

Revolutionizing Data Sharing Advances NP Research

nBS Workshop

The NoBS Consortium | GA 2026 Reims

1 – Introduction

Background information and workshop overview

A - NP Molecules (metabolites)

2 - Chemical Structures & Nomenclature

Identifiers, atom numbering, stereochemistry

3 - Why 3D Matters

About conSTITUtion, conFIGURAtion, and conFORMAtion

B- NoBS Portal & CORE FUNCTIONS *NEW*

4 - THE FRAMEWORK - Portal Architecture & Core Functionality

Architecture, modules, functionality

5 - THE COMPOUND - Compound Record Creation

Structure import, drawing, validation, and automatic numbering

6 - THE SPIN - NMR Data Integration & Interpretation

Assignment workflows, processing, publication-ready reporting

7 - THE MASS [M-rep] - MS Data Integration

MS1/MS2 import, mol. formula determination, adduct documentation

8 - THE CARBON FLOW [C-rep] - ¹³C NMR Dereplication

New tools for pure compounds and complex mixtures

9 - THE PROTONS [H-rep] - HiFSA / QM-NMR Workflows

Nuclear genotyping, spectral matching, structural validation, nmrXiv integration

C – Summary & Interactive Discussion

10 - **Community needs**, future developments, potential collaborations

Presenters:

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2026 Questionnaire

nobs.naturalproducts.net/

noBS Webpage



←You are welcome to participate!

