



ORAL PRESENTATIONS

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Visualising quality: the application of hyperspectral imaging to the quality control of herbal medicines

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Purpose: The quality control of complex herbal medicines is an ongoing process for which simple and rapid analysis methods are required. Hyperspectral imaging (HSI) has been used as a quality control method in the food and beverage, agricultural and pharmaceutical industries. HSI acquires both spectral and spatial information from a sample through an amalgamation of conventional spectroscopy and imaging. In combination with chemometric data analysis, models that can be used for quality control purposes can be developed. As a result, non-destructive analyses can be performed in a much shorter time compared to conventional analysis methods such as liquid chromatography. This study investigated the potential of shortwave infrared (SWIR) hyperspectral imaging and chemometric data analysis as a rapid quality control method for commercially important herbal medicines including Chinese star anise (*Illicium verum*), skullcap (*Scutellaria laterifolia*) and *Echinacea* species.

Methods: The sisuChema SWIR hyperspectral pushbroom imaging system was used to acquire images. The spectral range was 920-2514 nm with a resolution of 6-7 nm. Principal component analysis (PCA) score plots with mean centering were constructed and used in conjunction with the score images to remove unwanted background and edge effects where necessary. These score images and plots were then used to interactively assign classes to the data. Classification models using partial least squares discriminant analysis (PLS-DA) were constructed, optimised and used for prediction of external datasets.

Results: The constructed PLS-DA models showed distinct clusters associated with each species; Model 1: toxic *Illicium anisatum* (Chinese star anise) and *Illicium verum* (Japanese star anise); Model 2: *Echinacea angustifolia*, *Echinacea pallida* and *Echinacea purpurea*; Model 3: *Scutellaria laterifolia* (Skullcap), *Teucrium canadense* (American germander) and toxic *Teucrium chamaedrys* (European germander). The classification models exhibited good R^2X_{cum} and R^2Y_{cum} values and accurately predicted external datasets inserted into the model, producing a visually interpretable result. In addition, the species content of *Echinacea* herbal products was determined using the constructed models while the adulteration detection potential of HSI was investigated for skullcap.

Conclusions: From the results it is clear that hyperspectral imaging is ideally suited as a visual tool for the quality control of herbal raw material as it is a rapid, accurate, non-destructive method with high prediction ability.

Computational Antimalarial Drug Discovery: machine learning from public antimalarial screen data

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Purpose: There is a large amount of public malaria screen data that may not have been fully harnessed for antimalarial drug finding. This study used unsupervised machine learning algorithm to explore the pattern in public antimalarial screen data (PASD) and trained a Naive Bayesian and support vector machine model to learn from the same data.

Method: Principal Component Analysis (PCA) was carried out on PASD (56 molecular descriptors as features) using FactoMineR in R statistical software to explore patterns in the data. For supervised learning, we built a Naive Bayesian (NB) model from the molecular fingerprint (FCFP_6 fingerprint) of PASD using Pipeline Pilot software. Chemical features that correlate with activity were extracted and visualized. The data was also used to train a support vector machine (SVM) model using KNIME software and the predictive capacity evaluated with an independent test data.

Results: A plot of the first three principal components of the PCA analysis showed that there were no distinct clusters of the active and inactive compounds. From the Naive Bayesian (NB) model, we extracted chemical groups that are associated with activity. This may be used to design a virtual library or score a compound library before in-vitro antimalarial assay. Evaluation of the SVM model with an independent test data set showed that the model had good predictive capacity (sensitivity, 98.55%; specificity, 80% and accuracy, 74.75%).

Conclusions: PCA analysis showed that molecular descriptors used in this study could not discriminate between active and inactive compounds. The NB model of the data was able to identify chemical features that are potentially related to antimalarial activity. The SVM model of the data displayed good predictive ability.

Comparison of the estimation capabilities of response surface methodology and artificial neural network (ANN) in the development of an HPLC-ECD method for the analysis of captopril

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Purpose. There have been few studies in the literature where models developed based on response surface methodology (RSM) were applied to artificial neural networks (ANN). Our aim was to use the same experimental data, which have been used for RSM design in developing an HPLC method and to investigate the usefulness of ANN in modeling.

Methods: The network consists of an input layer, one hidden layer and an output layer. The inputs for the network include mobile phase pH, molarity and concentration of acetonitrile; output is the retention time (Rt). In order to determine the optimum number of hidden nodes, a series of topologies was used, in which the number of nodes was varied from 1 to 20. A commercial Microsoft Window's based neural network software package, STATISTICA 12 (StatSoft Inc) was used throughout this study. The software is a Windows®-based package, which supports numerous types of training algorithms. The experimental data were randomly divided into two sets using the option available in the software: Twenty of data sets were used as training data and 5 data sets were used as testing data and these were derived from central composite design. The training data was used to compute the network parameters. The testing data was used to ensure robustness of the network parameters. The algorithm used to train ANN in this study was the standard feed-forward multilayer perceptron (MLP) using incremental back-propagation (IBP) approach. The calculation began at the output layer and progressed backwards through the network to the input layer. One hidden layer was set for this study to provide adequate prediction. The model was validated by using the 'leave-one-out-method'. The learning period was completed at 1000 iterative training process.

Results: The performance of the ANNs was statistically measured by the coefficient of determination (R^2). The gradient descent/ IBP algorithm has a better performance relative to the radial basis function (RBF) network, because the best result derived from IBP algorithm with 3-8-1 topology has a maximum R^2 , which is close to 1 for both validation and testing sets. The optimized values of network for learning rate and momentum were 0.1 and 0.1, respectively. The predicted model fitted so well to the actual values for testing, validation sets and RSM data. The Rt predicted by the MLP coincided well with the experimentally observed values obtained using RSM.

Conclusions: The satisfactory prediction of the Rt for test and optimal runs by MLP in this study has clearly shown the applicability of ANN based estimation to method development.

How occurrence of 20 mutations affects the conformational behaviour and binding landscape of HIV-Protease: Perspectives from Molecular Dynamics and Network Analysis

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Purpose: The recent discovery and investigation of a HIV-1 protease with 20 mutations, displaying high levels of resistance towards all currently approved HIV protease inhibitors, has provided a detailed understanding of the binding energy and inhibitor interaction landscape with certain protease inhibitors. To date, however, there has been no report detailing the effect of these 20 mutations on the conformational element of the HIV protease enzyme. Here we provide a comprehensive study of the changes of the HIV protease conformation as a result of these extensive mutations.

Results: The apo conformation of the PR20 variant of the HIV protease displayed a tendency to remain in an open conformation for a longer period of time which drastically contrasts with the opening, closing and re-opening nature of wild type HIV protease. We also demonstrated that the unliganded conformation of PR20 variant of the HIV protease displayed a more rigid conformational nature. Detailed evaluation of the conformational landscape of the substrate bound as well as the darunavir bound conformations further substantiated this finding. Calculated MM/GBSA based binding free energies disclosed the difference in binding free energies in both systems, which correlate well with experimental outcomes. The per-residue footprint displayed a decreased overall energy contribution as a result of mutation, highlighting the effect of these mutations on binding free energies.

Conclusion: The findings reported in this study, will provide a foundation for the design of more potent inhibitors targeting multi-drug resistant proteases.

Using vodcasts to assess pharmacy students' patient counselling competence

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Purpose: A Pharmacy Practice Management module presented at 4th year level to pharmacy students at the University of the Western Cape incorporates content on interpersonal communication, adherence and patient counselling. Traditionally these aspects have been assessed using written reports or role-plays, or, since 2009, podcasts. However, increasing class sizes have necessitated the introduction of alternative assessment tools. 2014 saw the introduction of a vodcast to assess pharmacy students' patient counselling competence.

Methods: Each student was presented with a multi-item prescription and a description of a patient or other issue that would require special attention during the pharmacist-patient interaction (for example, physical disability, psychological interference or environmental interference). Each prescription contained at least one item that would be considered as presenting a considerable potential for non-adherence. Students were instructed in the use of open source video-editing software (iWisoft Free Video Converter) and the use of their own mobile phones to record the videos. Vodcasts were uploaded to the UWC online teaching platform and assessed against a specially designed rubric. At the end of the module, semi-structured focus groups were conducted to gauge the students' responses to this new assessment tool.

Results: On reflection, the vodcast provided, for the lecturer, a very useful tool to assess knowledge, behaviours and attitudes in an integrated manner in a simulated real-life setting. Assessment though, was found to be very time-consuming. Despite initial misgivings, students were positive about the experience in terms of building their confidence, and of requiring the integration of knowledge across pharmacy practice and pharmacology disciplines. They expressed a strong preference for Windows Movie Maker instead of the iWisoft software. Ambivalence was expressed regarding being required to video simulated vs real-life scenarios. They were generally enthusiastic about the further incorporation of assessment tools which reflected their lifestyle.

Conclusions: The overall positive experiences of both the lecturer and the students support the further use of vodcasts as a tool for assessing pharmacy students' knowledge, behaviours and attitudes within the pharmacist-patient interaction.

Experiential learning opportunities of fourth year pharmacy students during visits to hospital dispensaries and primary health care clinics

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Purpose: Training of pharmacy students involves a balance between teaching and practical components. Lectures are not sufficient to prepare students for eventual practice. The fourth year pharmacy students were assigned to variety of hospital dispensaries and primary health care clinics in the Johannesburg region on Tuesday and Thursday mornings from March until September 2012. They rotated between the sites each week. This study focuses on eliciting the opinions of students regarding their experiences in the hospital dispensaries and primary healthcare sites as well as establishing the activities they engaged in.

Methods: The students were asked to anonymously complete a questionnaire on an online survey platform. The information from the close-ended questions was captured using Microsoft Excel and quantitatively assessed, making use of descriptive analyses. The data obtained from the open-ended questions from the questionnaire were qualitatively analysed using content analysis to identify common themes. Ethics clearance for this study was obtained from the University of Witwatersrand Human Research Ethics Committee.

Results: Majority, 76.67%, of the class responded to the survey. Although, more than half the respondents felt that visiting these sites was enjoyable and beneficial, all the respondents felt that the clinical programme could be improved. The three common themes identified in the results were application and acquisition of knowledge, organization and structure as well as student involvement. The respondents made valuable suggestions with respect to improving the experiential learning programme in these three categories.

Conclusion: The responses indicated the attitude and approach of the fourth year students towards the clinical programme and provided useful insight into how the programme could be improved.

Integrating Evidence Based Medicine (EBM) as an Experiential Training Tool in Undergraduate Final Year Pharmacology Training in the B Pharm Degree

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Purpose: EBM was introduced as a new innovative approach to medical practice and education in the early 1990's. EBM skill development has in the past been focused on medical practitioners. The development of clinical pharmacist practitioners has meant that there is a need for EBM skills to reinforce decisions and recommendations when involved in direct patient care, or serving on National EDL advisory committees, Hospital Formulary Committees and budget driven PTC's. This presentation describes a proposed experiential application of EBM to enhance quality of clinical skills attained.

Methods/Model: The model presupposes a foundation of basic pharmacology up to 3rd year. The final 4th year of study is an integrated "pharmacotherapy" and clinical pharmacology approach. Central to this model is the use of EBM principles that guide clinical decision making. Students are assigned to patients on ward rounds in small groups. Cases are presented in class. Each case must have an identified clinical question (PICO), and be supported with data of systematic review (SR) or randomised controlled trial (RCT) parameters. Pharmacoeconomic analysis and appropriate clinical practice guidelines must be incorporated and referenced in presentations. Students must search and retrieve the best available clinical evidence from the literature and show critical appraisal of the study methods to ensure validity of the results. Clinical outcomes and discussion must be supported by current literature with evidence supporting clinical decisions like measureable outcomes e.g. Number Needed to Treat/Harm (NNT/H), Relative Risk Ratios (RRR), Odds Ratios (OR) from RCT and SRs. Learners must identify "Drug Related Problems (DRPs) and Medicine Errors (ME) and classify them as per requirements of Pharmacovigilance practice.

Results/Outcomes: The effectiveness of the proposed model will be assessed at the end of the academic year. Final formative assessment occurs via evaluation of at least 8 in-depth case studies worth 15% of final mark. Case study write ups incorporate the traditional "SOAP" model and build in clinical aspects of "PICO" as recommended for EBM style learning. Cases are submitted online, marked and made available for use as revision tools. Summative assessment for the experiential component is "open-book" style, patient case assessment. Retention summative assessment takes the traditional format of closed book assessment. Final summative assessment includes oral assessment with external examiners.

Conclusions: This proposed model of training and assessment format lessens traditional memorising. Added gain from group discussions and actual patient interaction allows for engaged concept reasoning, increased knowledge and skill base as well as enhanced professional attitude preparing the new health professional for integrating with ease into the EBM driven health system in SA.

Product-centred to patient-centred pharmacy care: Commentary from the academic pharmacist-patient interface

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Background: It is well documented that over the past 25 years, pharmacists been exhorted to shift from a product-centred to a patient-centred culture of care. In its *2020 Vision, FIP's Vision, Mission and Strategic Plan*, FIP promotes a patient-focused, medicines-centred healthcare system in which the modern pharmacist is a provider of patient care. Other organisations point to the growing demand for pharmacists' specialist skills in patient-centred pharmaceutical healthcare. Within the various descriptions of models of pharmacy care, is the term "patient-centred care" interpreted in the same way by pharmacy as it is in other areas of healthcare?

Looking at patients through a sociological lens casts a different perspective on the position that patients inhabit in society, and their desires, needs and expectations from the healthcare system. The long-dominant biomedical model of care still often prevails today, despite rigorous criticism by sociologists and efforts by international and national healthcare organisations to influence the manner in which healthcare is delivered, the degree to which patients are included or excluded in "clinical conversations", and the extent to which they are encouraged to participate in their own healthcare plans.

Method: Using an autoethnographic illness narrative approach, I will describe my oral cancer illness journey, with a focus on recent major operations, extended hospital stays and a resultant fundamentally altered functionality and quality of life. Through reflection on the quality of the many diverse models of care I experienced from various health professions, I will interrogate the meaning of "patient-centred care" and question how this concept is perceived in a pharmacy context.

Conclusion: Experiential evidence does not support a patient-centred model of pharmacy care.

Applying a behavioral model of medication adherence to educate HIV-infected patients to achieve a better therapeutic outcome in a public sector

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Purpose: Adherence to HAART is a major determinant of outcome to HIV infection. Good adherence to ART is necessary to achieve the best virological response, lowers the risk of development of drug resistance, and reduces morbidity and mortality. Therefore it's a pharmacist's role to educate the patients about HIV/AIDS and its management. The objective of this study is to determine factors associated with poor adherence to HAART and thereafter apply a behavioral model of medication adherence to educate HIV-infected patients to achieve a better therapeutic outcome.

Methods: A descriptive-cross-sectional study was conducted among ARV clinic attendees. Face-to-face exit interviews using a standardized questionnaire were used. Data were analysed using SPSS version 21. Pill counts were performed and the computed adherence rate of $\geq 95\%$ was considered acceptable. Univariate factors associated with poor adherence to HAART were assessed with ANOVA. A logistic regression model was used to determine independent predictors of poor adherence. A P value of ≤ 0.05 was considered as statistical significant.

Results: A total of 102 HIV-infected patients on HAART were recruited, 83.3% females and 16.7% males, with mean age of (\pm SD) 35.09 (\pm 9.3) years. Patients were on HAART for 24.68 (\pm 20.5) months. Univariate factors associated with poor adherence rates to HAART were: CD4+ T count > 350 cells/mm³ ($\chi^2=46$; $P=0.05$), age >35 years ($\chi^2=28.75$; $P=0.011$), primary educational background ($\chi^2=9.18$; $P=0.027$), HAART regimen 1A-TDF ($\chi^2=14.37$; $P=0.003$), and >4 combined tablets (including ARVs) received per dose ($\chi^2=11.87$; $P=0.001$). There was a linear correlation between age >35 years and primary educational background ($r=0.538$; $P<0.0001$). After adjusting for univariate confounders, primary educational background ($P=0.020$) and >4 combined tablets (including ARVs) received per dose ($P=0.026$) were identified as independent predictors of poor adherence to HAART. Thereafter "The Behavioral Model" based on: Subjective Norm, Attitude and Perceived Behavioral Control (SNAPBC) was applied.

Conclusion: Although there is an increase in the number of HIV-infected patients receiving HAART, patients will not adhere to their treatment once they start improving clinically. Therefore education towards adherence is required.

Antimicrobial resistance in military healthcare facilities and in patient stewardship

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Purpose: In the 1940s, the widespread availability of penicillin and the subsequent discovery of streptomycin led to a dramatic reduction in illness and death from infectious diseases. Today, the extensive use of antimicrobial drugs has resulted in drug resistance that threatens to reverse the medical advances of the last seventy years. Preventing the spread of infection and microbial resistance is a battle being fought not just in civilian healthcare settings worldwide but in the military healthcare system as well. This year *Staphylococcus aureus* resistance in the African region has so far been reported to be between 12-80% in both civilian and military healthcare facilities. A review of several articles on the level of antimicrobial resistance worldwide in military healthcare facilities was carried out. The purpose of the review was to determine antimicrobial stewardship in these military healthcare facilities

Methods: Searches for everything relevant to antimicrobial resistance, in healthcare facilities in general, and in military facilities in particular was carried out. The articles found, were then sorted out into a coherent view of the “state of the art” of antimicrobial resistance and antimicrobial stewardship

Results: Between 1980 and 2002 in one of the military healthcare facility, of the 3920 gram-negative strains that were isolated in Europe, antimicrobial resistance for some of gram negative such as *E. coli* increased by 9.2%, *Pseudomonas spp.* resistance increased by 8%, *Enterobacter spp.* resistance increased by 4%. In 2014 *Staphylococcus aureus* overall reported range of resistance in African region was between 12-80% in both military and government healthcare facilities. In Walter Reed Army Hospital, Washington DC, the frequency of aminoglycosides resistance among clinical bacteria isolates increased from less than 1% in 1976 to 13% of all isolates in later years. Macrolide resistance among *Streptococcus pneumoniae* isolates from various countries is severe, e.g. Hong Kong is 81%, and Japan is 71%. The rate of Methicillin resistance among *Staphylococcus aureus* is high in Japan at 71.6% and 73% in Hong Kong.

Conclusion: Although the rate of antimicrobial resistance increases in both military and government healthcare facilities, reviews indicated that there are no action plans taken about antimicrobial resistance. In United States of America it was suggested that high priority must be given to strategies that limit the emergence and dissemination of organism’s resistance to the important antimicrobials.