

Abstract

Small molecule NMR research today faces formidable challenges. Greater demand for new drug leads, lower-level impurity characterization, higher cryogen and magnet expenses, lab space limitations, and stronger global competition all combine to apply new pressures on both pharmaceutical and academic NMR researchers and managers. An expectation of greater productivity has become the norm, which calls for fresh scientific approaches and advances in analytical instrumentation. Innovations must include cost reduction, less human intervention, and better equipment reliability to meet the demands of the modern laboratory workplace. A viable analytical instrument today must pay for itself, and in less time than before.

Due in part to significant up-front investment in both specialized equipment and technical staff, NMR is slower to adapt to changing needs when compared to benchtop analysis platforms such as mass spectrometry and liquid chromatography. A simple, yet effective way to address this shortcoming is to provide a more advanced workflow of samples to and from the spectrometer. Deliberate omission of the NMR tube in favor of maintaining samples in micro well plates and vials provides new ways for NMR to couple directly and non-disruptively to the overall sample workflow of the organization. Modern and efficient liquid handling robots combined with microfluidic advances now make this practical and economical. Microflow NMR links upstream processes such as reaction monitoring, synthesis, and mass-directed fractionation, with downstream activities that include library management, structure verification, and regulatory/IP protocols, all via a web-based, vendor-neutral desktop interface. Overall, the approach strengthens the role of NMR in the analytical laboratory, and carries both financial and scientific value for NMR as an indispensable and highly utilized institutional resource. This poster specifically describes unique accomplishments in 2008 of scientists in both academia and industry in 5 important focus areas: molecular library management, impurities, metabolomics, natural products, and open access. Groups are running up to hundreds of samples per week employing automation that monitors itself. Easily-configured software links together visualization, elucidation, verification, and statistical analysis packages via electronic reporting. Open-access and dedicated research platforms both benefit, resulting in a significantly improved role for NMR in service to the organization and individual researcher [1, 2, 3].

1. Sorensen, Dan., et al., CoSMoS Conference, July 28-30, 2008, San Jose, CA.
2. Codina, Anna. SMASH 2008 Poster. Sept. 7-10, 2008, Santa Fe, NM.
3. Wolfender, Jean-Luc, et al., *J. Chromatography A*, 1180 (2008) 90-98.

