

LC-MS NMR: Building High Throughput Natural Products Libraries

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As pharmacognosy researchers search the planet for new molecules, they need better and faster tools to sift through their collected materials. Increasingly, the first method of choice is LC-MS (liquid chromatography coupled to mass spectrometry). But when LC-MS systems are configured with mass-directed fraction collectors, 95% of the fraction is typically available for capillary NMR analysis. This makes Protasis' CapNMR probes and One-Minute NMR automation system an easy add-on to any existing LC-MS system. We call it **LC-MS NMR**. Several current Protasis customers combine these rich sources of information (e.g., *mass from MS* and *structure, purity and amount from NMR*) to dereplicate known molecules rapidly and fully characterize their new libraries of New Molecular Entities. Valuable NMR results can be obtained on existing LC-MS fractions.

Examples from plant and marine natural products applications will be shown.

One-Minute NMR delivers the easiest operator interface and most flexible sample formats of any commercially available NMR automation system. It can run collected fractions directly in microplates or vial racks directly without the time and cost of tube filling. Chemists can reserve space on the system from their desktop, monitor sample processing from the lab bench and direct emailed results reports to their home or dorm room. Seamless integration with ACD/Labs databasing software is included.

The rich feature set of One-Minute NMR is discussed in detail along with cutting-edge new data processing features that re-define the standard for integrated, multi-user HT-NMR.