ISOTOPE
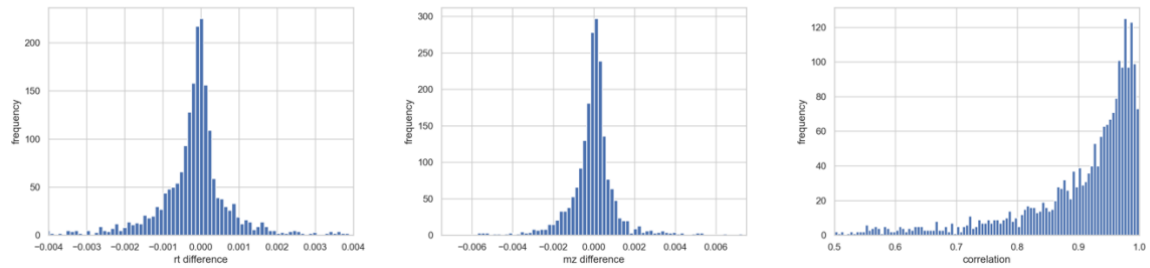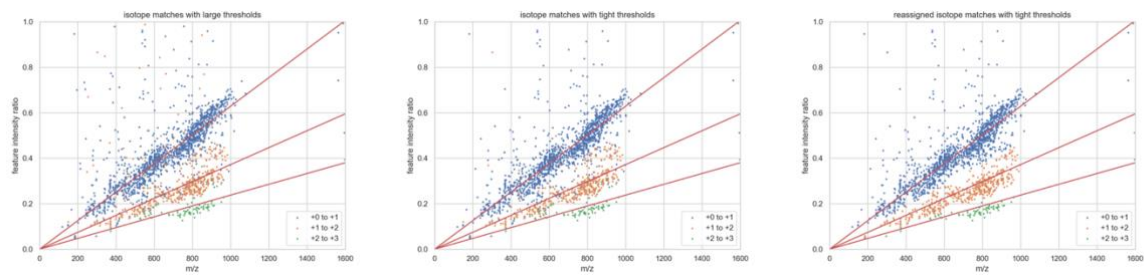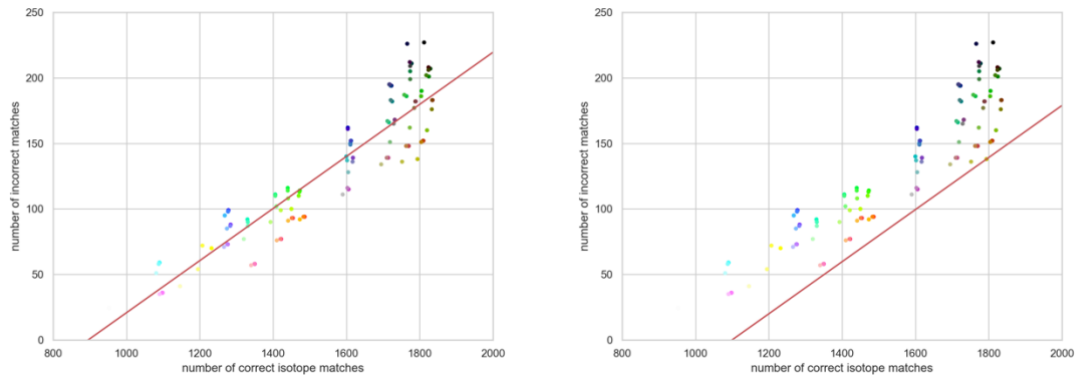

Intra-dataset distribution of rt difference, standardised mz difference and correlation for matched isotopes

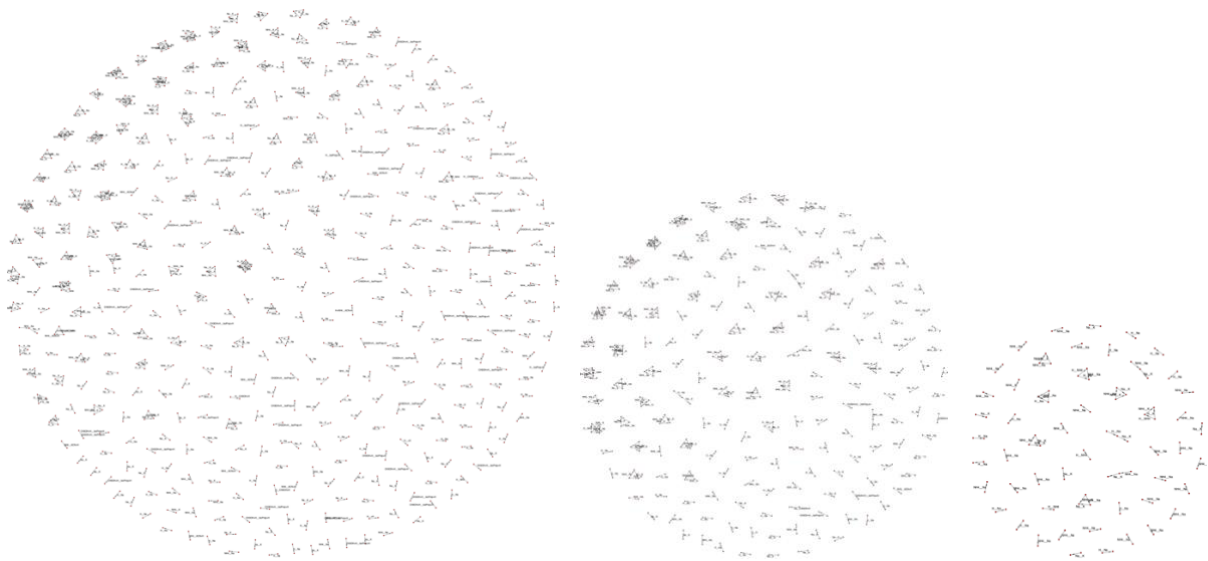Type of isotope matches with large rt, mz and correlation thresholds
Type of isotope matches with tight rt, mz and correlation thresholds
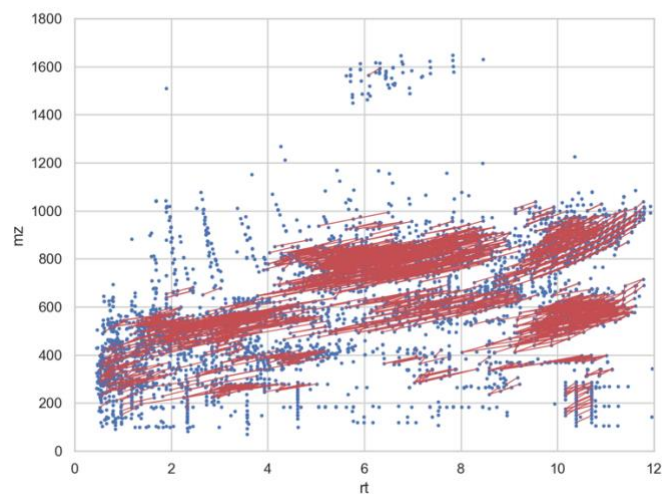Reassigned type of isotope matches with tight rt, mz and correlation thresholds

Linear regression to find the best set of thresholds. The colour of each point is RGB encoded thresholds.
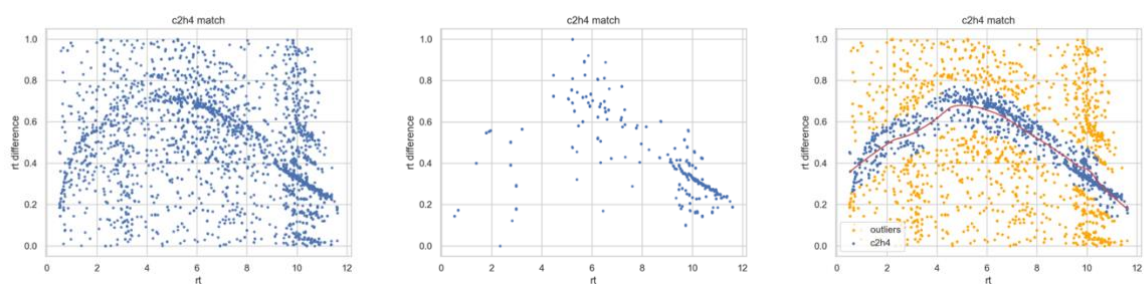
ADDUCT

Intra-dataset adduct matches in isotope layer +0, +1, +2 respectively.

Intra-dataset C2H4 match with large thresholds of mz and rt difference.

C2H4

C2H4 match with same or unknown adduct type (left)
C2H4 match with same adduct type (right)
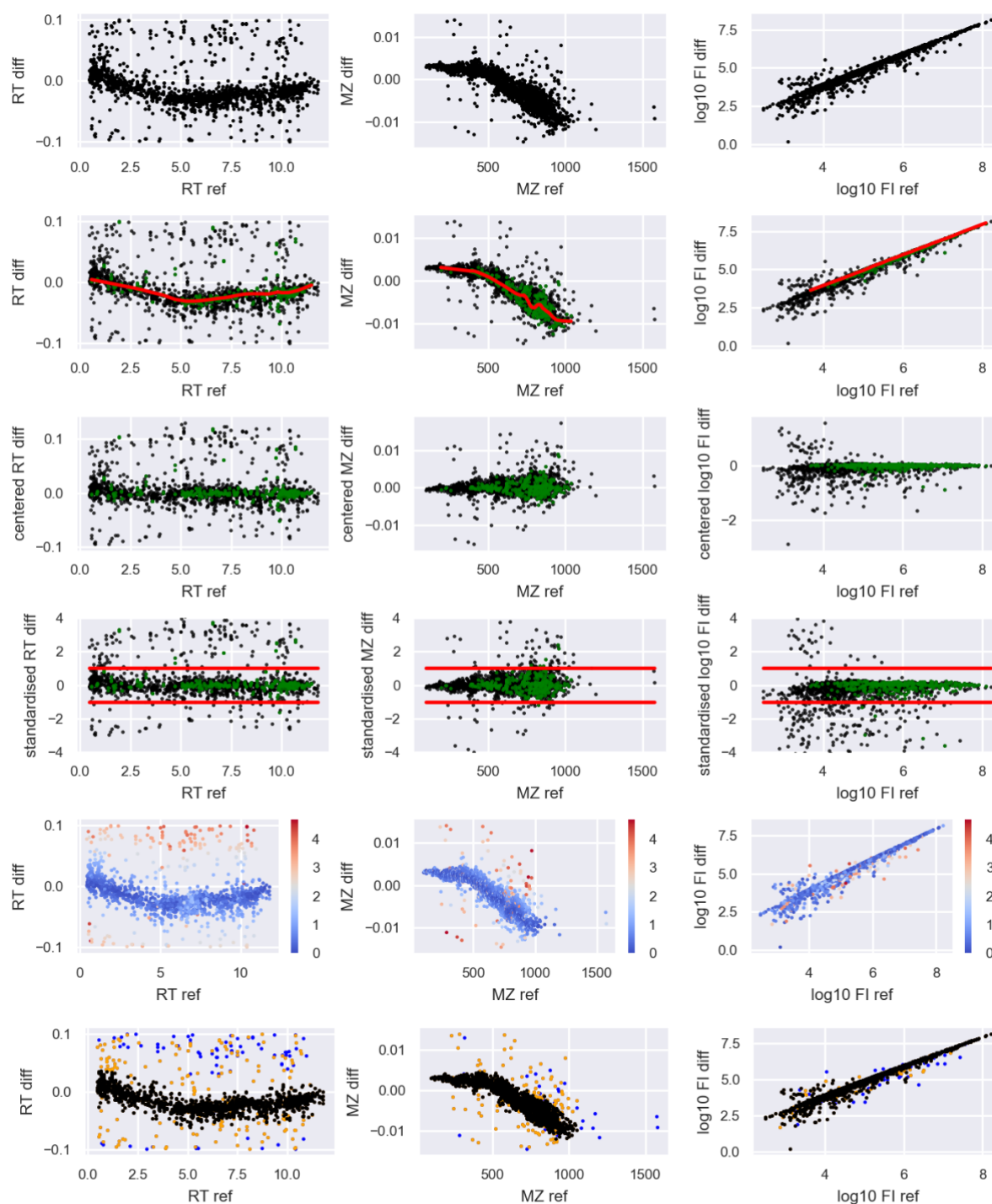LOWESS regression to select high probability C2H4 matches

WORKFLOW

Figure 1: 1st row: all possible matches, inter-dataset difference vs reference value in RT, MZ and log10FI domains. 2nd row: high probability matches in green and other matches in black, red line is LOWESS regression using only green dots. 3rd row: centred difference. 4th row: standardised difference by dividing 5MAD. 5th row: penalisation score for each match calculated by weighted sum of squared standardised difference of RT, MZ and log10FI. 6th row: multiple match in blue, poor match in orange and good match in black.