II. **Major research achievements and contributions, including patents or technical transfers.**

Our research focuses on computer-aided drug discovery and structural bioinformatics. We have developed a molecular docking tool (namely GEMDOCK) which is one of wide-used docking tools in the world. We cooperated with 10 research teams on diverse drug targets and experimental results demonstrate that our tools are useful for discovering lead compounds (e.g. dengue virus envelop protein, skimate kinases, and influenza virus neuraminidase), identifying functional sites (e.g. ß-lactoglobulin), and protein engineering (e.g. endo-chitosanase to exo-chitosanase). We published 7 papers on top journals in these fields and these papers were cited over 70 times since 2004. We get the 2007 National Innovation Award due to the achievement of *i*GEMDOCK which is graphic interface of GEMODCK. The *i*GEMDOCK was downloaded over 1,200 times and was used for education.

For structural bioinformatics, we have achieved successful results on protein structure prediction (PS^2), fast protein structure search (3D-BLAST), and structural protein-protein interaction networks (3D-partner). These results were published on the top journals (such as *Nucleic Acids Research* and *Genome Biology*) in these fields. A particularly exciting success is the development of the 3D-BLAST which is as fast as BLAST and has the features of BLAST (e.g. robust statistical basis, and effective and reliable search capabilities) for protein sequence search. 3D-BLAST is the first tool to search large protein structures (> 30000) within 3 seconds in the world. We believe that 3D-BLAST will be the most popular tool to elucidate the structural homology by large protein structure database search. The number of accessing this tool exceeds 5,100 from 44 countries and our papers were cited over 13 times since 2007. **All of these achievements (e.g. GEMDOCK and 3D-BLAST) are completed in Taiwan**. The achievements and contributions of some representative papers are summarized as follows:

Fast protein structure database search (representative papers 1~3)

Representative paper 1: **J.-M. Yang*** and C.-H. Tung, "Protein structure database search and evolutionary classification," *Nucleic Acids Research*, vol. 34, pp. 3646-3659, 2006. **(IF:6.954**; **Times Cited: 8**; Ranking 29/263 in BIOCHEMISTRY & MOLECULAR BIOLOGY**)**

Representative paper 2:C.-H. Tung, J.-W. Huang and **J.-M. Yang*,** "Kappa-alpha plot derived structural alphabet and BLOSUM-like substitution matrix for fast protein structure database search," *Genome Biology*, vol. 8, pp. R31.1-R31.16, 2007. **(IF: 6.589;** Times Cited: 2; Ranking 7/138 in BIOTECHNOLOGY & APPLIED MICROBIOLOGY**)**

Representative paper 3: C.-H. Tung and **J.-M. Yang*,** "fastSCOP: a fast web server for recognizing protein structural domains and SCOP superfamilies," *Nucleic Acids Research*, pp. W438-W443, 2007. **(IF: 6.954;** Times Cited: 3; Ranking 29/263 in BIOCHEMISTRY & MOLECULAR BIOLOGY**)**

BLAST is the most popular tool for protein function annotations by searching sequence databases. As more protein structures (e.g. 7273 structures are determined in 2007) become available and structural genomics efforts provide structural models in a genome-wide strategy, there is a growing need for fast and accurate methods, which own the advantages of BLAST, for discovering homologous proteins and evolutionary classifications of newly determined structures. In the representative papers 1 and 2**,** we have developed 3D-BLAST to address these issues. For protein structure database search, 3D-BLAST is the first tool that is as fast as BLAST and has the advantages of BLAST (e.g. a robust statistical basis, effective search and reliable database search capabilities). 3D-BLAST searches over 30,000 protein structures within 3 seconds and is ~20,000 times faster than two popular tools, CE and DALI. These research results are published in *Nucleic Acids Research* (IF:6.954) and *Genome Biology* (IF:6.589). Both papers are selected as the hot papers in the respective journals. This tool is available at http://3d-blast.life.nctu.edu.tw. In addition, the evolutionary classification databases, such as SCOP and

CATH, are valuable resources for understanding protein functions, structural similarity and evolutionary relationships. These two databases are updated intermittently (about six months) using manual and semi-automated methods; therefore, they cannot afford the annotations of new determined structures. To address this issue (in the representative paper 3**),** we developed an automated server (namely fastSCOP), which integrates 3D-BLAST and a detailed structural alignment tool, to recognize SCOP domains and SCOP superfamilies of a query structure within several seconds. 3D-BLAST and fastSCOP are useful for solving structure–function gap and producing manually tuned classification databases.

These two tools were accessed over 5,100 times from 44 countries from 2006. We believe that the 3D-BLAST a breakthrough tool and will be one of the most popular protocols for protein structure database search. These results have been widely discussed and were cited over 13 times since 2007. Some citation papers are listed as follows:

1. Alves, R., E. Vilaprinyo, and A. Sorribas. 2008. *Current Bioinformatics* **3:** 98-129.
2. Aung, Z. and K.L. Tan. 2007. *Drug Discovery Today* **12:** 732-739.
3. Dong, Q.W., X.L. Wang, and L. Lin. 2008. *Proteins-Structure Function and Bioinformatics* **72:** 353-366.
4. Giuseppe, P.O., F.O. Neves, A.L.T.O. Nascimento, and B.G. Guimaraes. 2008. *Journal of Structural Biology* **163:** 53-60.
5. Hetenyi, C., U. Maran, A.T. Garcia-Sosa, and M. Karelson. 2007. *Bioinformatics* **23:** 2678-2685.
6. Offmann, B., M. Tyagi, and A.G. de Brevern. 2007. *Current Bioinformatics* **2:** 165-202.
7. Tyagi, M., A.G. De Brevern, N. Srinivasan, and B. Offmann. 2008. *Proteins-Structure Function and Bioinformatics* **71:** 920-937.
8. Wu, F.M., J.H. Zhang, J.P. Sun, H. H.D., P. Ji, W.S. Chu, M.J. Yu, F.F. Yang, Z.Y. Wu, J.H. Wu, and Y.Y. Shi. 2008. *Proteins-Structure Function and Bioinformatics* **71:** 514-518.

Computer-aided drug discovery (representative papers 4 and 5)

Representative paper 4: **J.-M. Yang*** and C.-C. Chen, "GEMDOCK: A generic evolutionary method for molecular docking," *Proteins: Structure, Function, and Bioinformatics*, vol. 55, pp. 288-304, 2004. (**IF: 3.354**, **Times Cited: 28;** Ranking 18/69 in BIOPHYSICS)

Representative paper 5: **J.-M. Yang*** Y.-F. Chen, T.-W. Shen, B. S. Kristal, and D. F. Hsu*, "Consensus scoring criteria for improving enrichment in virtual screening," *Journal of Chemical Information and Modeling*, vol. 45, pp. 1134-1146, 2005. (**IF: 2.986; Times Cited: 25**; Ranking 6/92 in COMPUTER SCIENCE, INFORMATION SYSTEMS)

Practical application papers:

1. **J.-M. Yang*** and T.-W. Shen, "A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators," *Proteins: Structure, Function, and Bioinformatics*, vol. 59, pp. 205-220, 2005. (**IF: 3.354, Times Cited: 13;** Ranking 18/69 in BIOPHYSICS)
2. **J.-M. Yang*** "Development and evaluation of a generic evolutionary method for protein-ligand docking, " *Journal of Computational Chemistry*, vol. 25, pp. 843-857, 2004. (**IF: 4.297;** Ranking 17/127 in CHEMISTRY, MULTIDISCIPLINARY)
3. **[**flaviviruses envelop protein**]** **J.-M. Yang**, Y.-F. Chen, Y.-Y. Tu, K.-R. Yen, and Y.-L. Yang***,** "Combinatorial computation approaches identifying tetracycline derivates as flaviviruses inhibitors," *PLoS ONE*, pp. e428, 2007.
4. [ß-lactoglobulin] M.-C. Yang, H.-H. Guan, M.-Y. Liu, Y.-H. Lin, **J.-M. Yang**, W.-L. Chen, C.-J. Chen, and Simon J. T. Mao*, "Crystal structure of a secondary vitamin D_3 binding site of milk ß-lactoglobulin," *Proteins: Structure, Function, and Bioinformatics*, vol. 71, pp. 1197-1210, 2008. (**IF: 3.354;** Ranking 18/69 in BIOPHYSICS)
5. [endo-chitosanase to an exo-chitosanase] Y.Y. Yao, K.L. Shrestha, Y.J. Wu, H.J. Tasi, C.C. Chen, **J.-M. Yang**, A. Ando, C.Y. Cheng, Y.K. Li*, "Structural simulation and protein engineering to convert an endo-chitosanase to an exo-chitosanase," *Protein Engineering Design & Selection*, 2008, vol. 21, pp. 561-566. (**IF: 2.662;** Ranking 43/138 in BIOTECHNOLOGY & APPLIED MICROBIOLOGY)
6. [influenza virus neuraminidase] H.-C. Hung, C.-P. Tseng, **J.-M Yang**, Y.-W. Ju, S.-N. Tseng, Y.-S. Chao, H.-P. Hsieh, S.-R. Shih, J.T.-A. Hsu*, "Aurintricarboxylic acid inhibits influenza virus neuraminidase," *Antiviral Research*, 2008, in revision (**IF: 3.358;** Ranking 50/208 in PHARMACOLOGY & PHARMACY)
7. [ß-lactoglobulin] M.-C. Yang, H.-H. Guan, **J.-M. Yang**, C.-N. Ko**,** M.-Y. Liu, Y.-H. Lin, C.-J. Chen*, and Simon J. T. Mao*, " Rational design for crystallization of ß-Lactoglobulin and vitamin D3 complex: Reveal of a secondary binding site," *Crystal Growth & Design*, in revision (**IF: 4.046;** Ranking 1/25 in CRYSTALLOGRAPHY)

Structure-based virtual screening, pharmacophore model, post-screening analysis, and QSAR are

important tasks in drug discovery. We have developed a graphical environment (called *i*GEMDOCK) to integrate our in-house tools (e.g. GEMDOK) for each task. In the representative paper 4, we have developed the GEMDOCK tool for molecular recognition and virtual screening using our generic evolutionary method. This tool was evaluated over 300 protein-ligand complexes and four virtual screening targets. Experimental results show that GEMDOCK outperformed three popular tools, including DOCK, GOLD, and FlexX. This paper was cited over 28 times and the GEMDOCK tool was downloaded ~1200 times since 2004. Currently, the tool is one of population tools for virtual screening. GEMDOCK has been successfully applied to identify inhibitors for some target proteins, such as flaviviruses envelop protein (Professor Yang, YL in NCTU), influenza virus neuraminidases (Professor Hsu, TA in NHRI), helicobacter pylori shikimate kinase (Professor Wang, WC in NTHU), sulfotransferase and imidase (Professor Yang, YS in NCTU) and geranylgeranyl pyrophosphate synthase (Professor Liang PH, in Sinica). GEMDOCK was successful used to identify protein binding sites (e.g. beta-lactoglobulin with Professor Mao in NCTU) and to design functional sites (e.g. endo-chitosanase to an exo-chitosanase with Professor Li, YK in NCTU). Some of these results have been published in top journals.

The major weakness of virtual screening – the inability to consistently identify true positives (leads) - is likely due to our incomplete understanding of the chemistry involved in ligand binding and the subsequently imprecise scoring algorithms. We also enhanced and modified GEMDOCK by considering pharmacological preferences (pharmacological interactions and ligand preferences) to simultaneously serve as the scoring function. We demonstrate that this pharmacological model can interpret protein-ligand interacting mechanisms and improve screening accuracy. In addition, it has been demonstrated that combining multiple scoring functions (consensus scoring) improves enrichment of true positives. However, previous efforts at consensus scoring have largely focused on empirical results, but they are yet to provide theoretical analysis that gives insight into real features of combinations and data fusion for virtual screening. In the representative paper 5, we are the first team to establish a potential theoretical basis and demonstrate that combining multiple scoring functions improves enrichment of true positives only if (a) each of the individual scoring functions has relatively high performance, and (b) the individual scoring functions are distinctive. This paper was cited over 25 times since 2005.

We have published over 7 papers in the top journals in these fields. These papers were cited over 70 times since 2004. Some citation papers are listed as follows:

1. Celik, L., S. Sinning, K. Severinsen, C.G. Hansen, M.S. Moller, M. Bols, O. Wiborg, and B. Schiott. 2008. ***Journal of the American Chemical Society*** **130:** 3853-3865.
2. Coupez, B. and R.A. Lewis. 2006. ***Current Medicinal Chemistry*** **13:** 2995-3003.
3. Feher, M. 2006. ***Drug Discovery Today*** **11:** 421-428.
4. Joseph-McCarthy, D., J.C. Baber, E. Feyfant, D.C. Thompson, and C. Humblet. 2007. ***Current Opinion in Drug Discovery & Development*** **10:** 264-274.
5. Knox, A.J.S., M.J. Meegan, V. Sobolev, D. Frost, D.M. Zisterer, D.C. Williams, and D.G. Lloyd. 2007. ***Journal of Medicinal Chemistry*** **50:** 5301-5310.
6. Li, Z. and T. Lazaridis. 2007. ***Physical Chemistry Chemical Physics*** **9:** 573-581.
7. Radestock, S., M. Bohm, and H. Gohlke. 2005. ***Journal of Medicinal Chemistry*** **48:** 5466-5479.
8. Robeits, B.C. and R.L. Mancera. 2008. ***Journal of Chemical Information and Modeling*** **48:** 397-408.
9. Seifert, M.H.J., J. Kraus, and B. Kramer. 2007. ***Current Opinion in Drug Discovery & Development*** **10:** 298-307.
10. Shi, Y.H. 2007. ***Drug Discovery Today*** **12:** 440-445.
11. Thomsen, R. and M.H. Christensen. 2006. MolDock: ***Journal of Medicinal Chemistry*** **49:** 3315-3321.
12. van Dijk, A.D.J. and A. Bonvin. 2006. ***Bioinformatics*** **22:** 2340-2347.
13. Verdonk, M.L., G. Chessari, J.C. Cole, M.J. Hartshorn, C.W. Murray, J.W.M. Nissink, R.D. Taylor, and R. Taylor. 2005. ***Journal of Medicinal Chemistry*** **48:** 6504-6515.
14. Whittle, M., V.J. Gillet, and P. Willett. 2006. ***Journal of Chemical Information and Modeling*** **46:** 2193-2205.
15. Willett, P. 2006. ***QSAR & Combinatorial Science*** **25:** 1143-1152.
16. Wishart, D.S. 2005. ***Drug Metabolism Reviews*** **37:** 279-310.

III. Major academic awards or honors.

1. Win the 2007 National Innovation Award, iGEMDOCK: A graphical-automatic drug system for docking, screening and post-analysis.
2. Win outstanding Research Award at the National Chiao-Tung University, 2006
3. Promote to associate professor (2004/08-2007/07) and then to professor (2007/08-now) from assistant professor (2001/08-2004/07) within six years since I got Ph.D. degree (2001/01). All reviewers (14) consistently and strongly recommend (the highest grade) me for associate professor promotion and professor promotion. In addition, most of the reviewers have the similar comments, "Applicant's works are novel and continuous in computer-aided drug discovery and structural bioinformatics. In addition, his papers are high quality and are increasingly cited. The applicant has significant achievements and contributions in these two fields."
4. Win the prize of 2001 Best M.S. and Ph. D. Dissertation Award hosted by IICM (Institute of Information & Computing Machinery)
5. The bibliography was published in 2003 Marquis's Who's Who in Science and Engineering (7^{Th} edition).
6. Thesis Supervision Awards: Win the prize of 2004 Best M.S. and Ph. D. Dissertation Award hosted by IICM (Shen, TW; master student)
7. Thesis Supervision Awards: Win the prize of 2005 Best M.S. and Ph. D. Dissertation Award hosted by IICM (Tung CH; master student)

V. Other supporting materials, including Curriculum Vitae and publication list. List all works in order of publication date and mark corresponding author with an asterisk (*). In addition, please label each paper's impact factor and number of citations based on the *Journal Citation Reports* edition 2007.

1. 2001/8-2004/7: **Assistant Professor**, Department of Biological Science and Technology & Institute of Bioinformatics, National Chiao-Tung University.
2. 2004/8-2007/7: **Associate Professor**, Department of Biological Science and Technology & Institute of Bioinformatics, National Chiao-Tung University.
3. 2007/8-now: **Professor and Director**, Institute of Bioinformatics, National Chiao-Tung University.
4. 2005/8-2008/7: The **PI of Main Project of NSC Program for Interdisciplinary Research Project in Bioinformatics**. This Main Project consists of three sub-projects.
5. 2008/8-2011/7: T**he PI of Main Project of NSC Program for Interdisciplinary Research Project in Bioinformatics**. This Main Project consists of four sub-projects. (Main Project name: Comparative analysis of molecular interactions and pathways in biological systems)
6. 2008/5-2011/4: **The PI of NSC National Research Program for Genomic Medicine**. (Project name: Molecular interaction networks and 3D-domain interologs in medical applications)
7. 2007/2- now : Member of Bioinformatics Society Taiwan
8. Reviewer for the following journals:
    - *Nucleic Acids Research*
    - *Proteins: Structure, Function, and Bioinformatics*
    - *BMC Bioinformatics*

- *BMC Structural Biology*
- *Acta Pharmacologica Sinica*
- *Journal of Computational Chemistry*
- *Journal of Chemical Information and Modeling*
- *IEEE Transactions on Knowledge and Data Engineering*
- *Engineering Optimization*
- *Letters in Drug Design & Discovery*
- *Journal of Information Science and Engineering*

In the last five years (from 2003~2008), we published 22 SCI papers, 1 non-SCI paper (PLoS ONE), and 9 conference papers. Among these 22 SCI papers, the impact factor of five papers, which I am the corresponding author, exceeds 6.0 (Figure 1A) according to the Journal Citation Reports editor 2007. On average, we publish ~4 SCI papers each year and the impact factor of each paper is 3.59. The sum of impact factors is increasing from 2005 (6.34), 2006 (13.93), 2007 (20.52) to 2008/9 (18.84). The total number of citations is 192 since 2003 and the average number of citations is 6.2 for each paper (Figure 1B). My h-index is 9 since 2000.

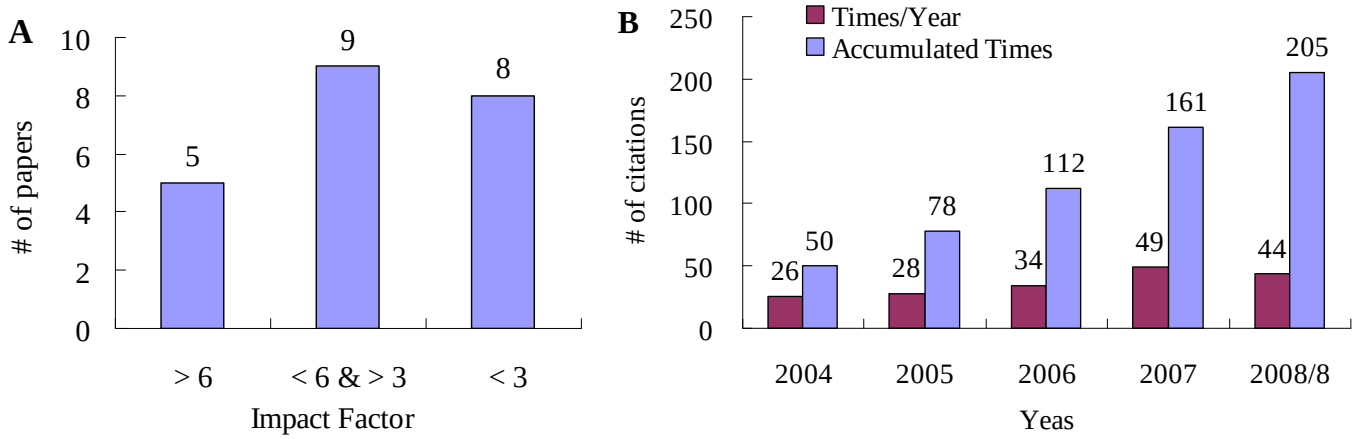


Figure 1. (A) The relationship between the number of papers and the impact factor and (B) the relationship between the number of citations and the publication year.

Journal Papers (* corresponding author) (order by publication date)

1. Y.-Y. Chiu, J.-K. Hwang, **J.-M. Yang***, "Soft energy function and generic evolutionary method for discriminating native from non-native protein conformations," *Journal of Computational Chemistry*, vol. 29, pp. 1364-1373, 2008 (**IF: 4.297)**
2. Y.-L. Chang, H.-K. Tsai, C.-Y. Kao, Y.-C. Chen, Y.-J. Hu, and **J.-M. Yang***, "Evolutionary conservation of DNA-contact residues in DNA-binding domains," *BMC Bioinformatics*, vol. 9 (S6), pp. S3.1~S3.9, 2008 (**IF: 3.493**).
3. C.-Y. Yang, C.-H. Chang, T.-C. Lin, Y.-L. Yu, S.-A. Lee, C.-C. Yen, **J.-M. Yang,** J.-M. Lai, Y.-R. Hong, T.-L. Tseng, K.-M. Chao, and C.-Y. Huang***,** "PhosphoPOINT: a comprehensive human kinase interactome and phospho-protein database," *Bioinformatics*, vol. 24, pp. i14-i20, 2008. (**IF: 5.039**)

4. M.-C. Yang, H.-H. Guan, M.-Y. Liu, Y.-H. Lin, **J.-M. Yang**, W.-L. Chen, C.-J. Chen, and Simon J. T. Mao*, "Crystal structure of a secondary vitamin D_3 binding site of milk ß-lactoglobulin," *Proteins: Structure, Function, and Bioinformatics*, vol. 71, pp. 1197-1210, 2008. (**IF: 3.354**)
5. Y.Y. Yao, K.L. Shrestha, Y.J. Wu, H.J. Tasi, C.C. Chen, **J.-M. Yang**, A. Ando, C.Y. Cheng, Y.K. Li*, "Structural simulation and protein engineering to convert an endo-chitosanase to an exo-chitosanase," *Protein Engineering Design & Selection*, vol. 21, pp. 561-566, 2008. (**IF: 2.662)**
6. C.-H. Tung, J.-W. Huang and **J.-M. Yang***, "Kappa-alpha plot derived structural alphabet and BLOSUM-like substitution matrix for fast protein structure database search," *Genome Biology*, vol. 8, pp. R31.1~R31.16, 2007. (**IF: 6.589;** Times Cited: 2)
7. C.-H. Tung and **J.-M. Yang***, "fastSCOP: a fast web server for recognizing protein structural domains and SCOP superfamilies," *Nucleic Acids Research*, pp. W438-W443, 2007. (**IF: 6.954;** Times Cited: 3)
8. Y.-C. Chen, Y.-S. Lo, W.-C. Hsu, and **J.-M. Yang***, "3D-partner: a web server to infer interacting partners and binding models, " *Nucleic Acids Research*, pp. W561-W567, 2007. (**IF: 6.954;** Times Cited: 2)
9. **J.-M. Yang**, Y.-F. Chen, Y.-Y. Tu, K.-R. Yen, and Y.-L. Yang***, "**Combinatorial computation approaches identifying tetracycline derivates as flaviviruses inhibitors," *PLoS ONE*, pp. e428.1-e428.12, 2007.
10. **J.-M. Yang*** and C.-H. Tung, "Protein structure database search and evolutionary classification," *Nucleic Acids Research*, vol. 34, pp. 3646-3659, 2006. (**IF: 6.954;** Times Cited: 8)
11. C.-C. Chen, J.-K. Hwang and **J.-M. Yang***, "$(PS)^2$: Protein structure prediction server," *Nucleic Acids Research*, pp. W152–W157, 2006. (**IF: 6.965;** Times Cited: 2)
12. **J.-M. Yang*** Y.-F. Chen, T.-W. Shen, B. S. Kristal, and D. F. Hsu, "Consensus Scoring Criteria for Improving Enrichment in Virtual Screening," *Journal of Chemical Information and Modeling*, vol. 45, pp. 1134-1146, 2005. (**IF: 2.986**; Times Cited: 25)
13. **J.-M. Yang*** and T.-W. Shen, "A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators," *Proteins: Structure, Function, and Bioinformatics,* vol. 59, pp. 205-220, 2005. (**IF: 3.354**; Times Cited: 13)
14. **J.-M. Yang*** and C.-C. Chen, "GEMDOCK: A generic evolutionary method for molecular docking," *Proteins: Structure, Function, and Bioinformatics*, vol. 55, pp. 288-304, 2004. (**IF: 3.354**; Times Cited: 28)
15. **J.-M. Yang*** "Development and evaluation of a generic evolutionary method for protein-ligand docking," *Journal of Computational Chemistry*, vol. 25, pp. 843-857, 2004. (**IF: 4.297;** Times Cited: 3)
16. H.-K. Tsai, **J.-M. Yang**, Y.-F. Tsai, and C-Y Kao, "An evolutionary algorithm for large traveling salesman problems," *IEEE Transactions on Systems Man and Cybernetics Part B-Cybernetics*, vol. 34, pp. 1718-1729, 2004. (**IF: 1.353;** Times Cited: 7)
17. H.-K. Tsai, **J.-M. Yang**, Y.-F. Tsai, and C-Y Kao, "An evolutionary approach for gene expression patterns," *IEEE Transaction on Information Technology in Biomedicine*, vol. 8, pp. 69-78, 2004. (**IF: 1.436;** Times Cited: 4)

18. H.-K. Tsai, **J.-M. Yang**, and C-Y Kao, "Issues of designing genetic algorithms for traveling salesman problems", vol. 8, pp. 689-697, *Soft Computing*, 2004. (**IF: 0.607**)
19. C.-C. Chuang, C-Y Chen, **J.-M. Yang**, P.-C. Lyu, J.-K. Hwang, "The detection of protein structural similarity using disulfide-binding patterns," *Proteins: Structure, Function, and Genetics*, vol. 53, pp. 1-5, 2003. (**IF: 3.354;** Times Cited: 22)
20. C.-S. Yu, J.-Y. Wang, **J.-M. Yang,** P.-C. Lyu, C.-J. Lin, J.-K. Hwang, "Fine-grained protein fold assignment by support vector machines using generalized n−peptide coding schemes and jury voting from multiple parameter sets," *Proteins: Structure, Function, and Genetics*, vol. 50, pp. 531-536, 2003. (**IF: 3.354;** Times Cited: 15)
21. Y.-W. Chu***** and **J.-M. Yang***, "Finding regularity in various types of secondary protein structures," *Journal of Information Science and Engineering*, vol. 19, pp.943-952, 2003. (**IF:0.202**)
22. E.-S. Lin, **J.-M. Yang**, and Y.-S. Yang, "Modeling the binding and inhibition mechanism of nucleotide and sulfotransferase using molecular docking," *Journal of the Chinese Chemical Society,* vol. 50, pp. 655-663, 2003. (**IF:0.643;** Times Cited: 1)
23. H.-K. Tsai, **J.-M. Yang**, Y.-F. Tsai, and C-Y Kao, "A heterogeneous selection genetic algorithm for traveling salesman problems," *Engineering Optimization*, pp. 297-311, 2003. (**IF:0.571;** Times Cited: 2)

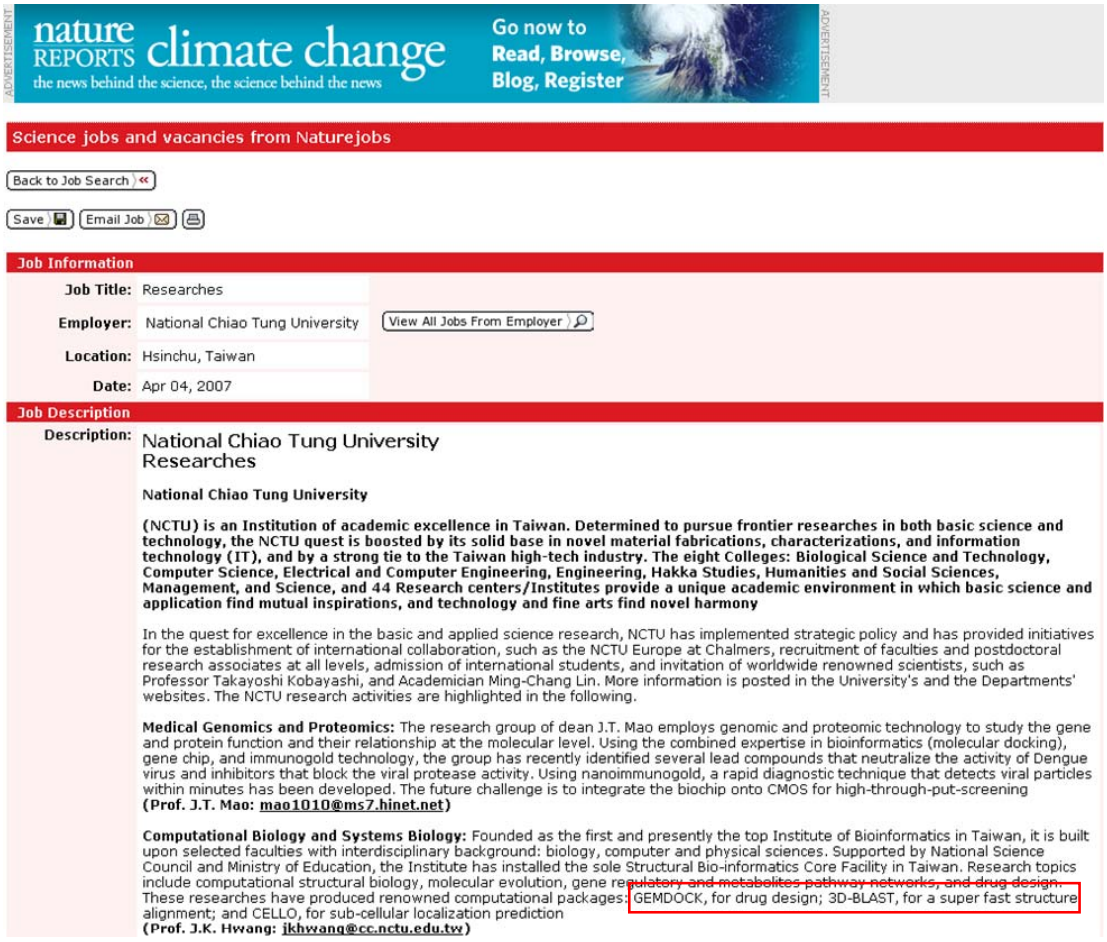
Conference Papers

1. K-C Hsu, Y-F Chen, and **J-M Yang***, "Binding affinity analysis of protein-ligand complexes," *2nd International Conference on Bioinformatics and Biomedical Engineering*, pp. 167-171, 2008.
2. J-W Huang, C-C Chen, and **J-M Yang***, "Identifying critical positions and rules of antigenic drift for influenza A/H3N2 viruses," *2nd International Conference on Bioinformatics and Biomedical Engineering*, pp. 249-252, 2008.
3. K.-P. Liu and **J.-M Yang*,** "A Gaussian evolutionary method for predicting protein-protein interaction sites," *Lecture Notes in Computer Science*, vol. 4447, pp. 143-153, 2007.
4. Y.-L. Chang, H.-K. Tsai, C.-Y. Kao and **J.-M. Yang***, "Evolutionary conservation of DNA-contact residues in DNA-binding domains," *International Multi-Symposiums on Computer and Computational Sciences* (IMSCCS07), pp. 9-16, 2007.
5. **J.-M. Yang***, L.-S. Chang, and K.-P. Liu, "ARPPI: A knowledge-based model for protein-protein interactions," *Sixth International Conference on Bioinformatics* (InCoB2007), 2007
6. Y.-C. Chen, H.-C. Chen and **J.-M Yang*,** "A 3D-domain annotated protein-protein interaction database," *Genome Informatics*, vol. 17, pp. 206-215, 2006.
7. Y.-Y. Chiu, J.-K. Hwang and **J.-M. Yang**, "GEMSCORE: A new empirical energy function for protein folding," *IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology* (*CIBCB 2005*), pp. 303-310, 2005.
8. Y.-C. Chen, **J.-M Yang**, C.-H. Tsai, C.-Y. Kao, "GEMPLS: A new QSAR method combining generic evolutionary method and partial least squares", *Lecture Notes in Computer Science*, vol.

3449, pp. 125-135, 2005.

9. Y.-C. Chen, **J.-M Yang**, C.-H. Tsai, C.-Y. Kao, "Comparative molecular binding energy analysis of HIV-1 protease inhibitors using genetic algorithm-based partial least squares method," *Lecture Notes in Computer Science*, vol. 3103, pp. 385-386, 2004.

Appendix A [nature reports]: 3D-BLAST and GEMDOCK are selected by National Chiao Tung University and reported on "Science jobs and vacancies from Nature jobs"



Science jobs and vacancies from Naturejobs

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Job Information

Job Title: Researches
Employer: National Chiao Tung University | View All Jobs From Employer
Location: Hsinchu, Taiwan
Date: Apr 04, 2007

Job Description

Description:

National Chiao Tung University
Researches

National Chiao Tung University

(NCTU) is an Institution of academic excellence in Taiwan. Determined to pursue frontier researches in both basic science and technology, the NCTU quest is boosted by its solid base in novel material fabrications, characterizations, and information technology (IT), and by a strong tie to the Taiwan high-tech industry. The eight Colleges: Biological Science and Technology, Computer Science, Electrical and Computer Engineering, Engineering, Hakka Studies, Humanities and Social Sciences, Management, and Science, and 44 Research centers/Institutes provide a unique academic environment in which basic science and application find mutual inspirations, and technology and fine arts find novel harmony

In the quest for excellence in the basic and applied science research, NCTU has implemented strategic policy and has provided initiatives for the establishment of international collaboration, such as the NCTU Europe at Chalmers, recruitment of faculties and postdoctoral research associates at all levels, admission of international students, and invitation of worldwide renowned scientists, such as Professor Takayoshi Kobayashi, and Academician Ming-Chang Lin. More information is posted in the University's and the Departments' websites. The NCTU research activities are highlighted in the following.

Medical Genomics and Proteomics: The research group of dean J.T. Mao employs genomic and proteomic technology to study the gene and protein function and their relationship at the molecular level. Using the combined expertise in bioinformatics (molecular docking), gene chip, and immunogold technology, the group has recently identified several lead compounds that neutralize the activity of Dengue virus and inhibitors that block the viral protease activity. Using nanoimmunogold, a rapid diagnostic technique that detects viral particles within minutes has been developed. The future challenge is to integrate the biochip onto CMOS for high-through-put-screening
(Prof. J.T. Mao: mao1010@ms7.hinet.net)

Computational Biology and Systems Biology: Founded as the first and presently the top Institute of Bioinformatics in Taiwan, it is built upon selected faculties with interdisciplinary background: biology, computer and physical sciences. Supported by National Science Council and Ministry of Education, the Institute has installed the sole Structural Bio-informatics Core Facility in Taiwan. Research topics include computational structural biology, molecular evolution, gene regulatory and metabolites pathway networks, and drug design. These researches have produced renowned computational packages: GEMDOCK, for drug design; 3D-BLAST, for a super fast structure alignment; and CELLO, for sub-cellular localization prediction
(Prof. J.K. Hwang: jkhwang@cc.nctu.edu.tw)

Appendix B: Top ten of the most cited papers in my search career since 2000

Use the checkboxes to remove individual items from this Citation Report or restrict to items processed between 1977 and 2008 Go	2004 ◄	2005	2006	2007	2008 ►	Total	Average Citations per Year
	26	28	34	49	44	205	20.50
1. Title: GEMDOCK: A generic evolutionary method for molecular docking Author(s): Yang JM, Chen CC Source: **PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS** Volume: **55** Issue: **2** Pages: **288-304** Published: **MAY 1 2004**	1	8	7	3	9	28	5.60
2. Title: Consensus scoring criteria for improving enrichment in virtual screening Author(s): Yang JM, Chen YF, Shen TW, et al. Source: **JOURNAL OF CHEMICAL INFORMATION AND MODELING** Volume: **45** Issue: **4** Pages: **1134-1146** Published: **JUL-AUG 2005**	0	0	6	9	10	25	6.25
3. Title: Relationship between protein structures and disulfide bonding patterns Author(s): Chuang CC, Chen CY, Yang JM, et al. Source: **PROTEINS-STRUCTURE FUNCTION AND GENETICS** Volume: **53** Issue: **1** Pages: **1-5** Published: **OCT 1 2003**	5	7	2	5	3	22	3.67
4. Title: Flexible ligand docking using a robust evolutionary algorithm Author(s): Yang JM, Kao CY Source: **JOURNAL OF COMPUTATIONAL CHEMISTRY** Volume: **21** Issue: **11** Pages: **988-998** Published: **AUG 2000**	4	1	0	1	0	16	1.78
5. Title: Fine-grained protein fold assignment by support vector machines using generalized npeptide coding schemes and jury voting from multiple-parameter sets Author(s): Yu CS, Wang JY, Yang JM, et al. Source: **PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS** Volume: **50** Issue: **4** Pages: **531-536** Published: **MAR 1 2003**	3	2	3	5	1	15	2.50
6. Title: A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators Author(s): Yang JM, Shen TW Source: **PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS** Volume: **59** Issue: **2** Pages: **205-220** Published: **MAY 1 2005**	0	2	4	5	2	13	3.25
7. Title: GEM: A Gaussian evolutionary method for predicting protein side-chain conformations Author(s): Yang JM, Tsai CH, Hwang MJ, et al. Source: **PROTEIN SCIENCE** Volume: **11** Issue: **8** Pages: **1897-1907** Published: **AUG 2002**	2	2	1	3	1	10	1.43
8. Title: A robust evolutionary algorithm for training neural networks Author(s): Yang JM, Kao CY Source: **NEURAL COMPUTING & APPLICATIONS** Volume: **10** Issue: **3** Pages: **214-230** Published: **2001**	2	0	3	2	2	10	1.43
9. Title: An evolutionary algorithm for the synthesis of multilayer coatings at oblique light incidence Author(s): Yang JM, Kao CY Source: **JOURNAL OF LIGHTWAVE TECHNOLOGY** Volume: **19** Issue: **4** Pages: **559-570** Published: **APR 2001**	4	1	2	0	2	10	1.25
10. Title: Protein structure database search and evolutionary classification Author(s): Yang JM, Tung CH Source: **NUCLEIC ACIDS RESEARCH** Volume: **34** Issue: **13** Pages: **3646-3659** Published: **2006**	0	0	0	3	5	8	2.67