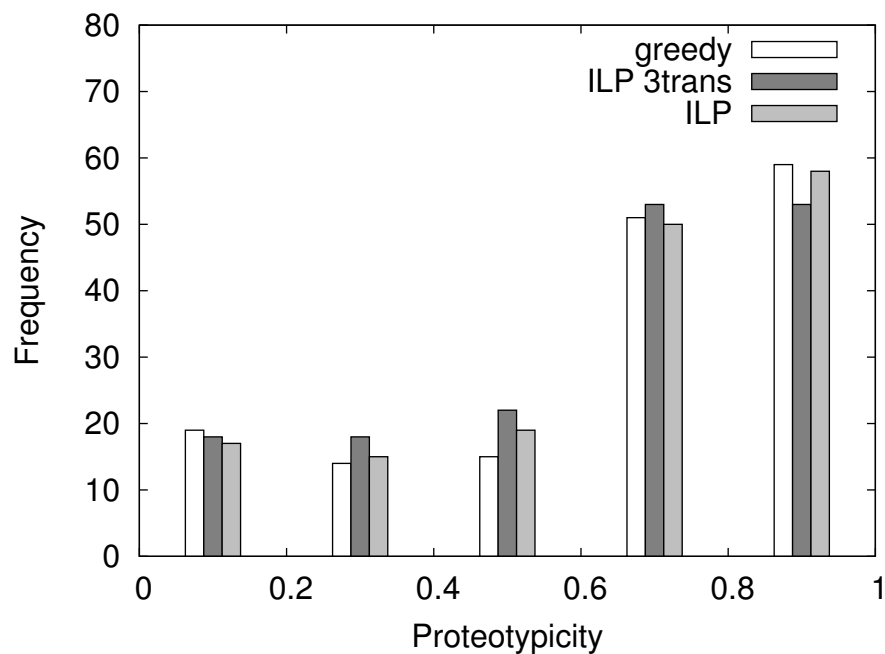


Supplemental material to the manuscript: Optimal de novo design of MRM experiments for rapid assay development in targeted proteomics

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1 Proteotypicity Histogram

Figure 1: Histogram of the proteotypicity values of the scheduled peptides. The greedy algorithm scheduled 474, the ILP with exactly three transitions allowed 492 and the ILP 502 transitions. The sum of the proteotypicity values of the peptides was 101.2 for the greedy, and 101.7 for the ILP variants.



2 Observed vs. Scheduled Peptides

Figure 2: The plot shows the ratio of observed vs. scheduled peptides of the greedy and ILP solutions for different proteotypicity values of the peptides. Although, the chance of observing peptides of high proteotypicity is greater than those with lower proteotypicity values, the difference of peptides with a proteotypicity > 0.6 are small.

