人工智慧驅動研究轉型

生命科學AI-深入實驗階段的創新工具

ELSEVIER
生命科學解決方案
Ryan Huang 黃恪涵

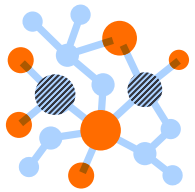
自然科學研究的三個階段

知識探索
Knowledge Discovery

實驗設計與執行

報告撰寫、發表

研究計畫提案



查詢、閱讀文獻
建立領域知識

內文圖標、實驗
數據的判讀
實驗設計
實驗執行

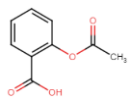
結果分析

報告與發表

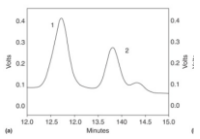
Generative AI Solutions

Elsevier Life Science AI offerings

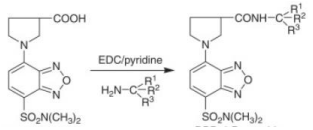
化學結構



實驗量測數據



化學反應式



基因

蛋白質

病毒

疾病機轉

治療疾病的機轉

實驗階段關鍵成功因子:

- ✓ 可信賴、高品質的實驗數據，進行研究決策。
- ✓ 創新的發現，科學的新穎性，創造新材料、新藥物!

Reaxys資料庫的演進

1881:
First edition of Beilstein Handbook of Organic Chemistry

1817:
First edition of Gmelin Handbook of organometallic and inorganic compounds

1988:
Beilstein and Gmelin database go online

1992:
CrossFire launched

Taiwan National License

2009:
Reaxys launched

2013/2014:
Complete revamp of Reaxys and content expansion

2016:
New Reaxys UI launched

2017:
New Reaxys Medicinal Chemistry (RMC) module

2020:
Reaxys Commercial Substances

2021:
Patent Expansion to 34 mil patent

2021:
Predictive Retrosynthesis (AI based Synthesis prediction)

Reaxys Academic Edition

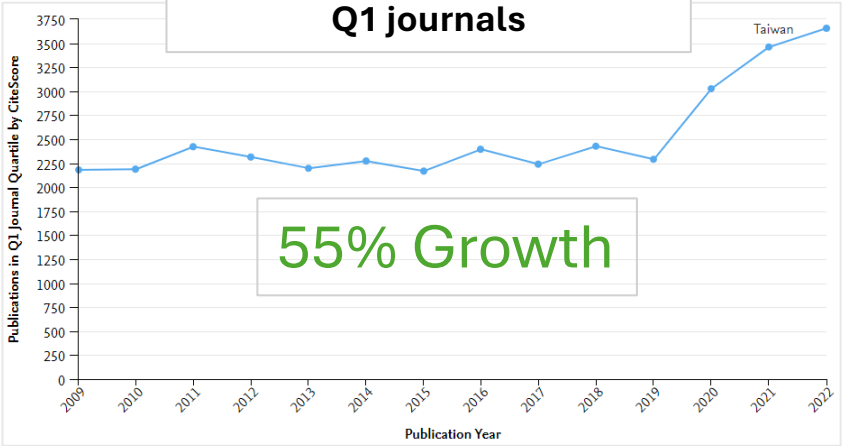
Research

Teaching & Learning

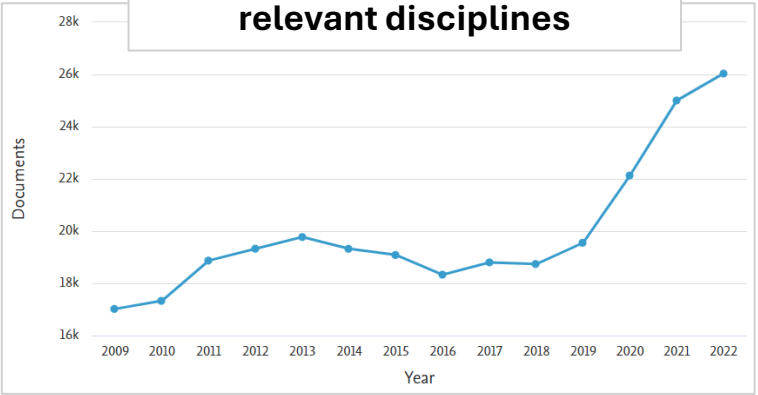
2023:
Reaxys Ecosystem
Integration of SicenceDirect & Scopus

2024:
Iktos-retroAI
Help chemist to make novel compounds in 10

Chemistry publications on Q1 journals



Research output of chemistry relevant disciplines

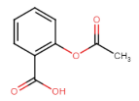


Reaxys的使用者邁入實驗設計與執行階段 – Reaxys AI被用來克服常見的合成瓶頸步驟

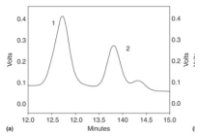
知識探索
Knowledge Discovery

實驗設計與執行

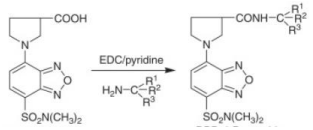
化學結構



實驗量測數據

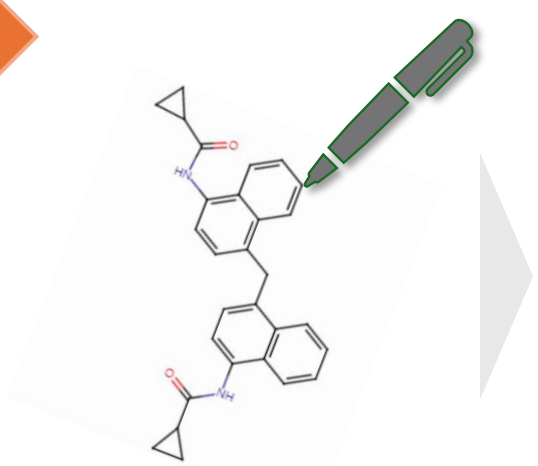


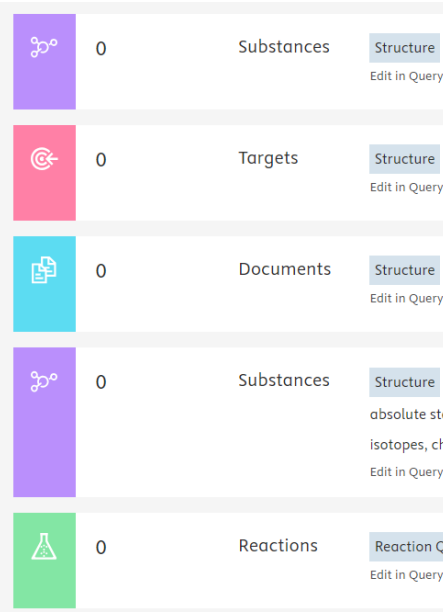
化學反應式



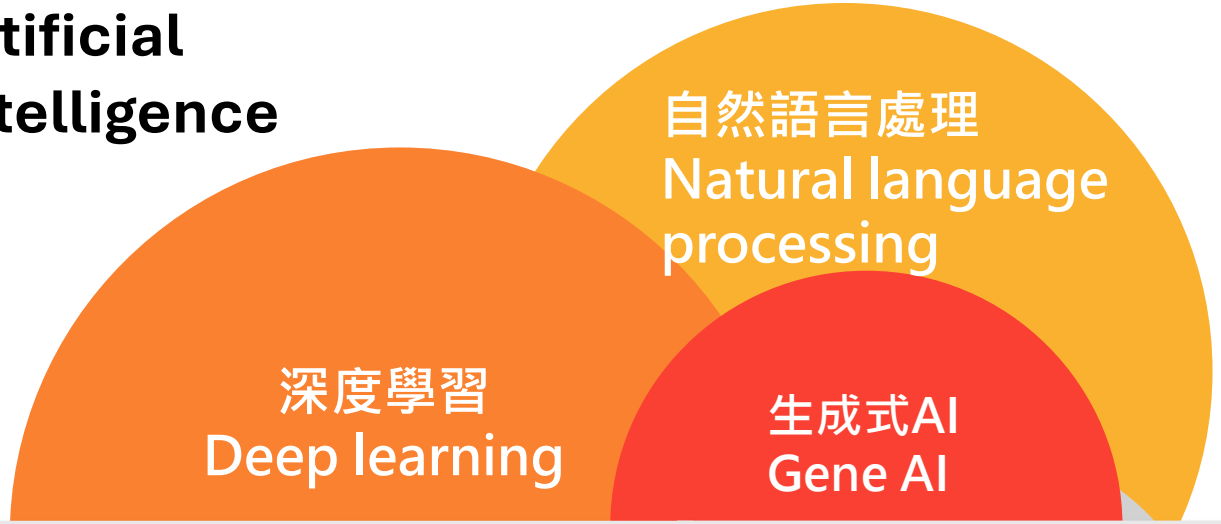
報告撰寫、發表

Elsevier Life Science AI offerings





不同的研究任務需要不同的AI解決方案



"我以為AlphaGo只是基於**計算機率**的**機器**，但當我看到它落子的步法，我改變想法了，它真的有**創意**!"

LEE SEDOL WINNER OF 18 WORLD GO TITLES

兩個深度學習 **AI 的著名案例**:

- **2016 AlphaGO AI** (Google DeepMind) beats human GO professional players with creativity moves.

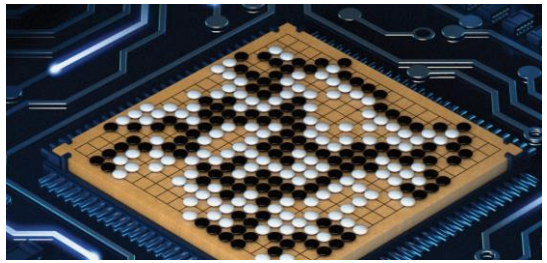


Image acquire from :AlphaGo - Google DeepMind

- 2024 Chemistry Nobel prize go to developers of **AlphaFold AI** that predicts protein structures

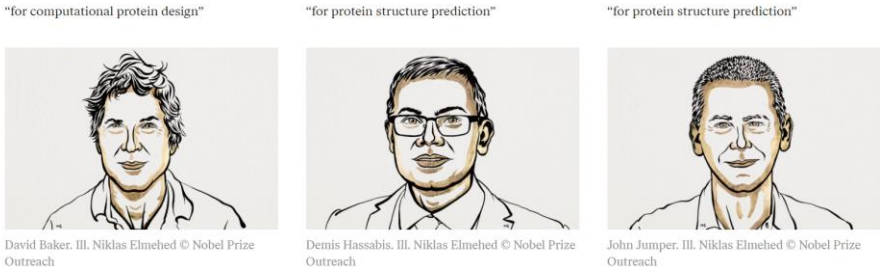
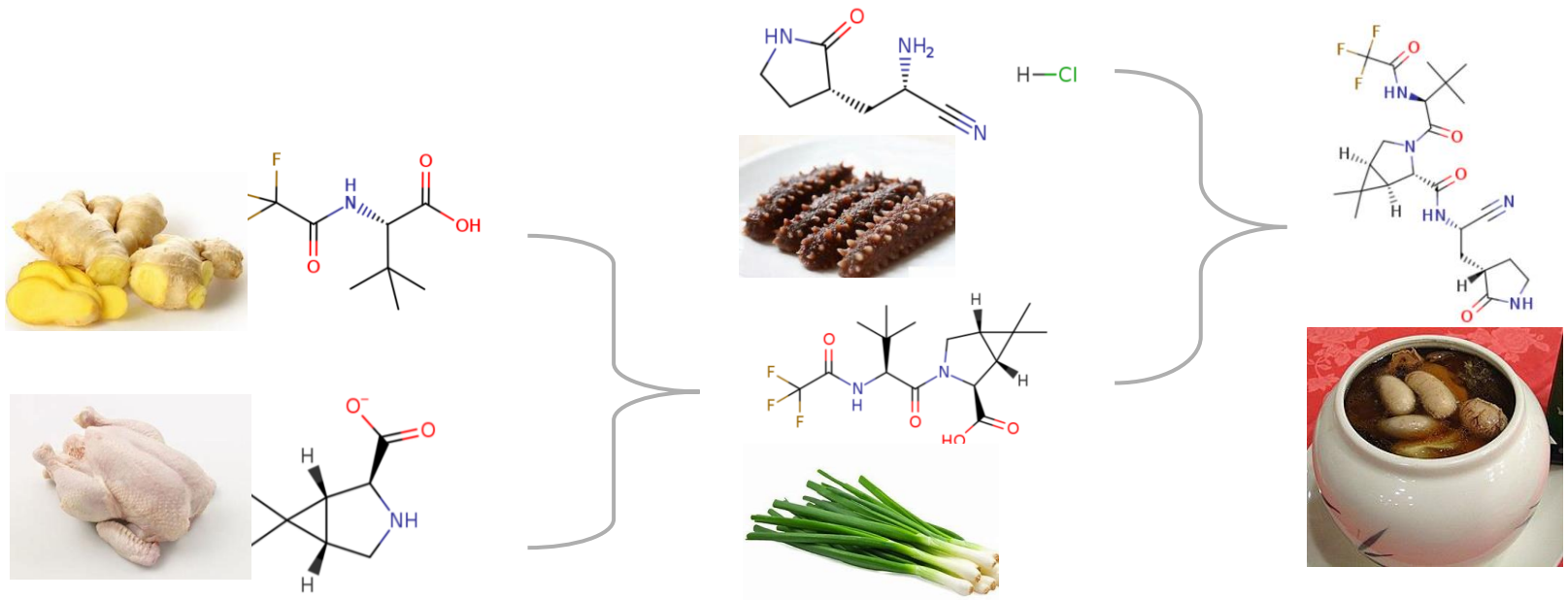


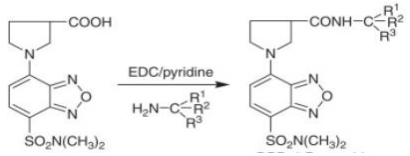
Image acquire from: All Nobel Prizes 2024 - NobelPrize.org

Reaxys AI 是基於上千萬條化學反應式的深度學習AI - 它被設計為化學家提供有創意的合成方法

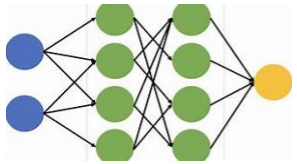
化學逆合成Retrosynthesis的藝術

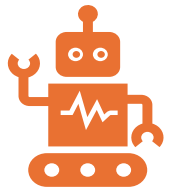


Reactions



Neural network





- 表現得像個化學家、看到一個陌生的化學結構。
- 在10分鐘之類想出數條逆合成的路徑。
- 優勢：不受限於個人經驗、跳脫框架的刺激研究者的思路。

在專業化學家中的Reaxys 逆合成 AI – 蘇黎世大學Prof. Carreira研究團隊

Takeaways, strengths and limitations of Reaxys predictive retrosynthesis

User friendly	The tool is user friendly and intuitive. If you are used to Reaxys this tool is easy to use
Robust routes	Robust predictions for drug like molecules. Chemists do need to review predicted routes and make small adjustments as required
Time saving	The tool provides time savings for designing synthesis routes and getting literature references and ideas for conditions that can be used
Innovative	Some suggested steps are very innovative and can be applied in a human assisted synthesis
Challenges	Challenged by complex molecules e.g. natural products so full routes might not be provided. However, it is possible to get innovative disconnections for some steps.

把專業AI的使用場景從實驗桌..

Research

..搬到教室

Teaching & Learning

導入ReaxysAI在教育中，培養主動學習與批判性思考

在課程的前半段，利用傳統教科書教導Retrosynthesis

在課程的後半段，我們讓學生把實作的未知分子放進去讓Reaxys AI預測，分組討論人腦想出來的合成方法與AI想出來的合成方法的優缺。

Integrating AI into education to foster active learning and critical thinking

Reaxys Predictive Retrosynthesis

Case study: Chung Shan Medical University (Taiwan)

Integrating scenario-based simulation into AI tool learning

Incorporating real-world scenarios, Professor Chu prompts students to immerse themselves as researchers in a pharmaceutical company, simulating the critical drug development journey from conception to synthesis. This approach accommodates diverse levels of comprehension, focus and enthusiasm for organic chemistry among students, making it an effective team effort. Over the initial eight weeks of the course, foundational concepts of organic synthesis reverse engineering are covered using classical retrosynthesis textbooks. Subsequently, students spend four weeks navigating the Reaxys software, engaging in simulations to design novel molecules and conceive artificial synthesis plans. The Reaxys AI tool then enters the picture. The final two to four weeks are devoted to group discussions evaluating the feasibility of the synthesized pathways.

— Professor Chih-Chien Chu
Department of Medical Applied Chemistry, Chung Shan Medical University (Taiwan)

ELSEVIER

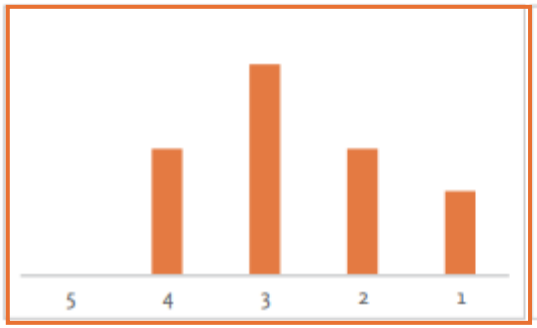
Read the story : Chung Shan Medical University_English_WEB (ctfassets.net)

養成次世代的科學家 – 與AI協作的核心能力

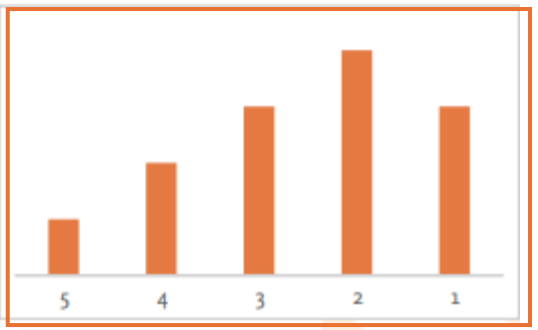
Student presentations on the use of Reaxys AI

80%

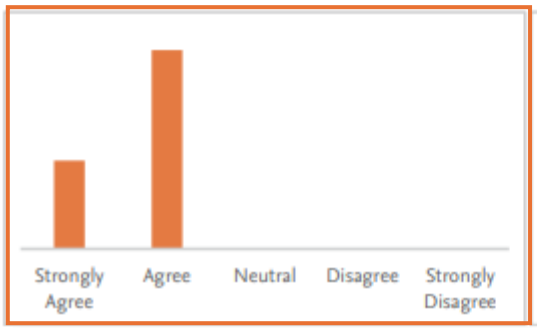
Of students acknowledged heightened interest and motivation in the course



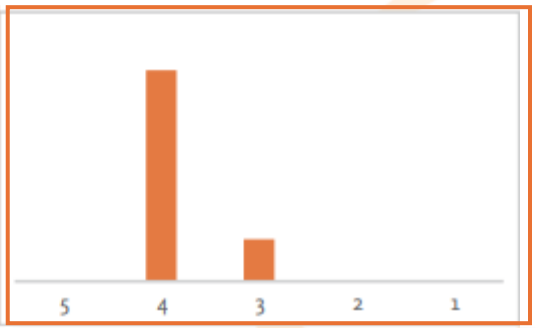
課前自評 – 學生的逆合成能力評估



還沒看見AI的方法 學生自評人腦合成方法



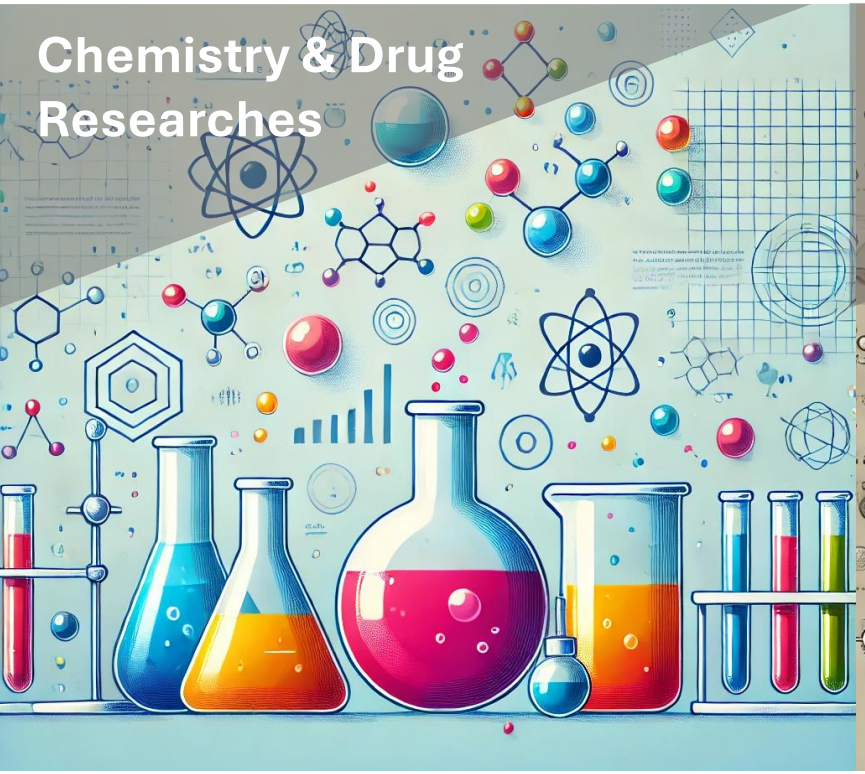
課後自評-學生對於逆合成AI能提升學習



課後自評-學生對於AI推測路徑的信任度

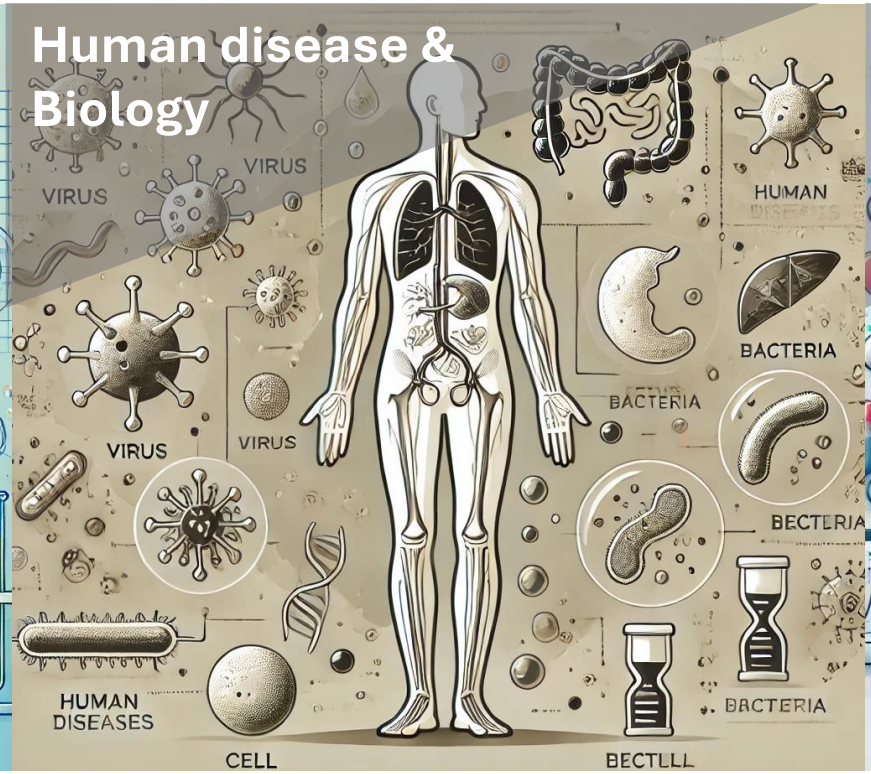
Read the story : [Chung Shan Medical University_English_WEB (ctfassets.net)]

Elsevier Life Science AI portfolio



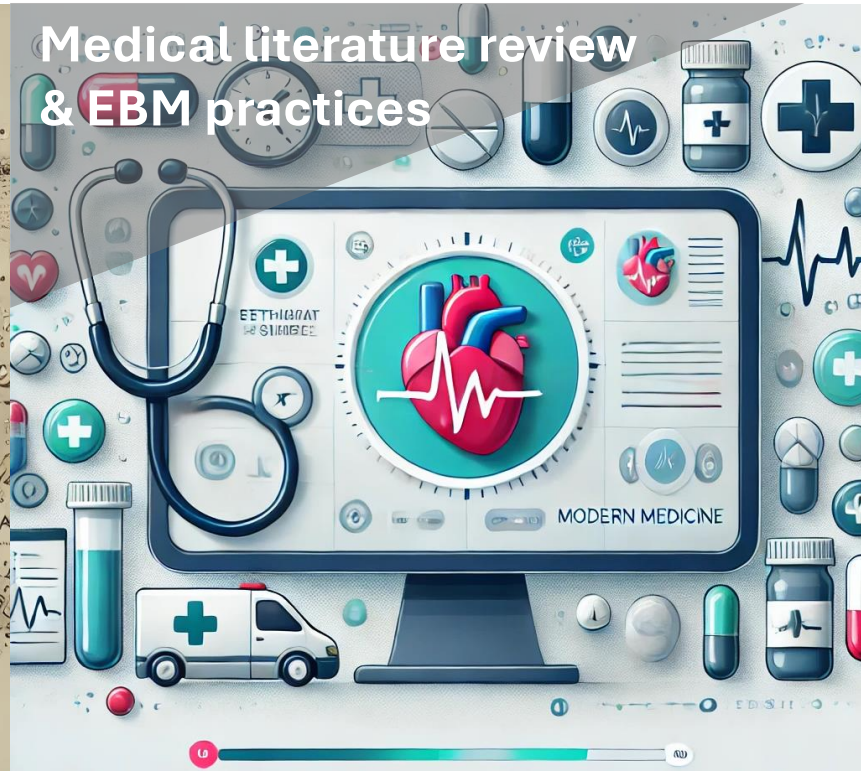
Reaxys predictive RT

- Deep learning
- 深入研究實驗階段的創意百寶箱
- 適合理學院、藥學院、工學院



EmBiology

- Natural language processing
- 互動式人類疾病知識圖譜，
- 適合醫學院、生命科學院、新藥研究團隊、轉譯中心



Embase AI

- Generative AI
- 2025推出 敬請期待