

Machine-learning-enhanced time-of-flight mass spectrometry analysis (12 min talk + 3 min discussion)

Thursday, 15 April 2021 11:45 (15 minutes)

Mass spectrometry is a widespread approach used to work out what the constituents of a material are. Atoms and molecules are removed from the material and collected, and subsequently, a critical step is to infer their correct identities based on patterns formed in their mass-to-charge ratios and relative isotopic abundances. However, this identification step still mainly relies on individual users' expertise, making its standardization challenging, and hindering efficient data processing. Here, we introduce an approach that leverages modern machine learning technique to identify peak patterns in time-of-flight mass spectra within microseconds, outperforming human users without loss of accuracy.

Poster title

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