

**Title:** Supplementary Data 1:

**Description:** List of all mass spectrometry runs (file names) used in this study.

**Title:** Supplementary Data 2:

**Description:** List of similar sequences (by substring) resulting in the same score. Six phosphorylation-enriched runs from Espadas et al. (2017) were used to generate this table.

**Title:** Supplementary Data 3:

**Description:** Output from PTM-Shepherd.

**Title:** Supplementary Data 4:

**Description:** Ion purity scores used in plotting Supplementary Figure 3. There are six tables corresponding to substitution-free Type 1, substitution-free Type 2, substitution-free Type 3, substitution-containing Type 1, substitution-containing Type 2, and substitution-containing Type 3 cases.