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Signal Processing Tools to Detect and Estimate Signal Peaks in ESI-TOF Mass spectrum

AzTE Case # M13-145

Inventors

Sai Buddi
Graduate Student
Electrical Engineering
Arizona State University

Thomas Taylor
Associate Professor
School of Mathematical and Statistical Sciences
Arizona State University

Randall Nelson
Research Professor
Molecular Biomarkers Lab
The Biodesign Institute
Arizona State University

Chad Borges
Associate Research Professor
Molecular Biomarkers Lab
The Biodesign Institute
Arizona State University

Douglas Cochran
Associate Professor
School of Electrical, Computer and Energy Engineering
Arizona State University

Intellectual Property Status:

Patent Pending

Contact

Yash Vaishnav, PhD, MBA

Vice President

Business Development, Life Sciences

Arizona Technology Enterprises, LLC (AzTE)

P: 480.884.1648

F: 847.971.2871

YASH@AZTE.COM

HEALTHSCIENCES@AZTE.COM

Invention Description

Since the FDA issued new regulations requiring that antidiabetic therapies not increase cardiovascular Disease (CVD) risk, there has been an increased emphasis in identifying panels of markers that are able to distinguish the types of CVD in the context of type 2 diabetes (T2D). ESI-TOF-MS (electrospray ionization time-of-flight mass spec) is an important and well established tool used to identify biomarkers; however, it produces data that requires the identification and quantification of signal peaks embedded in background noise. Current algorithms used to identify and quantify ESI-TOF-MS signal peaks are time consuming, and have difficulty with low amplitude peaks and processing large numbers of mass spectra.

Researchers at Arizona State University have developed novel signal processing methods for detection of signal peaks in mass spectrum data. These novel methods develop a theoretical description of the signal peak which matches the experimentally observed peak shape, and can be used for enhanced detection and amplitude estimate of low amplitude peaks. Background noise and unpredictable or uncontrolled signal variability is better characterized, both of which also enable enhanced detection of low amplitude peaks.

These novel methods utilize sound mathematical principles, can quickly process large numbers of mass spectra, and, unlike the existing methods, perform very well at low signal-to-noise ratio conditions.

Potential Applications

- Detect and estimate low amplitude signal peaks in mass spectra for biomarker discovery

Benefits and Advantages

- Enhanced detection and amplitude estimation of low amplitude peaks
- Eliminates pre-processing and deconvolution routines for ESI MS that may result in loss of information at low signal-to-noise ratios
- Employs a mathematically optimal scheme to detect signal peaks
- Utilizes robust mathematical models to determine signal shape
- Signal peaks are detected and their amplitude and area is estimated even when the signal-to-noise ratio is small
- Noise distribution is determined from experimental data with the use of goodness of fit tests
- Automatically estimates peak amplitude and area under curve
- Performs better than existing methods at low SNRs