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International Conference on

STD-AIDS AND INFECTIOUS DISEASES

September 03-04, 2018 | Bangkok, Thailand

DAY 1

Scientific Tracks & Abstracts

Day 1

SESSIONS

September 03, 2018

HIV/ AIDS | Transmitted Diseases & Infection | Proteomics | Biophysics | Enzyme Kinetics

Session Introduction

Session Chair
Rex Stockton
Indiana University
USA

Title: **The folding mechanisms prediction of Ig-like beta sandwich proteins based on inter-residue average distance statistics methods**
Panyavut Aumpuchin, Ritsumeikan University, Japan

Title: **Prediction of folding sites of β-trefoil proteins with irregular structures**
Risako Kimura, Ritsumeikan University, Japan

Title: **Estimation of relative binding free energy for the CDK2 protein-ligand system**
Kawano Takayuki, Ritsumeikan University, Japan

Title: **Immunodiagnostic test kits for rapid detection of fasciolosis and paramphistomosis**
Panat Anuracpreeda, Mahidol University, Thailand

Title: **Structural co-evolution of PACAP/GCGR from invertebrates to vertebrates**
B K C Chow, The University of Hong Kong, China

Title: **Towards high resolution GABAA receptor modular structure**
Hong Xue, Hong Kong University of Science and Technology, China

Title: **Categorization of metabolic pathways in bacteria**
A S Kolaskar, The Neotia University, India

Title: **Comprehensive analysis of the catalytic and structural properties of a mu-class glutathione s-transferase from Fasciola gigantica**
Jupitara Kalita, North Eastern Hill University, India

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THE FOLDING MECHANISMS PREDICTION OF IG-LIKE BETA SANDWICH PROTEINS BASED ON INTER-RESIDUE AVERAGE DISTANCE STATISTICS METHODS

Panyavut Aumpuchin and **Takeshi Kikuchi**
Ritsumeikan University, Japan

To understand the folding mechanism of a protein is one of the goals in bioinformatics study. Nowadays, it is enigmatic and difficult to extract the folding information from its amino acid sequence by using standard bioinformatics techniques or even experimental protocol which cost and time consuming. To overcome these problems, we aim to extract the initial folding unit for titin protein (Ig and fnIII domains) in the mean of inter-residue average distance statistics, average distance map (ADM) and contact frequency analysis (F-value). TI I27 and TNfn3 domains are represented for Ig-domain and fnIII-domain, respectively. Beta-strand two, three, five and six are significant for the initial folding processes of TI I27. On the other hands, the central strands of TNfn3 were predicted as a primary folding segment. Furthermore, known 3D structure and unknown 3D structure domains were investigated by structure or non-structure based multiple sequence alignment, respectively, to seek the conservation hydrophobic residue and predicted compact region through the evolution. Our results show well corresponded to experimental data, phi-value and protection factor of H-D exchange manner. It is confirming the significance of conserved hydrophobic residues near F-value peaks for structural stability by using hydrophobic packing. Again, our prediction methods could extract the folding mechanism by only its amino acid sequence.

BIOGRAPHY

Panyavut Aumpuchin has completed his master's degree in the field of Molecular Plant Pathology from Kasetsart University, Thailand. He is the PhD student of faculty of Life Sciences, Ritsumeikan University, Japan.

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PREDICTION OF FOLDING SITES OF B-TREFOIL PROTEINS WITH IRREGULAR STRUCTURES

Risako Kimura and **Takeshi Kikuchi**
Ritsumeikan University, Japan

Details of protein folding mechanism are still unknown. The solution to this problem is useful for elucidating the mechanism and treatment of diseases caused by misfolding. The relationship between the amino acid sequence and the structure of a protein is generally thought to be higher in structural similarity between proteins with high amino acid sequence identity. However, β-trefoil proteins are known to have a similar structure despite its low sequence identity among super families. In this study, we aim to obtain information on protein folding, targeting β-trefoil protein with a characteristic structure. We already clarified that the central unit is a folding core in β-trefoil protein with high structural symmetry in the previous. In this study, we predicted folding cores for β-trefoil proteins with irregular structures. The compact areas are predicted using a contact map based on inter-residue average distance statistics (average distance map). Then, high interaction residues are predicted by F-value analysis which calculates the contact frequency by using an effective potential derived from inter-residue average distance statistics. From these, we identify the points important in forming the 3D structure along given sequence. We also investigated the conservation of hydrophobic residues among sequences and attempted to clarify residues important for folding of β-trefoil proteins. Furthermore, the folding mechanisms of the β-trefoil proteins are simulated using the Go model and compared it with the obtained results by ADMs. Because of the ADM analyses, compact regions are found in the N-terminal unit and the C-terminal unit in a β-trefoil protein treated in this study. In the result of the F-value analyses, there is a peak of F-value plot in the central unit. After formation of units at both ends folding occurred, suggesting that the central unit interacts with them. Similar results were obtained in the results of the Go model simulations.

BIOGRAPHY

Risako Kimura has completed her Bachelor of Science from Ritsumeikan University, Japan. Currently, she is a graduate student of Bioinformatics course of Advanced Life Sciences from Ritsumeikan University, Japan.

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IMMUNODIAGNOSTIC TEST KITS FOR RAPID DETECTION OF FASCIOLOSIS AND PARAMPHISTOMOSIS

Panat Anuracpreeda
Mahidol University, Thailand

Statement of the Problem: Tropical fasciolosis caused by *Fasciola gigantica* infection and paramphistomosis caused by paramohistomes are the major diseases infecting ruminants and humans in the tropical regions of Africa and Asia including Thailand. Parasitological diagnosis of fasciolosis is often unreliable and possesses low sensitivity. Therefore, the detection of circulating parasite antigens is thought to be a better alternative for diagnosis of fasciolosis, as it reflects the real parasite burden.

Methodology & Theoretical Orientation: In this study, we have produced a monoclonal antibody (moAb) against native and recombinant antigens and developed both sandwich enzyme-linked immunosorbent assay (sandwich ELISA) and immunochromatographic (IC) test for rapid detection of circulating antigens in the sera or stool from mice experimentally and cattle naturally infected with *Fasciola gigantica* or paramphistomes.

Findings: The lower detection limits of sandwich ELISA and IC test were 3 pg/ml and 0.256 ng/ml, respectively. Sandwich ELISA and IC test could detect *F. gigantica* infection from day 1 to 35 post infection. In experimental mice, the sensitivity, specificity and accuracy were 95%, 100% and 98.6% (for sandwich ELISA), and 93%, 100% and 98.2% (for IC test), while in natural cattle they were 98.3%, 100% and 99.5% (for sandwich ELISA) and 96.7%, 100% and 99.1% (for IC test).

Conclusion & Significance: These two assay methods showed high efficiencies and precisions for diagnosis of fasciolosis and paramphistomosis.

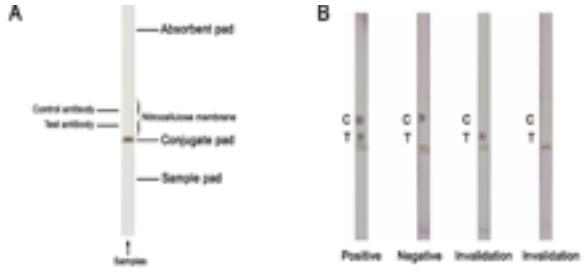

Figure.1: An immunochromatographic (IC) strip test is developed for diagnosis of fasciolosis by *F. gigantica*: experiment trial. (A) A schematic diagram of the immunochromatographic (IC) strip test showing several components: a sample pad, a conjugate pad, an immobilized nitrocellulose membrane (control and test antibody) and an absorbent pad. (B) The samples of the IC strip test for deciding the results: a positive result shows two red dots at the test and control regions, while a negative result exhibits only one red dot in the control region. The strip tests are invalid when there is no red dot at the control region.

Recent Publications

1. Anuracpreeda P, Kullanid Tepsupornkul, Chawengkirttikul R (2017). Immunodiagnosis of paramphistomosis using monoclonal antibody-based sandwich ELISA for detection of *Paramphistomum gracile* circulating 16 kDa antigen. Parasitology. 144: 899-903.
2. Anuracpreeda P, Amaya Watthanadirek, Chawengkirttikul R, Sobhon P (2017). Production and characterization of a monoclonal antibody specific to 16 kDa antigen of *Paramphistomum gracile*. Parasitol Res. 116: 167–175.
3. Anuracpreeda P, Chawengkirttikul R, Sobhon P (2016). Immunodiagnostic monoclonal antibody-based sandwich ELISA of fasciolosis by detection of *Fasciola gigantica* circulating fatty acid binding protein. Parasitology. 143: 1369-1381.
4. Anuracpreeda P, Chawengkirttikul R, Sobhon P (2016) Antigenic profile, isolation and characterization of whole body extract of *Paramphistomum gracile*. Parasite Immunol. 38: 431-438.

BIOGRAPHY

Panat Anuracpreeda is an Associate Professor of Mahidol University and belongs to Molecular Medical Biosciences Cluster. He is associated with Institute of Molecular Biosciences. He has his research interests in parasite immuno-molecular biology, advance hybridoma technology, advance immuno-molecular diagnostic assays and advance immuno-molecular therapy.

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STRUCTURAL CO-EVOLUTION OF PACAP/GCGR FROM INVERTEBRATES TO VERTEBRATES

B K C Chow
The University of Hong Kong, China

Statement of the Problem: G-protein coupled receptors (GPCRs), an essential molecular signaling device to connect extracellular stimulus and intracellular response, are currently one of the major targets for therapeutic drugs. Class B GPCRs are highly attractive therapeutic targets with several pathophysiological functions. In recent years, crystal structures of two full receptors (glucagon receptor and CRF receptor) and several other extracellular domains were released, enabling novel understanding of the interactions of this family of ligand-receptor at atomic level. The current knowledge base provides great opportunity to conduct comparative study and investigate the structural evolution of the receptor family by generating reliable homology model of class B1 GPCRs from various species. The comparison between primitive and advanced species provide insight into how communicating systems are built to support complicated operation of multiple tissues. Investigating these GPCRs with long evolutionary history can provide treasurable information for drug design. We intend to investigate the molecular evolution of class B1 GPCRs from structural perspective, with focus on ligand binding pocket. Comparative study of class B1 GPCRs has been a research focus of our lab for more than 10 years.

Methodology & Theoretical Orientation: We used data mining and bioinformatics analysis along with molecular cloning techniques to develop and clone ancestral PACAP/GCG receptor by using the information from the genome projects to isolate all putative ligand and receptor cDNAs from *B floridae* and *B belcheri* and further screen the receptor sequences from amphioxus. In quest to understand the pre-2WGD condition of PACAP and GCG receptor interaction with their receptor, we developed a photo-label probe analog to natural peptide, to test for the binding location on to the receptor. To understand and compare the structure of primitive receptor with the human receptors, we designed homology model of the receptor and further developed a receptor ligand complex. This complex will be validated by photoaffinity data provided by the help of photo labeled probe.

Conclusion & Significance: Investigating GPCRs with long evolutionary history by comparative approach will allow assessment of ligand binding domain of the receptor for intracellular signaling, which is a treasurable information.

Figure.1: Summary of molecular cloning of class B1 GPCRs and cognate ligands done by our group. Each red stars * indicate sequence reported in our publications.

Recent Publications

1. Ng SY (2012) Agnathan VIP, PACAP and their receptors: ancestral origins of today's highly diversified forms. PLoS One 7: e44691.
2. Ng SY (2011) Discovery of a new reproductive hormone in teleosts: pituitary adenylate cyclase-activating polypeptide-related peptide (PRP). Gen Comp Endocrinol 173: 405-410.

BIOGRAPHY

B K C Chow is a Chair Professor of the University of Hong Kong. He has his research interest in endocrinology of brain-gut peptides, pleiotropic activities of secretin in our body and evolution of GHRH/PACAP peptides and receptors.

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Hong Xue et al., J Genet Mol Biol 2018, Volume 2

TOWARDS HIGH RESOLUTION GABAA RECEPTOR MODULAR STRUCTURE

Hong Xue, Hoi Ming Li, Ata Ullah and **Sue Tsang**
Hong Kong University of Science and Technology, China

Type A gamma-butyric acid (GABAA) receptor is the main inhibitory neurotransmitter receptor family in the brain. Previous studies including those by us have associated GABAA receptor structural and functional variations with neuropsychiatric disorders such as schizophrenia. Differential expressions of alternative splicing isoforms of GABAA receptor beta-2 subunit different in electrophysiology properties have been found in a developmental stage and disease status dependent manner. High resolution structural information is required to provide in-depth knowledge about the mechanisms of associated neuropsychiatric disorders and a foundation for structure-based drug development. To enable detailed structural studies, we have previous established a platform for hyper expression and purification of recombinant GABAA receptor proteins. By systematic deletions coupled with secondary structure integrate analysis, two consecutive beta-rich structural domains spanning the entirety of the extracellular region and a part of the potential transmembrane portion of the receptor protein have been identified. In addition, through site-directed Ala substitution of all non-Ala amino acid residues within the second of the two domains, secondary structure determinant and benzodiazepine binding site residues have been identified. A beta-sandwich type of domain structure has been implicated from our series of studies, which represents a discrepancy with the current structure model of neurotransmitter-gated channel receptors. As a critical step in resolving the recombinant GABAA receptor protein structure at atomic level, we have recently achieved in sample preparation for Cryo-electro microscopic analysis (Figure 1). This will lead to high resolution structure for a important family of neurotransmitter receptors pivotal in schizophrenia and comorbid disorders and pave the way to new therapeutics for neuropsychiatric diseases.

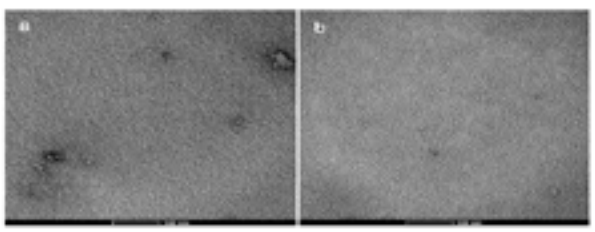

Figure.1: Transmission electron micrographs of purified recombinant protein fragments of GABAA receptor a1 subunit. (a) Electron micrograph of negatively stained C166-L296 protein fragment; (b) electron micrograph of negatively stained Q28-R248 protein fragment.

Recent Publications

1. Zhiwen Xu, Shisong Fang, Haifeng Shi, Hoiming Li, Jiun-Ming Wu, Hueih-Min Chen, Yiqun Deng, Yinglei Liao, Hui Zheng, Huaimin Zhu, Shui Ying Tsang and Hong Xue (2005). Topology characterization of a benzodiazepine-binding-rich domain of the GABAA receptor α1 subunit. Protein Science 14: 2622 – 2637.
2. Haifeng Shi, Shui Ying Tsang, Man Kit Tse, Zhiwen Xu and Hong Xue (2003). Recombinant extracellular domain of the three major subunits of GABAA receptor show comparable secondary structure and benzodiazepine binding properties. Protein Sci. 12:2642-2646.
3. Jun Hang, Haifeng Shi, Dongyang Li, Yinglei Liao, Dejun Lian, Yazhong Xiao, and Hong Xue (2000). Ligand binding and structural properties of segments of GABAA receptor α1 subunit overexpressed in Escherichia coli. J. Biol. Chem. 275: 18818-18823.
4. Xue, H, H Zheng, HM Li, A Kitmitto, H Zhu, P Lee and A Holzenburg (2000). A fragment of recombinant GABAA receptor α1 subunit forming rosette-like homo-oligomers. J. Mol. Biol. 296: 739-742.
5. Xue, H, J Hang, R Chu, Y Xiao, H Li, P Lee, and H Zheng (1999). Delineation of a membrane-proximal β-rich domain in GABAA receptor by progressive deletions. J. Mol. Biol. 285:55-61.

BIOGRAPHY

Hong Xue has obtained her first degree from the Shanghai Second Military Medical University in 1983, PhD from the Institute of Medical Sciences and Department of Biochemistry, University of Toronto in 1992, and carried out postdoctoral studies at the Department of Genetics, University of Glasgow before joining the Department of Biochemistry, Hong Kong University of Science and Technology (HKUST). Currently, she is Director of Applied Genomics Center of HKUST and Professor of the Division of Life Science at Hong Kong University of Science and Technology. Her group research focuses on the type-A gamma amino butyric acid (GABAA) receptor, the major inhibitory neurotransmitter receptor, including the structure, function, genetics and pharmacology aspects of GABAA receptor and its involvement in neuropsychiatric disorders such as schizophrenia.

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A S Kolaskar et al., J Genet Mol Biol 2018, Volume 2

CATEGORIZATION OF METABOLIC PATHWAYS IN BACTERIA

A S Kolaskar and **Shweta Kolhi**
The Neotia University, India

Fully sequenced bacterial genomes having more than ≥250 well annotated metabolic pathways were analysed to find out identical pathways in all these bacteria in more than 100 well annotated bacteria ≥250 well annotated pathways and fully sequenced genomes, 42 identical pathways were found in each of these bacteria. These pathways were called as stage I pathways or Fundamental pathways. The categorization of pathways was carried out by comparing compounds for each of the stage I pathways with compounds from remaining pathways. Pathways having common compounds with stage I pathways are categorized as stage II pathways. Following the logic of identifying common compounds between newly categorized pathways and the remaining pathways, this tool categorizes the metabolome iteratively. Categorization process is stopped when no common compounds exist between newly categorized pathways and remaining pathways. This was termed as metabolic categorization. In each metabolome, non-interacting pathways can be used to engineer bacteria without affecting other networks/ interacting pathways. The case study of *Escherichia coli* O157, having 433 annotated pathways, shows that 376 pathways interact directly or indirectly with 42 stage I pathways while 17 pathways are non-interacting. These 376 pathways are distributed in the stage II (285), stage III (76), stage IV (13) and stage V (two) category. This approach allows a better understanding of the complexity of metabolic networks. This approach suggests that stage I pathways could be the most ancient pathways and compounds that interact with maximum pathways maybe compounds with high biosynthetic potential, which can be easily identified. Further, it has been shown that interactions of pathways at various stages could be one to one, one to many, many to one, many to many mappings through interacting compounds. The granularity of the method being high, the impact of pathway perturbation on the metabolome and particularly sub-networks can be studied precisely. This can help in engineering a bacterium with desired characteristics.

BIOGRAPHY

A S Kolaskar has played a key role in shaping India's educational direction. Currently, he splits his time between being the Honorary Vice Chancellor at the University of Pune in India, the Director of the Bioinformatics Program for the American Type Culture Collection and an affiliate professor in the School of Computational Sciences at George Mason University. For the past 13 years, he has served as a professor and as Director of the Bioinformatics Center at the University of Pune. His main areas of research include theoretical molecular biophysics work and bioinformatics. He also has spent time in various management positions, from advising PhD students as a chairman of the post-graduate department at the University of Pune and as the chief investigator of large research and infra-structural grants and contracts from the Indian government. He has also been actively involved with international scientific organizations from the Technology Transfer Society to the American Association for the Advancement of Science and the Maharashtra Association for the Cultivation of Science. He has implemented major reforms in the university governance during his tenure as Vice Chancellor of the University of Pune, one of the largest universities in India.

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COMPREHENSIVE ANALYSIS OF THE CATALYTIC AND STRUCTURAL PROPERTIES OF A MU-CLASS GLUTATHIONE S-TRANSFERASE FROM *FASCIOLA GIGANTICA*

Jupitara Kalita, Rohit Shukla, Harish Shukla and **Timir Tripathi**
North Eastern Hill University, India

Glutathione S-transferases (GSTs) play an important role in the detoxification of xenobiotics. They catalyze the nucleophilic addition of glutathione (GSH) to nonpolar compounds, rendering the products water-soluble. Fascioliasis is a neglected tropical disease caused by the food-borne trematodes *Fasciola hepatica* and *Fasciola gigantica*. These parasites infect mammals through ingestion of aquatic plants or contaminated water having encysted metacercaria. GST plays important roles in maintaining the cellular homeostasis, protection against oxidative stress and detoxification of xenobiotics thereby helping in survival. In the present study, we have investigated the catalytic and structural properties of a mu-class GST from the liver *Fasciola gigantica* (FgGST1). This will help in understanding the structure-function relationship of GSTs in these flukes. The gst1 gene was amplified, cloned in pET23a vector and overexpressed in BL21(DE3) cells. The purified recombinant FgGST1 formed a homodimer and composed of ~25 kDa subunit. Kinetic analysis revealed that FgGST1 displays broad substrate specificity and shows high GSH conjugation activity towards 1-chloro-2,4-dinitrobenzene, 4-nitroquinoline-1-oxide, trans-4-phenyl-3-butene-2-one and peroxidase activity towards trans-2-nonenal and hexa-2,4-dienal. The FgGST1 was highly sensitive to inhibition by Cibacron blue. The cofactor(GSH) and inhibitor(Cibacron blue) were docked against FgGST1 and binding sites were identified. The molecular dynamics studies and principal component analysis indicated the stability of the systems and the collective motions, respectively. Unfolding studies suggest that FgGST1 is a highly cooperative molecule because, during GdnHCl-induced denaturation, a simultaneous unfolding of the protein without stabilization of any partially folded intermediate is observed. The protein is stabilized with a conformational free energy of about 10±0.3 kcal mol−1.

BIOGRAPHY

Jupitara Kalita is a PhD student in the Department of Biochemistry, NEHU, Shillong. She has completed her MSc in Biochemistry in the year 2014. Her research interest concerns the structure, function, folding and stability of GSTs in infectious liver flukes. Her thesis centers around understanding the structure-function relationship of GSTs. This includes biochemical and biophysical characterization of the proteins. Other than this, she is also working in a project which deals with interactions of mRNA export factors (proteins) and nuclear pores.

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DAY 2

Scientific Tracks & Abstracts

Day 2

SESSIONS

September 04, 2018

Identification of HIV | Prevention & Treatment | Infectious Diseases | Structural Biology & 3D Structures

Session Introduction

Session Chair
Rex Stockton
Indiana University
USA

Title: **STD-AIDS in Asia and world perspective**
S M Rasel Faruk, Kabir National Skin Center, Bangladesh

Title: **Tuberculosis determination using surface enhanced Raman spectroscopy and chemometric methods**
Raju Botta, National Electronics and Computer Technology Center, Thailand

Title: **Solute Binding Proteins and their cognate ligands: structure, function and their role in functional annotation**
Umesh Yadava, Deen Dayal Upadhyaya Gorakhpur University, India

Title: **The impacts of a demand-side VMMC incentives program on the male circumcision rate in 2 districts in Malawi: a synthetic control approach**
Suzi Joel, National AIDS Commission, Malawi

Title: **Blood mixture and the danger of discharge in patients experiencing heart medical procedure with extracorporeal dissemination**
Manuel Luque Oliveros, University of Sevilla, Spain

Title: **Invasive pulmonary aspergillosis in an immunocompromised patient: a case report**
Jamarkattel Sujan, Lincoln Medical Center, USA

S M Rasel Faruk, J Genet Mol Biol 2018, Volume 2

STD-AIDS IN ASIA AND WORLD PERSPECTIVE

S M Rasel Faruk
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In 2008, there were an expected 110 million common STIs among ladies and men in the United States. Of these, over 20% of diseases (22.1 million) were among ladies and men matured 15 to 24 years. In 30 unique microscopic organisms, infections, and parasites prompt more noteworthy than 1 million sexually transmitted contaminations every day. Chlamydia (with an expected 131 million new diseases yearly), gonorrhea (78 million contaminations), syphilis (5.6 million diseases) and trichomoniasis (143 million diseases) are four of the most widely recognized diseases around the world. The four most predominant STIs are trichomoniasis, chlamydial contaminations, gonorrhea and syphilis. High prevalence of gonorrhea 2.7%, chlamydial infection 8.0%, nonchlamydial nongonococcal urethritis 27.7%, active syphilis 6.9%, hepatitis B virus infection 9.1%, herpes simplex virus-2 infection 7.8%, and genital warts 13.2%.Vaginal infection with *T. vaginalis* at mid-gestation was significantly associated with low birth weight. Seropositivity to HSV-2 is higher in HIV-infected persons and adults of lower socioeconomic status. Most women (80%) with HSV-2 antibodies have no clinical manifestations. Untreated early syphilis in pregnant ladies results in perinatal demise in up to 40% of cases and if gained amid the four years going before pregnancy, prompts contamination of the baby in more than 70% of cases. Among the 4390 HIV-positive patients, the majority were men (92.9%). The most common age at diagnosis was 20–29 years (36.5%) followed by 30–39 (33.5%) and 40–49 (13.2%) years. Sexual contact (96.4%) was the predominant risk factor followed by injection drug use (1.9%). Among sexually acquired cases, 54.5% of patients reported they were men having sex with men (MSM) but the actual percentage of MSM was probably much higher, because male homosexuality remained a social taboo in Taiwan. Commercial sex has been an important factor in the spread of HIV/AIDS in Asia.

BIOGRAPHY

S M Rasel Faruk is a senior Consultant at Kabir National Skin Center, Panthapath, Dhaka, Bangladesh. He did his graduation from University of Dhaka, working as a Dermatologist, Sexologist, laser expert. His field of interest is STD, hair transplant and psoriasis. He is a national and international speaker on hair, laser, STD, sexology. He has many research papers in his credit.

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Raju Botta, J Genet Mol Biol 2018, Volume 2

TUBERCULOSIS DETERMINATION USING SURFACE ENHANCED RAMAN SPECTROSCOPY AND CHEMOMETRIC METHODS

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Recently applications of Raman spectroscopy have been increased to various fields, especially clinical diagnosis. Tuberculosis (TB) is one of the leading causes of mortality in the world. WHO estimated that 10.4 M people were detected as active TB and about 1.4 M people died in 2015. However, propagation of TB can be prevented by early diagnosis and treatments. Various methods have been used for diagnosis TB such as sputum smear microscopy (SSM), culture method, chest radiography, tuberculin skin testing, etc. The existing methods are poorly sensitive and time-consuming. So, there is a need to develop a rapid and sensitive method to detect TB. Surface enhanced Raman spectroscopy (SERS) is an alternative nondestructive method in terms of its rapid and sensitivity. Herein, two groups of serum protein samples, active TB (AT) and healthy control (HC) were selected for SERS analysis and spectra were measured with 785 nm laser. The measured spectra associated with vibrational modes of serum proteins. To analyze the data various multivariate statistical methods such as principal component analysis (PCA), support vector machine (SVM), decision tree (DT) and random forest (RF) were developed and tested their ability to discriminate the HC and AT samples. First two principal components (PC1, PC2) PCA scores showed clusters of AT and HC separately. A blind test has been done to validate the calibration model and test data currently falls under the same category. Results demonstrate the distinction between HC and AT samples.

BIOGRAPHY

Raju Botta has received his PhD in Physics from the University of Hyderabad, India in 2016. He is working as Postdoctoral Researcher in Carbon-based Devices and Nanoelectronics Laboratory (CNL), National Electronics and Computer Technology Center (NECTEC), National Science and Technology Development Agency (NSTDA), Thailand. His main research interests are surface-enhanced Raman scattering (SERS), nanostructures fabrication, PVD techniques, sensing application in biomedical, environmental, agriculture and aquaculture.

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Umesh Yadava, J Genet Mol Biol 2018, Volume 2

SOLUTE BINDING PROTEINS AND THEIR COGNATE LIGANDS: STRUCTURE, FUNCTION AND THEIR ROLE IN FUNCTIONAL ANNOTATION

Umesh Yadava
Deen Dayal Upadhyaya Gorakhpur University, India

The uptake of exogenous solutes is mediated by transport systems embedded in the plasma membrane and drive active transport even at μM to nM solute concentrations. In many of these systems a periplasmic Solute-Binding Protein (SBP) is utilized to bind their cognate ligands with high affinity and deliver them to the membrane bound translocator subunits. Active transport systems with SBP components are traditionally divided into three main families based on their energetic coupling mechanism, primary sequence and subunit composition: tripartite ATP-independent periplasmic transporters (TRAP), ATP binding cassette transporters (ABC) and tripartite tricarboxylate transporters (TTT). Knowledge of the cognate ligand for the SBP component of the transporter can provide crucial data for functional assignment of co-located or co-regulated genes. In the present study, the structural and functional characterizations of several solute binding proteins have been carried out. Proteins were cloned from genomic DNA, expressed by autoinduction and purified by a combination of Ni-NTA and size exclusion chromatography. The purified SBPs were screened using differential scanning fluorometry (DSF) and a >400 compounds ligand library. Two of the SBPs exhibited DSF hits that were novel for their respective transport family. Crystallization trials of proteins have been conducted with their respective DSF ligand hits. Those SBPs that have structures determined and their respective interactions with co-crystallized ligands will be presented. Co-crystallization with DSF determined ligands resulted in structures of Avi_5305 in complex with D-glucosamine and D-galactosamine, the first structure of an ABC SBP with an amino sugar.

BIOGRAPHY

Umesh Yadava has started his career as Lecturer at MGPG College, Gorakhpur in 2001. He joined Department of Physics, DDU Gorakhpur University in 2003. He is the recipient of DST Young Scientist under FAST Track Scheme, and UGC Raman Fellowship awards. He has one-year postdoctoral research experience at AECOM, New York, USA.

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THE IMPACTS OF A DEMAND-SIDE VMMC INCENTIVES PROGRAM ON THE MALE CIRCUMCISION RATE IN 2 DISTRICTS IN MALAWI: A SYNTHETIC CONTROL APPROACH

Suzi Joel
National AIDS Commission, Malawi

Background: The study aimed to evaluate the effect of incentives on improving the uptake of VMMC. The primary research question sought to find out whether provision of incentives can significantly increase VMMC uptake among in-school and out-of-school boys and young men aged 10 to 34 in Malawi. Uptake of VMMC among eligible 10-34 years old males has been slow and Malawi Government sought to identify evidence-based innovative solutions to increase VMMC uptake. In this light, the Malawi National AIDS Commission undertook a study of using incentives to create VMMC demand in Mchinji and Rumphi districts from October 2015 to April 2016. School heads and community-based mothers' groups offered vouchers to potential circumcision clients and their caretakers and a second set to hand out to their friends and caregivers – that covered the cost of transport for them and their caregiver for the procedures and two follow-up visits.

Methods: Synthetic control methods were used to estimate the causal effect of the program on the circumcision rate of males 10-34 years old. Information on VMMC rates for the two years before study onset, as well as district-level socio-demographic and health information, inform the synthetic counterfactual for each of the study districts. Permutation tests establish the robustness of the impact estimates.

Findings: The program led to a substantial increase in circumcisions: an additional 16.05 male circumcisions per 1,000 adult males in Rumphi, and an additional 9.15 in Mchinji. Overall, an individual who received a voucher was seven times more likely to be circumcised than someone who had not received one. Complementary qualitative findings suggest that mothers' groups were more effective in motivating young men due to personal attention and that caregivers and informal networks play an important supportive function in the circumcision decision.

Conclusions: Despite implementation challenges, the demand-side VMMC program is highly effective in increasing the circumcision rate from low baseline levels.

BIOGRAPHY

Suzi Joel is behavior change specialist currently heading HIV combination prevention and social and behavior change programmes for the Malawi National AIDS Commission. He holds a Master of Arts degree in Communication in Development from the University of Malawi and a first degree in Humanities Minoring in Demography from the same university. He has over 13 years of experience in HIV and health program and policy development and management, research and evaluation. He has conducted research and published five papers on non-biomedical HIV and integrated health programming. He has previously worked with Johns Hopkins University Center for Communication Programs in Malawi on several projects coordinating integrated health communication programmes.

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BLOOD MIXTURE AND THE DANGER OF DISCHARGE IN PATIENTS EXPERIENCING HEART MEDICAL PROCEDURE WITH EXTRACORPOREAL DISSEMINATION

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Purpose: Patients undergoing cardiac surgery with extracorporeal circulation (ECC) frequently present haemorrhages as a complication associated with high morbidity and mortality. One of the factors that influences this risk is the volume of blood infused during surgery. The objective of this study was to determine the optimal volume of autologous blood that can be processed during cardiac surgery with ECC. We also determined the number of salvaged red blood cells to be reinfused into the patient to minimize the risk of haemorrhage in the postoperative period.

Methods: This was an observational retrospective cross-sectional study performed in 162 ECC cardiac surgery patients. Data regarding the sociodemographic profiles of the patients, their pathologies and surgical treatments and the blood volume recovered, processed, and reinfused after cell salvage were collected. We also evaluated the occurrence of postoperative haemorrhage.

Results: The volume of blood infused after cell salvage had a statistically significant effect ($p<0.01$) on the risk of post-operative haemorrhage; the receiver operating characteristic sensitivity was 0.813 and the optimal blood volume cut-off was 1800 ml. The best clinical outcome (16.7% of patients presenting haemorrhages) was in patients that had received less than 1800 ml of recovered and processed autologous blood, which represented a volume of up to 580 ml reinfused red blood cells.

Conclusion: The optimum thresholds for autologous processed blood and red blood cells reinfused into the patient were 1800 and 580 ml, respectively. Increasing these thresholds augmented the risk of haemorrhage as an immediate postoperative period complication.

BIOGRAPHY

Manuel Luque Oliveros is attached to the surgical block of the University Hospital Virgen Macarena and Associate Professor in the Department of Nursing, Spain. He is Doctor by the University of Seville, with international research awards to his credit, and more than 200 publications in which high impact magazine is found.

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Note:

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INVASIVE PULMONARY ASPERGILLOSIS IN AN IMMUNOCOMPROMISED PATIENT: A CASE REPORT

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Background: We present a case of invasive pulmonary aspergillosis in an immunocompromised patient along with supportive diagnostic results that include serum biomarker assays, computed tomography imaging, and bronchoalveolar lavage fluid analysis.

Case Presentation: A 47 years old HIV/AIDS patient, non-compliant to antiretroviral therapy, presented with acute non-specific symptoms of malaise, mild productive cough, and subjective fever with chills without hemoptysis or chest pain. He had recently visited other hospitals prior to this visit and importantly was not diagnosed with Aspergilloma. During this hospitalization, his low grade intermittent fever was resistant to empirical broad spectrum antibiotic therapy. He was noted to have marked immunosuppression with 1 CD4+ lymphocytes/mm and a high viral RNA load. In addition, imaging studies revealed the presence of a thick walled cavitary mass at the right lung apex with centrilobular nodules consistent with aspergilloma, along with patchy ground glass opacities surrounding an alveolar infiltrate and consistent with the "Halo Sign" of invasive aspergillosis. Tuberculosis was ruled out. Serum aspergillus titers were positive. Bronchoscopy with bronchoalveolar lavage revealed dark fluid with suspended black particles and fluid analysis revealed high aspergillus titers. Microbiological cultures grew *aspergillus fumigatus*. The patient refused antifungal treatment with voriconazole and left against medical advice. Follow up revealed the patient expired two weeks later.

Discussion: The initial presentation of invasive aspergillosis, as in this patient, can be subtle and presents diagnostic challenges. Definitive identification requires culture of *Aspergillus* species from a normally sterile site along with histopathologic demonstration of hyphal tissue invasion. The diagnostic approach in patients with suspicious findings initially involves non-invasive modalities, such as fungal biomarkers, imaging studies and fungal cultures followed by invasive procedures, such as bronchoscopy and biopsy in select cases.

Conclusion: Despite advances in antiretroviral treatment, which have dramatically prolonged the survival of these patients, suspicion for aspergillosis in immunocompromised patients presenting with non-specific pulmonary symptoms should remain high, especially considering the risk of high mortality. Clinicians should be alert to the possibility of invasive fungal infections in such high-risk patients and be able to initiate early antifungal therapy for favorable outcomes.

BIOGRAPHY

Jamarkattel Sujan, worked in the department of Internal Medicine at Lincoln Medical Center, New York.

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