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Do We Still Need NMR to Identify Natural Products

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With the recent progresses made in metabolite profiling methods especially based on Liquid chromatography high resolution mass spectrometry methods (LC-HRMS), a question that arises is: Do we still need to fully identify natural products (NPs) using tedious isolation protocols from complex biological matrices and subsequent 1D and 2NMR characterisation for their unambiguous identification?
High resolution mass spectrometry (HRMS) and data dependent MS/MS analyses provide very valuable information on secondary metabolites for in-depth metabolome annotation studies [1]. The recent development of molecular network (MN) approaches for the mining of such data in combination with spectral database generated in silico [2] gives the possibility to establish relationships between metabolites thus significantly improving the efficiency of dereplication when combined with high quality chemotaxonomic data [3]. Such types of information can be generated with a few mg of extract only and are readily applicable to herbarium scale samples. These data massively acquired on many samples provides a new and efficient way to obtain detailed structural information on many metabolites at once and this considerably improves the dereplication process.
NMR is still required for complete de novo identification of new compounds and, in this case, MS-targeted micro-isolation of given NPs can be performed and sensitive 1D and 2D microNMR with microgram amounts of purified metabolites can be acquired. For bioactivity determination, many bioassays fit also to this scale. Using an ideal combination of methods it is this virtually possible to fully identify any bioactive principles in this way. Integration of other filters to this approach such as permeation studies on extracts additionally provide key information on the possible bioavailability of NPs prior to their isolation. Furthermore the link of a given bioactivity result to those previously reported for compounds similar to those identified can be rationalised through in silico chemical space approaches.
Ideally a combination all these state-of-the-art methods should enable to identify and localise valuable NP efficiently at the analytical scale. In such a way large scale MS-targeted isolation of valuable NPs only can become a very rational way to conduct investigations. Different recent applications of our metabolomics and phytochemical investigations will illustrated these aspects.
References
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