Bioinformatics and Drug Design
Research Group

Main Goals of BIDD:

- Development of Bioinformatics databases and software
- Development of Computer-aided drug design methods and software
- Tool development and mechanistic study of traditional Chinese medicine

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BIDD group was set up in 1997 aimed at development of tools for bioinformatics, computer-aided drug design, and study of traditional Chinese medicine. BIDD consists of 4 research staffs, 7 PhD and 4 MSc students. It is equipped with state-of-the-art computers (IBM Clusters, HP and SGI workstations), PCs, and bioinformatics software (SYBYL, Insight II, DS Modeling, Gaussian, and own developed INVDOCK, SVMProt, Pearls, MoViES).

Since 1997, BIDD has published 47 papers in SCI-listed scientific journals, obtained 1 US patent and filed 2 US patents, developed 3 bioinformatics and drug-design software packages, developed 6 bioinformatics databases with over 25,000 visits. Some US companies have expressed strong interest in our databases and tools.

BIDD’s research on traditional Chinese medicine has led to 1 US patent filing and 3 databases. Our works were published in the SCI highest ranked natural product and traditional medicine journals, and attracted media attention in Singapore. Channel U’s News at Ten and Lian He Zao Bao, the largest Chinese language newspaper in Singapore, reported our research on Aug 18 and 19 2002. Our technology has attracted interest from several investors and herbal medicine companies.
One paper has been extensively cited by in review journals including Current Opinion in Chemical Biology (2 papers), Current Opinion in Drug Discovery and Development (2 papers), Current Pharmaceutical Design (1 paper), Current Protein and Peptide Science (1 paper), Mol Biol Rep (1 paper).

Comments from scientific journal reviewers:

“This paper describes using Support Vector Machines method to predict functional families, the 46 Enzyme families. For this large number of families, the prediction is a difficult problem. The high accuracy obtained in the prediction is good. In this direction, the paper made a timely contribution.”

“The manuscript describes an application of the newly developed computer software INVDOCK to screen for bioactive compounds in Chinese medicinal plants. Considering the recent interests of the Chinese medicinal plants, proteinomics and gene therapy, the appearance of this screening method appears timely and appropriate.”

“It is admirable that the authors have undertaken to assess the usefulness of SVM-Prot with viral proteins. Insights provided by such tools would be of great value to virologists.”
Selected publications:

**Reviews:**


**Bioinformatics**


**Computer aided drug design**


Selected publications:

**Herbal medicine**


**Computational biology and Biophysics**


Software developed:


Bioinformatics databases developed:


Traditional Chinese medicine research tools developed:

- Traditional Chinese medicine information database
- Herbal ingredient and content database
- Natural product effect and consumption info system
- Traditional Chinese medicine recipe prediction and validation system

BIDD technology in herbal medicine had been selected as one of the three patents from NUS to present at “Global Entrepolis @ Singapore”, an Enterprise Exchange Expo of Singapore 2003 (http://www.globalentrepolis.com).
Inventions:

- Method and apparatus for computer automated detection of protein and nucleic acid targets of a chemical compound. United States patent US 6,519,611 B1
- Method and information system for the benefits and consumption of natural products, U.S. Provisional Application No. 60/512,479.

Several US, European, and Singapore companies have licensed or in talk with of BIDD about BIDD's technologies
国大应用电脑分析
以求提高中草药疗效

吴文华 报道

新加坡国立大学正在以电脑为工具，
发展新药和提高现有药物的疗效。

这包括计算机分析药物成分、对药物
副作用及毒性进行研究。

国大研究科学家发现，将电脑
用于中草药的分析和研究工作，
未来中草药的药效将能更早地被
发现，并可以更有效地用于临床研究。

中药治疗的方法和疗效都
处于不断的改革之中，但计算机
在中草药的分析和研究中也
扮演了重要的角色。

国大研究科学家发现，可借
助电脑对中草药成分进行分
析，并将其与现有的药物成分
相比，以提高中草药的疗效。

国大应用电脑分析
以求提高中草药疗效

国大计算科学系师生
合作设立五个数据库

有关的五个数据库是：
医药数据库、中草药成分数据库，
治疗目标数据库、副作用数据库和
中草药成分数据库。

治疗数据库的主要功能是收集和分析
药物成分，以作为中草药研究的参考。
副作用数据库则收集了各种药物的副
作用信息，以供研究者参考。

中草药成分数据库则收集了各种中
草药的成分，包括其化学成分和药
理作用。

治疗目标数据库则收集了各种
治疗目标的成分，包括其化学成分和药
理作用。

此外，国大还设立了中草药成分数据库，
该数据库则收集了各种中草药的成分，包括
其化学成分和药理作用。

国大研究人员希望，这五个数据库
能为中草药的研究提供更准确的
数据，以提高中草药的疗效。
Dr. Chen obtained his Ph.D. in statistical physics in the theoretical physics group of the Department of Mathematics UMIST UK in 1989. He obtained his M.Sc. in theoretical physics in the Institute of Theoretical Physics Chinese Academy of Sciences China in 1985. He got his BSc in applied physics in the Department of Physics of Dalian University of Technology China in 1982.

He began his research in biophysics and computational biology in the biophysics group of the Department of Physics of Purdue University USA in 1989 as a postdoctoral research associate. Since then he has published over 70 papers in international refereed journals, obtained 1 and filed 2 US patents, developed 3 bioinformatics and drug design software packages and 6 bioinformatics databases. He worked at ISIS pharmaceuticals USA using computer modeling to facilitate the design of antisense drugs. He joined National University of Singapore in 1997. He has been maintaining close collaborations with a number of companies in pharmaceutical industry and several Universities in USA, Japan, Singapore and China.

He has been a member of Singapore Traditional Chinese Medicine Taskforce and the committees for the development of National University of Singapore’s life science, medicinal chemistry, bioengineering programs. His research achievement is recognized by being selected in the 7th edition of Marquis Who’s Who in Science and Engineering.
Dr. Cao ZhiWei

Dr. Cao ZhiWei is an expert in molecular modeling of protein dynamics, informatics of medicinal herbs, and computational study of pharmacokinetic properties of drugs. Her research in molecular modeling of proteins has led to 3 publications in high-ranking bio-modeling journals. Her work on medicinal herbs has resulted in 1 US patent filed and 3 herbal databases developed. Her recent work on pharmacokinetics of drugs has led to 1 paper submitted and 2 others in preparation. She obtained her PhD in Oct 2003.

Dr. Ji ZhiLiang

Dr. Ji ZhiLiang is a highly productive and promising scientist. He has made major contributions in bioinformatics software development, data mining, database development, and drug property research. His achievement is best reflected by his publication of 8 papers in high-ranking bioinformatics and pharmacology journals. He is the leading developer of 2 bioinformatics databases and a major contributor of 3 other bioinformatics databases.

Mr. Chen Xin

Mr. Chen Xin is a bright and qualified young researcher with good research record in the application of machine learning methods in biology, mechanistic study of medicinal plants, and bioinformatics database development. He has 9 publications in high-ranking bioinformatics, natural product, and pharmacology journals. He is the leading developer of 2 bioinformatics databases and a major contributor of 3 other bioinformatics databases. His PhD thesis is currently under review and he is expected to get his PhD soon.
Dr. Cai CongZhong

Dr. Cai CongZhong is an expert in the application of machine learning methods in biology. After joining BIDD for only two years, he has played a central role in the development of bioinformatics software at BIDD. He has also used machine-learning methods for studying the function of novel proteins in real-case studies such as SARS virus and for the analysis of traditional Chinese medicine recipes. His excellent research work has led to 7 publications in high-ranking journals in just two years.

Dr. Xue Ying

Dr. Xue Ying is an experienced physical chemist using theoretical methods to derive descriptors of structural and physicochemical properties of molecules, which are essential component in computer-aided drug design methods. Her excellent work has led to two papers submitted and 2 manuscripts in preparation.

Mr. Yap ChunWei

Mr. Yap ChunWei is a promising young researcher with good knowledge in pharmacology and commanding skills in computer-aided drug design methods. He has been leading the effort for developing computational tools for prediction of pharmacokinetic and toxicological properties of drugs. He has also been involved in the development of bioinformatics databases. So far, he has 1 publication, 3 papers submitted, and 2 manuscripts in preparation.

Mr. Wang JiFeng

Mr. Wang JiFeng has played a central role in the development of traditional Chinese medicine database and investigation tools at BIDD. He is leading the study of the mechanism of medicinal herbs and Chinese medicine recipes. He has also contributed to the development of two bioinformatics databases and in the study of pharmacokinetic properties of drugs. He has 2 publications, 1 paper submitted and 3 manuscripts in preparation.
Ms. Sun Li Zhi

Ms. Sun Lizhi is a dedicated researcher with good record in bioinformatics database development and in the study of pharmacokinetic properties of drugs. She led the development of one bioinformatics database and played important role in the development of another database. Her effort has led to 4 publications in high ranking bioinformatics and pharmacology journals. She also has 1 paper submitted and 2 manuscripts in preparation. She obtained her MSc degree in April 2003.

Mr. Han LianYi

Mr. Han LianYi is a very bright and promising PhD student at BIDD. He has quickly learned computational skills and biological knowledge needed to develop bioinformatics and pharmainformatics software. After joining BIDD for slightly more than a year, he has become a major contributor of BIDD’s bioinformatics software development and has been leading the effort of using bioinformatics software for the prediction of the function of novel proteins in real-case studies such as SARS virus. He is currently the leading developer of BIDD’s pharmainformatics software. So far, he has 4 publications and 2 accepted papers in top ranking bioinformatics and pharmacology journals. Moreover, he has 4 other papers submitted for publication. This is a substantial achievement for a second-year PhD student.

Miss Zheng ChanJuan

As a second-year PhD student, Miss Zheng ChanJuan has already become an expert in pharmainformatics. She is leading the effort for comprehensive study and understanding of therapeutic targets and related biological pathways. She is a major contributor for the development of therapeutic target database and the leading developer of therapeutically relevant multiple pathways database. She has applied statistical methods to analyze therapeutic targets. She has also been involved in the development of other bioinformatics databases. Her effort has led to 3 publications and 2 papers submitted in high-ranking bioinformatics and pharmacology journals.