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RESEARCH INTEREST:

Chemical Biology, Proteomics/Metabolomics, Bioinformatics, High-throughput Screening

EDUCATION AND RESEARCH EXPERIENCE

- 12/2014 – present Research Associate, Department of Chemical Physiology, The Scripps Research Institute, La Jolla, CA. (advisor: Prof. John R. Yates III)
- 06/2009 – 09/2014 Ph.D., Department of Chemistry, Scripps Florida, Jupiter, FL. (advisor: Prof. Thomas J. Kodadek)
- 08/2008 – 05/2009 Graduate Student, Department of Biochemistry, University of Texas Southwestern Medical Center at Dallas, Dallas, TX
- 08/2004 – 06/2008 B.S. in Pharmaceutical Science (undergraduate research advisor: Prof. Junyi Liu), School of Pharmaceutical Science, Peking University, Beijing, China

TEACHING EXPERIENCE

- 02/2017 Guest lecturer, graduate course, “Biophysics: Bioinformatics in proteomics”, 3 hours, The Scripps Research Institute, La Jolla, CA.
- 10/2016 Guest lecturer, undergraduate course, “Research Methods: Mass spectrometry”, 9 (in class) + 6 (online) hours, Department of Biology, Occidental College, Los Angeles, CA.
- 09/2014 Guest lecturer, graduate course, “High-throughput screening with peptoid workshop”, 8 hours, Nanotechnology Institute, Chinese Academy of Science, Beijing, China.
- 09/2012 Teaching assistant, Biophysics and Spectroscopy class, Scripps Florida

AWARD AND FELLOWSHIP

- 2017 Postdoctoral Fellowship, Bridge Institute at University of Southern California
- 2014 Graduate Research Award, Richard and Helen DeVos Foundation
- 2008 Excellence in Research Award, Peking University
- 2006 Meritorious Winner, Interdisciplinary Contest in Modeling, Consortium for Mathematics and Its Applications (COMAP)

PUBLICATION (Total citation 450, H-index 10, as of Sep 2017)

1. **Gao, Y.;** Pinto, A.; Tan, D.; Ma, J.; Kolar, M.; Saghetalian, A.; Yates, J.R. “Dilu: a platform for accurate metabolomics data quantitation using high-resolution MS/MS data”, *Nature Communications* (submitted).
2. López-Aguilar, A.; **Gao, Y.;** Zu, G.; Tejairo, J.; Lebrilla, C.; Wu, P. “Glycan Changes And N-Acetyl Lactosamine Influence on CD8⁺ T Cells Activation After Acute LCMV Infection.”, *Journal of Immunology* (submitted).
3. **Gao, Y.;** Ma, J.; Saghetalian, A.; Yates, J.R. “Targeted Searches for Novel Peptides in Big Mass Spectrometry Data Sets”, *Nature Methods* (in revision).
4. Sarkar, M.; **Gao, Y.;** Pels, K.; Kodadek, T.J. “Design, Synthesis and Structure Elucidation of Diversity-Oriented Libraries with Stereochemically Defined Branched Backbones.”, *Organic & Biomolecular Chemistry* (in revision).
5. **Gao, Y.;** López-Aguilar, A.; Hou, X.; Yates, J.R.; and Wu, P. “A Chemoenzymatic Study Of O-GlcnaC-Modified Proteins in Effector and Memory CD8⁺ T Cells in a *Listeria Monocytogenes* Infection Model.”, *ACS Chemical Biology* (in press).
6. Xu, T.; Park, S.K.; Venable, J.D.; Wohlschlegel, J.A.; Diedrich, J.K.; Cociorva, D.; Lu, B.; Liao, L.; Hewel, J.; Han, X.; Wong, C.C.L.; Fonslow, B.; Delahunty, C.; **Gao, Y.;** Shah, H.; Yates, J.R. “ProLuCID: An improved SEQUEST-like Algorithm with Enhanced Sensitivity and Specificity.”, *Journal of Proteomics*, 2015, 129, 16-24.
7. Doran, T.; **Gao, Y.;** Simanski, S.; McEnaney, P.; Kodadek, T.J. “High Affinity Binding of Conformationally Constrained Synthetic Oligomers to An Antigen-Specific Antibody: Discovery of a Diagnostically Useful Synthetic Ligand for Murine Type 1 Diabetes Autoantibodies”, *Bioorganic & Medicinal Chemistry Letters*, 2015, 25(21), 4910-4917.
8. **Gao, Y.;** Kodadek, T.J. “Direct Comparison of Linear and Macrocyclic Compound Libraries as a Source of Protein Ligands”, *ACS Combinatorial Sciences*, 2015, 17 (3), 190–195. ***ACS Editors' Choice, Top 10 most downloaded paper in first half 2015.**
9. **Gao, Y.;** Amar, S.; Pahwa, S.; Fields, G.; Kodadek, T.J. “Rapid Lead Discovery Through Iterative Screening of One Bead One Compound Libraries”, *ACS Combinatorial Sciences*, 2015, 17 (1), 49–59. ***Top 10 most downloaded paper in first half 2015.**
10. Sarma, B.K.; Liu, X.; **Gao, Y.;** Kodadek, T.J. “Solid Phase Synthesis of 1,3,4-oxadiazin-5 (6R)-one and 1,3,4-oxadiazol-2-one Scaffolds from Acyl Hydrazides”, *Organic & Biomolecular Chemistry*, 2015, 13, 59.
11. Doran, T.; **Gao, Y.;** Mendes, K.; Dean, S.; Kodadek, T.J. “The Utility of Redundant Combinatorial Libraries in Distinguishing High and Low Quality Screening Hits”, *ACS Combinatorial Sciences*, 2014, 16 (6), 259–270. ***ACS Editors' Choice**
12. **Gao, Y.;** Kodadek, T.J. “Split-and-pool Synthesis and Characterization of Peptide Tertiary Amide Library”, *Journal of Visualized Experiments*, (88), e51299.
13. Rzuczek, S.G.; Gao, Y.; Tang, Z.; Thornton, C.; Kodadek, T.J.; Disney, M.D. “Features of Modularly Assembled Compounds That Impart Bioactivity Against an RNA Target”, *ACS Chemical Biology*, 2013, 8(10) 2312–2321.

14. **Gao, Y.**; Kodadek, T.J. “Synthesis and Screening of Stereochemically Diverse Combinatorial Libraries of Peptide Tertiary Amides”, *Chemistry & Biology* (now *Cell Chemical Biology*), Volume 20, Issue 3, 360-369.
15. Wang, X.; **Gao, Y.**; Xu, Y.; Liu, J. “An efficient preparation of a photolabile agent MNI-glu by regioselective nitration of 4-methoxyindoline derivative”, *Synthetic Communications*, 41(2009), 15, 4030-4038.
16. **Gao, Y.**; He, R.; He, Y.; Liu, T.; Qi, R.; Liu, G. “PEG-conjugated PAMAM dendrimers mediate efficient intramuscular gene expression”, *The AAPS Journal*, 11 (2009), 3, 395-405
17. **Gao, Y.**; He, Y.; Liu, T.; Qi, R. “Recent Advances of Dendrimers in Delivery of Genes & Drugs”, *Mini-Reviews in Medicinal Chemistry*, 8 (2008), 889-900.
18. Zhang, Q.; **Gao, Y.**; Zhai, Y.; Liu, F.; Gao, G. “Synthesis of sesbania gum supported dithiocarbamate chelating resin and studies on its adsorption performance for metal ions”, *Carbohydrate Polymers*, 73(2), 2008, 359–363.
19. Sun, H.; **Gao, Y.**; Zhai, Y.; Zhang, Q.; Liu, F.; Gao, G. “Recent Advances in Synthesis of Chiral Ionic Liquids”, *Progress in Chemistry*, 20 (2008), 698-712.
20. Zhai, Y.; **Gao, Y.**; Liu, F.; Zhang, Q.; Gao, G. “Synthesis of nanostructured TiO₂ particles in room temperature ionic liquid and its photocatalytic performance”, *Materials Letters*, 61 (2007), 5056–5058

PATENT

1. Gao, Y.; Thomas Kodadek. “Synthesis of Libraries of Peptide Tertiary Amides”, US Patent PCT/US2012/061963.
2. Li Li, Gao, Y.; Xiaowei Wang, Junyi Liu. “Synthesis of Non-Nucleoside Reverse Transcriptase Inhibitor Emivirine and Analogues”, China Patent # 201010136763.0.

PRESENTATION AND INVITED TALK

1. Big data to knowledge (BD2K) technical meeting online, 2016, oral presentation, “Learning from deep learning, a database-search engine for feature identification.”
2. American Society for Mass Spectrometry (ASMS) annual meeting at Indianapolis, 2017, poster, “GPGPU-based database-search engine for feature identification with DIA data.”
3. US-HUPO at San Diego, 2017, oral presentation, “Dilu: a high-resolution metabolomics quantification and identification platform.”
4. BD2K technical meeting online, 2016, oral presentation, “MSCompress: a stream compressor for lossless and lossy compression of mass data.”
5. Big data to knowledge (BD2K) Open Data Science Symposium at NIH, 2016, poster, “A improved proteomics data analysis workflow for DIA data”
6. ACS 251st meeting at San Diego, 2016, oral presentation, “Chemical probe for kinase substrate enrichment.”
7. BD2K site meeting at UCLA, 2015, poster, “Dilu: a better quantification tool for high resolution metabolomics data”

8. Mass Spectrometry: Application to the Clinical Lab (MSACL) at San Diego, 2015, poster, “Proteomics approach for small molecule identification and quantitation.”
9. Gordon Conference: High Throughput Chemistry & Chemical Biology at Colby-Sawyer College, 2013, poster, “Combinatorial libraries with privileged scaffold for high-throughput screening.”
10. 8th Peptoid Summit at University of California Berkeley, 2012, invited talk, “Conformational Restricted Foldamers: From Peptoid to Natural Product-Like Molecules”
11. ACS 244th meeting at Philadelphia, 2012, oral presentation “Synthesis and screening of stereochemically diverse combinatorial libraries of peptide tertiary amides”
12. ACS 240th meeting at Boston, 2010, oral presentation “Comparison study of cyclic and linear peptoid libraries for high throughput screening”

SOFTWARE DEVELOPMENT

- T2D Converter:** Convert ABI t2d format mass spectrometry data to MZML/MZXML/TXT in batch mode. Mainly used for MALDI-TOF based small molecule visualization.
- PCG-GUI:** Peptoid chemical structure generator with graphic user interface. Generate peptoid structure from mass spectrometry data after on-bead screening. Mainly used for screening hits structure elucidation and visualization.
- Dilu:** Novel platform that performs end-to-end metabolomics analysis based on high-resolution MS/MS data. This platform performs metabolomics data analysis from raw data conversion to peak picking, noise filtering, peak deconvolution, feature matching, feature quantitation and metabolite identification.
- PATS:** Post-acquisition targeted search engine for novel peptide identification in large proteomics dataset. Currently PATS can identify novel peptide and PTM from extremely large dataset (>10 TB raw data, >10,000 hours MS run) in minutes.

REFERENCE

Dr. Thomas Kodadek (Ph.D. advisor), kodadek@scripps.edu,

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