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Dereplication of analytical products

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Tatural products continue to play an important role in the discovery and development of new chemical entities as druglead compounds. Considerable effort is being expended by many groups worldwide on the isolation of natural products from terrestrial and marine macro- and micro-organisms. Natural products obtained from plants and micro-organisms often exhibit biological activities of interest for the discovery of new drugs as well as pharmaceutical and agrochemical products. For instance, over 60% of the anticancer drugs have been discovered directly from natural products or are semi-synthetic derivatives of these compounds. However, the research for new bioactive compounds is usually laborious and slow, once the biological evaluation processes are preceded by isolation, purification, and structural elucidation steps, which are usually expensive and time-consuming. This fact, in combination with the large number of known compounds, has led the scientific community to develop new technique DEREPLICATION. Dereplication is the process that allows for the rapid identification of bioactive metabolites in crude extracts by distinguishing previously identified compounds from novel ones. This technique avoids repetitive work of isolation of already known natural products, promoting chemical screening or metabolite profiling. This uses analytical techniques and database searching to determine the identity of an active compound at the earliest possible stage in the discovery process. In the past few years, advances in technology have allowed the development of tandem analytical techniques such as liquid chromatography mass spectrometry (LC-MS), LC-MS-MS, liquid chromatography nuclear magnetic resonance (LC-NMR), and LC-NMR-MS. LC-NMR, despite its lower sensitivity as compared to LC-MS, provides a powerful tool for rapid identification of known compounds and identification of structure classes of novel compounds.