TingJun Hou, Ph. D

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1 Education and Professional Experience:

2009-now **Department of Chemistry & Biochemistry, UCSD, San Diego, CA**
Research Scientist
Research partner: Prof. Wei Wang

2004-2008 **Department of Chemistry & Biochemistry, UCSD, San Diego, CA**
Postdoctoral research in Bioinformatics and Computational Biology
Research partner: Prof. Wei Wang

2002-2004 **College of Chemistry & Molecular Engineering, Peking University, Beijing**
Postdoctoral research in Molecular Modelling
Research partner: Prof. Xiaojie Xu

1999-2004 **Neotrident Company (the agent of Accelrys and MDL in China)**
Technical adviser (support for InsightII, Catalyst, Cerius2, MDL databases and information system)

2000-2004 **ChemBay (the agent of Tripos in China)**
Technical adviser (support for SYBYL)

1997-2002 **College of Chemistry & Molecular Engineering, Peking University, Beijing**
Ph. D. in Physical Chemistry
Dissertation: Development of New Methods for Computer-Aided Drug Design
Supervisor: Prof. Xiaojie Xu

1992-1997 **College of Chemistry & Molecular Engineering, Peking University, Beijing**
B. S. in Chemistry

2 Research Experience:

2004-present University of California, San Diego

- Determining the binding specificity and protein interacting partners of peptide-recognition protein domains by using binding free energy calculations and bioinformatics analysis.
- Studies of HIV-1 protease drug resistance by using molecular dynamics, free energy calculations, and molecular interaction field analysis.
- Development of an integrated intelligent system to predict the ADME/Tox properties, including logP, pKa, logD, solubility, Caco-2 permeability, logBB, intestinal absorption, bioavailability, CYP450 metabolism and toxicity by using artificial neutral networks, support vector machine, Bayesian networks, graphics information, etc.
- Development of a new molecular handling C++ template and a new user interface for AMBER 10.
- Development of an efficient entropy calculation method to estimate entropy for both small and macro-molecules.

2002-2004, Peking University

- Development of methods for protein/ligand docking and scoring functions used in virtual screening.
- Development of the efficient and reliable strategy of virtual database screening to identify drug leads.
- Application of molecular docking, 2D/3D-QSAR, pharmacophore modeling, virtual screening, molecular dynamics, free energy calculations, and other molecular modeling techniques for the development of potential drug candidates.
- Development of prediction models for logP, solubility, Caco-2 permeability, and Blood-brain partitioning.

1997-2002, Peking University

(1) Development of the general data structures and template libraries suitable for both computational programs and user interfaces. (2) Application of intelligent algorithms (genetic algorithms, Tabu search, simulated annealing) in molecular docking, conformational analysis and QSAR studies. (3) Development of a Chinese herb database.

3. Peer-reviewed Publications (Cited ~510 times by others, ISI SCI database)

[A] Invited reviews:

1. Youyong Li, **Tingjun Hou**, William A. Goddard III, Molecular modeling of structure-function of G Protein-Coupled Receptors with applications for drug design, *Current Medicinal Chemistry*, 2008, (invited review, in preparation)
2. **Tingjun Hou**, Yongyong Li, Wei Zhang, Junmei Wang, *In silico* predictions of intestinal absorption and bioavailability, *Combinatorial Chemistry & High Through Screening*, 2008, (in press)
3. **Tingjun Hou**, Junmei Wang, Structure–ADME relationship: still a long way to go? *Expert Opinion on Drug Metabolism and Toxicology*, 2009, (in press)
4. **Tingjun Hou**, Junmei Wang, Wei Zhang, Wei Wang, Xiaojie Xu, Recent advances in computational prediction of drug absorption and permeability in drug discovery, *Current Medicinal Chemistry*, 2006, *13*, 2653-2667.
5. Junmei Wang, **Tingjun Hou**, Xiaojie Xu, Recent advances in free energy calculations with a combination of molecular mechanics and continuum models, *Current Computer-Aided Drug Design*, 2006, 2, 287-306.
6. **Tingjun Hou**, Xiaojie Xu, Recent development and application of virtual screening in drug discovery: An overview, *Current Pharmaceutical Design*, 2004, *10*, 1011-1033.

[B] Published on International Journals:

7. **Tingjun Hou**, Zheng Xu, Wei Zhang, William A. McLaughlin, David A. Case, Yang Xu and Wei Wang, Characterization of domain-peptide interaction interface: a generic structure-based model to decipher the binding specificity of SH3 domains, *Molecular & Cellular Proteomics*, 2009, accepted.
8. **Tingjun Hou**, Wei Zhang, Jian Wang, Wei Wang, The prediction of HIV-1 protease drug resistance by analyzing the protease/drug decomposed interaction energy components, *Proteins: Structure, Function, and Bioinformatics*, 2008, in press.
9. **Tingjun Hou**, Wei Zhang, Case A. David, Wei Wang, Characterization of domain-peptide interaction interface: A case study on the amphiphysis-1 SH3 domain, *Journal of Molecular Biology*, 2008, 376, 1201-1214.
10. **Tingjun Hou**, William McLaughlin, Wei Wang, Evaluating the potency of HIV-1 protease drugs to combat resistance, *Proteins: Structure, Function, and Bioinformatics*, 2008, 71, 1163-1174.

11. William McLaughlin, Ken Chen, **Tingjun Hou**, Wei Wang, On the detection of functionally coherent groups of protein domains with an extension to protein annotation, *BMC Bioinformatics*. 2007, 8, 390.
12. **Tingjun Hou**, Junmei Wang, Youyong Li, ADME evaluation in drug discovery. 8. The prediction of intestinal absorption by a support vector machine, *Journal of Chemical Information and Modeling*, 2007, 47, 2408-2415.
13. **Tingjun Hou**, Yon Yu, Molecular dynamics and free energy studies on the wild-type and double mutant HIV-1 protease complexed with amprenavir and two amprenavir-related inhibitors: mechanism for binding and drug resistance, *Journal of Medicinal Chemistry*, 2007, 50, 1177-1188.
14. **Tingjun Hou**, Junmei Wang, Wei Zhang, Xiaojie Xu, ADME evaluation in drug discovery. 7. Prediction of oral absorption by correlation and classification. *Journal of Chemical Information and Modeling*.2007, 47, 208-218.

    (This paper is the 6th most assessed article of JCIM in 2007)
15. **Tingjun Hou**, Junmei Wang, Wei Zhang, Xiaojie Xu, ADME evaluation in drug discovery. 6. If the oral bioavailability in human can be effectively predicted by simple molecular properties-based rules? *Journal of Chemical Information and Modeling*. 2007, 47, 460-463.

    (This paper is the 10th most assessed article of JCIM in 2007)
16. Junmei Wang, Xiangqun Xie, **Tingjun Hou**, Xiaojie Xu, Fast Approaches for Molecular Polarizability Calculations. *Journal of Physical Chemistry* A 2007, 111, 4443-4448.
17. Junmei Wang, George Krudy, **Tingjun Hou**, George Holland, Xiaojie Xu, Development of Reliable Aqueous Solubility Models and Their Application in Drug-like Analysis. *Journal of Chemical Information and Modeling*. 2007, 47, 1395-1404.
18. **Tingjun Hou**, Ken Chen, William McLaughlin, Benzhuo Lu, Wei Wang, Analysis and prediction of peptide binding partners of the Abl SH3 domain. *PLoS Computational Biology* 2006, 2, 0046-0055.

    (This paper was recommended by Faculty 1000,

    http://www.f1000biology.com/article/id/1030930/evaluation)
19. **Tingjun Hou**, William McLaughlin, Benzhuo Lu, Ken Chen, Wei Wang, Prediction of Binding Affinities between the Human Amphiphysin-1 SH3 Domain and Its Peptide Ligands Using Homology Modeling, Molecular dynamics and Molecular Field Analysis. *Journal of Proteome Research* 2006, 5, 32-43.
20. William McLaughlin, **Tingjun Hou**, Wei Wang, Prediction of binding sites of SH2 domains using free energy estimates and sequence analysis. *Journal of Molecular Biology*. 2006, 357, 1322-1334.
21. Aihua Wu, Qi Chen, Ke Xia, **Tingjun Hou**, Xinghai Shen, Hongcheng Gao, Xiaojie Xu. Investigation on photophysical properties of a substituted 3H-indole-modified β-cyclodextrin I. Conformation in water and recognition mechanism as a chemosensor. *Journal of Photochemistry and Photobiology A-Chemistry*. 2006, 182, 174-180.
22. Benzhuo Lu, Xiaolin Chen, **Tingjun Hou**, J. Andrew McCammon, The calculation of the Maxwell stress tensor and the PB force on a solvated molecular surface using hypersingular boundary integrals, *Journal of Chemical Physics*. 2005, 123, 084904.
23. Wei Zhang, **Tingjun Hou**, Xiaojie Xu, New Born Radii Deriving method for Generalized Born Model. *Journal of Chemical Information and Modeling*, 2005, 45, 88-93.
24. **Tingjun Hou**, Wei Zhang, Huang Qin, Xiaojie Xu, An extended aqueous solvation model based on atom-weighted solvent accessible surface areas: SAWSA v2.0 model. *Journal of Molecular Modeling*, 2005, 11, 26-40.
25. Wei Zhang, **Tingjun Hou**, Xuebin Qiao, Xiaojie Xu, Some basic data structures and algorithms for chemical generic programming, *Journal of Chemical Information and Computer Sciences*, 2004, 44, 1571-1575.

(MORT, the new version of MHTL reported in this paper, was used in AMBER10 and release in 2008)

26. **Tingjun Hou**, Wei Zhang, Ke Xia, Xiaojie Xu, ADME evaluation in drug discovery. 5. Correlation of Caco-2 permeation with simple molecular properties, *Journal of Chemical Information and Computer Sciences*, 2004, 44, 1585-1600.

    (This paper is the 11th most assessed article of JCICS in 2004)

27. Wei Zhang, **Tingjun Hou**, Xuebin Qiao, Xiaojie Xu, Binding affinity of hydroxamate inhibitors of matrix metalloproteinase-2, *Journal of Molecular Modeling*, 2004, 10, 112-120.

28. **Tingjun Hou**, Ke Xia, Wei Zhang, Xiaojie Xu, ADME evaluation in drug discovery. 4. Prediction of aqueous solubility based on atom contribution approach, *Journal of Chemical Information and Computer Sciences*, 2004, 44, 266-275.

    (This paper is the 10th most assessed article of JCICS in 2004)

29. **Tingjun Hou**, Lili Zhu, Lirong Chen, Xiaojie Xu, Mapping the Binding Site of a Large Set of Quinazoline Type EGF-R Inhibitors Using Molecular Field Analyses and Molecular Docking Studies, *Journal of Chemical Information and Computer Sciences*, 2003, 43, 273-287.

30. **Tingjun Hou**, Xiaojie Xu, ADME Evaluation in Drug Discovery. 2. Prediction of Partition Coefficient by Atom-additive Approach Based on Atom-weighted Solvent Accessible Surface Areas, *Journal of Chemical Information and Computer Sciences*, 2003, 43, 1058-1067.

31. **Tingjun Hou**, Xiaojie Xu, ADME Evaluation in Drug Discovery. 3. Modeling Blood-Brain Barrier Partitioning Using Simple Molecular Descriptors. *Journal of Chemical Information and Computer Sciences*, 2003, 43, 2137-2152.

    (This database reported in this paper has been used by Bio-rad's KnowItAll system, http://www.bio-rad.com)

32. Wei Zhang, **Tingjun Hou**, Parameters for Generalized Born Model Consistent with RESP Atomic Partial Charge Assignment Protocol, *Journal of Physical Chemistry B*, 2003, 34, 9071-9078.

33. **Tingjun Hou**, Xiaojie Xu, ADME Evaluation in Drug Discovery. 1. Applications of Genetic Algorithms on the Prediction of Blood-brain Partitioning of a Large Set Drugs from Structurally Derived Descriptors, *Journal of Molecular Modeling*, 2002, 8 337-349.

34. **Tingjun Hou**, Xiaojie Xu, Predictions of binding of a diverse set of ligands to gelatinase-A by a combination of molecular dynamics and continuum solvent models, *Journal of Physical Chemistry B*, 2002, 106, 5527-5535.

35. **Tingjun Hou**, Xiaojie Xu, Empirical aqueous solvation models based on accessible surface areas with implicit electrostatics, *Journal of Physical Chemistry B*, 2002, 106, 11295-11304.

36. **Tingjun Hou**, Xiaojie Xu, Molecular docking simulations of a group of gelatinase-a inhibitors using molecular dynamics, *Journal of Computer-aided Molecular Design*, 2002, 16, 27-41.

37. Xuebin Qiao, **Tingjun Hou**, Wei Zhang, SenLi Guo, Xiaojie Xu, A 3D Structure Database of Bioactive Components from Chinese Traditional Medicinal Herb, *Journal of Chemical Information and Computer Sciences*, 2002, 42, 481-489.

38. Guo Senli, **Tingjun Hou**, Xiaojie Xu, Simulation of the phase behavior of the (EO)(13)(PO)(30)(EO)(13)(Pluronic L64)/water/p-xylene system using MesoDyn, *Journal of Physical Chemistry B*, 2002, 106, 11397-11403.

39. Huang Yanyi, Cheng Tianrong, Li Fuyou, Huang Chunhui, **Tingjun Hou**, Yu Anchi, Zhao Xinsheng, Xiaojie Xu, Photophysical studies on the mono- and dichromophoric hemicyanine dyes I. Photoelectric conversion from the dye modified ITO electrodes, *Journal of Physical Chemistry B*, 2002, 106, 10020-10030.

40. **Tingjun Hou**, Xiaojie Xu, A new molecular simulation software package – Peking University Drug Design System (PKUDDS) for structure-based drug design, *Journal of Molecular Graphics and Modeling*, 2001, 19, 455-465.

41. **Tingjun Hou**, Yu An, Binggen Ru, Bi Ruchang, Xiaojie Xu, Cysteine-indepent polymerization of metallothoneins in solutions and crystals, *Protein Science*, 2000, 9, 2302-2312.

42. **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Binding affinities for a series of selective inhibitors of gelatinase-A using molecular dynamics with a linear response method, *Journal of Physical Chemistry B*, 2001, 105, 5304-5315.
43. **Tingjun Hou**, Xiaojie Xu, The localization and adsorption of benzene and propylene in ITQ-1 zeolite: grand canonical Monte Carlo simulations, *Journal of Molecular Structure (THEO)*, 2001, 535, 9-23.
44. **Tingjun Hou**, Xiaojie Xu, The absorption of a series of aromatics in ITQ-1: Grand Canonical Monte Carlo simulations, *Journal of Molecular Catalysis A: Chemical*, 2001, 171, 103-114.
45. **Tingjun Hou**, Xiaojie Xu, Three-Dimensional quantitative structure activity relationship analysis of some cinnamamides, *Chemometrics and Intelligent Laboratory*, 2001, 56, 123-132.
46. Lili Zhu, **Tingjun Hou**, Xiaojie Xu, 3D QSAR analyses of novel tyrosine kinase phosphorylation inhibitors based on pharmacophore alignment, *Journal of Chemical Information and Computer Sciences*, 2001, 41, 1032-1040.
47. Lili Zhu, **Tingjun Hou**, Xiaojie Xu, Three-Dimensional Quantitative Structure-Activity Relationship Study on Paullones as CDKs inhibitors using CoMSIA and CoMFA, *Journal of Molecular Modeling*, 2001, 7, 223-230.
48. **Tingjun Hou**, Zhengming Li, Jie Liu, Xiaojie Xu, Three-dimensional quantitative structure activity relationship analysis of the new potent sulfonaylureas using Comparative Molecular Similarity Indices Analysis (CoMSIA), *Journal of Chemical Information and Computer Science*, 2000, 40, 1002-1009.
49. **Tingjun Hou**, Lili Zhu, Xiaojie Xu, Adsorption and diffusion of benzene in ITQ-1 type zeolite: Grand Canonical Monte Carlo and molecular dynamics simulation study, *Journal of Physical Chemistry B*, 2000, 104, 9356-9364.
50. **Tingjun Hou**, Youyong Li, Ning Liao, Xiaojie Xu, Three-dimension quantitative structure-activity relationship analysis of some cinnamamides using comparative molecular similarity indices analysis (CoMSIA), *Journal of Molecular Modeling*, 2000, 6, 438-445.
51. Youyong Li, **Tingjun Hou**, Kaixuan Wang, Senli Guo, The mesodyn simulation of pluronic water mixtures using the 'equivalent chain' method, *Physical Chemistry Chemical Physics*, 2000, 2, 2749-2753.
52. **Tingjun Hou**, Junmei Wang, Xiaojie Xu, Automatic docking of peptides and proteins using a hybrid method combined with genetic algorithm and tabu search, *Protein Engineering*, 1999, 12, 639-647.
53. **Tingjun Hou**, Junmei Wang, Ning Liao, Xiaojie Xu, Applications of genetic algorithms on the structure-activity relationships analysis of some cinnamamides, *Journal of Chemical information and computer science*, 1999, 39, 775-781.
54. **Tingjun Hou**, Junmei Wang, Xiaojie Xu, Applications of genetic algorithms on the structure-activity correlation study of a group of non-nucleoside HIV-1 inhibitors, *Chemometrics and Intelligent Laboratory system*, 1999, 45, 303-310.
55. Jummei Wang, **Tingjun Hou**, Xiaojie Xu, Automatic docking of peptides and proteins using genetic algorithm, *Chemometrics and Intelligent Laboratory system*, 1999, 45, 281-286.
56. Junmei Wang, **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Conformational analysis of peptides using Monte Carlo simulations combined with the genetic algorithm, *Chemometrics and Intelligent Laboratory system*, 1999, 45, 347-351.
57. Junmei Wang, Hua Zhang, Huixin He, **Tingjun Hou**, Xiaojie Xu, Theoretical studies on force titration of amino-group-terminated self-assembled monolayers, *Journal of Molecular Structure (THEO)*, 1998, 451, 295-303.

[C] In submitted

58. **Tingjun Hou**, William A. McLaughlin, Wei Wang, The prediction of the binding peptides of PKA RIIα using a hierarchical strategy, (submitted)

[D] Published on Chinese Journals:

59. **Tingjun Hou**, Xiaojie Xu, Calculations of free energies based on the combination of molecular dynamics simulations and continuum solvation model, *Progress in Chemistry*, 2004, 16, 153-158.
60. **Tingjun Hou**, Xiaojie Xu, Applications of genetic algorithms to computer-aided drug design, *Progress in Chemistry*, 2004, 16, 35-41.
61. Ke Xia, **Tingjun Hou**, Xiaojie Xu, Shen Xinhai, Molecular modeling of DPH-cyclodextrins nanotube-type aggregate, *Acta Physico-Chimica Sinica*, 2004, 20, 5-8.
62. Yongmei Pan, **Tingjun Hou**, Mingjuan Ji, Xiaojie Xu, MD simulations of PTP1B-inhibitor complex, *Acta Chimica Sinica*, 2004, 62, 148-152.
63. **Tingjun Hou**, Wei Zhang, Qin Huang, Xuebin Qiao, Xiaojie Xu, Empirical aqueous solvation model for protein based on accessible surface areas, *Acta. Phys. Chim. Sin.* 2003, 19, 723-726.
64. Wei Zhang, **Tingjun Hou**, Xuebin Qiao, Tingjun Hou, Parameters of GB/SA solvation models consistent with AMBER force field, *Acta Physico-Chimica Sinica*, 2003, 19, 289-292.
65. **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Molecular docking studies of the 4-anilinoquinazoline inhibitors with EGFR, *Acta Chimica Sinica*, 2002, 20, 221-227.
66. Lili Zhu**, Hou Tingjun**, Zhang Wei, Xu Xiaojie, Binding free energy calculations for MMP2-hydroxamate complexes, *Acta Chimica Sinica*, 2002, 60, 43-48.
67. **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Studies on interactions between EGFR and 4-anilinoquinazoline inhibitors, *Acta Chimica Sinica*, 2002, 60, 1023-1028.
68. **Tingjun Hou**, Wei Zhang, Xuebin Qiao, Xiaojie Xu, Prediction of binding free energies between benzamides and trypsin, *Acta Chimica Sinica*, 2002, 60, 1116-1121.
69. Xuebin Qiao, **Tingjun Hou**, Yu Huidong, Xiaojie Xu, Research and development of traditional Chinese medicine drugs information system based on networks, *Acta Physico-Chimica Sinica*, 2002, 18, 394-398.
70. Wei Zhang, **Tingjun Hou**, Xiaojie Xu, Binding preference of hydroxamate inhibitors of the matrix metalloproteinase-3, *Acta Chimica Sinica*, 60 (2002) 43.
71. **Tingjun Hou**, Yu An, Binggen Ru, Xiaojie Xu, Theoretical studies on the crystal packing form of MT-II from rat liver, *Chem. J. Chinese U*. 2002, 23, 271-274.
    Tingjun Hou, Xiaojie Xu, Aqueous solvation models based on accessible surface area calculations, *Acta Physico-Chimica Sinica*, 2002, 11, 1052-1056.
72. Xuebin Qiao, **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Prediction of Brain-blood partitioning using back progation network, *Acta Physica-Chimica Acta*, 2002, 18, 385-388.
73. Guo Senli, **Tingjun Hou**, Xiaojie Xu, Zhang Bin, Zhu Daoben, Crystal structure prediction of a new BEDT-TTF charge transfer salt, *Acta Physica-Chimica Acta*, 2002, 18, 289-291.
74. Lili Zhu, **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Molecular docking studies of the 4-anilinoquinazoline inhibitors with EGFR, *Acta Chimica Sinica*, 2002, 60, 43-48.
75. Xuebin Qiao, Bo Jiang, **Tingjun Hou**, Xiaojie Xu, Representation of Molecular Electrostatic Potentials Distribution on Surface of Proteins by Self-Organizing Feature Map, *Chinese Journal of Chemistry*, 2001, 19, 1172-1178.
76. **Tingjun Hou**, Xuebin Qiao, Xiaojie Xu, Research and development of 3D molecular structure database of traditional Chinese drugs, *Acta Chimica Sinica*, 2001, 59, 1788-1792.
77. **Tingjun Hou**, Xiaojie Xu, Recent Progress in Comparative Molecular Field Analysis (CoMFA), *Progress of Chemistry*, 2001, 13, 436-440.
78. Lili Zhu, **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Pharmacophore model analysis of novel tyrphostins, *Acta Chimica Sinica*, 2001, 59, 1078-1083.
79. Lili Zhu, **Tingjun Hou**, Xiaojie Xu,Molecular field analysis of two sets of non-peptide corticotropin-releasing hormone antagonists, *Acta. Chimica. SInica*, 2001, 59, 887-882.

80. **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Molecular docking simulations betweeen hydroxamtes and MMP-2, *Acta Chimica Sinica*, 2001, 59, 1184-1189.
81. **Tingjun Hou**, Lili Zhu, Xiaojie Xu, Mingjuan Ji, Ye Xueqi, Adsorption of some aromatic compounds in ITQ-1 zeolite: Grand canonical Monte Carlo simulations, *Chem. J. Chinese U.*, 2001, 22, 230-233.
82. Guo Senli, **Tingjun Hou**, Xiaojie Xu, Simulation of the phase separation of the pluronic L64/water/p xylene system using MesoDyn. *Acta Chimica Sinica*, 2001, 59, 2093-2098.
83. Wei Zhang, **Tingjun Hou**, Xiaojie Xu, Binding preference of hydroxamate inhibitors of the matrix metalloproteinase-3, *Acta Chimica Sinica*, 2001, 59, 2116-2121.
84. Changming Gu, **Tingjun Hou**, Xiaojie Xu, Comparative molecular field analysis of gamma-hydroxy butenolide endothelin antagonists, *Chem. J. Chinese U.* 2001, 22, 1864-1868.
85. **Tingjun Hou**, Yu An, Ruchang Bi, Binggen Ru, Xiaojie Xu, Studies on the metallothionein polymerization in different buffers, *Chem. J. Chinese U.* 2000, 21, 82.
86. **Tingjun Hou**, Junmei Wang, Youyong Li, Ning Liao, HongPeng Luo, Xiaojie Xu, An Automatic Conformation Selection Procedure using Genetic Algorithm in Comparative Molecular Field Analysis, *Computer and Applied Chemistry*, 2000, 17, 1
87. **Tingjun Hou**, Zenru Wu, Ning Liao, Zheng Li, Hongpeng Luo, Wang Jiaquan, Xiaojie Xu, Pharmacophore model and 3D-QSAR study of two kinds of HCV NS3 serine protease inhibitors, *Acta Physico-Chimica Sinica*, 2000, 16, 196-201.
88. **Tingjun Hou**, Yu An, Binggen Ru, Xiaojie Xu, Electrostatic interactions in three types of metallothioneins aggregates, *Acta Chimica Sinica*, 2000, 58, 313-318.
89. **Tingjun Hou**, Yu An, Binggen Ru, Xiaojie Xu, Theoretic studies on the mechanism of cations in metallothioneins polymerization, *Acta Physico-Chimica Sinica*, 2000, 16, 356-361.
90. **Tingjun Hou**, Yu An, Binggen Ru, Xiaojie Xu, Theoretic studies of dynamics stability to three kinds of metallothioneins, *Acta Physico-Chimica Sinica*, 2000, 16, 221-225.
91. **Tingjun Hou**, Yu An, Youyong Li, Binggen Ru, Xiaojie Xu, Studies on hydrophobic interactions of three kinds of metallothionein aggregates, *Acta Biophysica Sinica*, 2000, 1, 25.
92. **Tingjun Hou**, Xiaojie Xu, Adsorption of benzene in MCM-22 zeolite by grand canonical Monte Carlo simulation, *Acta Chimica Sinica*, 2000, 58, 1216-1220.
93. **Tingjun Hou**, Xiaojie Xu, Mingjuan Ji, Ye Xueqi, Diffusion of benzene in MCM-22 zeolite: A molecular dynamics study, *Acta Physico-Chimica Sinica*, 2000, 16, 701-707.
94. **Tingjun Hou**, Youyong Li, Yuangkang He, Xiaojie Xu, Substituents effect on the optical properties of benzonitrile and oligobenzonitriles. *Chinese Chemical Letters*, 2000, 11, 693-696.
95. Lili Zhu, **Tingjun Hou**, Xiaojie Xu, Computer simulation studies of the adsorption behaviors of xylenes in ITQ-1 zeolite, *Acta Physico-Chimica Sinica*, 2000, 16, 981-986.
96. Lili Zhu, **Tingjun Hou**, Xiaojie Xu, The Grand Canonical Monte Carlo simulations of benzene and propylene in ITQ-1 zeolite, *Chinese Chemical Letters*, 2000, 11, 623-626.
97. Youyong Li, **Tingjun Hou**, Wang Kanxuan, Guo Senli, Xiaojie Xu, Theoretical study of the mesoscopic morphology of the pluronics water mixtures, *Acta Chimica Sinica*, 2000, 58, 402-408.
98. **Tingjun Hou**, Junmei Wang, Xiaojie Xu, A comparison of three heuristic algorithms for molecular docking, *Chinese Chemical Letters*, 1999, 10, 651-618.
99. **Tingjun Hou**, Liu Hui, Xiaojie Xu, Localization and mobility of benzene in sodium-Y zeolite by Monte Carlo simulation, *Acta Chimica Sinica*, 1999, 57, 1004-1008.
100. Xiaojie Xu, **Tingjun Hou**, Junmei Wang, Lirong Chen. A new molecular design system - PUMDS based on intermolecular interactions, *Computer and Applied Chemistry*, 1999, 16, 334
101. **Tingjun Hou**, Mingjuan Ji, Liu Hui, Huang Xiaowei, Ye Xueqi, Xiaojie Xu, Molecular dynamics studies an thermal behavior of a FAU-type zeolite, *Chinese Chemical Letters*, 1999, 10, 515-518.

102. **Tingjun Hou**, Ning Liao, Luo Huopeng, Xiaojie Xu, An enhanced comparative molecular field analysis method using genetic algorithm, *Chinese Chemical Letters*, 1999, 10, 759-762.
103. **Tingjun Hou**, Junmei Wang, Youyong Li, Xiaojie Xu, Application of genetic algorithm to the QSAR research of pyrrolobenzothiazepinones and pyrrolobenzoxazepinones-novel and specific non-nucleoside HIV-1 reverse transcription inhibitors, *Chinese Chemical Letters*, 1998, 9, 651-654.

[E] Book Chapters:

104. **Tingjun Hou**, Xu Xiaojie, Recent development and application of virtual screening in drug discovery: An Overview. *in Frontier in Medicinal Chemistry*, Bentham Science Publishers, Vol 3, 2006, 675-703.
105. Xu Luo, "Chemical statistics", Science Publisher, 2002. (Chapter 16)
106. Xiaojie Xu, **Tingjun Hou**, Xuebin Qiao, Wei Zhang, "Computer-aided drug design: principle, methods and applications", Chemical Industrial Publisher, 2004. (Chapters 4 to 16)

4. Professional Activities:

- Reviewed papers for the following journals: *Journal of Medicinal Chemistry*, *Expert Opinion on Drug Metabolism & Toxicology*, *ChemMedChem*, *Molecular Pharmaceutics*, *Bioorganic & Medicinal Chemistry letters*, *Journal of Pharmacy and Pharmacology*, *Biomarker Insights*, *Medicinal Chemistry*, *Science in China*, *Acta Chimica Sinica*, *Acta Physico-Chimica Sinica*, etc.
- Developer for AMBER 10.
- Established and managed Wei Wang's group home page.
- Established and managed Xiaojie Xu's group PC cluster.

5. Awards:

- Award for outstanding thesis, Peking University, 2003.
- The first-level financial support for postdoctoral associates in China, sponsored by the Chinese Chemistry Society to only 10 first-level winners (only one for Chemistry) out of all postdoctoral associates in China, 2003
- Creative honor, Peking University, 2001
- The best 10 research undergraduates of Peking University, 2000
- JianHao honor, China. Awarded to 100 excellent graduates and undergraduates in China, 2000
- Guanghua Scholarship, 1999.

6. Memberships in Professional Organizations:

- Protein Society (2005 to present)
- American Chemistry Society (2006 to present)
- International Society for Computational Biology (ISCB) (2006 to present)

7. References:

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