274Y) Mutation on Peramivir: A bio-Computational Study from a Molecular Perspective

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Neuraminidase is a membrane glycoprotein enzyme found on the surface of influenza viruses and play a significant role in the release of the virus from the host cell. The existence of a resistant strain has an adverse impact on human health. The information relating to the resistance due to point mutations of H5N1 to Peramivir is a neglected topic in literature. In this study, a comprehensive understanding concerning the impact of this mutation that leads to Peramivir resistance to H5N1 is provided, from an atomistic perspective. Comprehensive molecular dynamic analysis of the wild type and the H274Y mutant revealed a diminished binding capacity of Peramivir. The mutants binding affinity energy dropped by ~2 kcal/mol in comparison to the wild type. The RIN profile further correlated to the binding free energy profile of Peramivir where the wild type residues TRP214, ASP212, TYR171, and ASN213 chains display

a hydrogen bond and van der Waals force interaction with the HIS193 while ARG143, ALA169, ASN213, TRY214, ILE292 and ASP212 side chain shows a hydrogen bond, pipi stack and van der Waals force interaction with TYR193, for the mutant complex. The computed van de Waals calculations were found to be -26.38 kcal mol⁻¹ and -32.34 kcal mol⁻¹ contributions for the mutant and the wild type, respectively. The remarkable difference of the $\Delta G_{gas} \sim 33,1798$ kcal/mol as a result of the point mutation confirmed that the H274Y mutant has a great potential to significantly affect the efficacy of Peramivir. Hence, H274Y mutation has adverse effects on the residue interaction network thus destabilizing the protein backbone and diminishing the Peramivir binding landscape. This study will open new avenues for the discovery and design of novel therapeutic agents that act against neuraminidase H5N1 resistance.

Speaker Biography

Ndumiso Buthelezi is a PhD candidate with keen interest in biological advancements through computer-aided drug design. He is currently at the UKZN Laboratory Medicine and Medical Sciences department at the Howard College Campus (Durban, South Africa) under the leadership of Dr. Kumalo and Dr. Mhlongo. He holds the qualifications: BSc Chemistry, BSc. Hons Advanced Chemistry and MMed Medical Biochemistry (Suma Cum Laude). His primary interests involve structure-based drug disease for infectious diseases and mutational effects on molecular systems. My research group interests on the molecular modelling of *Mycobacterium tuberculosis*



drug targets, design and development of inhibitors against tuberculosis.

In silico Analysis of Cytochrome P450 Monooxygenase CYP139 Family role in the Genus *Mycobacterium*

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Tuberculosis (TB) is one of the top infectious diseases causing numerous human deaths in the world. Despite enormous efforts, the physiology of the causative agent, *Mycobacterium tuberculosis*, is poorly understood. To contribute to better understanding the physiological capacity of these microbes, we have carried out extensive in silico analyses of the 1111 mycobacterial species genomes focusing on revealing the role of the orphan cytochrome P450 monooxygenase (CYP) CYP139 family. We have found that CYP139 members are present in 894 species belonging to three mycobacterial groups: *M. tuberculosis* complex (850-species), *Mycobacterium avium* complex (34-species), and non-tuberculosis mycobacteria (10-species), with all CYP139 members belonging to the subfamily "A". CYP139 members have unique amino acid patterns at the CXG motif. Amino acid conservation analysis placed this family in the 8th among CYP families belonging to different biological domains and kingdoms.

Biosynthetic gene cluster analyses have revealed that 92% of CYP139As might be associated with producing different secondary metabolites. Such enhanced secondary metabolic potentials with the involvement of CYP139A members might have provided mycobacterial species with advantageous traits in diverse niches competing with other microbial or viral agents, and might help these microbes infect hosts by interfering with the hosts' metabolism and immune system.

Speaker Biography

Mrs Syed matriculated from Reatlehile secondary school in Virginia, Free State in 1998. After matric (Grade 12) she went to Hillside View Collage (currently Motheo Collage) where she received her N6 National Certificate in Electrical Engineering (2004). Later in 2010 she joined University of Cincinnati, Ohio, USA, where she did Respiratory Care course (2010-2013). She continues with her studies at Central University of Technology, Bloemfontein, Free State where she received a B. Tech degree (2017) in Clinical Technology as a Pulmonologist.

Mrs Syed has done her training at the Universitas Academic Hospital, Bloemfontein, Free State, working at the Lung Function Unit (2016-2017). Her



responsibilities were including routine in lung function procedures in adults and children, e.g., Flow Volume Loops, Plethysmography (body-box), Exercise Test (6 Minutes' Walk Test) and Methacholine Challenge Test. She is currently student at University of KwaZulu-Natal, currently busy with her Master degree in Pharmaceutical Chemistry.

Cytochrome P450 Monooxygenase Prote

ome Analysis between the Genera Streptomyces and Mycobacterium

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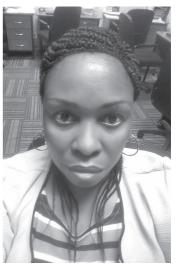
Analyses of P450 evolutionary patterns with respect to species and their ecological niches is gaining a great momentum and this type of study has been reported involving several organisms. Even though the impact of lifestyle has been reported, this characteristic however is hardly explored in bacteria. In this report, *Streptomyces* and *Mycobacterium*, belonging to the phylum *Actinobacteria*, were studied owing to their contrasting lifestyles and impact on human beings.

Genome-wide data mining and annotation of P450s was conducted in 48 *Streptomyces* species revealed the presence of 1625 P450s in their genomes and 34 fragment/pseudo P450s and were grouped into 144 P450 families and 377 P450 subfamilies. Furthermore, new P450 families and subfamilies were identified in both *Streptomyces* and Mycobacterial species. Comparative analysis of P450 profiles between the genera *Streptomyces* and *Mycobacterium* revealed different P450 profiles with few similarities. A significant difference in the number of member P450s in the commonly shared P450 families was observed between *Streptomyces* and *Mycobacterium*. Differences were also observed in the number of dominant P450 families as well as in the P450 profiles between the two genera in terms of type of families. In contrast to the P450 families highly populated in *Streptomyces* species, P450 families are involved in steroid and hydroxylation, suggesting that these P450 families possibly help mycobacterial species to assimilate the host compounds.

Based on the evidence presented in this study, the researcher hereby proposes that lifestyle or ecological niches play a key role in the evolution of P450 profiles in species belonging to the genera *Streptomyces* and *Mycobacterium*.

Speaker Biography

Senate Moshoeshoe first obtained a Diploma in Biomedical Science at National Health Training College, followed by B-Tech degree in Biomedical technology (Cum Laude) at Nelson Mandela Metropolitan University, Port Elizabeth. Thereafter she acquired her Bsc Honours Medical microbiology at University of Free State (UOFS), and M-Tech in Biomedical technology at Central University of Technology, Bloemfontein. She is currently completing her Doctor of health sciences degree at Central University of Technology. Working as Quality Manager (2014 - 2018) at Ministry of Health she became a certified Laboratory Auditor (ISO 15189:2012) and a SADCAS Technical Assessor



and thus conducted several Laboratory Audits in the SACD Region.

Senate lectured at UOFS (2007) then she moved to National Health Training College as a Senior lecturer (2010 - 2014), she is currently a Senior lecturer at Botho University. She has also worked in several Laboratories as a Technologist. Previous research work done was on incidence of aerobic spoilage in milk (2011) and *Listeria monocytogenes* (2009) at Central University of Technology, *Klebsiella pneumonia* (2007) at UOFS and antimicrobial properties of plant *Aloe ciliaris* (2005) at Nelson Mandela Metropolitan University.

In silico Analysis of Cytochrome P450 Monooxygenase Proteome in the Fungal class *Tremellomycetes*

<u>Olufunmilayo Olukemi Akapo¹</u>, Tiara Padayachee¹, Wanping Chen², Abidemi Paul Kappo¹, Jae-Hyuk Yu^{3,4} David R Nelson⁵, Khajamohiddin Syed¹

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Tremellomycetes, a fungal class in the subphylum *Agaricomycotina*, contain well-known opportunistic and emerging human pathogens. The azole drug fluconazole, used in the treatment of diseases caused by some species of *Tremellomycetes*, inhibits cytochrome P450 monooxygenase CYP51, an enzyme that converts lanosterol into an essential component of the fungal cell membrane ergosterol. Studies indicate that mutations and over-expression of CYP51 in species of *Tremellomycetes* are one of the reasons for fluconazole resistance. Moreover, the novel drug, VT-1129, that is in the pipeline is reported to exert its effect by binding and inhibiting CYP51. Despite the importance of P450s, the P450 repertoire in species of

Tremellomycetes has not been reported to date. This study intends to address this research gap. Comprehensive genome-wide P450 analysis revealed the presence of 203 P450s (excluding 16 pseudo-P450s) in 23 species of *Tremellomycetes* that can be grouped into 38 P450 families and 72 P450 subfamilies. Twenty-three

P450 families are new and three P450 families (CYP5139, CYP51 and CYP61) were conserved across 23 species of *Tremellomycetes*. Pathogenic cryptococcal species have 50% fewer P450 genes than non-pathogenic species. The results of this study will serve as reference for future annotation and characterization of P450s in species of *Tremellomycetes*.

Speaker Biography

Mrs Olufunmilayo Olukemi Akapo graduated from Rivers State University of Science and Technology, Nigeria where she obtained a BSc degree with a second class upper division. She obtained her MSc degree in Biochemistry from University of Zululand. She is presently a PhD candidate at University of Zululand (Biochemistry & Microbiology Department) under the Supervision of Prof Khajamohiddin Syed, a C1 rated NRF researcher who is well known across the world with P450s enzyme researches. Her research is focused on the role



of P450s in relation to Cryptococcal disease, a disease which affects majorly immunocompromised patients. She has been able to present her different researches in conference and symposium.

Plant Metabolites in the Management of Type 2 Diabetes: *Enzyme Kinetics* and *in silico* Consideration

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The global upsurge in the prevalence of diabetes mellitus (DM) has remained a key health threat with significant economic burden. Although, conventional oral hypoglycaemic drugs have been effective in the management of DM, high cost, non-compliance and significant adverse effects have undermined their usage. Little wonder, new and emerging evidence-based phytotherapeutic studies geared towards diabetes management are now exploring more affordable and easily accessible plant formulations. This paper presents the mechanism(s) of hypoglycaemic potential of plant metabolites through inhibition of the specific activities of carbohydrate metabolizing enzymes *in vitro* and *in silico*. Put together, besides being antioxidative, the results provided baseline evidence for antidiabetic application of the studied metabolites.

Speaker Biography

Dr. Sabiu Saheed is a South African National Research Foundation (NRF) Y-rated researcher and a Senior Lecturer at the Department of Biotechnology and Food Technology, Durban University of Technology (DUT). In addition to his interests in Human Genetics, Phytopharmacology and Molecular Biotechnology, Dr. Sabiu is a faculty representative on HIV/AIDS committee at DUT and also an Affiliate Researcher with the Next-Generation Sequencing (NGS) Unit of the University of the Free State (UFS), where the



focus of his research is on enteric viruses using whole genome sequencing and metagenomic approaches.

As his postdoctoral fellowship, Dr. Sabiu spent valuable time at both the Clinical

Biochemistry Laboratory and NGS Unit of the UFS, where he had respective exposure on Molecular Biotechnology and Viral Metagenomics. During this time, he was a member of the UFS committee that hosted Senior delegates on viral metagenomics of enteric viruses from the Centre for Disease Control and Prevention, Atlanta, USA, and also the secretary of the organizing committee of the Bill and Melinda Gates Foundation's Data and Bioinformatics Workshop hosted by UFS-NGS Unit. He enjoys teaching Biochemistry modules and has supervised postgraduate students. Dr. Sabiu has significant publications to his credit and also reviewing for more than ten good impact factor journals. He is a registered Professional Natural Scientist with the South African Council for Natural Scientific Professions, and a member of several national and international scientific organizations.

His interests in Community Development engagements in training the locals on the importance of standardized herbal preparations coupled with expertise in Phytopharmacology with keen focus on plant-derived secondary metabolites/ antioxidants had earned him the Action Research Grant Award. He has also had Travel Grant Awards to attend and present papers in international and national conferences. Most recent is the 2018 Knowledge, Interchange and Collaboration Travel Grant Award by the NRF.

Caught Between "Big Three" and Neglected Tropical Disease: Cryptosporidiosis

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Infectious diseases caused by intracellular parasitic organisms continue to cause chronic and debilitating conditions in the poorest most disadvantaged areas worldwide. Gastroenteritis is amongst the parasitic infection disease of concern and is caused by *Cryptosporidium* sp. Gastroenteritis is usually self-limiting in immunocompetent individuals, however, life-threatening complications are generally observed with immune-compromised patients particularly those with AIDS. Proteins involved in the redox systems have been shown to be crucial for the survival of the parasite, especially intracellular parasites including *Cryptosporidium*, *Plasmodium* and Schistosoma. These parasites use redox and the anti-oxidation systems to prevent cellular damage resulting from oxidative stress. Among the array of enzymes involved in the redox pathways is glutathione transferase (GST).

Transcriptome profile of the parasite has shown that GST transcription is present at all stages of the parasite's life attesting to the importance of GST in the parasite. Subsequently, targeting GST for rational drug discovery is viewed as a promising prospect using rational ligand design that can inhibit *Cryptosporidium* GST (Crypto-GST).

The only hindrance to this approach is the absence of detailed structural

and functional information on Crypto-GST. To this end, we undertook a bioinformatics approach and homology modelling to enhance our understanding of Crypto-GST in detail. Our results show that crypto species have a vast number of GSTs and can be divided into distinct groups. This finding indicates that designing one inhibitor will not cover all crypto species to annihilate cryptosporidiosis.

In responding to the global health crisis due to "big three" we have designed and synthesize novel peptidomimetic inhibitors of M. *tuberculosis* that use a novel mode of action. The peptides target the caseinolytic protease and disrupt the regulated protein degradation process essential for cell survival resulting in cell death. Our peptide was found to exhibit a Minimum Inhibitory Concentration (MIC) comparable to that of ethambutol.

Speaker Biography

Dr Tandeka Khoza is Biochemistry lecture at School of Life Science at University of KwaZulu Natal. Her research group is focused on caseinolytic protease (Clp) which are important in the pathogenesis and virulence of various bacterial pathogens including mycobacterium and Klebsiella pneumoniae. Her research is aimed at resulting in novel scientific approaches that can be used to diagnose and manage disease mechanisms at cellular and molecular level. She obtained her Msc in Biochemistry at the University of Witwatersrand studying proteins associated with Diabetes. This was followed by



a PhD in Structural biology, which was aimed at understanding the folding mechanism and three-dimensional structure of GSTs. This enzyme is implicated in the cancer development and chemotherapeutic resistance. Prior to joining UKZN, she was at the National Health Laboratory, Centre for HIV and STIs as a SPARC Post-Doctoral Fellowship where she was part of a research team that focuses on HIV broadly neutralising antibodies and their interplay with the evolving virus. She is currently completing a Master in Vaccinology with University of Lausanne which has broaden her knowledge into how vaccines are designed, developed, manufactured and implemented through public health programs. She also serves as a Chairperson for National Research Foundation: funding review panels as well as a member of GMO Advisory Committee Membership for Department of Agriculture, Forestry and Fisheries.

Phylogenetic Characterization, Diversity and Antibacterial Activity of Bioactive Compounds Produced by Novel Endophytic Fungi Isolated from *Sceletium tortuosum* L. (Kougoed)

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Throughout history, mankind has used plants as their primary source of sustainability, in agricultural commodities, clothing, fragrances, fertilizers, flavours, and providing shelter. There is a strong symbiotic relationship between the plant and its endophytes. Endophytes are harboured within the living plant tissues without causing neither diseases nor symptoms. They produce bioactive compounds that protect the host plants against attack of insects, pathogens and herbivores. The bioactive compounds might be utilized for pharmaceutical, agricultural, or biotechnological applications. This paper reported on the various endophytic fungi strains that were isolated from isolated from a medicinal plant, Sceletium tortuosum. The current study determined the antimicrobial properties and identify the chemical compounds of secondary metabolites produced by endophytic fungi isolated from S. tortuosum L. Sixty fungi were isolated from fifty S. tortuosum plants. Morphological characteristics and molecular identification (ITS1 and ITS4) and elongation factor (EF 1 and 2). Fusarium species (37%) followed Aspergillus (25%) and Penicillium (7%) species. Phylogenetic analysis was performed using nuclear ribosomal DNA sequences and three potentially new isolates (DR 019 Fusarium penzigii, DR 010 Phomopsis columnaris, DR 007 *Fusarium oxysporum* f. sp. *lycopersici*) were identified in the phylogenetic tree that was constructed. The chemical compounds were characterized by GC-MS. *Enterococcus faecalis* (ATCC S1299) and *Enterococcus gallinarum* (ATCC 700425) while *Bacillus cereus* (ATCC 10876) was the most susceptible against the fungal extracts. *F. oxysporum* (GG 008) with accession no. KJ774041.1 displayed significant antibacterial activity that was linked to high levels of 5-hydroxymethylfurfural (HMF) and octadecanoic acid as revealed by GCMS. This study revealed the presence of bioactive secondary metabolites with antibacterial activities from fungi isolated from *S. tortuosum* L. Our results offers basic data on the symbiotic/or mutualistic relationship between the medicinal plant *S. tortuosum* and its endophytic fungi, as well as novel species.

Speaker Biography

Dr Madira Manganyi obtained her M. Tech degree in Pharmaceutical Sciences (Tshwane University of Technology, South Africa) in 2013 with her undergraduate in molecular microbiology. She completed her PhD degree in 2018, at the Faculty of Natural and Agricultural Science, North-West University in South Africa. She is currently the youngest researcher in the NWU, Department of Microbiology. She joined the School of Biological Sciences at NWU, Mafikeng in 2015 as a Senior Laboratory Technician and



immediately registered for her PhD studies. Before joining NWU, she worked at the Agricultural Research Council (ARC), Mycology and specializing in fungal taxonomy of infectious diseases affecting agricultural commodities. Currently, she is a lecturer at NWU, Department of Microbiology. Her research focuses is on diversity of endophytic fungi possessing bioactive compounds isolated from medicinal plants. She presented her research data in various platforms including world renowned FEMS conference at the 7th Congress of European Microbiologists (FEMS 2017) in Valencia, Spain. Dr Madira Manganyi was the first to report these finding in the world. Her work promotes the use of novel fungi isolated from indigenous plants of South Africa as a tool for novel, new, affordable, efficacious, effective bioactive compounds with antimicrobial activities.

Tracking the Environmental Dissemination of Carbapenem-Resistant Klebsiella pneumoniae using Whole Genome Sequencing

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The emergence and dissemination of infections caused by carbapenemresistant Klebsiella pneumoniae (CRKP) are of great concern worldwide, as there are limited options for their treatment. Thus, in this study, whole-genome sequencing (WGS) was applied to assess CRKP distribution and dissemination from hospital settings to the aquatic environment in order to identify the extent of the problem. Samples were collected from hospital wastewaters and receiving water bodies. Susceptible K. pneumoniae and CRKP were enumerated and isolated using standard methods. Seventeen CRKP were DNA-sequenced using an Illumina HiSeq XTM platform. *De novo* assembly and annotation were performed using SPAdes and RAST, respectively. The study analysed antibiotic resistance traits (antibiotic resistant genes, mobile genetic elements, and virulence genes) in CRKP isolates. Although influent of wastewater harboured the highest CRKP, wastewater treatment plants were efficient in reducing the threat. In terms of resistance per matrix, benthic sediment proved to harbour more CRKP (22.88%) versus susceptible K. pneumoniae, as revealed by their resistant quotient analysis, while effluent of wastewaters (4.21%) and water bodies (4.64%) had the lowest CRKP loads. The disseminating CRKP consisted of six sequence types (ST) - ST307 (n=7), a novel ST3559 (n=5), ST15 (n=2), and one isolate of each of ST39, 152 and 298. All CRKP isolates harboured β -lactams (*bla*_{CTX-M-15} and *bla*_{OXA-1}), quinolone (*oqxA* and *oqxB*) and fosfomycin (fosA) resistance genes as well as virulence genes. This study highlights the dissemination of 'high' importance and novel STCRKP from hospital wastewater to waterbodies. This is concerning, particularly in the African context where a sizable number of people still rely on direct water resources for household use, including drinking. Further research is needed to systematically track the occurrence and distribution of these bacteria so as to mitigate their threat.

Speaker Biography

MD Ekwanzala is PhD candidate in the Water Research Unit of Tshwane University of Technology (Pretoria, South Africa). He holds a Baccalaureus of Technology in Biotechnology (Vaal University of Technology) and a Master of Technology in Water Science and Technology (TUT). He worked as a Microbiologist at MicroChem Lab Services. His doctoral research uses genomics and metagenomics approaches to track and characterize environmental resistome in a bid to develop a genomic webtool to geospatially link environmental and clinical isolates at genomic level. In this project, they



made use of whole genome and shotgun metagenomics sequencing to track and characterize South African hospital wastewater, municipal wastewater (in-fluent and effluent), activated sludge, surface water and benthic sediment. Concurrently, they are using an Ultra-Performance Liquid Chromatography System hyphenated with a Waters Synapt G2 instrument combined with a quadrupole time-of-flight mass spectrometer (UHPLC-QTOF-MS) to quantify most prescribed antibiotics in aquatic environment. He has authored five research articles in peer-reviewed journals.

Application of Next Generation Sequencing and Metagenomics in Deciphering the Respiratory and Enteric Virome

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High-throughput sequencing technologies have revolutionized how we think about viruses. We can now go beyond pathogenic viruses and have access to the thousands of viruses that inhabit our bodies without causing clinical symptoms. Besides learning their effect on health and disease, the potential to discover novel viruses or viruses with previously unappreciated tropism, is of significance, especially in illnesses of unknown origin.

Viral metagenomics through the use of high-throughput NGS techniques has the ability to elucidate the human virome, resolve diagnostic discrepancies by identifying viral agents, detect novel virus and/or identify co-infections where applicable, however, its capacity and proficiency in this regard is yet to be fully utilised.

Currently, complete composition of enteric and respiratory viruses (both pathogenic and commensals) remains largely unknown, especially in developing countries such as South Africa. Children and infants are at greater risk of enteric and respiratory illnesses from viral infections due to their developing immune system.

While RNA viruses are the most frequent cause of respiratory and enteric illnesses in children, the RNA virome in these cases are yet to be fully deciphered. More so, beside the inherent requirement for adequate sample preparation in NGS, optimisation of different enrichment method applicable to sample from different sites remains crucial for improved detection.

As a preliminary study, using an optimized protocol for the detection of enteric viruses, we successfully performed viral metagenomics on fecal sample from children diagnosed with gastroenteritis.

Metagenomic analysis revealed the presence of diverse population of human, other mammalian and plant viruses in all fecal samples. *Picornaviridae* and *Reoviridae* were the most abundant virus family identified. A polio virus was also identified but could be a vaccine derived strain. Our baseline study reveals a wide variety of RNA enteric viruses, suggesting that the infant's gut is indeed colonized by distinct viral populations.

Speaker Biography

Mr. Ogunbayo Ayodeji Emmanuel graduated from the University of South Africa where he obtained a BSc Degree in Biochemistry and Microbiology. He obtained his BMedSci Honours degree with specialization in Medical Microbiology and Virology at the University of the Free State. He pursued his MMedSci Degree in Medical Microbiology at the same University where he worked on novel method of detecting tuberculosis in children. During his MMedSci, he won the best poster presentation at the 7th Annual Free State Research Health day and the Master's people's choice award at the 2017, Three Minutes Thesis Competition. He was also sponsored by the National Research Foundation



(NRF) for specialized equipment related training at the National Institute for Communicable Disease (NICD) in Johannesburg. He is currently a PhD fellow at the Next Generation Sequencing (NGS) Unit, Division of Virology at the University of the Free State under the mentorship of Dr Martin Nyaga. His current research which is the first of its kind in Africa focuses on deciphering the composition and diversity of respiratory virome of children using NGS *via* metagenomics.

Diversity and Structure of the Endophytic Seed Mycobiome of Four Legumes using Illumina Sequencing

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A diverse group of microbiota are associated with plants and they are associated with different niches or vegetative and reproductive organs. With respect to the reproductive organs, seed carry microbial communities that can be beneficial or deleterious to the health and productivity of the newly emerging seedlings. Next Generation Sequencing technologies have enabled intensive characterization of the seed microbiome directly from seeds in the field. In this study we characterized the structure and diversity of endophytic fungi from seed in closed pods of Bambara groundnut, Cowpea, Dry beans and Soybeans directly collected from the field. DNA was extracted from seeds and the ITS2 region of the fungal internal transcribed spacer was sequenced using an Illumina MiSeq. Sequence analyses at 97% similarity resulted in the allocation of over 100 unique Molecular Operational Taxonomic Units (MOTUs). Variation in fungal community composition was found at genus level between seed from different legume crops, but each crop also contained their own unique endophytes. Plant pathogenic genera such as Fusarium and Alternaria were detected in all seed samples, as well as beneficial fungi, such as Trichoderma. Environmental sequencing can thus be an important tool for fungal community diversity description. Taxa can be compared and monitored more easily over time, assisting studies on the role of the seed microbiome during stages of growth development, and aiding strategies for disease prevention and increased plant health.

Speaker Biography

Gilmore Pambuka is a PhD candidate in the Department of Genetics at the University of the Free State (UFS) in Bloemfontein. He holds a BSc (Hons) in Agronomy from Midlands State University, Zimbabwe (2011) and an MSc in Plant Pathology from the University of KwaZulu-Natal (2015). His research for his Masters focused on isolation of biological control microorganisms for control of plant pathogens, plant-parasitic nematodes and, for plant health and growth promotion in various field crops. After completing his masters, he then went on to work in the private sector in Zimbabwe as a Research Agronomist/Plant pathologist and also as a trained Precision farming specialist, specializing in GPS



nutrient mapping. He left Zimbabwe in 2017 to further pursue his studies at the UFS under the mentorship of Dr M. Gryzenhout and Dr M. Nyaga. His PhD research looks into the plant microbiome, its interaction with its host and the environment in various indigenous and field crops in South Africa. Next Generation Sequencing Technologies (Next Generation Sequencing Unit, UFS) were employed using targeted sequencing and several bioinformatics tools to study and analyse microbial diversity and dynamics in different niches or habitats, with the aim of improving plant health and productivity.

Theory and Practice on Making Phylogenetic Trees

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Phylogenetic analysis is a basic but critical means of bioinformatics. Although it's easy to make a phylogenetic tree, it's not easy to make a suitable tree and interpret it. In this topic, general process to make phylogenetic trees, sequence alignment, commonly used tree-building methods, tree types and roles, and so on will be introduced. Then, I will share my experiences on making phylogenetic trees, including how to choose the suitable method and parameter, my favored software on sequence editing, alignment, tree-inferring and tree annotation, strategy to respond different tree types, and so on. This topic will help you a comprehensive understanding on making phylogenetic trees.

Speaker Biography

Dr Chen completed his B.Eng. in Food Science and Technology, and Ph.D. at Huazhong Agricultural University, Wuhan, China. He was a visiting scholar at the University of Wisconsin-Madison, USA (2012-2013). After his doctoral studies he worked as a Lecturer and then Associate Professor of food microbiology at Huazhong Agricultural University (2014-). Currently he is a Humboldt fellow at the University of Göttingen, Germany.

His interests focus on fungal development and secondary metabolism by means of bioinformatics,



genomics and molecular biology: 1) Regulation, and mechanism of development processes and secondary metabolites synthesis in industrial fungi, especially for Aspergillus spp. and Monascus spp., promoting their applications in industrial fermentation. 2) Phylogeny, structure analysis, evolution, and functional study of cytochrome P450 monooxygenase superfamily in fungi and beyond,

to understand and explore its important and diverse roles in development processes and secondary metabolites regulation and synthesis. Moreover, he has participated in many international research collaborations and his research work have been published in many high reputed journals such as Natural Product Reports, Studies in Mycology, Genome Biology, Chemical Science, and Biotechnology Advances.

The Burden of Bacterial Vaginosis in Women from Durban

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INTRODUCTION – Bacterial vaginosis (BV) represents the main cause of abnormal vaginal discharge in women of reproductive age, and has been linked to considerable gynecologic and obstetric morbidity. It has also been suggested that BV may be a sexually associated condition since many studies have shown that BV positive individuals share similar risk factors with that of STI infected individuals. This talk will provide data on the prevalence estimates of BV in pregnant and non-pregnant women from Durban. The association between BV and other STIs will also be described. Finally, the use of an ultrasensitive molecular based methods for the detection of BV associated microorganisms will be discussed.

RESULTS - In non-pregnant women, the prevalence of BV was 31%. Among these women, BV was significantly associated with incident *Trichomonas vaginalis* (14.6 per 100 PY, p=0.03) and *Chlamydia trachomatis* infections (15.8 per 100 PY, p=0.04). BV remained a significant predictor for *Trichomonas vaginalis* infections even after adjusting for potential confounders such as age and marital status (HR: 1.60, 95% CI: 1.00, 2.57, p=0.04). In another study, we found that non-pregnant who had a HSV-2 infection at enrolment were shown to be at increased risk for incident BV infections (adjusted hazard ratio 1.17, 95% CI 1.08, 1.27, p \leq 0.001). In addition, being of a young age, being unmarried and having a partner that has other partners were significantly associated with subsequent BV infection. In pregnant women, the prevalence of BV was estimated to be 49%. Within the pregnant women, there was no significant coinfection with other STIs. Through our research we have also provided the first evidence for the presence of BV-associated bacteria in urine of South African pregnant women using an ultrasensitive molecular based method.

DISCUSSION AND CONCLUSION - Women with BV infections should be counselled on the use of condoms and the risk of new STIs. Using digital droplet PCR (ddPCR) we were able to successfully detect BV associated microorganisms in urine. Comparison of the urine to vaginal swab samples, showed a good correlation between the two samples, recommending the future use of urine as a non-invasive sample for the detection of BV.

Speaker Biography

Dr. Nathlee Abbai completed her Masters in Medical Microbiology at the University of KwaZulu-Natal (UKZN) and then went on to complete a Ph.D in Microbial Biotechnology at the University of the Free State in Bloemfontein. Thereafter she had worked as a Postdoctoral fellow in the Department of Microbiology at the University of KwaZulu-Natal in Durban. After completion of the Postdoctoral fellowship, Dr Abbai joined the HIV Prevention Research Unit of the South African Medical Research Council as a Senior Scientist. At the SAMRC, Dr Abbai



was involved in the conduct of large scale clinical trials that investigated products to prevent HIV acquisition in high risk women.

In November 2015, Dr Abbai joined UKZN in Durban as a senior lecturer in the School of Clinical Medicine (SCM) and the Academic Head of the SCM Laboratory. Dr Abbai is a NRF-Rated scientist with a research interest in infectious diseases. Her ongoing research studies are directed towards reproductive tract infections and sexually transmitted diseases including HIV in women. More recently her research focus has been on such infections in pregnant women. She has ongoing studies that will provide data on the prevalence of viral and bacterial STIs in women attending antenatal care in Durban. Abbai is also involved in studies that will investigate potential drug resistance in some of STI pathogens. The mechanisms involved in drug resistance will also be identified by using sophisticated sequencing approaches.

Dr Abbai is a member of the South African Society for Microbiology and a member of the Biomedical Ethics Research Committee at UKZN. She also serves as reviewer for a number of local international journals such as the South African Medical Journal, Aids and Behaviour, PlosOne and the International Journal of STD and AIDS. As Academic Head of her laboratory, Dr Abbai has been the recipient of research equipment grants to develop her laboratory to a state-of-the-art facility to capacitate more young scientists.

Genetic Diversity of *Gardnerella vaginalis* in Pregnant Women Diagnosed with Intermediate and Positive Bacterial Vaginosis

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Bacterial vaginosis (BV) is main cause of abnormal vaginal discharge in women of reproductive age. *Gardnerella vaginalis* has been detected in almost all women with BV. However, there is limited information on the genetic diversity of *G. vaginalis* isolated from BV intermediate and positive cases.

Vaginal swabs were characterized by the Nugent method. A total of n=87 samples were included in the genetic analysis, (n=50 BV positive) and (n=37 BV intermediate). *G. vaginalis* was detected by PCR using bacterium specific 16S rRNA primers. All PCR positive amplicons were sequenced by the Sanger method and the edited sequence data was used for the phylogenetic analysis using the PHYLIP software. The copy numbers of *sialidase A* gene was quantified by droplet digital PCR. To assess the diversity of the *sialidase A* gene, Sanger sequencing was performed.

The bacterium specific 16S rRNA gene for *G. vaginalis* was shown to be present in all BV positive and BV intermediate samples tested by PCR. All PCR samples were successfully sequenced and the nucleotide BLAST results revealed 100% identify to *G. vaginalis*. The phylogenetic analysis revealed that there is no diversity in *G. vaginalis* present in BV positive and intermediate

cases. Furthermore, *sialidase* A was quantified by droplet digital PCR. The average number of copies per cell was much higher in BV positive group compared to the intermediate group. The phylogenetic tree of *sialidase* A gene sequences of intermediate and positive BV revealed two major clades which showed differences related to *sialidase* A copy number. Some of the intermediate cases showed high copy numbers for the virulence gene and clustered with the BV positive cases. We further demonstrate for the first time that the genetic information present within the *sialidase* A gene has a direct influence on BV status.

Speaker Biography

Silondiwe Philiswa Nzimande completed her grade 12 at Gcwalulwazi High School, Eshowe, KwaZulu Natal. She went on to do her BSc in Industrial and Applied Biotechnology at the University of KwaZulu Natal (2013-2016). After that she did BSc Honors in Medical Microbiology that she obtained cum laude at the University of KwaZulu Natal (2017). In her Honors project she investigated the diversity of HIV-1 LTR in acutely infected patient cohort. Currently, she is doing her master's in Clinical Medicine working on bacterial genetics. Her Masters project is novel since it is the first to explore the genetic diversity of positive and intermediate Gardnerella vaginalis strains in South African pregnant women.



Diagnostic Evaluation of a DNA Probe Assay for the Detection of Bacterial Vaginosis, *Trichomonas vaginalis* and *Candida* spp. in a Population of Pregnant Women in South Africa

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INTRODUCTION –Untreated reproductive tract infections pose a serious health risk to mother and child. The BD Affirm VPIII assay is a DNA probe-based assay designed as a point-of-care test for the diagnosis of Bacterial Vaginosis, Trichomoniasis and Candida. In this study we compared the detection of BV, *T.vaginalis* and *Candida* spp using the BD Affirm VPIII assay with the nucleic acid amplification test, the BD Max Vaginal assay, and report on prevalence.

RESULTS - 273 women attending antenatal care were enrolled in this study and had provided two self-collected vaginal swabs for testing on the BD Affirm VPIII and BD Max platforms. Sensitivity, specificity, positive predictive value (PPV), and negative predictive value (NPV) of the BD Affirm compared to the BD Max were calculated. The BD Affirm VPIII assay showed a moderate sensitivity (79.8%) and specificity (80.3%) for diagnosing BV. The assay had an excellent specificity for *Candida* and *T. vaginalis* of 97.4% and 100.0%, respectively, but exhibited poor sensitivities of 52.9% and 42.4%, respectively. The prevalence of Bacterial Vaginosis, Candidiasis and Trichomoniasis was 49.4%, 57.2% and 10.3%, respectively. A large proportion of women (78.8%) in this study did not have a discharge despite being positive for one or more pathogens.

DISCUSSION AND CONCLUSION - Overall, the BD Affirm VPIII assay performed better as a confirmatory test and may serve useful if used in

conjunction with other clinical parameters such as vaginal pH. The prevalence of Bacterial Vaginosis was higher than previously reported in the antenatal population in South Africa and the prevalence of Candidiasis and Trichomoniasis in this population was in keeping with previous reports. The high number of asymptomatic infections detected is of concern and indicates the need for the reevaluation of the syndromic management approach especially in the antenatal population.

Speaker Biography

Fazana Dessai is а qualified Biomedical Technologist registered with the Health Professions Council of South Africa. She has obtained a BTech degree in Biomedical Technology (cum laude) and is currently completing a Masters in Medical Science degree at UKZN. She is currently the Laboratory Manager of the School of Clinical Medicine Laboratory in College of Health Sciences at UKZN. She has previously been employed as a Laboratory Manager in the following laboratories at UKZN: K-RITH(2012-2014); the Department of Medical Microbiology (2007-2012); the Hasso Plattner Research Laboratory (2006-2007) and was the Head of Diagnostics at the CAPRISA



Laboratory (2006-2007). She has a Medical Microbiology background and a special interest in Sexually Transmitted Diseases.

Development of State-of-the-art Genomics and Bioinformatics Training Curricula for Health Professionals and Biomedical Researchers in LMICs

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Genomics and bioinformatics have accelerated since the advent of whole genome sequencing in the early 2000s in developed countries. However, for genomics and bioinformatics to be adopted for patient care and clinical practice, globally, there remains gaps in research, training and technology in many lowand middle-income countries (LMICs). Genomics research is required to inform policy while training in genomics and bioinformatics is necessary for all health professionals and biomedical researchers. For example, clinicians need to appreciate its usefulness, biomedical scientists must ensure accuracy of testing while bioinformatics should interpret genomics data correctly. In response to the above needs, we developed a curriculum for genomics and bioinformatics courses relevant for training health professionals and biomedical scientists in LMICs. Collaborators from universities and institutions interested in genomics and bioinformatics training carried out general needs' assessment for the curriculum, by identifying gaps in undergraduate and postgraduate training of health professionals and biomedical scientists. Draft curricula targeting postgraduate doctors, nurses, medical laboratory scientists and pharmacists were then developed. The draft training curriculum was developed by a team comprising members of four departments and one school of the University of Zimbabwe, College of Health Sciences (UZ): Department of Chemical Pathology, Department of Medical Laboratory Sciences (DMLS), Department of Medical Microbiology, Department of Psychiatry and School of Pharmacy, in collaboration with senior academics from Department of Biotechnology at Chinhoyi University of Technology (CUT), Zimbabwe and the School of Pharmacy and Pharmaceutical Sciences at the University at Buffalo (UB), State University of New York (SUNY), USA. A proposed state-of-the-art genomics and bioinformatics training curriculum targeting LMIC health professionals and biomedical researchers is however, just an initial step towards mainstreaming genomics and bioinformatics sciences in LMIC education and health care systems. In order, to ensure relevance and access, the primary focus of genomics and bioinformatics science for clinical practice in LMIC should not only spearhead training but also drive programs aimed at advocacy and collaborative capacity building (human and technological) among partnering departments and institutions

Speaker Biography

Danai Zhou is a senior lecturer of Clinical Biochemistry and Genetics at University of Zimbabwe (UZ) and is registered as a Clinical Scientist by the Medical Laboratory and Clinical Scientists' Council of Zimbabwe. She studied in Zimbabwe, for a BSc Hons in Applied Biology and Biochemistry and an MSc in Clinical Chemistry. During her PhD study, at University of Oslo, Norway, she published papers describing human variants (CYP2B6/CYP1A2 and APOB) and HIV drug resistance mutations. She is currently a recipient of a two-year competitive NIH Fogarty International



Centre, HIV Research Training Program (HRTP) Postdoctoral fellowship. Her postdoctoral research focuses on Pharmacogenomics of antiretroviral drugs and comprises training visits to the University at Buffalo, State University of New York (UB), USA. While at the UB, she has shadowed senior academics and researchers involved in Pharmacogenomics and Bioinformatics research at the New York State Centre of Excellence, Bioinformatics and Life Sciences; Roswell Park Cancer Center and UB, Jacobs Medicine School. Back home in Zimbabwe, she continues to coalesce a group of collaborators at the UZ, UB and other institutions to collaborate towards the development of a curriculum and Genomics and Bioinformatics Centre of Excellence, targeting health professionals and biomedical scientists from LMICs.

Identification of Secondary Metabolites Using Various Analytical Methods

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Secondary metabolites produced by bacteria or fungi are organic compounds. These compounds unlike primary metabolites not involved in the normal growth, reproduction and/or development of the organism. These secondary metabolites have several applications as flavorings, pigments, recreational drugs and mainly as medicines. For example, morphine has applications as pain killer, salicylic acid as analgesic, anti-inflammatory, and penicillin as antibiotic medicines. These organic compounds can be identified using various analytical methods such as UV-Visible spectroscopy, Fourier-Transform Infrared spectroscopy, Gas Chromatography – Mass Spectrometry, and High Performance Liquid Chromatography methods. My talk entails of these various analytical techniques that are used to identify the secondary metabolites.

Speaker Biography

VSR Rajasekhar Pullabhotla received his bachelor's degree in chemistry, physics and mathematics from Andhra University, India in 1995. Then he received his master's degree, MSc (Eng) in petrochemicals at the Jawaharlal Nehru Technological University, Hyderabad, India. Then he started his research on the heterogeneous oxidation catalysis of aliphatic hydrocarbons at the University of KwaZulu-Natal, Durban, South Africa and received his PhD in 2008. He continued the study of heterogeneous catalysis as a postdoctoral fellow at the same place. He



continued his research on nanomaterials synthesis as a postdoctoral fellow at the University of Zululand. In 2011, he joined the same University as a Lecturer. Since 2016 he has been an Associate Professor. Prof Pullabhotla has co-authored

44 publications and 1 monograph in peer reviewed journals. Through his research activities he has supervised 3 PhD, 4 MSc, 12 Hons and currently supervising 4 PhD, 5 MSc, 1 Hons projects. He has examined several PhD and MSc thesis from UKZN, DUT and other overseas universities. Through his research he has established the collaborations not only in South Africa, also in Singapore, India and USA. He is a reviewer for various journal (Catalysis Today, Journal of Environmental and Chemical Engineering, Journal of Materials Sciences and Applications, American Journal of Materials Research and AASCIT Materials). He is a rated researcher by National Research Foundation (NRF), South Africa. His research interests are mainly directed towards heterogeneous catalysis, oxidation reactions, wastewater research and nanomaterials.

Prof Pullabhotla is the principal investigators of the Catalysis Research Group at University of Zululand. He is a talented materials researcher with strong heterogeneous catalysis and nanomaterials research background. As catalysis plays an important role globally, Prof Pullabhotla's research has been carried out in heterogeneous catalysis, a multidisciplinary science that involves analytical, inorganic, organic, surface chemistry and chemical engineering. From the different areas of research (Oxidation reactions, catalysis and nanomaterials) Prof Pullabhotla have worked on, he still feels that there is a lot of scope to study on the catalytic oxidation reactions using molecular ozone, oxidative degradation of toxic compounds and the transformations of various organic compounds into value added products. His research interests foster on studying the use of the nanomaterials as catalysts in these organic transformation reactions.

Catalytic Oxyfunctionalisation of 1,2-Dichlorobenzene Using Mn Loaded Catalysts

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The ozone initiated oxidation of 1,2-dichlorobenzene catalysed manganese supported on metal oxide (γ -Al₂O₃ and SiO₂) at ambient temperature and pressure conditions is reported in this study. Wet impregnation method was used to synthesize various percentages of Mn loading viz. 2.5%, 5%, 7.5% and 10% on supports like γ -Al₂O₃ and SiO₂. The as-synthesized catalysts were calcined for 6 hours at 300°C in order to remove impurities. The catalysts were then characterised by FT-IR, SEM, EDX, TEM and XRD techniques. Before the catalytic testing, oxidation reactions were performed in the absence of the catalysts. The ozonation reaction was also studied by using activated charcoal, bare γ -Al₂O₃ and SiO₂ supports to investigate their catalytic activities in this reaction.

All the reactions were conducted at an oxygen flow rate of 0.5 LPM and 40% current in an impinger glass reactor using 25 mL pure 1,2-dichlorobenzene and 1.25 g of the catalysts. The Mn/γ -Al₂O₃ and Mn/SiO_2 were found to be more active than γ -Al₂O₃, SiO₂ support and activated charcoal. The 5% Mn/SiO₂ catalyst was found to be the active catalysts during all the ozonation reactions. Therefore, it can then be concluded that the activity of the catalysts is

attributed to manganese loaded in catalysts support $(\gamma-Al_2O_3 \text{ and } SiO_2)$. The reaction products were characterized by Gas Chromatography - Mass Spectroscopy (GC-MS) and FT-IR for quantitative and qualitative identification of the products.

Speaker Biography

Nomthandazo Mkhize completed her grade 12 at Drakensberg Comprehensive High School, Estcourt, KwaZulu Natal. She then enrolled at the University of Zululand to do her Bsc degree in Chemistry and Hydrology (2015-2017). After



completing her Bsc degree in Chemistry and Hydrology, she did Bsc Honours in Chemistry at the University of Zululand in year 2018. She is currently doing her Masters of Science degree at the University of Zululand, her research project entails to investigate a more active and selective metal doped metal oxide catalyst towards the degradation of 1,2-dichlorobenzene into a value added products.

Catalytic Oxidation of Cyclohexane Using Metal Supported Catalysts and Ozone at Ambient Temperature and Pressure Conditions

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Oxidation of cyclohexane to a mixture of cyclohexanol and cyclohexanone (KA oil) is one of the imperative reactions in industries. This is mainly because KA oil is the prominent intermediate for the production of nylon plastics. On the other hand, nylon plastics are used for the production of tyre cords, textile, military vests, hosiery, insecticides and herbicides. However, the industrial oxidation of cyclohexane employs homogenous catalysts at high temperature and pressure conditions. This has been associated with several disadvantages such as the instability of the catalysts at high temperatures, poor selectivity to KA oil and difficulty of separating the catalyst from the reaction mixture. In this manner, the current study entails to use metal supported heterogeneous catalysts at ambient temperature and pressure conditions. The metal supported catalysts were prepared using wet impregnation technique. Their physiochemical properties were studies with FT-IR, XRD, SEM-EDX, TEM and ICP-OES. Cyclohexane was oxidised in an impinger reactor equipped with porous bubbler for 1 hour. The aliquots were collected after 30 minutes and 1 hour and analysed in GC-MS and FT-IR. Cyclohexanol and cyclohexanone were obtained after 30 minutes. However, after 1 hour only cyclohexanone was obtained. This suggest

that cyclohexanol is first formed and then further oxidised to cyclohexanone. The results obtained further suggest that ambient conditions enhance the selectivity toward the KA oil.

Speaker Biography

Siphumelele Thandokwazi Mkhondwane matriculated from Siyaphambili high school, Harding, KwaZulu Natal. He then enrolled toward BSc Biochemistry and Chemistry at University of Zululand, which he obtained in 2016. Thereafter, He completed his BSc honours in Chemistry at



University of Zululand in 2017. In 2018, He started persuading toward Master of Science degree in chemistry (heterogeneous catalysis) at University of Zululand under the supervision of Professor V.S.R. Pullabhotla. In the current year, he was granted an opportunity to present his MSc research project at a symposium, Science Centre, University of Zululand, which was organised by Faculty of Science and Agriculture, where he obtained award for best oral presentation. Currently, He is persuading toward his MSc degree in Chemistry, which entails to establish an environmentally and economically benign contemporary approach for liquid phase oxidation of cyclohexane to KA oil over heterogeneous catalysts.

Improvement of Thermal Properties of Carboxylesterases by Protein Domain Shuffling

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Carboxylesterase (CESTs) are α/β hydrolases that catalyse the hydrolysis and synthesis of ester bonds. They have attracted considerable attention because of their potential applications in various industries such as food, pharmaceutical, detergents, textileand cosmetic industries. However, the properties of native enzymes do not always meet the requirements for industrial applications, which has prompted studies aimed at improving enzyme properties through protein engineering. In this study, we report on the construction of 2 hybrid enzymes by PCR-aided shuffling of the C- and the N-terminal domains from the Bacillus pumilus and Bacillus licheniformis CESTs (parent enzymes) and the kinetic and structural characterization. Upon construction, the hybrid genes were expressed in Escherichia coli, purified to homogeneity, and characterised with respect to kinetic (thermal activity and stability) and structural properties (Circular dichroism spectroscopy). The results of hybrid enzyme characterization showed a difference in thermo-stability and -activity when compared to parent enzymes. Furthermore, hybrid2 displayed a temperature optimum of 60°C when compared to the parental enzymes whose temperature optimum ranged between 45 and 50°C respectively. Hybrid2 was also observed to be stable at 80°C, with a halflife of 120 min at 80°C. The improvement in the thermal properties of hybrid2 was further confirmed by the Circular dichroism and fluorescence spectroscopy data which showed a modification in the secondary and tertiary structure of the protein. The thermal properties of hybrid2 reported here show that the protein domain shuffling can be used as a method for improving the kinetic properties of enzymes.

Speaker Biography

I am a Ph.D (Biotechnology) graduate from the University of the Free State, currently employed as a Senior Lecturer in the Department of Biochemistry, North West University, Mafikeng Campus. Areas of interest: Enzymology, microbial physiology and environmental transcriptomics/ metatranscriptomics.



Evaluation of Cytochrome P450 Gene Expression in Zebrafish (*Danio rerio*) Liver Treated with Oleanoic acid

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Diabetes management requires an integrated approach that includes the early intervention to prevent or delay its appearance. This uses a combination of therapies to control glycaemia and lipidemia in its stages. Although many drugs with different modes of action are available, novel natural antidiabetic agents, with insulin-sensitizing effects and preventive actions are receiving more research attention. The target is not solely the reduction of hyperglycaemia but also to address the metabolic syndrome as a whole. Natural products from plants that are reported to be antidiabetic are pentacyclic triterpenes such as oleanolic acid, however the metabolism of such plant secondary metabolites is poorly understood. This research aimed at closely evaluate the effects of oleanolic acid as an antidiabetic agent on cytochrome P450 of interest, CYP1B1, CYP1D1 of the zebrafish (Danio rerio) as an alternative in treatment option for type 2 diabetes. The objectives were to induce hyperglycaemia on selected zebrafish, to evaluate gene expression of (CYP1B1 and CYP1D1) using quantitative RT-PCR. It was observed that hyperglycaemia was induced in the fish, CYP1B1 gene was up-regulated in diabetic zebrafish treated with oleanolic acid, compared to the control group. Contrary, CYP1D1 was down regulated in diabetic (glucose/ sick) and treated zebrafish.

Speaker Biography

Sandile Fuku completed his Doctoral studies in Biomedical Technology from the Central University of Technology and is currently a Senior Lecturer in the Department of Biochemistry, at North-West University. Currently, his research is on epigenetic regulation in metabolic syndromes, particularly focusing on diabetics and cancer. He has published work in cancer treatment, diabates and phytochemistry.



CGPMB-2019: PARTICIPANTS' BIOGRAPHIES

Zinhle Edith Chiliza

University of Zululand, KwaZulu-Natal, South Africa

Miss Chiliza went to Umlazi Commercial High School in Durban, KwaZulu-Natal, South Africa (2008-2012). She registered at the University of Zululand, KwaDlangezwa, KwaZulu-Natal, South Africa, for a bridging program (Science Foundation) in 2013, her BSc. degree in Biochemistry and Microbiology (2014-2016), enrolled for Honours degree in Microbiology in 2017, and she is currently doing her MSc in M

Ntokozo Minenhle Zondo

University of Zululand, KwaZulu-Natal, South Africa

Miss Ntokozo Minenhle Zondo completed her high school grade in rural area KwaZulu Natal at Mjindi Secondary school 2013, and attend her tertiary school at University of Zululand in 2014 to do Bsc in Biochemistry and Microbiology completed in 2017. Then she pursues her study to do honors in the same institution in Biochemistry in 2018. On her honors she was dealing with identification of P450s in sixty mycobacterial species. She is currently doing her M.Sc. in Biochemistry now trying to understand the role of P450s using an in silico approach in mycobacterial

species at University of Zululand, KwaDlangezwa, KwaZulu-Natal.

Fanele Mnguni

University of Zululand, KwaZulu-Natal, South Africa

Fanele mnguni did her high school in Masakhane high school (2009-2013), in Empangeni and further her studies at the University of Zululand where she did her BSc degree finished in 2016, and further enrolled for Honours degree in 2017 at the same institution, currently she is doing her MSc degree in Microbiology, under the supervision of Prof Syed. Her Masters work is titled Comprehensive comparative analysis of P450s in the genus *Streptomyces*, where she hopes to finish this year.







Tiara Padayachee

University of Zululand, KwaZulu-Natal, South Africa

Miss Padayachee completed matric in 2014 as a prefect, with one distinction in life science and received her academic colours at Empangeni High School, Empangeni, South Africa. During her high school career she was academically chosen to travel to London, United Kingdom, England for two weeks. In 2015, she studied BVet at the University of Pretoria for one year before registering to study Biochemistry and Zoology at the

University of Zululand in 2016. She completed her BSc Degree (Biochemistry and Zoology) in 2018 and obtained her degree with a distinction. She is currently an honours student at the University of Zululand, Department of Biochemistry and Microbiology, Faculty of Science and Agriculture, University of Zululand, KwaDlangezwa, KwaZulu-Natal.

Nomfundo Nzuza

University of Zululand, KwaZulu-Natal, South Africa

Miss Nzuza started High school at Ubambiswano High in 2011. In 2013 she was part of Childcare South Africa Organisation, in 2015 she became the Head girl of the school and completed her Matric. After completing her Matric she enrolled at the University of Zululand in eMpangeni (KwaDlangezwa) main campus in the faculty of Science and Agriculture for the BSc degree and became

the Deputy Secretary of the Botany Society for the period (2016/2017). In 2018 she became the peer helper and assisted students during registration and she was also the peer leader facilitating the First Time Entering Students (FTENS) group and this was also the year she completed her BSc Biochemistry and Microbiology degree. She is currently registered for BSc Honours in Biochemistry in the same institution.

Nsikelelo Allison Malinga

University of Zululand, KwaZulu-Natal, South Africa

Nsikelelo A Malinga is an honours (BSc. Biochemistry) graduate from the University of Zululand and is currently pursuing his masters in Bioinformatics at the University of Zululand. He is currently a permanent staff member of the University of Zululand serving as Projects Officer







and he has also previously served in a temporal contract position as Operations Manager at the UniZulu Science Centre. He has received training on Project Management under the MAPPP9 programme. He has also been previously appointed to serve as a volunteer at the UniZulu Science Centre under the Department of Science and Technology's National Youth Service Programme (NRF/SAASTA)

Malinga also completed an internship programme with the National Research Foundation (NRF/RISA) being based at Durban University of Technology under the department of Biotechnology.

He has also been highly active in an international student organisation known as ENACTUS which aims at using the power of entrepreneurial action to transform lives and shape a better, more sustainable world for all through the initiation of projects for the neighboring communities to their institutions. For this organization, he has served as a Head of External Affairs where his main responsibilities where to ensure publicity and communications of the organisation within the institution.

Makhosazana Jabulile Khumalo

University of Zululand, KwaZulu-Natal, South Africa

Miss Khumalo completed her matric at wetsie Secondary School (2013), KwaZuluNatal. After her matric she studies Augmented Programme in Physics and Life Sciences (2014-2015) at the University of Zululand, KZN, South Africa; she obtained her Degree in BSc Biochemistry and Microbiology, Faculty of science and Agriculture at University of Zululand (2018) and Currently she is an Honors student in Biochemistry on the topic entitled "In silico analysis of P450s natural product synthesis in the phylum cyanobacteria".



Felecity kgotlelelo Mashile

University of Zululand, KwaZulu-Natal, South Africa

Miss Mashile completed her matric at Orhovelani High school (2013). Thereafter, she went to the University of Zululand and did Bsc foundation science (2014). She completed her Bsc Biochemistry and Microbiology degree 2018. After her degree, she is doing her honors degree in Biochemistry at the University of Zululand (2019).



Lungile Zethembiso Vuyiswa Dube

University of Zululand, KwaZulu-Natal, South Africa Miss Dube completed her matric on 2013 at Velangaye Comprehensive High School located at Nkandla rural area. After her matric she went to the University of Zululand on 2014 and started doing Bachelor of Science in foundation and then on 2015 she did her degree in Biochemistry and Microbiology still at University of Zululand and completed her degree in 2018. Now she's doing her honors in Bichemistry in the same institute.

Martin Naicker

University of Zululand, KwaZulu-Natal, South Africa

Martin completed his matric at Stanger Manor Secondary School (2013). He then went on to complete a bsc degree in biochemistry and microbiology at the University of Zululand (2018). He is currently doing his honors in biochemistry at the University of Zululand (2019).

Busisiwe Minenhle Xaba

University of Zululand, KwaZulu-Natal, South Africa

Miss Busisiwe Minenhle Xaba completed her matric in 2015, and then she started studying at University of Zululand, KwaDlangezwa, KwaZulu-Natal in 2016 and she completed her BSc Degree in Biochemistry and Microbiology in 2018, and she is currently doing BSc Honors in Biochemistry at the University of Zululand, Department of Biochemistry and Microbiology, Faculty of Science and Agriculture, KwaDlangezwa, KwaZulu-Natal.

Keamogetswe Nicole Riet

University of Zululand, KwaZulu-Natal, South Africa

Keamogetswe Nicole Riet Matriculated from St Boniface High School in 2014 and started university in the year 2015. She holds a BSc Majoring in Genetics and Physiology (2017) and an Honors degree in Behavioral Genetics (2018) from the University of the Free State (UFS). Her







honors project was based on studying genes that are associated with anxiety. She is currently doing her first year of a master's program in biomedical sciences at Central university of Technology (CUT). Her research project is supervised by Dr M. Sechoacha from pharmacology UFS and co supervised by Dr M. Nyaga from Next generation Sequencing (NGS) UFS. The focus of the project is on targeted treatment for prostate cancer with the use of pharmacogenomics, using Next Generation Sequencing Technologies for gene targeting.

Paballo Motloung

University of Zululand, KwaZulu-Natal, South Africa

Paballo Motloung, matriculated high school in 2013 from Ntsu Secondary School (Bethlehem), Free State. She holds a BSc in Biochemistry & Genetics (2016) and BSc Honours in Genetics (2018), at the University of the Free State in Bloemfontein. Her honours project focused on Genetic diversity and differentiation on game ranch farms focusing mainly on giraffes. Of current, she is registered for a Master of Health Sciences (Biomedical

technology) degree at the Central University of Technology in Bloemfontein under the supervision of Dr Mamello (Pharmacology), Dr Nyaga (Virology & NGS) and Mr Abrahams (Medical Sciences). Her research project focuses on the applications of Pharmacogenomics and Next Generation Sequencing to reduce drug resistance in Prostate Cancer treatment by targeting genes responsible for cancer proliferation as well as genes responsible for resistance.

Nokwanda Samantha Ngcobo

University of Zululand, KwaZulu-Natal, South Africa

Nokwanda Samantha Ngcobo was born and raised in Durban KwaZulu-Natal and matriculated from Ridge Park College in 2014. She graduated at the University of Zululand with a dual degree in Biochemistry and Microbiology. She remained at the aforementioned intuition to complete her Honours degree in Microbiology in 2018. Nokwanda is currently pursuing her Master's degree in Microbiology focusing on bioinformatics related research at the university.





Fikile Thubelihle Mthiyane

University of Zululand, KwaZulu-Natal, South Africa Miss F.T Mthiyane was born in KwaZulu-Natal in a small rural town Mtubatuba and went to Nkodibe Secondary School in Mtubatuba (2009-2013). She then enrolled at the University of Zululand in 2014 where she did a bridging course(Science Foundation) and in 2015 she did her drgree in Biochemistry and Microbiology(2015-2017), in 2018 she enrolled for her BSc Honour's degree in Microbiology and in 2019 she is enrolled for her BSc Master's in Microbiology.

Ntombizethu Nokuphiwa Msomi

University of Zululand, KwaZulu-Natal, South Africa Msomi Nokuphiwa Ntombizethu completed high school education at Mqhawe secondary school in the year 2011. I started tertiary education at the university of Zululand in 2014 doing a science excess programme known as science foundation which I completed on that year and started my degree in Biochemistry and Microbiology in 2015 and completed it on 2017 and I went on to do honours in microbiology in 2018 where I was testing the antimicrobial ability of the *Amaranthus spinosus* plant against pathogenic bacteria. I am currently registered for Masters in Microbiology.



Amanda Valentin Shangase

University of Zululand, KwaZulu-Natal, South Africa Miss Amanda Valentine Shangase completed matric at Savannah Park secondary school completed matric in 2010, thereafter went to university of Zululand and did Bsc Augumented (2012). Due to financial challenges gaped in 2015 and 2016 and completed Bsc in Biochemistry and Microbiology. I am currently doing honors degree in Biochemistry at University of Zululand.





Mbalenhle Sizamile Mfeka

University of Zululand, KwaZulu-Natal, South Africa

Mbalenhle is an MSc candidate finishing the last year of her Biochemistry degree. She is a recipient of the National research foundation Sarchi Chair awarded student support and the NRF Freestanding Innovation and Scarce Skills Masters Scholarship. She has put an enormous amount of effort to obtaining a decent academic record alongside being steered to be highly skilled in planning and conducting complex projects while developing critical rationales and analytical skills through a significant amount of independent research

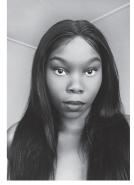
granted throughout her degree. Being a content creator saw her being drawn to the therapeutic target discovery and drug design side of biochemistry. The fulfilment and self-satisfaction of contributing to the well-being of thousands of lives seem the like the best motive to dedicating a lifetime to the world of science. This has led her down a rabbit hole of Cryptosporidium studies to try an alleviate cryptosporidiosis through as Glutathione-S-transferase approach.

Vuyokazi Nongogo Armscor-Protechnik Laboratories, Pretoria, Gauteng, South Africa

Ms Vuyokazi Nongogo obtained her Master's degree in Microbiology at the University of Fort Hare in 2015. Her research experience includes medicinal plants (2011) which was for her honours degree and water quality monitoring which was funded by Water Research Commission for her MSc. From her MSc work, she was able to publish 2 papers which described Vibrio species isolated from final effluents. After completion of her MSc, she was employed by SAPS as a Forensic Analyst. Currently she is employed as a Scientist at Protechnik Laboratories, a division of ARMSCOR. Her research group focuses on biowarfare, bioterrorism and biodefense

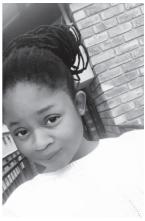


research in which she works closely with the Department of Defence.



Mukhanu Cynthia Armscor-Protechnik Laboratories, Pretoria, Gauteng, South Africa

Miss Mukhanu Cynthia completed matric in 2014 at LigegeSecondary school. Started her degree in 2015 at the University of Venda doing Bachelor of Science in Microbiology and Biochemistry. She completed her degree in 2017. Miss Mukhanu then joined Armscor in 2018, working under the division of research and development known as Protechnik Laboratories. On her journey of being trained as Scientist she is well experience in Next Generation Sequencing, Real-time PCR and other molecular biology techniques. She has worked with cyanobacteria, cyanotoxins and detection of drug resistance using bioautography technique. Now she currently continuing with her honors degree



at University of South Africa focusing on the antimicrobial activity of medicinal plants against gastrointestinal diseases.

Nasiphi Siyanda Mtyelwa

Armscor-Protechnik Laboratories, Pretoria, Gauteng, South Africa

Mtyelwa is a junior scientist who holds a B Sc honours degree in microbiology obtained from University of Fort Hare Alice campus in 2016. From 2015 to 2016 She worked as a intern for South African Agency for Science Advancement (SAASTA) at FOSST Discovery Center where she developed communications skills through working with learners on science projects. She later started working at Protechnik Laboratories, late 2016. After participating in different project work at Protechnik Laboratories



whilst showing interest and devotion, Nasiphi has advanced her research skills by knowing which information is valuable in solving a problem. Nasiphi has has experience in molecular techniques such as real-time PCR, Next generation Sequencing and conducting bioautography using Thin layer chromatography.

Dr Nontuthuko Rosemary Ntuli University of Zululand, KwaZulu-Natal, South Africa

Nontuthuko Ntuli obtained her PhD degree at the University of Zululand in 2014. Her research interest is on agro-morphological, nutritional and genetic variation among indigenous and traditional leafy vegetables as well as fruit trees. She has ongoing collaborations with various departments within the university as well as other academic and research institutions. She has graduated four MSc students. Nontu has presented and published several papers both locally and internationally. She is Senior Lecturer in the Department of Botany, University of Zululand.



Note: Academic/administrative staff members participated in the conference is not listed.



NOTES





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