Project Title:

Harnessing Machine Learning for Identification and Development of Novel Platinum-based Anticancer Drugs

PI: Professor Maria BABAK of CityUHK

Co-I: Professor Oleg KIRIUKHIN of CityUHK

Project Abstract/Proposal Summary:

In the rapidly evolving field of drug discovery, machine learning (ML) has emerged as a game-changer. Yet, its potential in exploring metal-based compounds, particularly platinum anticancer compounds, has been largely untapped due to a lack of organized data. In our groundbreaking study, we've bridged this gap by creating an unprecedented database of over 4000 unique platinum anticancer compounds. This first-in-class database not only contains information about the cytotoxicity of platinum-based compounds but also includes data on their physico-chemical properties, amounting to over 15,000 entries in total. We've harnessed this comprehensive database to train an ML model that can predict the anticancer activity of new platinum metal complexes. Our model's predictions have been experimentally validated, highlighting its promising potential for future use in anticancer drug discovery. This study resulted not only in the creation of the comprehensive metal-based complex search engine but also underscores the transformative role of ML in drug discovery, opening new avenues for the exploration of metal-based compounds.