*C*omputational *M*olecular *D*esign & *M*etabolomics

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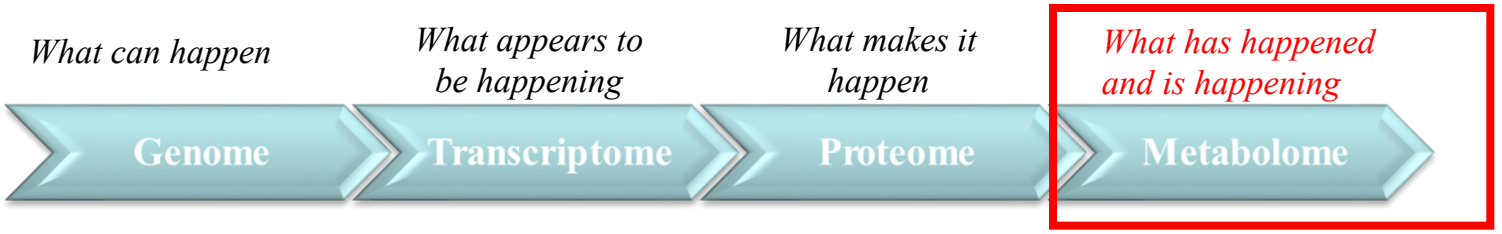
研究

AI in drug discovery and Bimedical advancement

研究主題一：診斷

代謝體學

基因型



表現型

nature Vol 463|7 January 2010

OPINION

nature publishing group npg

代謝體

未來十年會改善人類生活的14學科之一 (*Nature*'s 2020 vision)

14學科 — 搜尋、個人化醫療、藥物開發、微生物學、 精神健康…

14學科中之個人化醫療、藥物開發、微生物學、精神健康認為自己的領域要突破需要代謝體的協助

研究主題一：代謝體學

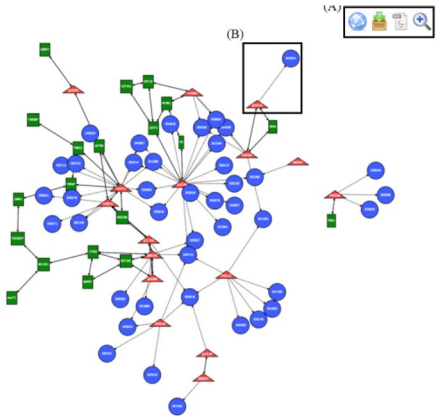
圖譜計算、系統生物網路計算

Software

Highly accessed | Open Access

3Omics: a web-based systems biology tool for analysis, integration and visualization of human transcriptomic, proteomic and metabolomic data

Tien-Chueh Kuo[12], Tze-Feng Tian[23] and Yufeng Jane Tseng[123]*



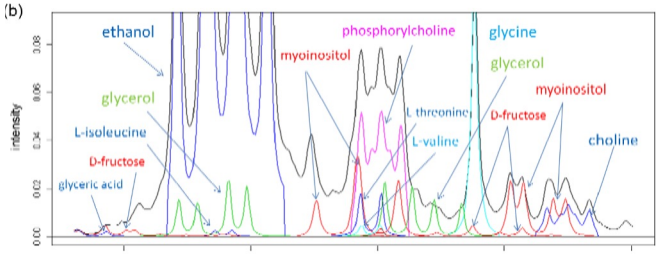
analytical chemistry — Article — pubs.acs.org/ac

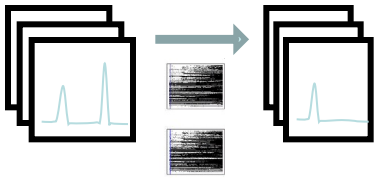
Batch Normalizer: A Fast Total Abundance Regression Calibration Method to Simultaneously Adjust Batch and Injection Order Effects in Liquid Chromatography/Time-of-Flight Mass Spectrometry-Based Metabolomics Data and Comparison with Current Calibration

analytical chemistry — Article — pubs.acs.org/ac

Distribution-Based Classification Method for Baseline Correction of Metabolomic 1D Proton Nuclear Magnetic Resonance Spectra

Kuo-Ching Wang,[†,∥,⊥,#,▽] San-Yuan Wang,[‡,∥] Ching-hua Kuo,[§,∥] and Yufeng J. Tseng*[,†,‡,§,∥]

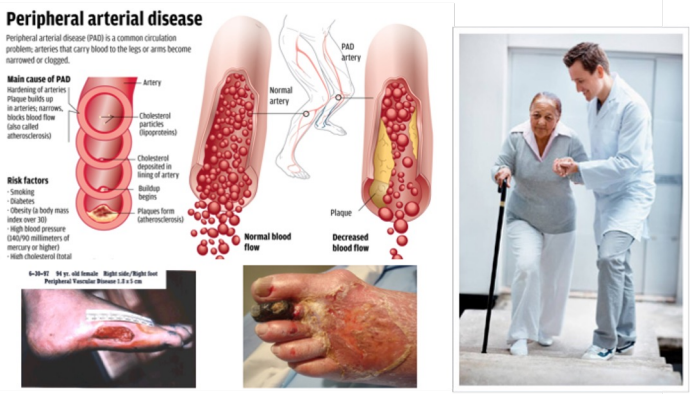


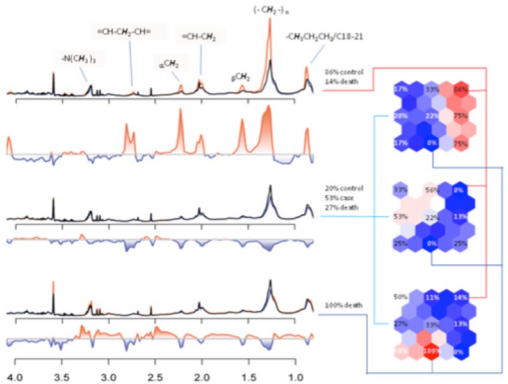


- 發展可分析混和物的質譜與核磁共振光譜演算法
- 2011國際代謝體年會最佳論文獎
- 最多理論計算發表到分析化學最好的期刊「Analytical Chemistry」
- 系統生物網路計算 3Omics –Highly Accessed Article [BMC Systems Biology (2013)]

研究主題一：代謝體學

鑑定臨床上診斷、治療的生物指標





周邊動脈疾病

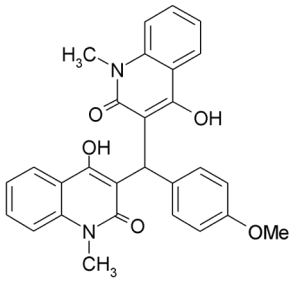
- **三成死亡率**
- **全球最大的周邊動脈疾病血液樣本**
- 全球唯一團隊

- FDA同級的台大代謝體核心實驗室
- 世界上第一個可預知一年後周邊動脈疾病死亡率的生物指標
- 開啟台灣學界代謝體本領域研究

Lab Focus

診斷

- **找尋生物指標**
- **圖譜、系統生物網路計算**
- **精準醫學**



分子結構計算

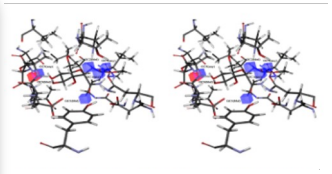
治療

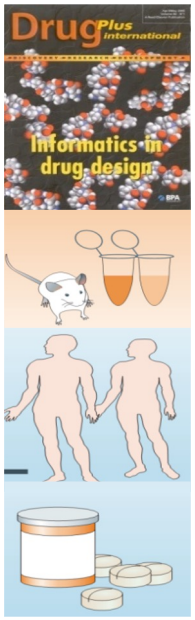
- **電腦藥物設計**
- **電腦藥物篩選**
  –計算模型取代生物實驗標準
- **AI應用於藥物開發**

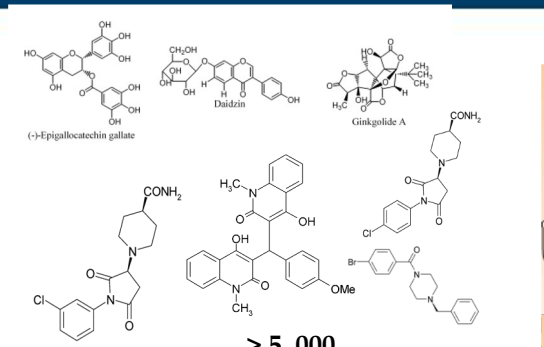
電腦輔助藥物設計

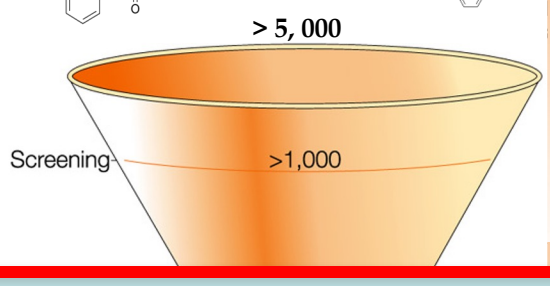
10 years

7 Years

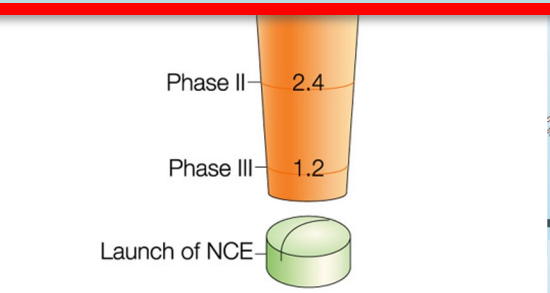




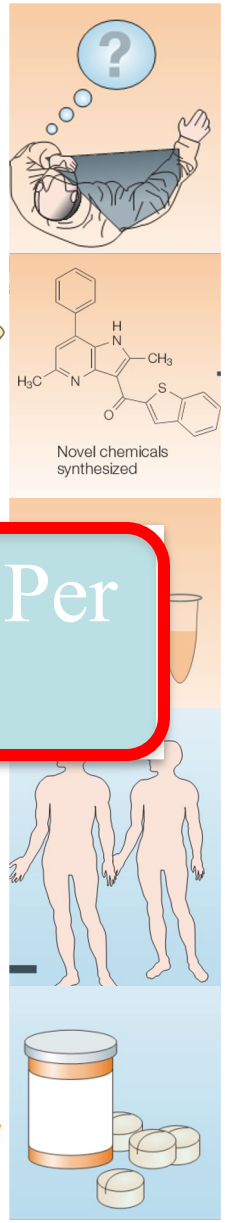




US $ 1.7 Billion Per Drug



Nature Reviews | Drug Discovery



20 years

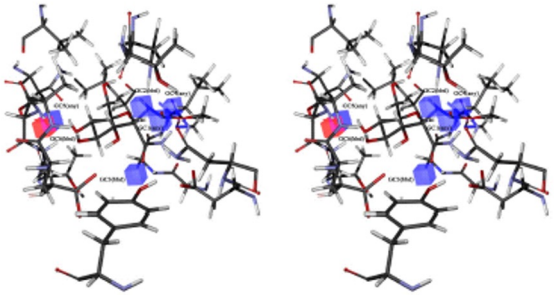
7 Years

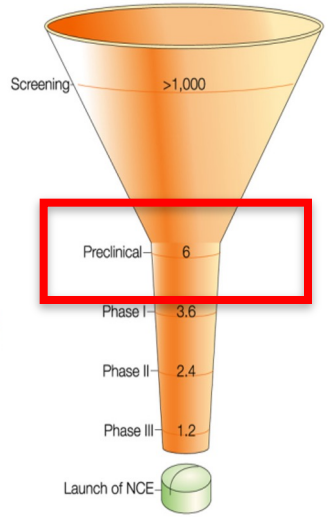
傳統藥物開發

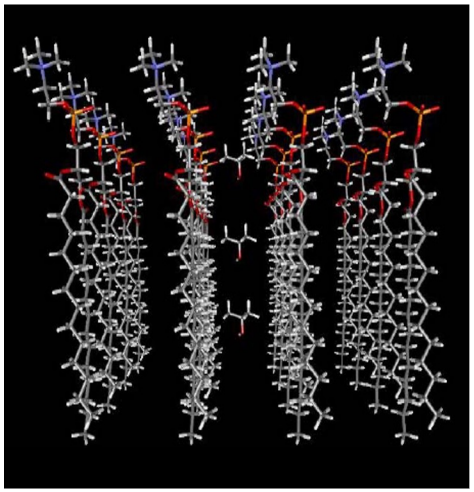
研究主題二：電腦藥物設計

減少毒性

美國國家衛生研究院唯一臨床前電腦預測藥物篩選之計畫
(2006-2009，總共10個領域得到支持)



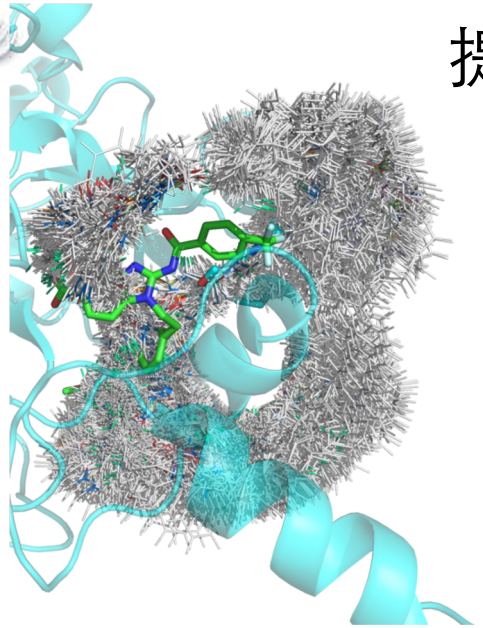


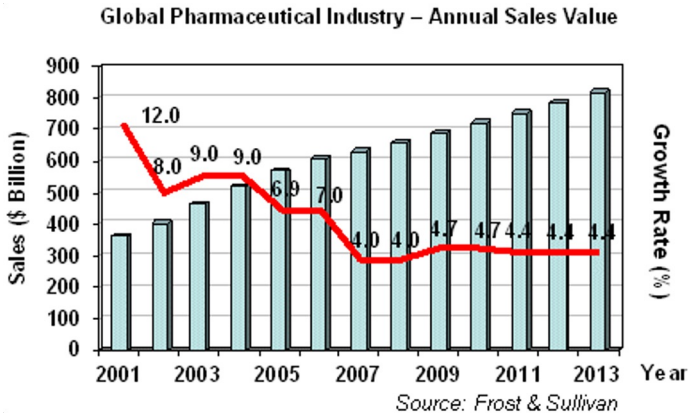


- 已成為國際業界標準:
  - 美國知名製藥公司採用的電腦藥物篩選模型(2007-)
- 計算模型**取代**生物實驗
  - 口腔腸道藥物吸收、皮膚致敏毒性、皮膚吸收、皮膚滲透的計算模型
  - 歐盟在2012年啟用禁止生物測試化學物質經由皮膚吸收毒性法規

研究主題二：電腦藥物設計

提高結構活性、獲得藥物專利

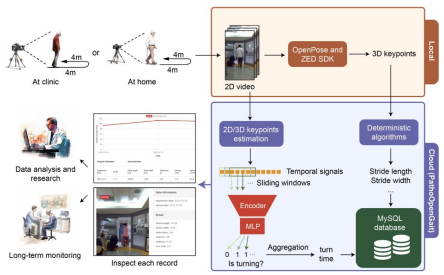




- 藥物要能獲利是要有藥品結構專利
- 一年全球獲准上市的藥物不超出17種
  - 在一個治療類別裡第一個上市的藥物 (first in the class)可以拿下一半的全球市場15至20年

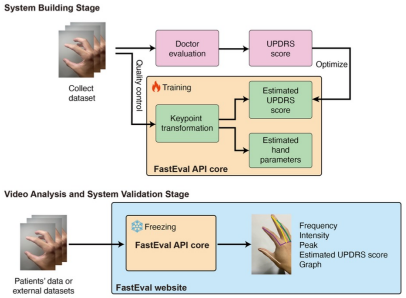
研究主題三：**AI for Healthcare**

We leverage computer vision, nature language processing, and machine learning methods to understand human movement and behavior, toward scalable and accessible healthcare solutions.



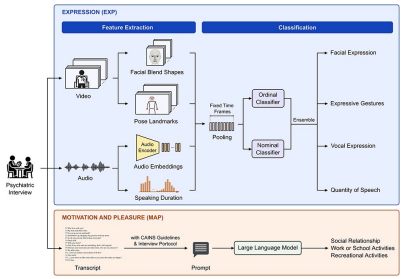
PathoOpenGait
(*IEEE JBHI 2024*)

Open-source cloud-enabled platform for pathological gait analysis.
— Semi-supervised learning + cloud inference for scalable gait evaluation.



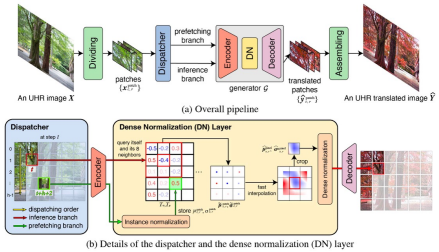
FastEval Parkinsonism
(*npj Digital Medicine 2024*)

Instant video-based online assessment system for Parkinsonian motor symptoms.
— First real-time, deep-learning–assisted evaluation platform.



AI for Schizophrenia
(*Schizophrenia Bulletin 2025*)

Gen AI + ML for automated symptom assessment.
— First attempt to quantify negative symptoms using LLM/AIGC methods.



Dense Normalization
(*ECCV 2024*)

Ultra-high-resolution unpaired image-to-image translation via dense normalization.
— Enabling data augmentation for large images in healthcare scenarios.

Computational Molecular Design & Metabolomics Lab

研究主題四：AI Agent

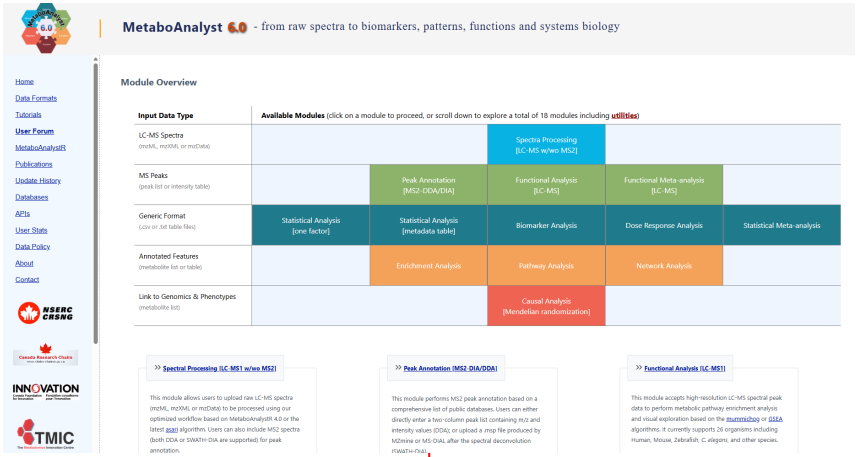
We employ AI agents to assist users in analyzing mass spectrometry data through reliable databases, reducing complex manual procedures and facilitating deeper data interpretation.

User Upload data

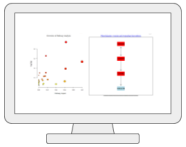
Assist in using specific or designated tools after analyzing the content

Help Upload the data for user

MetaboAnalyst 6.0

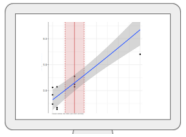


Choose the analysis approach according to the data



Pathway Analysis

Enrichment Analysis



Dose Response Analysis

Retrieve the results after the analysis is completed

Interpret and analyze the retrieved results

Further explain and discuss with the user

User Accept data

Figure resource : https://share.google/images/8ypUS5MHfwSeXMD01
MetaboAnalyst 6.0 : https://www.metaboanalyst.ca/faces/ModuleView.xhtml

研究主題四：AI Agent

We use AI agent to help users explore and understand toxic chemicals they are curious about, by gathering and interpreting information from academic literature and chemical databases, enabling deeper insights into the substances of interest.

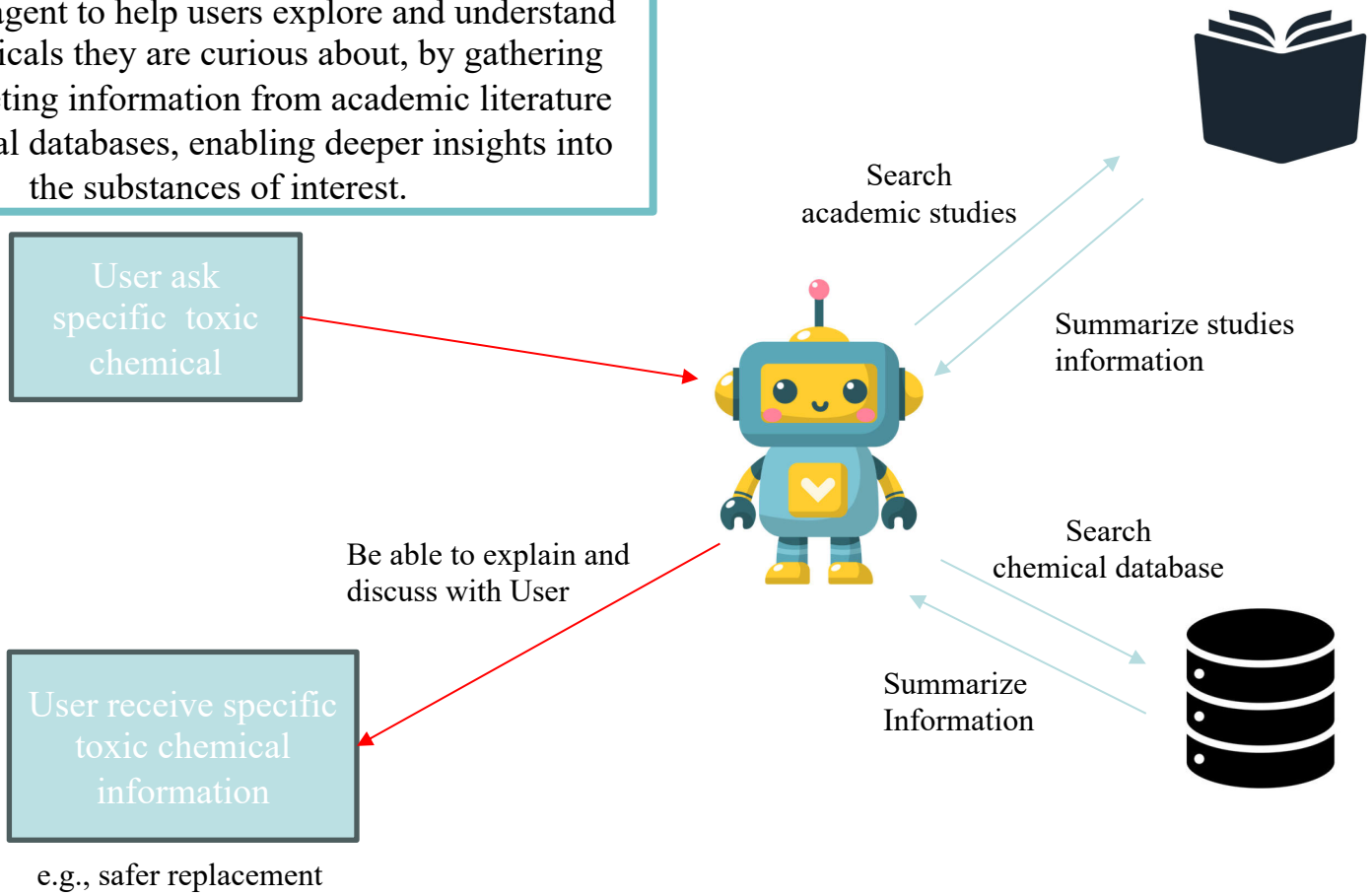
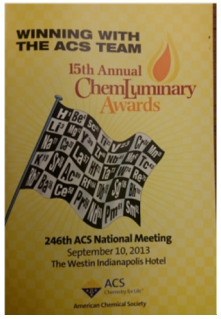


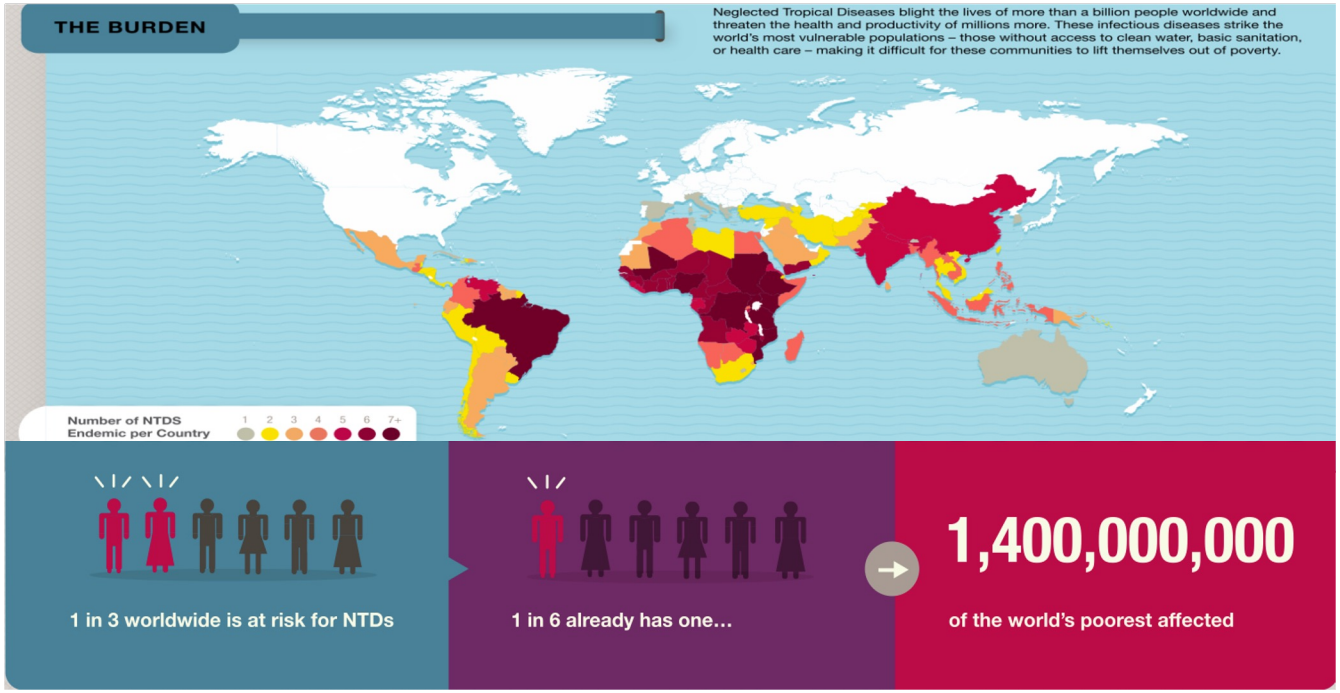
Figure resource :
https://share.google/images/thOzC0Te9PccKQHFD
https://share.google/images/iY2BLgx1KsKWUQukw

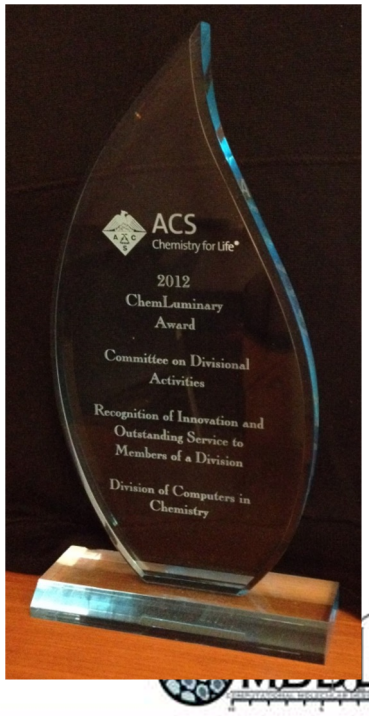
國際服務

「Teach Discover Treat （TDT)」initiatives



- 集合全球學界開發忽略性疾病藥物 (neglected disease) since 2010
- 病人眾多，但集中在藥廠不關心的非歐美地區，無現有有效的藥
- 「台大，Novartis，Merck， UC」 Founder (4) , Scientific Board Member
- **2012 美國化學協會創新研究獎** ACS IPG innovation award
- **2013 美國化學協會創新服務獎** ACS Chemluminary award





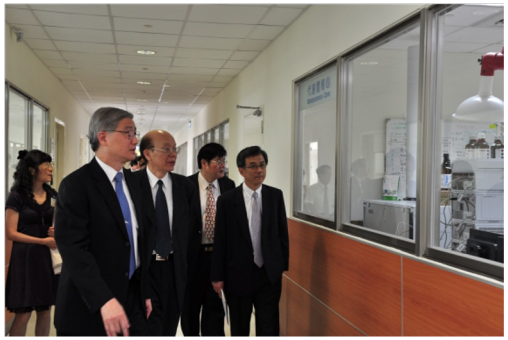
跨國跨院服務

跨院系服務

- 藥物研究中心
- 基因體醫學研究中心代謝體核心
  - 設立台大醫學院代謝體核心實驗室
  - 國科會代謝體核心實驗室

跨國服務

- 跨國頂尖癌症研究中心 (i-Rice) [2012年迄今]



WELCOME

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