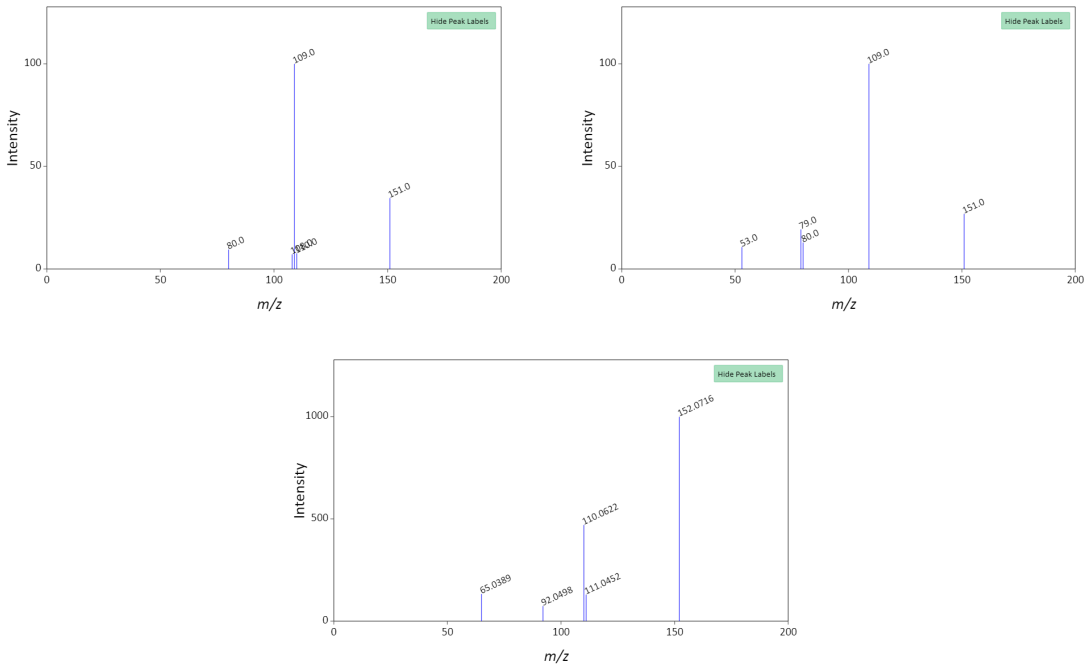
PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

Developing an R cheminformatics toolkit: functions and recipes to manage MS spectra

There are many types of chemical information of which digital processing is not currently standardized. An example of this is the case of MS spectra: many hardware manufacturers use proprietary formats which are hardly interoperable, while some text-based open formats are available but not commonly used. At the same time, it is unlikely that a spectra contains a single species, but databases only cover pure substances. Last, measurement error and instrumental differences don't make it easy to compute whether two spectra belong to the same analyte or not.
This proposal consists in identifying, systematizing and completing existing functions in R packages to contribute, with improved functions and example recipes for MS processing, to an R toolkit for cheminformatics.

Three different MS Spectra of acetaminophen from many collected at https://pubchem.ncbi.nlm.nih.gov/compound/1983



OFFERED POSITION: 1 Master research project (6-9 months)

For more information, contact Dr. Jordi Cuadros, jordi.cuadros@iqs.url.edu, or Dr. Roger Estrada, roger.estrada@iqs.url.edu.