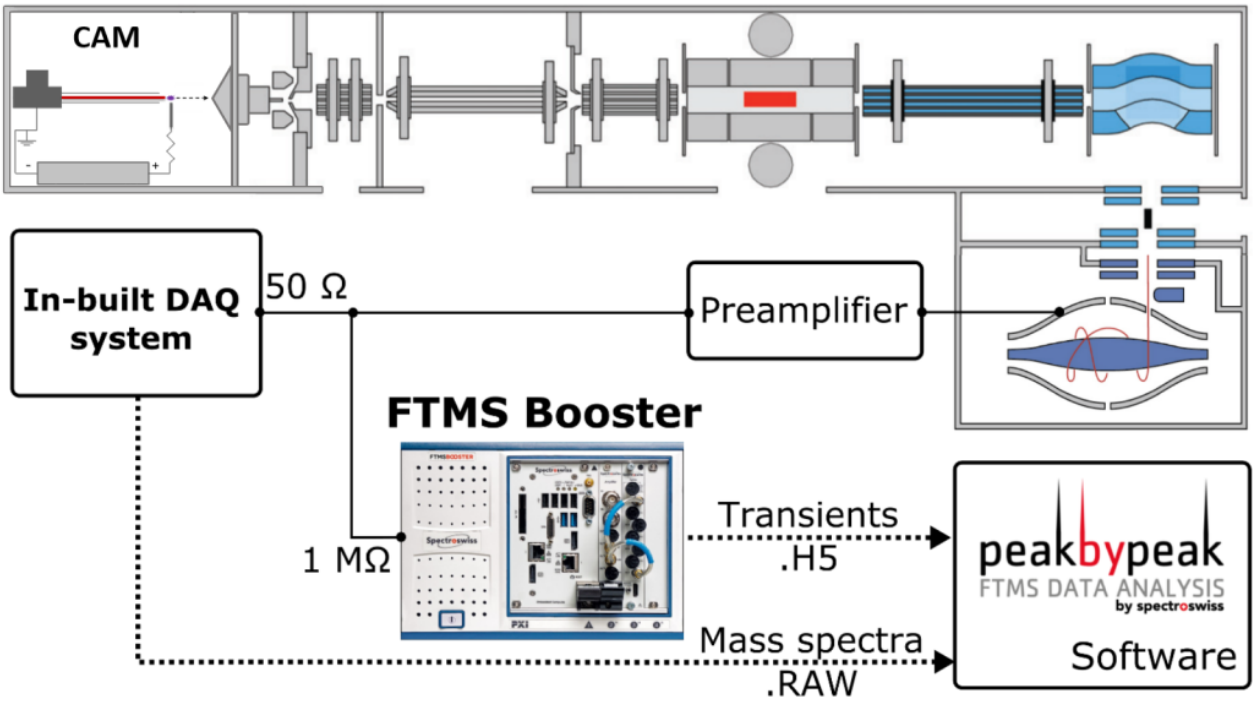
The Swiss Army Knife of Operando Chemical Mass Spectrometry: EWMS Spectroscopy

Vasily Grebennikov[1,2], Adrian Wichser[1], Davide Bleiner[1,2]

[1]Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, 8600 Dübendorf, Switzerland

[2]University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland.
Author email: adrian.wichser@empa.ch



Mass Spectrometry is split into traditional categories such as elemental (or inorganic) and molecular (mainly organic), despite more and more application are cross-field. This is due to the different kind of ionization sources, harder for elemental, e.g. ICP, or softer for molecular, e.g. APCI, ESI. However it is desirable to develop new analytical platform that offer the required flexibility between elemental and molecular analysis. Furthermore, traditional mass spectrometry can only indirectly infer the molecular structure. This happens as a jigsaw puzzle on the fragments. In the case of complex mixture of many isomers and compounds, e.g. wastewater samples with halogenated pollutants, such data analysis is virtually impossible. Thereafter, there should be "orthogonal dimensions" of analysis that besides the mass-to-charge would give the collisional cross-section. The latter happen in ion mobility.

In particular, FAIMS is an effective method for adding a new dimension to separation, namely the compensation voltage of a sample. This new dimensionality allows for the separation of constitutional isomers, enabling the study of complex mixtures as previously mentioned. Furthermore, due to the non-destructive nature of FAIMS, it provides valuable insights into molecular studies, as opposed to fragmentation studies, which are often complicated and challenging to follow.

In turn, the analytical characteristics of mass-to-charge data should also correspond to the sample complexity. These include resolution, mass accuracy, sensitivity, and dynamic range. To maximize the analytical performance of our Orbitrap-based MS set-up, we interfaced it with a high-performance data acquisition and processing system, FTMS Booster.

Aim of this project was to develop a unique "Swiss Army Knife" that would combine all the needs above. As chemistry continues to evolve, so will the complexity of chemical samples, rendering normal mass spectrometers obsolete as they may not provide enough information about an analyte. Therefore, the development of new dimensionalities provided by mass spectrometers is crucial to keep up with the demands of modern chemical analysis.

Randy W. Purves *et al., Rev. Sci. Instrum.* 69, 4094–4105, **1998,** https://doi.org/10.1063/1.1149255
Kenneth Marcus *et al.*, *Mass Spectrom. Rev.* 42, 652-673, **2023,** https://doi.org/10.1002/mas.21720
Deslignière, E., Yin, V.C., Ebberink, E.H.T.M. *et al., Nat Methods,* **2024**, https://doi.org/10.1038/s41592-024-02207-8