

## 摘要

隨著電腦資訊的迅速進步，資訊取得的方式有了巨大的改變。過去資料的取得往往都是從教科書上或是科學家的著作上擷取。過去的研究者在圖書館尋找資料時，必須依照書籍的領域、學術著作或是一般著作、期刊或是研究論文、類別、科目開始找起。過去的搜尋方式過程繁複，十分耗費時間。隨著科技的進步，實體書逐漸式微，有著逐漸被電子書所取代的趨勢。電腦的資訊處理功能日益強大，研究者能夠藉由輸入關鍵字，便能快速找到想要的書籍。因此，我們希望建立一個方便使用者搜尋資料的網路資料庫，來幫助研究者節省尋找資料的時間。

過去疾病相關的資料庫還不是很多，而更多的是分子生物資料庫。由於醫學上的需要以及資料取得的方便性，目前的疾病相關資料庫建立者大多是經由與醫院合作，資料庫的資料為了方便醫師查詢，建立的內容大多偏向疾病症狀和治療方式。對於研究者來說，許多研究疾病的研究者更需要的是造成疾病的源頭、引發疾病的蛋白質相關資訊，例如序列和參與路徑。我們希望提供一個能夠查詢與疾病有關的蛋白質資料及藥物的資料庫。我們從現有的各大蛋白質資料庫中尋找其關聯性。我們以 **The Protein Data Bank (PDB)** 的蛋白質結構及序列為主體，並提供 **KEGG** 的蛋白質代謝路徑。我們同時也希望為疾病建立針對疾病的藥物資料庫，接著從廣泛的文獻及大型資料庫蒐集資料，例如 **PubChem**、**KEGG**、**DrugBank**、**Therapeutic Target Database**、**LigandBox**、**Drugs.com** 及 **Wikipedia**。

我們將蒐集來的資料，依照我們希望提供的功能做分類及整理，大致上分作藥物的結構及其化合物相關資訊、藥物的藥效、藥物的結合情形，以及參考文獻。我們建立資料庫是希望一方面能協助研究者更加快速且方便進行藥物設計，另一方面希望加速生醫科學的發展。

# Abstract

With the rapid advances in computer and information, the acquired way of information it has drastic changes. In the past, scientists obtain information are often capture from the writings of the scientists or textbook. Previous researchers search for information in library who should be refer to the subject, academic works, journals, research papers to find the data we need. The way for search is complicated and time-consuming in the past. With the advancement of technology, e-books have a tendency to replace real book gradually. Processing of computer information become more and more powerful. Researchers will be able to find the required information quickly by internet. Therefore, we want to establish a convenience web database for users to find some data they want easily.

Disease-related databases are few in the past. Due to the need and convenience of the medical information obtained. Most of current disease-related databases set up via cooperation with the hospital. For the purpose of convenience of the physician queries, information of database established to disease symptoms and treatment. Information of the structure of the disease, caused by protein-related diseases are more important to many researchers who study diseases, such as the sequence and their pathways. We want to build a database including disease-associate proteins and

drugs. We are looking for the relationship between databases we refer to, and we built a list of drugs as index of drug. SDRPD is based on protein and structure of pdb.list, and then we built the page of protein respectively. At the same time, we built the page of drug. The source data of drug database which form PubChem, KEGG, DrugBank, Therapeutic Target Database, LigandBox, Drugs.com and Wikipedia.

According to function and classification, we collect the information for drug and separated them by classification, like the information of the drug, the structure of the drug, the pharmacology, the data of binding, and literature. We want to establish a database which not only provide some help to researchers for drug design quickly and conveniently, but also make the development of biotechnology science speed up.

