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MS2Snoop: a R package for automatic extraction and curation of MS/MS spectra in metabolomics

Kévin Wagner^{1,2}, Lain Pavot³, Franck Giacomoni³, Guillaume Marti^{2,4}, Yann Guitton⁵, Laurent Debrauwer^{1,2}, Emilien Jamin^{1,2}, Jean-François Martin^{1,2}

¹ Toxalim (Research Center in Food Toxicology), Toulouse University, INRAE, ENVT, INP-Purpan, Toulouse, France

² MetaboHUB-MetaToul, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France

³ Université Clermont Auvergne, INRAE, UNH, Plateforme d'Exploration du Métabolisme, MetaboHUB Clermont, Clermont-Ferrand, France

⁴ Metatoul-AgromiX Platform, LRSV, Université de Toulouse, CNRS, UT3, INP, Toulouse, France

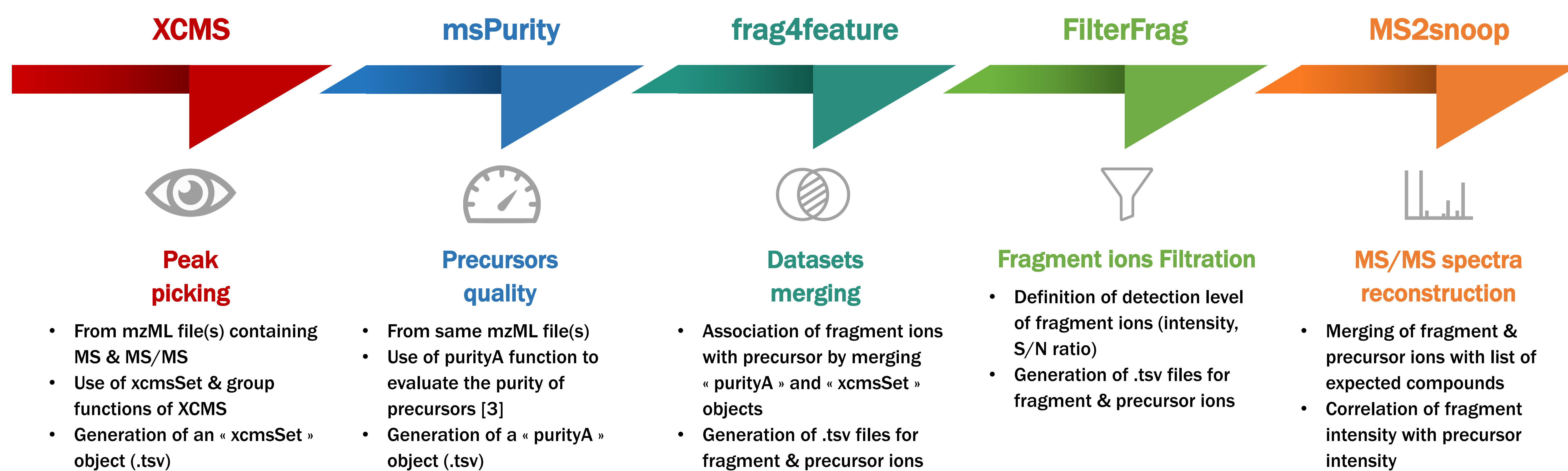
⁵ Oniris, INRAE, LABERCA, Nantes, France

Introduction

Omics approaches including metabolomics generate huge datasets requiring powerful processing tools. In the field of non-targeted mass spectrometry metabolomics, HRMS data mining has been the subject of much work, with the development of powerful interactive tools, including Workflow4Metabolomics (W4M) [1-2]. One of the main bottlenecks of current workflows lies in the complexity of the interpretation of results, in particular a lack of reliable MS/MS spectral reference databases (DBs) to be used for confident identification (level 1 and 2 according to the metabolomics standard initiative). Creating reliable and well curated spectral DBs remains a laborious and challenging task, but necessary to ensure the quality of the reference spectra. In this work, we present a tool inspired by expert manual curation allowing the export of MS/MS data from both targeted and data dependent (DDA) fragmentation methods to laboratory spectral DBs, named "MS2Snoop".

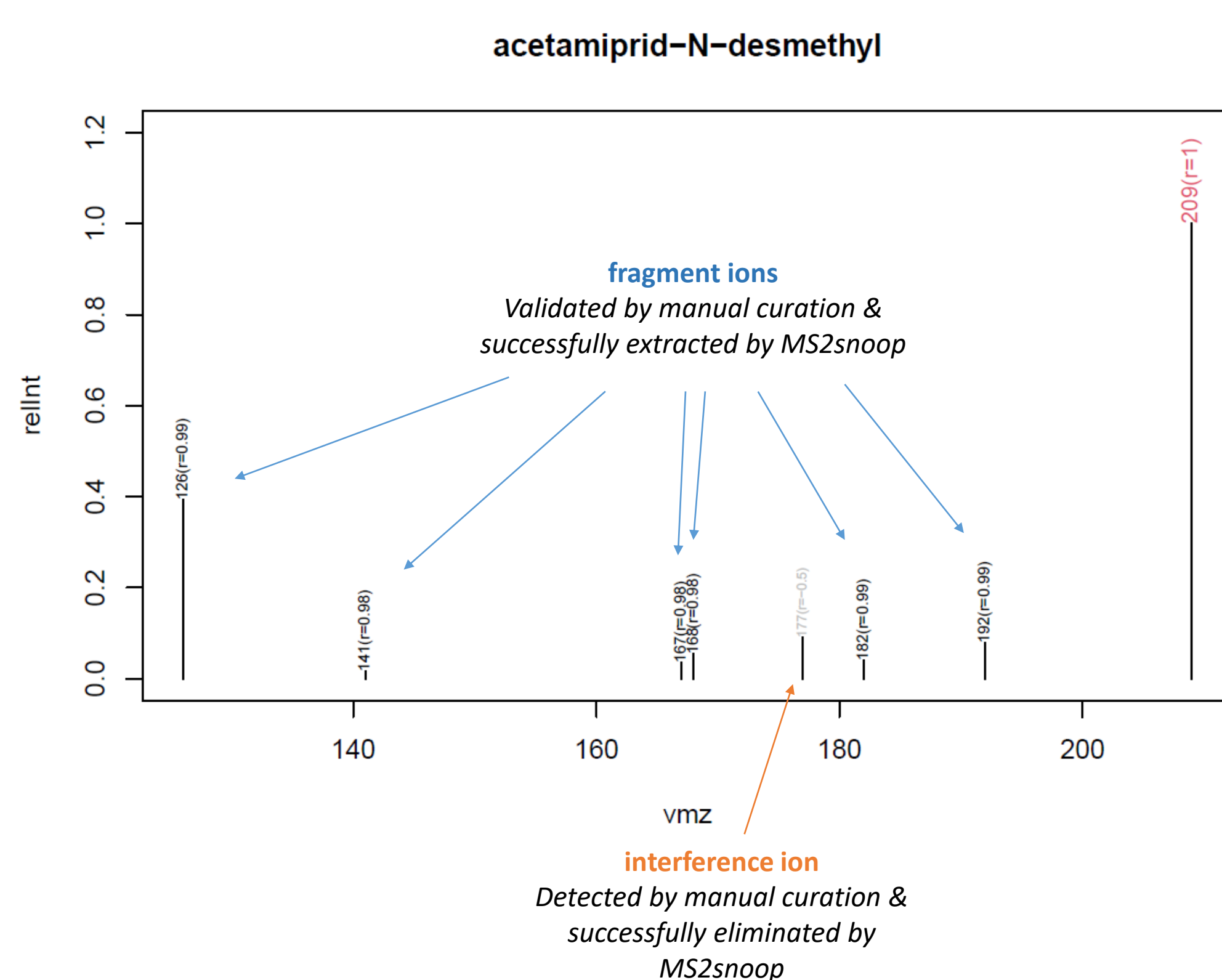
MS2snoop

Workflow (R):

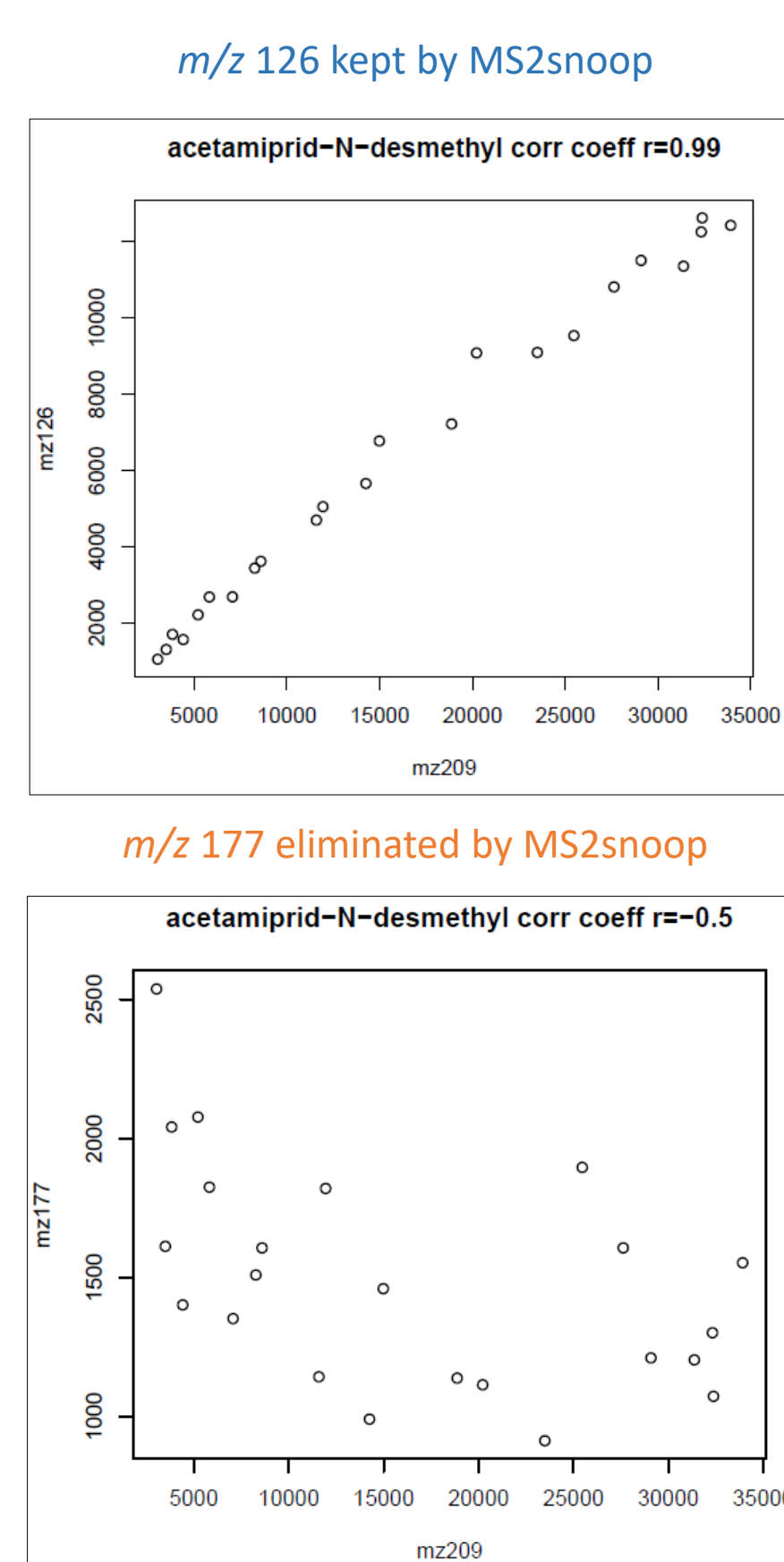


Examples of applications

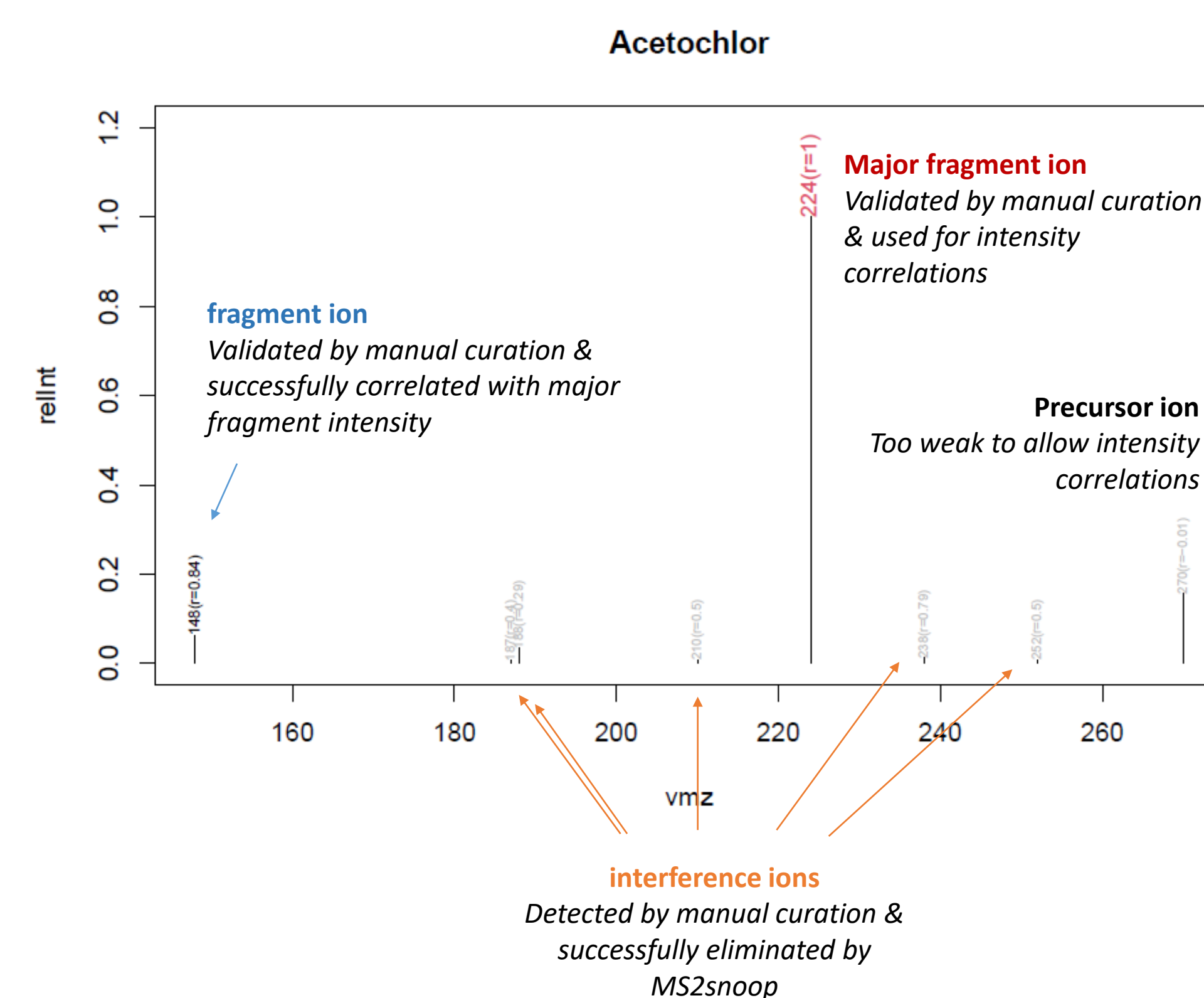
Targeted MS/MS by resonant CID achieved on a LTQ-Orbitrap XL using ESI in the positive mode



Curation by correlation between precursor ion intensity & fragment ion intensities



Successful application to the particular case of acetochlor with a very weak precursor ion intensity



Conclusions

MS2Snoop already allows extracting and cleaning MS/MS datasets using commonly used metabolomics data processing steps as a starting point, then combined with inputs of a list of expected compounds and MS/MS raw data deconvoluted by MSPurity. Firstly developed and validated with targeted MS/MS spectra from about 30 compounds, MS2Snoop is compatible with DDA spectra, although limited by the number of MS/MS scans acquired. This package will allow high throughput extraction of MS/MS spectra in order to feed the PeakForest project [4]. Preliminary results obtained with MS2Snoop allowed considering it as a valuable tool for confident annotation of metabolites on chromatographic methods coupled to non-targeted mass spectrometry.

A beta version of this original package is already publicly available on W4M (<https://workflow4metabolomics.org/>) and recent update allows fragments ions formula annotation with Sirius.

References

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