Shao-Gang Li, Ph.D.

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Research Experience:

Nov. 2012 - Present Postdoctoral fellow, in Prof. Joel S. Freundlich's Lab, Center for Emerging and Re-emerging Pathogens; Department of Pharmacology & Physiology; Rutgers University-New Jersey Medical School

- Designed and synthesized 88 thienopyrimidines, 23 of which are active against *Mycobacterium tuberculosis* (MIC ≤ 10 μg/mL). Improved *in vivo* stability of the lead compound through metabolomics-informed approach.
- Synthesized 25 novel carbapenems (analogs of meropenem and imipenem). 15 of these have MIC≤ 10 μg/mL against *M. tuberculosis*. Structure-based design techniques were utilized to improve both select pathogen and broad-spectrum efficacy.
- Synthesized novel antitubercular triazines analogs. Improved solubility and cell permeability through a medicinal chemistry heuristic-based approach.

Sep. 2007-July 2012 Dissertation research, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences.*Advisor*: Professor Yikang Wu

- Completed the first total synthesis of the natural product demethyl cezomycin.
- Developed a novel tandem ring-opening 1,5-hydrogen transfer reaction of cyclopropane.
- Created a novel allyl transfer coupled with a Grob fragmentation reaction.
- Developed regioselective reduction of the C–C double bonds inα, β-unsaturated acyl 4-substituted oxazolidin-2-ones and oxazoline-2-thiones.

Jan. 2007-June 2007 Undergraduate research, Nanjing University
Advisor: Professor Li-Min Zheng

- Performed microwave-assisted preparation of mixed-valent manganese phosphonate clusters

Education

Sep. 2007-July 2012 Ph.D. in Organic Chemistry
Advisor: Professor Yikang Wu
Shanghai Institute of Organic Chemistry,
Chinese Academy of Sciences, China

Sep. 2003-July 2007 B.S. in Chemistry
Advisor: Professor Li-Min Zheng
Nanjing University, Nanjing, China

Skills and Competences:

- Extensive experience in organic synthesis, which includes total synthesis of natural products and synthesizing novel antibacterial compounds with a range of chemotypes. Skilled in designing multi-step synthesis and overcoming synthetic hurdles encountered during these

syntheses.

- Substantial experience in the development of new reactions and new methodologies.
- Skilled in SAR studies and optimizing compounds to enhance whole-cell biological activity and metabolic stability. Experienced in collaborating with biologists and computational chemists and with utilizing metabolomics and modeling data to help guide drug discovery.
- Familiar with BSL2/BSL3 studies: MIC assay, development of drug resistant mutants, and DNA extraction from *M tuberculosis*.
- Expertat modern analysis, purification, and structural identification techniques, including NMR, IR, LC/MS, and HPLC. Trained multiple lab members how to perform all of these techniques.
- Skilled in utilizing SciFinder, Reaxys, and ChemOffice.

Publications:

1. Li, J-T.; Ma, Y-S.; Li, S-G.; Cao, D-K.; Li, Y-Z.; Song, Y.; Zheng, L-M. Mixed-valent manganese phosphonateclusters prepared under microwave-assisted and ambient conditions. *Dalton Trans*., **2009**, 5029-5034.
2. Li, S-G.; Jin, J-W.; Wu, Y. Regio-selective reduction of the C–C double bonds in α, β-unsaturated acyl 4-substituted oxazolidin-2-ones and oxazoline-2-thiones. *Tetrahedron* **2011**, *68*, 846-850.
3. Li, S-G.; Wu, Y. Synthesis and Absolute Configuration of Demethyl (C-11) Cezomycin. *Chem-Asian J.,* **2013**, 2792-2800.
4. Han, W-B.; Li, S-G.; Lu, X-W.; Wu, Y. Facile Conversion of Cyclopropanols into Linear Conjugate Enones. *Eur. J. Org. Chem.*, **2014**, 3841-3846.
5. Li, S-G.; Vilchèze, C.; Chakraborty, S.; Wang, X.; Kim, H.; Anisetti, M.; Ekins, S.; Rhee, K. Y.; Jacobs Jr. W. R.; Freundlich, J. S. Evolution of a thienopyrimidine antitubercular relying on medicinal chemistry and metabolomics insights. *Tetrahedron Letter*, **2015**, 3246-3250.
6. Perryman, A.L.; Yu, W.; Wang, X.; Ekins, S.; Forli, S.; Li, S-G.; Freundlich, J. S.; Tonge, P. J.; Olson, A. J. A Virtual Screen Discovers Novel, Fragment-Sized Inhibitors of Mycobacterium tuberculosis InhA. *J. Chem. Inf. Model.*, **2015**, 645–659.
7. Forbes, L.; Ebsworth-Mojica, K.; DiDone, L.; Li, S-G.; Freundlich, J.S.; Connell, N.; Dunman, P.M.; Krysan, D.J.A High Throughput Screening Assay for Anti-Mycobacterial Small Molecules Based on Adenylate Kinase Release as a Reporter of Cell Lysis. *PLoS One*, doi:10.1371/journal.pone.0129234. PMID: 26098625.
8. Li, S-G.; Chen, H.-J.; Yang, Y.-Y.; Wu, W.-J.; Wu, Y. A Novel Allyl Transfer Coupled with A Grob Fragmentation, *Chem-Asian J.,* **2015**, 2333-2336.
9. Ekins, S.; Madrid, P. B.; Sarker, M,; Li, S-G.; Mittal, N.; Kumar, P.; Wang, X., Straton, T. P.; Zimmerman, M.; Talcott, C.; Bourbon, P.; Travers, M.; Yadav, M.; Freundlich, J. S. Combining Metabolite-Based Pharmacophores with Bayesian Machine Learning Models for Mycobacterium tuberculosis Drug Discovery. *PLoS One*, DOI:10.1371/journal.pone.0141076. PMID: 26517557.
10. Kumar, P.; Kaushik, A. K.; Lloyd, E. P.; Li, S-G.; Mattoo, R.; Ammerman, N. C.; Bell, D. T.; Perryman, A. L.; Zandi, T. A., Ekins, S.; Ginel, S. L.; Townsend, C. A.; Freundlich, J. S.; Lamichhane, G. Non-classical transpeptidases yield insight into new antibacterials *Nat. Chem. Biol.* doi:10.1038/nchembio.2237 PMID: 27820797