

Artificial Intelligence (AI) Provides Ease-of-Use in TOF-SIMS Data Reduction

Mass spectrometry imaging by TOF-SIMS can be challenging, especially for new operators and analysts. Even veteran practitioners have difficulty with peak assignments from time to time as the data shown in Figure 1 illustrates. The problem can be compounded when an analyst has data from many samples. PHI provides a solution using AI to improve ease-of-use in TOF-SIMS data reduction. The algorithm involves a supervised approach for both feature identification (i.e., organic, atomic and isotope peaks) and classification (i.e., high or low confidence). The AI algorithm provides an AI Score of zero to 99% to classify the spectral calibration as “high confidence” or “low confidence”. High confidence is defined as > 90% and low confidence is < 80%. See Figure 2 for an illustration representing the algorithm’s behavior.

Key Features of AI Score

- Simple go / no-go feedback of spectral calibration confidence
- Feedback window with flags for multiple raw file playback
- Ease-of-use for new operators or analysts

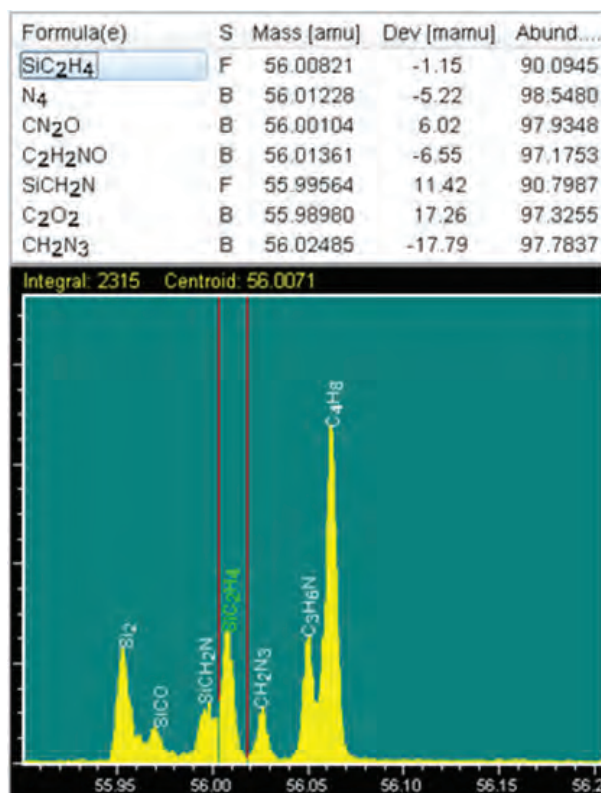


Figure 1: Many peaks at the same nominal m/z is a challenge.

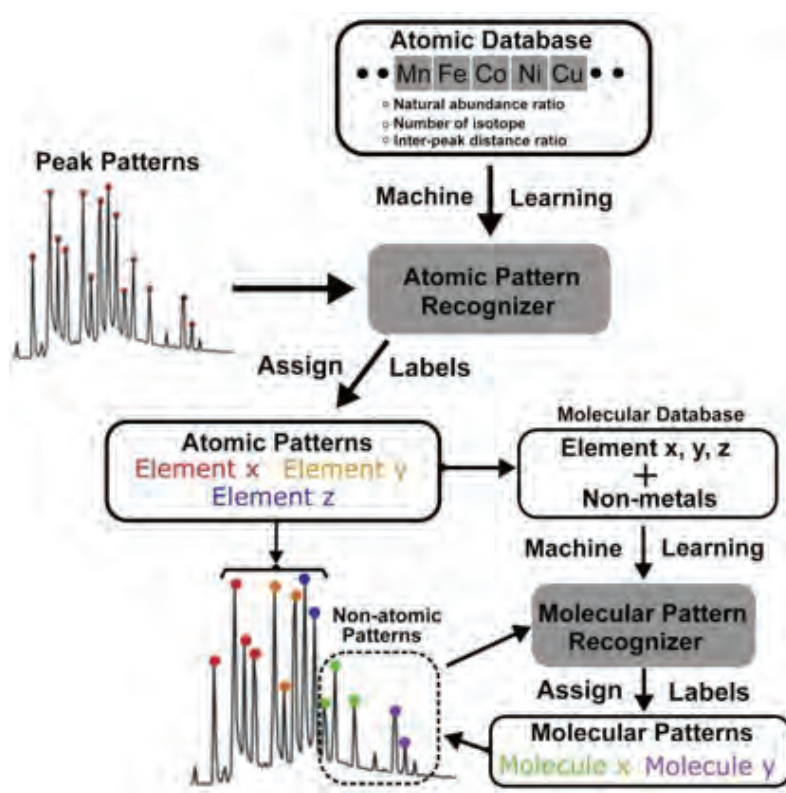


Figure 2: Schematic illustration of the AI processing. Image from Y. Wei, et al., *Patterns* 2 (2021) 100192.

Figure 3: The 98% AI Score indicates high confidence in the calibration of the as-collected spectral data.

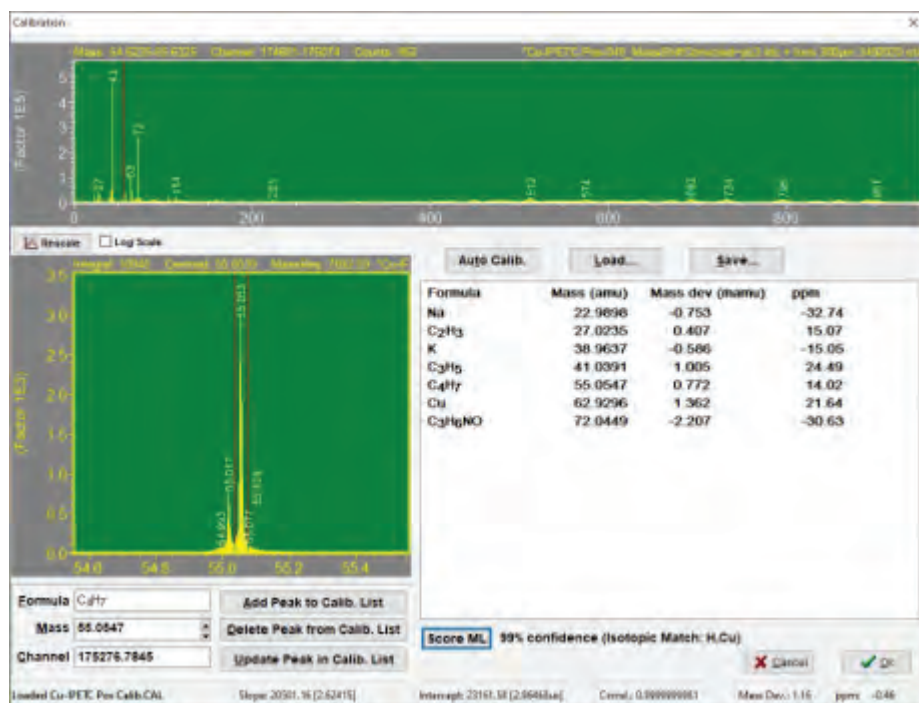
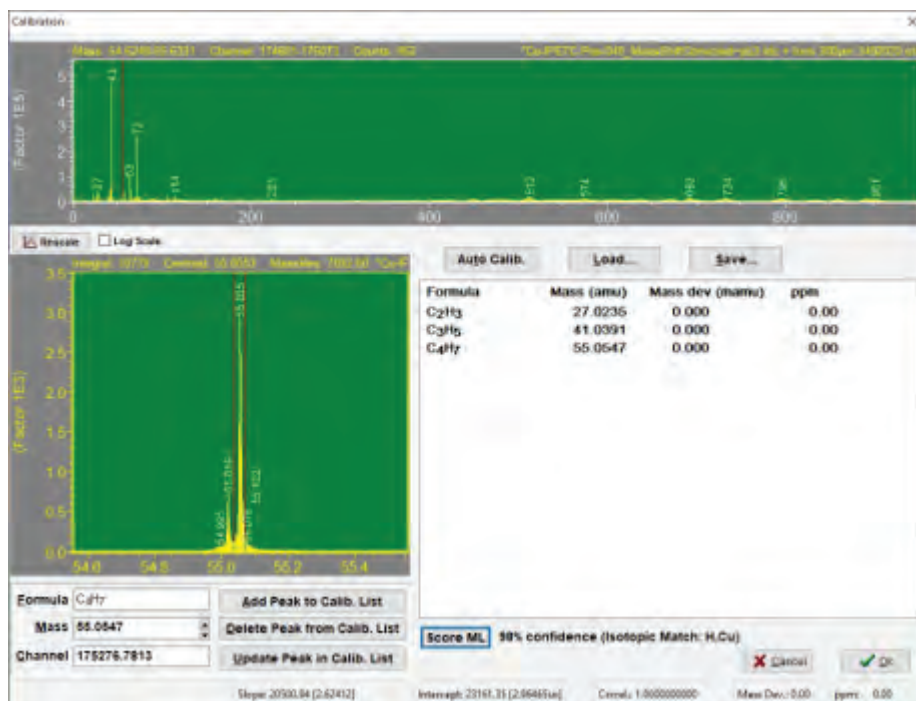


Figure 4: The 99% AI Score indicates high confidence in the added putative compositional peak assignments.

The example data shown in Figures 3 & 4 illustrate the feedback provided by the AI Score, an indication of the confidence level of correct peak assignments in the mass calibration.

Physical Electronic has developed an AI algorithm for the processing of TOF-SIMS mass spectral data. We continue our efforts to provide features that enable the work of analysts and to enhance productivity. If you would like to participate in further developments, please contact us for follow up.