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ChromAnnot a webserver for deep LC-HRMS/MS chromatogram annotation

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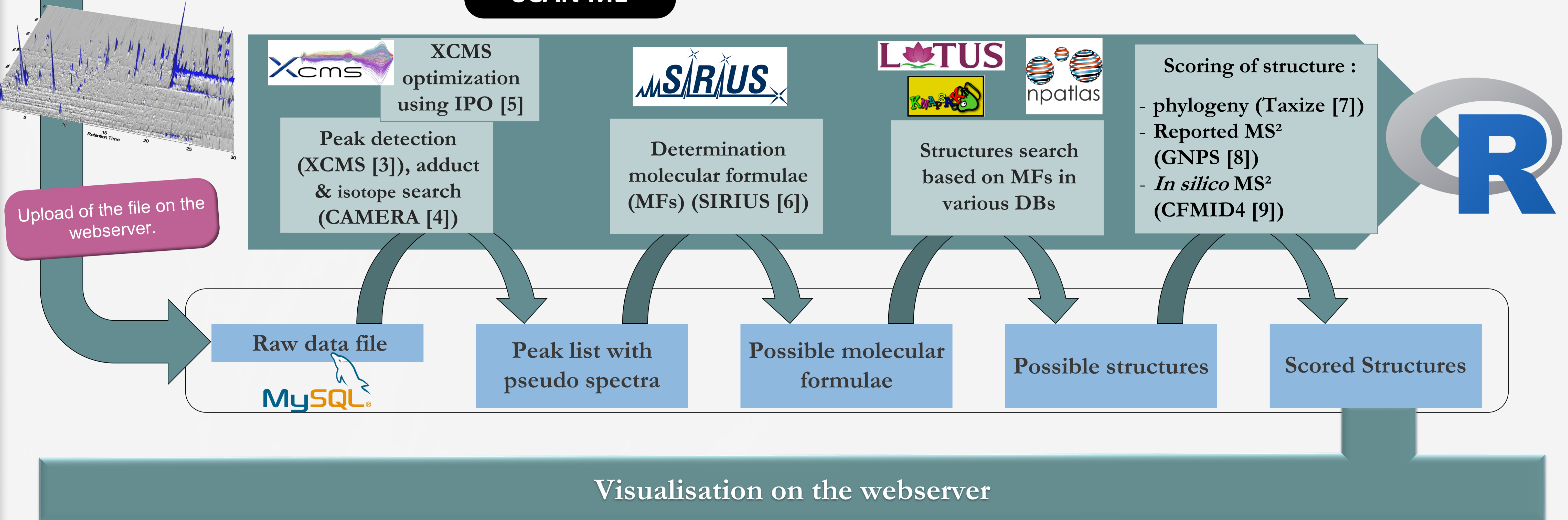
Background

In metabolomic strategy, LC-HRMS/MS feature annotation is usually performed on those highlighted by the statistical analysis. This step is particularly challenging due to the lack of knowledge about all compounds presented in chemical profiles [1]. In addition, such an annotation step based on spectral data is very time consuming.

Therefore, the annotation is many times unsuccessful. However, full LC-HRMS/MS chromatogram could be a very valuable step for data interpretation, not only focusing on altered features observed in metabolomic studies but also on unaltered ones. To achieve such an annotation on an entire LC-HRMS/MS profile, the only reasonable solution remains the automation of the full process.



At the ISOMer laboratory, we developed an entirely automated annotation strategy going from raw LC-HRMS/MS data (in open format) to full peak annotation [2]. In addition, the workflow was integrated into a web-based interface to ease exploring the annotation results. The ChromAnnot webserver is accessible at <https://chromannot.univ-nantes.fr/>.



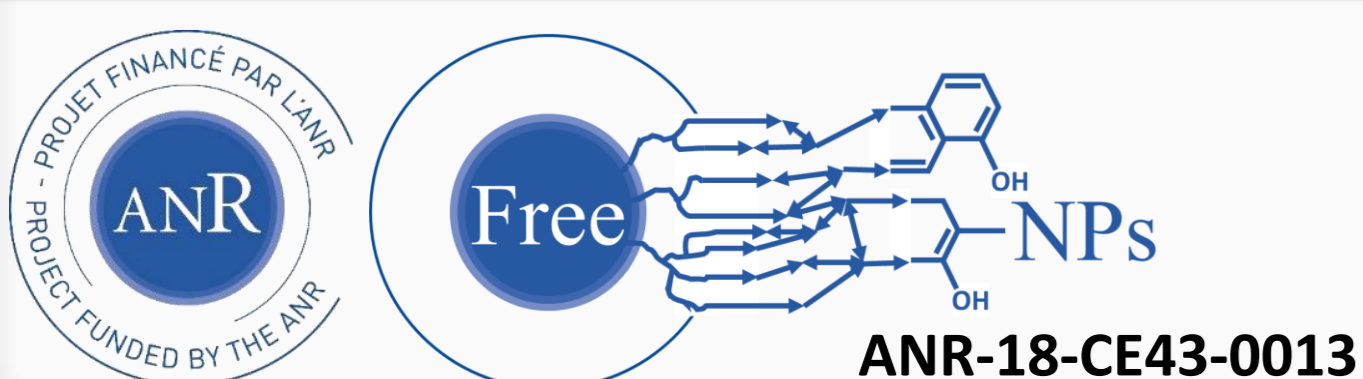
Visualisation on the webserver

Conclusion

Once the complete workflow is achieved on a file, it provides for all peaks (if spectral quality are sufficient), spectral interpretation, molecular formulae, annotations for most peaks. The only limitation is the availability of chemical structures within the data bases. The full processes can take hours to days depending on the depth of signal annotation (intensity limit) and chromatogram complexity.

As expected, even in model organisms like *Penicillium chrysogenum* (strain Winsconsin 54-1255) annotation is rather limited. This highlights the fact that there is still many compounds to be discovered.

Funding



References

[1] Analytical Chemistry 2019, 91 (1), 704. 10.1021/acs.analchem.8b05112; [2] Phytochemistry Letters 2017, 21, 297. 10.1016/j.phytol.2016.12.025; [3] BMC Bioinformatics 2008, 9, 504. 10.1186/1471-2105-9-504; [4] Analytical Chemistry 2012, 84 (1), 283. 10.1021/ac202450g; [5] BMC Bioinformatics 2015, 16, 118. 10.1186/s12859-015-0562-8; [6] Bioinformatics 2009, 25 (2), 218. 10.1093/bioinformatics/btn603; [7] F1000Research 2013, 2, 191. 10.12688/f1000research.2-191.v2; [8] Nature biotechnology 2016, 34, 828. 10.1038/nbt.3597; [9] Analytical Chemistry 2021. 10.1021/acs.analchem.1c01465

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