

Reverse and Random Decoy Methods for False Discovery Rate Estimation in High Mass Accuracy Peptide Spectral Library Searches

Zheng Zhang^{1*}, Meghan Burke¹, Yuri A. Mirokhin¹, Dmitrii V. Tchekhovskoi¹, Sanford P. Markey¹, Wen Yu², Raghothama Chaerkady³, Sonja Hess³, Stephen E. Stein^{1*}

¹Mass Spectrometry Data Center, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland 20899 USA

²Research Bioinformatics, MedImmune LLC, One MedImmune Way, Gaithersburg, Maryland 20878 USA

³Antibody Discovery and Protein Engineering, Protein Sciences, MedImmune LLC, One MedImmune Way, Gaithersburg, Maryland 20878 USA

Correspondence to:

*E-mail: zheng.zhang@nist.gov Tel: +1 301 975 5828.
steve.stein@nist.gov. Tel: +1 301 975 2505.

KEYWORDS: *peptide mass spectral library, target-decoy approach, PeptideProphet algorithm, false discovery rate*

ABBREVIATIONS: **FDR**, false discovery rate; **SLS**, Spectral library searching; **SDS**, sequence database searching; **LC-MS/MS**, liquid chromatography-tandem mass spectrometry; **PSM**, peptide-spectrum match; **NIST**, National Institute of Standards and Technology; **NCBI**, National Center for Biotechnology Information; **NIH/NCI**, National Institutes of Health/National Cancer Institute; **CPTAC**, Clinical Proteomic Tumor Analysis Consortium; **HCD**, higher-energy collisional dissociation; **iTRAQ**, isobaric tags for relative and absolute quantitation; **IDs**, identifications; **SUI**, sequence uniqueness index.

