

# AY1920 Semester 1 Postgraduate Seminar 23 September 2019 S4 Level 2, PPS Hub 9.00 - 10.30 am

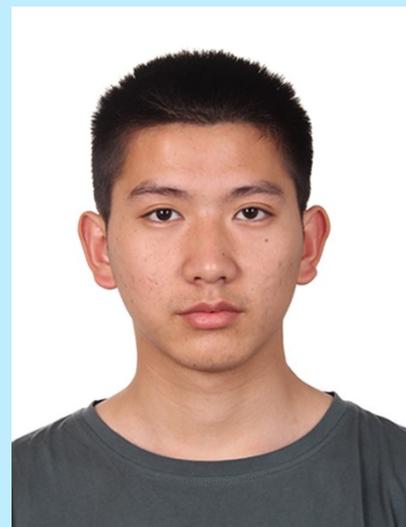
## Program

9 - 9.10 am	Opening Address (Prof Eric Chan)
9.15 - 9.45 am	Mr He Weidong
9.45 - 10.15 am	Ms Joanne Teh
10.15 am	Closing Remarks & End

**ALL ARE WELCOME**

\* mandatory for all PG students

# Development of Artificial Neural Network Models for Target Prediction



**Mr He Weidong**  
Supervisor: Prof Chen Yu Zong

**ABSTRACT** Recent years have seen a great number of exploratory applications of machine learning methods in the drug design process, especially in prediction of molecule-target relationship. However, since most advanced methods originated from other areas, such as computer vision and nature language processing, it is still challenging making the best of them in the drug design field. In this study, we developed several artificial neural networks to predict targets of small molecules. They were compared with each other in terms of prediction accuracy, and we explored possible techniques to improve their performance. The intrinsic causes of differences in their performance were also discussed to enlighten future improvement.

**BIOGRAPHY** Mr. He Weidong is a postgraduate in the BIDD (Bioinformatics and Drug Design) group under Professor Chen Yu Zong in the Department of Pharmacy at the National University of Singapore. He got a bachelor's degree of biology at Zhejiang University of China and developed interests in programming and bioinformatics in the fourth year of his undergraduate studies. He updated the chemical family database CFam, and has been focusing on development of machine learning models to predict useful pharmaceutical properties of small molecules, such as inhibition against specific disease target and aqueous solubility. Models involved including support vector machine and artificial neural networks.

# Impact of Die Wall Material on the Mechanical Properties of Tablets

**Ms TEH Liam Chee**

**Supervisor: A/Prof Paul Heng**

**Co-Supervisors:**

**A/Prof Chan LW & Dr Celine Liew**



**ABSTRACT** Tablet quality can be affected by material, configuration and design of the tooling which comprise punches and dies. Much research attention had centred around punches, with very little reported on the dies. Dies with modified bore lining materials or inserts are available for special applications. However, the influence of such die types on tablet properties and the compaction process has not been well studied. Often, the reason for selecting dies with harder lining material is for improved wear resistance. In this study, flat-faced and convex-faced tablets were produced from paracetamol granules using dies with different bore inserts. Tablet properties and response parameters of the compaction process were evaluated to understand the impact of die mechanical and surface properties on the compacts formed. Compaction pressure was found to have the greatest impact on tablet elastic recovery ( $r \geq 0.96$ ,  $p < 0.01$  in all bivariate correlations) and thus affecting the tensile strength. Choice of die inserts could impact the mechanical properties of convex-faced tablets, particularly at high compaction pressures.

**BIOGRAPHY** TEH Liam Chee received her M. Eng (Bioprocess) degree from Faculty of Chemical Engineering, Universiti Teknologi Malaysia (UTM) where she developed a directly compressible herbal formulation for tableting. Liam Chee is currently pursuing her PhD at Department of Pharmacy, National University of Singapore, under the supervision of A/Prof Paul Heng Wan Sia and co-supervision of A/Prof Chan Lai Wah and Dr Celine Valeria Liew. Her research interest focuses on tablet compaction particularly in the field of tableting die configuration. Her work involves preparation of tablets from pharmaceutical powders, characterisation of tablet physicommechanical properties and analysis of compaction profiles in order to elucidate the influence of tableting die configurations on pharmaceutical powder compaction and tablet quality.