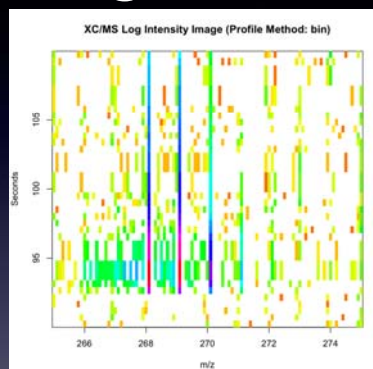
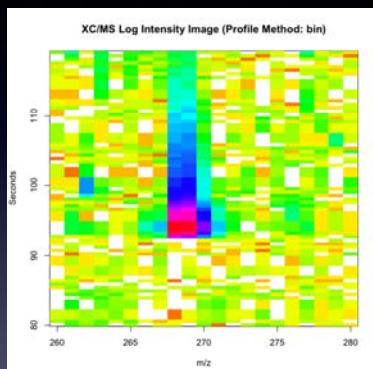


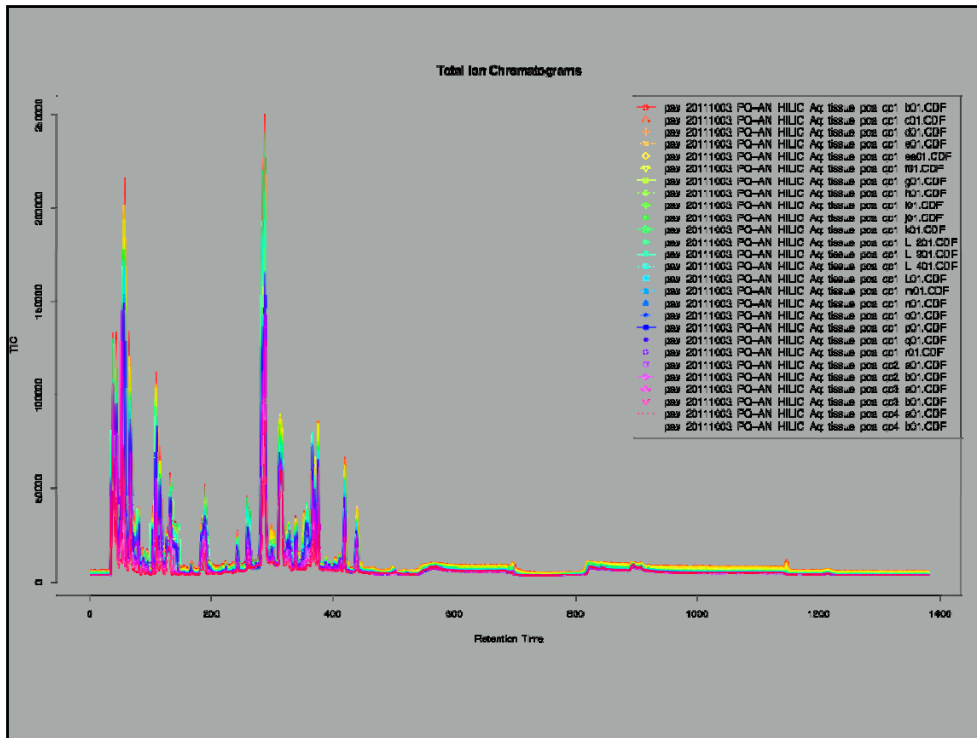
# XCMS Parameters in 20 mins

H. Paul Benton

## Peak Picking

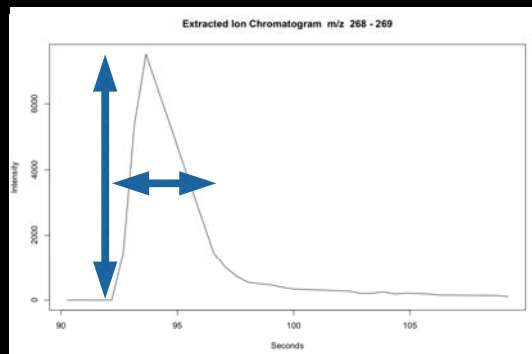


- Look at your data!



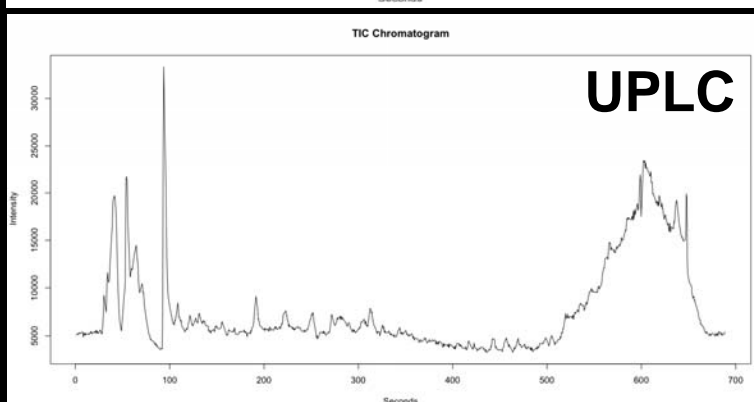
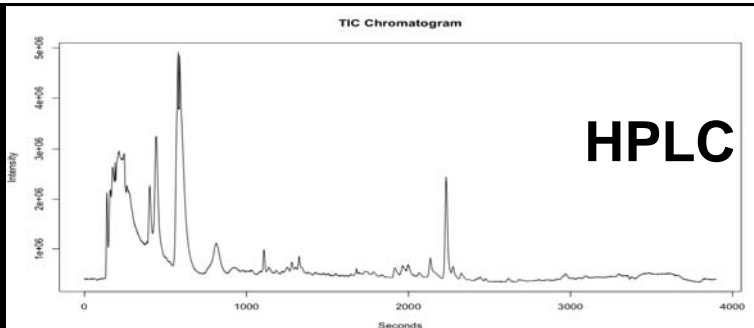
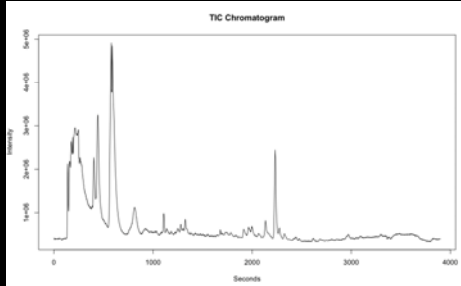
# Matched Filter

- Profile Data - profMethod
  - binlinBase - profile data
  - bin - centroid data
- profStep - Bin Size
- Peak Width - FWHM

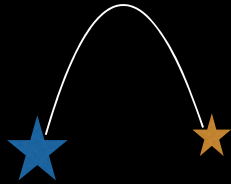


# CentWave

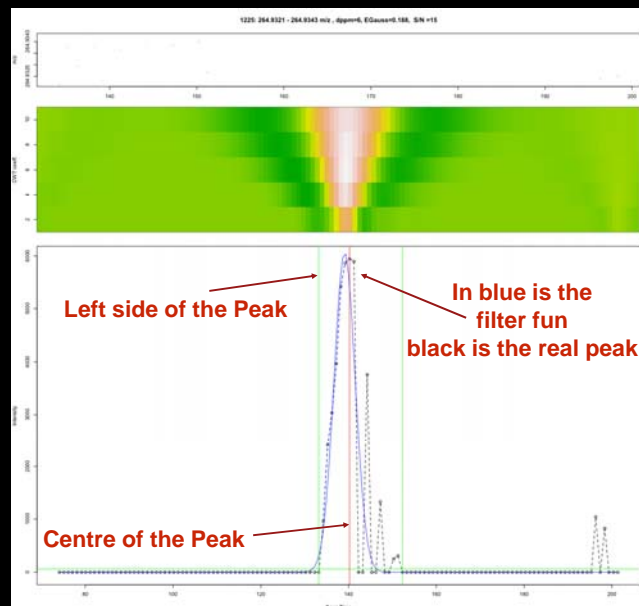
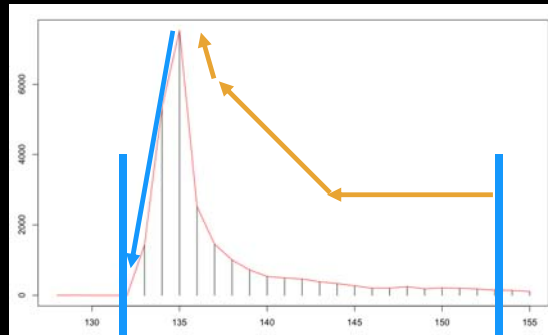
- Peak Width
- HPLC
- UPLC
- CentWave still finds bins its just dynamically finding bins (ROI)
- Tracking missiles - ppm



Tracking Missiles is like tracking LC-MS traces

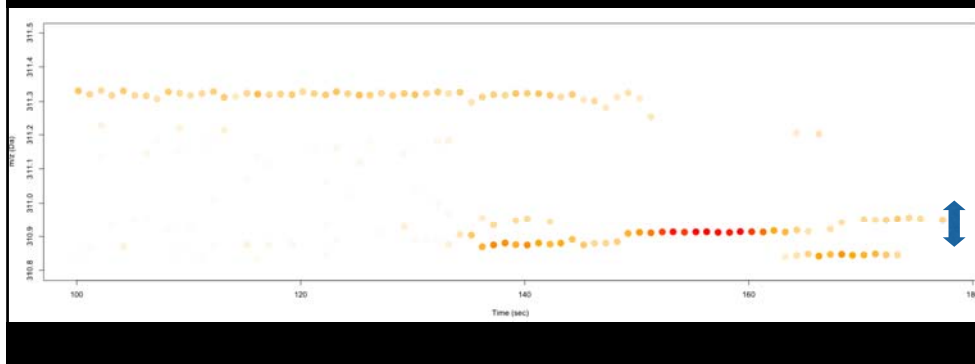


Trace backward along the trace  
This will define the area of the 'bin'



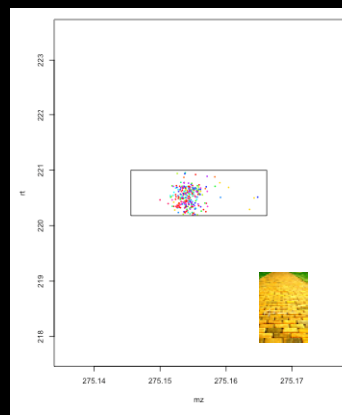
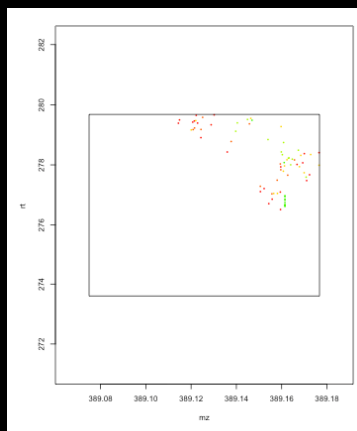
# CentWave - ppm

Determines how much  $m/z$  variation from the start of the ROI/peak there can be in ppm

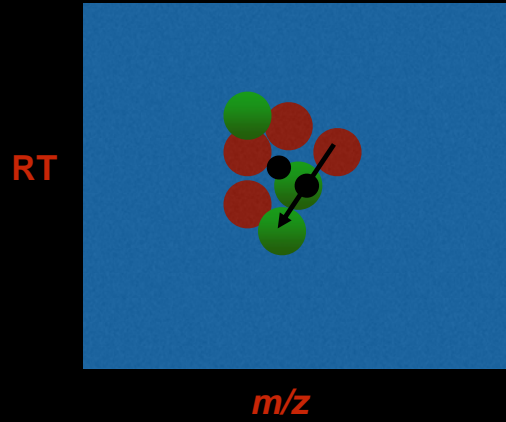


# Grouping

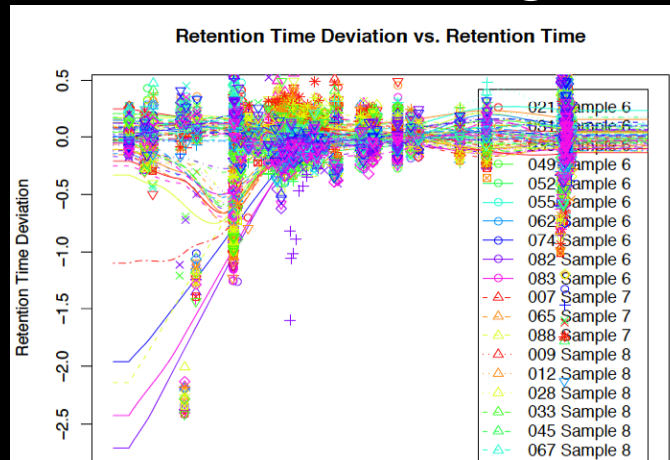
- Grouping -
  - Kernel Density
    - $bw = 30$
    - $mzwid = 0.25$
  - Nearest Neighbor



# Group.nearest



# Retention Time alignment

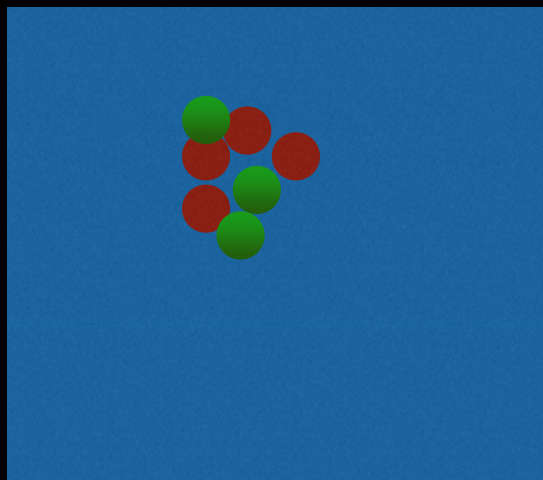


Good Spread of 'well behaved features'

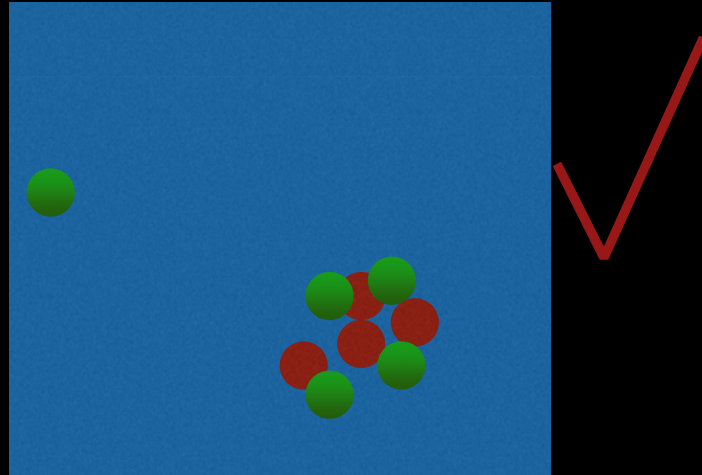
# Retcor.loess

- Original algorithm
- missing & extra
- span - Smoothing : relaxes the amount of weigh a each 'well behaved peak' group

Missing =1



# Extra = 1



## Question?

- Lunch Time !
- Some documentation on parameters -
  - <https://xcmsonline.scripps.edu/docs/usermanual.pdf> - last page
  - <http://www.bioconductor.org/packages/release/bioc/manuals/xcms/man/xcms.pdf>