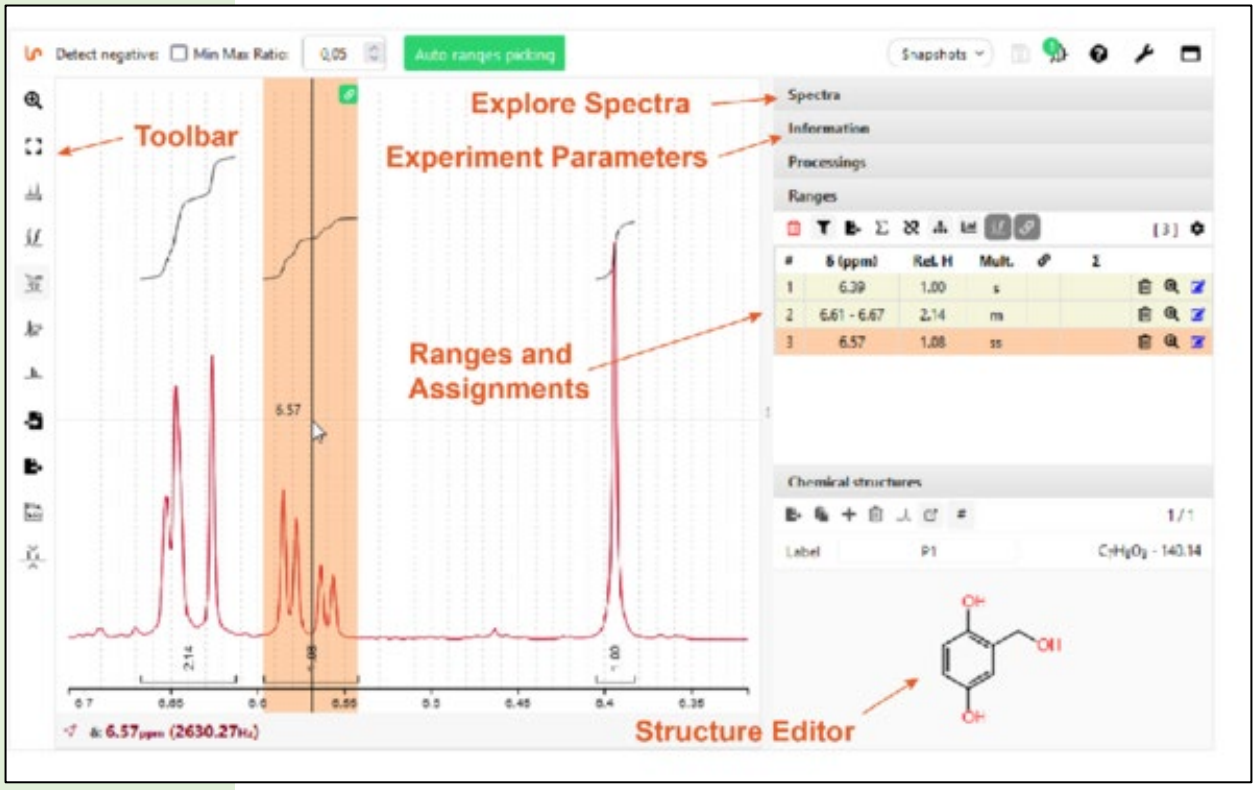
eWorkshop

Society for Medicinal Plant and Natural Product Research

NMR Data Processing, Assignment, and FAIR Data Publishing with NMRium

Online, January 30, 2026
15:00 – 17:00 (CET)
9:00 – 11:00 (EST-U.S.)
22:00 – 24:00 (CST-China)



NMR Data Processing, Assignment, and FAIR Data Publishing with NMRium

NMRium is a versatile web-based application for the processing, analysis, and data management of NMR spectra — entirely within your browser. NMRium provides powerful tools for spectrum processing, multiplet assignment, reference database creation, and FAIR-compliant data publishing to Zenodo. This workshop will combine theoretical insights with hands-on activities, leading participants through real examples from basic spectrum processing to advanced analysis and data sharing.

Workshop outline:

1. **Data Management Overview** – Principles and best practices for storing, organizing, and sharing NMR datasets to ensure long-term accessibility and compliance with FAIR data standards.

2. **Basic 1D NMR Spectrum Processing and Assignment (Ethyl Vinyl Ether)** – Step-by-step demonstration of basic processing and peak assignment on a simple spectrum to introduce the workflow and interface.

3. **Advanced Spectral Assignment Using 1D and 2D Spectra (Ibuprofen)** – Practical strategies for correlating 1D and 2D spectral information (COSY, HSQC, HMBC, etc.) to achieve more complex structural assignments.

4. **STOCSY Analysis** – Exploration of an array of 1D NMR data and demonstration of Statistical Total Correlation Spectroscopy (STOCSY) to reveal relationships between molecules in real-world forensic NMR data.

5. **E-Learning Exercises** – Guided and self-paced practice tasks for reinforcing skills learned during the session.

6. **Publishing Data to Zenodo** – Walk-through the available direct integration of NMRium with functions for the publishing of processed datasets to Zenodo, ensuring that data are findable, accessible, interoperable, and reusable (FAIR).

By the end of this workshop, participants will be able to:

- **Process and assign 1D and 2D NMR spectra using NMRium**
- **Create and publish FAIR-compliant NMR datasets with minimal effort**

Chairman
Dr. Emerson F. Queiroz, University of Geneva, Switzerland

Speaker

✓ **Dr. Luc Patiny, Zakodium Sàrl, Lonay, Switzerland**

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Society for Medicinal Plant and Natural Product Research

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Organization

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Registration

This eWorkshop is offered free of charge.
Please use this link to registrer. You will receive a Zoom link via e-mail afterwards – please check your spam-folder. If you do not receive the link, please contact events@ga-online.org (Cornelia Kern).

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