

# Zhibo Yang

## Zhibo Yang

**Associate Professor** (Analytical Chemistry)

University of Oklahoma

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## RESEARCH EXPERIENCE

### Associate Professor

Jul. 2018 – Present

*University of Oklahoma, Norman, OK*

### Assistant Professor

Aug. 2012 – Jun. 2018

*University of Oklahoma, Norman, OK*

### Postdoctoral

Oct. 2008 – Jul. 2012

*University of Colorado, Boulder, CO*

Mentors: Dr. Veronica M. Bierbaum, Dr. Theodore P. Snow

### Postdoctoral

Oct. 2005 – Sept. 2008

*Pacific Northwest National Laboratory, Richland, WA*

Mentors: Dr. Julia Laskin, Dr. Jean H. Futrell

## EDUCATION

### Ph.D. Physical Chemistry

Aug. 2000 – Sept. 2005

*Wayne State University, Detroit, MI*

Mentor: Dr. Mary T. Rodgers

### M.S. Physical Chemistry

Sept. 1997 – Jul. 2000

*University of Science and Technology of China, Hefei, China*

Mentor: Peiyan Lin

### B.S. Geochemistry (Major) and

Material Chemistry (Minor)

Sept. 1992 – Jul. 1997

*University of Science and Technology of China, Hefei, China*

Mentor: Jiangfeng Chen

## AWARDS and HONORS

- Finalists for Phase I of *Follow that Cell Challenge*, NIH, 2015
- Outstanding Member of *Chinese American Society for Mass Spectrometry*, 2015
- *ASMS (American Society for Mass Spectrometry) Research Award*, 2014
- *Travel Award of Early Career Scientist* to attend Astrobiology Graduate Student Conference (AbGradCon), Sweden, 2010
- *Best Student Paper in International Journal of Mass Spectrometry* (**Z. Yang**, M. T. Rodgers, *Int. J. Mass Spectrom.* **2005**, 241, 225-242.)
- *Dan Trivich Memorial Award for Research in Physical Chemistry*, 2005
- *Summer Dissertation Fellowship*, 2005
- *Chairs' Fund Fellowship* to attend 2005 Gordon Conference in Biological Molecules in the Gas Phase, Lewiston, ME
- *Chairs' Fund Fellowship* to attend 2005 Gordon Conference in Gaseous Ions: Structures, Energetics & Reactions, Ventura, CA
- *Heller Graduate Fellowship*, 2004

## PROFESSIONAL SOCIETIES

Member of the *American Society for Mass Spectrometry (ASMS)*

# Zhibo Yang

Member of the *American Chemical Society (ACS)*

Member of the *American Society of Pharmacognosy (APS)*

## RESEARCH HIGHLIGHT IN THE MEDIA

(1) Invited guest for a state-wide OCAST radio show, Oklahoma Innovations (June 30th, 2015), for public science education based on the research supported by OCAST grant ([http://www.ok.gov/ocast/News\\_Media/Radio\\_Show/](http://www.ok.gov/ocast/News_Media/Radio_Show/)).

(2) Single cell MS studies reported by *Chemistry World*, *Chemical & Engineering News*, Proteo Monitor, Genomeweb, and Bioanalysis Zone (2014).

(3) Astrochemistry research reported by NCSA (National Center for Supercomputing Applications), and the interview was published in the *ACCESS* magazine and on the *iSGTW* (International Science Grid This Week) website (2011).

## TEACHING

CHEM 1415 (*General Chemistry II*)

Fall 2016, 2017, 2019

CHEM 4023 (*Instrumental Method-Chemical Analysis*)

Fall 2012–2015

CHEM 5120 (*Physical and Chemical Separations*)

Spring 2013–current

## RESEARCH FUNDING

(1) OU new faculty startup funding.

(2) VPR Supplemental Equipment Funding, OU (awarded: \$139,400)

(3) Junior Faculty Fellowship, OU, 2013–2014 (awarded: \$14,000)

(4) Faculty Enrichment Grant, OU, 2013 (awarded: \$1,200)

(5) Travel Assistance Program, OU, 2013–2016 (awarded: \$4,800)

(6) Faculty Investment Program, OU, 2013–2015 (awarded: \$30,000)

(7) Honors Research Assistant Program (HRAP) for undergraduate student research, OU, 2014–2018 (total awarded: \$ 4,500)

(8) ASMS (American Society for Mass Spectrometry) Research Award, 2014 (sponsored by Waters Corporation, \$35,000)

(9) OCAST (Oklahoma Center for the Advancement of Science and Technology), Health Research–FY2014 Competition (PI: Zhibo Yang; total awarded: \$135,000)

(10) NIH (R01GM116116), 8/2015–7/2020 (PI: Zhibo Yang; Co-I: Chuanbin Mao; Collaborator: Anthony Burgett; total awarded: \$1,486,000)

(11) NSF EPSCoR REU, 5/2016–8/2016 (PI: Zhibo Yang; Co-PI: Marc Libault; total awarded: \$5,000)

(12) NIH (R21CA204706-01), 6/2016–5/2019 (PI: Anthony Burgett; Co-I: Zhibo Yang; Collaborator: Jonathan E. Heinlen; total awarded: \$588,000)

(13) NSF (1634630), 8/2016–7/2019 (PI: Zhibo Yang; former PI: Boris Wawrik; total awarded: \$462,000)

(14) NSF MRI (1626372), 9/2016–8/2019 (PI: Robert Cichewicz; Co-PIs: Laura Bartley, Marc Libault, Zhibo Yang, Si Wu; total awarded: \$416,500)

(15) NIH DSP (Diversity Supplements Program) for undergraduate student research, supplement to R01GM116116, 9/2017–8/2019 (PI: Zhibo Yang; total awarded: \$44,000)

## SCIENTIFIC COMMUNITY SERVICE

(1) Peer-reviewer: *Analyst*, *Analytical Biochemistry*, *Analytical and Bioanalytical Chemistry*, *Analytical Chemistry*, *Analytical Methods*, *Astrobiology*, *Applied Surface Science*, *Cellular and Molecular Biology Letters*, *Chemical Science*, *Computational and Theoretical Chemistry*, *European Journal of Mass Spectrometry*, *Frontiers in Plant Science*, *International Journal of Mass Spectrometry*, *Journal of American Chemical Society*, *Journal of American Society of Mass Spectrometry*, *Journal of Molecular Graphics and Modeling*, *Journal of Physical Chemistry*, *Journal of Visualized Experiments*, *Mass Spectrometry*, *Molecular Physics*, *Organic & Biomolecular Chemistry*, *PLOS ONE*, *RSC Advances*, and *Scientific Reports*.

(2) *Ad hoc* Reviewer: NSF, NASA, ACS PRF, Research Grants Council (RGC) of Hong Kong, China

(3) Panelist: *NASA panel review meetings*.

## Zhibo Yang

- (4) Conference Session Chair: ASMS, APS, Lake Arrowhead Ion Chemistry Conference, SciX.
- (5) Guest Editor: *Frontiers in Plant Science*

### DEPARTMENTAL and UNIVERSITY SERVICE

- (1) Chair of Graduate Student Recruiting Committee (2017-current).
- (2) Member of Graduate Student Recruiting Committee (2013-2016).
- (3) Core-member of Center for Bioanalysis (2014-current).

### Patent

- (1) Yang, Z., US Patent for Cellular probe device, system and analysis method Patent (Patent # 10,000,789), Approved: 2018.

### Publications

#### Column Article (non-peer reviewed)

1. W. Rao, N. Pan, **Z. Yang\***, “Single-Cell MS and High-Spatial-Resolution MS Imaging Under Ambient Conditions Using a Novel Sampling Device”, *LCGC North America* **2015**, *33*, 414–419.

#### Editorial Article (peer reviewed)

1. A. Svatoš\*, Y. J. Lee, and **Z. Yang**, “Single Plant Cell Metabolomics”, *Front. Plant Sci.*, **2020**, *11*, 161.

#### Book Chapter

1. N. Pan, W. Rao, **Z. Yang\***, “Single-Probe Mass Spectrometry Analysis of Metabolites in Single Cells. In: Shrestha B. (eds) *Single Cell Metabolism*”, *Methods in Molecular Biology*, **2020**, vol. 2064. Humana, New York, NY.

2. X. Tian, Z. Zou, Z. Yang\*, “Extract Metabolomic Information Using the Single-probe Mass Spectrometry Imaging Experiment Combined with Advanced Data Analysis”, *Mass Spectrometry Imaging of Small Molecules*, Springer, Berlin, Germany.

#### Peer-reviewed Publications

##### **Research Publications after Joined OU**

81. C. Huang, W. Rodgers, R. Liu, Y. Liu, E. Sherman, **Z. Yang**, X. Zhang\*, “Tetraspanin CD82 as a Principle for the Organization of Cell Membrane Spatial Heterogeneity”, manuscript under preparation.

80. M. Sun, X. Chen, **Z. Yang\***, “Irinotecan-Resistant Colorectal Cancer Cells Possesses Molecular Characteristics Similar to Cancer Stem Cells Through Modulation of SCD1”, manuscript under preparation.

79. X. Chen, M. Sun, **Z. Yang\***, “Single Cell Mass Spectrometry Analysis of Drug-resistant Cancer Cells: Metabolomics Studies of Synergetic Effect of Combinational Treatment”, manuscript under preparation.

78. R. Bensen, S. Standke, D. Colby, N. Kothapalli, A. Le, M. A. Patten, A. Tripathi, J. Heinlen, **Z. Yang\***, A. Burgett\*, “Single Cell Mass Spectrometry Quantification of Anticancer Drugs: Proof of Concept in Cancer Patients”, *ACS Pharmacol. Transl. Sci.*, in press.

77. R. Liu, **Z. Yang\***, “Single Cell Metabolomics Using Mass Spectrometry: Techniques and Data Analysis”, *Anal. Chim. Acta*, **2021**, *1143*, 124-134.

76. Z. Pei, J. Yang, J. Deng, Y. Mao, Q. Wu, **Z. Yang**, B. Wang, C. M. Aikens, W. Liang\*, and Y. Shao\*, “Visualization and Analysis of Energy Densities: II. Linear-Response Time-Dependent Density Functional Theory Calculations”, *Phys. Chem. Chem. Phys.*, **2020**, *22*, 26852-26864.

75. J. Yang, Z. Pei, J. Deng, Y. Mao, Q. Wu, **Z. Yang**, B. Wang, C. M. Aikens, W. Liang\*, and Y. Shao\*, “Visualization and Analysis of Energy Densities: I. Real-Time Time-Dependent Density Functional Theory Simulations”, *Phys. Chem. Chem. Phys.*, **2020**, *22*, 26838-26851.

74. Y. Zhu, W. Wang, **Z. Yang\***, “Combining Mass Spectrometry with Paternò-Büchi Reaction to Determine Double-bond Positions in Lipids at the Single-cell Level”, *Anal. Chem.* **2020**, 92, 11380-11387.
73. M. Liu, Y. Zhang, J. Yang, X. Cui, Z. Zhou, H. Zhan, K. Ding, X. Tian, **Z. Yang**, K. A. Fung, B. H. Edil, R. G. Postier, M. S. Bronze, M. E. Fernandez-Zapico, M. P. Stemmler, T. Brabletz, Y. Li, C. W. Houchen, M. Li\*, “ZIP4 Increases Expression of Transcription Factor ZEB1 to Promote Integrin  $\alpha\beta 1$  Signaling and Inhibit Expression of the Gemcitabine Transporter ENT1 in Pancreatic Cancer Cells”, *Gastroenterology*, **2020**, 158, 679–692.
72. Y. Tao, N. Bellonzi, Y. Mao, Z. Pei, Z. Zou, **Z. Yang**, Y. Shao\*, “Constructing Spin-Adiabatic States for the Modeling of Spin-Crossing Reactions. I. A Shared-Orbital Implementation”, *Int. J. Quantum Chem.* **2020**, 120, e26123.
71. R. Liu, M. Sun, G. Zhang, Y. Lan, **Z. Yang\***, “Towards Early Monitoring of Chemotherapy-Induced Drug Resistance Based on Single Cell Metabolomics: Combining Single-probe Mass Spectrometry with Machine Learning”, *Anal. Chim. Acta*, **2019**, 1092, 42-48.
70. X. Tian, B. Xie, Z. Zou, Y. Jiao, L. Lin, C. Chen, C. Hsu, J. Peng\*, **Z. Yang\***, “Multimodal Imaging of Amyloid Plaques: Fusion of the Single-probe Mass Spectrometry Image and Fluorescence Microscopy Image”, *Anal. Chem.* **2019**, 91, 12882-12889.
69. Y. Zhu, R. Liu, **Z. Yang\***, “Redesigning the T-probe for Mass Spectrometry Analysis of Online Lysis of Non-adherent Single Cells”, *Anal. Chim. Acta*, **2019**, 1084, 53-59.
68. N. Pan, S. Standke, N. R. Kothapalli, M. Sun, R. C. Bensen, A. Burgett, **Z. Yang\***, “Quantification of Drug Molecules in Live Single Cells using the Single-probe Mass Spectrometry Technique”, *Anal. Chem.* **2019**, 91, 9018-9024.
67. S. Standke, D. Colby, R. Bensen, A. Burgett\*, **Z. Yang\***, “Integrated Cell Manipulation Platform Coupled with the Single-probe for Mass Spectrometry Analysis of Drugs and Metabolites in Single Suspension Cells”, *J. Vis. Exp.*, **2019**, 148, e5987.
66. X. Tian, G. Zhang, Z. Zou, **Z. Yang\***, “Anticancer Drug Affects Metabolomic Profiles in Multicellular Spheroids: Studies Using Mass Spectrometry Imaging Combined with Machine Learning”, *Anal. Chem.* **2019**, 91, 5802-5809.
65. R. Liu, G. Zhang, M. Sun, X. Pan, **Z. Yang\***, “Integrating A Generalized Data Analysis Workflow with the Single-probe Mass Spectrometry Experiment for Single Cell Metabolomics”, *Anal. Chim. Acta*, **2019**, 1064, 71-79.
64. B. L. Roberts, Z. C. Severance, R. C. Bensen, A. T. Le, N. R. Kothapalli, J. I. Nuñez, H. Ma, S. Wu, S. J. Standke, **Z. Yang**, W. J. Reddig, E. L. Blewett, A. W. G. Burgett\*, “Transient Compound Treatment Induces a Multigenerational Reduction of Oxysterol-Binding Protein (OSBP) Levels and Prophylactic Antiviral Activity”, *ACS Chem. Biol.* **2019**, 14, 276-287 (ACS Editors' Choice).
63. M. Sun, **Z. Yang\***, “Metabolomic Studies of Live Single Cancer Stem Cells Using Mass Spectrometry”, *Anal. Chem.* **2019**, 91, 2384-2391.
62. S. Standke, D. Colby, R. Bensen, A. Burgett\*, **Z. Yang\***, “Mass Spectrometry Measurement of Single Suspended Cells using Combined Cell Manipulation System and the Single-probe Device”, *Anal. Chem.* **2019**, 91, 1738-1742.
61. R. Liu, G. Zhang, **Z. Yang\***, “Towards Rapid Prediction of Drug-resistant Cancer Cell Phenotypes: Single Cell Mass Spectrometry Combined with Machine Learning”, *Chem. Comm.* **2019**, 55, 616-619.
60. R. Liu, N. Pan, Y. Zhu, **Z. Yang\***, “T-Probe: An Integrated Microscale Device for Online In Situ Single Cell Analysis and Metabolic Profiling Using Mass Spectrometry”, *Anal. Chem.* **2018**, 90, 11078–11085.
59. M. Sun, **Z. Yang**, B. Wawrik\*, “Metabolomic Fingerprints of Individual Algal Cells Using the Single-Probe Mass Spectrometry Technique”, *Front. Plant Sci.*, **2018**, 9:571.
58. X. Tian, G. Zhang, Y. Shao\*, **Z. Yang\***, “Towards Enhanced Metabolomic Data Analysis of Mass Spectrometry Image: Multivariate Curve Resolution and Machine Learning”, *Anal. Chim. Acta*, **2018**, 1037, 211-219.
57. L. Du, A. L. Risinger, C. A. Mitchell, J. You, B. W. Stamps, N. Pan, J. B. King, J. C. Bopassa, S. I. V. Judge, **Z. Yang**, B. S. Stevenson, and R. H. Cichewicz\*, “A Unique Amalgamation of Primary and

Secondary Structure Attributes Transform Peptaibols into Potent Bioactive Cell-Penetrating Peptides”, *Proc. Natl. Acad. Sci.* **2017**, *114*, E8957-E8966.

56. B. Wawrik\*, D. A. Bronk, S. E. Baer, L. Chi, M. Sun, J. T. Cooper, **Z. Yang**, “Bacterial Utilization of Creatine in Seawater”, *Aquat. Microb. Ecol.* **2017**, *80*, 153–165.

55. M. Sun, X. Tian, **Z. Yang\***, “Microscale Mass Spectrometry Analysis of Extracellular Metabolites in Live Tumor Spheroids”, *Anal. Chem.* **2017**, *89*, 9069–9076.

54. N. Pan, W. Rao, S. J. Standke, **Z. Yang\***, “Using Dicationic Ion-Pairing Compounds to Enhance the Single Cell Mass Spectrometry Analysis with the Single-Probe”, *Anal. Chem.* **2016**, *88*, 6812–6819.

53. W. Rao, N. Pan, **Z. Yang\***, “Applications of the Single-Probe: Mass Spectrometry Imaging and Single Cell Analysis under Ambient Conditions”, *J. Vis. Exp.* **2016**, *112*, e53911, doi:10.3791/53911.

52. C. M. Nichols, Z.-C., Wang, **Z. Yang**, W. C. Lineberger, V. M. Bierbaum\*, “Experimental and Theoretical Studies of the Reactivity and Thermochemistry of Dicyanamide:  $N(CN)_2^-$ ”, *J. Phys. Chem. A*, **2016**, *120*, 992–999.

51. W. Rao, N. Pan, X. Tian, **Z. Yang\***, “High-Resolution Ambient MS Imaging of Negative Ions in Positive Ion Mode: Using Dicationic Reagents with the Single-Probe”, *J. Am. Soc. Mass Spectrom.* **2016**, *27*, 124–134 (Highlighted article).

50. W. Rao, N. Pan, **Z. Yang\***, “High Resolution Tissue Imaging using the Single-probe Mass Spectrometry under Ambient Conditions”, *J. Am. Soc. Mass Spectrom.* **2015**, *26*, 986–993.

49. **Z. Yang\***, N. Pan, “Computational Studies of Ion-neutral Reactions of Astrochemical Relevance: Formation of Hydrogen Peroxide, Acetamide, and Amino Acetonitrile”, *Int. J. Mass Spectrom.* **2015**, *378*, 364–368.

48. N. Pan, W. Rao, N. Kothapalli, R. Liu, A. Burgett\*, **Z. Yang\***, “The Single-probe: A Miniaturized Multifunctional Device for Single Cell Mass Spectrometry Analysis”, *Anal. Chem.* **2014**, *86*, 9376–9380.

47. N. J. Demarais; **Z. Yang**, T. P. Snow, V. M. Bierbaum\*, “Gas-Phase Reactions of Polycyclic Aromatic Hydrocarbon Cations and their Nitrogen-containing Analogues with H atoms”, *Astrophys. J.* **2014**, 784:25 (7pp).

46. C. A. Cole, N. J. Demarais, **Z. Yang**, T. P. Snow, V. M. Bierbaum\*, “Heterocyclic Anions of Astrobiological Interest”, *Astrophys. J.* **2013**, 779:181 (9pp).

45. C. M. Nichols, **Z. Yang**, V. M. Bierbaum\*, “Gas-phase organic reactions of the atomic oxygen radical cation”, *Int. J. Mass Spectrom.* **2013**, *353*, 1–6.

44. N. J. Demarais, **Z. Yang**, T. P. Snow, V. M. Bierbaum\*, “Chemistry of HCNH: Mechanisms, Structures, and Relevance to Titan’s Atmosphere”, *Struct. Chem.* **2013**, *24*, 1957–1963.

43. C. M. Nichols, **Z. Yang**, B. B. Worker, D. R. Hager, N. M. M. Nibbering, V. M. Bierbaum\*, “Gas-phase Reactions of the Atomic Oxygen Radical Cation with Halogenated Compounds”, *Phys. Chem. Chem. Phys.* **2013**, *15*, 561–567.

#### **Research Publications Before Joined OU**

42. Z. Lin, D. Talbi, E. Roueff, E. Herbst\*, N. Wehres, C. A. Cole, **Z. Yang**, T. P. Snow, V. M. Bierbaum, “Can Interstellar Propene ( $CH_3CHCH$ ) Be Formed via Gas-Phase Reactions?”, *Astrophys. J.* **2013**, 765:80 (5pp).

41. J. Laskin\*, **Z. Yang**, C. Lam, I. K. Chu, “Entropy Effects on the Proton and Radical Mobility in Gas-Phase Peptide Ions”, *Int. J. Mass Spectrom.* **2012**, 316-318, 252–258.

40. J. M. Garver, **Z. Yang**, N. Wehres, C. M. Nichols, B. B. Worker, V. M. Bierbaum\*, “The  $\alpha$ -effect in Elimination Reactions and Competing Mechanisms in the Gas Phase”, *Int. J. Mass Spectrom.* **2012**, 330–332, 182–190.

39. C. A. Cole, N. Wehres, **Z. Yang**, D. L. Thomsen, T. P. Snow, V. M. Bierbaum\*, “A Gasphase Formation Route to Interstellar Trans-methyl Formate”, *Astrophys. J.* **2012**, 754:L5 (4pp).

38. J. M. Garver, **Z. Yang**, C. Nichols, B. Worker, S. Gronert, V. M. Bierbaum\*, “Resolving the  $\alpha$ -effect in Gas Phase S2 Reactions: A Marcus Theory Approach”, *Int. J. Mass Spectrom.* **2012**, 316–318, 244–250.

37. **Z. Yang**, M. T. Rodgers\*, “Tautomerization in the Formation and Collision-Induced Dissociation of Alkali Metal Cation-Cytosine Complexes”, *Phys. Chem. Chem. Phys.* **2012**, *14*, 4517–4526.

36. N. J. Demarais, **Z. Yang**, O. Martinez Jr., N. Wehres, T. P. Snow, V. M. Bierbaum\*, “Gas Phase Reactions of Polycyclic Aromatic Hydrocarbon Anions with Molecules of Interstellar Relevance”, *Astrophys. J.* **2012**, 746:32 (6pp).
35. **Z. Yang**, C. A. Cole, O. Martinez Jr., M. Y. Carpenter, P. Snow, V. M. Bierbaum\*, “Experimental and Theoretical Studies of Reactions between H Atoms and Nitrogen-containing Carbanions”, *Astrophys. J.* **2011**, 739:19 (10pp).
34. J. Laskin\*, **Z. Yang**, “Energetics and Dynamics of Dissociation of Deprotonated Peptides: Fragmentation of Angiotensin Analogs”, *Int. J. Mass Spectrom.* **2011**, 308, 275–280.
33. J. M. Garver, **Z. Yang**, S. Kato, S. W. Wren, K. M. Vogelhuber, W. C. Lineberger, V. M. Bierbaum\*, “Gas Phase Reactions of 1,3,5-Triazine: Proton Transfer, Hydride Transfer and Anionic s-Adduct Formation”, *J. Am. Soc. Mass Spectrom.* **2011**, 22, 1260–1272.
32. J. Laskin\*, **Z. Yang**, A. S. Woods, “Competition between Covalent and Noncovalent Bond Cleavages in Dissociation of Phosphopeptide-Amine Complexes”, *Phys. Chem. Chem. Phys.* **2011**, 13, 6936–6946.
31. J. M. Garver, N. Eyet, S. M. Villano, **Z. Yang**, V. M. Bierbaum\*, “Mechanistic Investigation of S<sub>N</sub>2 Dominated Gas Phase Alkyl Iodide Reactions”, *Int. J. Mass Spectrom.* **2011**, 301, 151–158.
30. J. Laskin\*, **Z. Yang**, T. Song, C. Lam, I. K. Chu, “The Effect of the Basic Residue on the Energetics, Dynamics, and Mechanisms of Gas-Phase Fragmentation of Protonated Peptides”, *J. Am. Chem. Soc.* **2010**, 132, 16006–16016.
29. **Z. Yang**, B. Eichelberger, M. Y. Carpenter, O. Martinez Jr., T. P. Snow, V. M. Bierbaum\*, “Experimental and Theoretical Studies of Reactions between H Atoms and Carbanions of Interstellar Relevance”, *Astrophys. J.* **2010**, 723, 1325–1330.
28. **Z. Yang**\*, T. P. Snow, V. M. Bierbaum\*, “Computational Studies of Gas Phase Reactions of Carbon Chain Anions with N and O Atoms”, *Phys. Chem. Chem. Phys.* **2010**, 12, 13091–13098.
27. O. Martinez Jr., **Z. Yang**, N. J. Demarais, T. P. Snow, V. M. Bierbaum\*, “Gas-Phase Reactions of Hydride Anion, H<sup>-</sup>”, *Astrophys. J.* **2010**, 720, 173–177.
26. **Z. Yang**\*, B. Eichelberger, O. Martinez Jr., M. Stepanovic, T. P. Snow\*, V. M. Bierbaum\*, “The Influence of Spin Effects on the Gas Phase Reactions of Carbanions with N and O Atoms”, *J. Am. Chem. Soc.* **2010**, 132, 5812–5819.
25. J. Laskin\*, **Z. Yang**, C. M. Dominic Ng, I. K. Chu, “Fragmentation of  $\alpha$ -Radical Cations of Arginine-Containing Peptides”, *J. Am. Soc. Mass Spectrom.* **2010**, 21, 511–521.
24. O. Martinez Jr., **Z. Yang**, N. B. Betts, T. P. Snow, V. M. Bierbaum\*, “Experimental Determination of the Rate Constant for the Associative Detachment Reaction H<sup>-</sup> + H  $\rightarrow$  H<sub>2</sub> + e at 300 K”, *Astrophys. J.* **2009**, 705, L172–L175.
23. **Z. Yang**, E. R. Vorpapel, J. Laskin\*, “Influence of the Charge State on the Structures and Interactions of Vancomycin Antibiotics with Cell-Wall Analogue Peptides: Experimental and Theoretical Studies”, *Chem. Eur. J.* **2009**, 15, 2081–2090.
22. **Z. Yang**, E. R. Vorpapel, J. Laskin\*, “Experimental and Theoretical Study of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues”, *J. Am. Chem. Soc.* **2008**, 130, 13013–13022.
21. **Z. Yang**, C. Lam, I. K. Chu, J. Laskin\*, “The Effect of the Secondary Structure on Dissociation of Peptide Radical Cations: Fragmentation of Angiotensin III and Its Analogues”, *J. Phys. Chem. B* **2008**, 112, 12468–12478.
20. J. Laskin\*, **Z. Yang**, I. K. Chu, “Energetics and Dynamics of Electron Transfer and Proton Transfer in Dissociation of Metal<sup>III</sup>(salen)-Peptide Complexes in the Gas-Phase”, *J. Am. Chem. Soc.* **2008**, 130, 3218–3230.
19. **Z. Yang**, N. S. Rannulu, Y. Chu, M. T. Rodgers\*, “Bond Dissociation Energies and Equilibrium Structures of Cu<sup>+</sup>(MeOH)<sub>x</sub>, x=1–6, in the Gas Phase: Competition Between Solvation of the Metal Ion and Hydrogen Bonding Interactions”, *J. Phys. Chem. A* **2008**, 112, 388–401.
18. C. Ruan, **Z. Yang**, M. T. Rodgers\*, “Influence of the d Orbital Occupation on the Nature and Strength of Binding Copper Cation- $\pi$  Interactions: Threshold Collision-Induced Dissociation and Theoretical Studies”, *Phys. Chem. Chem. Phys.* **2007**, 9, 5902–5918.

## Zhibo Yang

17. C. Ruan, **Z. Yang**, M. T. Rodgers\*, “Cation- $\pi$  interactions with a  $\pi$ -Excessive Nitrogen Heterocycle: Structures and Absolute Binding Energies of Alkali Metal Cation-Pyrrole Complexes”, *Int. J. Mass Spectrom.* **2007**, 267, 233–247.
16. J. Laskin\*, **Z. Yang**, C. Lam, I. K. Chu, “Charge-Remote Fragmentation of Odd-Electron Peptide Ions”, *Anal. Chem.* **2007**, 79, 6607–6614.
15. **Z. Yang**, C. Ruan, H. Ahmed, M. T. Rodgers\*, “Probing the Potential Energy Landscape for Dissociation of Protonated Indole via Threshold Collision-Induced Dissociation and Theoretical Studies”, *Int. J. Mass Spectrom.* **2007**, 265, 388–400.
14. **Z. Yang**, O. Hadjar, J. Laskin\*, “Effect of the surface morphology on the energy transfer in ion-surface collisions”, *Int. J. Mass Spectrom.* **2007**, 265, 124–129.
13. **Z. Yang**, M. T. Rodgers\*, “The Influence of Thio-Substitution on Noncovalent Interactions of Uracil with Alkali Metal Ions. Threshold Collision-Induced Dissociation and Theoretical Studies”, *J. Phys. Chem. A* **2006**, 110, 1455–1468.
12. **Z. Yang**, M. T. Rodgers\*, “Influence of Methylation on the Properties of Uracil and Its Noncovalent Interactions with Alkali Metal Ions. Threshold Collision-Induced Dissociation and Theoretical Studies”, *Int. J. Mass Spectrom.* **2005**, 241, 225–242.
11. C. Ruan, **Z. Yang**, N. Hallowita, M. T. Rodgers\*, “Cation-Pi Interactions with a Model for the Side Chain of Tryptophan: Structures and Absolute Binding Energies of Alkali Metal Cation Indole Complexes”, *J. Phys. Chem. A* **2005**, 109, 11539–11550.
10. **Z. Yang**, M. T. Rodgers\*, “Influence of Halogenation on the Properties of Uracil and Its Noncovalent Interactions with Alkali Metal Ions. Threshold Collision-Induced Dissociation and Theoretical Studies”, *J. Am Chem. Soc.* **2004**, 126, 16217–16226.
9. **Z. Yang**, M. T. Rodgers\*, “Theoretical Study of the Unimolecular and Bimolecular Tautomerization of Cytosine”, *Phys. Chem. Chem. Phys.* **2004**, 6, 2749–2757.
8. N. Rannula, R. Amunugamma, **Z. Yang**, M. T. Rodgers\*, “Influence of *s* and *d* Orbital Occupation on the Binding of Metal Ions to Imidazole”, *J. Phys. Chem. A* **2004**, 108, 6385–6396.
7. Y. Chu, **Z. Yang**, M. T. Rodgers\*, “Solvation of  $\text{Cu}^+$  by Acetone. Structures and Sequential Binding Energies of  $\text{Cu}^+(\text{acetone})$ ,  $x = 1-4$  from Collision-Induced Dissociation and Theoretical Studies”, *J. Am. Soc. Mass Spectrom.* **2002**, 13, 453–468.
6. L. Xiao, P. Lin\*, W. Wang, **Z. Yang**, Y. Fu, S. Yu, “A Novel Preparation Route of Three-way Catalysts”, *Top. Catal.* **2001**, 16/17, 107–113.
5. **Z. Yang**, P. Lin\*, W. Wang, S. Yu, “Study of  $\text{CeO}_2\text{-ZrO}_2$  Solid Solution Promoter Modified by Nd”, *Chinese J. Catal.* (In Chinese) **2001**, 22, 365–369.
4. **Z. Yang**, P. Lin\*, L. Xiao, S. Yu, “ $\text{CeO}_2\text{-ZrO}_2$  Solid Solutions Prepared by Modified Sol-Gel Method and Their Characteristics”, *J. Funct. Mater.* (In Chinese) **2000**, 31, 657–659.
3. L. Xiao, P. Lin\*, **Z. Yang**, W. Wang, “The Phase Purity and Effects on Three-way Catalysts of  $\text{CeO}_2\text{-ZrO}_2$  Solid Solutions”, *J. Mol. Catal.* (In Chinese) **2000**, 14, 81–86.
2. L. Xiao, P. Lin\*, **Z. Yang**, G. Bian, “The Effect of  $\text{ZrO}_2$  on the  $\text{Rh}/\gamma\text{-Al}_2\text{O}_3$  Catalyst for NO Catalytic Reduction”, *Chinese J. Chem. Phys.* (In Chinese) **2000**, 13, 329–335.

### **Publication Based on Undergraduate Research**

1. X. Zhang\*, Z. Xie, **Z. Yang**, “A Discussion on Discriminating the Production Sites of the Ancient Pottery by Using Isotopic Ratios”, *Acta Geoscientia Sinica* (In Chinese) **1997**, 18, 307–309.

### **Oral Presentations**

#### Independent Research at OU

73. **Z. Yang**\*, “Metabolomics Studies of Live Single Cells Using the Single-Probe Coupled to Mass Spectrometry”, online seminar, Department of Chemistry & Biochemistry, University of Maryland, College Park, MD, November 24, 2020.

## Zhibo Yang

72. **Z. Yang\***, “Mass Spectrometry Analysis of Live Single Cells: From Qualitative to Quantitative Analysis”, online seminar, Department of Pharmaceutical Sciences, College of Pharmacy, University of Illinois at Chicago, Chicago, IL, October 7, 2020.
71. **Z. Yang\***, “Metabolomics Studies of Live Single Cells Using the Single-Probe Coupled to Mass Spectrometry”, online seminar, Department of Chemistry, Vanderbilt University, Nashville, TN, September 14, 2020.
70. **Y. Lan, T. Nguyen, R. Liu, S. S. Kane, L. McCall\*, Z. Yang\***, “Single cell mass spectrometry metabolomics studies of cell heterogeneity in the infection of Chagas disease”, 68<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Online Meeting, June 1-12, 2020.
69. **Z. Yang\***, “The Single-Probe: A Microscale Device for Mass Spectrometry Analysis of Single Cells and Tissue”, Department of Chemistry, Wichita State University, Wichita, KS, February 25-26, 2020.
68. **X. Chen, Z. Yang\***, “Metabolomics Studies of Irinotecan-Resistant Cells under Metformin Treatment”, 2020 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 17–19, 2020.
67. **Y. Zhu, W. Wang, Z. Yang\***, “Mass Spectrometry Determination of Double-Bond Positions in Lipids at the Single-Cell Level”, 2020 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 17–19, 2020.
66. **Z. Yang\***, “Mass Spectrometry Analysis of Live Single Cell: From Qualitative to Quantitative Studies”, Moffitt Cancer Center, Tampa, FL, January 31, 2020.
65. **Z. Yang\***, “Extract Metabolomic Information Using Mass Spectrometry Imaging Experiments Combined with Advanced Data Analysis”, 35<sup>th</sup> Asilomar Conference on Mass Spectrometry, Pacific Grove, CA, Oct. 11-15, 2019.
64. **Z. Yang\***, “Mass Spectrometry Analysis of Live Single Cell: From Qualitative to Quantitative Studies”, Pfizer, Groton, CT, September 16, 2019 (Invited).
63. **Z. Yang\***, “Single-probe: A Miniaturized Device for Ambient Mass Spectrometry Analysis of Live Single Cells and Tissues”, College of Chemistry and Chemical Engineering, Lanzhou University, China, July 8, 2019 (Invited).
62. **S. Beasley, M. Sun, Z. Yang\***, “Single-Cell Metabolomic analysis of Metastatic and non-Metastatic Cell Line Pairs Using Mass Spectrometry”, 67<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, Jun. 2-6, 2019.
61. **X. Tian, G. Zhang, Z. Zhu, and Z. Yang\***, “Metabolomic Studies of Tissues Using Mass Spectrometry Imaging Strengthened by Machine Learning and Image Fusion”, 2019 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 18–20, 2019.
60. **S. Standke, N. Pan, R. Bensen, D. Colby, M. Sun, A. Burgett, and Z. Yang\***, “Quantitative Analysis of Drug Compounds in Single Cells”, 2019 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 18–20, 2019.
59. **Z. Yang\***, “Mass Spectrometry Analysis of Live Single Cancer Stem Cells”, SELECTBIO Single Cell Analysis Summit, Coronado Island, CA, Oct. 2-3, 2018 (Invited).
58. **Z. Yang\***, “Microscale Bioanalysis Using Mass Spectrometry: From Single Cells to Tissues”, Chemistry Department, Missouri State University, Springfield, MO, Sept. 12-13, 2018.
57. **Z. Yang\***, “Single Cell Mass Spectrometry: From Qualitative to Quantitative Studies”, 22<sup>nd</sup> International Mass Spectrometry Conference, Florence, Italy, Aug. 23-31, 2018 (Keynote speaker).
56. **Z. Yang\***, “Live Single Cell Mass Spectrometry: Towards Quantitative Analysis”, College of Chemistry, Nankai University, Tianjing, China, July 8, 2018 (Invited).
55. **Z. Yang\***, “Live Single Cell Mass Spectrometry: Towards Quantitative Analysis”, College of Chemistry, Beijing Normal University, China, July 5, 2018 (Invited).
54. **M. Sun; N. Pan; S. Standke; Z. Yang\***, “Live Single Cell Mass Spectrometry: Towards Quantitative Analysis”, 15<sup>th</sup> Taiwan Society for Mass Spectrometry Annual Conference, Taipei, China, Jul. 16-20, 2018.
53. **X. Tian; G. Zhang; W. Yang; C. Mao; Z. Yang\***, “Combining Machine Learning and Multivariate Curve Resolution for Mass Spectrometry Imaging Data Analysis: From Spheroids to Tumors”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.



## Zhibo Yang

52. **N. Pan**; S. Standke; M. Sun, N. R. Kothapalli; A. Burgett, Z. Yang\*, “Quantification of Anticancer Drug in Live Single Cancer Cells Using the Single-Probe MS Technique”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.
51. **Z. Yang\***, “Live Single Cell Mass Spectrometry: Towards Quantitative Analysis”, 255<sup>th</sup> ACS National Meeting, New Orleans, LA, Mar. 22, 2018 (Invited).
50. **Z. Yang\***, “Combining the Single-probe Mass Spectrometry Imaging with Advanced Data Analysis”, 255<sup>th</sup> ACS National Meeting, New Orleans, LA, Mar. 21, 2018 (Invited).
49. **Z. Yang\***, “Mass Spectrometry for Microscale Bioanalysis: Single Cells, Tissues, and Multicellular Spheroids”, Department of Chemistry, Wesleyan University, Middletown, CT, Feb. 16, 2018 (Invited).
48. **M. Sun**, R. Liu, Z. Yang\*, “Mass Spectrometry Analysis of Living Single Cancer Stem Cells”, 2018 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 12–14, 2018.
47. **R. Liu**, G. Zhang, M. Sun, Z. Yang\*, “Live Single Cell Metabolomic Analysis Using Single-Probe Mass Spectrometry: Towards Understanding the Nexus Between Cell-to-Cell Heterogeneity and Metabolic Phenotypes”, 2018 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 12–14, 2018.
46. M. Sun, X. Tian, **Z. Yang\***, “Microscale Mass Spectrometry Analysis of Live *in vitro* Tumors”, SciX, Reno, NV, Oct. 8-13, 2017 (Invited).
45. **S. Standke**, N. Pan, N. R. Kothapalli, A. Le, A. Burgett, Z. Yang\*, “Quantification of Ant-Cancer Compounds in Single Bladder Cancer Cells using the Single-probe MS Technique First Time Quantification of Anti-cancer Compounds in Individual Bladder Cancer Cells”, SciX, Reno, NV, Oct. 8-13, 2017 (Invited).
44. **Z. Yang\***, “Towards Quantitative Mass Spectrometry Analysis of Live Single Cells Using the Single-Probe Device”, SELECTBIO 2017, RNA-Seq, Single Cell Analysis & Single Molecule Analysis, Coronado Island, CA, Oct. 5-6, 2017 (Invited).
43. N. Pan, S. Standke, N. R. Kothapalli, J. E. Heinlen, **Z. Yang\***, A. W. G. Burgett\*, “Towards Quantitative Mass Spectrometry Analysis of Chemotherapy Drugs in Single Bladder Cancer Cells in Patients”, Oklahoma Prostate and Urologic Cancers Research Retreat, Oklahoma City, OK, September 21, 2017.
42. **Z. Yang\***, “Microscale Mass Spectrometry: Single Cell, Tissue Imaging, and Artificial Tumor”, Department of Chemistry, University of Science and Technology of China, China, July 5, 2017 (Invited).
41. **Z. Yang\***, “Microscale Mass Spectrometry: Single Cell, Tissue Imaging, and Artificial Tumor”, College of Chemistry and Chemical Engineering, Lanzhou University, China, June 29, 2017 (Invited).
40. **Z. Yang\***, “Microscale Mass Spectrometry: Single Cell, Tissue Imaging, and Artificial Tumor”, College of Chemistry, Beijing Normal University, China, June 23, 2017 (Invited).
39. **N. Pan**, S. Standke, Z. Yang\*, “Quantification of Anticancer Drug in Live Single Cancer Cells using the Single-probe Device”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.
38. **X. Tian**, W. Rao, Z. Yang\*, “Mass Spectrometry Profiling of *in vitro* Tumors Using the Single-probe Device”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.
37. **Z. Yang\***, “Quantitative Mass Spectrometry Analysis of Live Single Cells Using the Single-Probe Device”, Stephenson Cancer Center (SCC) Preclinical Translational Cancer Research Program, University of Oklahoma Health Sciences Center, OK, March 8, 2017.
36. **Z. Yang\***, “Mass Spectrometry Detection of Chemotherapy Drugs in Single Bladder Cancer Cells in Patients”, 2017 Annual Cancer Research Symposium, University of Oklahoma Health Sciences Center, OK, January 27, 2017.
35. **M. Sun**, N. Pan, and Z. Yang\*, “Single-Probe MS Analysis of Intercellular Metabolites in Live *In Vitro* Tumors”, 2017 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 13–17, 2017.
34. **X. Tian**, W. Rao, Z. Yang\*, “Mass Spectrometry Profiling of Live 3D Artificial Tumors Using the Single-Probe Device”, SciX, Minneapolis, MN, Sept. 18-23, 2016 (Invited).

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33. N. Pan, S. Standke, W. Rao, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “Quantitative Analysis of Live Single Cells Using Single-probe Mass Spectrometry Techniques”, SciX, Minneapolis, MN, Sept. 18–23, 2016 (Invited).
32. **N. Pan**, W. Rao, H. Yu, N. R. Kothapalli, M. Sun, A. Burgett, Z. Yang\*, “Quantifying Concentrations of Molecules in Live Single Cells using the Single-probe MS Technique”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
31. **Z. Yang\***, “The Single-Probe: An Integrated Device for Mass Spectrometry Analysis of Live Single Cells and Tissue Imaging”, Department of Chemistry, University of Californian, Riverside, April 14, 2016 (Invited).
30. **W. Rao**, N. Pan, X. Tian, S. Standke, and Z. Yang\*, “Single-Probe Ambient MS Imaging and Single Cell MS Analysis: Using Dicationic Compounds to Detect Negatively Charged Metabolites in the Positive Ionization Mode”, 2016 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 15–17, 2016.
29. **Z. Yang\***, “The Single-probe: A Miniaturized Device for Mass Spectrometry Single Cell Analysis and Tissue Imaging”, Seminar, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, China, Nov. 4<sup>th</sup>, 2015 (Invited).
28. **Z. Yang\***, “The Single-probe: A Miniaturized Device for Mass Spectrometry Single Cell Analysis and Tissue Imaging”, 16<sup>th</sup> International Beijing Conference and Exhibition on Instrumental Analysis (BCEIA 2015), Beijing, China, Oct. 27–30, 2015 (Invited).
27. N. Pan, W. Rao, R. Liu, N. R. Kothapalli, A. W. Burgett, **Z. Yang\***, “The Single-probe Mass Spectrometry for Single Cell Analysis and Biological Tissue Imaging”, American Society of Pharmacognosy 2015 Annual Meeting, Copper Mountain, CO, July 25–29, 2015.
26. **R. Liu**, N. Pan, Z. Yang\*, “T-probe: A Novel Device to Implement Online *in situ* Single Cell Analysis Using Mass Spectrometry”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.
25. N. Pan, W. Rao, N. Kothapalli, R. Liu, A. Burgett, **Z. Yang\***, “The Applications of Single-probe Mass Spectrometry: Single Cell Analysis and Biological Tissue Imaging”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.
24. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “The Single-Probe: A Microscale Sampling and Ionization Device For Mass Spectrometry Single Cell Analysis, Tissue Imaging, and Detection of Sulfated Proteins”, Michigan Mass Spectrometry Discussion Group, Detroit, MI, May 8, 2015 (Invited).
23. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “The Single-probe: A Microscale Sampling and Ionization Device for Mass Spectrometry Single Cell Analysis and Tissue Imaging”, Pittcon, New Orleans, LA, March 8–11, 2015 (Invited).
22. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “The Single-Probe: A Microscale Sampling and Ionization Device For Mass Spectrometry Single Cell Analysis, Tissue Imaging, and Detection of Sulfated Proteins”, Center for Bioanalysis Symposium, the University of Oklahoma, Norman, OK, February 20, 2015.
21. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “Applications of the Single-Probe MS to Bioanalysis: From Single Cells and Tissues”, Mesilla Chemistry Workshop, Mesilla, NM, February 7–10, 2015 (Invited).
20. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “The Single-Probe: A Miniaturized Sampling and Ionization Device for Mass Spectrometry Studies of Single Cells and Tissue Imaging”, 2015 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 16–18, 2015.
19. **R. Vowcicefski**, N. Pan, Z. Yang\*, “Development of Single-Probe MS and Its Application to the Detection of Sulfated Peptides”, 2015 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 16–18, 2015.

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18. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. Kothapalli, A. Burgett, **Z. Yang\***, “Single-probe: A novel multifunctional device for mass spectrometry studies of single cells, biological tissues, and sulfated proteins”, 248<sup>th</sup> ACS National Meeting, San Francisco, CA, Aug. 10–14, 2014 (Invited).
17. **Z. Yang\***, “Mass Spectrometry: Fundamentals and Applications”, Departmental Seminar, Lanzhou University, China, Jun. 25, 2014 (Invited).
16. **N. Pan**, W. Rao, N. Kothapalli, R. Liu, A. Burgett, **Z. Yang\***, “Single-probe Mass Spectrometry: a Novel Method for Single Cell Analysis”, 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, Jun. 15–19, 2014.
15. **N. Pan**, **Z. Yang\***, “Single-probe Mass Spectrometry for Single Cell Analysis: Development and Applications”, 2014 Lake Arrowhead Conference on Gas Phase Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, Jan. 17–19, 2014.
14. **Z. Yang\***, “Computational Studies of Ion-neutral Reactions of Astrochemical Relevance: Hydrogen Peroxide and Amino Acetonitrile”, 40<sup>th</sup> FACSS/SciX, Milwaukee, WI, Sept. 29, Oct. 04 (Invited).
13. **Z. Yang\***, “Gas Phase Ion Chemistry: Mass Spectrometry and Theoretical Studies of Structures, Energetics, and Reaction Mechanisms”, Physical Chemistry Seminar, Wayne State University, Detroit, MI, Sept. 27, 2012 (Invited).

### Graduate and Postdoc Research:

12. **Z. Yang**, C. Cole, O. Martinez Jr., N. Demarais, M. Y. Carpenter, T. P. Snow, and V. M. Bierbaum\*, “Gas Phase Carbanion-Neutral Reactions of Astrochemical Relevance”, University of Colorado Astrobiology Seminar, Boulder, CO, Oct. 5, 2011 (Invited).
11. **Z. Yang**, O. Martinez Jr., B. Eichelberger, M. Y. Carpenter, T. P. Snow, and V. M. Bierbaum\*, “Gas Phase Reactions of Carbanions with H Atoms”, AbGradCon, Tällberg, Sweden, Jun. 14–18, 2010 (Invited).
10. **Z. Yang**, O. Martinez Jr., B. Eichelberger, M. Carpenter, T. P. Snow, and V. M. Bierbaum\*, “Gas Phase Reactions of Carbanions with H Atoms”, 58<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Salt Lake City, UT, May 23–27, 2010.
9. **Z. Yang**, B. Eichelberger, O. Martinez Jr., M. Stepanovic, T. P. Snow, and V. M. Bierbaum\*, “The Influence of Spin Effects on the Gas Phase Reactions of Carbanions with N and O Atoms”, 2010 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 15–17, 2010.
8. **Z. Yang**, B. Eichelberger, O. Martinez Jr., M. Stepanovic, T. P. Snow, and V. M. Bierbaum\*, “Gas Phase Reactions of Carbanions with N and O Atoms”, 57<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Philadelphia, PA, May 31–Jun. 4, 2009.
7. **Z. Yang**, C. Lam, I. K. Chu and J. Laskin\*, “Surface Induced Dissociation of Peptide Radical Anions”, 56<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Denver, CO, Jun. 1–5, 2008.
6. **Z. Yang** and J. Laskin\*, “Experimental and Theoretical Study of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues”, 55<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 3–7, 2007.
5. **Z. Yang** and Julia Laskin\*, “Experimental and Theoretical Study of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues”, Fundamental and Material Science Division Seminar, PNNL, WA, May 4, 2007.
4. **Z. Yang** and M. T. Rodgers\*, “The Influence of Modification (Halogenation, Methylation, and Thiolation) on the properties of Uracil and its Noncovalent Interactions with Alkali Metal Ions: Collision-Induced Dissociation and Theoretical Studies”, Physical Chemistry Seminar, WSU, MI, Mar. 26, 2005.
3. **Z. Yang** and M. T. Rodgers\*, “The Influence of Halogenation on the Alkali Metal Ion Affinities of Uracil: Threshold CID and Theoretical Studies”, 2004 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 17–19, 2004.
2. **Z. Yang** and M. T. Rodgers\*, “Theoretical Studies of Cytosine Tautomerization in the Gas Phase”, WSU Department of Chemistry Graduate Student Symposium, Oct. 2003.
1. **Z. Yang** and M. T. Rodgers\*, “Collision-Induced Dissociation and Theoretical Studies of  $\text{Cu}^+(\text{EtOH})_n$  ( $n = 1 - 6$ ) and  $\text{M}^+\text{L}$  ( $\text{M} = \text{Na}$  and  $\text{K}$ ;  $\text{L} = \text{Hypoxanthine}$ ,  $\text{Guanine}$ ,  $\text{Purine}$ , and  $\text{Cytosine}$ )”, Physical Chemistry Seminar, WSU, MI, Mar. 2002.

**Poster Presentations**

Independent research at OU

53. **Z. Zou**, P. Yu\*, X. Tian, Z. Yang\*, “Analysis of Metabolites Relevant to Growth of Retinal Blood Vessels using the Single-probe MS Imaging Combined with Fluorescence Microscopy”, 68<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Online Meeting, June 1-12, 2020.
52. **X. Chen**, Z. Yang\*, “Single Cell MS Metabolomics Studies of Anticancer drug-resistant Cells: understanding synergetic effect of mono- and combinational treatments”, 68<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Online Meeting, June 1-12, 2020.
51. **Y. Zhu**, W. Wang, Z. Yang\*, “Determination of double-bond position in unsaturated lipids: reactive single cell mass spectrometry studies”, 68<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Online Meeting, June 1-12, 2020.
50. S. Standke, R. Bensen, D. Colby, A. Le, N. Kothapalli, J. Heinlen, A. Burgett\*, **Z. Yang\***, “Quantitative Analysis of Anticancer Drug in Live Single Suspension Cells: From Cell Lines to Patient Samples.”, 67<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, Jun. 2-6, 2019.
49. **Y. Zhu**, Z. Yang\*, “MS determination of double bond position of lipids at single-cell level”, 67<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, Jun. 2-6, 2019.
48. **X. Tian**, Z. Zou, B. Xie, J. Peng\*, Z. Yang\*, “Metabolomic Studies of Amyloid Plaques in Mouse Brain with Alzheimer Disease Using Mass Spectrometry Imaging Strengthened by Image Fusion”, 67<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, Jun. 2-6, 2019.
47. **R. Liu**, J. Li, A. Chen, Z. Yang\*, “Revealing Concurrent Change of Heterogeneity and Subpopulations of Cancer Cells Using Single Cell Metabolomics”, 67<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, Jun. 2-6, 2019.
46. R. Liu, G. Zhang, J. Li, A. Chen, and **Z. Yang\***, “Single Cell Metabolomics: Combined Mass Spectrometry Experiments and Advanced Data Analysis”, 2019 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 18–20, 2019.
45. **M. Sun**, Z. Yang\*, “Metabolomic Analysis of Live Single Cancer Stem Cells Using Mass spectrometry”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.
44. **S. Standke**, R. Bensen, N. R. Kothapalli, A. Le, A. Burgett, Z. Yang\*, “Investigating Single Cell Pharmacodynamics of Anti-Cancer Compounds Using Quantitative Single Cell Mass Spectrometry”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.
43. **D. Colby**, S. Standke, N. R. Kothapalli, A. Burgett, Z. Yang\*, “Mass Spectrometry Analysis of Non-Adherent Single Cancer Cells: Towards Studies of Patient Cells Obtained from Liquid Biopsy”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.
42. **R. Liu**, G. Zhang, M. Sun, X. Pan, Z. Yang\*, “Single Cell Metabolomics Using Single-probe Mass Spectrometry: Understanding the Nexus between Cell to Cell Heterogeneity and Metabolic Phenotypes of Live Cancer Cells”, 66<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Diego, CA, Jun. 3-7, 2018.
41. X. Tian, G. Zhang, Y. Shao\*, **Z. Yang\***, “Towards Enhanced Metabolomic Data Analysis of Mass Spectrometry Image: Multivariate Curve Resolution and Machine Learning”, 2018 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 12–14, 2018.
40. **S. Standke**, N. Pan, N. Rama Kothapalli, A. T. Le, C. A. Malinky, A. W. Burgett, Z. Yang\*, “Towards Quantification of Anti-Cancer Compounds in Individual Patient Bladder Cancer Cells”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.
39. **R. Liu**, Y. Zhu, N. Pan, Z. Yang\*, “Application of T-probe to MS Metabolomics analysis of live single cells”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.
38. **M. Sun**, X. Tian, Z. Yang\*, “Single-Probe MS Analysis of Extracellular Metabolites in Live *In vitro* Tumors”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.

37. **Y. Zhu**, R. Liu, Z. Yang\*, “The T-probe: A Novel Device for Rapid MS Analysis of Non-Adherent Live Single Cells”, 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4–8, 2017.
36. **S. J. Standke**, N. Pan, N. R. Kothapalli, E. Gyan, D. H. Puccetti, A. W. Burgett\*, Z. Yang\*, “Mass Spectrometry Detection of Drugs in Single Bladder Cancer Cells from Patients”, 2017 Annual Cancer Research Symposium, University of Oklahoma Health Sciences Center, OK, January 27, 2017.
35. X. Tian, W. Rao, **Z. Yang\***, “Mass Spectrometry Profiling of Live 3D Artificial Tumors Using the Single-Probe Device”, 2017 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 13–17, 2017.
34. **Y. Zhu**, R. Liu, Z. Yang\*, “The T-Probe: A Novel Device for MS Analysis of Non-Adherent Live Single Cells”, 2017 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 13–17, 2017.
33. S. J. Standke, N. Pan, N. R. Kothapalli, E. Gyan, D. H. Puccetti, **A. W. Burgett\***, **Z. Yang\***, “Mass Spectrometry Detection of Drugs in Single Bladder Cancer Cells from Patients”, NIH 17<sup>th</sup> Annual Innovation Molecular Analysis Technologies (IMAT) Principle Investigators' (PI) Meeting, Bethesda, MD, December 1–2, 2016.
32. **S. Standke**; N. Pan; N. R. Kothapalli; A. W. Burgett, Z. Yang\*, “Anti-Cancer Drug Detection at the Single Cell Level”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
31. **M. Sun**; N. Pan; B. Wawrik; Z. Yang\*, “Detection of Creatine from Single Algae Cells using Mass Spectrometry”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
30. **R. Vowcicefski**; N. Pan; Z. Yang\*, “Generating Radical Cations of Aromatic Hydrocarbons through Reactive ESI Using the Single-Probe”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
29. **Y. Guan**; R. Vowcicefski; W. Rao; N. Pan; A. Burgett; Z. Yang\*, “Use of Tricationic Ion-Pairing Compounds for the Detection of Nucleotides from Single Cells”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
28. **X. Tian**; W. Rao; N. Pan; H. Yu; D. Karamichos; Z. Yang\*, “Applications of Single-Probe Device for Ambient Mass Spectrometry Imaging Analysis: Human Corneas and 3D Artificial Tumors”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
27. **W. Rao**; N. Pan; H. Yu; X. Qu; C. Mao; Z. Yang\*, “MS Profiling of Molecular Composition Inside live 3D Artificial Tumors Using the Single-Probe Device”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
26. **R. Liu**; Y. Zhu; N. Pan; Z. Yang\*, “Microfabrication and Evaluation of the T-Probe: A Novel Device for Online in situ Live Single Cell MS Analysis”, 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5–9, 2016.
25. **X. Tian**, W. Rao, N. Pan, and Z. Yang\*, “Ambient Mass Spectrometry Imaging Analysis of Human Cornea using the Single-Probe”, 2016 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 15–17, 2016.
24. **M. Sun**, N. Pan, B. Wawrik, Z. Yang\*, “Single Cell Mass Spectrometry Analysis of Marine Algae: Detection of Creatine”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.
23. **R. Vowcicefski**, N. Pan, Z. Yang\*, “Single-probe Ionization Device: Application to the Detection of Sulfated Peptides”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.
22. **W. Rao**, N. Pan, Z. Yang\*, “High-Resolution Ambient MS Imaging of Negative Ions in Positive Ion Mode: Using Dicationic Reagents for Surface Micro-Extraction with the Single-probe”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.

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21. **N. Pan**, W. Rao, Z. Yang\*, “Single-probe Mass Spectrometry: a Novel Method for Single Cell Analysis”, 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31–June 4, 2015.
20. **R. Liu**, N. Pan, Z. Yang\*, “T-probe: A Novel Device to Implement In Situ Online Single Cell Analysis using Mass Spectrometry”, 2015 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, January 16 -18, 2015.
19. **R. Vowcicefski**, N. Pan, Z. Yang\*, “Novel Ionization Method of Sulfated Peptides Using The Single-Probe Ionization Source”, 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, Jun. 15–19, 2014.
18. **W. Rao**, N. Pan, R. Liu, Z. Yang\*, “High resolution ambient MS imaging of mouse tissue by surface micro-extraction using the Single-probe”, 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, Jun. 15–19, 2014.
17. N. Pan, W. Rao, R. Vowcicefski, R. Liu, N. R. Kothapalli, A. W. Burgett, **Z. Yang\***, “Single-Probe: A Novel Sampling and Ionization Device for Mass Spectrometry Studies of Single Cells, Biological Tissues, and Sulfated Biomolecules”. 62<sup>nd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Baltimore, MD, Jun. 15–19, 2014.
16. **Z. Yang\***, “Computational Studies of Ion-neutral Reactions of Astrochemical Relevance: Formation of Hydrogen Peroxide and Amino Acetonitrile”, 61<sup>st</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 9–13, 2013.

### Graduate and Postdoc Research:

15. **Z. Yang**, J. M. Garver, N. Wehres, C. M. Nichols, B. B. Worker, S. Gronert, V. M. Bierbaum\*, “Intrinsic Reactivity and a-effect in Elimination Reactions and Competing Mechanisms in the Gas-phase”, 22<sup>nd</sup> International Symposium on Gas Phase Kinetics, Boulder, CO, June 18–22, 2012.
14. **Z. Yang**, J. M. Garver, N. Wehres, C. M. Nichols, B. B. Worker, S. Gronert, V. M. Bierbaum\*, “Intrinsic Reactivity and a-effect in Elimination Reactions and Competing Mechanisms in the Gas-phase”, 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, BC, Canada, May 20–25, 2012.
13. **Z. Yang**, N. J. Demarais, C. A. Cole, O. Martinez Jr., M. Y. Carpenter, T. P. Snow\*, V. M. Bierbaum\*, “Gas Phase Carbanion-Neutral Reactions of Astrochemical Relevance”, 59<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Denver, CO, June 6–9, 2011.
12. **Z. Yang**, O. Martinez Jr., B. Eichelberger, M. Y. Carpenter, T. P. Snow\*, V. M. Bierbaum\*, “Gas Phase Reactions of Carbanions with Atomic Species”, 2011 Gordon Conference (Gaseous Ions: Structures, Energetics & Reactions), Galveston, TX, Feb. 27–Mar. 4, 2011.
11. **Z. Yang**, O. Martinez Jr., B. Eichelberger, M. Y. Carpenter, T. P. Snow\*, V. M. Bierbaum\*, “Gas Phase Reactions of Carbanions with Atomic Species”, 2010 NASA Laboratory Astrophysics Workshop, Gatlinburg, TN, Oct. 25–28, 2010.
10. **Z. Yang** and J. Laskin\*, “Experimental and Theoretical Study of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues”, 2007 Gordon Conference (Biological Molecules in the Gas Phase: Mass Spectrometry, High-Resolution Spectroscopy, and Theory), Lewiston, MA, Jul. 22–27, 2007.
9. **Z. Yang**, O. Hadjar, J. Laskin\*, “Effect of the surface morphology on the energy transfer in ion–surface collisions”, 54<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Seattle, WA, May. 28–Jun 1, 2006.
8. **Z. Yang** and M. T. Rodgers\*, “The Influence of Modification on the properties of Uracil and its Noncovalent Interactions with Alkali Metal Ions. Collision-Induced Dissociation and Theoretical Studies”, 2005 Gordon Conference (Biological Molecules in the Gas Phase), Lewiston, MA, Jul. 24–29, 2005.
7. **Z. Yang** and M. T. Rodgers\*, “Tautomerization in the Formation and Collision-Induced Dissociation of Alkali Metal Ion-Nucleobases (Cytosine, Guanine, and Hypoxanthine) Complexes”, 2005 Gordon Conference (Gaseous Ions: Structures, Energetics & Reactions), Ventura, CA, Feb. 27–Mar. 4, 2005.

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6. **Z. Yang** and M. T. Rodgers\*, “Tautomerization in the Formation and Collision-Induced Dissociation of Alkali Metal Ion-Cytosine Complexes”, 2004 Anachem/SAS Symposium, Nov. 8<sup>th</sup>, 2004.
5. **Z. Yang** and M. T. Rodgers\*, “Tautomerization in the Formation and Collision-Induced Dissociation of Alkali Metal Ion-Cytosine Complexes”, WSU Department of Chemistry Graduate Student Symposium Oct. 2004.
4. **Z. Yang** and M. T. Rodgers\*, “Metal Ion-Nucleobase Interactions: Guided Ion Beam Mass Spectrometry and Theoretical Studies”, 2003 Conference on Ion Chemistry and Mass Spectrometry, Lake Arrowhead, CA, Jan. 17–19, 2003.
3. **Z. Yang** and M. T. Rodgers\*, “Metal Ion-Nucleobase Interactions: Guided Ion Beam Mass Spectrometry and Theoretical Studies”, WSU Department of Chemistry Graduate Student Symposium, Sept. 2002.
2. **Z. Yang** and M. T. Rodgers\*, “Collision-Induced Dissociation and Theoretical Studies of  $M^+L$  ( $M^+ = Na^+$  and  $K^+$ ;  $L =$  Hypoxanthine, Guanine, Purine, and Cytosine)”, WSU Department of Chemistry Graduate Student Symposium, Aug. 2001.
1. Yun Chu, **Z. Yang**, and M. T. Rodgers\*, “Cation-Solvent Complexes in the Gas Phase: Bond Dissociation Energies and Equilibrium Structures of  $Cu^+(MeOH)_x$  and  $Cu^+(EtOH)_x$ ,  $x = 1-5$ ”, 49<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Chicago, IL, May 27–31, 2001.

(**Presenters** are in bold; \* Indicates PI or corresponding author.)