

ALL about QMSA

A Collection of Presentations, Tutorials and focused reports on essential features related to QMSA (Quantum Mechanical Spectral Analysis),

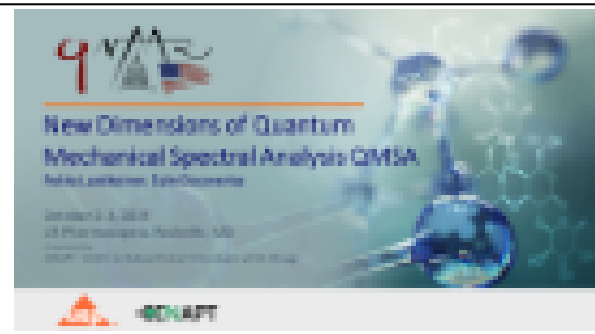
Ready for teaching and learning

by

Spin Discoveries Ltd

QMSA ..hmm?

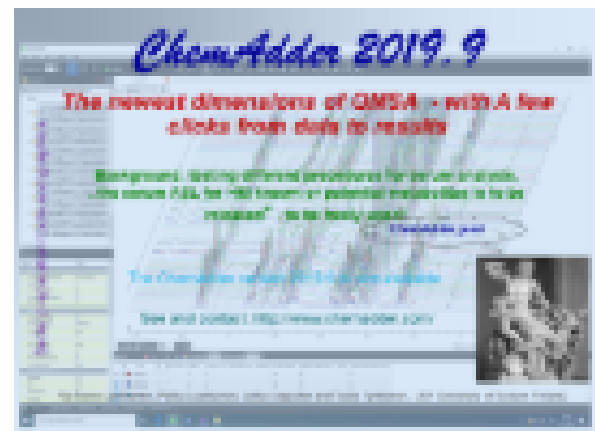
PRESENTATIONS & TUTORIALS



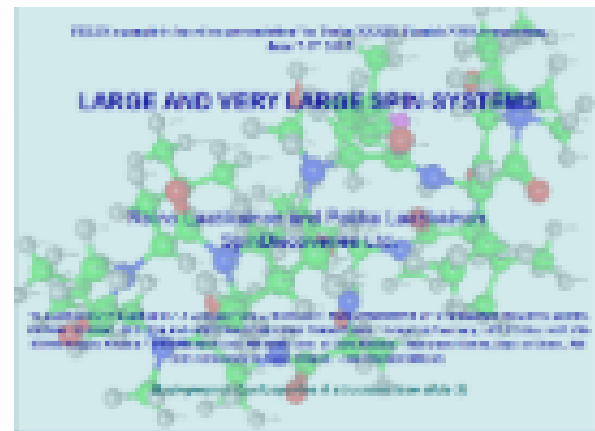
New Dimensions of QMSA
(USP summit)



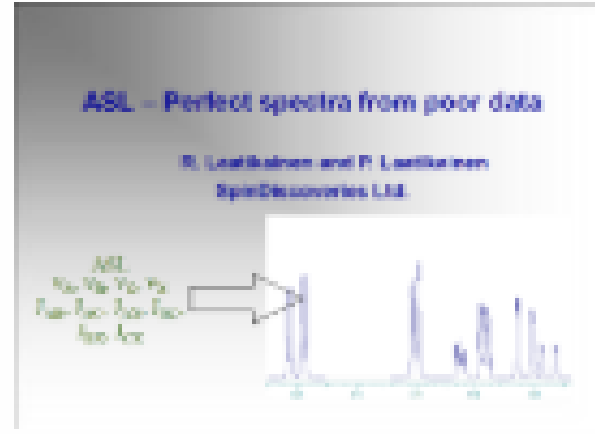
QMSA Basics



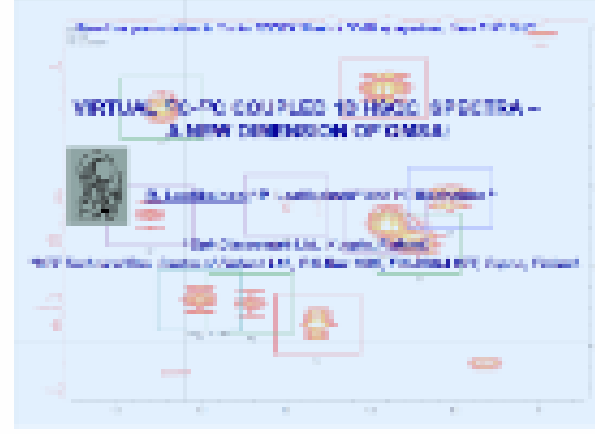
ChemAdder 2019



Large and Very Large Spin
Systems



ASL – Perfect Spectra from Poor
data



Virtual ¹³C-¹³C Coupled 1D HSQC
Spectra



Quantitative NMR



Quantitative NMR in Profiling
of Biorefinery Products (Abowe
project)



Millions of Transitions



qQMSA, Superior Tool for Analysis
of Biofluids



Basic tutorial 1

In this tutorial we start with very basics of spectral analysis with ChemAdder. The contents are: manually created spin systems, spin particle determination, shift and proton assignments, adding J-couplings, spectrum simulation and parameter iteration.

Basic tutorial 2

In this tutorial we learn automatic spin system determination directly from molecule structure. We also get familiar with spin particle type of '1*2*1'.

Basic tutorial 3

In this tutorial we learn integration. Also the integrals aren't always integrals exactly. We learn also how the responses can be made unfixed.

Intermediate tutorial 1

In this tutorial we analyze simple aromatic molecule. We also learn how to add heteronuclear coupling.

Intermediate tutorial 2

In this tutorial we have our first raw spectrum. We learn phase and baseline correction. We also use J-couplings to determine the molecule structure.

Advanced tutorial 1

In this tutorial we use ChemAdder to determine concentrations of different compounds in simple mixture.

Advanced tutorial 2

In this tutorial we determine ratio of α- and β-glucose.



EUROMAR 2025
OULU

Oulu's police: the famous statue in Oulu

QMSA Letters

A collection of focused research reports about QMSA

QMSA Letters 2022

History of QMSA

Reino Laatikainen¹, University of Eastern Finland, Kuopio, Finland
Pekka Laatikainen², Spin Discoveries Ltd, Kuopio, Finland
Updated July 6th, 2025

QMSA Letters 2023

Removal of ¹³C Effects for Impurity qQMSA. How Quantitative is DISPEL – Comparison with Gentle ¹³C Decoupling Method?

Reino Laatikainen¹, Jari Rakkila², Pekka Laatikainen³, Henri Martonen⁴ and Tuula Tynkkynen⁵
¹ Spin Discoveries Ltd., Kuopio, Finland
² Abo Academi, Turku, Finland (presently Bruker Biospin)
³ University of Eastern Finland, Kuopio, Finland
Updated July 5th, 2025

QMSA Letters 2025

Why QMSA and ChemAdder

Reino Laatikainen¹, Pekka Laatikainen², Henri Martonen³
¹University of Eastern Finland, Finland, ²Spin Discoveries Ltd, Kuopio, Finland
Last update July 1st, 2025

QMSA Letters 2025

Spin-layers and packing of large spin-networks

Reino Laatikainen¹, Pekka Laatikainen² and Henri Martonen³
Spin Discoveries Ltd., Kuopio, Finland
Updated July 6th, 2025

QMSA Letters 2025

Diversity of NMR Line-Shapes

¹Reino Laatikainen, Pekka Laatikainen and Henri Martonen
²USP Team: Sami Pandel, Christine Castagna, Justa Breck and Ben Shapiro
³UEF: Tuula Tynkkynen
⁴Spin Discoveries Ltd., Kuopio, Finland
⁵USP: US Pharmaceuticals, USA
⁶UEF: University of Eastern Finland
Updated July 5th, 2025

QMSA Express 2022

Response Factors (RF) are not always one !

Reino Laatikainen¹, Pekka Laatikainen², Henri Martonen³ and Tuula Tynkkynen⁴
¹Spin Discoveries Ltd., Kuopio, Finland
²University of Eastern Finland, Kuopio, Finland
Updated July 5th, 2025

QMSA Letters 2024

Anatomy of a 60 MHz Benchtop NMR Spectrum – Dissection Out of Coil correction

R. Laatikainen¹, S. Pandel², B. Shapiro³, J. Zhang⁴, J. Hein⁵ and P. Laatikainen⁶
¹ Spin Discoveries Ltd., Kuopio, Finland
² USP (US Pharmaceuticals), Rockville, 12601 Twinbrook Parkway, MD 20852, USA
³ University of British Columbia, Department of Chemistry, Vancouver, BC V6T 1Z4, Canada
Updated July 5th, 2025

QMSA Letters 2025

The IT Supported QMSA for pNMR (purity NMR)

Reino Laatikainen, Pekka Laatikainen and Henri Martonen
Spin Discoveries Ltd., Kuopio, Finland
Updated July 6th, 2025

QMSA Letters 2024

The effects of C, Si, Cl and S isotopes in ¹H NMR spectra – not that simple – for perfectionists

Reino Laatikainen¹, Pekka Laatikainen² and Henri Martonen³
¹ Spin Discoveries Ltd., Kuopio, Finland
² University of Turku, Turku, Finland
Updated July 5th, 2025

QMSA Letters 2025

The Art of QMSA
Almost Complete Complete QMSA – the Concepts of NMR-Purity and Impurity

Reino Laatikainen¹, Pekka Laatikainen², Henri Martonen³, Tuula Tynkkynen⁴ and Jari Rakkila⁵
¹ Spin Discoveries Ltd., Kuopio, Finland, ²University of Eastern Finland, Finland, ³Abo Academi, Finland (presently Bruker Biospin)
Updated July 5th, 2025

QMSA Letters 2025

Prior Knowledge* and Constraints

Reino Laatikainen, Pekka Laatikainen and Henri Martonen
Spin Discoveries Ltd., Kuopio, Finland
Updated July 6th, 2025

*WIKIPEDIA: Prior knowledge refers to what a learner already knows before learning new information. That is, it's the information and educational context already present before new instruction. Prior knowledge is important as it serves as a foundational building block for new knowledge. ... (not WIKIPEDIA) the phrase has also an ultimate meaning



Brotherman: the famous statue in Kuopio

SAVE 90% !

QMSA Letters 2025

The NMR-Purity and the new dimensions and standards of purity

Reino Laatikainen, Pekka Laatikainen and Henri Martonen
Spin Discoveries Ltd., Kuopio, Finland
Updated July 12th, 2025