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Do we still need to isolate Natural Products for their identification? - A paradigm shift in pharmacognosy.

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The recent rapid innovations made in metabolite profiling and bioassays may lead to a change of paradigm in NP research. Indeed having at hand full or partial of structure of possibly all metabolites in given natural extract open the possibility to perform pharmacognosy studies from a more holistic perspective. A question thus arise: *do we still need to isolate Natural Products for their identification*?

The increasing amount of accurate metabolome data that can be acquired from massive sample sets, including high-resolution mass spectrometry analyses (data dependent HRMS/MS), allows natural extracts to be mapped to an unprecedented level of accuracy [1]. To this end, the creation of integrated databases linking the valuable published knowledge provided by pharmacognosy with recent metabolite profiling data through appropriate computer tools could be extremely useful for future development in NP research [2].

In this context we push forward our applications and further development of UHPLC-HRMS/MS molecular network (MN) approaches [3,4] to provide enhanced annotation confidence level though multiple scores, notably taxonomy and MN structural consistency, and we are benchmarking this. We will discuss how far we are from the unambiguous identification of NPs by these approaches and how such advances could significantly accelerate NP research in future. Various recent applications of our research in metabolomics and phytochemistry will illustrate these aspects.

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References

[1] Wolfender JL et al. *Anal. Chem.* 2019; 91:704-742.
[2] Allard PM et al. *Curr. Opin. Biotechnol.* 2018; 54:57-64.
[3] Allard PM et al. *Anal. Chem. 2016*; 88:3317-23.
[4] Allard PM et al. *Curr. Opin. Chem. Biol.* 2017; 36:40-49.