

Analytical Chemistry Seminar

Thursday, October 18, 2023
3:00 – 4:00 PM, BRWN 4102

“Mass Spectrometry in Studying Reaction Kinetics”



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Abstract

Mass spectrometry is an established tool in reaction monitoring and studying reaction intermediates.^[1] The nonlinear ionization response and, thus, the inability to obtain quantitative information about concentrations and kinetics partly cast a shadow on the advantage of the great sensitivity and large dynamic range of mass spectrometry in mechanistic research. To access the quantitative kinetic information about reactions in solution, we have been developing the Delayed reactant labeling method.^[2] In the lecture, I will introduce the method, explain possible applications, and show how we used the method to study equilibria in solution,^[3] solve reaction mechanisms, and predict the reaction selectivity.^[4]

References

- [1] J. Mehara, J. Roithova, Identifying reactive intermediates by mass spectrometry. *Chem. Sci.* **2020**, *11*, 11960.
- [2] L. Jašíková, M. Anania, S. Hybelbauerová, J. Roithová, Reaction Intermediates Kinetics in Solution Investigated by Electrospray Ionization Mass Spectrometry: Diaurated Complexes. *J. Am. Chem. Soc.* **2015**, *137*, 13647–13657.
- [3] Q. Duez, P. Tinnemans, J. A. A. W. Elemans, J. Roithová, Kinetics of ligand exchange in solution: a quantitative mass spectrometry approach. *Chem. Sci.* **2023**, Advance Article.
- [4] R. Hilgers et al., Monitoring Reaction Intermediates to Predict Enantioselectivity Using Mass Spectrometry. *Angew. Chem. Int. Ed.* **2022**, *61*, e202205720.

BIO: Jana Roithova graduated from Charles University in the Czech Republic (1998). Her PhD thesis focused on reaction dynamics (2003) and she learned mass spectrometry techniques with Prof. Schwarz (Berlin). In 2007 – 2018, she served as a professor at Charles University. Since 2018, she holds a chair in spectroscopy and catalysis at Radboud University in the Netherlands. *Email:* j.roithova@science.ru.nl