Dong, Xueming

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Education

Ph.D., Analytical Chemistry, Purdue University, West Lafayette, IN 2013-2019
Research Advisor: Frank Brown Distinguished Professor Hilkka I. Kenttämaa
Thesis: Development of Tandem Mass Spectrometric Methods for Characterizing Asphaltenes and Differentiating Small Organic Isomers

M.Sc., Biotechnology, Nanyang Technological University, Singapore 2010-2012
Research Advisor: Dr. Kai Tang
Research focus: biomarker discovery, proteomics, and protein structure study

B.Sc., Biology, Nanyang Technological University, Singapore 2005-2009

Research Experience

Nanyang Technological University, Singapore 2023-Present
Assistant Professor/Director of Mass Spectrometry Facility

- Structural proteomics
  - Native mass spectrometry
  - Hydrogen-deuterium exchange mass spectrometry
- Clinical proteomics
  - Acoustic levitation mass spectrometry
  - Immuno-MRM mass spectrometry
- Organic proteomics

Frederick National Laboratory for Cancer Research, Frederick, MD 2022-2023
Scientist-CLIA Proteomics

- Developed, implemented, and validated proteomics diagnosis methods for serum thyroglobulin under CLIA regulation.
- Automated multiple popular proteomics sample preparation pipelines.

National Renewal Energy Laboratory, Golden, CO 2019-2022
Post-Doctoral Researcher
Principle Investigator: Dr. Gregg Beckham; Team Leader: Dr. Brenna Black; Manager: Dr. Ed Wolfrum

- Method development for a novel automated identification of native lignin and lignin valorization products in collaboration with bioinformatic scientists
  - Ultrahigh performance liquid chromatography (UPLC) methods development for separation of complex mixture
  - Energy-resolved tandem mass spectrometry (ERMS) for in-depth fragmentation of candidate ions
  - Ion mobility mass spectrometry (IM-MS) for validation and filtering of candidate structures
- Developed methods for identification of polymer degradation products
  - UPLC-IM-ERMS and UPLC-IM-MS/MS for unknown compound identification
- Development of an indirect LC/MS-NMR for unambiguous identification of unknown compounds

Purdue University, West Lafayette, IN 2013-2019
Graduate Student Researcher
Research Advisor: Dr. Hilkka I. Kenttämaa
Academic research:

- Developed methods based on ERMS method for differentiation of isomeric ions of small organic molecules that cannot be addressed via conventional CAD methods.
- Developed a method based on in-source CAD (IS-CAD) for unbiased semi-quantitative analysis of multicore compounds in asphaltenes.
- Developed a method based on IS-CAD for structural elucidation of compounds in coals and during coal catalytic upgrading.
- Maintenance of several LC-UV/vis and LC-MS systems.

Industrial collaboration:

- AstraZeneca and Merck:
  - Unknown drug metabolite identification and differentiation
- The Pioneer Oil Company and Jonathan Amy Facility for Chemical Instrumentation:
  - Developed methods for high-throughput quantification and characterization of polymers and surfactant via HPLC coupled with UV/vis detector charged aerosol detector.
  - Developed methods for geological tracer detection and quantification via LC-MS
  - Proposed, designed, applied for funding, and validated a low-cost, transparent miniaturized coreflood system (TMCF) for rapid evaluation of candidate formulations for chemically enhanced oil recovery.
- ConocoPhillips:
  - Developed a desorption atmospheric-pressure chemical ionization (APCI) method for structural characterization of unknown insoluble solids formed during petroleum refining.
  - GCxGC/electron ionization (EI)/TOF MS characterization of unknown precipitations generated during natural gas refining.
- Chevron:
  - Developed a LC-MS method for quantification and structural characterization of organic compounds desoption onto surfaces of oil reservoir rocks.

Nanyang Technological University, Singapore 2010-2012

Research Advisor: Dr. Kai Tang; Dr. Valerie Lin

- Biomarker Discovery
  - Developed a high-throughput and cost-effective sample preparation method for population screening of inherited blood disease biomarkers in newborn infants.
  - Developed, optimized, and validated a method, for high-throughput peptide biomarker detection via UHPLC/nanoESI, coupled with a Thermo LTQ Orbitrap XL MS.
- Protein structure study via hydrogen deuterium exchange (HDX) MS:
  - Designed, built, optimized, and validated a semi-automated HDX device.
  - Determined the binding site of cyclic diguanylate to a DNA regulating protein FimX by using in-house developed HDX- LQIT/orbitrap MS.
- Proteomics:
  - Discovered novel lysine methylation sites on progesterone receptor in breast cancer cell lines by using HPLC-LQIT/orbitrap MS.
  - Reaction monitoring for synthesis of an antibiotic-resistant bacteria reporter by using HPLC-LQIT/orbitrap MS and MALDI/TOF MS.

B.Sc., Biology Nanyang Technological University, Singapore 2005-2009

- Protein structure study via HDX-MS

Awards and Honors

Singapore Ministration of Education Scholarship 2005-2009

Oral Presentations (*Speaking Author)

1. **Xueming Dong*** et al. High-resolution Broad Mass Range Collisional-Energy Scanning Tandem Mass Spectrometry for Structural Characterization of Asphaltene Molecular Ions", 64th Annual Conference of American Society of Mass Spectrometry, *San Antonio, TX*, **2016**.
2. **Xueming Dong*** et al. "Beam-Type Energy-Resolved Collisionally Activated Dissociation in a Linear Quadrupole Ion Trap/Orbitrap Mass Spectrometer for Characterization of Isobaric Aromatic Ions Derived from Asphaltene Samples." Ohio Mass Spectrometry Symposium, *Columbus, OH*, **2016**.
3. Johnston, Cliff*, **Xueming Dong**, Ravikiran Yerabolu, Bryan Clayton, Nathan Schultheiss, and Hilkka Kenttämaa. "Molecular interactions of crude oil with clay minerals." *Abstracts of Papers of The American Chemical Society* **2017**; 254:1155,

Publications (* Corresponding Author; ¥ Co-First Author)

1. Kevin P. Sullivan¥, Allison Z. Werner¥, Kelsey J. Ramirez¥, Lucas D. Ellis¥, Jeremy Bussard, Brenna A. Black, David G. Brandner, Felicia Bratti,1 Bonnie L. Buss, **Xueming Dong,** Stefan J. Haugen, Morgan A. Ingraham,1 Mikhail O. Konev, William E. Michener, Joel Miscall, Isabel Pardo, Sean P. Woodworth, Adam M. Guss, Yuriy Román-Leshkov, Shannon S. Stahl,* Gregg T. Beckham*, "Tandem chemical oxidation and biological funneling for upcycling of mixed plastic waste." *Science*, **2022**, 378 (6616)): 207-211.
2. Yuyang Zhang, Wanru Li, Haoran Lei, **Xueming Dong**, and Hilkka Kenttämaa*, "Differentiation of Seven Isomeric n-Pentylquinoline Radical Cations Based on Energy-Resolved Medium-Energy Collision-Activated Dissociation.", *Journal of the American Society for Mass Spectrometry,* **2023**, 34, 1:48-63
3. **Xueming Dong¥**, Heather Mayes¥, Kris Morreel, Rui Katahira, Yanding Li, John Ralph, Brenna Black*, Gregg Beckham*, "Energy-Resolved Mass Spectrometry as a Tool for Identification of Lignin Depolymerization Products", *ChemsusChem*, **2023**. e2202201441
4. Heather B. Mayes¥, **Xueming Dong¥**, Grace Dorgan, Rui Katahira, John Ralph, Brenna A. Black*, and Gregg T. Beckhama*, "LigninWrangler: An open-source program for modelling lignin and its decomposition products and identifying these species in mass spectrometry data", Manuscript in preparation, to be submitted to *Nature Communication*.
5. **Xueming Dong**, Yuyang Zhang, Jacob Milton, Ravikiran Yerabolu, Leah Easterling, Hilkka I Kenttämaa*. "Investigation of the relative abundances of single-core and multicore compounds in asphaltenes by using high-resolution in-source collision-activated dissociation and medium-energy collision-activated dissociation mass spectrometry with statistical considerations." *Fuel*, **2019**, 246:126-132.
6. Xing Fan, Xiao-Yun Zhang, **Xueming Dong*,** Jun-Jie Liao, Yun-Peng Zhao, Xian-Yong Wei. "Structural Insights of Four Thermal Dissolution Products of Dongming Lignite by Using In-Source Collision-Activated Dissociation Mass Spectrometry." *Fuel*, **2018**, 230, 78-82.
7. Xing Fan*, **Xueming Dong**, Wen-Han Wei, Zhen-Yu Gao, Hong-Cun Bai, Wen-Long Mo. "Monitoring single-heteroatom loss during deoxygenation and denitrogenation of soluble organic matter in coal using mass spectrometric methods." *Fuel*, **2021**, 292, 120294.
8. Kawthar Z Alzarieni, Joann P Max, Mckay Easton, Jacob R Milton, Xin Ma, **Xueming Dong**, Chungang Gu, Hilkka I Kenttämaa*. "Identification of the carboxylic acid functionality in protonated drug metabolite model compounds by using tandem mass spectrometry based on ion-molecule reactions coupled with high performance liquid chromatography." *Int. J. Mass Spectrom.*, **2021**, 463, 116551.
9. Jifa Zhang, Yuan Jiang, Leah F Easterling, Anton Anstner, Wanru Li, Kawthar Z Alzarieni, Xueming Dong, Joseph Bozell, Hilkka I Kenttämaa*. "Compositional analysis of organosolv

poplar lignin by using high-performance liquid chromatography/high-resolution multi-stage tandem mass spectrometry." *Green Chem*., **2021**, 23, 2, 983-1000.

10. Chu-Fan Wang, Xing Fan*, **Xueming Dong**, Hong-Cun Bai, Peter N Kuznetsov, Peng Liang, Zhen-Xue Liu, Xian-Yong Wei. "Insights into the structural characteristics of four thermal dissolution extracts of a subbituminous coal by using higher-energy collisional dissociation." *Fuel*, **2020**, 282, 118844.
11. Yang-Yang Xu, **Xueming Dong**, Xing Fan*, Hao Xu, Mei Zhong, Feng-Yun Ma, Xian-Yong Wei. "Evaluation of detailed molecular structures for sequential thermal dissolution extracts of a subbituminous coal using a tandem mass spectrometric method." *J. Energy Inst.*, **2020**, 93, 6, 2415-2420
12. Rayan Murtada, Kimberly Fabijanczuk, Kaylee Gaspar, **Xueming Dong**, Kawthar Zeyad Alzarieni, Kimberly Calix, Edgar Manriquez, Rose Mery Bakestani, Hilkka I Kenttämaa*, Jinshan Gao. "Free-radical-mediated glycan isomer differentiation." *Anal. Chem.* **2020**., 92, 20, 13794-13802.
13. **Xueming Dong**, Fei Wang, Xing Fan*, Yun-Peng Zhao, Xian-Yong Wei, Rui-Yu Wang, Feng-Yun Ma, Jing-Mei Liu, Bei Li. "Evaluation of elemental composition obtained by using mass spectrometer and elemental analyzer: A case study on model compound mixtures and a coal-derived liquid." *Fuel*, **2019**, 245, 392-397.
14. Guo Yu, Xing Fan*, **Xueming Dong**, Rui-Yu Wang, Yun‐Peng Zhao, Hong-Cun Bai, Tian-Sheng Zhao, Qing-Jie Guo, Xian-Yong Wei. "Insight into molecular characteristics of a Chinese coal via separation, characterization, and data processing." *J. Sep. Sci.*, **2020**, 43, 4, 839-846.
15. **Xueming Dong**, Xing Fan*, Chu‐Fan Wang, Binoy K Saikia, Rui‐Yu Wang, Yao Lu, Hong-Cun Bai, Xian-Yong Wei. "A novel evaluation method developed for the denitrogenation and deoxygenation on molecules in coal during catalytic treatments." *ChemistrySelect*, **2019**, 4, 46, 13582-13588.
16. Fei Wang[¥], **Xueming Dong**[¥], Xing Fan[*], Yun-Peng Zhao, Guo-Sheng Li, Chu-Fan Wang, Xian-Yong Wei, Feng-Yun Ma, Mei Zhong. "In-source collision activated dissociation for coal/biomass-based model compounds and structural characterization of a coal extract." *Fuel*, **2018**, 234, 1033-1043.
17. Ya-Ru Yu, Xing Fan*, Lu Chen, **Xueming Dong**, Yun-Peng Zhao, Li B, Xian-Yong Wei, Feng-Yun Ma, Aisha Nulahong. "Mass Spectrometric Evaluation of the Soluble Products of a Coal using Cluster Analysis Methods." *Fuel*, **2019**, 236, 1037-1042.
18. Yerabolu, Ravikiran, Raghavendhar R. Kotha, Edouard Niyonsaba, **Xueming Dong**, Jeremy M. Manheim, John Kong, James S. Riedeman, Hilkka I. Kenttämaa[*]. "Molecular profiling of crude oil by using Distillation Precipitation Fractionation Mass Spectrometry (DPF-MS)." *Fuel*, **2018**, 234, 492-501.
19. Guo-Sheng Li, **Xueming Dong**, Xing Fan[*], Chun-Yan You, Ge Wu, Yun-Peng Zhao, Yao Lu, Xian-Yong Wei, Fen-Yun Ma. "Evaluation of Coal-Related Model Compounds Using a Tandem Mass Spectrometry." *Rapid Commun Mass Spectrom.*, **2018**, 32, 16, 1462-1472.
20. Xing Fan, Guo-Sheng Li, **Xueming Dong**, Jiang J, Xian-Yong Wei, Hilkka I. Kenttämaa[*]. "Tandem Mas Spectrometric Evaluation of Core Structures of Aromatic Compounds after Catalytic Deoxygenation." *Fuel Process Technol.*, **2018**, 176, 119-23.
21. Ling-Wen Ding, Qiao-Yang Sun, De-Chen Lin, Wenwen Chien, Norimichi Hattori, **Xueming Dong**, Sigal Gery, Manoj Garg, Ngan B Doan, Jonathan W Said, Jin-Fen Xiao, Henry Yang, Li-Zhen Liu, Xuan Meng, R YJ Huang, Kai Tang, H Phillip Koeffler[*]. "LNK (SH2B3): paradoxical effects in ovarian cancer." *Oncogene*, **2015**, 34, 111, 1463-1474
22. John Takyi-Williams, **Xueming Dong**, Haiqing Gong, Yang Wang, Wenying Jian, Chuan-Fa Liu, Kai Tang[*]. "Application of Paper Spray-MS in PK Studies Using Sunitinib and Benzethonium as Model Compounds." *Bioanalysis*, **2015**, 7, 413-423.

23. Hwa Hwa Chung, Siu Kwan Sze, Amanda Rui En Woo, Yang Sun, Kae Hwan Sim, **Xueming Dong**, Valerie C. L. Lin*. "Lysine Methylation of Progesterone Receptor at Activation Function 1 Regulates both Ligand-independent Activity and Ligand Sensitivity of the Receptor." *J. Biol. Chem.*, **2014**, 289, 704-5722.
24. Qing Shao, Yan Zheng, **Xueming Dong**, Kai Tang*, Xiaomei Yan, and Bengang Xing*. "A Covalent Reporter of β - Lactamase Activity for Fluorescent Imaging and Rapid Screening of Antibiotic - Resistant Bacteria." *Chem. Eur. J.*, **2013**, 19, 903-10910.
25. Yaning Qi, Linghui Xu, **Xueming Dong**, Yin Hoe Yau, Chun Loong Ho, Siew Lee Koh, Susana Geifman Shochat, Shan-Ho Chou, Kai Tang*, and Zhao-Xun Liang*. "Functional Divergence of FimX in PilZ Binding and Type IV Pilus Regulation." *J. Bacteriol.*, **2012**, 194, 922-5931.
26. Yaning Qi, Mary Lay Cheng Chuah, **Xueming Dong**, Kailing Xie, Zhen Luo, Kai Tang, and Zhao-Xun Liang*. "Binding of Cyclic Diguanylate in the Non-catalytic EAL Domain of FimX Induces a Long-range Conformational Change." *J. Biol. Chem.*, **2011**, 286, 910-2917.

Review Service

1. Fuel
2. Journal of Proteome Research
3. Energy Conversion and Management
4. International Journal of Oil, Gas and Coal Technology
5. Journal of Spectroscopy

Teaching

Purdue University:

- CHM 115 Head Teaching Assistants 2013-2014
- CHM 115 Teaching Assistant 2012-2013

University Service

- Purdue Chemistry Week Volunteer 2014-2016
- New graduate student mentor 2017-2017

Professional Association

- American Society for Mass Spectrometry 2014-