



Mestrelab Research
chemistry software solutions

Processing and Analysis in Mnova 12
Focus on requirements for qNMR

Mike Bernstein – February, 2018

“Fit for Purpose” qNMR

How accurate and precise do you need your qNMR result?

Sample preparation (weighing accuracy)

Spectrum acquisition conditions (delay, number of scans)

Processing and analysis



“High performance qNMR ($u < 0.5$)



High purity ($u < 2.0$)



Regular purity ($u < 5.0$)

Processing

FT

64K data points minimum for 1H up to 600 MHz (guide)
Zero-fill (up to 2X only)


Apodisation

Exponential (0.1-0.3 Hz)
Stanning function

Phase correction

Manual
Automatic (Regions, Global)

Baseline correction

Polynomial (3)
Bernstein polynomial (3)
Whittaker smoother 

Integration

Manual/Automatic

Used by Mnova Purity for Ref. Compound integration

Multiplets analysis

Manual/Automatic

Nuclides/multiplet may be improved by AutoAssignment

Can be affected by Ref Standard (CRM) if not in blind region

Used by Mnova Purity for Compound integration and nuclides



Sum integration

Manual/Auto
Ranges Growth factor



Global Spectrum Deconvolution (GSD)

Uses peak pick options



qGSD

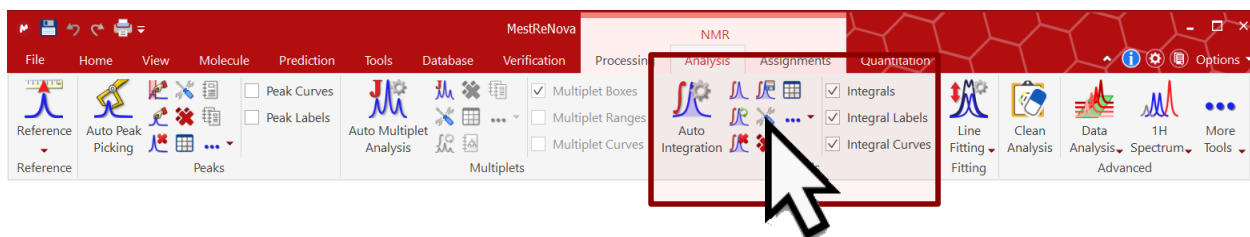
Uses peak pick options



Edited sum*

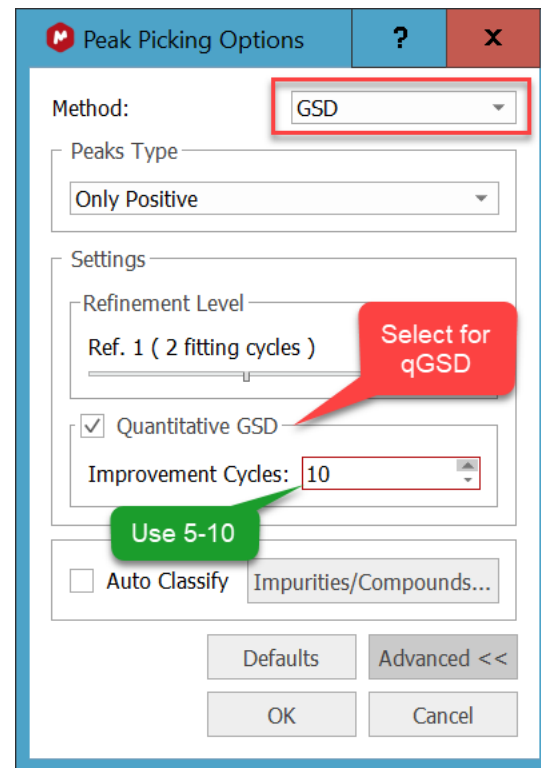
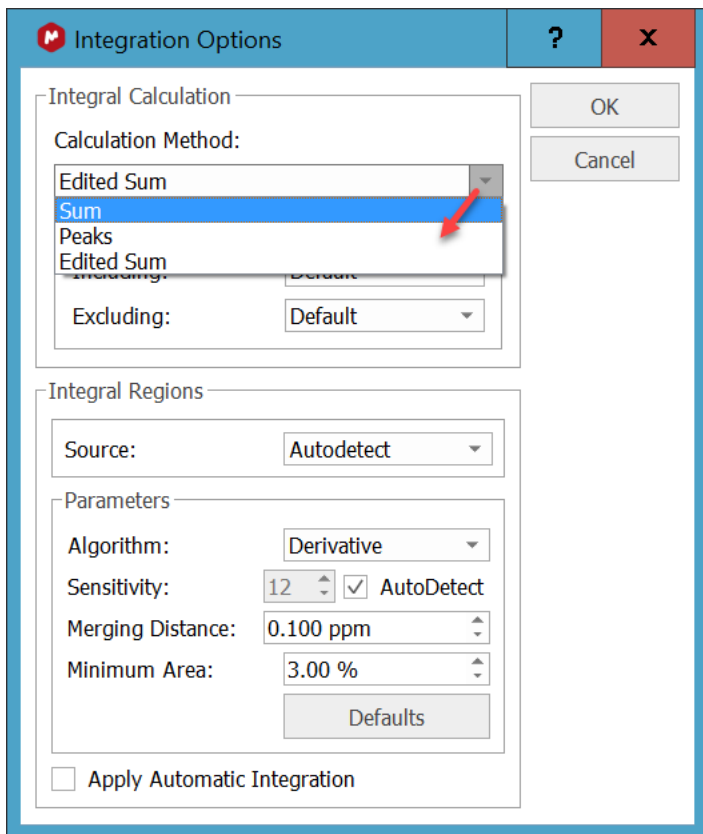
Hybrid method
Sum and GSD to remove unwanted signal contributions

Integration options

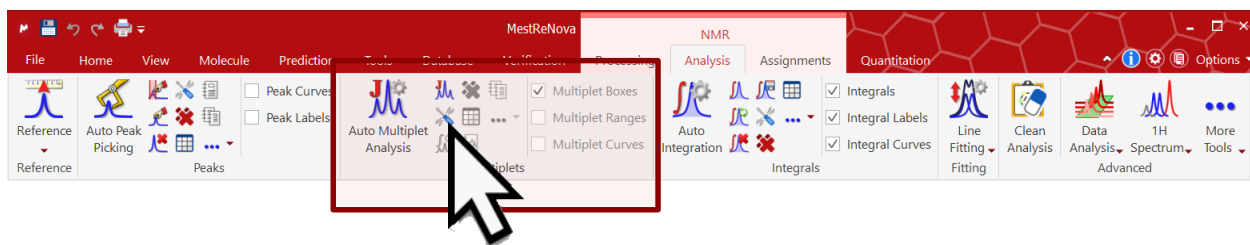


Sum and Edited Sum
Use the options shown here

Peaks must be selected for GSD or qGSD
integration. They use these options:

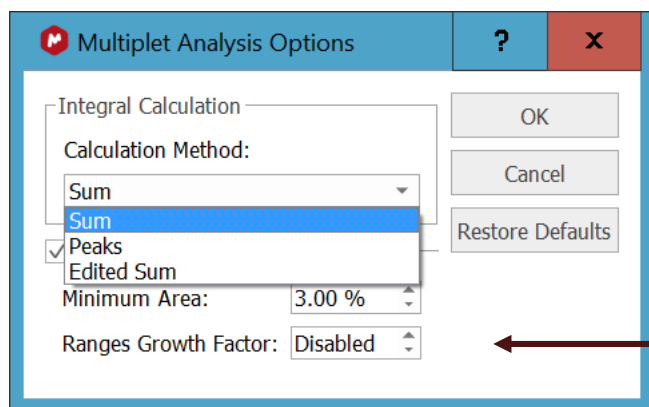


Multiplet integration



Sum and Edited Sum

Use the options shown here



The “Ranges Growth Factor” can be set here.

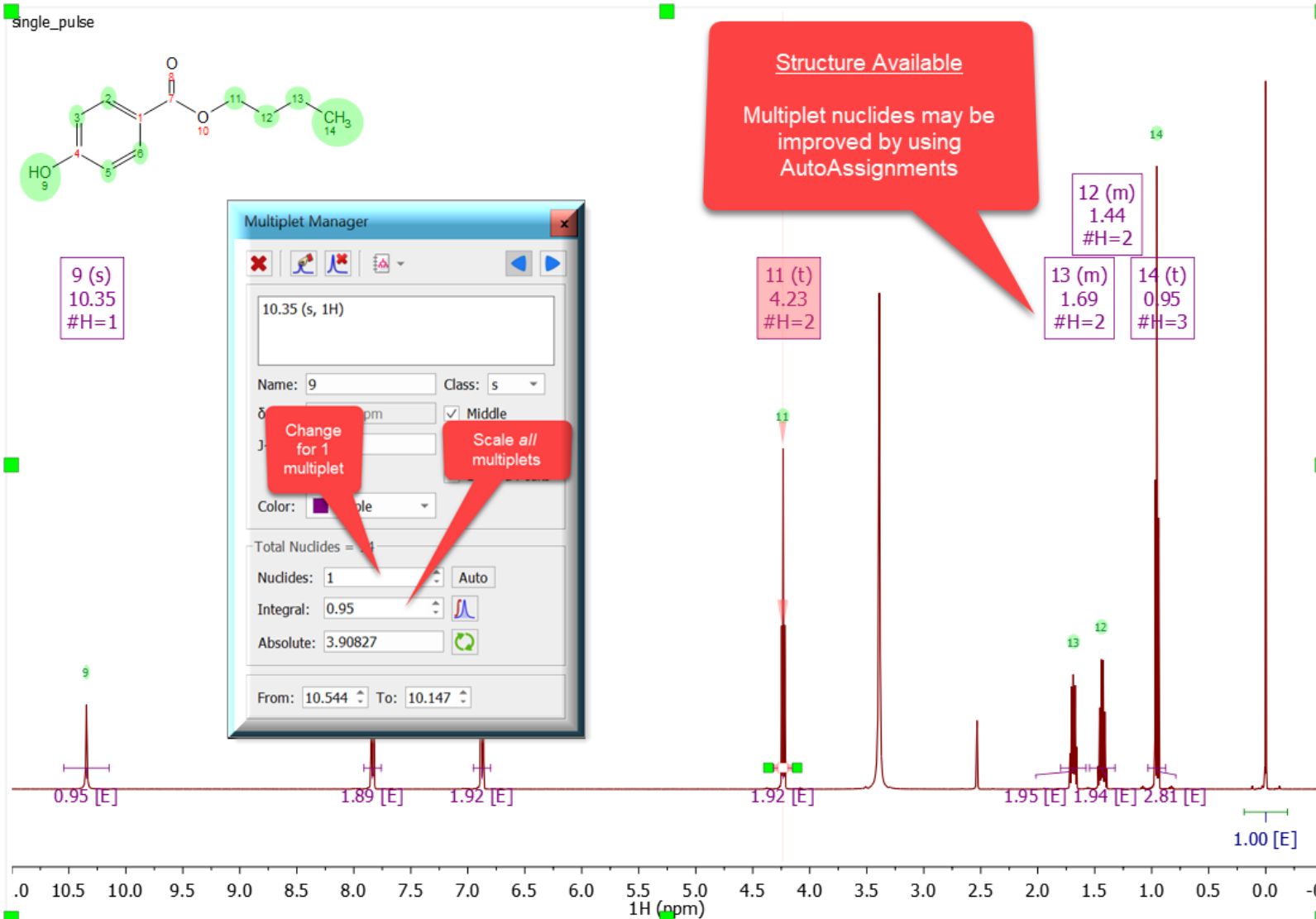
Use a value of about 15-20 for qNMR so the integral region is wider

Peaks must be selected for GSD or qGSD integration.

They use the options as for Peaks

Nuclides per multiplet

For qNMR Purity



[Stanning: A new NMR apodization function](#)

[A Novel qNMR Technique: Quantitative Global Spectrum Deconvolution \(qGSD\)](#)

[Basis on qNMR: Integration Rudiments \(Part I\)](#)

[Peak Integration Methods in qNMR](#)

[qNMR Purity Recipe Book \(1 – Sample Preparation\)](#)

[qNMR Purity Recipe Book \(2 – NMR Acquisition\)](#)

[qNMR Purity Recipe Book \(3 – Data Processing\)](#)

[Getting REALLY fussy about integration](#)

[Basics for qNMR – John Gauvin \(DSM\)](#)

[Getting picky with qNMR – John Gauvin \(DSM\)](#)

[Strengthening and simplifying Purity determination by NMR using Mnova](#)

[Mnova qNMR - Purity Determination \(22nd May 2013\)](#)