chem-bla-ics

Recovering full mass spectra from GC-MS data #2

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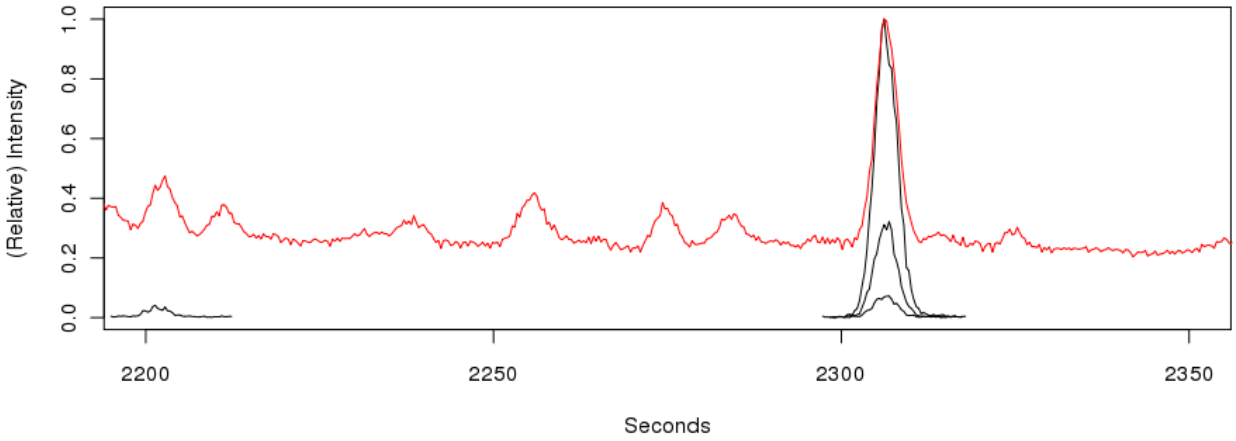
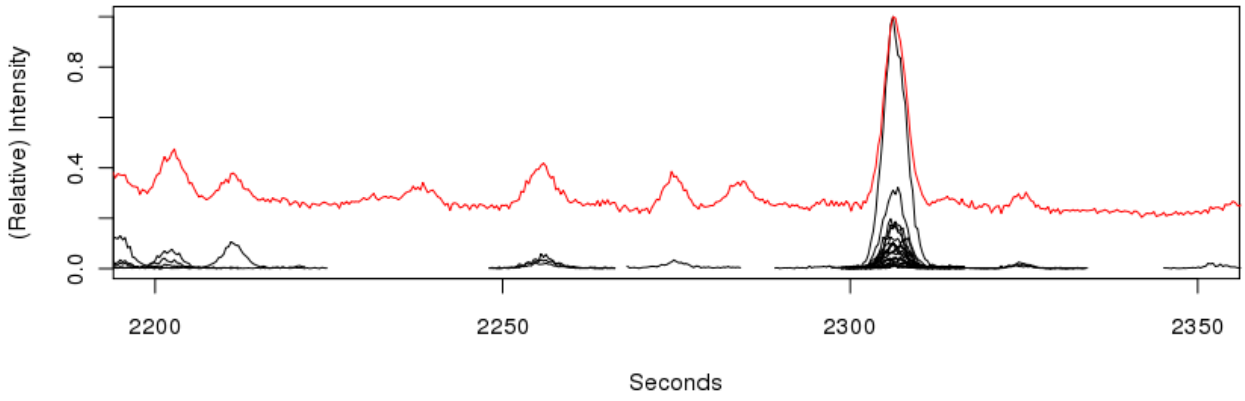
Steffen reminded me over email that the particular machine only has a 1 dalton accuracy, and that the 150ppm parameter setting is somewhat inappropriate. As seen yesterday , it works fine for larger peaks, but fails for low intensity peaks. So, I reran the `centWave` peak detection with 750, 1000 and 1250 ppm, and that indeed make XCMS recover many more metabolites, and, also important, with more extracted ion chromatograms per metabolite, yielding a more accurate mass spectrum. At the same time, I notice that profiles are not as clean as before, but that's where the peak fitting with (Modified) Gaussians come into play.

The original 150ppm results:



The 750ppm results:



And for 1000ppm (1250ppm did not further improve):

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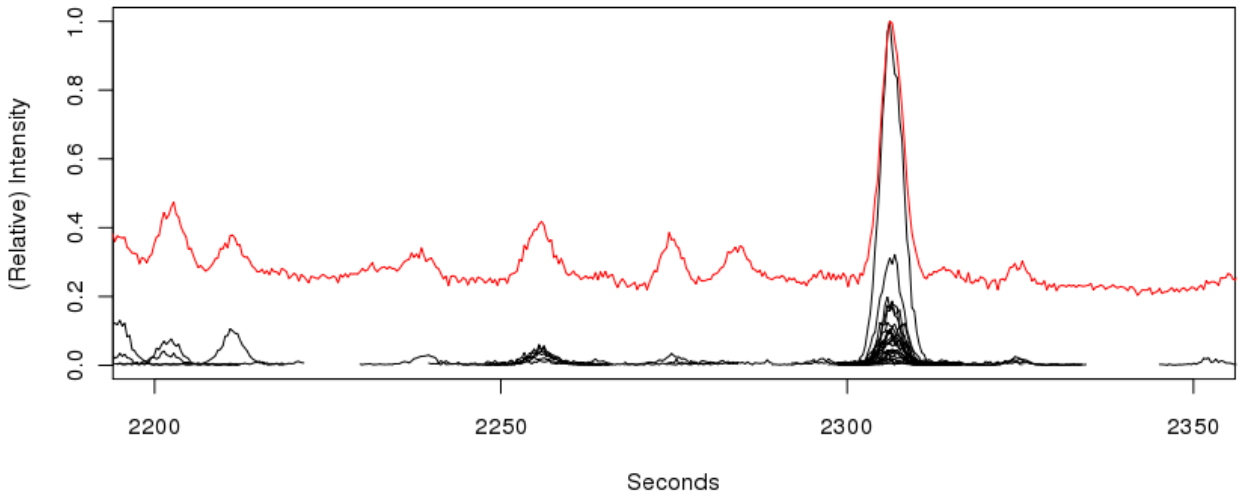
(Relative) Intensity
0.0
0.2
0.4
0.6
0.8
1.0
2200
2250
2300
2350
Seconds