TingJun Hou, Ph. D

College of Pharmaceutical Sciences,

Zhejiang University, Hangzhou, Zhejiang 310058, China

Telephone: 0512-65882039

Email: tingjunhou@zju.edu.cn or tingjunhou@hotmail.com

WWW: http://cadd.suda.edu.cn

1 Education and Professional Experience:

2013-now **College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, China**
Full professor in Computational Biology and Computer-aided Drug Design

2009-2012 **College of Pharmaceutical Sciences and Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, China**
Full professor in Computational Biology and Computer-aided Drug Design

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

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

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. Professional Activities:

- Member of editorial board: *Journal of Cheminformatics*
  Member of editorial board: *Theoretical Biology & Medical Modelling*
  Member of editorial board: *Genomics, Proteomics & Bioinformatics*
  Member of editorial board: *Journal of Pharmaceutics*
  Member of editorial advisory board: *Mini-Reviews in Medicinal Chemistry*
  Member of editorial advisory board: *Current Pharmaceutical Design*
  Member of editorial advisory board: *Current Computer-aided Drug Design*
  Member of editorial advisory board: *Medicinal Chemistry*
  Guest Editor: *Combinatorial Chemistry and High Throughput Screening*
- Reviewed papers for the following journals: *JACS, Drug Discovery Today, Molecular Pharmaceutics, Journal of Medicinal Chemistry, Journal of Chemical Information and Modeling, Journal of Pharmacy and Pharmacology, Journal of Computational Chemistry, Current Medicinal Chemistry, Expert review of clinical pharmacology, Expert Opinion on Drug Metabolism & Toxicology, Journal of Computer-aided Molecular Design, Bioinformatics, Proteins: Structure, Functions, and Bioinformatics, Journal of Physical Chemistry B, Journal of Physical Chemistry A, Biopolymer: Peptide Science, Journal of Molecular Graphics and Modeling, Retrovirology, PLoS One, Journal of Molecular Modeling, Chemical Biology & Drug Design, ChemMedChem, BMC Biology, Bioorganic & Medicinal Chemistry, Journal of Computer-aided Molecular Design, Mini-reviews in Medicinal Chemistry, Current Computer-aided Drug Design, Biomaker Insights, Letters in Drug Design & Discovery, Science in China, Progress in Biochemistry and Biophysics, Progress in Chemistry, Acta Chimica Sinica, Acta Physico-Chimica Sinica, Structure Chemistry (China), etc.*

- Developer for AMBER.

3. Research Experience:

[Computer-aided Drug Design]

- Development of an integrated intelligent system to predict the ADME/Tox properties and drug-likeness, including logP, pKa, logD, solubility, Caco-2 permeability, logBB, intestinal absorption, bioavailability, P-gp, CYP450 metabolism, hERG blockage and toxicity by using artificial neutral networks, support vector machine, Bayesian networks, graphics information, etc.
- Studies of HIV-1 protease drug resistance by using molecular dynamics, free energy calculations, and molecular interaction field analysis.
- Development of a new molecular handling C++ template and a new user interface for AMBER 10.

[Bioinformatics and Computational Biology]

- Determining the binding specificity and protein interacting partners of peptide-recognition protein domains by using binding free energy calculations and bioinformatics approaches.
- Development of methods for protein/ligand docking and scoring functions used in virtual screening.

Peer-reviewed Publications

[A] Invited reviews (*corresponding author):

1. Peichen Pan, Mingyun Shen, Huidong Yu, Youyong Li, Dan Li, **Tingjun Hou***, Advances in the development of Rho-associated protein kinase (ROCK) inhibitors, *Drug Discovery Today*, 2013, 18, 1323–1333.
2. Lei Xu, Youyong Li, Huiyong Sun, Xuechu Zhen, Chunhua Qiao, Sheng Tian, **Tingjun Hou***, Current developments of macrophage migration inhibitory factor (MIF) inhibitors, *Drug Discovery Today*, 2013, 18, 592-600..
3. Sichao Wang, Youyong Li, Lei Chen, **Tingjun Hou***, Advances on predicting hERG blockage in silico, *Current Topics in Medicinal Chemistry*, 2013, 13, 1317-1326.
4. Lei Chen, Youyong Li, Huidong Yu, Liling Zhang, **Tingjun Hou***, Computational models for predicting substrates and inhibitors of P-glycoprotein, *Drug Discovery Today*, 2012, 17, 343-351.
5. Fangliang Gan, Biyin Cao, Depei Wu, Zixing Chen, **Tingjun Hou***, Xinliang Mao*, Exploring Old Drugs for the Treatment of Hematological Malignancies, *Current Medicinal Chemistry*, 2011, 18, 1509-1514.
6. Youyong Li*, **Tingjun Hou**, Computational simulation of Drug delivery at molecular level, *Current Medicinal Chemistry*, 2010, 17, 4482-4491.
7. **Tingjun Hou***, Junmei Wang, Youyong Li*, Recent progress of *in silico* predictions of oral bioavailability, *Combinatorial Chemistry & High Throughput Screening*, 2011, 5, 362-372.
8. Junmei Wang, **Tingjun Hou**, Advances of computational predictions of solubility, *Combinatorial Chemistry & High Throughput Screening*, 2011, 5, 328-338.
9. 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*, 2010, 17, 1167-1180.
10. **Tingjun Hou***, Yongyong Li, Wei Zhang, Junmei Wang, In silico predictions of intestinal absorption and bioavailability, *Combinatorial Chemistry & High Through Screening*, 2009, 12, 497-506.

11. **Tingjun Hou***, Junmei Wang, Structure–ADME relationship: still a long way to go? *Expert Opinion on Drug Metabolism and Toxicology*, 2008, 4, 759-771.
12. **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.
13. 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.
14. **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:

15. Lei Xu, Yu Zhang, Longtai Zheng, Chunhua Qiao, Youyong Li, Dan Li, Xuechu Zhen*, **Tingjun Hou***, Discovery of novel inhibitors targeting macrophage migration inhibitory factor via structure-based virtual screening and bioassays, *Journal of Medicinal Chemistry*, 2014, 57, 3737-3745.
16. Juan Tang, Jingyu Zhu, Yu Yang, Zubing Zhang, Guodong Chen, Jie Li, Chunhua Qiao, **Tingjun Hou***, Xinliang Mao*, A virtual screen identified C96 as a novel inhibitor of phosphatidylinositol 3-kinase that displays potent preclinical activity in multiple myeloma in vitro and in vivo, *Oncotarget*, 2014, accepted.
17. Huiyong Sun, Youyong Li, Sheng Tian, Lei Xu, **Tingjun Hou***, Assessing the Performance of MM/PBSA and MM/GBSA Methods. 4. Accuracies of MM/PBSA and MM/GBSA Methodologies Evaluated by Various Simulation Protocols using PDBbind Data Set, *PCCP*, 2014, accepted.
18. Xiaotian Sun, Zhiwei Feng, **Tingjun Hou**, Youyong Li , The Mechanism of Graphene Oxide as an Enzyme Inhibitor from Molecular Dynamics Simulations, *ACS Applied Materials & Interfaces*, 2014, In press.
19. Zhenyu Guo, Oleg Prezhdo, **Tingjun Hou**, Xue Chen, Shuit-Tong Lee, Youyong Li, Fast Energy Relaxation by Trap States Decreases Electron Mobility in TiO2 Nanotubes: Time-Domain Ab Initio Analysis", *Journal of Physical Chemistry Letter*, 2014, 5, 1642.
20. Yedong Wang, Meiyu Wang, Huixin Qi, Peichen Pan, **Tingjun Hou**, Jiajun Li, Guangzhao He, Hongjian Zhang, Pathway-Dependent Inhibition of Paclitaxel Hydroxylation by Kinase Inhibitors and Assessment of Drug-Drug Interaction Potentials, *Drug Metabolism and Disposition*, 2014, in press.
21. Xuwen Wang, Peichen Pan, Youyong Li, Dan Li, **Tingjun Hou***, Insight into the prominent performance of CX-4945 derivatives: guidance for rational design of CK2 inhibitors, *Molecular Biosystems*, 2014, 10, 1196-1210.
22. Dan Li, Lei Xu, Youyong Li, Sheng Tian, Huiyong Sun, **Tingjun Hou***, ADMET Evaluation in Drug Discovery. 13. Development of in silico Prediction Models for P-glycoprotein Substrates, *Molecular Pharmaceutics*, 2014, 11, 716-726.
23. Yan Guan, Huiyong Sun, Youyong Li, Peichen Pan, Dan Li, **Tingjun Hou***, The competitive binding between inhibitors and substrates of HCV NS3/4A protease: a general mechanism of drug resistance, *Antiviral Research*, 2014, 103, 60-70.
24. Jingyu Zhu, Peichen Pan, Youyong Li, Man Wang, Dan Li, Binyin Cao, Xinliang Mao*, **Tingjun Hou***, Theoretical studies on beta and delta isoform-specific binding mechanisms of phosphoinositide 3-kinase inhibitors, *Molecular Biosystems*, 2014, 10, 454-466.

25. Biyin Cao, Jie Li, Jingyu Zhu, Mingyun Shen, Kunkun Han, Zubin Zhang, Yang Yu, Yali Wang, Depei Wu, Suning Chen, Aining Sun, Xiaowen Tang, Yun Zhao, Chunhua Qiao, **Tingjun Hou**, Xinliang Mao, The Antiparasitic Clioquinol Induces Apoptosis in Leukemia and Myeloma Cells by Inhibiting Histone Deacetylase Activity, *Journal of Biological Chemistry*, 2013, 288, 34181-34189.
26. Peichen Pan, Lin Li, Youyong Li, Dan Li*, **Tingjun Hou***, Insights into susceptibility of antiviral drugs against the E119G mutant of 2009 influenza A (H1N1) neuraminidase by molecular dynamics simulations and free energy calculations, *Antiviral Research*, 2013, 100, 356–364.
27. Jie Li, Biyin Cao, Shunye Zhou, Jingyu Zhu, Zubin Zhang, **Tingjun Hou**, Xinliang Mao, Cyproheptadine-induced myeloma cell apoptosis is associated with inhibition of the PI3K/AKT signaling, *European Journal of Haematology*, 2013, 91, 514-521.
28. Sheng Tian, Huiyong Sun, Youyong Li, Dan Li, Tingjun Hou*, Development and evaluation of an integrated virtual screening strategy by combining molecular docking and pharmacophore searching based on multiple protein structures, *Journal of Chemical Information and Modeling*, 2013, 53, 2743-2756.

    (One of the most read article in the last one month)
29. Huilong Dong, **Tingjun Hou**, Xiaotian Sun, Youyong Li*, Shuit-Tong Lee, The structures and properties of Si/SiOR2R core/shell quantum dots studied by density-functional tight-binding calculations, *Applied Physics Letters*, 2013, 103, 123115.
30. Huiyong Sun, Youyong Li*, Dan Li, Tingjun Hou*, Insight into Crizotinib Resistance Mechanisms Caused by Three Mutations in ALK Tyrosine Kinase using Free Energy Calculation Approaches, *Journal of Chemical Information and Modeling*, 2013, 53, 2376–2389.

    (One of the most read article in the last one month)
31. Liang Wu, **Tingjun Hou**, Youyong Li, K. S. Chan, Shui-Tong Lee, First-Principles Study on Migration and Coalescence of Point Defects in Mono-layer Graphene, *Journal Physical Chemistry C*, 2013, 117, 17066–17072.
32. Qian Zhang, Junmei Wang, Ginés D. Guerrero, José M. Cecilia, José M. García, Youyong Li, Horacio Pérez-Sánchez, **Tingjun Hou***, Accelerated Conformational Entropy Calculations Using Graphic Processing Units, *Journal of Chemical Information and Modeling*, 2013, 53, 2057–2064.
33. Wenkang Huang, Shaoyong Lu, Zhimin Huang, Xinyi Liu, Linkai Mou, Yu Luo, Yanlong Zhao, Yaqin Liu, Zhongjie Chen, Tingjun Hou, Jian Zhang, Allosite: a method for predicting allosteric sites, *Bioinformatics*, 2013, 29, 2357-2359.
34. Mingyun Shen, Shunye Zhou, Youyong Li, Dan Li, **Tingjun Hou***, Theoretical study on the interaction of pyrrolopyrimidine derivatives as LIMK2 inhibitors: insight into structure-based inhibitor design, *Molecular Biosystems*, 2013, 9, 2435 - 2446.

    (Inside cover story; Hot paper recommended by referees)
35. Sheng Tian, Youyong Li, Dan Li, Xiaojie Xu, Junmei Wang, Qian Zhang, **Tingjun Hou***, Modeling compound-target interaction network ofTraditional Chinese Medicines for type II diabetes mellitus: insight for polypharmacology and drug design, *Journal of Chemical Information and Modeling*, 2013, 53, 1787–1803.

    (One of the most read article in the last one month)
36. Lei Xu, Huiyong Sun, Youyong Li, Junmei Wang, **Tingjun Hou***, Assessing the Performance of MM/PBSA and MM/GBSA Methods. 3. The Impact of Force Fields and Ligand Charge Models, *Journal of Physical Chemistry B*, 2013, 117, 8408–8421.
37. Xiaohui Yu, **Tingjun Hou**, Youyong Li, Xuhui Sun, Shuit-Tong Lee, Effective Band Gap Reduction of Titanium Oxide Semiconductors by Codoping from First-Principles Calculations, International Journal of Quantum Chemistry, 2013, 23, 2546–2553.
38. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Transport of nucleosides in vcCNT facilitated by sodium gradients from Molecular Dynamics, *Molecular Biosystems*, 2013, 9, 2142-2153.

39. Yanfei Zhao, **Tingjun Hou**, Youyong Li, K. S. Chan, Shuit-Tong Lee, Effective increasing of optical absorption of TiO2 by introducing trivalent titanium, *Appl. Phys. Lett.* 2013, 102, 171902.

40. Wei Cui, Yuanhua Cheng, Lingling Geng, Densheng Liang, **Tingjun Hou***, Mingjuan Ji*, Unraveling the Mechanism of PTP1B by Free Energy Calculation Based on Umbrella Sampling, *Journal of Chemical Information and Modeling*, 2013, 53, 1157-1167.

(One of the most read article in the last one month)

41. Lei Xu, Youyong Li, Huiyong Sun, Dan Li,**Tingjun Hou***, Structural basis of the interactions between CXCR4 and CXCL12/SDF-1 revealed by theoretical approaches, *Molecular Biosystems*, 2013, 9, 2107-2117.

(One of the most read article in the last one month)

42. Jiangyong Gu, Qian Li, Lirong Chen, Youyong Li, **Tingjun Hou**, Gu Yuang, Xiaojie Xu, Platelet Aggregation Pathway Network-Based Approach for Evaluating Compounds Efficacy, *Evidence-Based Complementary and Alternative Medicine*, 2013, ID 425707.

43. Shunye Zhou, Youyong Li, **Tingjun Hou***, Feasibility of using molecular docking-based virtual screening for searching dual target kinase inhibitors, *Journal of Chemical Information and Modeling*, 2013, 53, 982-996.

(One of the most read article in the last one month)

44. Peichen Pan, Youyong Li, Huidong Yu, **Tingjun Hou***, Molecular principle of topotecan resistance by topoisomerase I mutations through molecular modeling approaches, *Journal of Chemical Information and Modeling*, 2013, 53, 997-1006.

45. Mingyun Shen, Huidong Yu, Youyong Li, Pixu Li, Peichen Pan, Shunye Zhou, Liling Zhang, Shang Li, Simon Ming-Yuen Lee*, **Tingjun Hou***, *Discovery of Rho-kinase inhibitors by docking-based virtual screening, Molecular Biosystems, 2013, 9, 1511-1521.*

(One of the most read article in the last one month)

46. Mingyun Shen, Shunye Zhou, Youyong Li, Peichen Pan, Liling Zhang, **Tingjun Hou***, Discovery and Optimization of Triazine Derivatives as ROCK1 Inhibitors: Molecular Docking, Molecular Dynamics Simulations and Free Energy Calculations, *Molecular Biosystems*, 2013, 9, 361-374.

47. Sheng Tian, Youyong Li, Junmei Wang, Xiaojie Xu, Lei Xu, Xiaohong Wang, Lei Chen, **Tingjun Hou***, Drug-likeness Analysis of Traditional Chinese Medicines: 2. Characterization of Scaffold Architectures for Drug-like compounds, Non-drug-like compounds, and Natural compounds from Traditional Chinese Medicines, *Journal of Chemoinformatics*, 2013, 5, 5.

48. Mingyun Shen, Sheng Tian, Youyong Li, Qian Li, Xiaojie Xu, Junmei Wang, **Tingjun Hou***, Drug-likeness analysis of Traditional Chinese Medicines: 1. Property distributions of Drug-like compounds, Non-drug-like compounds and Natural compounds from Traditional Chinese Medicines, *Journal of Chemoinformatics*, 2012, 4, 31.

(One of the most read article in the last one month)

49. Qian Zhang, Wei Zhang, Youyong Li, Junmei Wang, Liling Zhang, **Tingjun Hou***, A rule-based algorithm for automatic bond type perception, *Journal of Chemoinformatics*, 2012, 4, 26.

(One of the most read article in the last one month)

50. Lin Li, Youyong Li, Liling Zhang, **Tingjun Hou***, Theoretical studies on the susceptibility of oseltamivir against variants of 2009 A/H1N1 influenza neuraminidase, *Journal of Chemical Information and Modeling*, 2012, in press.

51. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Structure-based drug design for dopamine D3 receptor, *Combinatorial Chemistry & High Throughput Screening, 2012, accepted.*

52. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Unidirectional peristaltic movement in multisite drug binding pocket of AcrB from molecular dynamics simulations, *Molecular Biosystems*, 2012, 8, 2699-2709.

53. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Concerted movement in pH-dependent gating of FocA from molecular dynamics simulations, *Journal of Chemical Information and Modeling*, 2012, 52, 2119-2131.

54. Sheng Tian, Junmei Wang, Youyong Li, Xiaojie Xu, **Tingjun Hou***, Drug-likeness analysis of Traditional Chinese Medicines: 3. prediction of drug-likeness using machine learning approaches, *Molecular Pharmaceutics*, 2012, 9, 2875-2886.

55. Ming Liu, **Tingjun Hou**, Zhiwei Feng, Youyong Li, The flexibility of P-glycoprotein for its poly-specific drug binding from molecular dynamics, *Journal of Biomolecular Structure and Dynamics*, 2012, accepted.

56. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Concerted movement in pH-dependent gating of FocA from molecular dynamics simulations, *Journal of Chemical Information and Modeling*, 2012, accepted.

57. Zhiwei Feng, **Tingjun Hou**, Youyong Li, Unidirectional peristaltic movement in multisite drug binding pocket of AcrB from molecular dynamics simulations, *Molecular Biosystems*, 2012, accepted.

58. Lei Xu, Youyong Li, Lin Li, Shunye Zhou, **Tingjun Hou***, Understanding microscopic binding of macrophage migration inhibitory factor with phenolic hydrazones by molecular docking, molecular dynamics simulations and free energy calculations, *Molecular Biosystems*, 2012, 8, 2260-2273.

    (Hot paper highlighted by Molecular Biosystems)

59. Jing Zhang#, **Tingjun Hou# (co-first authors)**, Yang Liu, Gang Chen, Xiao Yang, Jun S. Li, Wei Wang, Systematic investigation on interactions for HIV drug resistance and cross-Resistance among protease inhibitors, *Journal of Proteome Science and Computational Biology*, 2012, in press.

60. Dongyue Cao, Junmei Wang, Rui Zhou, Youyong Li, Huidong Yu, **Tingjun Hou***, ADMET evaluation in drug discovery. 11. PharmacoKinetics Knowledge Base (PKKB) - a comprehensive database of pharmacokinetic and toxic properties for drugs, *Journal of Chemical Information and Modeling*, 2012, 52, 1132-1137.

    (The most read article in the last one month)

61. Junmei Wang, **Tingjun Hou**, Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations, *Journal of Chemical Information and Modeling*, 2012, 52, 1199-1212.

62. Yinxiang Wei, YuanFang Ma, Qing Zhao, Zhiguang Ren, Yan Li, **Tingjun Hou***, Hui Peng*, New Use for an old drug: inhibiting ABCG2 with sorafenib, *Molecular Cancer Therapeutics*, 2012, 11, 1693-1702.

63. Yanfei Zhao, **Tingjun Hou**, Liang Wu, Youyong Li, and Shuit-Tong Lee, Density functional calculations on silicon carbide nanostructures, *Journal of Computational and Theoretical Nanoscience*, 2012, in press.

64. **Tingjun Hou***, Nan Li, Youyong Li, Wei Wang, Characterization of domain-peptide interaction interface: prediction of SH3 domain-mediated protein-protein interaction network in yeast by generic structure-based models, *Journal of Proteome Research*, 2012, 11, 2982-2995.

65. Chongqian Zhang, **Tingjun Hou**, Youyong Li, Structure-Based Development of Antagonists for Chemokine Receptor CXCR4, *Current Computer-aided Drug Design*, 2012, in press.

66. Zhiwei Feng, **Tingjun Hou**, Youyong Li, The studies on the interactions between β2 adrenergic receptor and Gs protein by molecular dynamics simulations, *Journal of Chemical Information and Modeling*, 2012, 52, 1005-1014.

67. Sichao Wang, Youyong Li, Junmei Wang, Lei Chen, Liling Zhang, Huidong Yu, **Tingjun Hou***, ADME Evaluation in Drug Discovery. 12. Development of Binary Classification Models for Prediction of hERG Potassium Channel Blockage, *Molecular Pharmaceutics*, 2012, 9, 996-1010.

68. Xiaohui Yu, **Tingjun Hou**, Xuhui Sun, Youyong Li, The influence of defect on Mo-doped TiO2 by First Principles Studies, *ChemPhysChem*, 2012, 13, 1514-1521.

69. Junwei Xue, **Tingjun Hou**, Youyong Li, Optimal parameters for morphology of bulk heterojunction solar cells from simulations, *Applied Physics Letters*, 2012, 100, 053307.

70. Zheng Xu#, **Tingjun Hou**#(co-first author), Nan Li#, Yang Xu, Wei Wang, Proteome-wide detection of Abl1 SH3 binding peptides by integrating computational prediction and peptide microarray, *Molecular & Cellular Proteomics*, 2012, 11, O111.010389.

71. Jingyu Zhu, Youyong Li, Huidong Yu, Liling Zhang, Xinliang Mao, **Tingjun Hou***, Insight into the structural requirements of narlaprevir-type inhibitors of NS3/NS4A protease based on HQSAR and molecular field analyses, *Combinatorial Chemistry & High Throughput Screening*, 2012, 15, 439-450.

    (cover story)

72. Sheng Tian, Youyong Li, Junmei Wang, Jian Zhang*, **Tingjun Hou***, ADME Evaluation in Drug Discovery. 9. Prediction of Oral Bioavailability in Human based on Molecular Properties and Structural Fingerprints, *Molecular Pharmaceutics*, 2011, 2011, 8, 841-851.

    (One of the most read article in the last one month)

73. Nan Li, **Tingjun Hou**, Wei Wang, Characterization of PDZ domain-peptide interaction interface based on energetic patterns, *Proteins: Structure, Function, and Bioinformatics*, 2011, 79, 3208-3220.

74. Junmei Wang, **Tingjun Hou***, Application of Molecular Dynamics Simulations in Molecular Property Prediction II: Diffusion Coefficients, *Journal of Computational Chemistry*, 2011, 32, 3505-3519.

75. Junmei Wang, **Tingjun Hou***, Application of Molecular Dynamics Simulations in Molecular Property Prediction I: Density and Heat of Vaporization, *Journal of Chemical Theory and Computation*, 2011, 7, 2151-2165.

76. **Tingjun Hou***, Youyong Li, Wei Wang*, Prediction of peptides binding to the PKA RIIα subunit using a hierarchical strategy, *Bioinformatics*, 2011, 27, 1814-1821.

77. Yi Wang, **Tingjun Hou**, Sheng Tian, Shui-Tong Li, Youyong Li, Influence of doping effect on zinc oxide by first principles studies, *Journal of Physical Chemistry C*, 2011, 115, 7706-7716.

78. Lei Chen, Youyong Li, Qin Zhao, Hui Peng*, **Tingjun Hou***, ADME Evaluation in Drug Discovery. 10. Predictions of P-Glycoprotein Inhibitors using Recursive Partitioning and Naïve Bayesian Classification Techniques, *Molecular Pharmaceutics*, 2011, 8, 889-900.

79. **Tingjun Hou***, *In silico* predictions of ADME/T properties: progress and challenges, Combinatorial *Chemistry & High Throughput Screening*, 2011, 5, 306-306. (editorial materials)

80. Junmei Wang, Piotr Cieplak, Jie Li, **Tingjun Hou**, Ray Luo, and Yong Duan, Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability, *Journal of Physical Chemistry B*, 2011, 115, 3091-3099.

81. William A. McLaughlin, **Tingjun Hou**, Susan S. Taylor, Wei Wang, The identification of novel cyclic AMP-dependent protein kinase anchoring proteins using bioinformatic filters and peptide arrays, *Protein Engineering Design & Selection*, 2011, 24, 333-339.

82. Xinliang Mao, **Tingjun Hou**, Wenjiang Wang, Biyin Cao, Zhihua Li, Rose Hurren, Suzanne Trudel, Aaron D. Schimmer, The tricyclic anti-depressant amitriptyline inhibits D-cyclin transactivation and induces myeloma cell apoptosis by inhibiting histone deacetylases, *Molecular Pharmacology*, 2011, 79, 672-680.

83. **Tingjun Hou***, Junmei Wang, Youyong Li, Wei Wang*,Assessing the performance of the MM/PBSA and MM/GBSA methods: I. The accuracy of binding free energy calculations based on molecular dynamics simulations, *Journal of Chemical Information and Modeling*, 2011, 51, 69-82.

    (The most read article of JCIM in the last 12 months)

84. **Tingjun Hou***, Junmei Wang, Youyong Li, Wei Wang*, Assessing the performance of the MM/PBSA and MM/GBSA methods: II. The accuracy of ranking poses generated by molecular docking calculations, *Journal of Computational Chemistry*, 2011, 32, 866-877.

(Top ten most-cited paper in JCC from 2011)

85. Yaxue Zhao, Xuefeng Lu, Chaoyie Yang, Zhimin Huang, **Tingjun Hou***, Jian Zhang*, Computational Modeling Toward Understanding Agonist Binding on Dopamine 3, *Journal of Chemical Information and Modeling*, 2010, 50, 1633-1643.

86. Jing Zhang†, **Tingjun Hou**† (Co-first authors), Wei Wang, Jun S. Liu, A Bayesian Method for Detecting Combinatorial Mutation Patterns Responsible for HIV Drug Resistance, *Proceedings of the National Academy of Sciences*, 2010, 107, 1321-1326.

87. Junmei Wang, **Tingjun Hou**, Drug and Drug Candidate Building Block Analysis, *Journal of Chemical Information and Modeling*, 2010, 50, 55-67.

(The 5th most read article of JCIM in the past 12 months)

88. Wei Cui, Zhuo, Wei, Quan Chen, Yuanhua Chen, Lingling Geng, Jiang Zhang, Jianhua Chen*, **Tingjun Hou***, Mingjuan Ji*, Structure-based design of peptides with cytotoxicity on tumor cells, *Journal of Chemical Information and Modeling*, 2010, 50, 380-387.

(cover story)

89. Dawson, Marcial I, Ye Mao,…,**Tingjun Hou**,…,Zhang Xiaokun, Derivation of a Retinoid X Receptor Scaffold from Peroxisome Proliferator-Activated Receptor gamma Ligand 1-Di(1H-indol-3-yl)methyl-4-trifluoromethylbenzene, CHEMMEDCHEM, 2009, 4, 1106-1119.

90. Junmei Wang, **Tingjun Hou**, Xiaojie Xu, Aqueous Solubility Prediction Based on Weighted Atom Type Counts and Solvent Accessible Surface Areas, *Journal of Chemical Information and Modeling*, 2009, 49, 571-581.

91. **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, 8, 639-649..

92. **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*, 2009, 74, 837-846.

93. **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.

94. **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.

95. 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.

96. **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.

97. **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.

98. **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)

99. **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)

100. Junmei Wang, Xiangqun Xie, **Tingjun Hou**, Xiaojie Xu, Fast Approaches for Molecular Polarizability Calculations. *Journal of Physical Chemistry* A 2007, 111, 4443-4448.

101. 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.

102. **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)

103. **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.

104. 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.

105. 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.

106. 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.

107. 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.

108. **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.

109. 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)

110. **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)

111. 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.

112. **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)

113. **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.

114. **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.

115. **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)

116. 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.

117. **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.

118. **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.

119. **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.

120. **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.

121. 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.

122. 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.

123. 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.

124. **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.

125. **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.

126. **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.

127. **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.

128. **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.

129. **Tingjun Hou**, Xiaojie Xu, Three-Dimensional quantitative structure activity relationship analysis of some cinnamamides, *Chemometrics and Intelligent Laboratory*, 2001, 56, 123-132.

130. 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.

131. 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.
132. **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.
133. **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.
134. **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.
135. 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.
136. **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.
137. **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.
138. **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.
139. Jummei Wang, **Tingjun Hou**, Xiaojie Xu, Automatic docking of peptides and proteins using genetic algorithm, *Chemometrics and Intelligent Laboratory system*, 1999, 45, 281-286.
140. 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.
141. 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] Published on Chinese Journals:

142. **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.
143. **Tingjun Hou**, Xiaojie Xu, Applications of genetic algorithms to computer-aided drug design, *Progress in Chemistry*, 2004, 16, 35-41.
144. Ke Xia, **Tingjun Hou**, Xiaojie Xu, Shen Xinhai, Molecular modeling of DPH-cyclodextrins nanotube-type aggregate, *Acta Physico-Chimica Sinica*, 2004, 20, 5-8.
145. Yongmei Pan, **Tingjun Hou**, Mingjuan Ji, Xiaojie Xu, MD simulations of PTP1B-inhibitor complex, *Acta Chimica Sinica*, 2004, 62, 148-152.
146. **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.
147. 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.
148. **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Molecular docking studies of the 4-anilinoquinazoline inhibitors with EGFR, *Acta Chimica Sinica*, 2002, 20, 221-227.

149. Lili Zhu**, Hou Tingjun**, Zhang Wei, Xu Xiaojie, Binding free energy calculations for MMP2-hydroxamate complexes, *Acta Chimica Sinica*, 2002, 60, 43-48.
150. **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Studies on interactions between EGFR and 4-anilinoquinazoline inhibitors, *Acta Chimica Sinica*, 2002, 60, 1023-1028.
151. **Tingjun Hou**, Wei Zhang, Xuebin Qiao, Xiaojie Xu, Prediction of binding free energies between benzamides and trypsin, *Acta Chimica Sinica*, 2002, 60, 1116-1121.
152. 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.
153. Wei Zhang, **Tingjun Hou**, Xiaojie Xu, Binding preference of hydroxamate inhibitors of the matrix metalloproteinase-3, *Acta Chimica Sinica*, 60 (2002) 43.
154. **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.
155. 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.
156. 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.
157. 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.
158. 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.
159. **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.
160. **Tingjun Hou**, Xiaojie Xu, Recent Progress in Comparative Molecular Field Analysis (CoMFA), *Progress of Chemistry*, 2001, 13, 436-440.
161. Lili Zhu, **Tingjun Hou**, Lirong Chen, Xiaojie Xu, Pharmacophore model analysis of novel tyrphostins, *Acta Chimica Sinica*, 2001, 59, 1078-1083.
162. 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.
163. **Tingjun Hou**, Wei Zhang, Xiaojie Xu, Molecular docking simulations betweeen hydroxamtes and MMP-2, *Acta Chimica Sinica*, 2001, 59, 1184-1189.
164. **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.
165. 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.
166. Wei Zhang, **Tingjun Hou**, Xiaojie Xu, Binding preference of hydroxamate inhibitors of the matrix metalloproteinase-3, *Acta Chimica Sinica*, 2001, 59, 2116-2121.
167. Changming Gu, **Tingjun Hou**, Xiaojie Xu, Comparative molecular field analysis of gamma-hydroxy butenolide endothelin antagonists, *Chem. J. Chinese U.* 2001, 22, 1864-1868.
168. **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.
169. **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

170. **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.
171. **Tingjun Hou**, Yu An, Binggen Ru, Xiaojie Xu, Electrostatic interactions in three types of metallothioneins aggregates, *Acta Chimica Sinica*, 2000, 58, 313-318.
172. **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.
173. **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.
174. **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.
175. **Tingjun Hou**, Xiaojie Xu, Adsorption of benzene in MCM-22 zeolite by grand canonical Monte Carlo simulation, *Acta Chimica Sinica*, 2000, 58, 1216-1220.
176. **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.
177. **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.
178. 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.
179. 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.
180. 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.
181. **Tingjun Hou**, Junmei Wang, Xiaojie Xu, A comparison of three heuristic algorithms for molecular docking, *Chinese Chemical Letters*, 1999, 10, 651-618.
182. **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.
183. 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
184. **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.
185. **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.
186. **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:

187. Junmei Wang, **Tingjun Hou**, Recent Advances on in silico ADME Modeling, *Annual Reports in Computational Chemistry*, Elsevier, Volume 5, 2009, (in press)
188. **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.
189. Xu Luo, "Chemical statistics", Science Publisher, 2002. (Chapter 16)
190. Xiaojie Xu, Tingjun Hou, Xuebin Qiao, Wei Zhang, "Computer-aided drug design: principle, methods and applications", Chemical Industrial Publisher, 2004. (Chapters 4 to 16)

191. *Molecular* Conceptor *courseware*, Synergix Ltd. 2008. (Contributing the chapter: introduction to chemoinformatics).

6. Awards:

- Science and technology advancement award of Chinese Universities, Second Class (rank 2), 2008
- 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.

7. Memberships in Professional Organizations:

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