

行政院國家科學委員會專題研究計畫 成果報告

結構生物資訊核心設施 I (子計畫十)

計畫類別：整合型計畫

計畫編號：NSC92-3112-B-009-003-Y

執行期間：92年07月01日至93年12月31日

執行單位：國立交通大學生物科技研究所

計畫主持人：黃鎮剛

共同主持人：呂平江

報告類型：完整報告

報告附件：出席國際會議研究心得報告及發表論文

處理方式：本計畫可公開查詢

中 華 民 國 94 年 3 月 28 日

- 一、計畫名稱：臺灣生物資訊學-結構生物資訊核心
- 二、計畫編號：92-3112-B-009-003-Y
- 三、計畫主持人：黃鎮剛 / 呂平江
- 四、經費預算：3,500,000
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- 建立一個整合性結構分析工具，結合公共分析工具(CE, SSAP, MODELER, Predator, , ...)與我們所發展的分析工具（如支鍊預測工具、蛋白質分類工具、蛋白質結合子 docking 系統。）
- 建立一個整合性蛋白質結構與分類資料庫，結合公共資料庫(PDB, SCOP, CATH,FSSP,DSSP, SWISSPROT, ...)與我們所構建的加值資料庫（如蛋白質結構亂度資料庫 StEQ，雙硫鍵類型與結構料庫 SSDB，等）
- 發展自動化管路分析系統，由基因體序列預測及分類蛋白質 3D 結構

The structure bioinformatics core is available from <http://bioinfo.life.nctu.edu.tw/index.php>. The snapshot of the webpage is shown in Fig. 1.

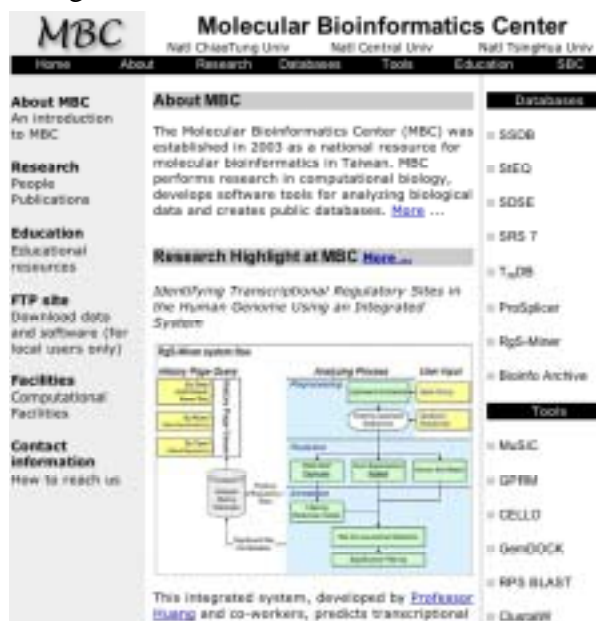


Fig. 1 the snapshot of the structure bioinformatics core
The currently available bioinformatics services:

CELLO: subcellular localization prediction server (Fig.2)

Website: <http://cello.life.nctu.edu.tw>

Usage: CELLO presently handles protein sequences from Gram-negative bacteria and Eukaryotic proteins only for version 2.1. We provide other prediction services for other organisms later.

Reference: Yu CS, Lin CJ, Hwang JK, Predicting Subcellular Localization of Proteins For Gram-Negative Bacteria by Support Vector Machines Based on n-Peptide Compositions. *Protein Science* (2004), 13, 1402-1406

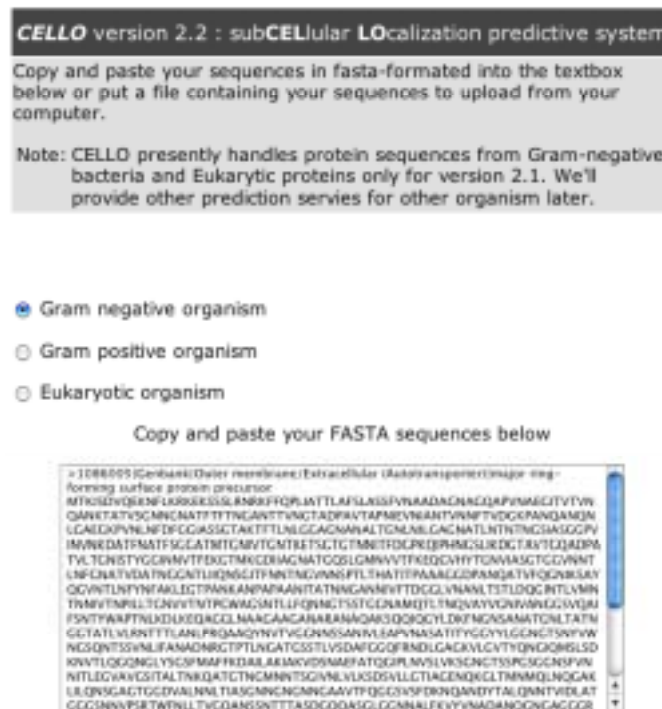


Fig. 2 The snapshot of the homepage of CELLO

SSDB: Database of disulfide patterns (Fig.3)

Website: <http://e106.life.nctu.edu.tw/~ssbond/>

Usage: The disulfide bonding patterns can be used to discriminate structure similarity. Our method, based on the hierarchical clustering scheme, is applicable to proteins with two or more disulfide bonds and is able to detect the structural similarities of proteins of low sequence identities (<25%). Our results show the surprisingly close relationship between disulfide-bonding patterns and proteins structures.

Reference: C-C. Chuang, C-Y Chen, J.-M. Yang, P.-C. Lyu, J.-K. Hwang, Relationship between protein structures and disulfide-bonding patterns. *Proteins: Structure, Function and Genetics* (2003), 53, 1-5.

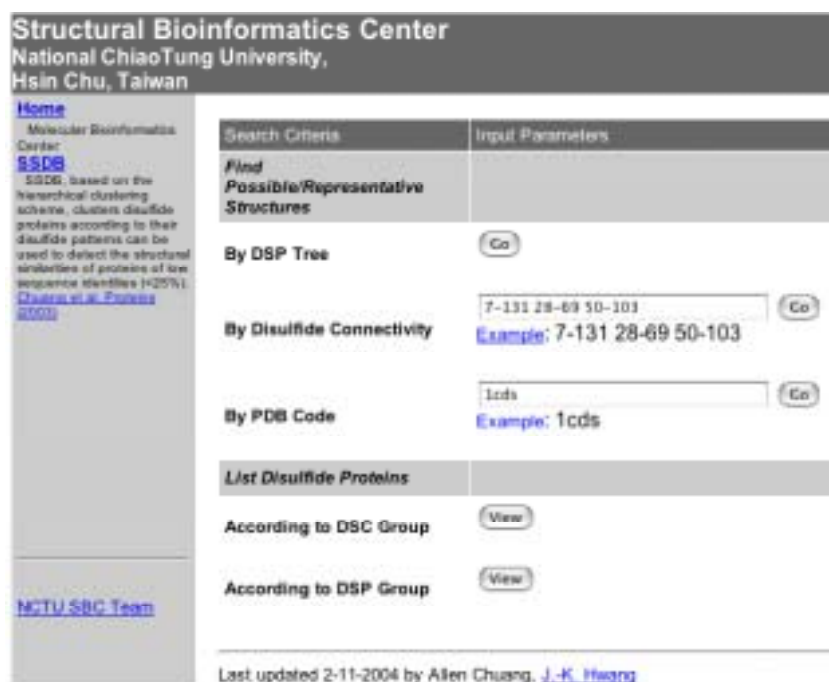


Fig. 3 The snapshot of the homepage of SSDB

SDSE: Sequence derived structural entropy (Fig.4)

Website: <http://sdse.life.nctu.edu.tw/>

Usage: To compute the structural entropy directly from protein sequences. The structural entropy is useful in identifying locally stable sequence fragment and in assisting protein structure design.

Reference: (1) Chan CC, Liang HK, Hsiao NW, Ko MT, Lyu PC, Hwang JK. The relationship between local structural entropy and protein thermostability. *Proteins: Structure, Function and Bioinformatics* (2004) 57, 684-691. (2) Liang HK, Huang CM, Ko MT, Hwang JK. The Amino Acid-Coupling Patterns in Thermophilic Proteins. *Proteins: Structure, Function and Bioinformatics* (2005), forthcoming.

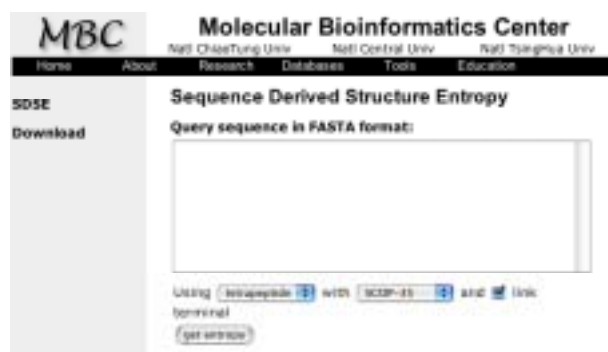


Fig. 4 The snapshot of the homepage of SDSE

PS²: Protein Structure Prediction Server (Fig.5)

Website: <http://ps2.life.nctu.edu.tw/>

Usage: Automated comparative protein structure prediction server using consensus sequence-profile alignment.

Reference: Chen *et al.* submitted.

Fig. 5 The snapshot of the homepage of PS2

The mirror sites

We have also provided the mirror site services: PDB mirror site:

<http://pdb.life.nthu.edu.tw/>, SCOP mirror site: <http://scop.life.nthu.edu.tw/> ; The

PredictProtein server: <http://biobug.life.nthu.edu.tw/predictprotein/index2.html>

(一) 研究成果

詳細項目(含智財、技轉及國際合作項目)請另填“國家型計畫成果檔”

| 類別 | 已發表論文 | 準備中/投稿中論文 | 研討會發表之論文 | 專利 | 專利(申請中) | 技術轉移 |
|----|-------|-----------|----------|----|---------|------|
| 篇數 | 2 | 1 | 3 | 0 | | |