

Press Release

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Shimadzu's Formula Predictor LCMS System Identifies Unknowns with Greater Certainty Using High Mass Accuracy MSⁿ Data

Answering researchers' need for improved accuracy and speed in identification of unknown components, Shimadzu Corporation, one of the world's leading developers of analytical instrumentation, has developed a new system featuring its award-winning LCMS-IT-TOF mass spectrometer. Using information-rich MSⁿ data, the patent-pending Formula Predictor software takes advantage of multiple levels of fragmentation, isotope pattern verification, and unique fragmentation filtering techniques to accurately determine the correct formula for unknown components.

Traditional approaches for deducing empirical formulae from mass spec data often depend on very high mass accuracy, which carries a correspondingly high cost, and considerable time input from the user to eliminate low-probability structures. Shimadzu's new system reduces or eliminates this need for tedious, manual processing of target candidates. In many cases, the software can reduce the collection of target compounds from a high number of possible candidates to predicting the most likely empirical formula with just a simple mouse click.

The first LCMS system to fully utilize the information-rich content of MSⁿ data in formulae prediction, Shimadzu's LCMS-IT-TOF

addresses the needs of biomarker discovery, trace amount impurity identification, and natural products research.

Features of the LCMS-IT-TOF include:

- High mass accuracy MSⁿ analysis. The high level of accuracy helps scientists process their data with greater confidence by performing accurate database searching and enabling workflows and data interpretation to greater precision.
- High-sensitivity, full-spectrum TOF analyzer providing low femtomole/picogram detection of multiple components in a single analysis.
- Constant mass accuracy and mass resolution in all MS modes.
- Fast data acquisition, up to 10 spectra per second, for efficient peak detection and compatibility with ultrafast HPLC separations.
- High-speed polarity switching (switching time of 100 milliseconds)

Kozo Shimazu, Corporate Officer & Deputy General Manager Analytical & Measuring Instruments Division for Mass Spectrometry & Life Sciences at Shimadzu Corporation, stated: “Our formula prediction software has been developed to help researchers working in compound verification to identify unknown compounds correctly with higher confidence. We believe that this software further strengthens the unique technology of the LCMS-IT-TOF in delivering an integrated solution to identify or verify empirical formulae.”

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