

FAIMS-MS analysis of self-assembling supramolecular complexes in the gas phase

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What is FAIMS?

- Field asymmetric waveform ion mobility spectrometry (FAIMS) is a gas phase ion separation technique, that utilises an oscillating high frequency (RF) waveform (Figure 1 (b)), known as the dispersion field (DF), at atmospheric pressure.
- The rapid separation of gas phase ions is a result of differences in ion mobility in a buffer gas in alternating low and high electric fields.
- A small DC voltage known as the compensation field (CF) is superimposed on the DF to transmit selected analytes (Figure 1 (a)).
- FAIMS provides orthogonal separation to mass spectrometry (MS)

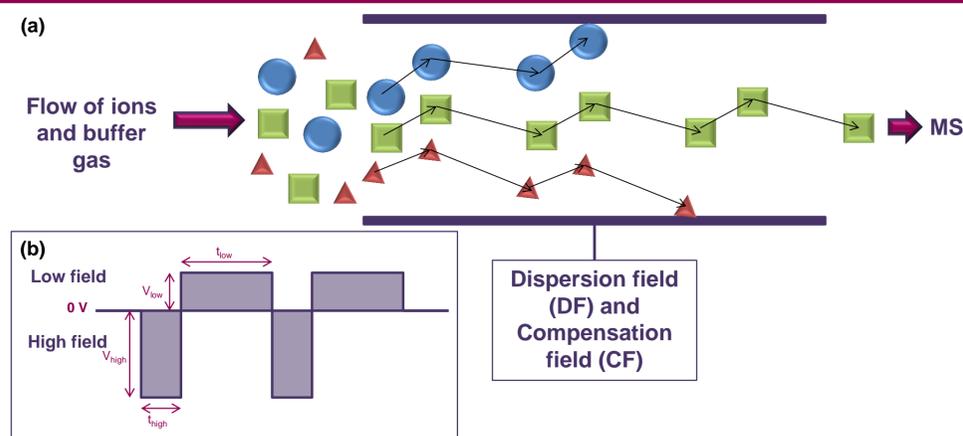


Figure 1: (a) Ion transmission through planar FAIMS electrodes at fixed DF and CF; (b) oscillating asymmetric waveform

Supramolecular Complexes

- Complexes that self-assemble around a cation were observed using FAIMS-MS (Figure 2).

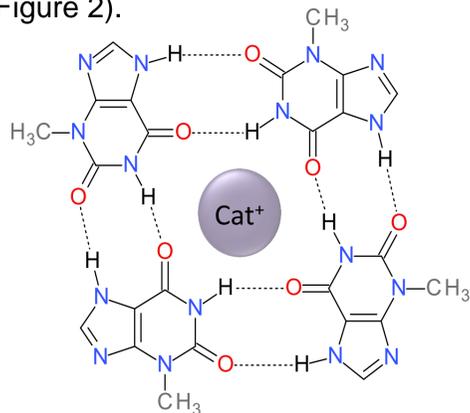


Figure 2: Structure of 3-methylxanthine (3-MX) non-covalently bound tetramer $[(3\text{-MX})_4 + \text{Cat}^+]$ with stabilising cation (NH_4^+ , Na^+ or K^+)

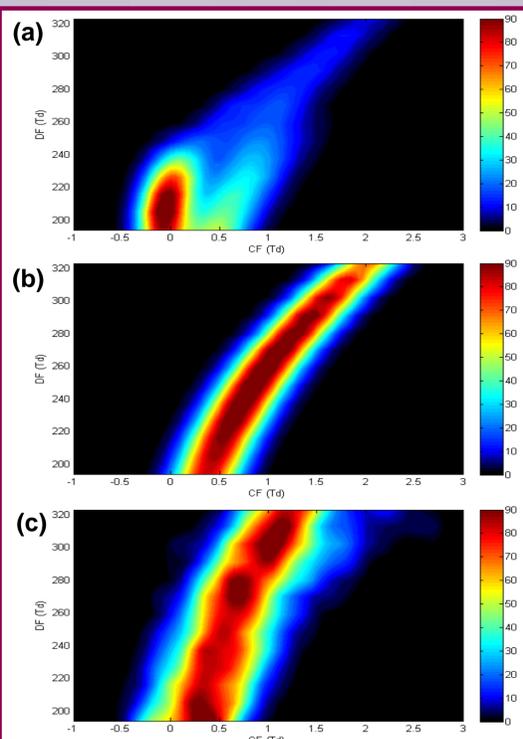


Figure 3: 3D heat map (where intensity is on the colour scale) of (a) $[(3\text{-MX}) + \text{Na}]^+$, (b) $[(3\text{-MX})_4 + \text{Na}]^+$ and (c) $[(3\text{-MX})_{12} + 2\text{Na-H}]^+$

Supramolecular Complexes

- Non-tetrameric complexes were less abundant and became less stable at increasing DFs, such as the 3-MX monomer (Figure 3 (a)).
- The tetrameric based complexes were found to be stable through the FAIMS device (Figure 3 (b)) up to the highest DFs.
- Higher-ordered tetrameric based complexes were shown to dissociate at higher DF values (Figure 3 (c)), broadening the heat map profile.
- Mass spectra of these complexes were enhanced using FAIMS (Figure 4).

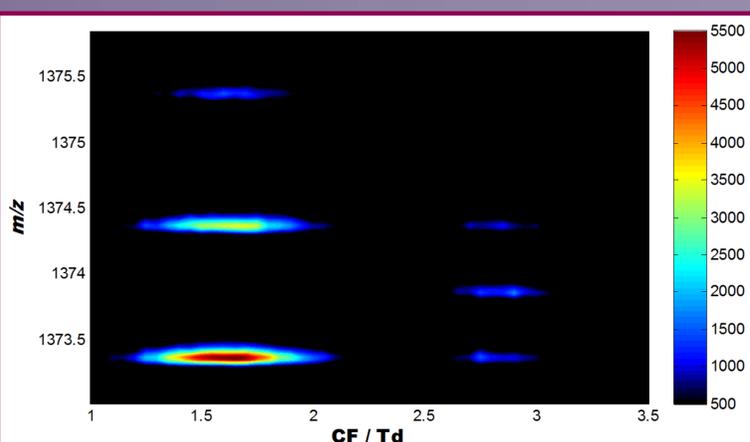


Figure 5: FAIMS-MS separation of 3-MX (+Na⁺) singly and doubly charged complexes which overlap at m/z 1373.4

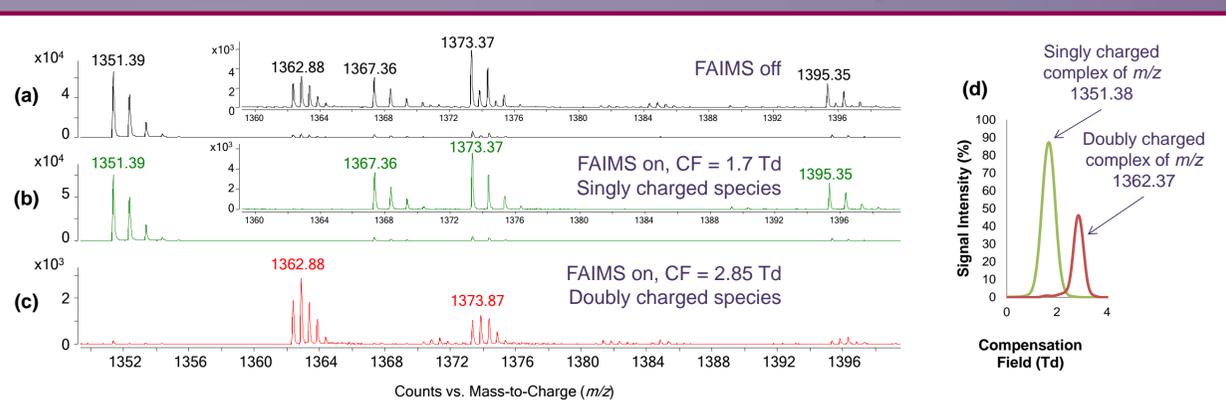


Figure 4: Charge state separation of 3-MX (+Na⁺) complexes using FAIMS (DF = 323 Td); (a) no FAIMS, (b) FAIMS selection of the singly charged species (CF = 1.7 Td) and (c) FAIMS selection of the doubly charged species (CF = 2.85 Td); (d) FAIMS CF scan at DF = 323 Td (selected ion responses)

FAIMS-MS Results

- FAIMS-MS can be used to resolve different charge states (Figure 4) by selecting either the singly (Figure 4 (b)) or doubly (Figure 4 (c)) charged complexes.
- FAIMS also demonstrates a 2-3 fold improvement in signal-to-noise ratio for low intensity complexes (Figure 4).
- Complexes of overlapping mass-to-charge (m/z) in the mass spectrum, can be resolved using FAIMS pre-selection (Figure 5).

Conclusions

The hyphenation of FAIMS-MS has shown the potential to aid in the deconvolution of complicated mass spectra of supramolecular non-covalent complexes.

Acknowledgements

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