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何鴻燊博士醫療拓展基金會
Dr. Stanley Ho Medical Development Foundation

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“揚帆追夢、創啟未來”2022年度獲資助研究項目
“SET SAIL FOR NEW HORIZONS, CREATE THE FUTURE” FUNDED PROJECT FOR 2022

胡元佳教授
Prof. Yuanjia HU

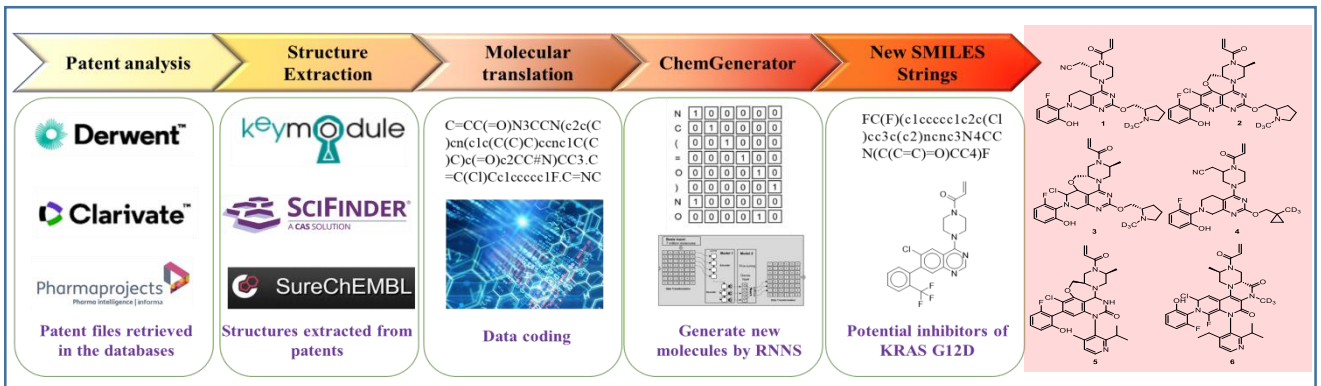
胡元佳，澳門大學中華醫藥研究院、健康科學學院教授；擔任中華醫藥研究院醫藥管理課程主任、健康科學學院公共衛生及醫藥管理學系副主任；主持科研項目25項，在*Nature Biotechnology*等國際期刊發表學術論文150餘篇。

Yuanjia HU is a Professor at the Institute of Chinese Medical Sciences (ICMS) and the Faculty of Health Sciences (FHS), University of Macau (UM). He is the Assistant Director (Medicinal Administration Education Development) at ICMS, and Associate Head of the Department of Public Health and Medicinal Administration, FHS. He has led 25 scientific research projects and published more than 150 academic papers in international journals such as *Nature Biotechnology.*

KRAS G12D小分子抑製劑專利化合物數據挖掘和分子生成
Data Mining and Molecular Generation of KRAS G12D Small Molecule Inhibitor Patent Compounds

KRAS G12D是一個重要但仍待探索的癌症靶點。我們的研究通過跟踪挖掘KRAS抑製劑領域領先機構的專利，確定KRAS G12D抑製劑的核心專利，並進行分子翻譯、結構提取，建立分子全景及骨架演化路徑。基於分子描述符、機器學習和QSAR模型，利用ChemGenerator生成313,867種可能具有KRAS G12D抑制活性的新型虛擬化合物，該研究可為先導化合物的篩选和結構優化提供新的起點，也可為後續抗癌活性實驗研究提供參考。

KRAS G12D is an important but still unexplored cancer target. Our study identifies the core patents of KRAS G12D inhibitors by tracking the patents of leading organizations in the KRAS inhibitor field, performs molecular translation and structure extraction, and establishes molecular landscape and scaffold evolution pathways. Based on molecular descriptors, machine learning and QSAR models, ChemGenerator was used to generate 313,867 novel virtual compounds with possible KRAS G12D inhibitory activity. This study can provide a new starting point for the screening and structural optimization of lead compounds, as well as a reference for subsequent experimental studies on anticancer activity.



數據挖掘及分子生成
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