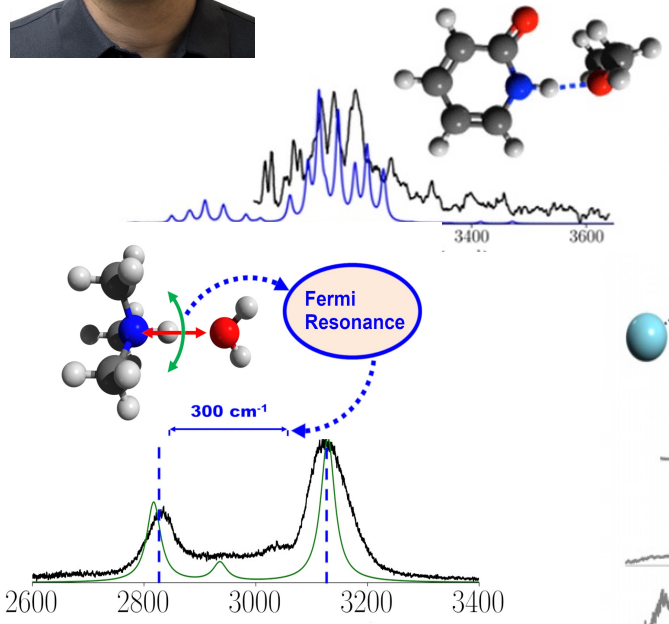
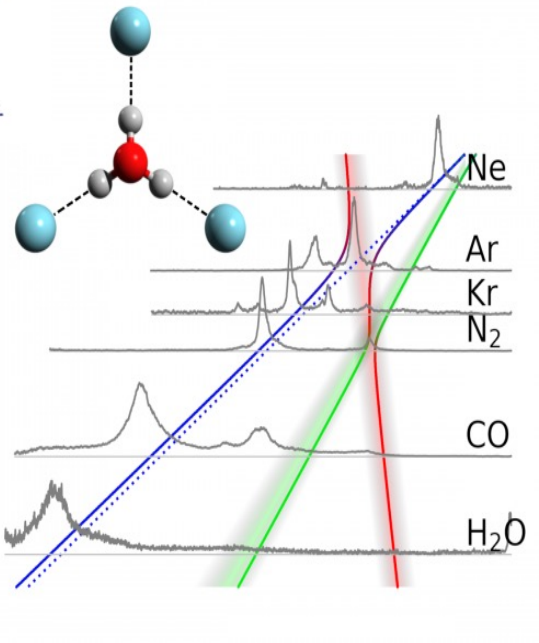
Molecular and Material Modeling Lab

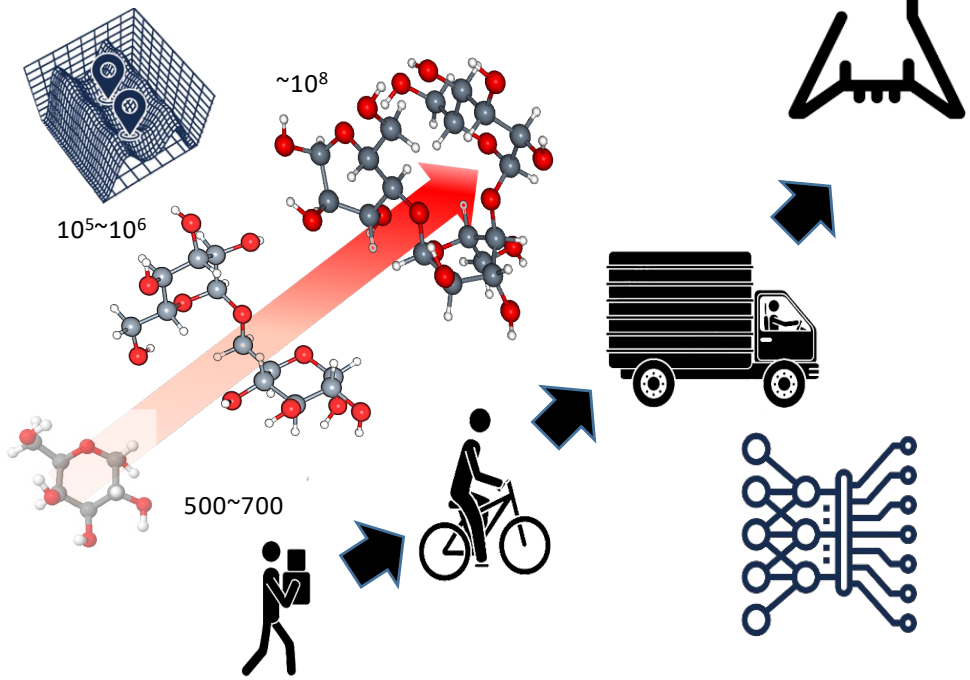
Jer-Lai Kuo, Institute of Atomic and Molecular Science, AS



Two NH stretch in amines have very different Fermi-Resonance (FR) patterns. Our *ab initio* anharmonic algorithms (A^3) do not require empirical parameters and are able to extract simple physical pictures behind the experimental spectra and thus reduce the chance of mis-interpretation. The parameter-free reduced Hamiltonians can be use to understand physical phenomena and make predictions to guide design of experimental observations.



Complex vibrational features in experimentally observed spectra of solvated H_3O^+ lead us to understand the coupling between OH stretch and other degrees of freedom. Using *ab initio* anharmonic algorithms, we are able to assign the observed complex spectral features and to reveal simple pictures of the interplay between FR and CB in both mid- and near-IR.



We utilize deep-learning neural network potential (DL-NNP) to accelerate the exploration of energy landscape of mono-saccharides (500~1000 conformers) and di-saccharides (~10^5-10^6) with the cost comparable to semi-empirical methods & the accuracy of a decent DFT methods. We are working to improve the efficiency of sampling schemes so that we can simulate systems containing sugar, peptides and nuclear acids. We believe DL-NNP can give a boost (by several orders of magnitude) to simulations of bio-molecules that requires first-principle accuracy.

洪上程博士實驗室

有機化學、醣化學、化學生物學

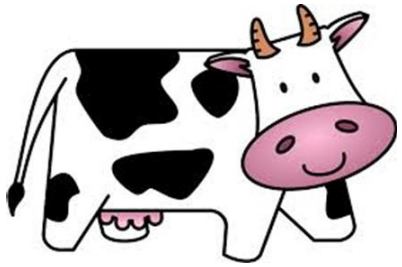
- 發展醣之「一鍋化」保護和鏈結方法。
- 開發自動化液相醣合成儀。
- 合成細胞表面醣分子庫和醣蛋白。
- 探討醣與疾病有關之蛋白質的作用關係。
- 發展新立體控制方法以合成線形天然物。

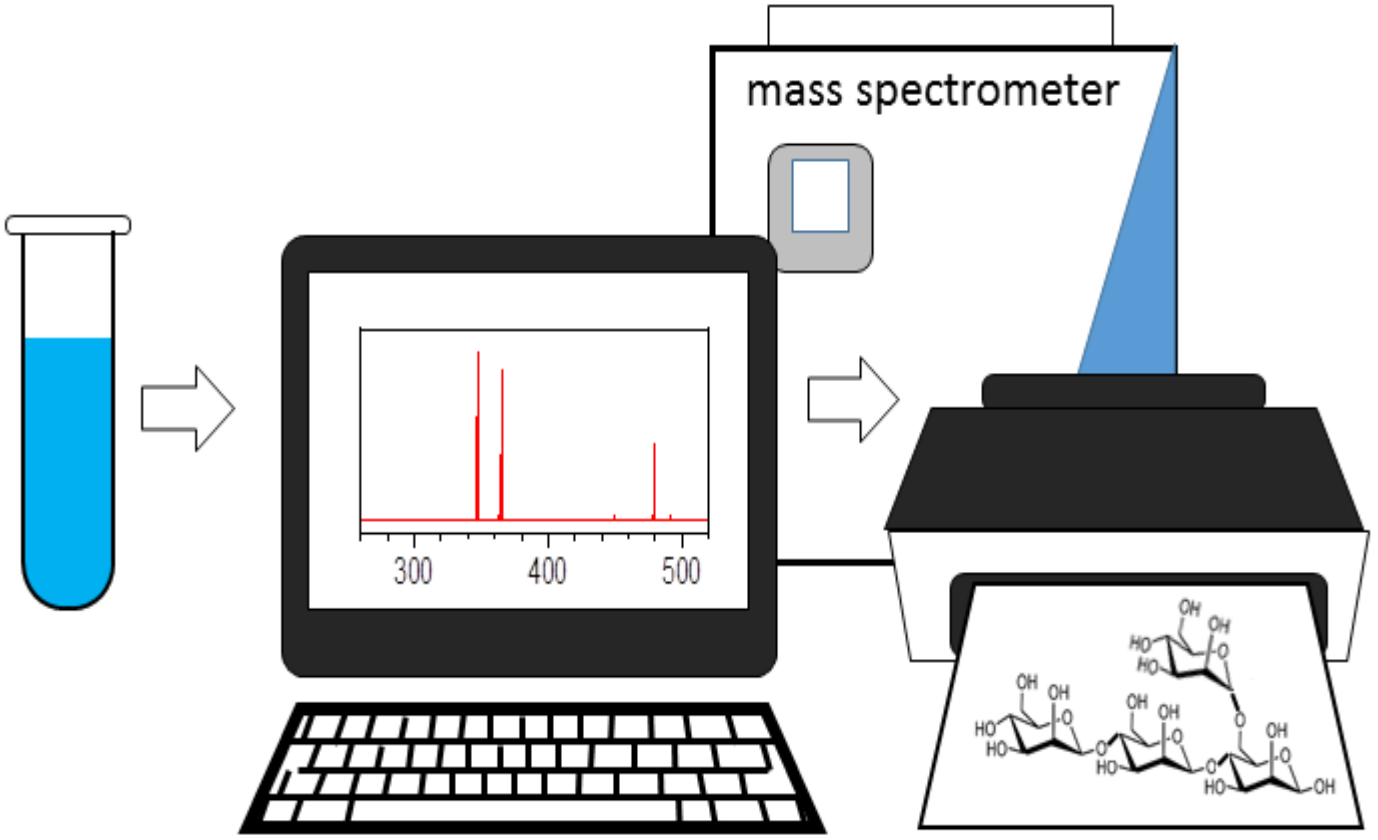
Carbohydrate Mass Spectrometry Lab

Chi-Kung Ni (倪其焜)

Experimental methods

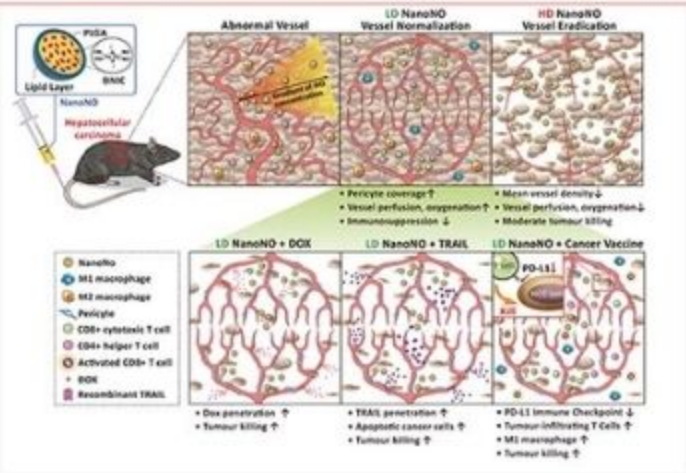
- Extraction of carbohydrate from biological samples
- Separation of carbohydrate isomers
- Structural determination of carbohydrates by mass spectrometry





陳韻晶實驗室 專注於創新藥物與奈米型藥劑的開發

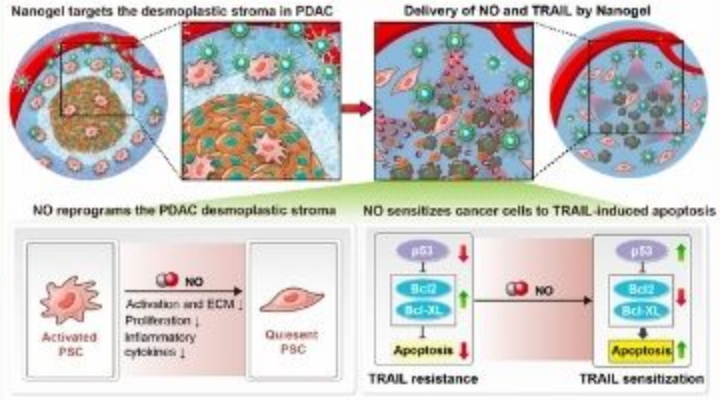
打通腫瘤血管，讓藥效更深入



Nature Nanotech 2018

用藥物「疏通」腫瘤內異常血管，提高藥物傳遞效率.

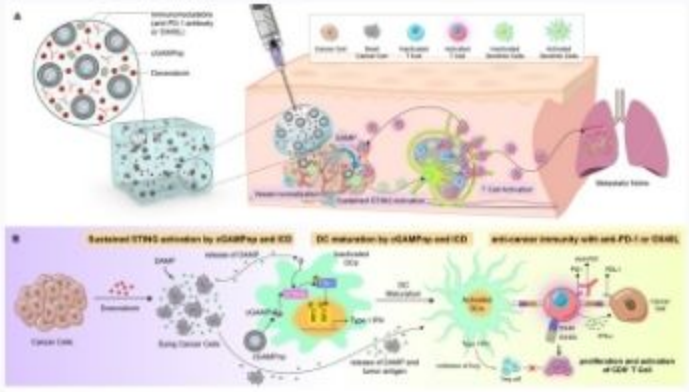
破解胰臟癌屏障，強化免疫治療



Gut, 2022

運用奈米載體精準釋放藥物，改變腫瘤微環境.

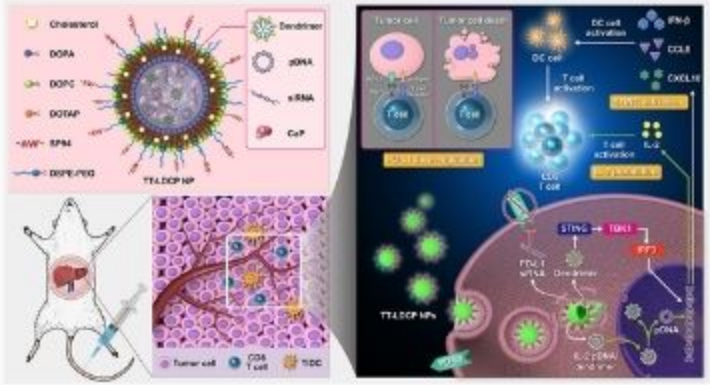
智慧型水膠疫苗，啟動癌症免疫防禦



Advanced Functional Materials 2024
ACS Nano 2024

開發「溫感可注射水膠」，讓腫瘤疫苗長效釋放

基因療法新革命，精準啟動活化免疫細胞



Hepatology. 2018, Science Advances 2020
Journal of Controlled Release, 2022

運用奈米載體輸送基因藥物，精準調控免疫細胞行為