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Mass Spectrometry Software Improves Data Evaluation (20120293, Dr. Timothy Griffin)

IP Status: Issued US Patent; **Application #:** 14/090,961

Peptide and Metabolite Identification with Mass Spectrometry Software

The Proximity-based Intensity Normalization (PIN) software offers improved evaluation of mass spectrometry data to identify molecules of biological interest. The algorithm dramatically improves the accuracy in the evaluation of mass spectrometry data, making it useful not only for protein identification, but metabolite and peptide identification. In accurately quantifying signals in mass spectrometry data, normalization is important to account for variation introduced by sample handling, sample loading and instrument response. PIN uses relative, rather than global scaling factors to achieve this aim, eliminating extraneous artifacts.

Uses Include Biomarker Discovery, Pharmaceutical Studies and Personlized Medicine

Using PIN reduces the coefficient of variation by more than 50% (compared with 9-25% for current methods) and the Pooled Estimate Variance (PEV) by 69-78% (compared with 9-38% for current methods). The result of using PIN is that complex peptide mixtures with statistically significant biological variation are observed which are often missed by conventional normalization techniques. Potential applications include biomarker discovery, pharmaceutical studies and personalized medicine.

BENEFITS OF MASS SPECTROMETRY PROXIMITY-BASED INTENSITY NORMALIZATION (PIN):

- PIN enables large scale peptidomic studies to go beyond identification of proteins to peptides and metabolites.
- The algorithm reduces systematic bias and random variability while retaining biological variability.
- PIN reduces the coefficient of variation by 50% and the Pooled Estimate Variance (PEV) by up to 78%.
- Potential applications are biomarker discovery, pharmaceutical studies and personalized medicine.

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