



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

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

Acquisition

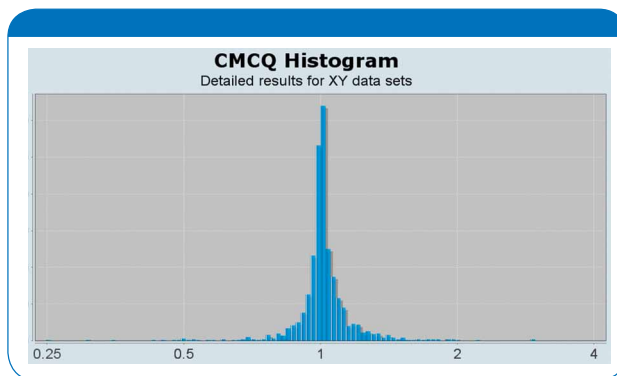
- Experimental parameters for standard NMR experiments in deuterated solvents, and typical screening samples in non-deuterated DMSO

Analysis

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

Report

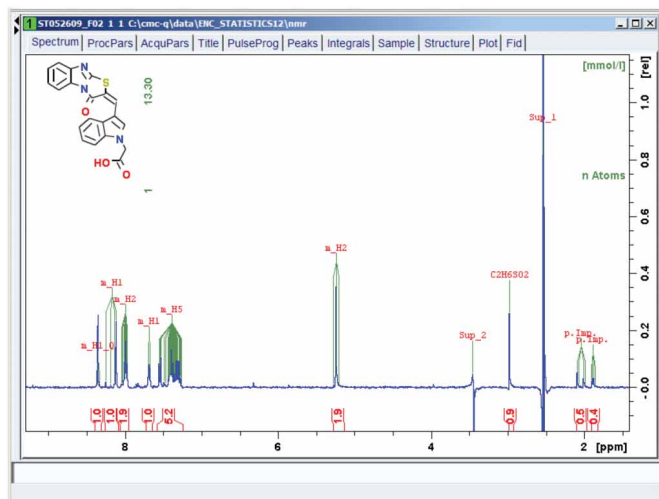
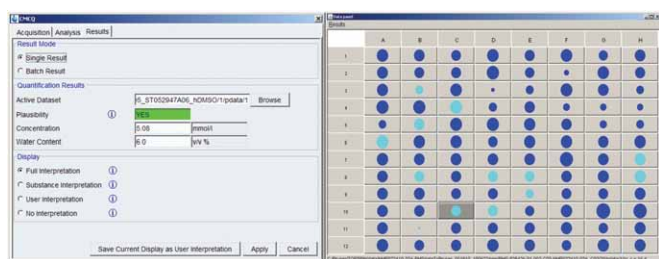
- Automatic report generation with easy viewing and editing, exportable to Excel or text file formats



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

Index	Status	Structure	Sum formula	Mass	Structure used	Spectrum	Water [v/v]	Conc [mM]	Proton	Shift [ppm]
1										
2			C19Q1M02S	255.1293	yes	CMCQ_LibCompound1_1_1	34	74.3	1	1.51
3			C10H14N02SF	231.0794	yes	CMCQ_LibCompound2_1_1	34	150.1	6	0.73
4			C10H13N03SC0	286.9993	yes	CMCQ_LibCompound3_1_1	34	242.3	2	1.55
5			C8H6N02SC0	263.9527	yes	CMCQ_LibCompound4_1_1	34	92.3	1	7.95
6			C12H19N02S	241.1366	yes	CMCQ_LibCompound5_1_1	34	150.1	6	0.80

● Bruker BioSpin

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