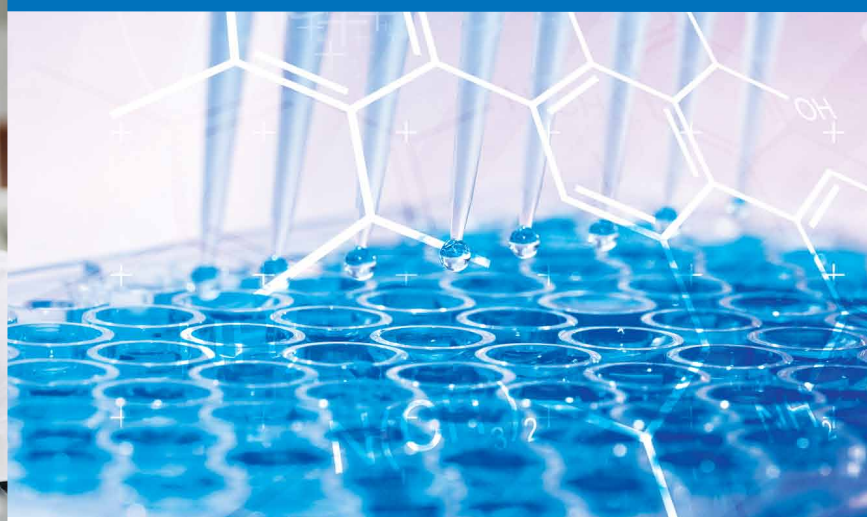


Automatic Concentration Determination Of Compound Libraries by NMR

CMC-q™ Complete Molecular Confidence - Quantification

Complete Molecular Confidence for quantification (CMC-q) is a complete workflow solution that facilitates automatic NMR-based quality assurance in batches.

- Controls experiment setup
- Manages data acquisition and processing
- Automatically analyzes the data
- Easy-to-use viewer for browsing and editing results
- Export results to Excel or text files

- CMC-q provides quick access to automated NMR quality assurance and quantification of larger batches of samples. Delivering accurate, precise information on sample concentration and water content in typical screening samples, CMC-q also marks questionable structures and provides a suggestion for spectral assignment. This is ideally complemented with LC-MS information such as derived from Bruker's SmartFormula program.

- Operating on a file-in, file-out basis, the user supplies an input file describing the samples to be measured, and receives an output file of results.

- The spectra interpretation function can also analyze individual datasets and prepare spectra for publication or for further analysis.

CMC-q Workflow

Setup

Acquisition

Analysis

Report

Setup

- Sample preparation from well plates
- Samples accompanied by SD Files
- SD Files used for experiment set up

Acquisition

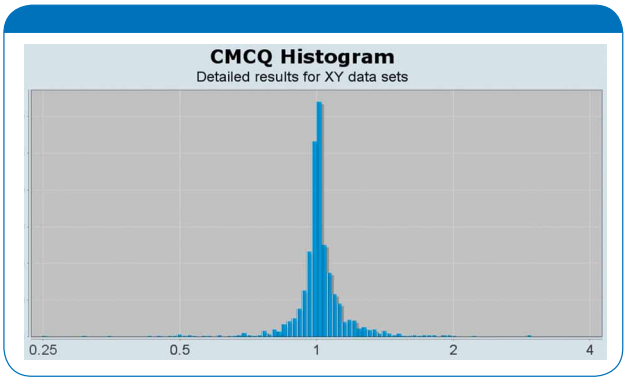
- Experimental parameters for standard NMR experiments in deuterated solvents, and typical screening samples in non-deuterated DMSO

Analysis

- Automatic NMR analysis of concentration, water content (for typical liquid store samples in non-deuterated DMSO), and plausibility with suggestion for assignment

Report

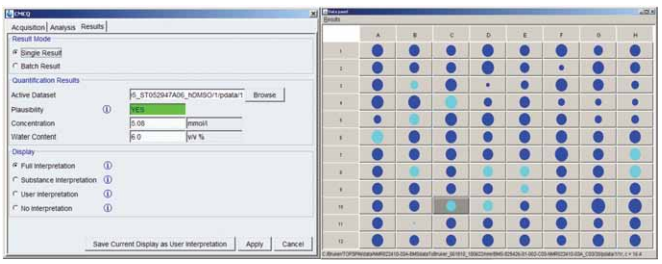
- Automatic report generation with easy viewing and editing, exportable to Excel or text file formats

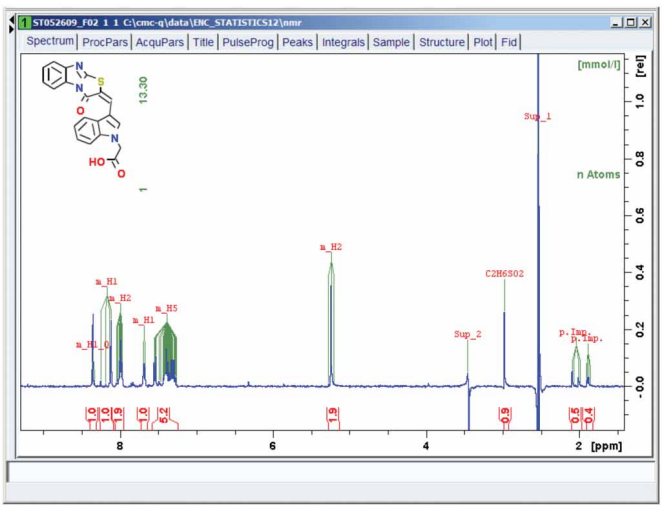


Quality of results

- CMC-q analysis assigns concentrations to over 95% of all datasets
- CMC-q also finds over 85% of the structures plausible, which the human expert found consistent.
- On these, more than 90% of the automatically assigned concentrations deviate only 20% or less from the manual expert result.
- This data was collected on ca. 2500 expert-interpreted spectra
- The compounds are commercial Lipinsky rule compounds from TimTec's APEX screening library and compounds from Actelion's own compound library
- Typically, 6-8ul samples in non-deuterated DMSO where used and data was acquired on 400 MHz instruments equipped with 1 mm MicroProbes and SampleJets. The turnover was a few minutes per sample.

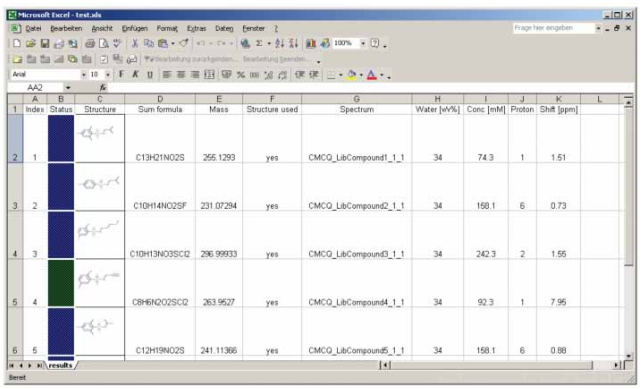
Single and multiple result view





Single and multiple result view

- Overview window of scaled dots representing concentration levels
- Dot color indicates structural plausibility status
- Overview of water content
- Concentration values that fall outside defined thresholds (low and high) can be highlighted
- Modify integral ranges, assignments and other results easily in the interactive CMC-q viewer
- User interaction can be logged



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ACTELION