

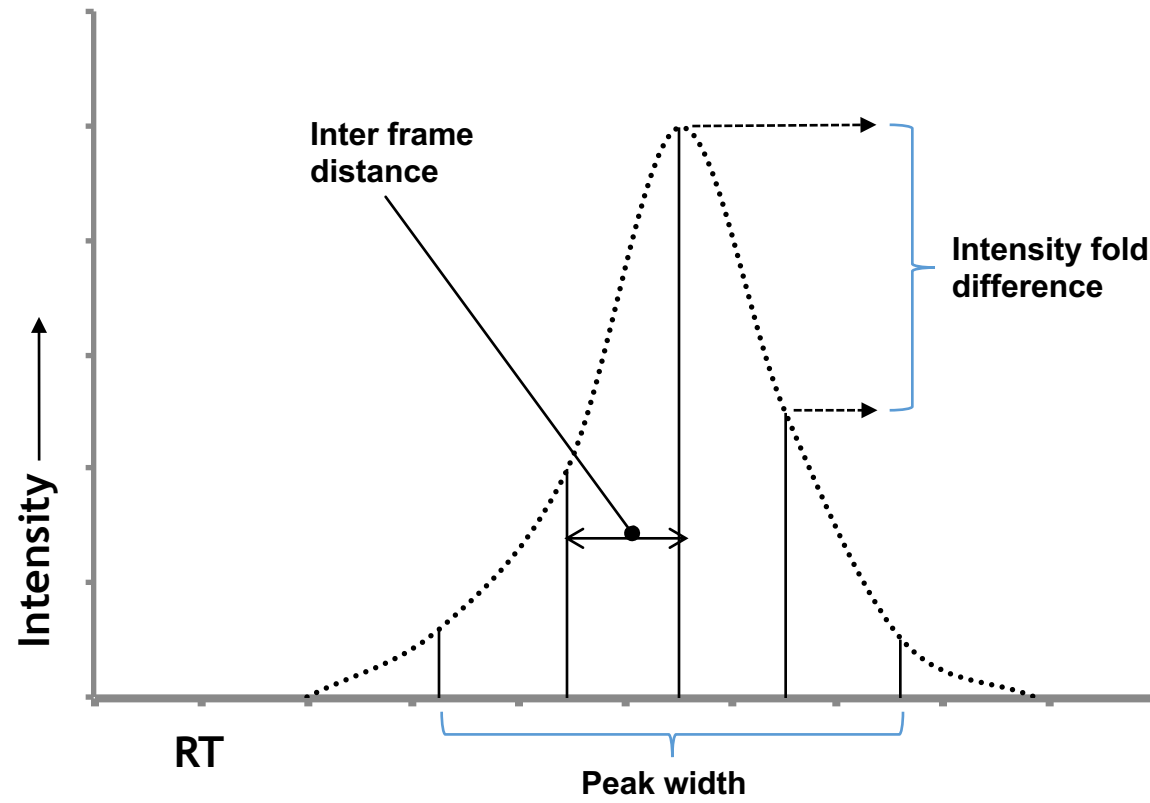
## Supplementary Figure Legends

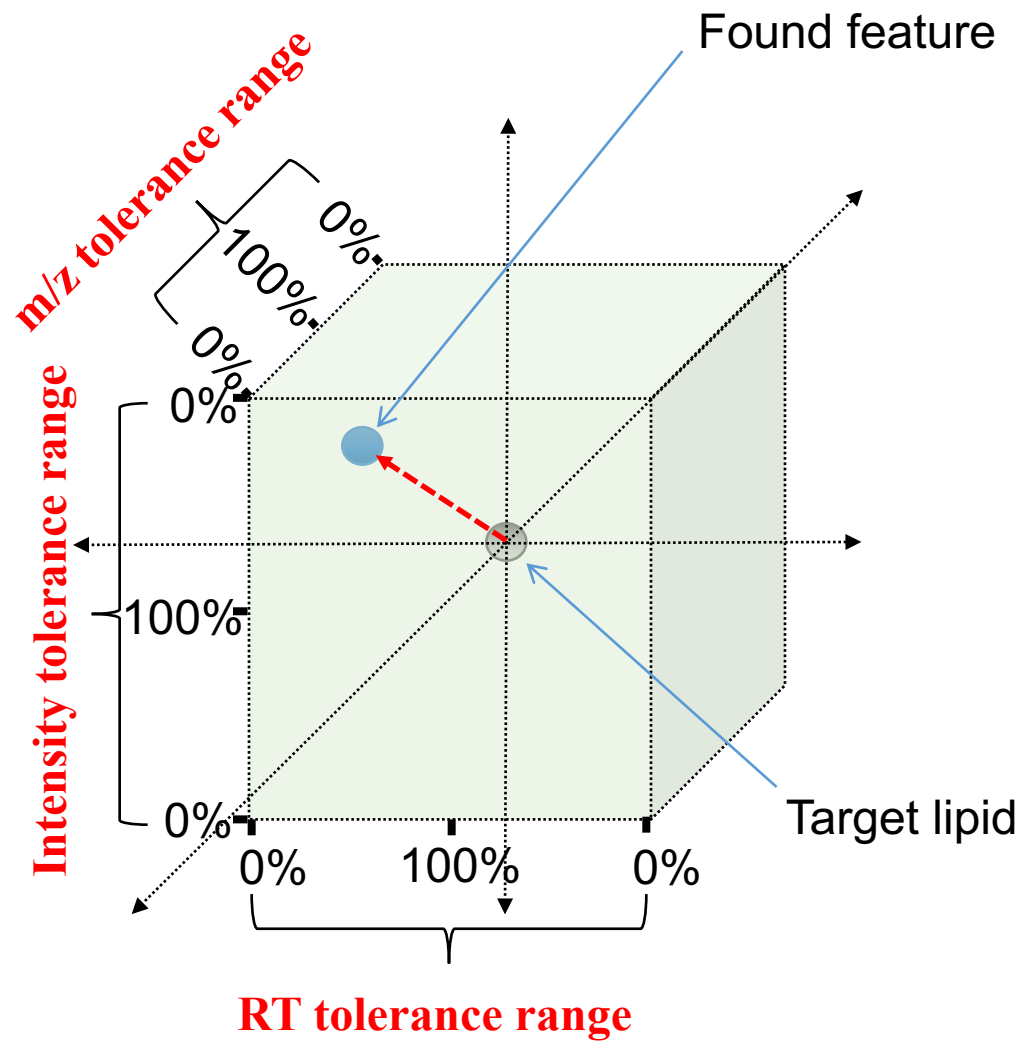
**Supplementary Figure 1. Building a peak in PeakFilter.** A representation of a single peak made up of 5 frames. The 3 key features that govern how a feature is categorized are (1) The inter frame distance, known as 'peakAdjacentFrameMaxRT' in LipidFinder governs how close the next frame can be in order to be considered part of the same peak; (2) the intensity fold difference, known as 'peakMinFoldCutOff' in LipidFinder governs how sharp the peak can be to be considered a lipid-like peak; (3) the maximum peak width, known as 'peakMaxRTWidth' in LipidFinder governs how wide a peak can get before it tails into contaminant.

**Supplementary Figure 2. The scoring mechanism in the PeakFilter optimization process.** The curated peak (CP) is the center point of a 3d cuboid search space, any features found within this search space will be a hit and will be scored on it's vector proximity to the CP.

**Supplementary Figure 3. Algorithmic representation of the 1opt Hill climbing algorithm used in the PeakFilter optimisation process.**

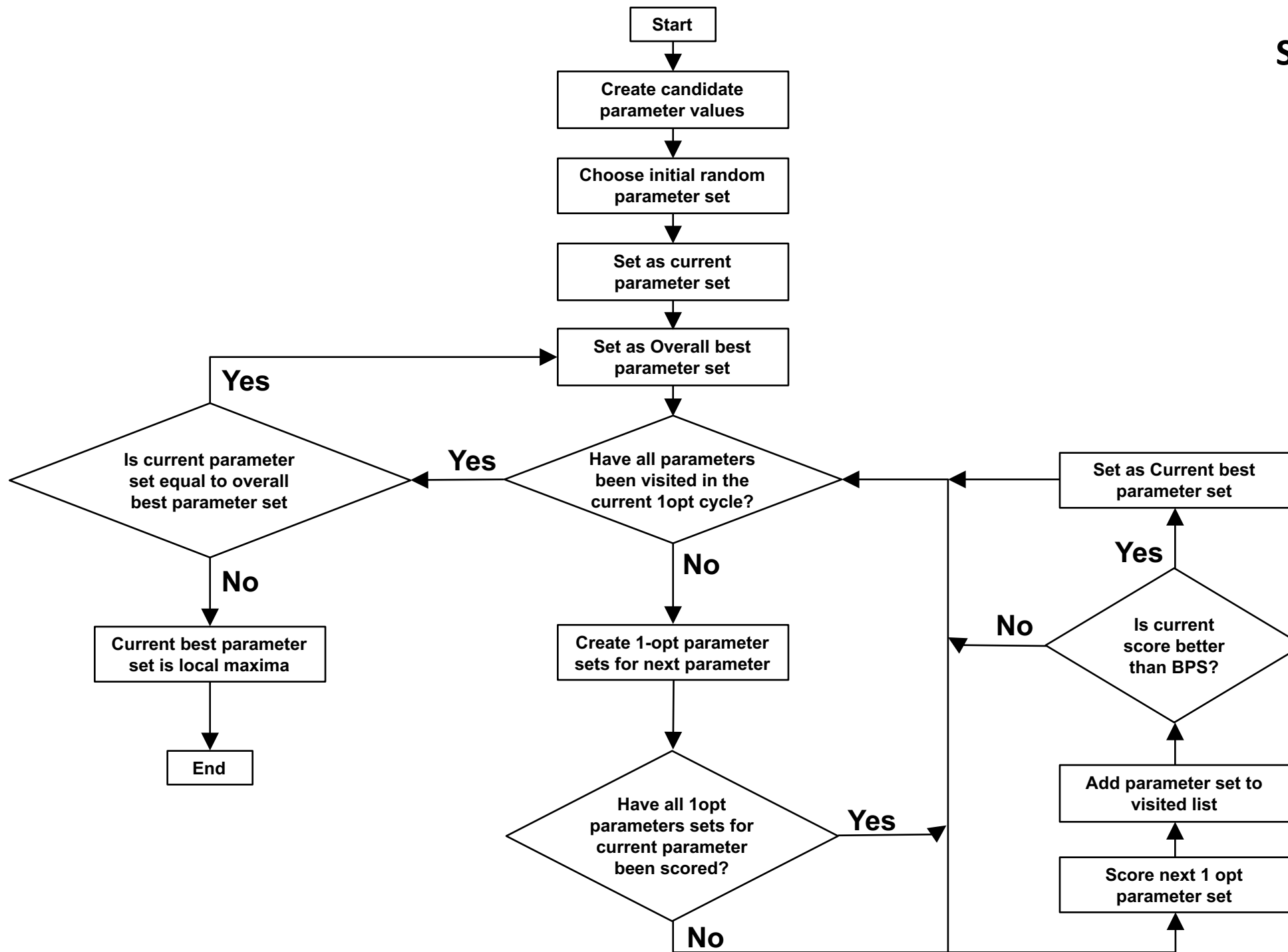
**Supplementary Figure 4. Peak filter data clean up.** *Panel A Broad retention time contaminant removal* The similar intensity contaminants (left plot) are removed leaving the higher intensity outlier lipid-like peaks (right plot). *Panel B. Retention time correction.* The table is a portion of a dataset and illustrates the correction of retention time for 'Rep\_4'. *Panel C Outlier correction* The table is a portion of a dataset and illustrates outlier correction, 'Rep\_4' is an outlier and is removed from the dataset. *Panel D The diagram illustrates the relationship between a mass cluster and its feature clusters.*

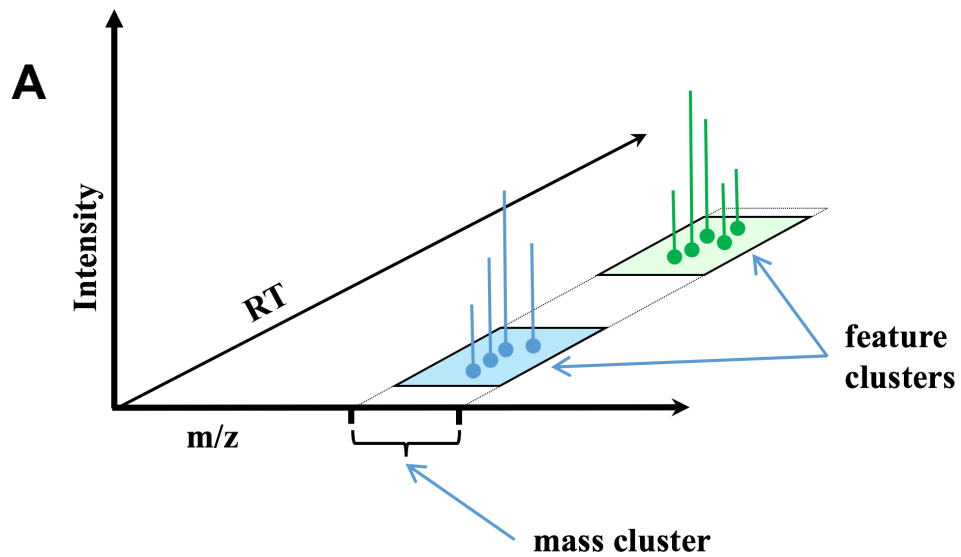




$$\text{Score} = \sqrt{3 - \sqrt{(\% \text{ proximity RT})^2 + (\% \text{ proximity m/z})^2 + (\% \text{ proximity intensity})^2}}$$

$$\frac{\sum_{i=1}^N \text{Score}_i}{N}$$





**B**

MZ	Time	Rep_1	Rep_2	Rep_3	Rep_4
157.1236	13.95	580.6	678.6	666.6	0
157.1236	14.19	0	0	0	529.6

MZ	Time	Rep_1	Rep_2	Rep_3	Rep_4
157.1236	13.95	580.6	678.6	666.6	529.6
157.1236	14.19	0	0	0	0

**C**

MZ	Time	Rep_1	Rep_2	Rep_3	Rep_4
157.1235	19.25	491	465	402	171.6

MZ	Time	Rep_1	Rep_2	Rep_3	Rep_4
157.1235	19.25	491	465	402	0

**D**

