How to Make Short Work of Your *Medicinal Chemistry* Samples

Implementing Open-Access HT-NMR in an Active Department using One-Minute NMR™

Your Department Full of Eager Synthesis Chemists

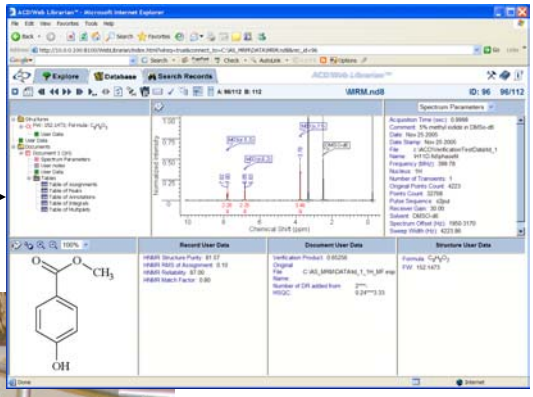
Now you can go from sample to results in one step. One-Minute NMR lets you transfer your prepared samples directly from your HPLC to a fast liquid handler for NMR analysis. Now you can load plates and vials directly.

Chemists and their managers will immediately appreciate the indispensable convenience of walk-away, unattended operation, with special support for overnight samples. When you consider shorter sample prep times, tiny sample withdrawals from valuable libraries, scant reagent and solvent consumption, elimination of the cost and effort to fill tubes plus improved magnet utilization due to faster spectral acquisition, this is a system that easily justifies itself in any NMR facility with multiple users or many samples.

Did I Make What I Thought I Made?

"For quality control of chemical libraries, 1D NMR spectra are acquired under full automation from 384-well plates on as many as 130 compounds within 24 hours using 128 scans per spectrum and a sample-to-sample cycle time of about 11 min. Because of the low volume requirements and high mass sensitivity of the microflow NMR system, 30 nmol of a typical small molecule is sufficient to obtain high quality, well-resolved, 1D proton or 2D COSY NMR spectra in approximately 6 or 20 min of data acquisition time per experiment, respectively."

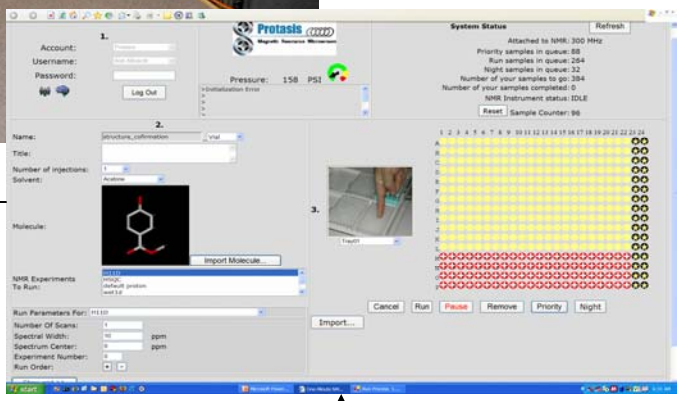
Bernhard Geierstanger, The Genomics Institute of the Novartis Research Foundation, ***Analytical Chemistry,*** **October, 2005**,



View acquired spectra and compare match and purity scores using ACD/Lab's Web Librarian. Results are emailed to each user. Flexible scripts allow any experiments using your spectrometer commands.

Sample Cleanup (e.g., HPLC, filtering)

Reconstitute And Boost Concentration In Deuterated Solvent



The workflow diagram shown is used in major pharmaceutical companies to process thousands of samples per month.

Log in samples quickly and monitor analytical progress from any web browser. Or import sample lists directly from your HPLC or other instruments. Support for 96 or 384 well microplates and your choice of low-volume vials. Supports up to three solvents.

HTSC

Get Structure Confirmation, %Yield and Purity

NMR Provides Quality Assurance for Molecular Libraries

Protasis High Throughput NMR Structure Confirmation System

Typical Configuration

- ✓ **Protasis CapNMR™ ICG Probe**
- ✓ **Protasis One-Minute NMR™ Software**
  - **Talks to Varian or Bruker Spectrometers**
  - **Seamless Interface to ACD Structure Confirmation Software**
  - **Accurate %Yield and Purity in a single step with ERETIC**
- ✓ **Protasis MultiSolvent HTSL + DSCM**
- ✓ **CTC/LEAP PAL Liquid Handler**
- ✓ **Vacuum Centrifuge**
- ✓ **Varian or Bruker Spectrometer**
- ✓ **400 MHz Shielded Magnet**

Get an optimized solution that can power your entire department! This Protasis High Throughput NMR Structure Confirmation System is supporting a sample workload of 2500+ samples per month in a departments with 150+ synthesis chemists.

Protasis can help you assemble a complete, dedicated multi-user NMR system for your Medicinal Chemistry department to serve all of your synthesis chemists. It is capable of processing hundreds of samples per day in up to three different solvents. Multiple methods can be defined for each sample using flexible, editable scripts that are sent to your spectrometer over a standard LAN.

The Protasis One-Minute NMR platform is a great way to introduce NMR automation to your synthesis chemists. You can mix and match laboratory-standard microplates and microvials freely on the fast, reliable CTC/LEAP liquid handlers that have proven themselves so well in mass spectrometry applications. Samples can be loaded directly from any HPLC system without the additional cost or time required to transfer samples to NMR tubes.

Protasis CapNMR probes are already sensitive and fast. To take full advantage of this revolutionary capability, Protasis adds convenient fully-automated sample loading using a standard injection loop. You can walk away with confidence knowing that your precious sample will be positioned accurately in the center of the NMR flowcell. Then your complete set of experiments can be executed and monitored efficiently by One-Minute NMR software.

Once acquired, One-Minute NMR can automatically send your 1D spectra to ACD/Lab's Structure Confirmation algorithm to determine match and purity scores. If you need more information, it will automatically schedule additional 2D experiments. A report with links to the results is emailed to each user. All acquired spectra can be reviewed in exquisite detail using ACD/Lab's spectral viewers.

The Protasis Structure Confirmation System is the highest performing system available for active departments that are building and certifying molecular libraries. Use mass spectrometry to provide molecular weight. But use One-Minute NMR to provide high-certainty structure confirmation, % yield and purity so that you can fully characterize your valuable molecules.

HTSC-2006-LC **High Throughput NMR Structure Confirmation System** **CALL**

Efficient NMR Automation: ***One-Minute NMR***