XIN YAN

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Appointment

2018-present	Assistant Professor, Department of Chemistry, Texas A&M University

Professional Preparation

Postdoctoral fellow	Stanford University, Chemistry, March 2016 - July 2018 Advisor: Professor Richard N. Zare
Ph.D.	Purdue University, Analytical Chemistry, December 2015 Advisor: Professor R. Graham Cooks Dissertation Title: "Novel analytical and preparative mass spectrometric methodologies in reaction monitoring and acceleration "
M.S.	Purdue University, Health Sciences, May 2011
B.S.	Fudan University, Pharmacy, June 2004

Awards/Honors

2023	Okeanos-CAPA Young Investigator Award at the Chemistry & Biology Interface
2022	NSF Faculty Early Career Development Program (CAREER) Award
2022	Montague-Center for Teaching Excellence Scholar Award
2022	CASMS young investigator award
2021	NIH Maximizing Investigators' Research (MIRA) Award
2021	American Society for Mass Spectrometry (ASMS) Research Award
2019	Selected to participate in the Cottrell Scholars Collaborative Workshop
2016	M. G. Mellon Award in Analytical Chemistry
2015	Thomas W. Keough Scholar Award
2014	Henry B. Hass Fellowship
2013	1st International Mass Spectrometry School Fellowship
2013	Eastman Fellowship Award in Analytical Chemistry
2012	Midwest Chapter of the Society of Cosmetic Chemists Scholarship
2011	Ross Fellowship

Publications (*signifies corresponding authors)

42. T. Yang, S. Tang, S. Kuo, D. Freitas, M. Edwards, H. Wang, Y. Sun, **X. Yan***, Lipid Mass Tags via Aziridination for Probing Isomeric Structures and Accurate Quantification, *Angew. Chem. Int. Ed*., **2022,** *61*, e202207098. DOI: 10.1002/ange.202207098.
41. H. Cheng, T. Yang, M. Edwards, S. Tang, S. Xu*, **X. Yan***, Picomole-Scale Transition Metal Electrocatalysis Screening Platform for Discovery of Mild C–C Coupling and C–H Arylation

through in situ Anodically Generated Cationic Pd, *J. Am. Chem. Soc.* **2022,** *144,* 1306–1312. DOI: 10.1021/jacs.1c11179.

40. Y. Zhu, S. Schrecke, S. Tang, M.T. Odenkirk, T. Walker, L. Stover, J. Lyu, T. Zhang, D. Russell, E. S. Baker, **X. Yan**, A. Laganowsky. Cupric Ions Selectively Modulate TRAAK–Phosphatidylserine Interactions. *J. Am. Chem. Soc.* **2022**, *144*, 7048–7053. DOI: 10.1021/jacs.2c00612
39. X. Chen. S. Tang, D. Freitas, E. Hirtzel, H. Cheng, **X. Yan***, Characterization of Glycerophospholipids at Multiple Isomer Levels via Mn(II)-Catalyzed Epoxidation, *Analyst,* **2022,** *147,* 4838 – 4844. DOI: 10.1039/D2AN01174C
38. S. Tang, X. Chen, Y. Ke, F. Wang, **X. Yan***, Voltage-Controlled Divergent Cascade of Electrochemical Reactions for Characterization of Lipids at Multiple Isomer Levels Using Mass Spectrometry, *Anal. Chem*. **2022**, *94*, 12750–12756. DOI: 10.1021/acs.analchem.2c02375.
37. S. Kuo, S. Tang, D. H. Russell*, **X. Yan***, Characterization of Lipid Carbon–Carbon Double-Bond Isomerism via Ion Mobility-Mass Spectrometry (IMS-MS) Combined with Cuprous Ion-Induced Fragmentation, *Int. J. Mass Spectrom.* **2022**, 479, 116889. DOI: 10.1016/j.ijms.2022.116889
36. K. S. Yang, S. Kuo, L. R. Blankenship, Z. Z. Geng, S. G. Li, D. H. Russell, **X. Yan**, S. Xu, W. R. Liu*, Repurposing Halicin as a potent covalent inhibitor for the SARS-CoV-2 main protease, *CRCHBI*, **2022**, *2*, 100025. DOI: 10.1016/j.crchbi.2022.100025.
35. D. Kuai, H. Cheng, K. Kuan, **X. Yan***, Accelerated Five-Component Spiro-Pyrrolidine Construction at The Air-Liquid Interface, *Chem. Commun,* **2021**, *57*, 3757-3760. DOI: 10.1039/D1CC00574J. *Published in the special issue of 2021 Emerging Investigators.*
34. S. Tang, L. Fan, H. Cheng, **X. Yan***, Incorporating Electro-Epoxidation into Electrospray Ionization Mass Spectrometry for Simultaneous Analysis of Negatively and Positively Charged Unsaturated Glycerophospholipids. *J. Am. Soc. Mass Spectrom.,* **2021**, *32*, 2288-2295. DOI: 10.1021/jasms.0c00356. *Published in the 2021 'Emerging Investigators' focus section.*
33. D. Freitas, X. Chen, H. Cheng, A. Davis, B. Fallon, **X. Yan***. Recent Advances of In-Source Electrochemical Mass Spectrometry. *ChemPlusChem*, **2021**, *86*, 434-445. DOI: 10.1002/cplu.202100030
32. **X. Yan***, Emerging microdroplet chemistry for synthesis and analysis, *Int. J. Mass Spectrom*., **2021**, *468*, 116639. DOI: 10.1016/j.ijms.2021.116639
31. D. A. Murphy, H. Cheng, T. Yang, **X. Yan**, I. M. Adjei*, Reversing Hypoxia with PLGA-Encapsulated Manganese Dioxide Nanoparticles Improves Natural Killer Cell Response to Tumor Spheroids. *Mol. Pharmaceutics*, **2021**, 18, 2935–2946. DOI: 10.1021/acs.molpharmaceut.1c00085
30. H. Cheng, S. Tang, T. Yang, S. Xu, **X. Yan***, Accelerating Electrochemical Reactions in a Voltage-Controlled Interfacial Microreactor. *Angew. Chem. Int. Ed*., **2020**, *59*, 19862-19867. DOI: 10.1002/anie.202007736. *Published as a Hot Paper; Highlighted in ChemistryViews.*
29. S. Tang, H. Cheng, **X. Yan***. On-Demand Electrochemical Epoxidation in Nano-Electrospray Ionization Mass Spectrometry to Locate Carbon-Carbon Double Bonds. *Angew. Chem. Int. Ed.*, **2020**, *59*, 209-214. DOI: 10.1002/anie.201911070
28. Z. Wei, Y. Li, R. G. Cooks*, **X. Yan***, Accelerated Reaction Kinetics in Microdroplets: Overview and Recent Developments. *Annu. Rev. Phys. Chem.*, **2020**, *71*, 31-51. DOI: 10.1146/annurev-physchem-121319-110654
27. **X. Yan**, X. Zhao, Z. Zhou, A. McKay, A. Brunet, R. N. Zare*, Cell-Type-Specific Metabolic Profiling Achieved by Combining Desorption Electrospray Ionization Mass Spectrometry Imaging and Immunofluorescence Staining. *Anal. Chem*. **2020**, *92*, 13281-13289. DOI: 10.1021/acs.analchem.0c02519
26. E. Gnanamani, **X. Yan**, R. N. Zare*. Chemoselective N-Alkylation of Indoles in Aqueous Microdroplets. *Angew. Chem. Int. Ed*. **2020**, *59,* 3069-3072. DOI: 10.1002/anie.201913069

25. X. Zhang, X. Ren, K. Chingin, J. Xu, **X. Yan**, H. Chen*. Mass spectrometry distinguishing C=C location and cis/trans isomers: A strategy initiated by water radical cation. *Anal. Chim. Acta*, **2020**, *1139*, 146-154. DOI: 10.1016/j.aca.2020.09.027
24. Z. Jiang, K. Pflug, S. M. Usama, D. Kuai, **X. Yan**, R. Sitcheran, K. Burgess*. Cyanine-Gemcitabine Conjugates as Targeted Theranostic Agents for Glioblastoma Tumor Cells. *J. Med. Chem.*, **2019**, *62*, 9236-9245. DOI: 10.1021/ACS.JMEDCHEM.9B01147

Prior to Texas A&M University

23. S. Banerjee, A. C. Y. Wong, **X. Yan**, B. Wu, H. Zhao, R. J. Tibshirani, R.N. Zare*, J. D. Brooks*. Early detection of unilateral ureteral obstruction by desorption electrospray ionization mass spectrometry. *Sci. Rep*., **2019**, *9*, 11007. DOI: 10.1038/s41598-019-47396-x
22. D. Gao, F. Jin, **X. Yan**, and R. N. Zare*. Selective synthesis in microdroplets of 2-phenyl-2,3-dihydrophthalazine-1,4-dione from phenyl hydrazine with phthalic anhydride or phthalic acid. *Chem. Eur. J*. **2019**, *25*, 1466-1471. DOI: 10.1002/chem.201805585
21. **X. Yan**, Y. Lai, R. N. Zare*, Preparative microdroplet synthesis of carboxylic acids from aerobic oxidation of aldehydes, *Chem. Sci.,* **2018**, *9,* 5207-5211. DOI: 10.1039/C8SC01580E
20. Z. Zhou, **X. Yan**, Y. Lai, R. N. Zare*, Fluorescence polarization anisotropy in microdroplets, *J. Phys. Chem. Lett.*, **2018**, *9*, 2928-2932. DOI: 10.1021/acs.jpclett.8b01129
19. R. G. Cooks*, **X. Yan**. Mass Spectrometry for Synthesis and Analysis. *Annu. Rev. Anal. Chem*., **2018**, *11*, 1-28. DOI: 10.1146/annurev-anchem-061417-125820
18. **X. Yan***, X. Li, R. G. Cooks*. Ambient ionization mass spectrometry measurement of aminotransferase activity. *J. Am Soc. Mass. Spectrom*., **2017**, *28*, 1175-1181. DOI: 10.1007/s13361-016-1591-x
17. **X. Yan**, H. Y. Cheng, S. Banerjee, R. N. Zare*. Two-phase reactions in microdroplets without the use of a catalyst. *Angew. Chem. Int. Ed.,* **2017**, *56*, 3562-3565. DOI: 10.1002/anie.201612308
16. H. Cheng, **X. Yan**, R. N. Zare*. Two new devices for identifying electrochemical reaction intermediates with desorption electrospray ionization mass spectrometry. *Anal. Chem*., **2017**, *89*, 3191-3198. DOI: 10.1021/acs.analchem.6b05124
15. S. Banerjee, E. Gnanamani, **X. Yan**, R. N. Zare*. Can all bulk-phase reactions be accelerated in microdroplets? *Analyst*, **2017**, *142*, 1399-1402. DOI: 10.1039/C6AN02225A
14. X. Li, **X. Yan**, R. G. Cooks*. Functionalization of saturated hydrocarbons using nitrogen ion insertion reactions in mass spectrometry. *Int. J. Mass Spectrom*. **2017**, *418*, 79-85. DOI: 10.1016/j.ijms.2016.11.017
13. **X. Yan**, R. M. Bain, R. G. Cooks*. Reaction acceleration in microdroplets revealed by mass spectrometry. *Angew. Chem. Int. Ed.,* **2016**, *55*, 12960-12972. DOI: 10.1002/anie.201602270
12. **X. Yan**, R. M. Bain, Y. Li, R. Qiu, T. G. Flick, R. G. Cooks*. On-line inductive electrospray ionization mass spectrometry as a process analytical technology tool to monitor the synthetic route to Anagliptin. *Org. Process Res. Dev*. **2016**, *20*, 940-947. DOI: 10.1021/acs.oprd.6b00039
11. R. M. Bain, **X. Yan**, S. A. Raab, S. T. Ayrton, T. G. Flick, R. Graham Cooks*. On-line and off-line chiral analysis of reaction mixtures using the kinetic method. *Analyst*, **2016**, *141*, 2441-2446. DOI: 10.1039/C6AN00100A
10. Y. Li, **X. Yan**, R. G. Cooks*. The role of the interface in thin film and droplet accelerated reactions studied by competitive substituent effects. *Angew. Chem. Int. Ed.,* **2016**, *55*, 3433-3437. DOI: 10.1002/anie.201511352
9. **X. Yan**, E. Sokol, X. Li, G. Li, S. Xu, R. G. Cooks*. On-line reaction monitoring and mechanistic studies by mass spectrometry: Negishi cross-coupling, hydrogenolysis and reductive amination. *Angew. Chem.Int. Ed*., **2014**, *23*, 5931-5935. DOI: 10.1002/anie.201310493

8. R. D. Espy, M. Wleklinski, **X. Yan**, R. G. Cooks*. Beyond the flask: reactions on the fly in ambient mass spectrometry. Trends *Anal. Chem.,* **2014**, *57*,135-146. DOI: 10.1016/j.trac.2014.02.008
7. R. Bain, C. J. Pulliam, **X. Yan**, K. Moore, R. G. Cooks*. Mass spectrometry in organic synthesis: Claisen-Schmidt base-catalyzed condensation and Hammett equation. *J. Chem. Ed*., **2014**, *91*,1985-1989. DOI: 10.1021/ed500288m
6. **X. Yan**, R. Augusti, X. Li, R. G. Cooks*. Chemical reactivity assessment using reactive paper spray mass spectrometry: Katritzky reaction. *ChemPlusChem*, **2013**, *78*, 1142-1148. DOI: 10.1002/cplu.201300172
5. **X. Yan**, Y. Zhou, S. Liu*. Optical imaging of tumors with copper-labeled rhodamine derivatives by targeting mitochondria. *Theranostics*, **2012**, *2*, 988-998. DOI: 10.7150/thno.4818
4. Y. Zhou, Y. Kim, **X. Yan**, O. Jacobson, X. Chen, S. Liu*. ^{64}Cu-labeled lissamine rhodamine B: a promising PET radiotracer targeting tumor mitochondria. *Mol. Pharm*., **2011**, *8*, 1198-1208. DOI: 10.1021/mp200025m
3. S. Xu, **X. Yan**, Y. Chen, P. Xia, Z. Qian, D. Yu, Yi Xia, Z. Yang, S. L. Morris-Natschke, K.H. Lee*. Anti-AIDS agents 84. Synthesis and anti-human immunodeficiency virus (HIV) activity of 2'- monomethyl-4-methyl- and 1'-thia-4-methyl-(3'R,4'R)-3',4'-di-O-(S)-camphanoyl-(+)-cis-khellactone (DCK) analogs. *Bioorg. Med. Chem.,* **2010**, *18*, 7203-7211. DOI: 10.1016/j.bmc.2010.08.031
2. **X. Yan**, S. Xu, J. Wang, Y. Chen, P. Xia*. Methyl 3β-methoxycarbonyl-4,4-dimethyl-17-oxo-16α-(3-oxobutyl)-16β-carboxylate. *Acta Crystallogr. Sect. E,* **2009**, *E65*, o1283. DOI: 10.1107/S1600536809017243
1. S. Xu, **X. Yan**, Q. Zhang, P. Xia*, Y. Chen. Unexpected rearrangement in the reaction of 7-mercapto-4-methylcoumarin with 1-mono- and 1,1-dimethyl propargyl alcohols. *Synth. Commun*., **2007**, *37,* 3801-3808. DOI: 10.1080/00397910701571615

Patents

5. Tandem Mass Tag for Lipid Quantitation, US Patent application number: US 63/171,846
4. On-Demand Electrochemical Reactions in Nano-Electrospray Ionization Mass Spectrometry for Biomolecular Analysis, United States provisional patent application number: 62/924,889.
3. Reaction monitoring, US Patent US20180047552A1.
2. Synchronization of ion generation with cycling of a discontinuous atmospheric interface, PCT international application number: 13/887,911.1.
1. Ambient surface cleaning and sampling with continuous mass spectrometric analysis, PCT international application number: 62/036,186.

Membership in Professional Societies

American Chemical Society Division of Analytical Chemistry;
American Society for Mass Spectrometry

Invited Seminars and Conference Talks

- Department of Chemistry, University of Texas at Austin, Austin, TX, January 26, 2023
- CAPA Symposium, University of South Florida, Tampa, FL, December 22, 2022
- Department of Chemistry, University of Wisconsin-Madison, Madison, WI, October 27, 2022

- School of Chemistry, University of New South Wales (UNSW) Sydney, October 19, 2022
- Department of Chemistry, Purdue University, West Lafayette, September 27, 2022
- 70th ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 4, 2022
- Department of Chemistry, Prairie View A&M University, Prairie View, TX, April 29, 2022
- Department of Chemistry and Environmental Science, New Jersey Institute of Technology, November 10, 2021
- Chinese American Society for Mass Spectrometry Conference, August 8, 2021
- Mass Spectrometry & Advances in the Clinical Lab, April 22, 2021
- Department of Chemistry, Wayne State University, April 13, 2021
- Department of Veterinary Physiology and Pharmacology Seminar Series, Texas A&M University, College Station, TX, February 20, 2020
- GRC Liquids in Complex Environments, Driving Reactions, Assembling and Pushed to Their Limits, Holderness, NH, August 5, 2019
- 67th ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, June 3, 2019
- Department of Chemistry, Texas A&M University, College Station, TX, April 22, 2019
- GRC Gaseous Ions: Structures, Energetics and Reactions, Ventura, CA, Feb, 18, 2019
- Ions at Work Symposium, College Station, TX, October 5, 2018
- GRC Molecular Structure Elucidation - Enabling Development of Novel Therapeutics Through Innovative Analytical Technologies and Methods, Newry, ME, August 12, 2018