Virscidian

3 Tech Note

Optimizing Peak Area Thresholds in AS-MS Background Filtering

The percentage difference in the peak area between the original hit and a background peak is another key parameter in cross-hit analysis. It defines the acceptable variation in peak areas for identifying background hits. When set improperly, this threshold can allow false positives, skewing your results.

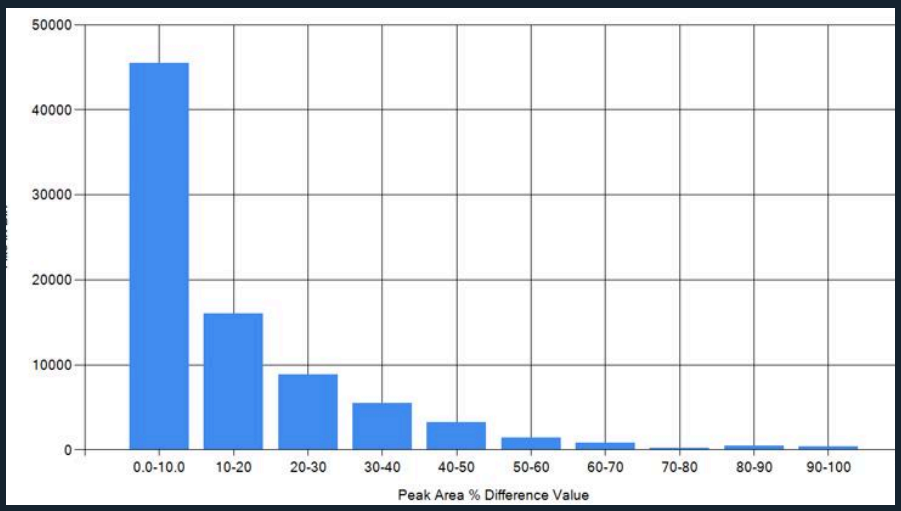
How much difference should there be in the peak area between the original hit and the potential cross-hit? It turns out that this is a key parameter and, if it's set improperly, you can see a significant increase in your false positives.

Experimental

Using a 250,000 compound AS-MS library spread across 96 wells, Virscidian scientists worked to determine what defined "similar" with respect to peak areas when searching for possible cross-hits.

Key Finding

After analysis of the 82,314 background ions, scientists discovered that a threshold of ±55% difference in peak areas between background ions and the potential hits captured approximately 97% of all the potential cross-hits.



Recommended Practice

Using Virscidian's automated cross-hit filter with an area difference threshold of around 55% maximizes background cross-hit filtering while preserving true hits. Tighter thresholds increase false positives; looser ones offer diminishing returns.