PotencyMR

- Quick Start Guide

User Manual

Version 003

Innovation with Integrity

NMR

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1 Introduction

This quick start documentation gives hints about how to use PotencyMR. Please refer to the PotencyMR manual for detailed information. Please refer as well to the IconNMR manual, the CMC-assist manual and the TopSpin manuals.

2 License

PotencyMR requires both a Topspin license and a PotencyMR license. CMC-assist is part of PotencyMR but doesn't need a license at the spectrometer.

PotencyMR license request: please contact your Bruker sales representative or email to our PotencyMR support at *qnmr@bruker.com*.

Once you have an order number, or if you want a demo license:

TopSpin and PotencyMR licenses can be ordered online from: *https://www.bruker.com/nmr_license_requests.html*.

A short instruction on installing the license will be sent together with the license. In addition, a description how to order and install a license can be found in the help menu of Topspin (**Help | Manuals (docs) | General | CodeMeter License Management**).

3 Sample Preparation

Prepare a sample containing the analyte and the internal reference standard (reference). The following information is needed when setting up the potency determination experiment:

- Purity of the reference
- Weight of reference and of analyte in mg
- Structure of the analyte (mol file). Only needed for the automatic analysis.
- Sample's solvent. A tip to get rid of exchangeable protons: add D2O (50µl in 600µl dDMSO)

For each reference's integral region:

- The left and right borders in ppm
- The proton number
- The multiplicity (optional)

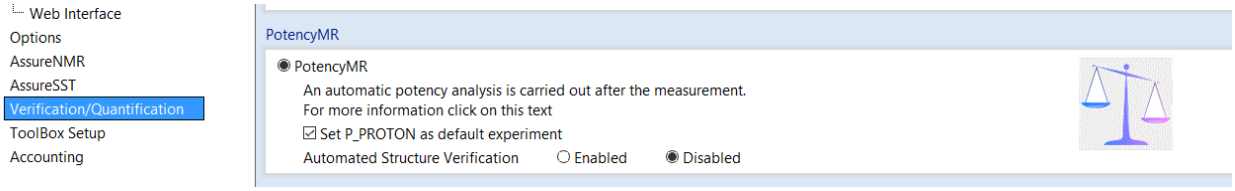
Optional: prepare and measure a 1H spectra of the analyte and the reference separately, in order to identify regions with no overlapping between the analyte and the reference. Overlap would lead to large errors.

4 Automated Potency Determination: Measurement

Start TopSpin:

Start IconNMR with the TopSpin command: **iconc**

Select PotencyMR settings:

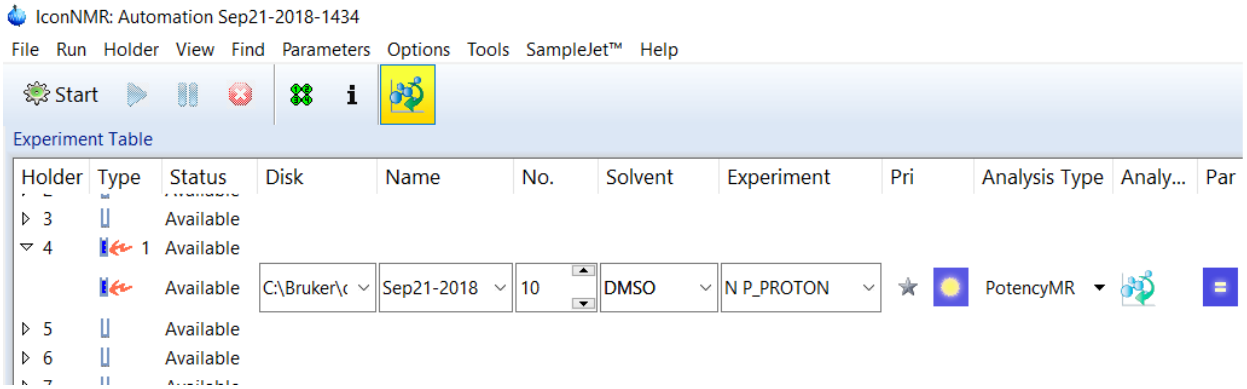


Create a new experiment for the holder with the sample. Select solvent and enter a name for the experiment.

The parameter sets listed in the table below are intended for use with PotencyMR. Please refer to the PotencyMR manual for further information.

Name	Pulse Sequence	Description
P_PROTON	zg	^{1}H-qNMR experiment with 90deg excitation pulse
P_PROTON30	zg30	^{1}H-qNMR experiment with 30deg excitation pulse
P_PROTON_IG	zgig	^{1}H{13C}-qNMR experiment with 90deg excitation pulse
P_PROTON30_IG	zgig30	^{1}H{13C}-qNMR experiment with 30deg excitation pulse

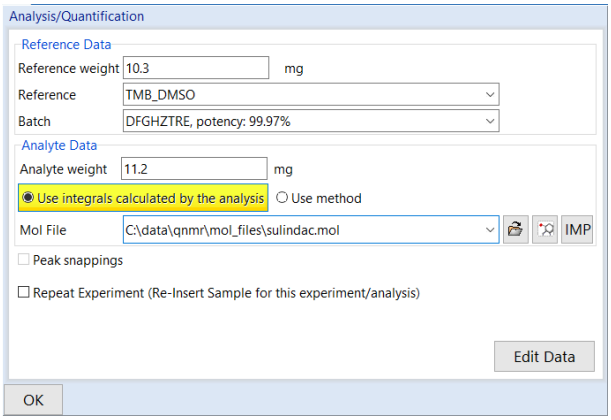
Table 4.1: Bruker library parameter sets for use with PotencyMR



Fill the analysis settings (automatic analysis or method) by clicking on:

Fill the internal standard data in the **Reference Data** section. The batch is a reference with a given potency. A reference and a batch need to be defined to run a potency calculation.

Fill the analyte data and choose to identify automatically the analyte integrals or to use a method:



Select **Repeat experiment** if the sample needs to be ejected and reinserted to redo the tuning/matching and shimming.

Click **Edit Data**, if you are an IconNMR supervisor, to create/delete reference, batch and method. There, it is possible to select peak snappings to automatically adjust the center of the predefined integrals in the Reference and in the method.

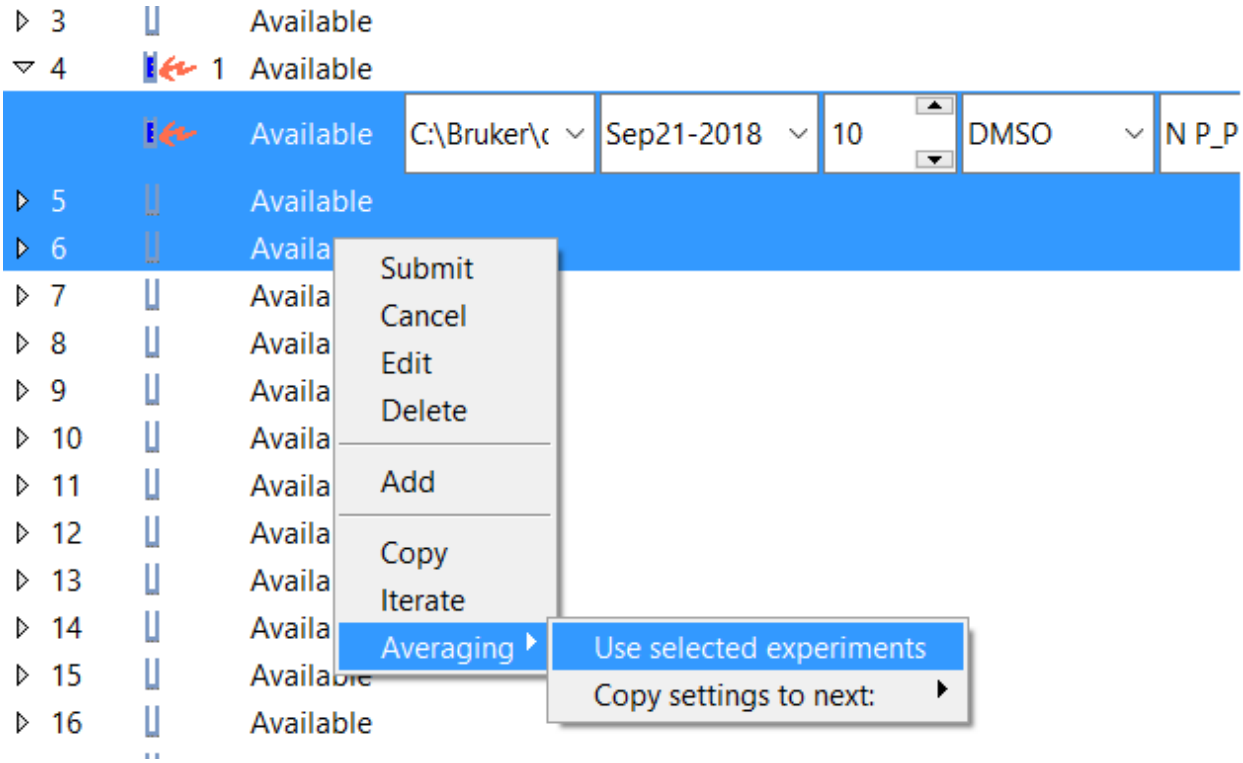
Click **OK** to close the analyse settings, Click **Start** in IconNMR, if not already started, and click on **Submit**.

Access the potency determination report in excel format, either in the measured dataset or directly in IconNMR by right clicking on the finished experiment in the preceding experiments panel. There, it is also possible to open the dataset in CMC-assist and visualize the spectrum.

5 Automated Potency Determination: Replicate Measurements

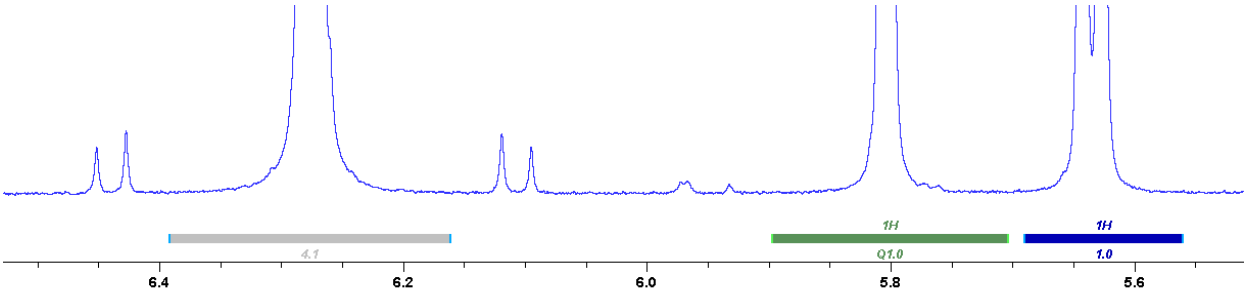
The average potency of several samples prepared in duplicate, triplicate... can be automatically calculated by following the steps below: Setup the first experiment as described before. Don't submit it.

Select the replicate by selecting the first experiment with a left click and then, press **Ctrl** key and select the holders where the replicate samples are. Then right click, select **Averaging | Use selected experiments:**

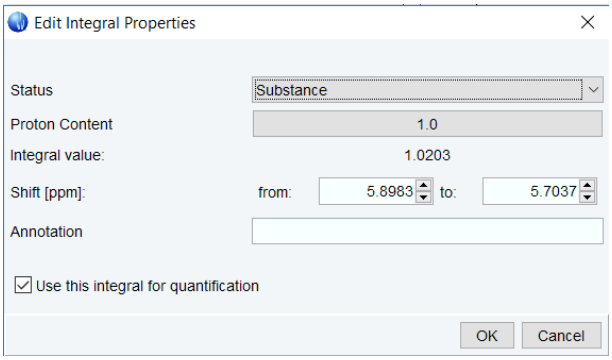


6 Method Development and Manual Potency Determination in CMC-assist

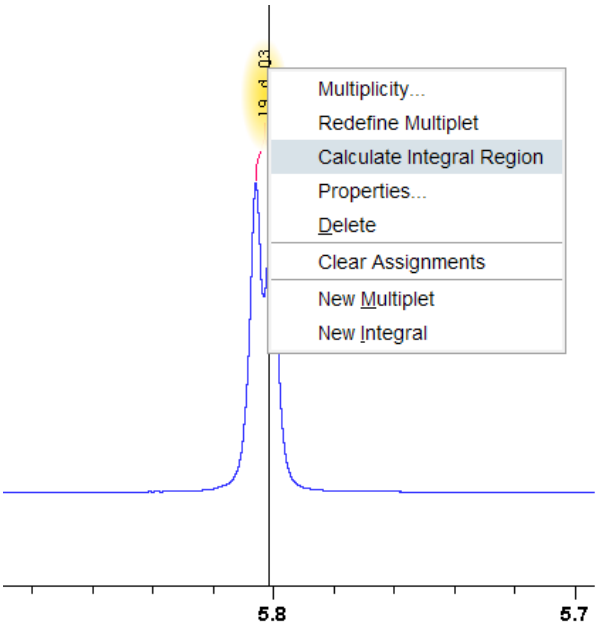
Method can be created in CMC-assist using a spectrum of the analyte. Only integrals in green are used in the potency calculation, they are from the analyte. The integral from the internal standard is defined in the reference data.



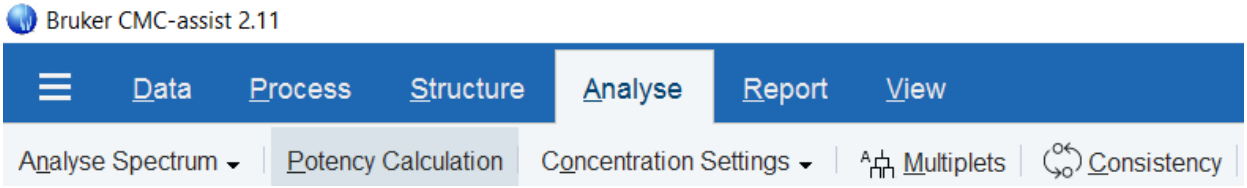
Right click on an integral bar to edit the integral properties:



Right click on a multiplet to select calculate integral region using a python script. A default script is provided to calculate based on a factor of the full width at half maximum of the peak:



A manual potency determination is done by opening the potency calculation settings, like in IconNMR. The settings are opened by using **Analyse | Potency Calculation**:



7 Contact

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