

## Deju Ye

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### EDUCATION

- 09/2009–Present Postdoctoral Fellow in Chemical Biology and Molecular Imaging, Department of Radiology, School of Medicine, **Stanford University**, CA, USA.  
*Research Advisor:* Prof. Jianghong Rao
- 09/2004–07/2009 Ph.D. in Medicinal Chemistry and Drug Design, **Shanghai Institute of Materia Medica**, Chinese Academy of Science, Shanghai, China.  
*Dissertation:* “Drug Design, Synthesis and Pharmacological Research of Privileged Structures”  
*Supervisors:* Prof. Hong Liu and Prof. Hualiang Jiang
- 09/2000–07/2004 B.S. in Chemistry, School of Chemistry and Chemical Engineering, **Nanjing University**, Jiangsu, China.

### RESEARCH EXPERIENCE

09/2009–Present **Postdoctoral research in Molecular Imaging Groups at Stanford (MIPS).**

Major responsibility was developing multimodality molecular imaging probes for enzyme activity detection in cells and *in vivo*.

- Researched on a biocompatible reaction and apply it to self-assemble small molecule fluorescence probes into nanoparticles for imaging of enzyme activity in living cells.
- Developed caspase-3 sensitive near-infrared (NIR) probes for non-invasive optical monitoring of chemotherapy-induced tumor cell death *in vivo*.
- Researched on caspase-activatable Gd-based magnetic resonance imaging (MRI) probes for high-resolution imaging of tumor apoptosis in living mice.
- Real-time monitoring of stem cell death after implantation in rat using caspase-activatable MRI probes (Collaboration with Prof. Heike Daldrup-Link at Stanford).
- Develop a “smart”  $^{19}\text{F}$ -MRS/ $^1\text{H}$  MRI dual-function probe for detection of protease activity.
- Develop reactive oxygen species (ROS)-responsive  $^{19}\text{F}$ -MRI probes for imaging of inflammation *in vivo*.
- Participate in the development of  $^{18}\text{F}$ -labeled nano-aggregation probe for positron emission tomography (PET) imaging of drug-induced tumor apoptosis.

09/2004–07/2009 **Graduate research in Drug Discovery and Design Center (DDDC), Shanghai Institute of Materia Medica, Chinese Academy of Science.**

Major responsibility was drug design, synthesis and pharmacological research of privileged structures on several disease targets, and development of efficient methods for the synthesis of sialic acid derivatives and gold-catalyzed coupling reaction to assemble heterocycles.

- Designed zanamivir analogues as neuraminidase (NA) inhibitors for anti-avian influenza agents.
- Developed xanthine derivatives as potent anti-tumor agents with an integration of inverse *in silico* screening for potential target identification.
- Developed potent 5-lipoxygenase (5-LOX) inhibitors via a combination of focused library design, virtual screening, chemical synthesis and bioassay.
- Discovery of novel thiophene derivatives as selective and cell permeable protein-tyrosine phosphatase 1B (PTP1B) inhibitors by using virtual screening and structure-based drug design.
- Participated in preclinical development of anti-HIV drug **DC32**: synthesized and optimized its prodrugs to improve pharmacokinetics (PK) profiles.
- Developed an efficient approach for the asymmetric synthesis of sialic acid derivatives, sialic acid dimers and  $\alpha$ -sialosides.
- Developed a green chemistry approach for rapid synthesis of *N*-heterocyclic compounds via Au(I)- and Ag(I)-catalyzed coupling reactions in water.

### **RESEARCH PROGRAM**

- 2009–Present Multimodality imaging of enzyme activity *in vitro* and *in vivo*. Center for Cancer Nanotechnology Excellence and Translation, an NCI-NIH U54 grant (# 1U54CA151459), and the NCI ICMIC@Stanford (1P50A114747-06).
- 2005–2009 Research in the development of zanamivir and its analogues as anti-AIV drugs. State Key Program of Basic Research of China (Grant 2006BAI01B02), National Natural Science Foundation of China (Grants 20721003), and a grant from the Korea Healthcare Technology R&D project, Ministry for Health, Welfare Family Affairs, Republic of Korea. (A085105).
- 2005–2007 Research in the development of 5-LOX inhibitors. The Key Project from the Shanghai Science and Technology Commission (Grant 02DJ14006).
- 2006-2009 New drug research program: 863 Hi-Tech Program of China (Grants 2006AA020402 and 2006AA020602), and International Collaboration Projects (grants 2007DFB30370 and 20720102040)

### **PUBLICATIONS**

*Peer Reviewed Journal Articles (H-index: 14 based on citations from Web of Science)*

1. **Deju Ye**, Adam J. Shuhendler, Lina Cui, Ling Tong, Sui Seng Tee, Grigory Tikhomirov, Dean W. Felsher and Jianghong Rao. Bioorthogonal Cyclization-mediated *In Situ* Self-Assembly of Small-Molecule Probes for Imaging Caspase Activity in Living Mice. *Nat. Chem. Accepted*.
2. **Deju Ye**, Gaolin Liang, Man Lung Ma, and Jianghong Rao. Controlling Intracellular Macrocyclization for the Imaging of Protease Activity. *Angew. Chem. Int. Ed.* **2011**, *50*, 2275–2279. (IF = 13.734)
3. **Deju Ye**, Woo-Jin Shin, Ning Li, Wei Tang, Enguang Feng, Jian Li, Pei-Lan He, Jian-Ping Zuo, Hanjo Kim, Ky-Youb Nam, Weiliang Zhu, Baik-Lin Seong, Kyoung Tai No, Hualiang Jiang, and Hong Liu. Synthesis of C-4 Modified Zanamivir Analogs as Neuraminidase Inhibitors and Their Anti-AIV activities. *Eur. J. Med. Chem.* **2012**, *54*, 764-770. (IF = 3.499)
4. **Deju Ye**, Yu Zhang, Fei Wang, Mingfang Zheng, Xu Zhang, Xiaoming Luo, Xu Shen, Hualiang Jiang, and Hong Liu. Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. *Bioorg. Med. Chem.* **2010**, *18*, 1773–1782. (IF = 2.903)
5. **Deju Ye**, Jinfang Wang, Xu Zhang, Yu Zhou, Xiao Ding, Enguang Feng, Haifeng Sun, Guannan Liu, Hualiang Jiang, and Hong Liu. Gold-catalyzed intramolecular hydroamination of terminal alkynes in aqueous media: efficient and regioselective synthesis of indole-1-carboxamides. *Green Chem.* **2009**, *11*, 1201–1208. (IF = 6.828)
6. **Deju Ye**, Xu Zhang, Yu Zhou, Dengyou Zhang, Lei Zhang, Hengshuai Wang, Hualiang Jiang, and Hong Liu. Gold- and Silver-Catalyzed Intramolecular Hydroamination of Terminal Alkynes: Water-Triggered Chemo- and Regioselective Synthesis of Fused Tricyclic Xanthines. *Adv. Synth. Catal.* **2009**, *351*, 2770–2778. (IF = 5.535)
7. **Deju Ye**, Wenfeng Liu, Dengyou Zhang, Enguang Feng, Hualiang Jiang, and Hong Liu. Efficient Dehydrative Sialylation of C-4-Aminated Sialyl-hemiketal Donors with Ph<sub>2</sub>SO/Tf<sub>2</sub>O. *J. Org. Chem.* **2009**, *74*, 1733–1735. (IF = 4.564)
8. **Deju Ye**, Jiang Wang, Kunqian Yu, Yu Zhou, Hualiang Jiang, Kaixian Chen, and Hong Liu. Current Strategies for the Discovery of K(+) Channel Modulators. *Curr. Top. Med. Chem.* **2009**, *9*, 348–361. (IF = 3.702)
9. **Deju Ye**, Guanghui Deng, Wenfeng Liu, Yu Zhou, Enguang Feng, Hualiang Jiang, and Hong Liu. Simultaneous 2-O-Deacetylation and 4-Amination of Peracetylated Neu5Ac: Application to the Synthesis of (4→4)-Piperazine Derivatives Linked Sialic Acid Dimers. *Tetrahedron* **2008**, *64*, 6544–6550. (IF = 2.803)
10. **Deju Ye**, Jian Li, Jian Zhang, Hong Liu, and Hualiang Jiang. Simultaneous stereoselective 4-amination with cyclic secondary amines and 2-O-deacetylation of peracetylated sialic acid derivatives. *Tetrahedron Lett.* **2007**, *48*, 4023–4027. (IF = 2.397)
11. **Deju Ye**, Jinfang Wang, Dengyou Deng, Enguang Feng, Hualiang Jiang, and Hong Liu. Advances in O-Sialylation. *Progress in Chemistry* **2010**, *22*, 91–100. (IF = 0.670)
12. **Deju Ye**, Xiaomin Luo, Jianhua Shen, Weiliang Zhu, Xu Shen, Hualiang Jiang, and Hong Liu. Discovery potential drug leads via docking, synthesis and bioassay. *Progress in Chemistry* **2007**, *19*, 1939–1946. (IF = 0.670)

13. Bin Shen, Jongho Jeon, Mikael Palner, **Deju Ye**, Adam Shuhendler, Frederick T. Chin, and Jianghong Rao. Positron Emission Tomography Imaging of Drug-Induced Tumor Apoptosis with a Caspase-Triggered Nano-aggregation Probe. *Angew. Chem. Int. Ed.* **2013**, *52*, 10511-10514 (inside cover paper). (IF = 13.734)
14. Gaolin Liang, John Ronald, Yuanxin Chen, **Deju Ye**, Prachi Pandit, Man Lung Ma, Brian Rutt, and Jianghong Rao. Controlled Self-Assembling of Gadolinium Nanoparticles as Smart Molecular Magnetic Resonance Imaging Contrast Agents. *Angew. Chem. Int. Ed.* **2011**, *50*, 6283–6286. (IF = 13.734)
15. Enguang Feng, Woo-Jin Shin, Xuelian Zhu, Jian Li, **Deju Ye**, Jiang Wang, Mingyue Zheng, Jian-Ping Zuo, Kyoung Tai No, Xian Liu, Weiliang Zhu, Wei Tang, Baik-Lin Seong, Hualiang Jiang, and Hong Liu. Structure-Based Design and Synthesis of C-1- and C-4-Modified Analogs of Zanamivir as Neuraminidase Inhibitors. *J. Med. Chem.* **2013**, *56*, 671-684. (IF = 5.614)
16. Enguang, Feng, **Deju Ye**, Jian Li, Dengyou Zhang, Jinfang Wang, Fei Zhao, Rolf Hilgenfeld, Mingyue Zheng, Hualiang Jiang, and Hong Liu. Recent Advances in Neuraminidase inhibitor Development as Anti-influenza Drugs. *ChemMedChem* **2012**, *7*, 1527-1536. (IF = 2.835)
17. Diliang Guo, Tao Chen, **Deju Ye**, Jinyi Xu, Hualiang Jiang, Kaixian Chen, Hui Wang, and Hong Liu. Cell-Permeable Iminocoumarine-Based Fluorescent Dyes for Mitochondria. *Org. Lett.* **2011**, *13*, 2884–2887. (IF = 6.142)
18. Xu Zhang, Yu Zhou, Hengshuai Wang, Diliang Guo, **Deju Ye**, Yungen Xu, Hualiang, Jiang, and Hong Liu. An Effective Synthetic Entry to Fused Benzimidazoles via Iodocyclization. *Adv. Synth. Catal.* **2011**, *353*, 1429–1437. (IF = 5.535)
19. Xu Zhang, Yu Zhou, Hengshuai Wang, Diliang Guo, **Deju Ye**, Yungen Xu, Hualiang, Jiang, and Hong Liu. Silver-catalyzed intramolecular hydroamination of alkynes in aqueous media: efficient and regioselective synthesis for fused benzimidazoles. *Green Chem.* **2011**, *13*, 397–405. (IF = 6.828)
20. Lei Zhang, **Deju Ye**, Yu Zhou, Guannan Liu, Enguang Feng, Hualiang Jiang, and Hong Liu. Regioselective Synthesis of 3-Benzazepinones and Unexpected 5-Bromo-3-benzazepinones. *J. Org. Chem.* **2010**, *75*, 3671–3677. (IF = 4.564)
21. Dengyou Zhang, **Deju Ye**, Enguang Feng, Jinfang Wang, Jianmei Shi, Hualiang Jiang, and Hong Liu. Highly alpha-Selective Synthesis of Sialyl Spirohydantoin by Regiospecific Domino Condensation/O→N Acyl Migration/N-Sialylation of Carbodiimides with Peracetylated Sialic Acid. *J. Org. Chem.* **2010**, *75*, 3552–3557. (IF = 4.564)
22. Haifeng Sun, **Deju Ye**, Hualiang Jiang, Kaixian Chen, and Hong Liu. One-Pot Approach for C-C Bond Formation through Ruthenium-Amido Complex Catalyzed Tandem Aldol Reaction/Hydrogenation. *Synthesis* **2010**, *15*, 2577–2582. (IF = 2.500)
23. Yu Zhou, Yun Zhai, Jian Li, **Deju Ye**, Hualiang Jiang, and Hong Liu. Metal-free tandem reaction in water: An efficient and regioselective synthesis of 3-hydroxyisoindolin-1-ones. *Green Chem.* **2010**, *12*, 1397–1404. (IF = 6.828)

24. Enguang Feng, He Huang, Yu Zhou, **Deju Ye**, Hualiang Jiang, and Hong Liu. Metal-Free Synthesis of 2-Substituted (N, O, C) Benzothiazoles via an Intramolecular C-S Bond Formation. *J. Comb. Chem.* **2010**, *12*, 422–429. (IF = 4.933)
25. Yu Zhou, Yun Zhai, Xun Ji, Guannan Liu, Enguang Feng, **Deju Ye**, Linxiang Zhao, Hualiang Jiang, and Hong Liu. Gold(I)-Catalyzed One-Pot Tandem Coupling/Cyclization: An Efficient Synthesis of Pyrrolo-/Pyrido[2,1-b]benzo[d][1,3]oxazin-1-ones. *Adv. Synth. Catal.* **2010**, *352*, 373–378. (IF = 5.535)
26. Xiaodong Zhang, **Deju Ye**, Haifeng Sun, Diliang Guo, Jiang Wang, He Huang, Xu Zhang, Hualiang Jiang, and Hong Liu. Microwave-assisted synthesis of quinazolinone derivatives by efficient and rapid iron-catalyzed cyclization in water. *Green Chem.* **2009**, *11*, 1881–1888. (IF = 6.828)
27. Xiao Ding, **Deju Ye**, Fang Liu, Guanghui Deng, Guannan Liu, Xiaomin Luo, Hualiang Jiang, and Hong Liu. Efficient Synthesis of alpha-Aryl-/Heteroaryl-Substituted beta-Amino Acids via Ni(II) Complex through the Suzuki Coupling Reaction. *J. Org. Chem.* **2009**, *74*, 5656–5659. (IF = 4.564)
28. Guannan Liu, Yu Zhou, **Deju Ye**, Dengyou Zhang, Xiao Ding, Hualiang Jiang, and Hong Liu. Silver-Catalyzed Intramolecular Cyclization of o-(1-Alkynyl)benzamides: Efficient Synthesis of (1H)-Isochromen-1-imines. *Adv. Synth. Catal.* **2009**, *351*, 2605–2610. (IF = 5.535)
29. Yu Zhou, Enguang Feng, Guannan Liu, **Deju Ye**, Jian Li, Hualiang Jiang, and Hong Liu. Gold-Catalyzed One-Pot Cascade Construction of Highly Functionalized Pyrrolo[1,2-a]quinolin-1(2H)-ones. *J. Org. Chem.* **2009**, *74*, 7344–7348. (IF = 4.564)
30. Enguang Feng, He Huang, Yu Zhou, **Deju Ye**, Hualiang Jiang, and Hong Liu. Copper(I)-Catalyzed One-Pot Synthesis of 2H-1,4-Benzoxazin-3-(4H)-ones from o-Halophenols and 2-Chloroacetamides. *J. Org. Chem.* **2009**, *74*, 2846–2849. (IF = 4.564)
31. Guanghui Deng, **Deju Ye**, Lingyan He, Yu Zhou, Jiang Wang, Hualiang Jiang and Hong Liu. Synthesis of (S)-, (R)- and (rac)-2-amino-3,3-bis(4-fluorophenyl)propanoic acids and an evaluation of the DPP IV inhibitory activity of denagliptin diastereomers. *Tetrahedron* **2008**, *64*, 10512–10516. (IF = 2.803)
32. Jian Li, **Deju Ye**, Hong Liu, Xiaomin Luo, and Hualiang Jiang. Microwave-assisted dehalogenation of a-haloketones by zinc and ammonium chloride in alcohol. *Synth. Commun.* **2008**, *38*, 567–575. (IF = 1.060)
33. Mingfang Zheng, Mingyue Zheng, **Deju Ye**, Yangmei Deng, Shuifeng Qiu, Xiaomin Luo, Kaixian Chen, Hong Liu, and Hualiang Jiang. Indole derivatives as potent inhibitors of 5-lipoxygenase: Design, synthesis, biological evaluation, and molecular modeling. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 2414–2420. (IF = 2.338)
34. Zhiyi Yao, **Deju Ye**, Hong Liu, Kaixian Chen, and Hualiang Jiang. Transformation of aryl acyloln O-alkyl and O-phenyl derivatives to ketones. *Synth. Commun.* **2007**, *37*, 149–156. (IF = 1.060)

35. Yuan Huang, **Deju Ye**, Qing Sun, Jianyi Shen. Surface modification and characterization of vapor grown carbon fibers. *Chin. J. Inorg. Chem.* **2006**, 22, 403–410. (IF = 0.720)

***Papers in preparation and to be submitted.***

36. **Deju Ye**, Prachi Pandit, Paul Kempen, Eddy Li, Liqing Xiong, Robert Sinclair, Brian Rutt, and Jianghong Rao. Activatable MRI Probes Using Controlled Macrocyclization for Self-Assembly of Gadolinium Nanoparticles. *To be submitted.*
37. **Deju Ye**, Adam J. Shuhendler, Prachi Pandit, Kimberly D. Brewer, Brian Rutt, and Jianghong Rao. Imaging chemotherapy-induced tumor cell apoptosis with gadolinium-based "smart" MRI probes *in vivo*. *To be submitted.*
38. Hossein Nejadnik\*, **Deju Ye**\*, Olga, Lenkov, John Martin, Jessica Doing, Rostislav Castillo, Nikita Derugin, Barbara Sennino, Jianghong Rao, Heike Daldrup-Link. MR imaging of stem cell apoptosis transplanted in rats with a caspase-activatable Gd-based contrast agent. (\*Co-first author). *To be submitted.*
39. **Deju Ye**, Kimberly D. Brewer, Adam J. Shuhendler, Brian Rutt, and Jianghong Rao. A "smart"  $^{19}\text{F}$ -MRS/ $^1\text{H}$  MRI dual-function probe for detection of caspase-3 activity. *In preparation.*
40. **Deju Ye**, Miao Hao, Tao Chen, Honglin, Li, Dengyou, Zhang, Hui Wang, Hualiang Jiang, Hong Liu. Design, Synthesis, and Biological Evolution of Novel 8-Phenylxanthine Derivatives in Human Cancer Cells. *In preparation.*
41. **Deju Ye**, Mingyue Zheng, Hualiang Jiang, Hong Liu. Discovery of novel xanthine analogues as potent 5-lipoxygenase inhibitors through rational drug design. *In preparation.*

**PATENTS**

1. Jianghong Rao, **Deju Ye**, Adam Shuhendler, Jonho Jeon, Bin Shen, Frederick T. Chin. Caspase-3 imaging probes. (US Patent, application number: 61/869233).
2. Hong Liu, Hui Wang, Hualiang Jiang, **Deju Ye**, Miao Hao, Tao Chen, Hengshuai Wang, Jinfang Wang, Kaixian Chen. Preparation and application of 8-phenyl xanthine compounds. CN Patent, 201010183800.3.
3. Hong Liu, Hualiang Jiang, Yu Zhou, Mingyue Zheng, **Deju Ye**, Xiaoming Luo, Weiliang Zhu, Kaixian Chen. Preparation and application of pyrazole derivatives as 5-LOX inhibitors. CN Patent, 200810035186.9.
4. Hong Liu, Hualiang Jiang, Yu Zhou, Mingyue Zheng, **Deju Ye**, Xiaoming Luo, Weiliang Zhu, Kaixian Chen. Preparation and application of 5-LOX inhibitors. CN Patent, 200810200408.8.

**CONFERENCE ABSTRACTS**

***Oral Presentations***

1. “Controlled in situ nano-aggregation of caspase-3/7 activatable fluorescent and MRI probes for dual-modality imaging of tumor cell death”, 2013 World Molecular Imaging Congress. Savannah, GA, USA, Sep 2013. (Highlight lecture).
2. “Controlled self-assembly of nanostructures for imaging protease activity”, Molecular Imaging Program at Stanford (MIPS) Philips Molecular Imaging Seminar Series, Stanford University, CA, USA, Aug 2011.

### ***Poster Presentations***

3. Sep 2012: Poster at 2012 World Molecular Imaging Congress (P105). Dublin, Ireland.
4. Sep 2011: Poster at NCI Alliance Nano 2011 meeting. Boston, MA, USA.
5. Sep 2011: Poster at 2011 World Molecular Imaging Congress (P036). San Diego, CA, USA.
6. Mar 2011: Poster at 3<sup>rd</sup> Annual CBIS Symposium. Stanford University.
7. Jul 2008: Poster at the 6<sup>th</sup> International Symposium for Chinese Medicinal Chemists (p253). Shanghai, China.
8. Jun 2008: Poster at the 26<sup>th</sup> Chinese Chemical Society (CCS) Congress (03-P-79). Tianjin, China.

### **HONORS AND AWARDS**

- 2013: Travel Awards at 2013 World Molecular Imaging Congress (WMIC), Savannah, GA, USA.
- 2012: The 1<sup>st</sup> Place Poster Awards at 2012 World Molecular Imaging Congress (WMIC), Dublin, Ireland (Co-first author with Adam Shuhendler in Prof. Jianghong Rao lab).
- 2011: The 5<sup>th</sup> Place NCI Alliance Nano 2011 Poster Award, Boston, USA
- 2009: Excellent Graduate Student of Chinese Academy of Science
- 2008: The 2<sup>nd</sup> Prize of Excellent Paper in the Organic Chemistry Session of the 26<sup>th</sup> Chinese Chemical Society (CCS) Congress, Tianjin, China

### **REFERENCES**

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