

# Spectrus JS



**ACD/Labs**

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# Spectrus JS – Overview

- Browser-based NMR processing software developed by ACD/Labs
- The NMR analyst only requires a web browser and access to the internet
- Hosted on your organizational intranet or (private) cloud
- For individual users, there is no need to perform installation and/or software updates
- Data pick-up from shared NMR server possible



# Spectrus JS – Home Page

Sign in to Spectrus JS Trial

ACD/Labs  
Spectrus JS

Username or email \*

Password \*

Remember me

Login

[Forgot Password?](#)

Authentication through active directory (Windows login) possible

# Spectrus JS – Home Page

The screenshot shows the Spectrus JS Home Page in a web browser. The page features a table of datasets with columns for Name, Last Modified, and a filter input. A yellow box highlights the 'NMR Projects' section, and a '+ Create New Dataset' button is visible at the bottom.

Name	Last Modified	filter by name
Dihydropyridin - Unprocessed	Mar 17, 2023	...
Felodipine - NMR Data	Feb 10, 2023	...
Felodipine - LC-MS Data	Jan 26, 2023	...
Dihydropyridin - Fully Processed	Dec 20, 2022	...
GC-MS_Eugenol	Dec 1, 2022	...
LC-MS_Verapamil_Rat_0min	Nov 28, 2022	...

**NMR Projects**

[+ Create New Dataset](#)

# Spectrus JS – Dashboard

The image displays the Spectrus JS dashboard interface, which is used for NMR data processing and analysis. The interface is divided into several main sections:

- Processing Tools:** A sidebar on the left contains various tools for data manipulation, including "Add Widget", "Upload/Open Data", "Download Dataset", "Undo", "Redo", "Fourier Transform", "Phase Correction", "Baseline Correction", "Solvent & Reference", "Signal Analysis", "Pick by Level", "Assignment", "Annotation", and "Report".
- NMR Spectra:** The central panel shows a 1D NMR spectrum with intensity (absolute) on the y-axis (scaled by  $10^8$ ) and chemical shift ( $\delta$  in ppm) on the x-axis. A prominent peak is labeled "TMS" at 0 ppm. Other peaks are visible in the aromatic region (6-8 ppm) and aliphatic region (2-4 ppm).
- NMR Tables:** Below the spectrum, there are tabs for "Multiplet Report", "Spectral Data Table", and "Peaks Table". The "Spectral Data Table" is currently active, displaying the text:  $^1\text{H}$  NMR (400 MHz, CHLOROFORM-d, 47°C):  $\delta$  =
- NMR Project Structure(s):** The right-hand panel shows the chemical structure of the sample, which is a benzyl-substituted piperidine derivative. The structure is labeled with "HN" and "O".

Yellow callout boxes highlight the "Processing Tools", "NMR Spectra", "NMR Tables", and "NMR Project Structure(s)" sections. The interface also includes a browser window at the top and an "Options" button in the bottom right corner.

# Spectrus JS – Fourier Transformation Options

**Fourier Transform Options**

Apply Fourier Transform

Initial:

Final:

FID Shift (pts):

Cyclical

**Window Function** | **Linear Prediction**

Function Type:

	LB	Tm (sec)
<input checked="" type="checkbox"/> EM:	<input type="text" value="0.15"/>	<input type="text" value="0"/>
<input type="checkbox"/> GM:	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="checkbox"/> Sine:	<input type="text" value="0"/>	<input type="text" value="0"/>
<input type="checkbox"/> Sq. Sine:	<input type="text" value="0"/>	<input type="text" value="0"/>

FT can be applied at any stage of analysis without losing any data.

**Close** **Apply**

Options

# Spectrus JS – Phase Correction Options

The screenshot displays the Spectrus JS interface for the compound Dihydropyridin. A modal dialog titled "Phase Correction Options" is open, showing the following settings:

- Phase 0:  with minus and plus adjustment buttons.
- Phase 1:  with minus and plus adjustment buttons.
- A **Flip Phase** button.
- Two checkboxes:  Fine Tuning and  Linear Phase Correction.

Instructions within the dialog:

- To change **Phase 0**, drag over the spectral plot.
- To change **Phase 1**, hold Shift and drag.
- To change the pivot point, move the red line on the spectrum.

At the bottom of the dialog are **Close** and **Apply** buttons.

The background shows the <sup>1</sup>H NMR spectrum (400 MHz, CHLOROFORM-d, 47°C) with a TMS peak at 0 ppm. The chemical structure of dihydropyridin is shown in the Structure panel on the right.

Options

# Spectrus JS – Baseline Correction Options

**Baseline Correction Options**

**Corrected Region**

- Complete Spectrum
- Selected Region (ppm):

**Manual Correction**

Points Connection:  Multiple Points  Cubic Spline

**Automatic Correction**

- Polynomial
- FID Reconstruction
- Spectrum Averaging

Polynomial Order:

**Recalculate Curve**

To add a point to the baseline, click the spectral plot.  
To delete a point on the baseline, select it.  
To correct the baseline, move the baseline point.

**Close** **Apply**



# Spectrus JS – Solvent and Referencing Options

The screenshot displays the Spectrus JS software interface. The main window shows a 1H NMR spectrum of dihydropyridin with a TMS peak at 0 ppm. The chemical structure of dihydropyridin is shown in the Structure panel. The 'Solvent & Reference Options' dialog box is open, allowing users to configure the software's behavior.

**Solvent & Reference Options**

- Apply to All Spectra of Project

Find	Search Options	Action
<input checked="" type="checkbox"/> Reference	TMS	▼
<input checked="" type="checkbox"/> Solvent	CHLOROFORM-d	▼

- DMSO Satellites
- Residual Solvents

**Close** **Apply**

# Spectrus JS - Spectrum Prediction

The screenshot displays the Spectrus JS web application interface for the compound Dihydropyridin. The main window is titled "Dihydropyridin - Unprocessed".

**Left Panel (Tools):**

- Add Widget
- Upload/Open Data
- Download Dataset
- Undo Redo
- Fourier Transform
- Phase Correction
- Baseline Correction
- Solvent & Reference
- Signal Analysis
- Pick by Level
- Assignment
- Annotation
- Report

**Center Panel (Spectra):**

The main plot shows the  $^{13}\text{C}$  NMR spectrum with Intensity (absolute) [e+9] on the y-axis and chemical shift  $\delta$  (ppm) on the x-axis. The x-axis ranges from 220 to 0 ppm. Key peaks are labeled: TMS at 0 ppm and CHLOROFORM-d at approximately 77 ppm. The spectrum shows several peaks in the aromatic region (120-140 ppm) and aliphatic region (30-40 ppm).

Navigation options below the plot include:  $^1\text{H}$ ,  $^{13}\text{C}$  APT, HSQC, HMBC, COSY, NOESY.

**Right Panel (Structure):**

The chemical structure of Dihydropyridin is shown, featuring a benzene ring attached to a six-membered ring containing an NH group and a carbonyl group. The structure is labeled with "HN" and "O".

**Bottom Panel (Data):**

Multiplet Report x Spectral Data Table Peaks Table

$^{13}\text{C}$  NMR (101 MHz, CHLOROFORM-d, 47°C):  $\delta =$

Options

Two callout boxes highlight the "Signal Analysis" icon in the top toolbar and the "Structure" panel's "Signal Analysis" icon, indicating the integration of the two views.

# Spectrus JS - 1D NMR Predictions

The screenshot displays the Spectrus JS web application interface for the compound Dihydropyridin. The interface includes a sidebar with various processing tools, a central plot area, and a structure panel on the right. A dropdown menu is open, showing the following options:

- Chemical Shifts
- 1D NMR Spectra (highlighted by a mouse cursor)
- 2D NMR Spectra
- Calculation Method

The 1D NMR Spectra dropdown is further expanded to show the following nuclei options:

- 1H
- 13C
- 15N
- 19F
- 31P

The background interface shows the chemical structure of Dihydropyridin, a 1H NMR spectrum with a TMS peak at 0 ppm, and a 13C NMR spectrum. The sidebar contains tools such as Add Widget, Upload/Open Data, Download Dataset, Undo/Redo, Fourier Transform, Phase Correction, Baseline Correction, Solvent & Reference, Signal Analysis, Pick by Level, Assignment, Annotation, and Report.

# Spectrus JS – 2D NMR Predictions

The screenshot displays the Spectrus JS web application interface for the compound Dihydropyridin - Unprocessed. The interface includes a sidebar with various processing tools such as Fourier Transform, Phase Correction, and Signal Analysis. The main area shows a 1D NMR spectrum with a TMS peak at 0 ppm. A dropdown menu is open, highlighting the '2D NMR Spectra' option. The menu lists several 2D NMR techniques: HSQC, HSQC-DEPT, HMBC, and COSY. The '2D NMR Spectra' option is currently selected, and a sub-menu is visible, listing 'Chemical Shifts', '1D NMR Spectra', '2D NMR Spectra', and 'Calculation Method'. The '2D NMR Spectra' option is highlighted in the sub-menu. The chemical structure of Dihydropyridin is shown in the Structure panel on the right, and the 1D NMR spectrum is shown in the Spectra panel.

Chemical Shifts

1D NMR Spectra

2D NMR Spectra

Calculation Method

HSQC

HSQC-DEPT

HMBC

COSY

# Spectrus JS - Prediction Algorithms

The screenshot displays the Spectrus JS software interface for the compound Dihydropyridin. The left sidebar contains a menu with the following items: Add Widget, Upload/Open Data, Download Dataset, Undo, Redo, Fourier Transform, Phase Correction, Baseline Correction, Solvent & Reference, Signal Analysis, Pick by Level, Assignment, Annotation, and Report. The main window shows a chemical structure of Dihydropyridin and a spectrum. A dropdown menu is open, listing prediction algorithms: Corrected Weighted Average Experimental, Average Experimental, Weighted Average Experimental, Tabular (Incremental), and Neural Network (marked with a checkmark). A secondary dropdown menu is also open, listing: Chemical Shifts, 1D NMR Spectra, 2D NMR Spectra, and Calculation Method (highlighted by a mouse cursor).

Chemical Shifts

1D NMR Spectra

2D NMR Spectra

Calculation Method

Corrected Weighted Average Experimental

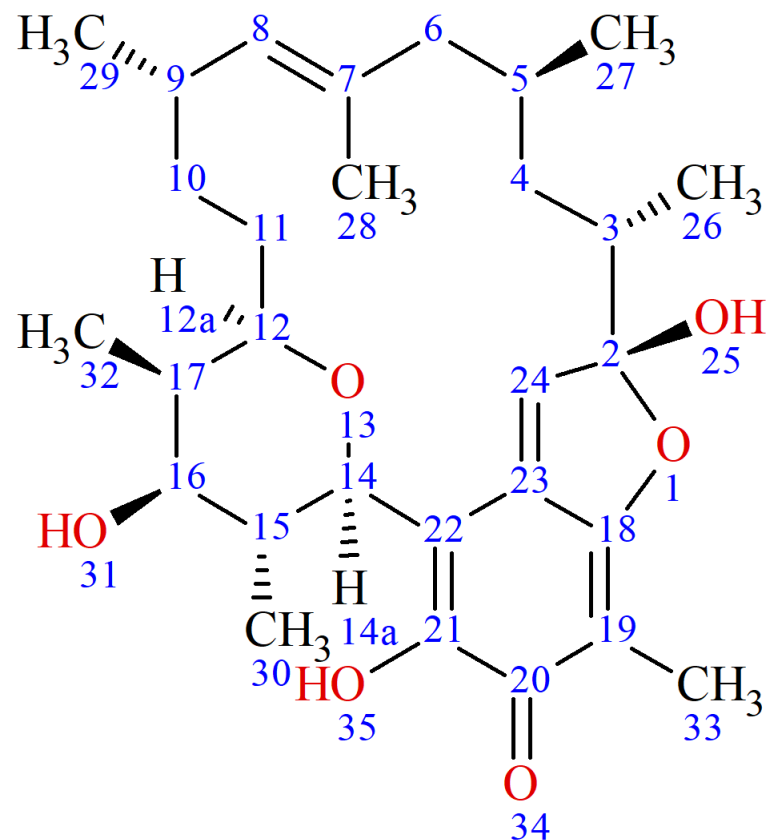
Average Experimental

Weighted Average Experimental

Tabular (Incremental)

Neural Network ✓

# Spectrus JS – Predicted <sup>13</sup>C APT



Internal database with <sup>1</sup>H and <sup>13</sup>C data of  
~300k structures

Atom No.	<sup>1</sup> H Shift	Ref
3	2.25	1
4	1.23 <=>	1
4	1.39 <=>	1
5	1.79	1
6	1.53 <=>	1
6	2.02 <=>	1
8	4.47	1
9	2.24	1
10	1.08 <=>	1
10	1.25 <=>	1
11	1.12 <=>	1
11	1.36 <=>	1
12a	3.39	1
14a	4.19	1
15	1.6	1
16	3.39	1
17	1.75	1
24	7.01	1
26	0.53	1
27	0.83	1

Formula: C<sub>29</sub>H<sub>42</sub>O<sub>6</sub>

FW: 486.6402

Name: (1R,9S,10S,12S,14E,16S,19R,20R,21S,22R)-3,9,21-trihydrox-

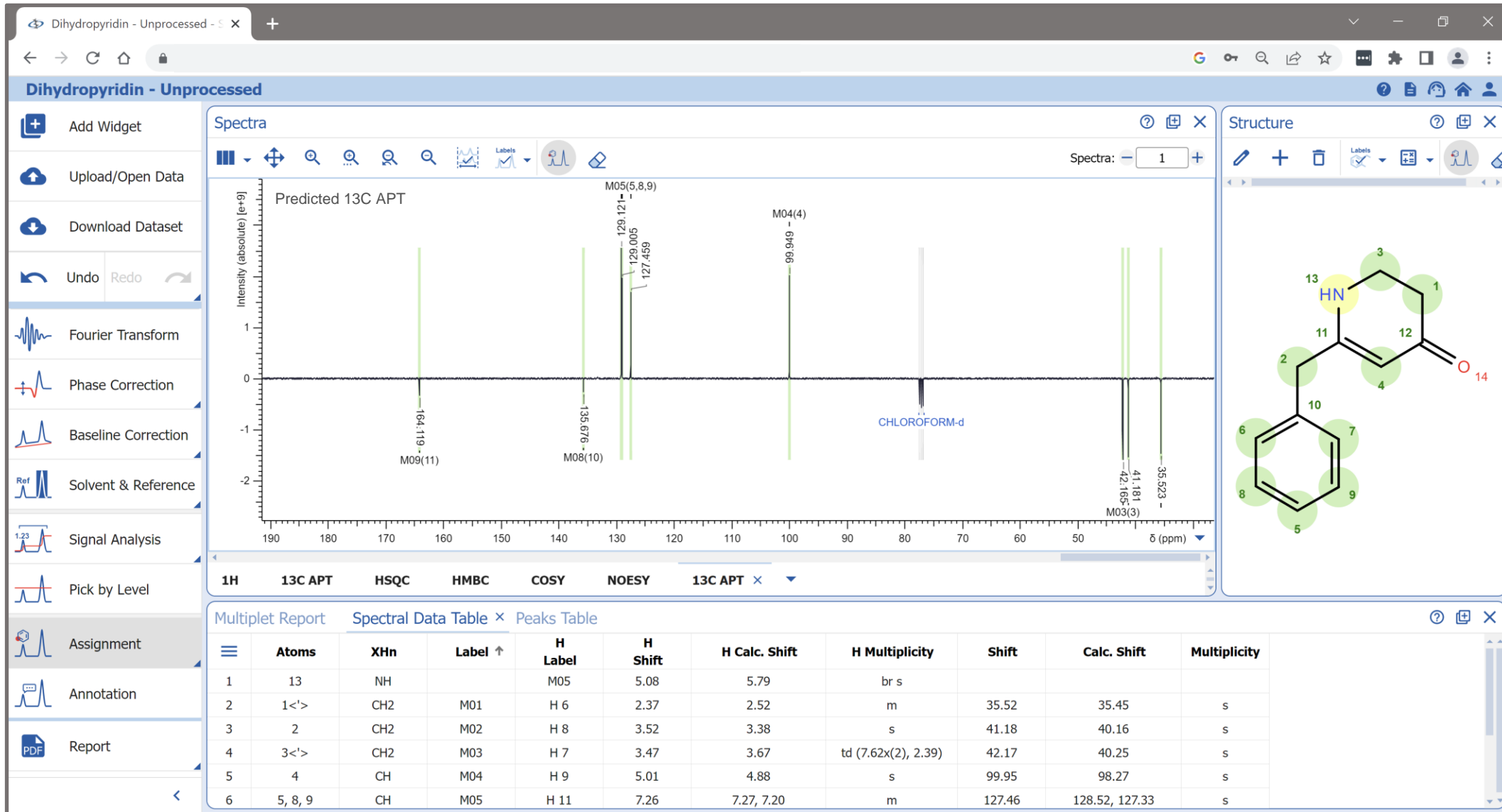
Trivial Name: kendomycin

Ref: J. Nat. Prod.,2020,v.83,p.965(HNMR: HSQC; 600 MHz; 300 K)

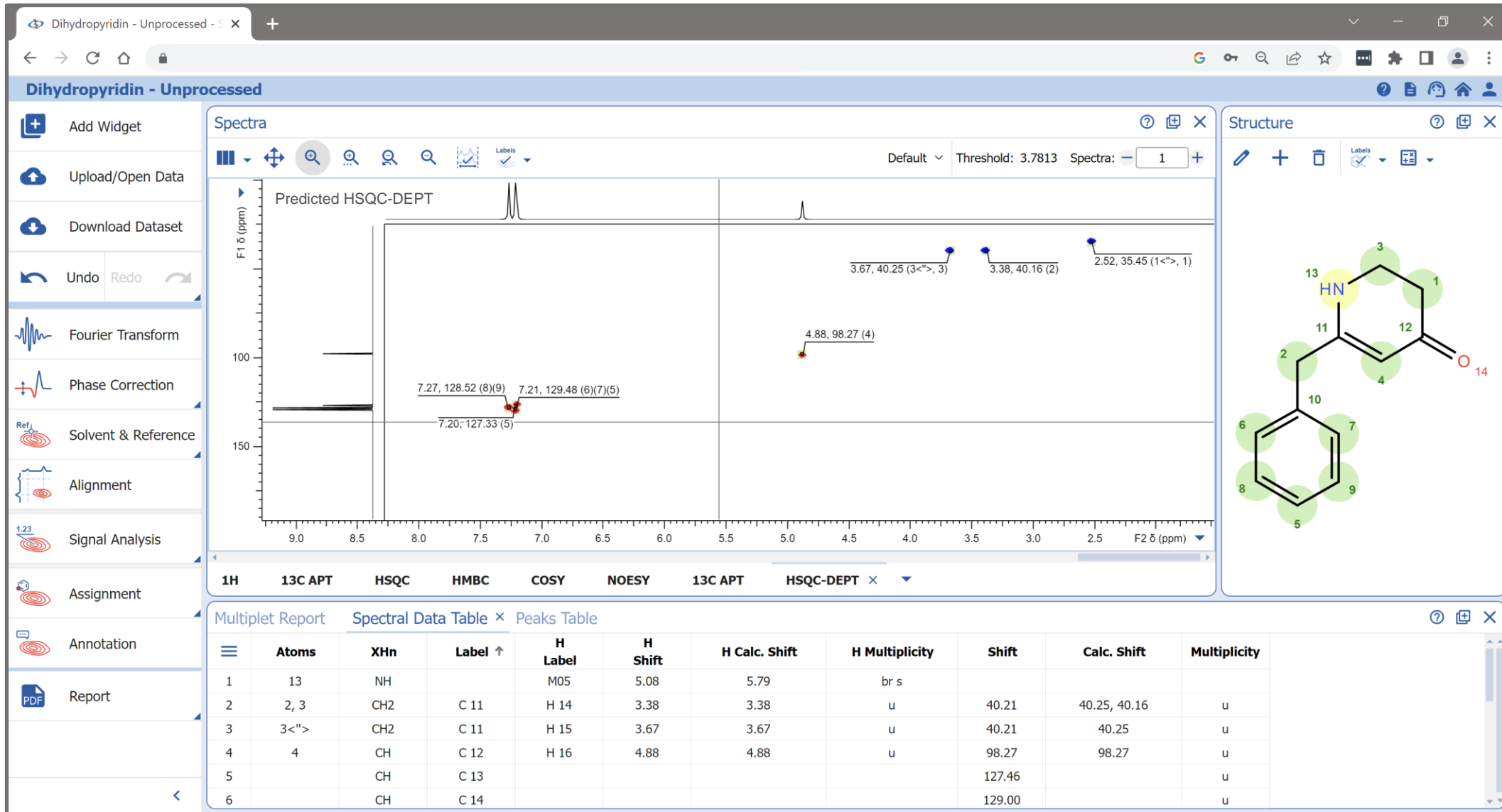
Monoisotopic Mass: 486.298139

[M+H]<sup>+</sup>: 487.305415

# Spectrus JS – Predicted $^{13}\text{C}$ APT

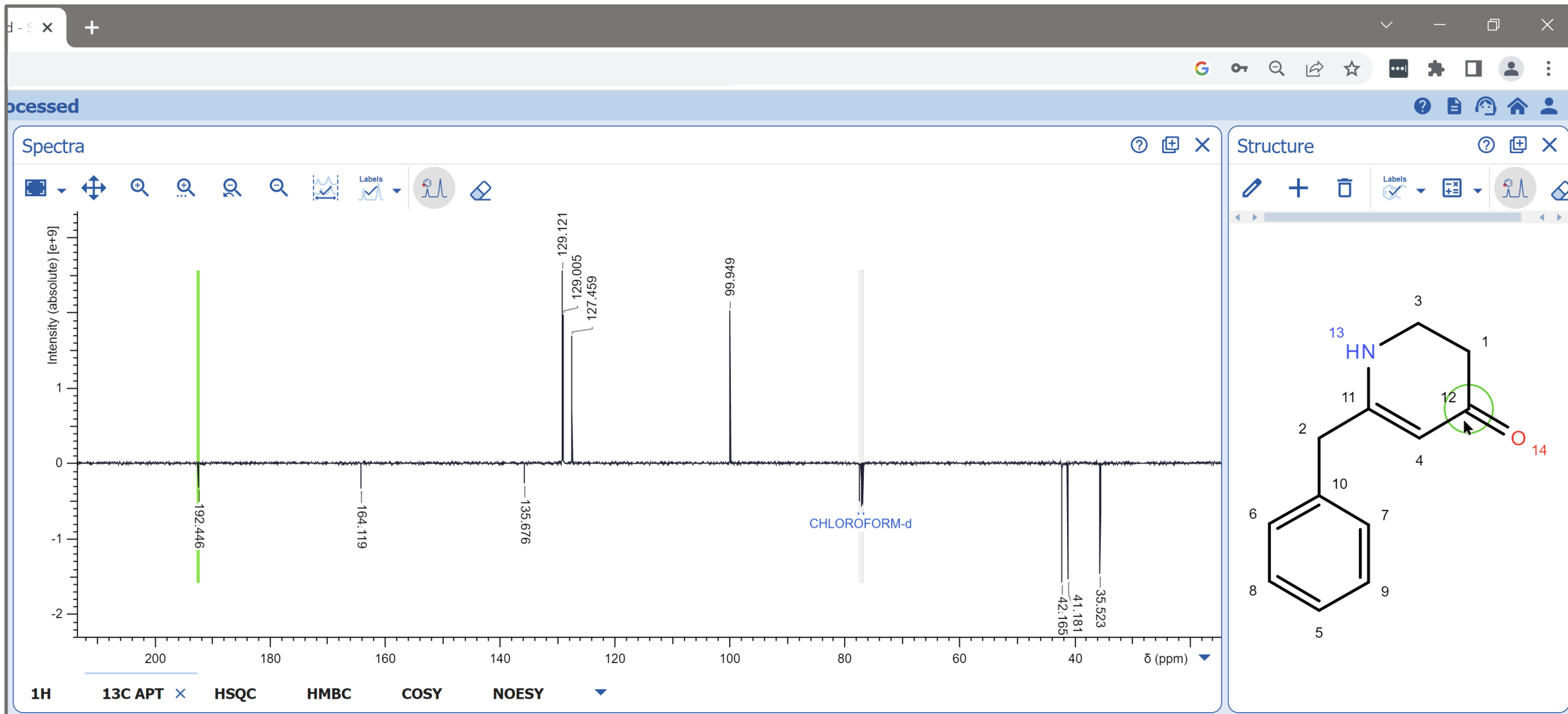


# Spectrus JS – Predicted HSQC-DEPT

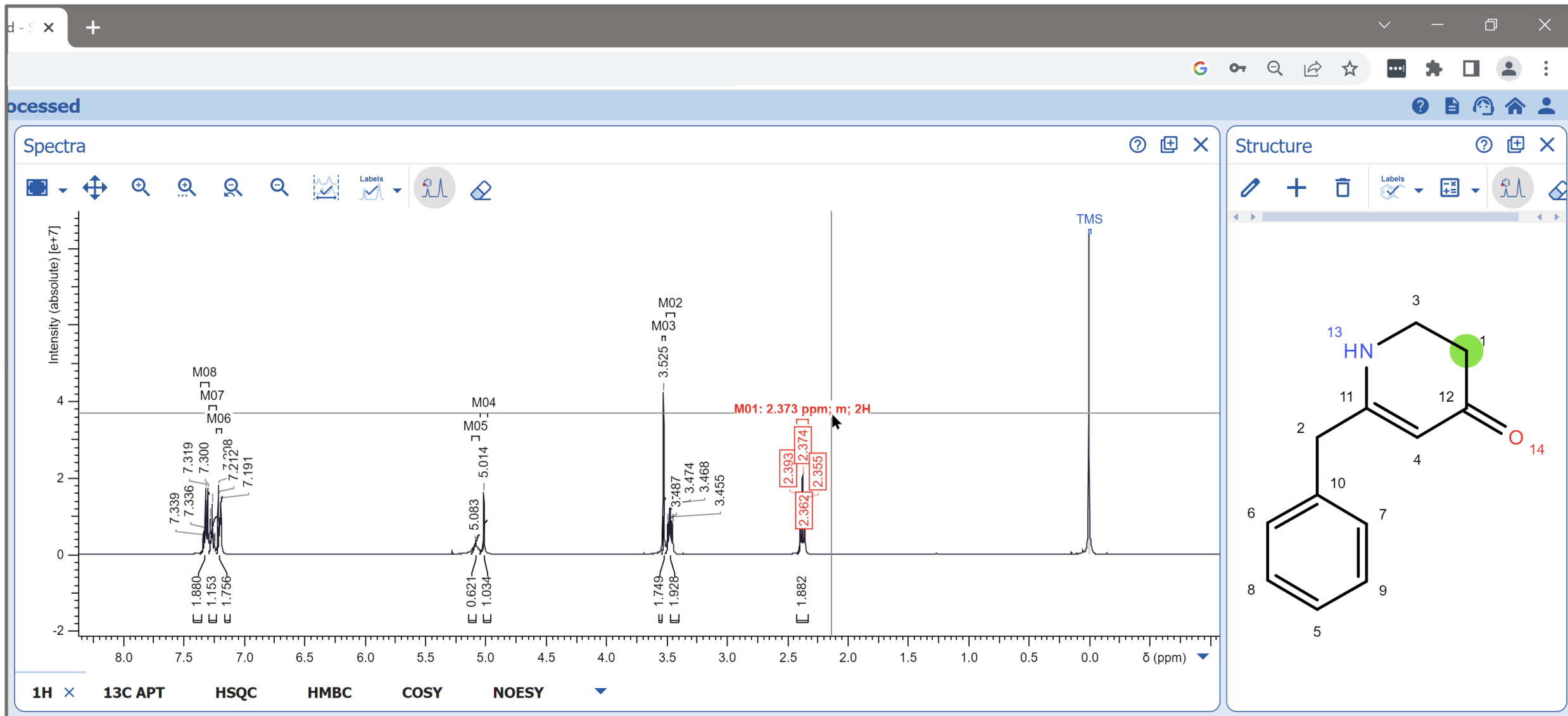




# Spectrus JS – Manual Assignment $^{13}\text{C}$



# Spectrus JS - Manual Assignment $^1\text{H}$



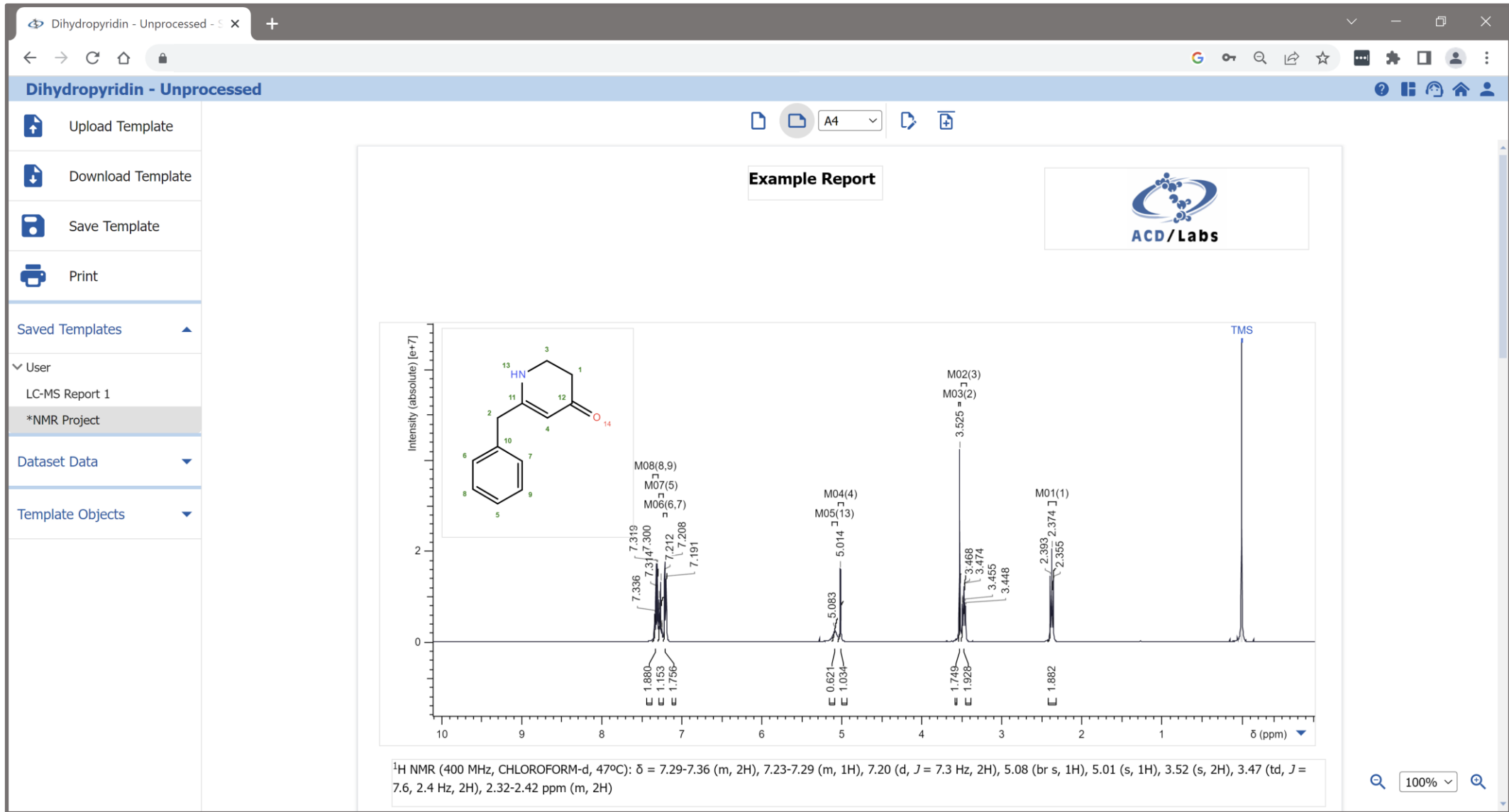
# Spectrus JS – Report Editor

The screenshot displays the Spectrus JS Report Editor interface for a sample named "Dihydropyridin - Unprocessed". The interface is divided into several sections:

- Left Panel:** A vertical toolbar with various processing and analysis tools, including "Add Widget", "Upload/Open Data", "Download Dataset", "Undo/Redo", "Fourier Transform", "Phase Correction", "Baseline Correction", "Solvent & Reference", "Signal Analysis", "Pick by Level", "Assignment", "Annotation", and "Report".
- Center Panel:** A 1D <sup>13</sup>C NMR spectrum plot. The y-axis is labeled "Intensity (absolute) [e+9]" and the x-axis is labeled "δ (ppm)" ranging from 220 to 0. The spectrum shows several peaks, with a prominent one at approximately 130 ppm and another at approximately 77 ppm labeled "CHLOROFORM-d". A peak at 0 ppm is labeled "TMS".
- Right Panel:** A "Structure" panel showing the chemical structure of the compound, which is a dihydropyridin derivative with a benzyl group and a carbonyl group. The structure is shown in a 3D perspective view.
- Bottom Panel:** A "Multiplet Report" section with tabs for "Multiplet Report", "Spectral Data Table", and "Peaks Table". The text below the tabs reads: "<sup>13</sup>C NMR (101 MHz, CHLOROFORM-d, 47°C): δ =".

Two blue document icons are highlighted with black boxes. One icon is located in the top right corner of the interface, and the other is located in the center of the spectrum plot area. A black arrow points from the top-right icon to the center icon.

# Spectrus JS - Report Editor



# Spectrus JS – Summary

- Compatible with every operating system and browser
- Intuitive interface
- Easy to operate for both 1D and 2D NMR processing
- Prediction of 1D and 2D NMR experiments
- Effortless report generation

[Click here for a free trial version.](#)

Questions?

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