

## המעבדה לכימיה אורגנית ואי-אורגנית

# סמינר

יום ב', 31.10.2022 בשעה 11:30, בחדר הסמינרים

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בנושא:

Harnessing mass spectrometry for interrogating  
reactive intermediates

## Harnessing mass spectrometry for interrogating reactive intermediates

**Abstract:** Electrospray ionization mass spectrometry (ESI-MS) is an important tool for mechanistic studies in organic and organometallic chemistry. It allows investigation of reaction mixtures including monitoring of reactants, products, and intermediates, studying properties of the intermediates and their reactivity. Studying the reactive species in the gas phase can be advantageously combined with theoretical calculations. My talk will give a general introduction into the ESI-MS and how it can be used for mechanistic studies, followed by recent investigations of aryl-corrins—a class of B12 derivatives that embodies “antivitamin” properties and represents a biologically important class of compounds. I will present experimental measurements of the bond strength in a series of aryl-corrins,<sup>1</sup> as well as on the structural properties of arylcobinamides. Quantum chemical calculations for the interpretation of experimental spectra as well as for the comparison with the bond strengths will also be discussed.

1 A. Tsybizova, C. Brenig, C. Kieninger, B. Kräutler, and P. Chen, *Chemistry – A European Journal* 27, 7252 (2021).

