## Introduction to the research topics of Protein Crystallography Research Group, MCB UJ



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## Abstract

- 1. Small Molecule Inhibitors of PD-1/PD-L1 immune checkpoint
- 2. PEX inhibitors in Chagas Disease
- 3. Kinase inhibition in diabetes

Our primary interest encompasses characterization of protein-small molecule interactions to facilitate rational optimization of therapeutically relevant inhibitors. I will present our major interests in recent years including: (i) Characterization of small molecule and macrocyclic inhibitors of PD-1/PD-L1 immune checkpoint (~20 min); (ii) Development of PEX inhibitors in Chagas Disease (~15 min); (iii) Kinase inhibition in diabetes (~5 min).

Topic (i) will include brief introduction to the role of PD-1/PD-L1 pathway in cancer, characterization of the binding mode and activity of BMS compounds, and characterization of the interaction mode and in vitro action of macrocyclic inhibitors. Topic (ii) includes introduction to Chagas disease and peroxisomes in Trypanosoma parasites. Inhibitors of peroxisomal transport capable of reducing parasitaemia will be discussed primarily form the structural point of view. Topic (iii) includes brief overview of our approach to possible alleviation of diabetes by targeting diabetes related kinases (the work of NAWA fellow dr Anna Czarna).