# Spectrus JS

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# Spectrus JS – Overview

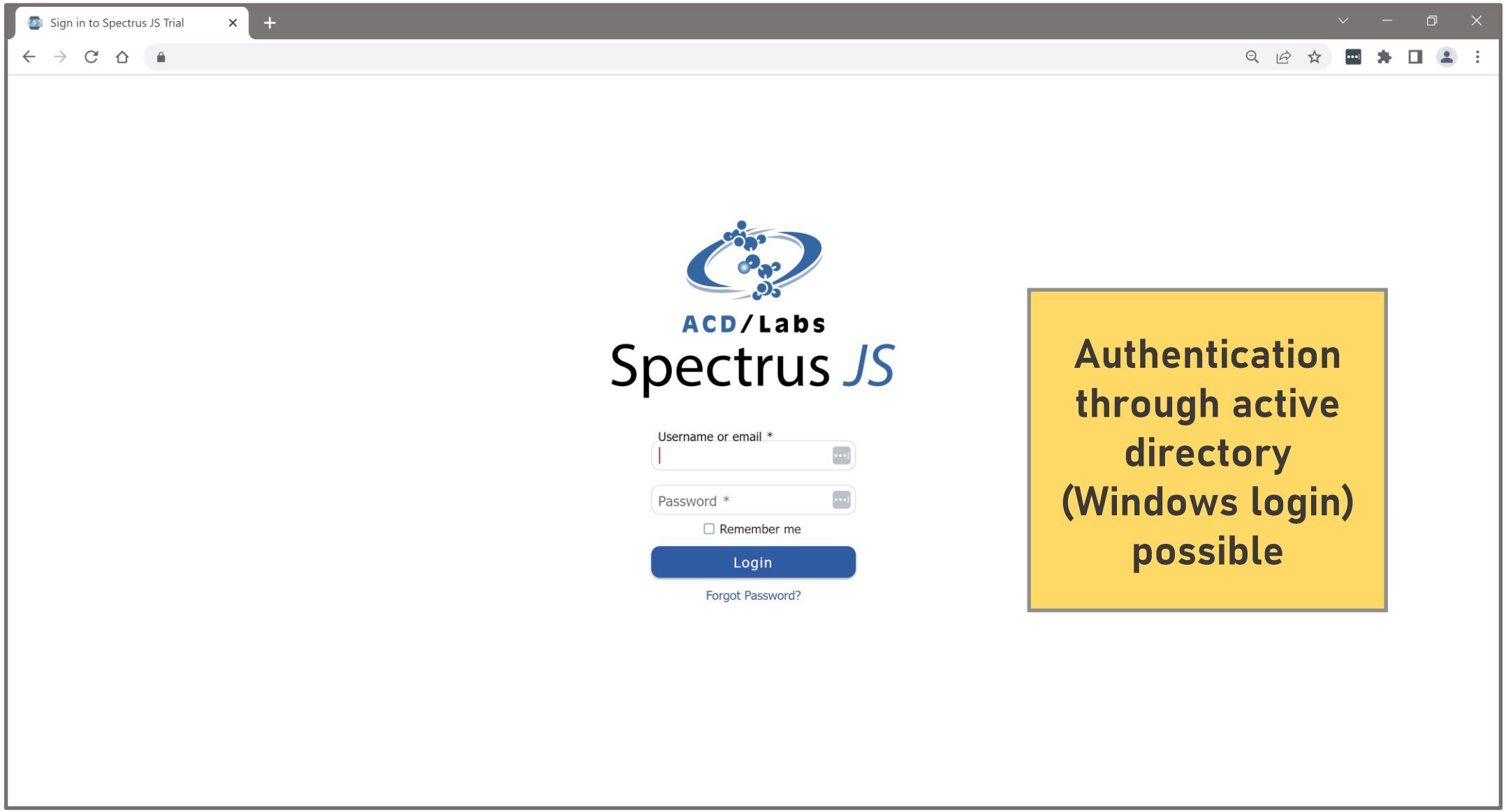
- Browser-based NMR processing software developed by ACD/Labs
- The NMR analyst only requires a web browser and access to the internet
- Hosted on your organizational intranet or (private) cloud
- For individual users, there is no need to perform installation and/or software updates
- Data pick-up from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





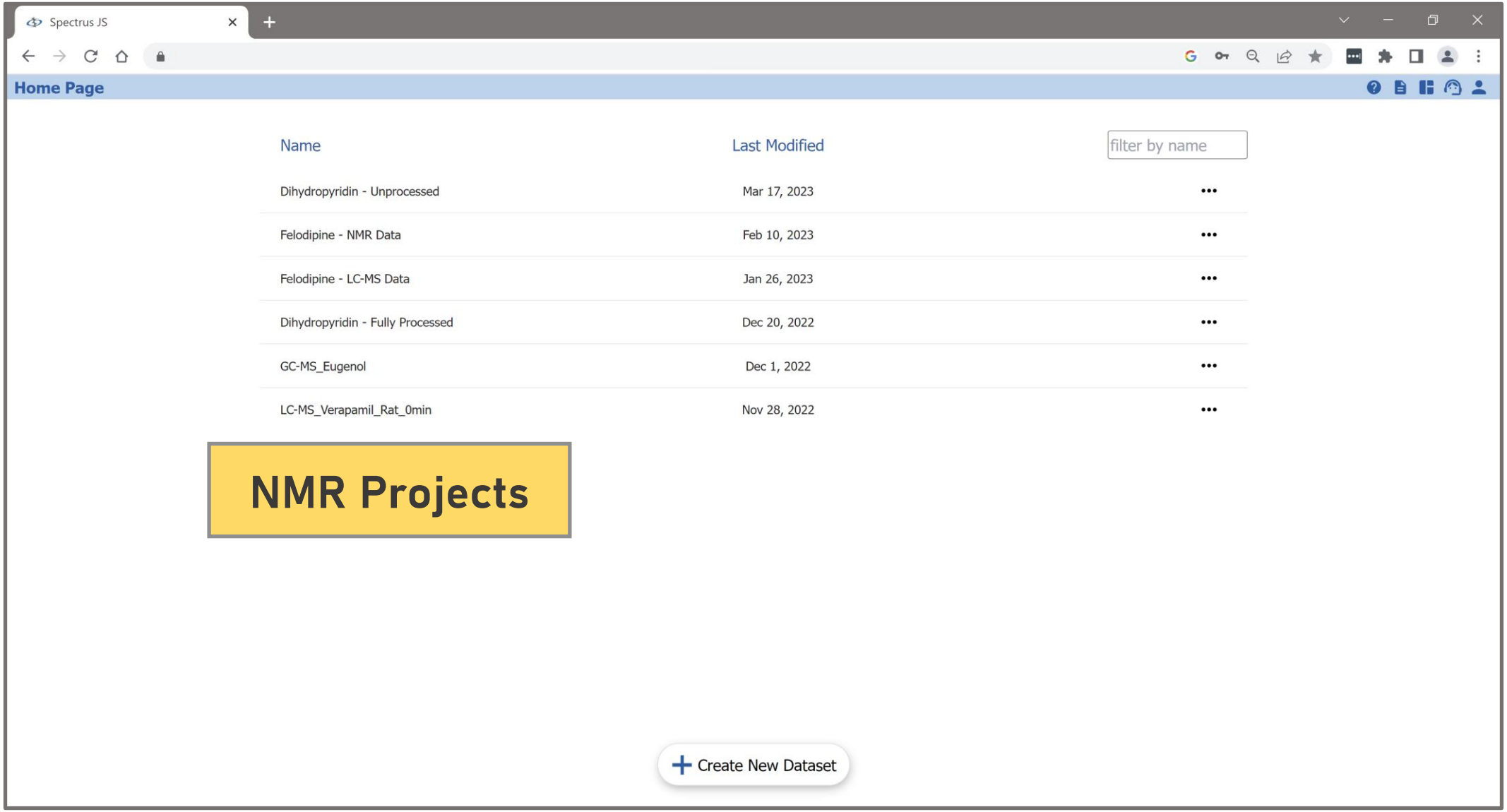


# Spectrus JS – Home Page




**Authentication through active directory (Windows login) possible**

# Spectrus JS – Home Page

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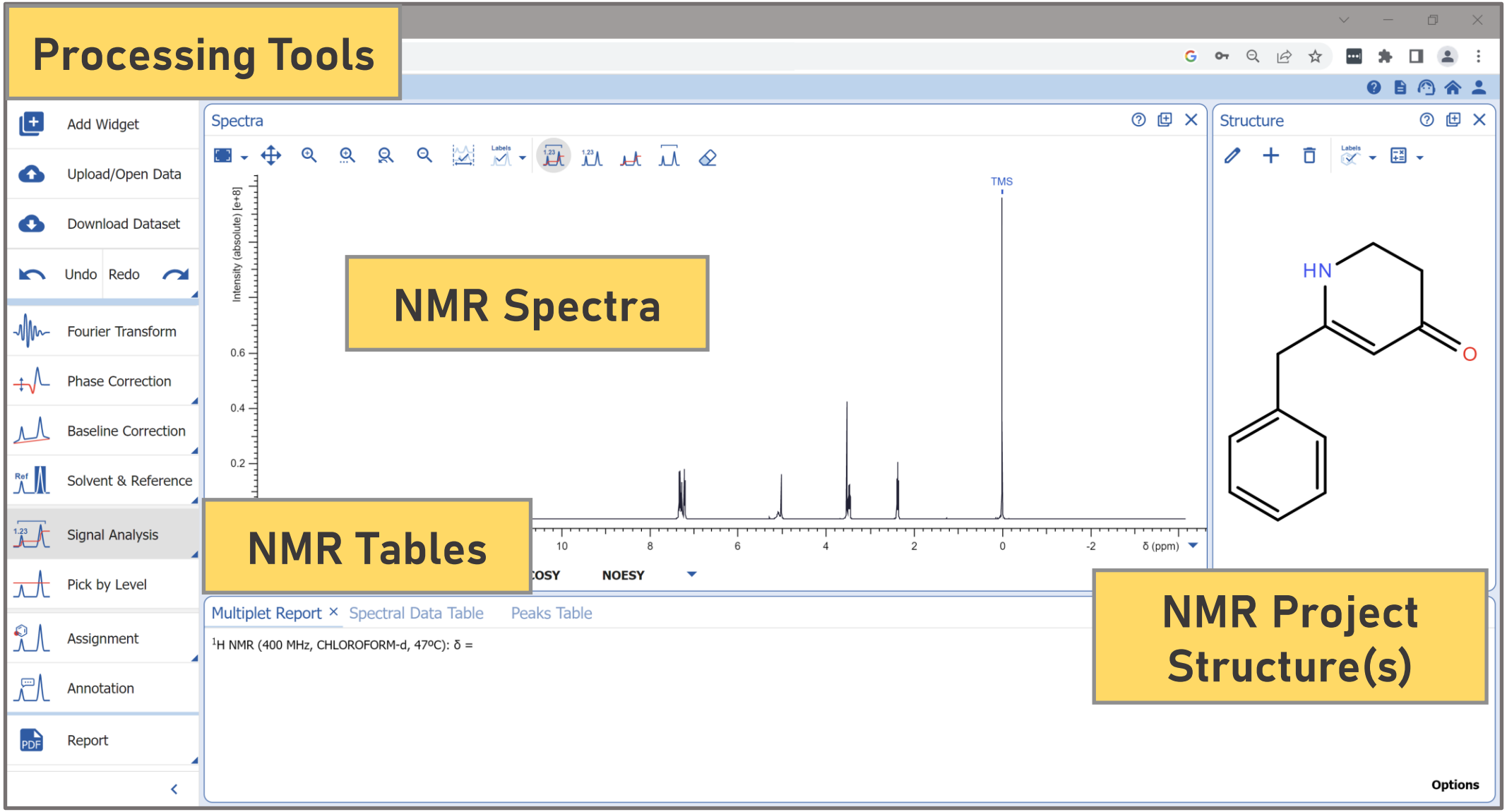
# Spectrus JS – Dashboard

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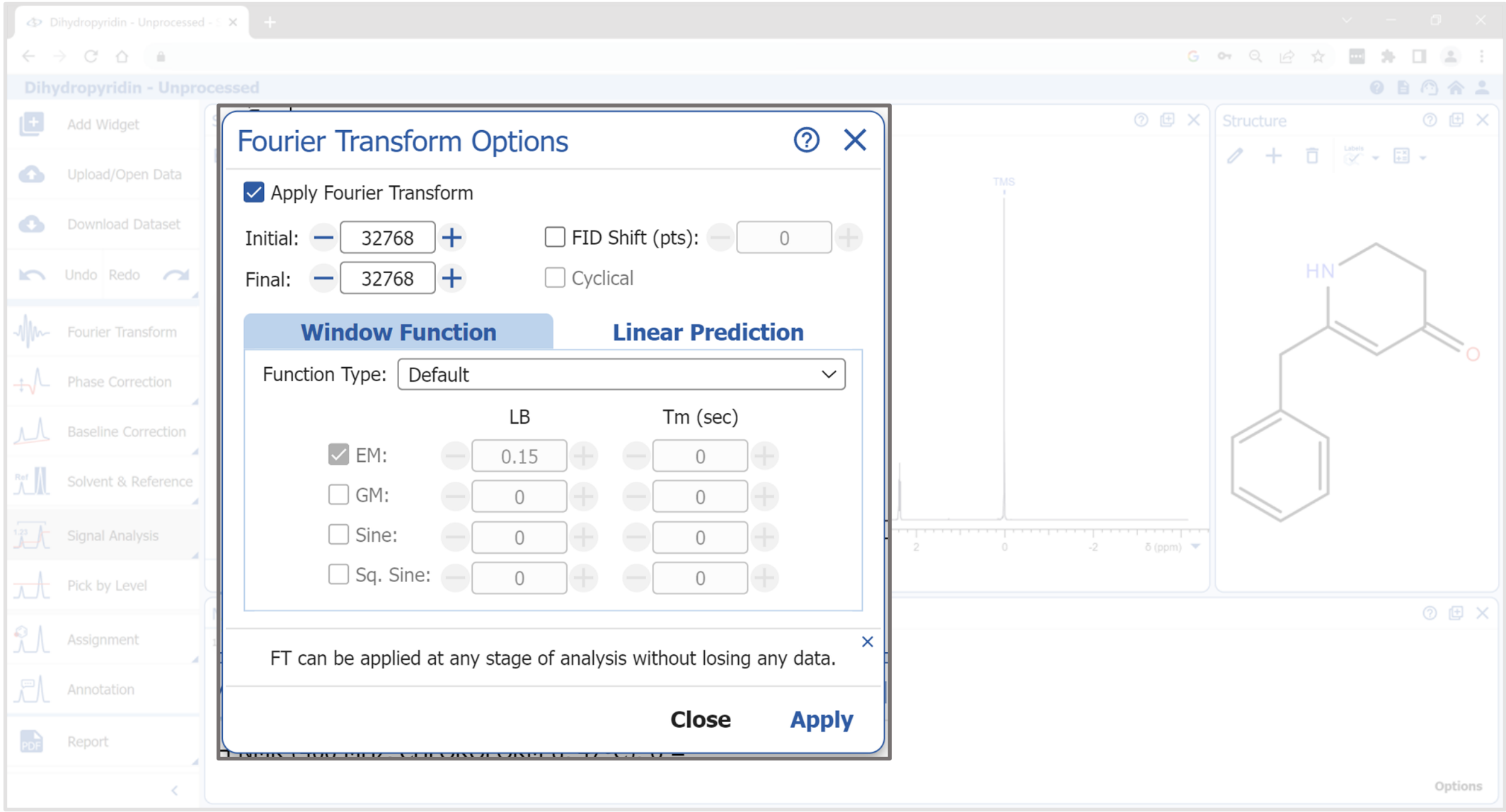
# Spectrus JS – Fourier Transformation Options

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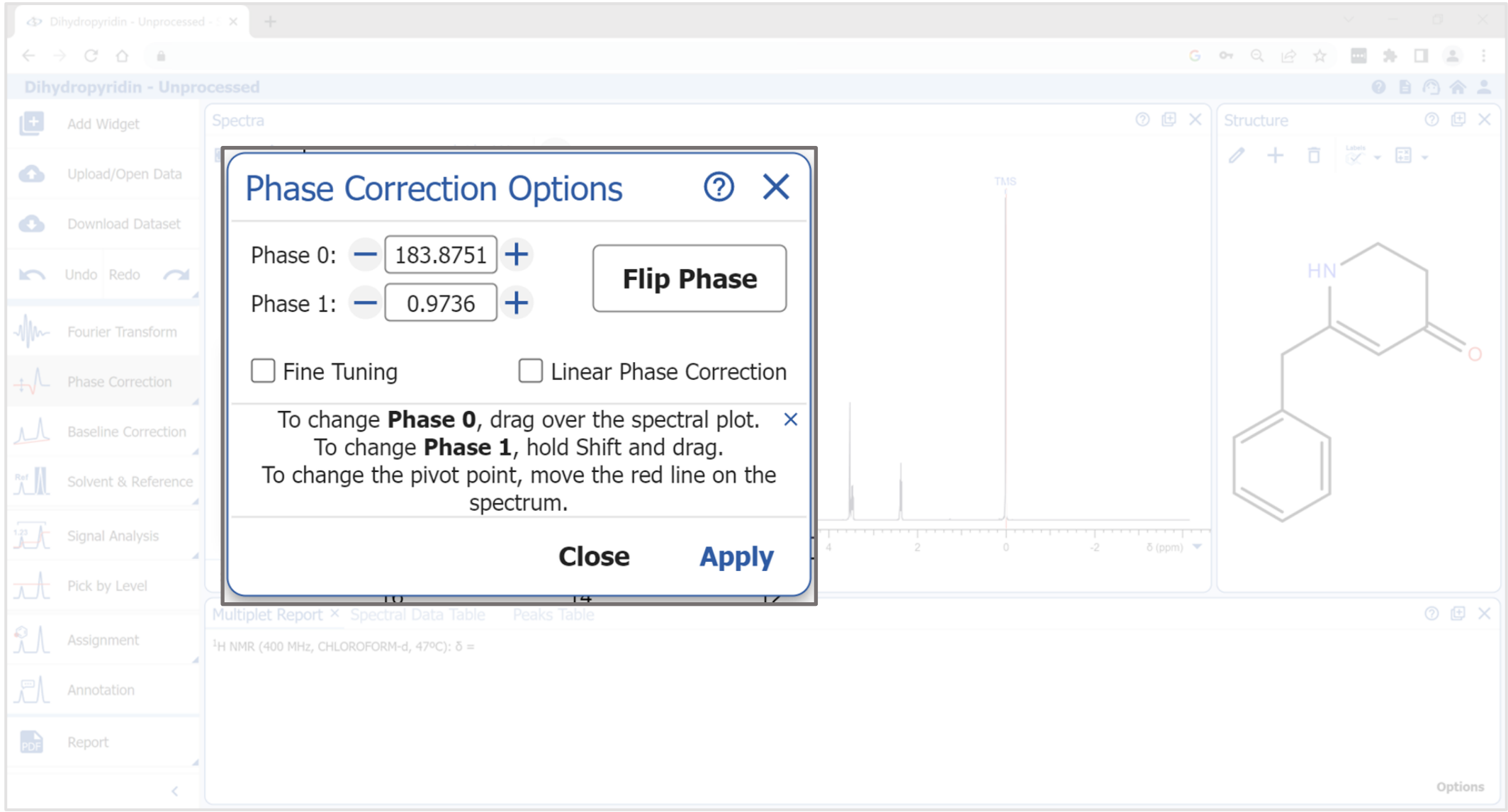
# Spectrus JS – Phase Correction Options

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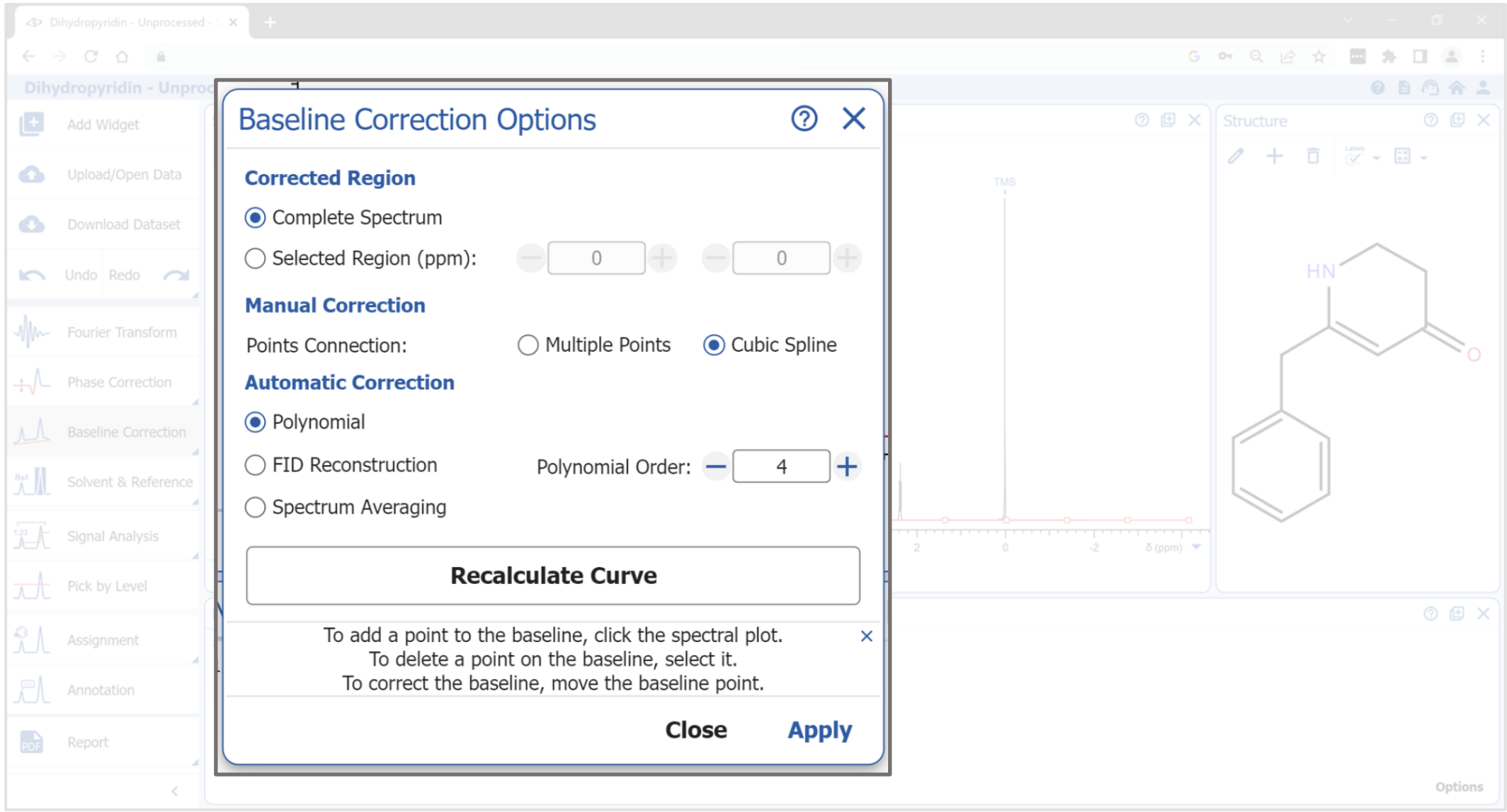
# Spectrus JS – Baseline Correction Options

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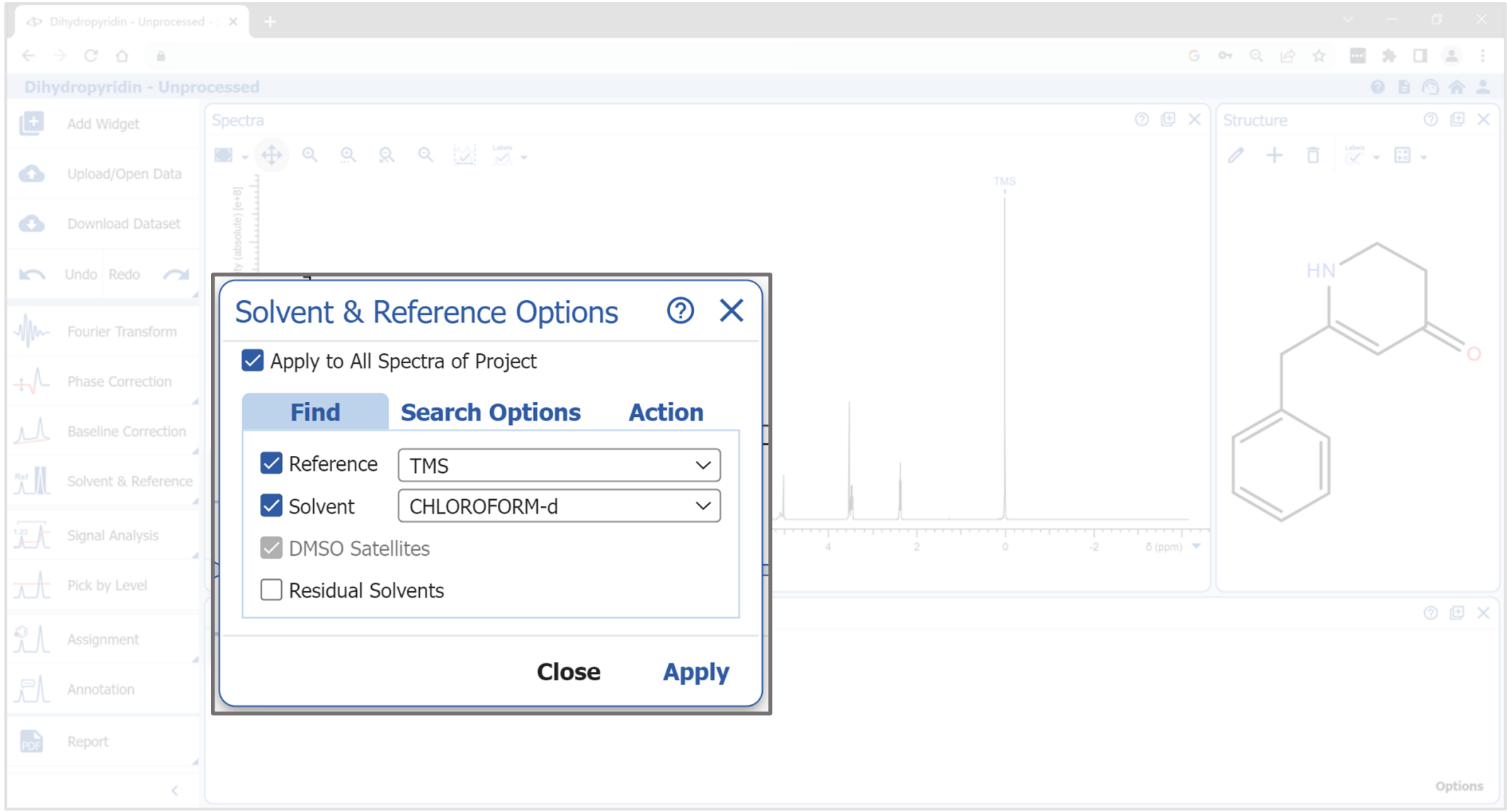
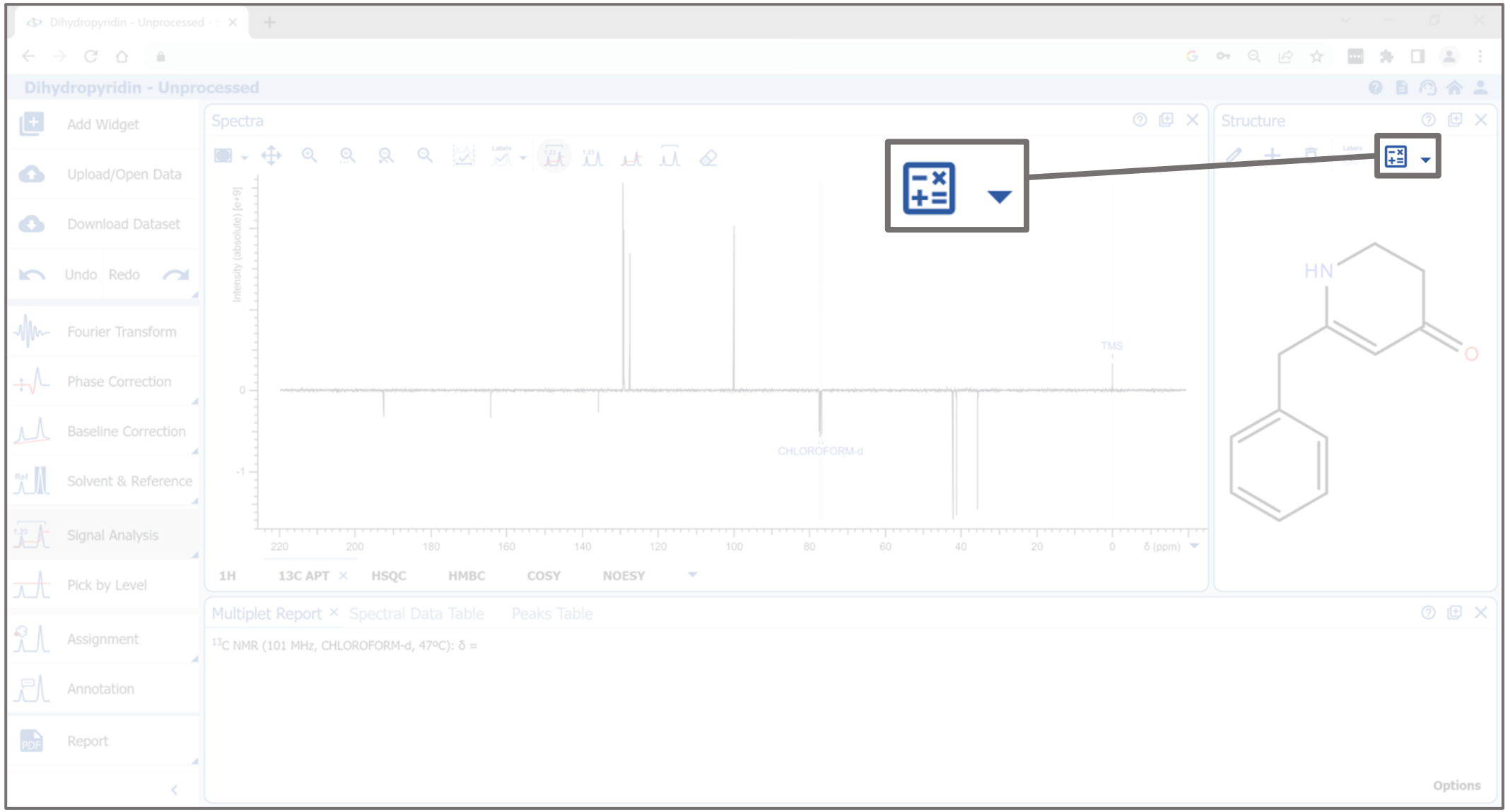
# Spectrus JS – Solvent and Referencing Options



# Spectrus JS – Spectrum Prediction

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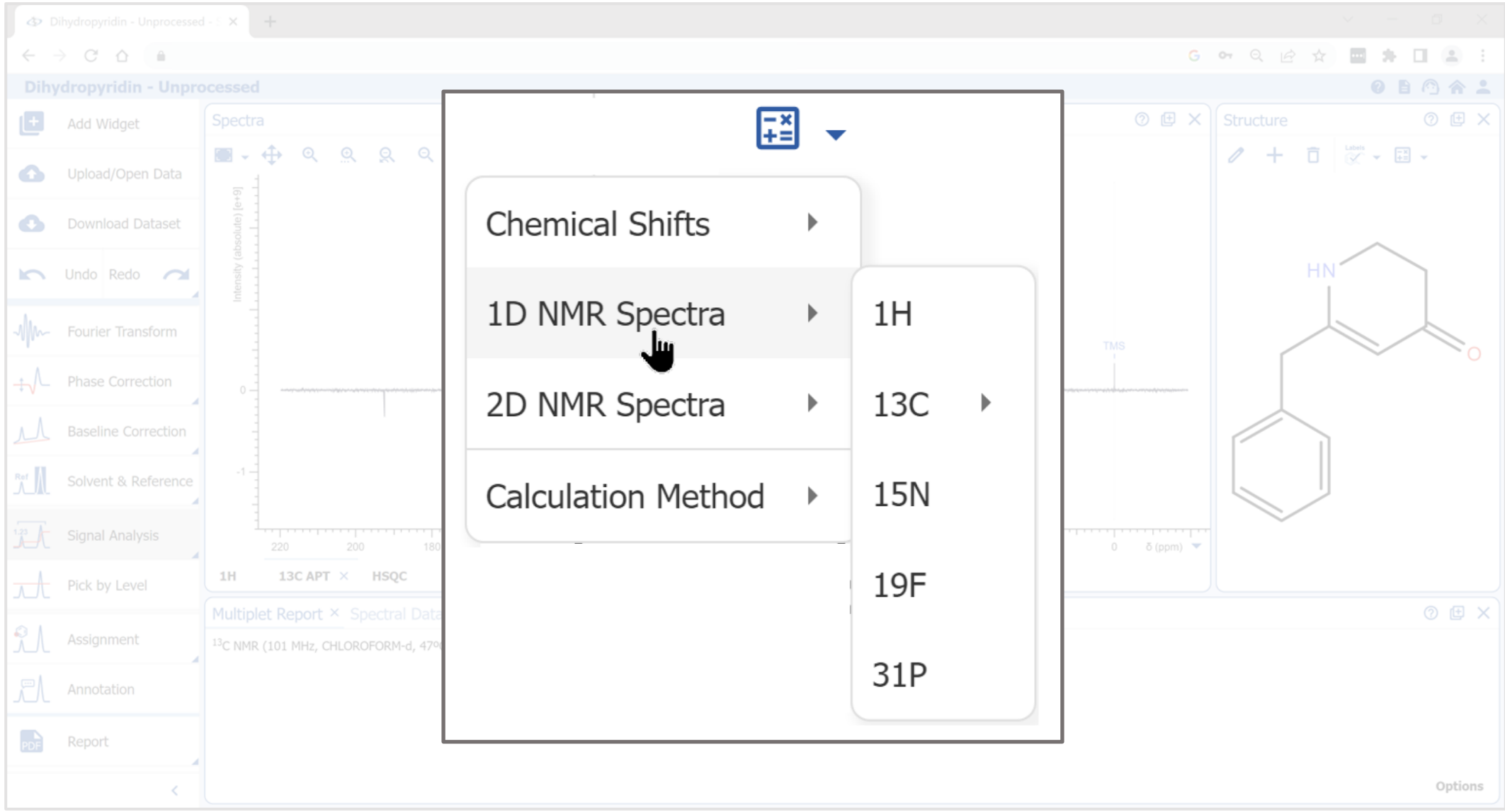
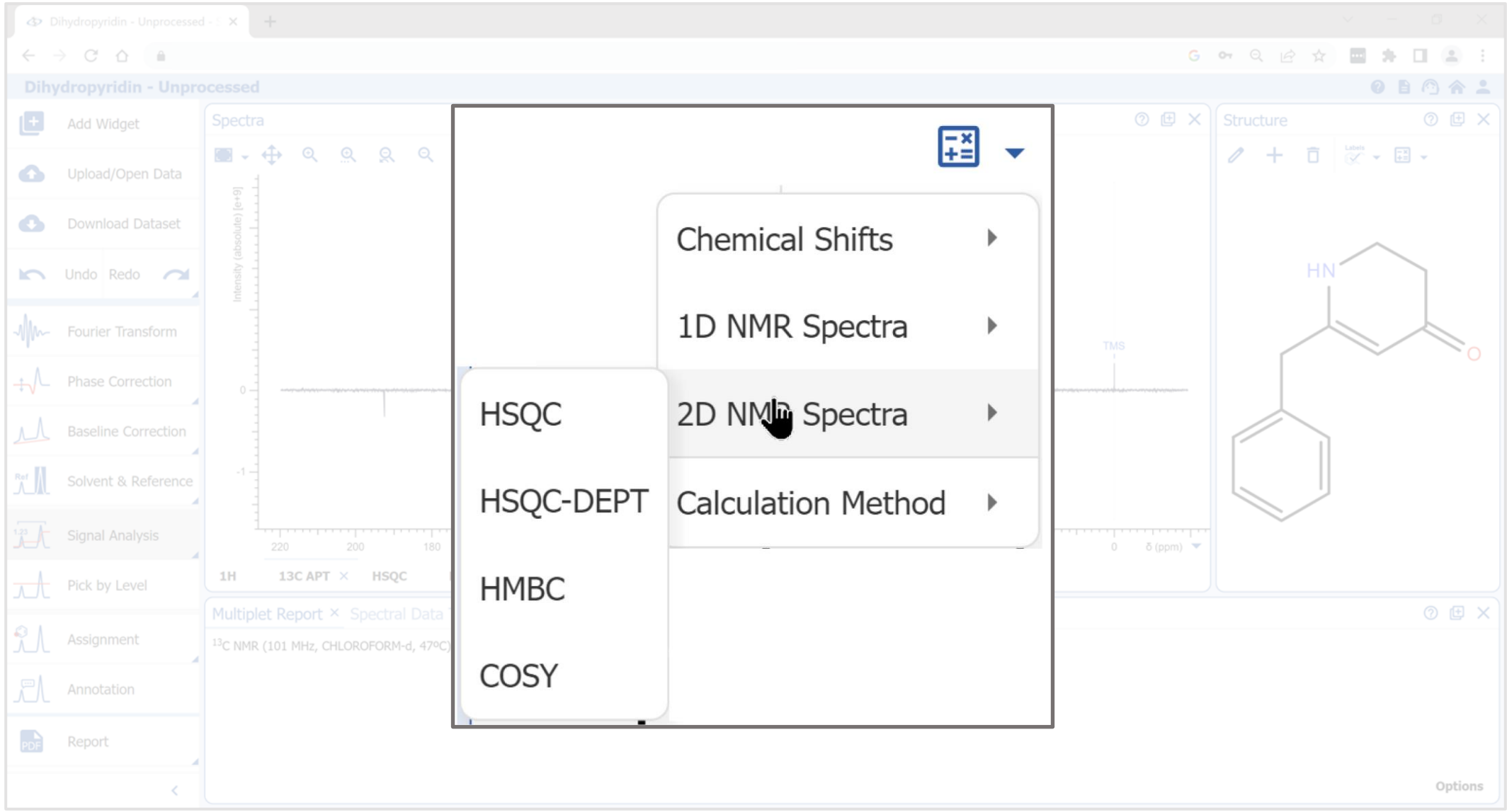
# Spectrus JS – 1D NMR Predictions



# Spectrus JS – 2D NMR Predictions

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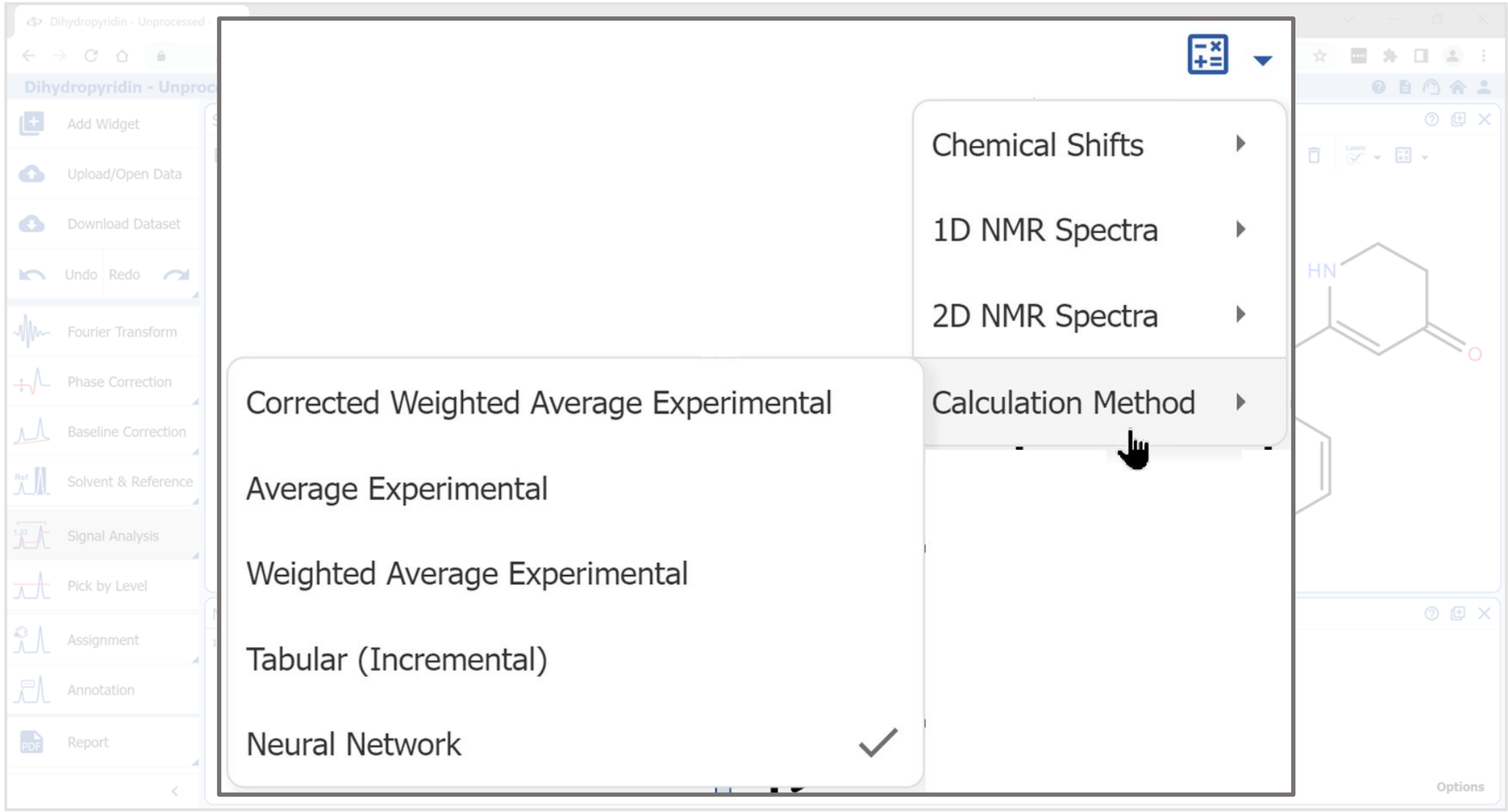
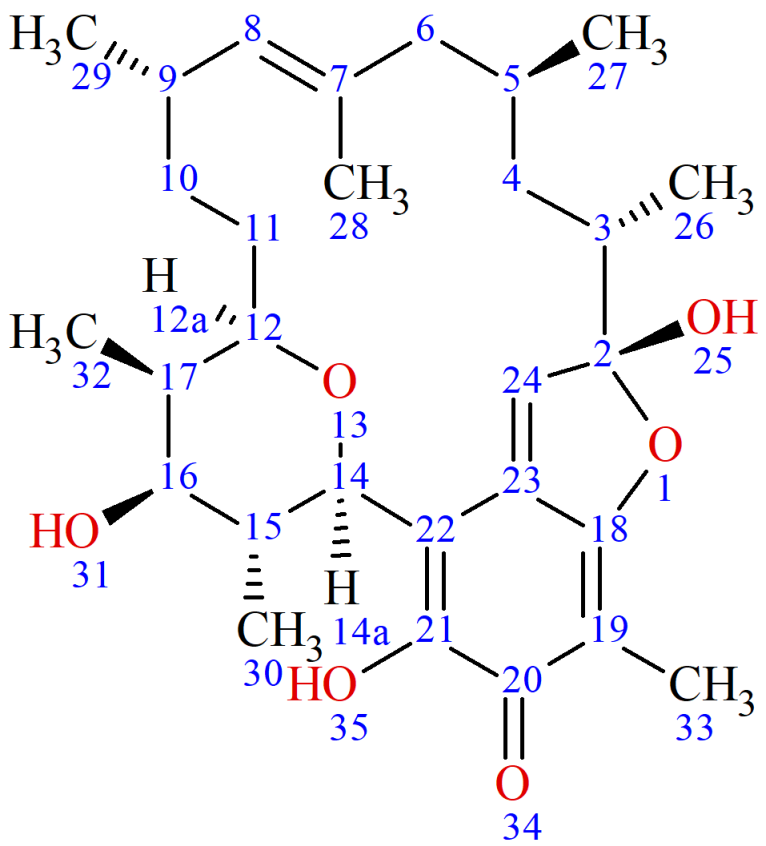
# Spectrus JS – Prediction Algorithms



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




Internal databse with $^{1}H$ and $^{13}C$ data of ~300k structures

| Atom No. | 1H 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: $C_{29}H_{42}O_6$

FW: 486.6402

Name: (1*R*,9*S*,10*S*,12*S*,14*E*,16*S*,19*R*,20*R*,21*S*,22*R*)-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]+: 487.305415

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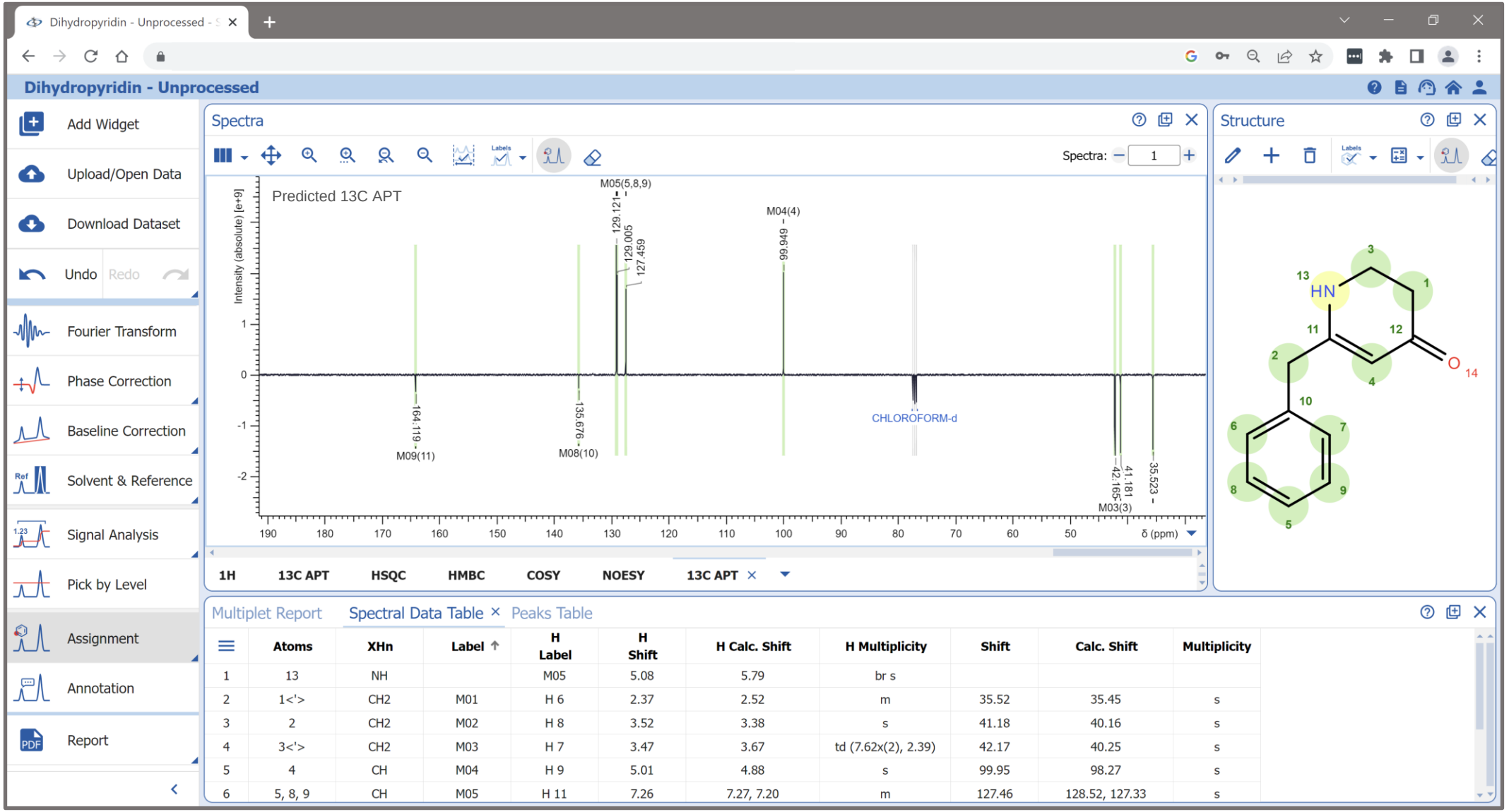
# Spectrus JS – Predicted $^{13}$C APT




| | Atoms | XHn | Label | H Label | H Shift | H Calc. Shift | H Multiplicity | Shift | Calc. Shift | Multiplicity |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 13 | NH | | M05 | 5.08 | 5.79 | br s | | | |
| 2 | 1<'> | CH2 | M01 | H 6 | 2.37 | 2.52 | m | 35.52 | 35.45 | s |
| 3 | 2 | CH2 | M02 | H 8 | 3.52 | 3.38 | s | 41.18 | 40.16 | s |
| 4 | 3<'> | CH2 | M03 | H 7 | 3.47 | 3.67 | td (7.62x(2), 2.39) | 42.17 | 40.25 | s |
| 5 | 4 | CH | M04 | H 9 | 5.01 | 4.88 | s | 99.95 | 98.27 | s |
| 6 | 5, 8, 9 | CH | M05 | H 11 | 7.26 | 7.27, 7.20 | m | 127.46 | 128.52, 127.33 | s |

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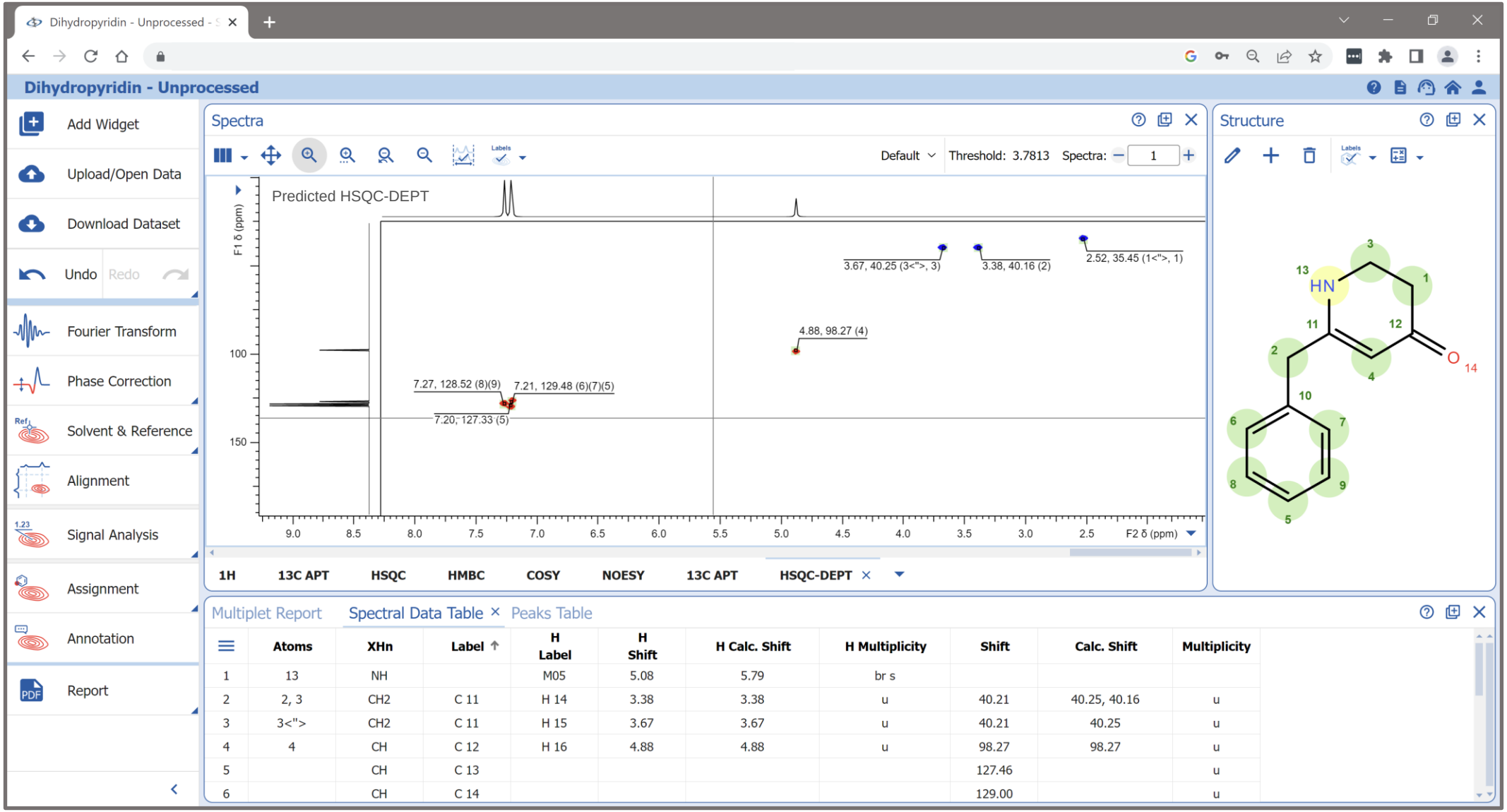
# Spectrus JS – Predicted HSQC-DEPT




| | Atoms | XHn | Label | H Label | H Shift | H Calc. Shift | H Multiplicity | Shift | Calc. Shift | Multiplicity |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 13 | NH | | M05 | 5.08 | 5.79 | br s | | | |
| 2 | 2, 3 | CH2 | C 11 | H 14 | 3.38 | 3.38 | u | 40.21 | 40.25, 40.16 | u |
| 3 | 3<"> | CH2 | C 11 | H 15 | 3.67 | 3.67 | u | 40.21 | 40.25 | u |
| 4 | 4 | CH | C 12 | H 16 | 4.88 | 4.88 | u | 98.27 | 98.27 | u |
| 5 | | CH | C 13 | | | | | 127.46 | | u |
| 6 | | CH | C 14 | | | | | 129.00 | | u |

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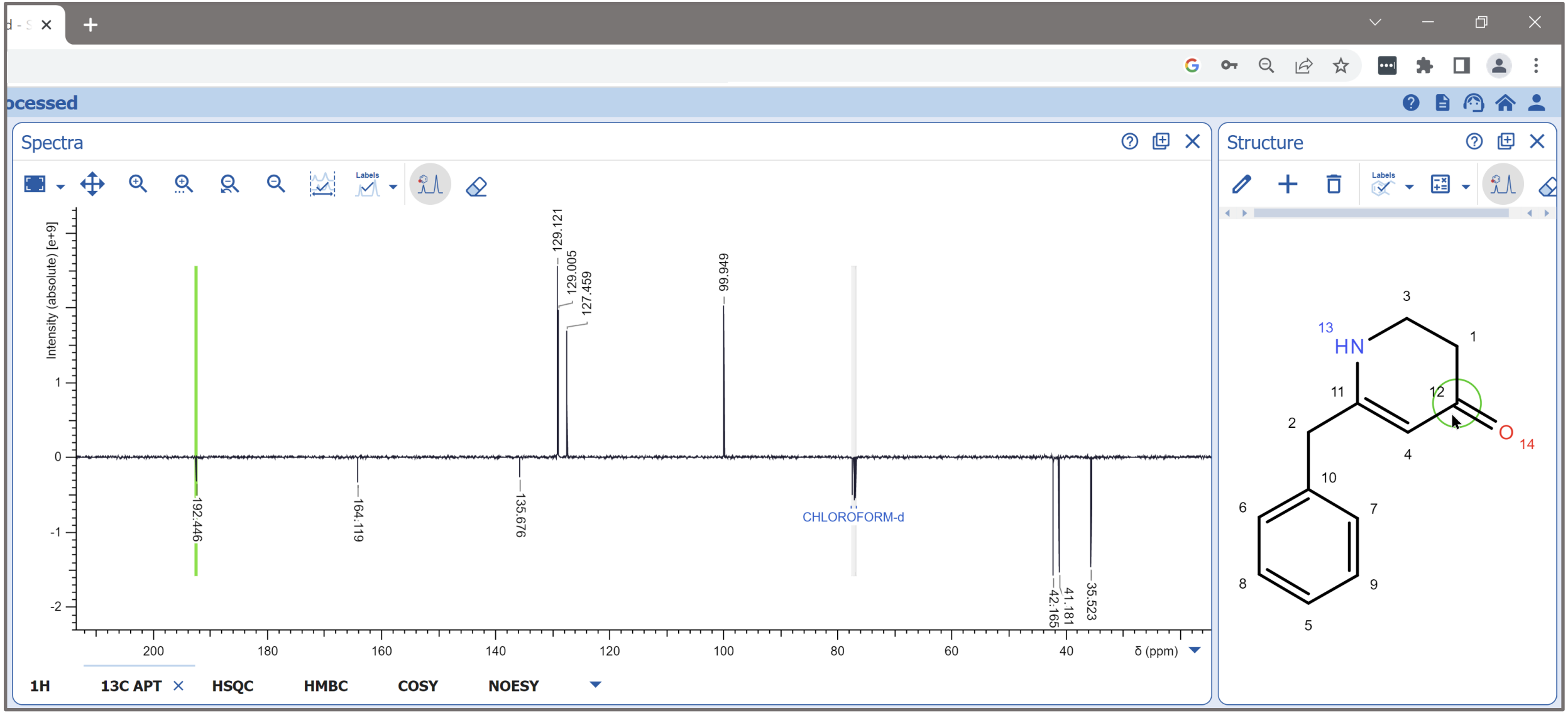
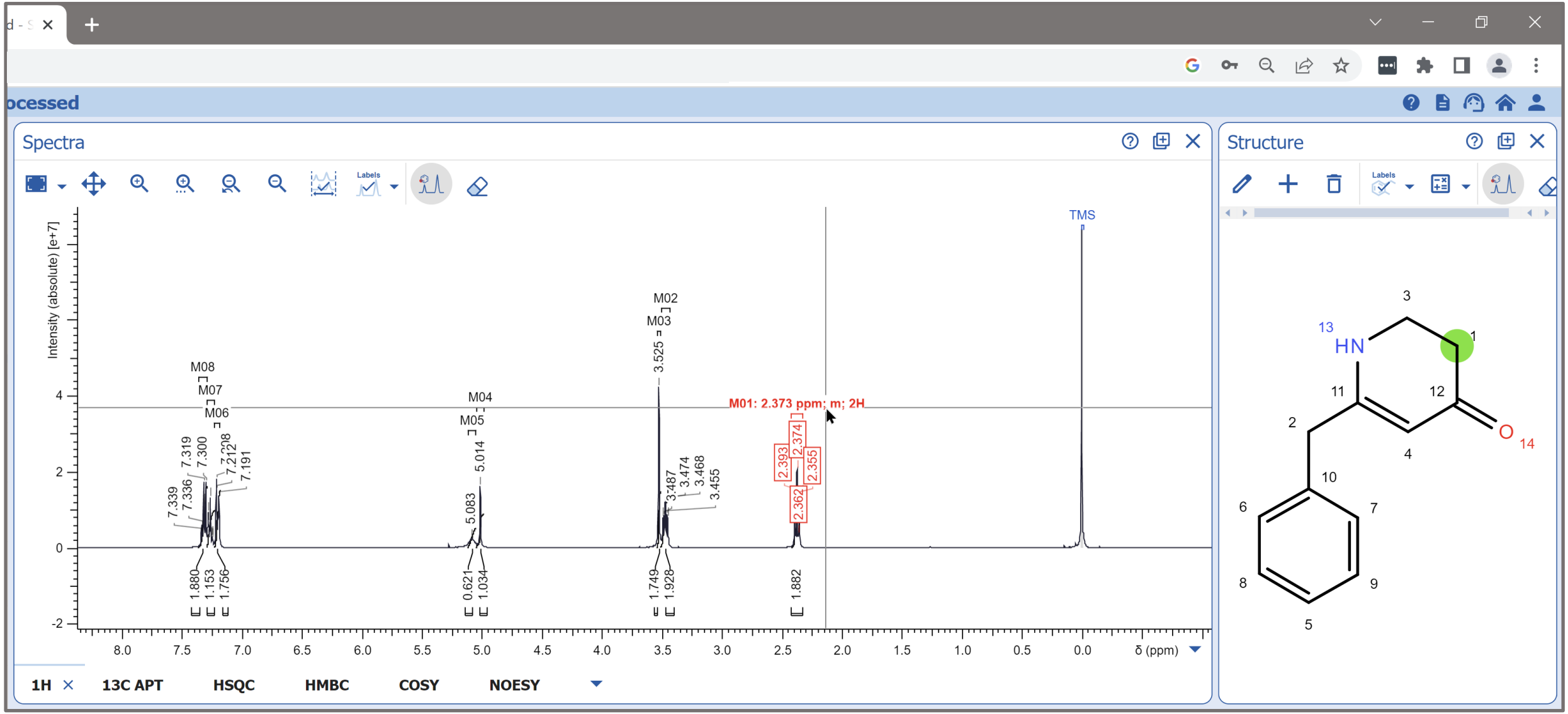
# Spectrus JS – Manual Assignment $^{13}C$



# Spectrus JS – Manual Assignment $^{1}H$

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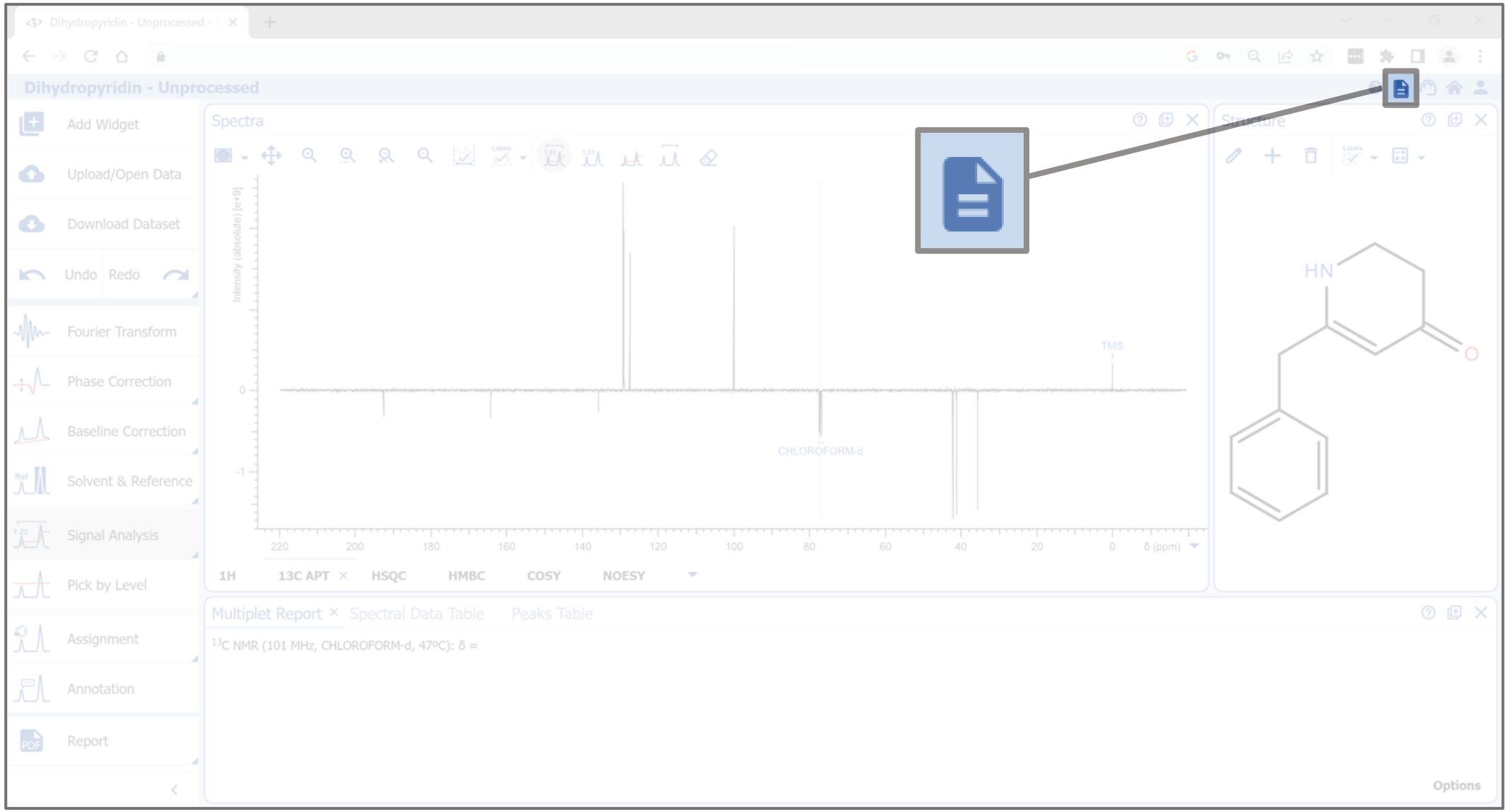
# Spectrus JS – Report Editor

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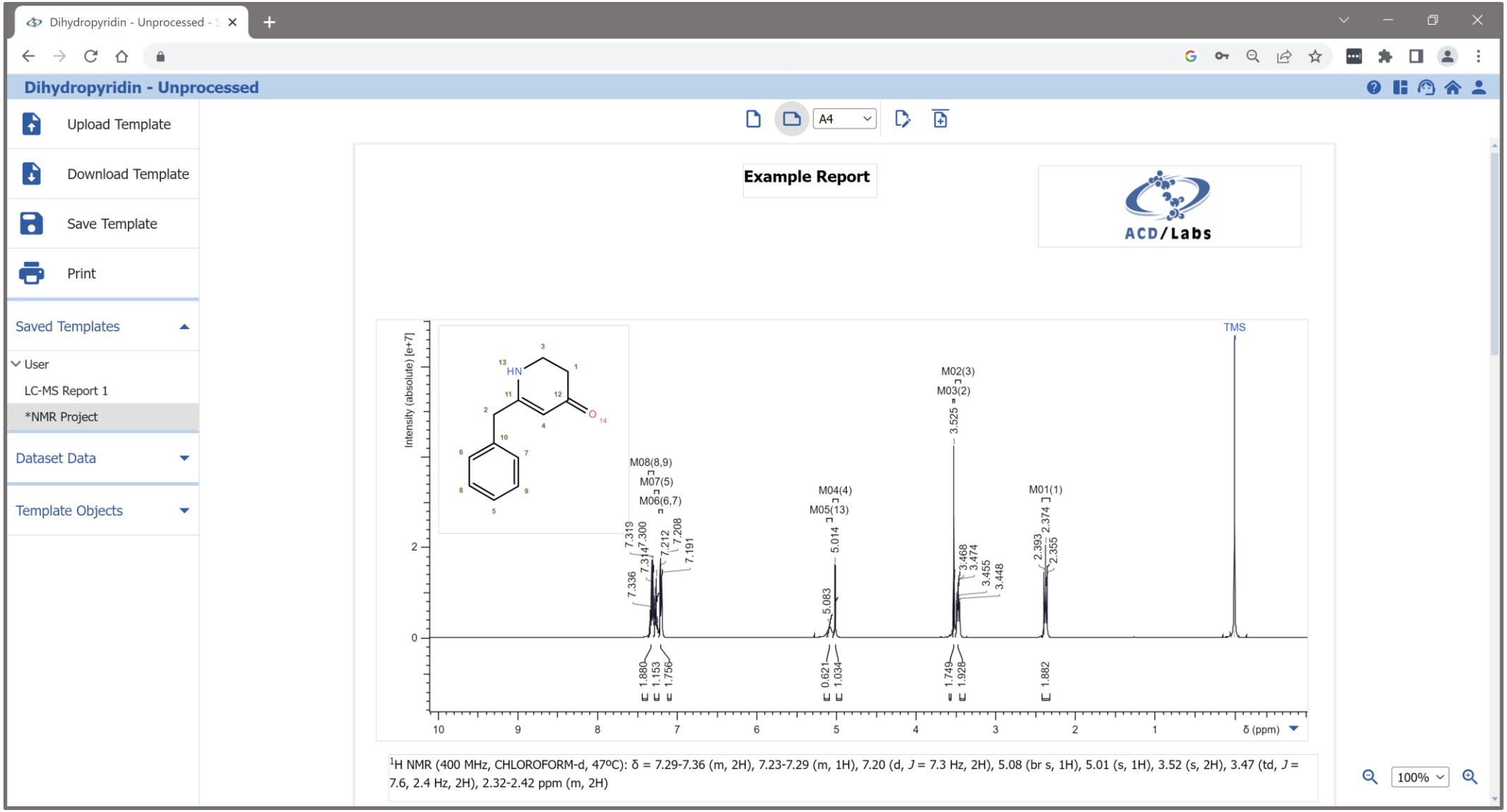
# Spectrus JS – Report Editor



# 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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