Supplementary Information for: A development platform for rapidly creating mass spectrometry proteomics computational tools

*Damon May, Wendy Law, Matt Fitzgibbon, Qiaojun Fang and Martin McIntosh**

Molecular Diagnostics Program, Fred Hutchinson Cancer Research Center

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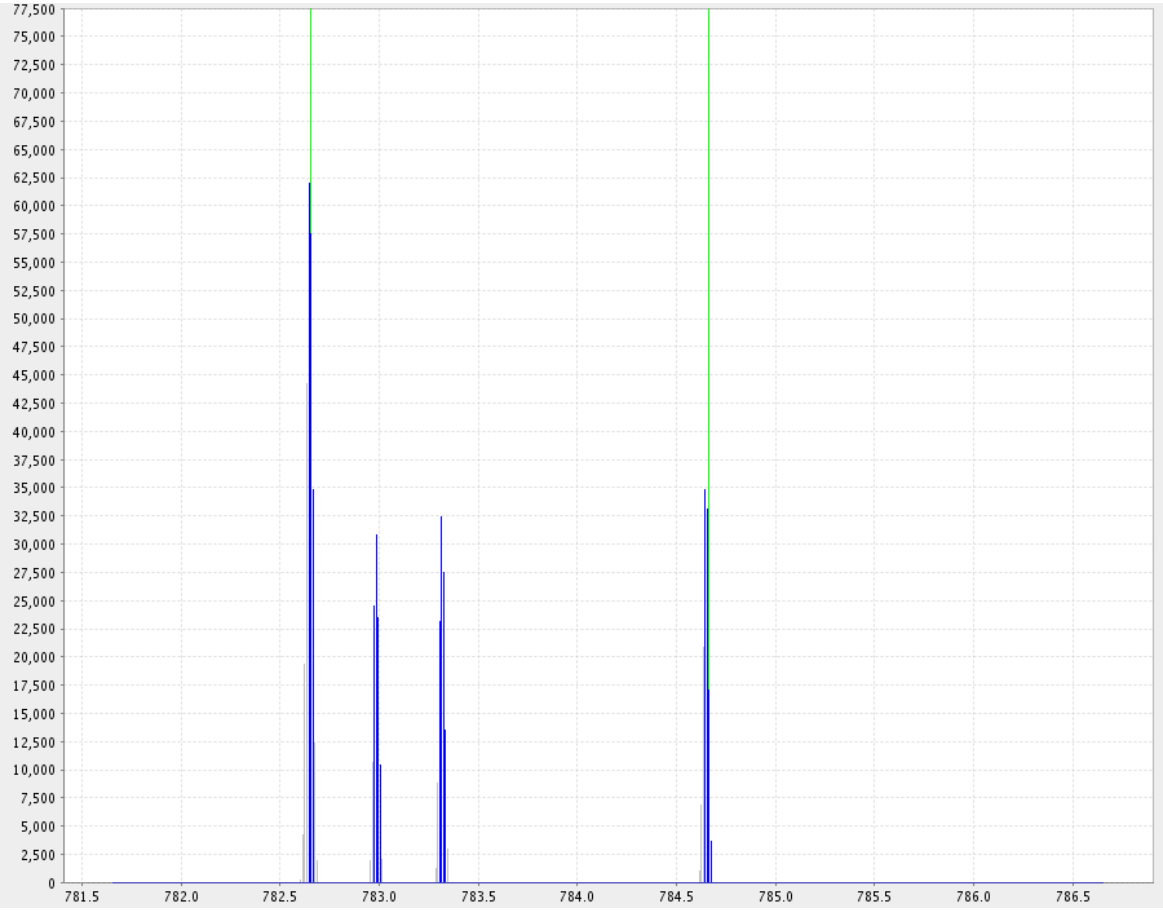
Charts Describing Categories of 'Bad' Events

In the manuscript, six categories of 'Bad' quantitative events are described. These charts provide examples of quantitative events that are typical of each category.

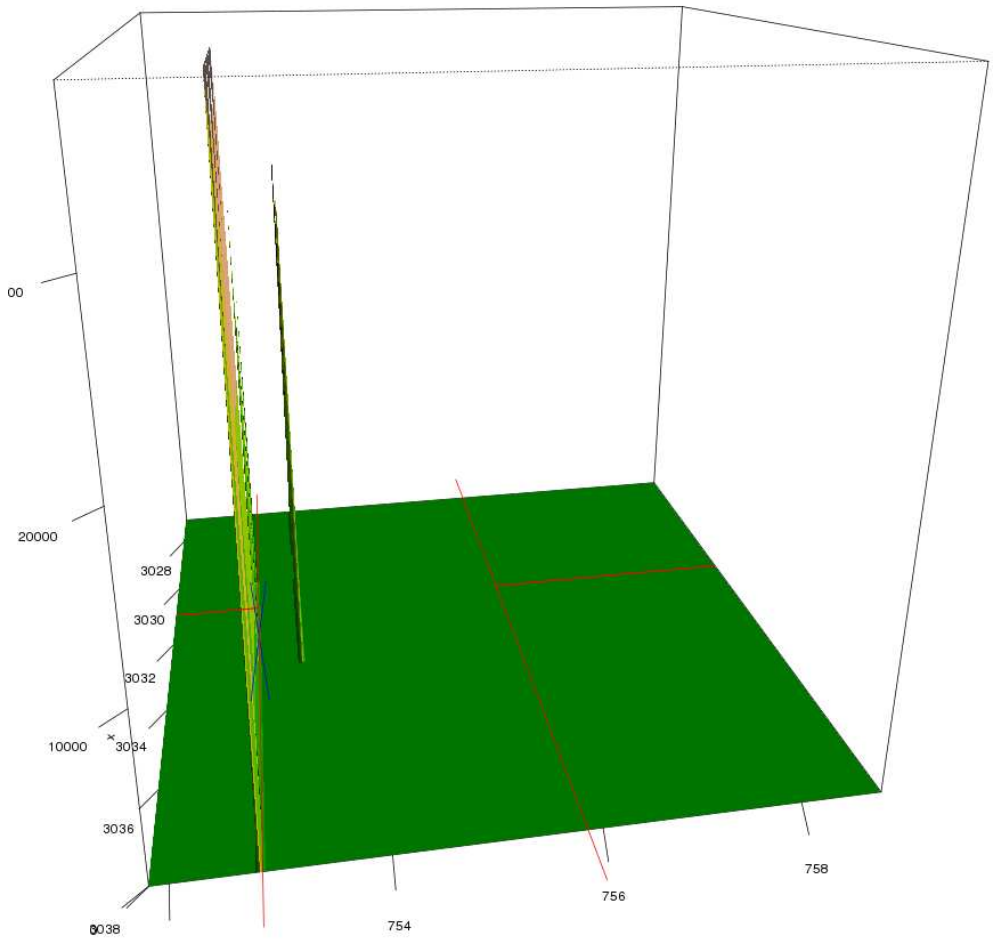
1. Questionable Isotopic Distribution

In this example, the intensity-sum chart shows two attributes that make this quantitative event questionable. First, the isotopic distribution of the light peaks is very different from the theoretical distribution (Mass is 2344.9, so second peak should be highest). Second, the second and third peaks aren't seen at all in the heavy isotope, which is particularly worrying since the second peak should be most abundant.



2. Only Light Ion Identified

In this example, there are two abundant peaks for the light ion, but none for the heavy ion. In the context of this 1:1 experiment this probably indicates a bad identification: the peptide is most likely not actually a Cysteine-containing peptide. In a real experiment this might indicate a bad identification, or it might indicate presence of the peptide in one sample and not the other.

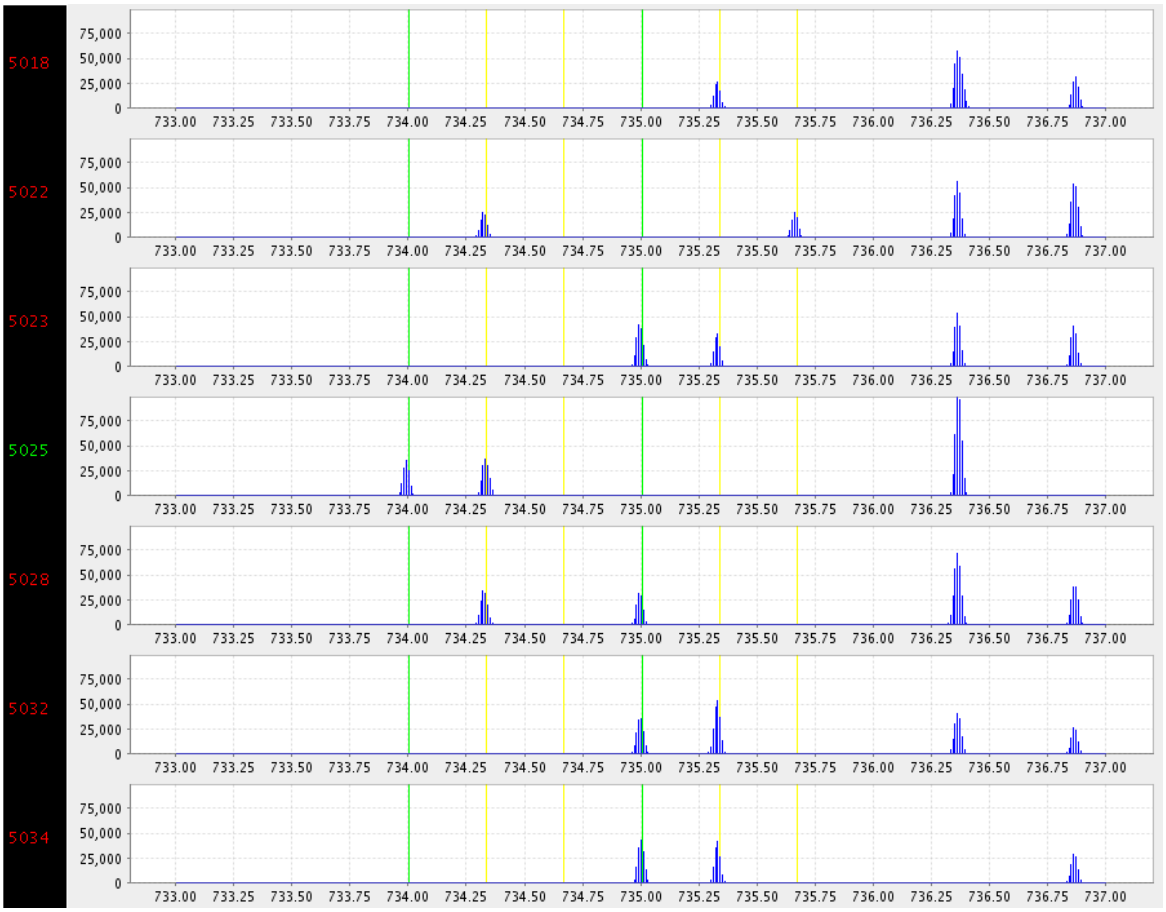


3. Identified C13 Peak

In this example, the observed peptide monoisotope is actually at the m/z location of the theoretical C13 peak of the identified peptide. This is strong, but not conclusive, evidence for a bad identification. Regardless of the correctness of identification, however, the quantitation value is not correct for the identified peptide.

4. Long-eluting peptide quantitated based on too few scans

This peptide is clearly visible in both heavy and light forms in multiple scans. However, the quantitation algorithm used only scan 5025 (scan number in green) for quantitation. In doing so, it missed the heavy peaks entirely.



5. Coeluting peptides affect quantitation

The light peaks of this peptide appear to be enhanced by the peaks of a coeluting peptide three Daltons lighter. The amount of contribution by this fourth peak of the lighter peptide is difficult to determine, but it is likely significant, since the lighter peptide is much more abundant than the peptide being quantitated.

6. Too low intensity relative to noise

In this case, the peptide being quantitated is extremely low-intensity, with peaks having a similar intensity to nearby peaks that are likely noise. In this case only one peak from the light version is quantitated, and no peaks from the heavy, so this event is questionable for multiple reasons.