

Supporting Information

Optimization and Modeling of Quadrupole Orbitrap Parameters for Single-Cell Proteomics

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Keywords:

shotgun proteomics; tandem mass spectrometry; LC-MS/MS; Orbitrap; ion injection time; mass isolation window, single-cell proteomics, trace proteomics

Table S1. Protein identification for 10ng CHO lysate using benchmark and optimal instrumental parameters (separate xlsx file).

Table S2. GO enrichment analysis of proteins identified in Supplementary Table S1 (separate xlsx file).

Fig S1. Numbers of MS2 scans and PSMs as a function of ITmax for trypsin digest of 1 ng CHO-cell lysate acquired by Q-Exactive HF. Page S-3

Fig. S2. Percentage of uniquely detected peptides in CHO-cell lysate digests of 1, 10, and 100 ng as a function of IW. Page S-4

Fig. S3. Protein groups detected from 1, 10, and 100 ng of trypsin digest of CHO-cell lysate at regular (2E4) and low (2E3) threshold of MS2 fragmentation defined in Q-Exactive HF at MS2 ITmax of 50 ms and IW of 2.0 Th. Page S-5

Fig. S4. Number of MS2 scans, PSMs, peptide and protein groups obtained from 1, 10, and 100 ng of trypsin digest of CHO-cell lysate with a minimum S/N of 3.0 in the Orbitrap for more reliable detection compared to the default S/N of 1.5. Page S-6

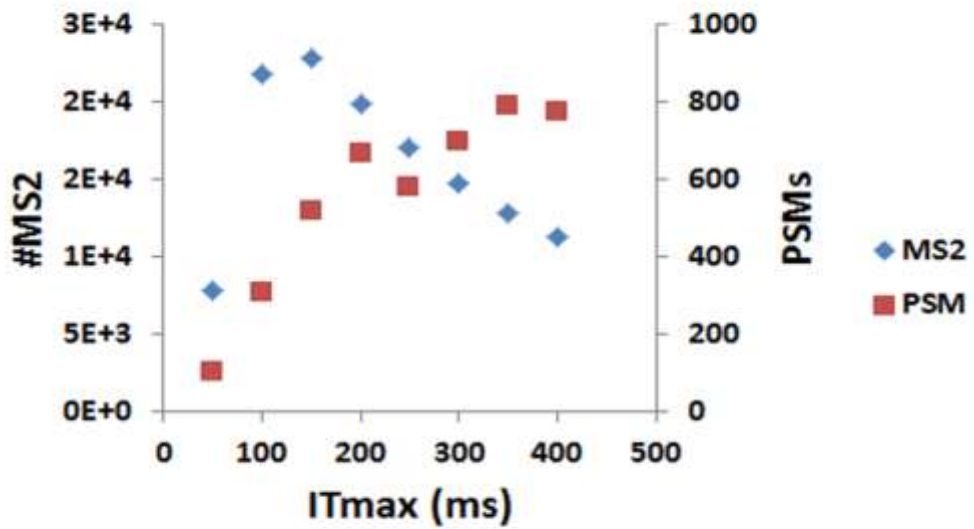


Fig. S1. Numbers of MS2 scans and PSMs as a function of ITmax for trypsin digest of 1 ng CHO-cell lysate acquired by Q-Exactive HF.

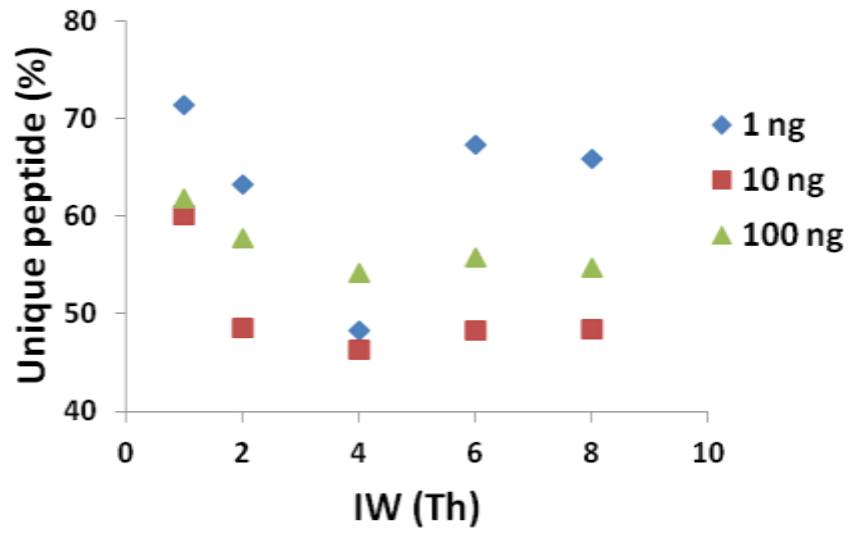


Fig. S2. Percentage of uniquely detected peptides in CHO-cell lysate digests of 1, 10, and 100 ng as a function of IW.

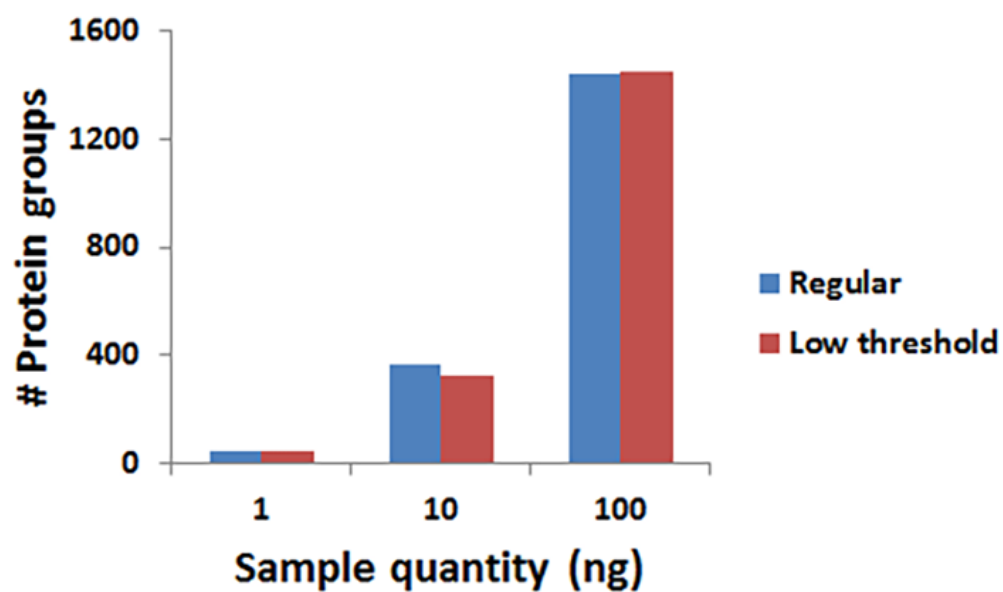


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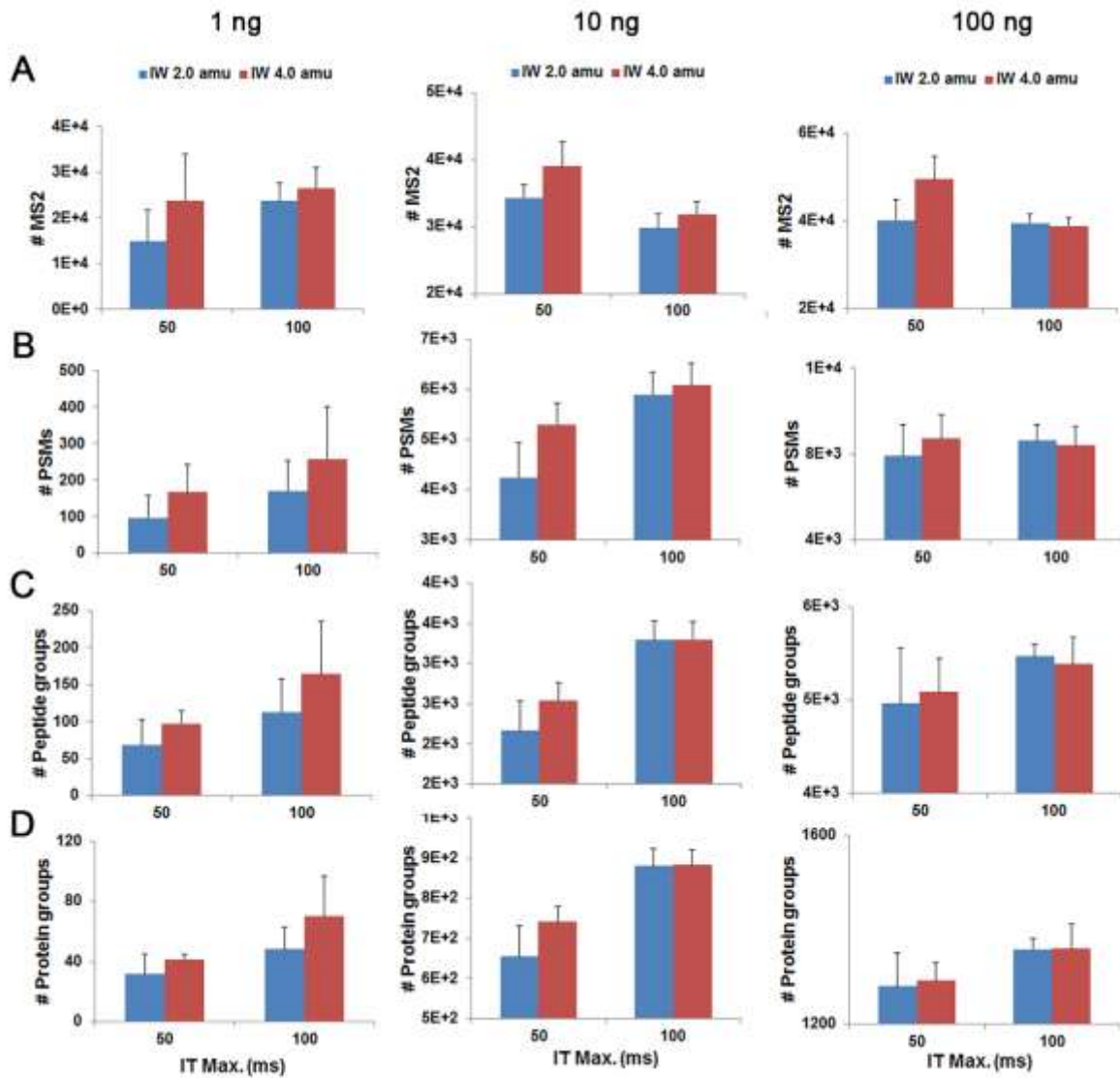


Fig. S4. Number of MS2 scans, PSMs, peptide and protein groups obtained from 1, 10, and 100 ng of trypsin digest of CHO-cell lysate with a minimum S/N of 3.0 in the Orbitrap for more reliable detection compared to the default S/N of 1.5. The error bar is the standard deviation of the mean.