

CURRICULUM VITAE

Y. Z. Chen

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Research interests:

Drug discovery: pharmainformatics, virtual screening, ADME-Tox prediction, drug combination, target discovery

Computational biology: bioinformatics, systems biology, proteomics, biomarker discovery, immunology

Nano-science: Nano-systems simulation

Herbal medicine: herbal informatics, molecular mechanisms, combination therapies

Art and Science: digital art of proteins, protein music

Academic qualifications:

B.Sc. 1982 Dalian University of Technology, China

M.Sc. 1985 Institute of Theoretical Physics, Academia Sinica, China

Ph.D. 1989 University of Manchester, Institute of Science and Technology, U.K

Career history:

2007 Jan - Present Tenured Professor, Dept. of Pharmacy, National Univ of Singapore

2008 July – Present Member, International Scientific Committee, International Centre for Science & High Technology, UNIDO, Trieste, Italy

2006 Jan – 2006 Dec Tenured Associate Professor, Dept. of Pharmacy, National Univ. of Singapore

2004-Present Adjunct Professors, Shanghai Center Bioinfo Tech, Xiamen Univ, SiChuan Univ, ChongQing Univ

2003-2005 Head, Dept of Computational Science, National Univ of Singapore

2000-2005 Tenured Associate Professor, Dept of Computational Science, National Univ of Singapore

2000-Present Fellow, Singapore-MIT alliance.

1998-2000 Senior Lecturer, Dept of Computational Science, National Univ of Singapore

1997-1998 Lecturer, Dept of Computational Science, National Univ of Singapore

1997-1997 Research Scientist, ISIS Pharmaceuticals, Carlsbad, CA, USA

1994-1996 Research Assistant Scientist, Biophysics Group, Dept of Phys, Purdue University, Indiana, USA

1989-1993 Post-Doc Fellow, Biophysics Group, Dept of Phys, Purdue University, Indiana, USA

Research accomplishments:

Publications: 16 invited reviews, 155 papers in international refereed journals.

Inventions and developments:

Patents:

- Target identification method (Sole inventor, US Patent 6,519,611).
- Biological pathway and molecular simulation system (Principal inventor, U.S. Regular Patent Appl.10/674,586)
- Herb/food effects and consumption information system (Principal inventor, U.S. Provisional Appl. 60/512,479)

Products:

- Target discovery software INVDOCK, jointly developed and marketed by Bridgeway Hypersystems Co Ltd China
- Microarray biomarker discovery software MASDA, jointly developed and marketed by Bridgeway Co Ltd China
- Oligonucleotide toxicity prediction software ONSET, jointly developed with ISIS Pharmaceuticals USA
- Machine learning software for virtual screening, ADMET prediction, target discovery, applied in separate joint drug discovery projects with Asia Medicine Co Ltd (Hainan), SiChuan Univ, Shanghai CDC, China
- Web-based protein function prediction software SVMProt (<http://jing.cz3.nus.edu.sg/cgi-bin/svmprot.cgi>)
- Databases of therapeutic & ADMET targets, binding kinetics (http://bidd.nus.edu.sg/group/cjttd/TTD_ns.asp)
- Web-based protein art and music servers (<http://amas.cz3.nus.edu.sg/art/>)

Awards, honours, editorships, conference chairmanships, invited speakers

- Outstanding Scientist Award 2007, Science Faculty, National Univ of Singapore
- Marquis Who's Who in Science and Engineering. 7th, 8th, 9th edition 2003-2006; Marquis Who's Who in Medicine and Health Care 6th edition 2006; Marquis Who's Who in Asia 1st edition 2007
- Member, International Scientific Committee, International Centre for Science & High Technology, UNIDO, Trieste, Italy
- Editorial board of Current Proteomics, Protein and Peptide Lett, Bioinformation, Int J of Integrative Biology
- Featured in "Protein art and music" Singapore Unified Morning News, 6/5/2005; "Protein music". Shanghai Evening News, 3/7/2005; "Computer study of Chinese medicine". Singapore Unified Morning News, 19/8/2002
- Invited podium speaker, PSWC 2007 Pharmaceutical Sciences World Congress, Amsterdam, 23 April 2007

- Invited speaker, Symposium on *Chem Vision in Life Science*, KRICT, Korea, 25 August 2006
- Invited speaker, ICS-UNIDO Workshop, Bangkok, 4-6 May 2009
- Invited speaker, 3rd Asian Pacific ISSX regional meeting, Bangkok 10-12 May 2009
- Invited speaker, 3rd Cross-Strait Theoretical and Computation Chemistry Conference, Chengdu 23-25 April 2009
- Co-chair, platform session *computational methods & molecular dynamics*, 45th Annual Meeting of American Biophysical Society, Boston, USA. February 21, 2001.
- Organizer and chair, *Minisymposium in math modeling in molecular biology and drug design*, Pacific Rim Dynamics Systems Conferences, Hawaii, USA. 9-13 August, 2000
- Invited speaker, AIMECS'99 *International Medicinal Chemistry Symposium*, Beijing, China. 13 Sept. 1999.
- Invited speaker, Annual meeting of American physical society, San Jose, USA. 24 March, 1995.
- Member, Singapore TCM Taskforce, Singapore Science Center TCM exhibition committee
- Member, National Univ of Singapore Taskforces on Computational Biology, medicinal chemistry program development committee, life science curriculum committee, bioengineering program development committee

Funding:

PI of 11 Singapore ARF grants; 1 China NSF, 1 Hong Kong K.C.Wong grant; Co-PI of 1 China 863 grant

Teaching:

Graduate courses taught: Computer aided drug design, Molecular modelling, Bioinformatics, Computational biology, Biotechnology, Simulation Methods, Biophysics

Undergraduate courses taught:

Computer aided drug design, Medicinal chemistry, Computational chemistry, Bioinformatics, Simulations, Parallel and Distributed Computing, Computational physics, Computational Science (On-line lecture notes adopted by Education Curriculum Center, The Mathworks, UK in 2004-2006)

Representative publications (all as the sole corresponding author):

1. What are next generation innovative therapeutic targets? Clues from genetic, structural, physicochemical and systems profile of successful targets. F. Zhu, L.Y. Han, ... **Y.Z. Chen**. *J Pharmacol Exp Ther*. 2009 (accepted)
2. Synergistic therapeutic actions of herbal ingredients and their mechanisms from molecular interaction and network perspectives X. H. Ma, C.J. Zheng, ... **Y. Z. Chen**. *Drug Discov Today*. 2009 (accepted).
3. Mechanisms of drug combinations from interaction and network perspectives J. Jia, F. Zhu, X.H. Ma, Z.W. Cao, Y.X. Li and **Y.Z. Chen**. *Nature Rev. Drug Discov.*, 8(2):111-28(2009)
4. Derivation of Stable Microarray Cancer-differentiating Signatures by a Feature-selection Method Incorporating Consensus Scoring of Multiple Random Sampling and Gene-Ranking Consistency Evaluation. Z.Q. Tang, L.Y. Han, H.H. Lin, J. Cui, J. Jia, B.C. Low, B.W. Li, **Y.Z. Chen**. *Cancer Res*. 67:9996-10003 (2007).
5. Support vector machine approach for predicting druggable proteins: Recent progress in its exploration and investigation of its usefulness. L.Y. Han, , ... , and **Y.Z. Chen**. *Drug Discov Today* 12: 304-313 (2007)
6. PharmGED: Pharmacogenetic Effect Database B. Xie,... , and **Y. Z. Chen**, *Clin. Pharmacol. Ther.* 81: 29 (2007)
7. Therapeutic Targets: Progress of Their Exploration and Investigation of Their Characteristics. C.J. Zheng, L.Y. Han, C. W. Yap, Z. L. Ji, Z. W. Cao and **Y. Z. Chen**. *Pharmacological Reviews* 58, 259-279 (2006)
8. Prediction of p-glycoprotein substrates by support vector machine approach. Xue, Y.; Yap, C. W.; Sun, L. Z.; Cao, Z. W.; Wang, J. F.; **Chen, Y. Z.** *J. Chem. Inf. Comput. Sci.* 44, 1497-505 (2004)
9. SVM-Prot: Web-Based Support Vector Machine Software for Functional Classification of a Protein from Its Primary Sequence. C.Z. Cai, L.Y. Han, Z.L. Ji, X. Chen, **Y.Z. Chen**. *Nucleic. Acids Res.* 31: 3692-3697 (2003)
10. TTD: Therapeutic Target Database. X. Chen, Z.L. Ji, and **Y. Z. Chen**, *Nucleic. Acids. Res.*, 30, 412 (2002)
11. Ligand-Protein Inverse Docking and Its Potential Use in Computer Search of Putative Protein Targets of a Small Molecule. **Y. Z. Chen** and D. G. Zhi, *Proteins*, 43, 217 (2001)

Selected publications:

Drug Discovery (all but one as the sole corresponding author):

Pharmainformatics

1. PharmGED: Pharmacogenetic Effect Database B. Xie,... , and **Y. Z. Chen**, *Clin. Pharmacol. Ther.* 81: 29 (2007).
2. PEARLS: Program for Energetic Analysis of Receptor-Ligand System. L.Y. Han, H.H. Lin, Z. R. Li, C.J. Zheng, Z.W. Cao, B. Xie, and **Y. Z. Chen**. *J. Chem. Inf. Model.* 23:445-450 (2006)
3. DART: Drug Adverse Reaction Target Database. Z. L. Ji, L. Y. Han, C. W. Yap, L. Z. Sun, X. Chen, and **Y Z. Chen**. *Drug Safety* 26, 685-690 (2003).
4. Absorption, distribution, metabolism, and excretion-associated protein database. L. Z. Sun, Z. L. Ji, X. Chen, J. F. Wang, and **Y. Z. Chen**, *Clin. Pharmacol. Ther.* , 71, 405 (2002).

Virtual screening and ADME-Tox prediction:

1. Comparative analysis of machine learning methods in ligand-based virtual screening of large compound libraries. X.H. Ma, J. Jia, F. Zhu, ...and **Y. Z. Chen**. *Comb. Chem. High Throughput Screen.* 2008 (accepted).
2. Evaluation of Virtual Screening Performance of Support Vector Machines Trained by Sparsely Distributed Active Compounds. X.H. Ma, R. Wang, S.Y. Yang, ... and **Y. Z. Chen**. *J Chem Inf Model.* 48(6):1227-1237 (2008)
3. A support vector machines approach for virtual screening of active compounds of single and multiple mechanisms from large libraries at an improved hit-rate and enrichment factor. L.Y. Han, X.H. Ma, ..., **Y.Z. Chen**. *J Mol Graph Model* 26(8):1276-1286 (2008)
4. Machine Learning Approaches for Predicting Compounds That Interact with Therapeutic and ADMET Related Proteins. H. Li, C.W. Yap, ...and **Y.Z. Chen**. *J. Pharm. Sci.* 96:2838-2860 (2007).
5. In Silico Prediction of Pregnane X Receptor Activators by Machine Learning Approaches. C.Y. Ung, H. Li, C.W. Yap and **Y.Z. Chen**. *Mol. Pharmacol.* 71:158-168 (2007).
6. Formulation Development of Transdermal Dosage Forms: Quantitative Structure Activity Relationship Model for Predicting Activities of Terpenes that Enhance Drug Penetration Through Human Skin. L. Kang, C.W. Yap, PFC Lim, Y.Z. Chen, P C L Ho, YW Chan, GP Wong and S Y Chan. *J. Controlled Release* 120:211-219 (2007)
7. Classification of a Diverse Set of Tetrahymena Pyriformis Toxicity Chemical Compounds from Molecular Descriptors by Statistical Learning Methods Y. Xue, ...and **Y.Z. Chen**. *Chem. Res. Toxicol.* 19: 1030-1039 (2006).
8. Effect of Selection of Molecular Descriptors on the Prediction of Blood-Brain Barrier Penetrating and Non-penetrating Agents by Statistical Learning Methods. H. Li, C. W. Yap, C. Y. Ung, Y. Xue, Z. W. Cao, and **Y. Z. Chen**. *J. Chem. Inf. Model.* 45: 1376-1384 (2005)..
9. Prediction of Cytochrome P450 3A4, 2D6, 2C9 Inhibitors and Substrates by Using Support Vector Machines. C.W. Yap, **Y.Z. Chen** *J. Chem. Inf. Model.* 45: 982-992 (2005).
10. Prediction of Genotoxicity of Chemical Compounds by Statistical Learning Methods. H. Li, Y. Xue, C.Y. Ung, C.W. Yap, Z.R Li, and **Y.Z. Chen**. *Chem Res Toxicol.* 18:1071-1080 (2005).
11. Effect of molecular descriptor feature selection in support vector machine classification of pharmacokinetic and toxicological properties of chemical agents. Xue, Y.; Li, Z.....; **Chen, Y. Z.** *J. Chem. Inf. Comput. Sci.* 44: 1630-1638(2004)
12. Prediction of torsade-causing potential of drugs by support vector machine approach. Yap, C. W., Cai, C. Z., Xue, Y., and **Chen, Y. Z.** *Toxicol. Sci.* 79: 170-177 (2004).

Drug combinations and multi-targeting:

1. Synergistic therapeutic actions of herbal ingredients and their mechanisms from molecular interaction and network perspectives X. H. Ma, C.J. Zheng, ... **Y. Z. Chen**. *Drug Discov Today.* 2009 (accepted).
2. Mechanisms of drug combinations: interaction and network perspectives J. Jia, F. Zhu, X.H. Ma, Z.W. Cao, Y.X. Li and Y.Z. Chen. *Nature Rev. Drug Discov.*, 8(2):111-28(2009)

Target discovery:

1. What are next generation innovative therapeutic targets? Clues from genetic, structural, physicochemical and systems profile of successful targets. F. Zhu, L.Y. Han, ... Y.Z. Chen. *J Pharmacol Exp Ther.* 2009 (accepted)
2. Support vector machine approach for predicting druggable proteins: Recent progress in its exploration and investigation of its usefulness. L.Y. Han, , ..., and **Y.Z. Chen**. *Drug Discov. Today* 12: 304-313 (2007).
3. Computer prediction of drug resistance mutations in proteins. Z. W. Cao, L. Y. Han, C. J. Zheng, Z. L. Ji, X. Chen, H. H. Lin and **Y. Z. Chen** *Drug Discov. Today* 10:521-529 (2005)
4. Ligand-Protein Inverse Docking and Its Potential Use in Computer Search of Putative Protein Targets of a Small Molecule. **Y. Z. Chen** and D. G. Zhi, *Proteins*, 43, 217 (2001).
5. Prediction of Potential Toxicity and Side Effect Protein Targets of a Small Molecule by a Ligand-Protein Inverse Docking Approach. **Y. Z. Chen**, C. Y. Ung, *J. Mol. Graph. Mod.*, 20, 199-218 (2001).

Computational Biology (all but two as the sole corresponding author, one as co-corresponding author):

Systems biology, biomarker discovery, proteomics:

1. Pathway sensitivity analysis for detecting pro-proliferation activities of oncogenes and tumor suppressors of EGFR-ERK pathway at altered protein levels H. Li, C. Y. Ung, ... **Y. Z. Chen**. *Cancer.* 2009 (accepted)
2. Simulation of Crosstalk between Small GTPase RhoA and EGFR-ERK Signaling Pathway via MEKK1. H. Li, C. Y. Ung, X. H. Ma, B. W. Li, B. C. Low, Z. W. Cao and **Y. Z. Chen**. *Bioinformatics*, 25(3):358-64(2009)
3. Simulation of the Regulation of EGFR Endocytosis and EGFR-ERK Signaling by Endophilin-Mediated RhoA-EGFR Crosstalk. C.Y. Ung, H. Li, ..., B.C. Low and **Y.Z. Chen**. *FEBS Lett.* 582:2283-2290 (2008)
4. Derivation of Stable Microarray Cancer-differentiating Signatures by a Feature-selection Method Incorporating Consensus Scoring of Multiple Random Sampling and Gene-Ranking Consistency Evaluation. Z.Q. Tang, L.Y. Han, H.H. Lin, J. Cui, J. Jia, B.C. Low, B.W. Li, **Y.Z. Chen**. *Cancer Res.* 67:9996-10003 (2007).

- Advances in exploration of machine learning methods for predicting functional class and interaction profiles of proteins and peptides irrespective of sequence homology J. Cui, L.Y. Han, H.H. Lin, Z.Q. Tang, Z.L. Ji, Z.W. Cao, Y.X. Li, and **Y.Z. Chen**. *Curr. Bioinformatics* 2: 95-112 (2007).
- Effect of training datasets on support vector machine prediction of protein-protein interactions. S.L. Lo, C. Z. Cai, **Y.Z. Chen** and Maxey C. M. Chung. *Proteomics* 5:876-884 (2005)

Bioinformatics

- PROFEAT: A Web Server for Computing Structural and Physicochemical Features of Proteins and Peptides from Amino Acid Sequence. Z.R. Li, H.H. Lin, L.Y. Han, ... and **Y.Z. Chen**. *Nucleic Acids Res.* 34, W32-7 (2006)
- MoViES: Molecular Vibrations Evaluation Server for Analysis of Fluctuational Dynamics of Proteins and Nucleic Acids. Z.W. Cao, Y. Xue, ..., and **Y. Z. Chen**, *Nucleic. Acids Res.* 32. W679-W685 (2004)
- TRMP: A Database of Therapeutically Relevant Multiple-Pathways. C.J.Zheng, H. Zhou, B. Xie, L.Y. Han, C.W. Yap, and **Y. Z. Chen**, *Bioinformatics*. 20:2236-41(2004)
- KDBI: Kinetic Data of Bio-molecular Interactions Database. Z. L. Ji, X. Chen, ..., and **Y. Z. Chen**. *Nucleic. Acids. Res.* 31: 255-257 (2003).
- ADME-AP: A database of ADME associated proteins. L. Z. Sun, Z. L. Ji, X. Chen, J. F. Wang, and **Y. Z. Chen**. *Bioinformatics*, 18:1699-1700 (2002).

Protein function:

- Prediction of the Functional Class of Lipid-Binding Proteins from Sequence Derived Properties Irrespective of Sequence Similarity. H.H. Lin, L.Y. Han, ... , and **Y.Z. Chen**. *J. Lipid Res.* 47(4):824-31 (2006)
- Prediction of Transporter Family by Support Vector Machine Approach H. H. Lin, L.Y. Han, C.Z. Cai, Z. L. Ji, and **Y.Z. Chen**. *Proteins*. 62 (1): 218-31 (2006)
- Prediction of Functional Class of the SARS Coronavirus Proteins by a Statistical Learning Method.C.Z. Cai, L.Y. Han, X. Chen, Z.W. Cao, **Y.Z. Chen**. *J. Proteome Res.* 4 (5): 1855-1862 (2005).
- Prediction of Functional Class of Novel Viral Proteins by a Statistical Learning Method Irrespective of Sequence Similarity. L.Y.Han, C.Z Cai, Z. L. Ji, **Y.Z. Chen**. *Virology* 33:136-143(2005)
- Predicting Functional Family of Novel Enzymes Irrespective of Sequence Similarity: A Statistical Learning Approach. L.Y.Han, C.Z.Cai, Z.L.Ji, Z.W.Cao, J.Cui, **Y.Z.Chen**. *Nucleic Acids Res.* 32: 6437-6444(2004)
- Enzyme Family Classification by Support Vector Machines. C.Z. Cai, ..., **Y.Z. Chen**. *Proteins*. 55,66-76 (2004).
- Prediction of RNA-Binding Proteins from Primary Sequence by Support Vector Machine Approach. L.Y. Han, C.Z. Cai, S. L. Lo, Maxey C. M. Chung, **Y. Z. Chen**. *RNA*. 10: 355-368. (2004).

Immunology

- Genome-Scale Search of Tumor-Specific Antigens by Collective Analysis of Mutations, Expressions and T-Cell Recognition. J. Jia, Cui. J. , ... **Y. Z. Chen**. *Mol. Immunol.* 2009 (accepted).
- AAIR: Antibody Antigen Information Resource. Z.Q. Tang, ..., **Y.Z. Chen**. *J. Immunol.* 178: 4705 (2007)
- Prediction of MHC-Binding Peptides of Flexible Lengths from Sequence-Derived Structural and Physicochemical Properties. J. Cui, L. Y. Han, ..., and **Y. Z. Chen**. *Mol. Immunol.* 44: 866-877 (2007).
- Computer Prediction of Allergen Proteins from Sequence-Derived Protein Structural and Physicochemical Properties J. Cui, L.Y. Han, ..., and **Y.Z. Chen** . *Mol. Immunol.* 44: 514-520 (2007).
- MHC-BPS: MHC-Binder Prediction Server for Identifying Peptides of Flexible Lengths from Sequence-Derived Physicochemical Properties. J. Cui, L.Y. Han, ..., and **Y.Z. Chen** *Immunogenetics* 58:607-13 (2006)

Biomolecular Modeling

- Correlation between Normal Modes in The 20-200cm⁻¹ Frequency Range and Localized Torsion Motions Related to Certain Collective Motions in Proteins. Z. W. Cao, ...and **Y. Z. Chen**. *J. Mol. Graph. Mod.* 21,309-319 (2003).
- Spontaneous base flipping in DNA and its possible role in methyltransferase binding. **Y.Z. Chen**, V. Mohan, and R. H. Griffey, *Phys. Rev. E*62, 1133-1137 (2000).
- Effect of backbone zeta torsion angle on low energy single base opening in B-DNA crystal structures. **Y.Z. Chen**, V. Mohan, and R.H. Griffey, *Chem. Phys. Lett.* 287, 570 (1998)
- Theory of DNA melting based on the Peyrard-Bishop model. Y.L. Zhang, W.M. Zheng, J.X. Liu, **Y.Z. Chen**, *Phys. Rev. E*56, 7100-7115 (1997).
- Premelting base pair opening probability and drug binding constant of a daunomycin--Poly d(GCAT)-Poly d(ATGC) complex. Y.Z. Chen and E.W. Prohofsky, *Biophys. J.* 66, 820 (1994).
- The role of a minor groove spine of hydration in stabilizing Poly(dA)-Poly(dT) against fluctuational interbase H-bond disruption in the premelting temperature regime. Y.Z. Chen & E.W. Prohofsky, *Nucleic. Acids. Res.* 20, 415 (1992)
- Energy flow considerations and thermal fluctuational opening of DNA base pairs at a replicating fork: Unwinding consistent with observed replication rates. **Y.Z. Chen**, W. Zhuang & E.W. Prohofsky, *J. Biomol. Struct. Dynam.*

Nano-science:

1. Simulation of DNA Electrophoresis in Systems of Large Number of Solvent Particles by Coarse-Grained Hybrid Molecular Dynamics Approach. R. Wang, J.S. Wang, ... **Y. Z. Chen**. *J Comput Chem*. 30(4):505-13(2009).
2. Dissipative particle dynamics simulations of electroosmotic flow in nano-fluidic devices. D Duong-Hong, JS Wang, G.R. Liu, Y.Z. Chen J.Y. Han, and N.G. Hadjiconstantinou. *Microfluid. Nanofluid.* 4, 219 (2008)
3. Continuum transport model of Ogston sieving in patterned nanofilter arrays for separation of rod-like biomolecules. ZR Li, G.R. Liu, Y.Z. Chen, J.S. Wang, ..., Y Cheng, and J.Y. Han. *Electrophoresis* 29, 329 (2008)

Herbal Medicine (all but one as the sole corresponding author, one as the joint corresponding author):

1. Synergistic therapeutic actions of herbal ingredients and their mechanisms from molecular interaction and network perspectives X. H. Ma, C.J. Zheng, ... **Y. Z. Chen**. *Drug Discov Today*. 2009 (accepted).
2. Are Herb-Pairs of Traditional Chinese Medicine Distinguishable from Others? Pattern Analysis and Artificial Intelligence Classification Study of Traditionally-Defined Herbal Properties. C.Y. Ung, ... and **Y.Z. Chen**. *J. Ethnopharmacol.* 111:371-377 (2007)
3. Database of traditional Chinese medicine and its application to studies of mechanism and to prescription validation. X Chen, H Zhou, ... and **YZ Chen** *Br. J. Pharmacol.* 149:1092-1103 (2006).
4. Usefulness of Traditionally-Defined Herbal Properties for Distinguishing Prescriptions of Traditional Chinese Medicine from Non-Prescription Recipes C.Y. Ung, ... and **Y.Z. Chen**. *J. Ethnopharmacol.* 109: 21-28 (2006).
5. Traditional Chinese Medicine Information Database. Z. L. Ji, H. Zhou, J. F. Wang, L. Y. Han, C. J. Zheng, and **Y. Z. Chen**. *J. Ethnopharmacol.* 103:501 (2006)..
6. TCM-ID: Traditional Chinese Medicine information database. J. F. Wang, H. Zhou, L. Y. Han, C.J. Zheng, C.Y. Kong, C.Y. Ung, H. Li, Z.W. Cao , X. Chen and **Y. Z. Chen**, *Clin Pharmacol. Ther.* 78:92-93 (2005).
7. A Computer Method for Validating Traditional Chinese Medicine Herbal Prescriptions. J. F. Wang, C. Z. Cai1, C. Y. Kong, and **Y. Z. Chen**. *Am. J. Chin. Med.* 33:281-297(2005).
8. Computer Automated Prediction of Putative Therapeutic and Toxicity Protein Targets of Bioactive Compounds from Chinese Medicinal Plants. **Y. Z. Chen** and C. Y. Ung, *Am. J. Chin. Med.*, 30, 139 (2002).

Invited Reviews (all as the sole corresponding author):

1. Trends in the Exploration of Anticancer Targets and Strategies in Enhancing the Efficacy of Drug Targeting. F. Zhu, C.J. Zheng, L.Y. Han, ... **Y.Z. Chen**. *Curr Mol Pharmacol.* 1(3):213-232(2008)
2. Advances in Machine Learning Prediction of Toxicological Properties and Adverse Drug Reactions of Pharmaceutical Agents. X.H. Ma, ..., Y.Q. Wei and **Y.Z. Chen**. *Current Drug Safety*. 3(2):100-114 (2008).
3. Advances in exploration of machine learning methods for predicting functional class and interaction profiles of proteins and peptides irrespective of sequence homology J. Cui, L.Y. Han, ..., and **Y.Z. Chen**. *Curr. Bioinformatics* 2: 95-112 (2007).
4. Progress and Problems in the Exploration of Therapeutic Targets. C.J. Zheng, L.Y. Han, C. W. Yap, B. Xie, and **Y. Z. Chen** *Drug Discovery Today* 11: 412-420 (2006).
5. Information of ADME-associated proteins and potential application for pharmacogenetic prediction of drug responses. C.J. Zheng, L.Y. Han, ..., and **Y. Z. Chen**. *Curr. Pharmacogenomics* 4:87-103 (2006).
6. Recent progresses in the application of machine learning approach for predicting protein functional class independent of sequence similarity. L.Y. Han, J. Cui, ..., and **Y.Z. Chen** *Proteomics*. 6: 4023-4037 (2006).
7. Application of Support Vector Machines to in silico Prediction of Cytochrome P450 Enzyme Substrates and Inhibitors. C. W. Yap, Y. Xue, Z. R. Li, and **Y. Z. Chen** *Curr. Top. Med. Chem.* 6:1593-1607 (2006)
8. Prediction of Compounds with Specific Pharmacodynamic, Pharmacokinetic or Toxicological Property by Statistical Learning Methods. C. W. Yap, Y. Xue..., and **Y. Z. Chen**. *Mini. Rev. Med. Chem.* 6:449-459 (2006).
9. Computer prediction of drug resistance mutations in proteins, Z. W. Cao, L. Y. Han, C. J. Zheng, Z. L. Ji, and **Y. Z. Chen**. *Drug Discovery Today*, 10:521-529 (2005)
10. Trends in Exploration of Therapeutic Targets. C.J. Zheng, L.Y. Han, C. W. Yap, B. Xie, and **Y. Z. Chen**, *Drug News & Perspectives* 18:109-127 (2005)
12. Drug ADME-Associated Protein Database as a Resource for Facilitating Pharmacogenomics Research. C.J. Zheng, L. Z. Sun, L. Y. Han, Z. L. Ji, X. Chen, and **Y. Z. Chen**. *Drug Dev. Res.* 62:134-142 (2004).
13. Internet Resources for Proteins Associated with Drug Therapeutic Effects, Adverse Reactions, and ADME. Z. L. Ji, L. Z. Sun, X. Chen, ..., and **Y. Z. Chen**, *Drug Discovery Today*, 8,526-529. (2003).
14. Can an In-Silico Drug-Target Search Method be Used to Probe Potential Mechanisms of Medicinal Plant Ingredients? X. Chen, C. Y. Ung, and **Y. Z. Chen**. *Nat. Prod. Rep.* 20: 432-444 (2003).

PhDs trained:

Student Name	Year of PhD award	Research Field	Current Position
Guo Yong Jian	2000 (MSc)	Computational Biology	Lead Bioinformatics Developer, NIAID, NIH, USA
Cao Zhi Wei	2004	Bioinformatics	Professor, Department Head, Tongji University; Assistant Director, Shanghai Center for Bioinformation Technology, China
Ji Zhi Liang	2004	Bioinformatics, Computer aided drug design	Professor, Deputy Department Head, Xiamen Univ, China
Chen Xin	2004	Bioinformatics, Computer aided drug design	Associate Professor, Deputy Head of Department, Zhijiang Univ, China
Yap Chun Wei	2006	Computer aided drug design	Assistant Professor, National Univ of Singapore
Han Lian Yi	2006	Bioinformatics, Computer aided drug design	Staff Scientist, Pubchem, NCBI, NIH, USA
Zheng Chan Juan	2006	Computer aided drug design, Bioinformatics	Research Fellow, CDD, CBB, NCBI, NIH, USA
Lin Hong Huang	2007	Bioinformatics, Computer aided drug design	Staff Scientist, Harvard Univ Medical School, USA
Li Hu	2007	Computer aided drug design, Bioinformatics	Research Fellow, Boston University, USA
Cui Juan	2008	Bioinformatics	Research Associate, Univ of Georgia, USA
Tan Zhi Qun	2008	Bioinformatics	Research Associate, George Town Univ, USA
Ung Choong Yong	2008	Computer aided drug design, Bioinformatics	Research Associate, National University of Singapore
Zhang Hai Lei	2008	Bioinformatics	Research Associate, Harvard Univ Medical School, USA

Statistics of publications in 2001-2009:

Journal	Impact factor	No of Papers	Journal	Impact factor	No of papers
Nature Reviews Drug Discovery	23.308	1	Cancer Research	7.672	1
Pharmacological Reviews	18.823	1	Nucleic Acids Research	6.954	8
Clinical Pharmacology & Therapeutics	8.033	3	Physical Review Letters	7.489	1
Drug Discovery Today	6.761	5	Journal of Proteome Research	5.675	1
Natural Product Reports	7.325	1	Journal of Immunology	6.068	1
Drug Metabolism Reviews	5.754	1	RNA	6.145	1
Molecular Pharmacology	4.088	1	Bioinformatics	5.039	4
Current Topics in Medicinal Chemistry	4.400	1	Proteomics	5.479	3
Journal of Controlled Release	4.756	1	BMC Bioinformatics	3.493	2
Journal of Pharmacology & Exp Ther	4.006	1	Proteins	3.354	3
British Journal of Pharmacology	3.767	1	Molecular Immunology	3.742	3
Journal of Chemical Info & Comp Science	3.423	5	New Phytologist	5.249	1
Toxicological Science	3.367	1	Journal of Lipid Research	4.336	1
Chemical Research in Toxicology	3.508	2	Virology	3.080	1
Drug Safety	3.673	1	Immunogenetics	2.741	1
Journal of Molecular Graphics & Modeling	1.932	5	Biopolymers	2.545	1
Journal of Pharmaceutical Science	2.942	2	Physical Review E	2.010	9

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