

Recovering full mass spectra from GC-MS data #2

Egon Willighagen 

Published June 5, 2008

Citation

Willighagen, E. (2008). Recovering full mass spectra from GC-MS data #2. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/j9rb9-ns27>

Keywords

Metabolomics, Rstats

Abstract

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.

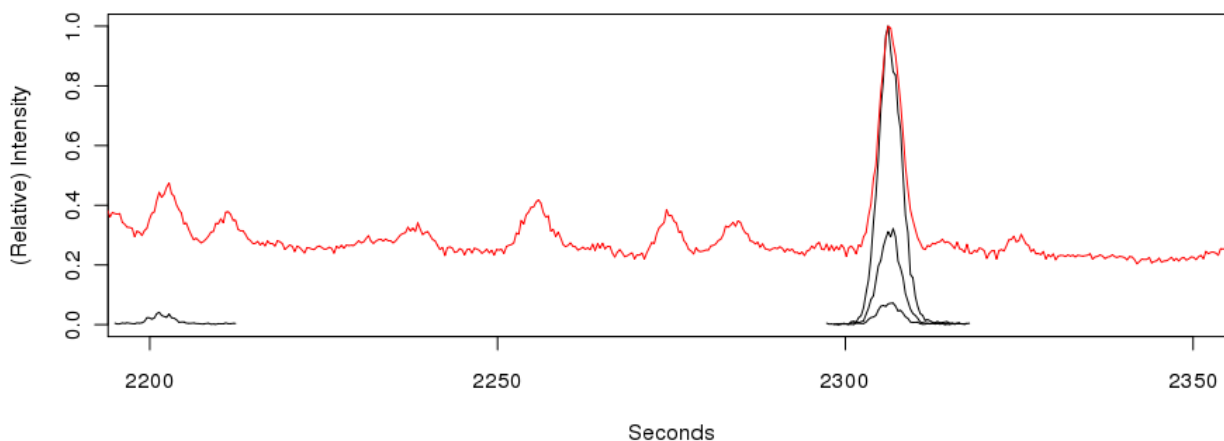
Copyright

Copyright © Egon Willighagen 2008. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

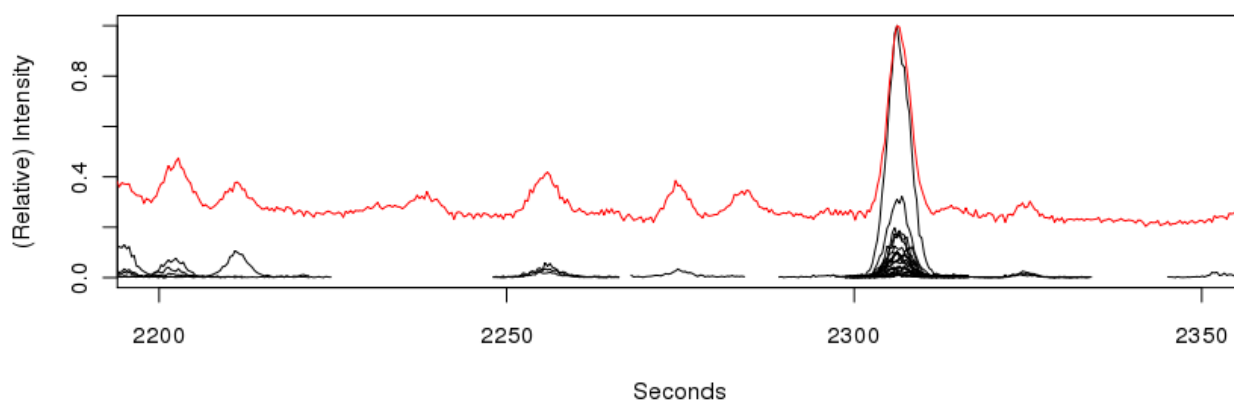
chem-bla-ics

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):

chem-bla-ics

