



Coupling Assignment and Improved Multiplet Analysis for 1D Spectra

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Advanced Chemistry Development, Inc. (ACD / Labs)

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Coupling Constants

Why?

Multiplet
Analysis

Coupling
Assignment

Automatic

Manual

Tables

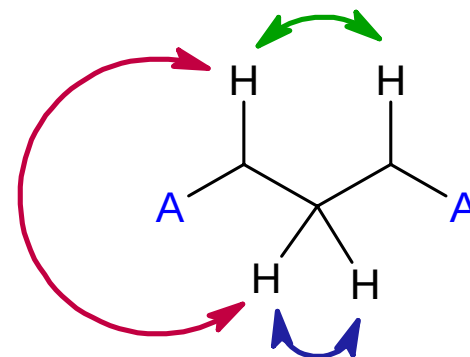
Visualizations

Summary



Useful for:

- Matching against predicted
- Showing spin systems
- Guiding assignment or contributing to the match factor



We now take advantage of this information

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Specific New Features

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- Improved Multiplet Analysis
 - Obtains and uses more coupling constants for a more accurate result
- Assign coupled multiplets
- Use of coupling values in match factor
- Showing couplings on the structure

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Improved Multiplet Analysis

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- Resolve overlapping multiplets
- Correctly identify coupling in the presence of small impurities

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Improved Multiplet Analysis

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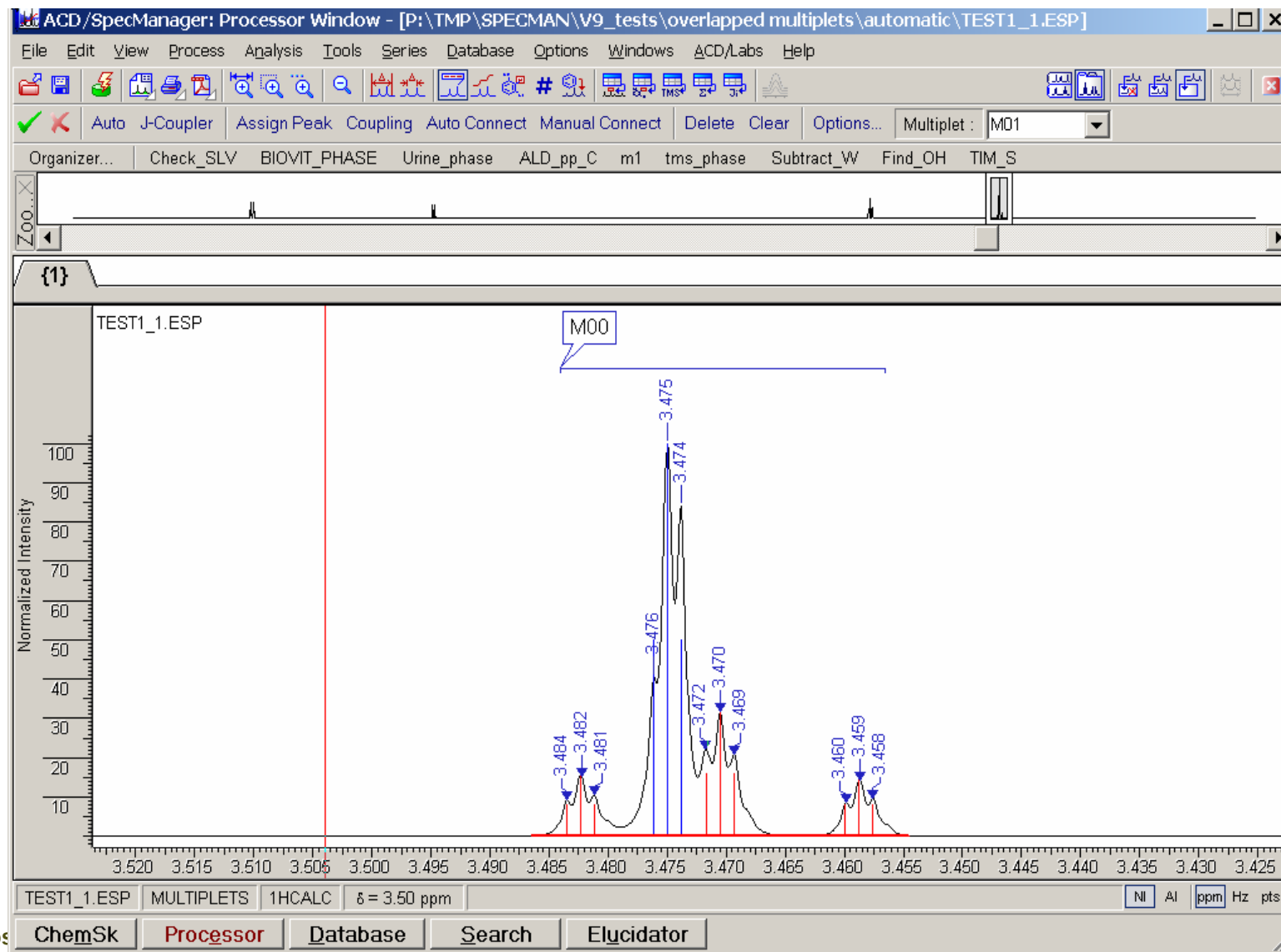
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Improved Multiplet Analysis

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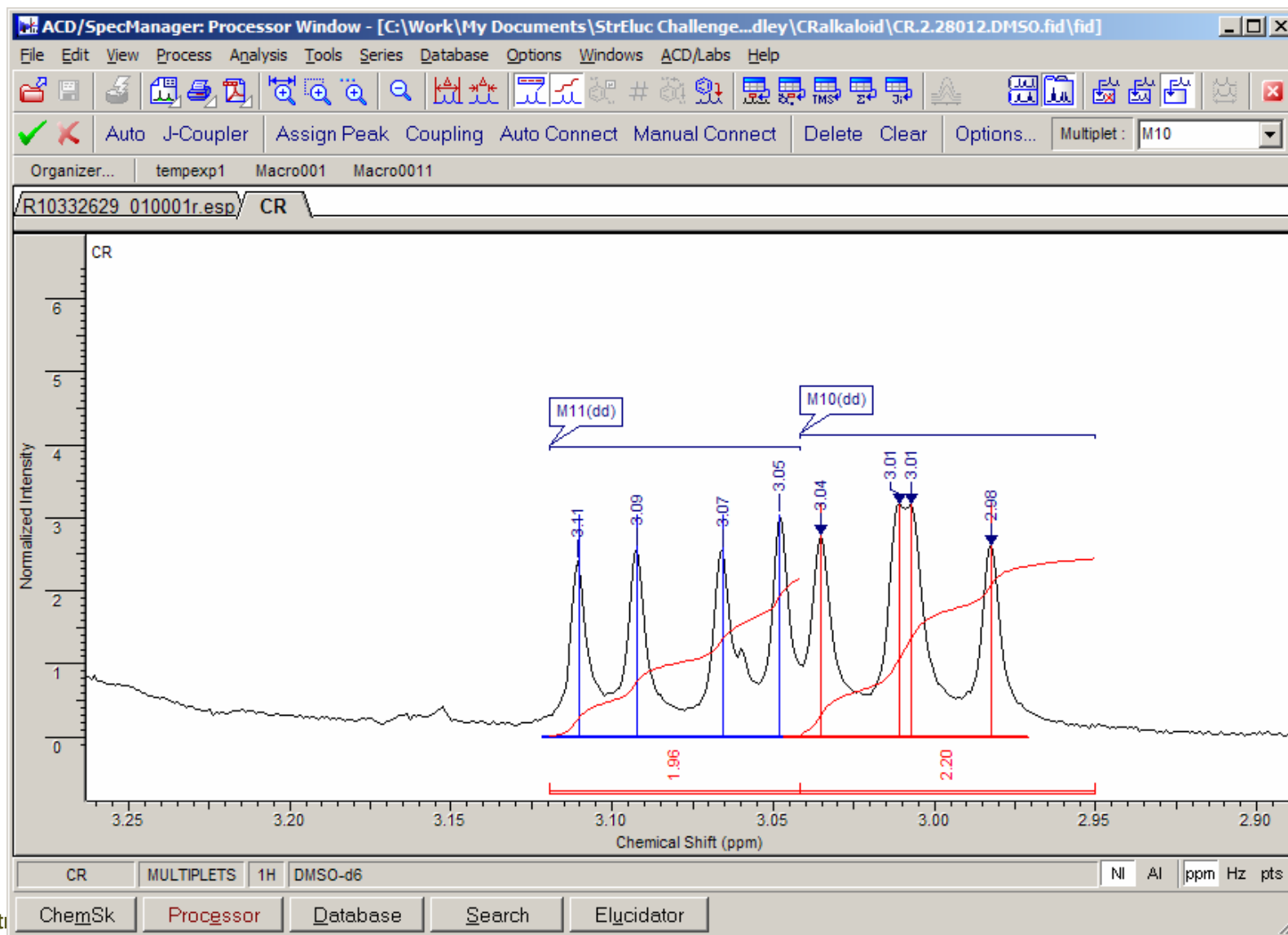
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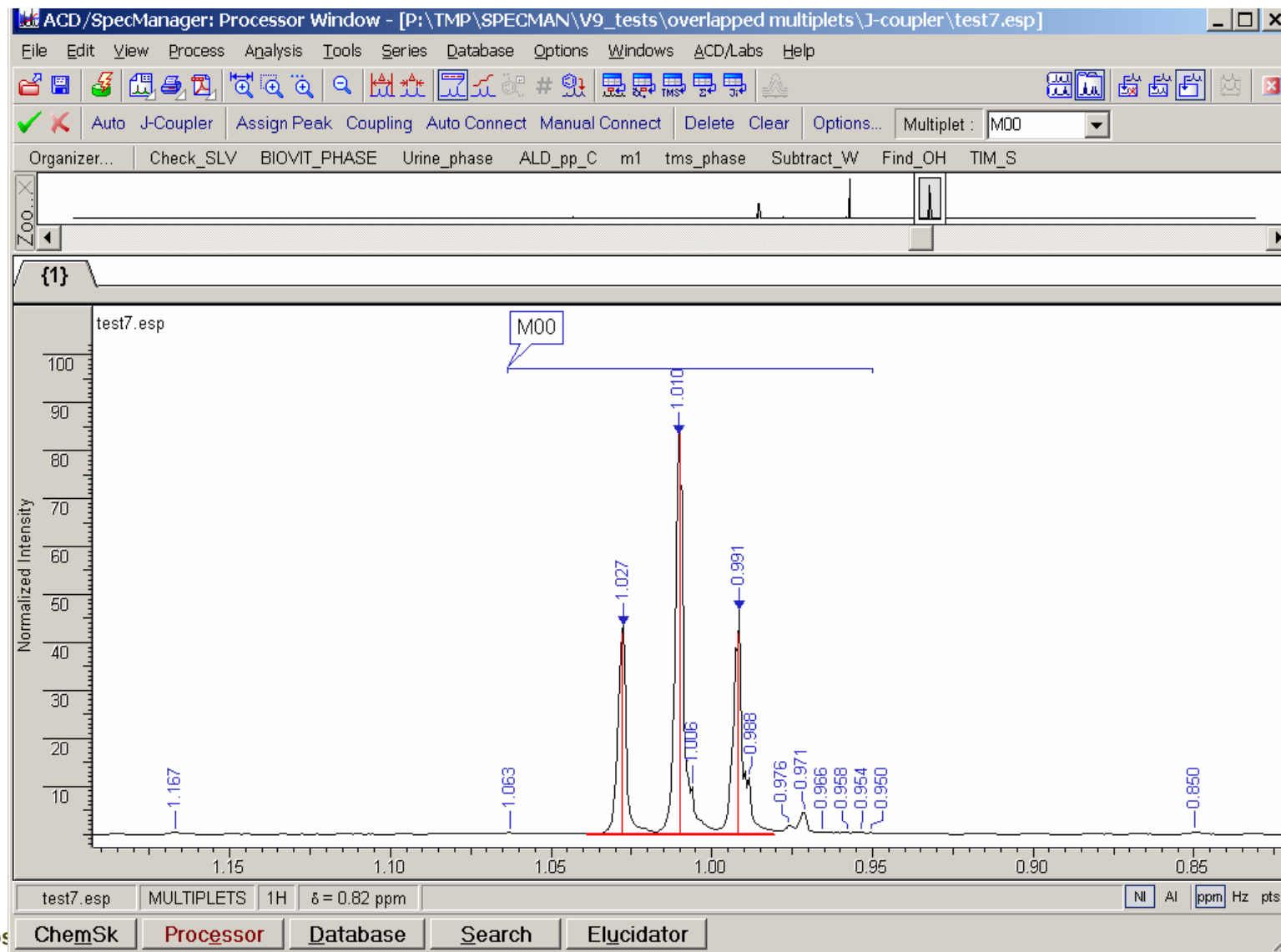
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Improved Multiplet Analysis

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- 🌀 More intelligent coupling detection
- 🌀 Extract more coupling constants
- 🌀 Identify more multiplets

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Coupled Multiplets

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- 🌀 Coupling assignment can be done:
 - 🌀 Automatically
 - 🌀 Manually
- 🌀 Flexible in both modes
 - 🌀 Assign either way
- 🌀 See the couplings on the structure!

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The Automatic Algorithm

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- Couplings are analyzed and categorized
- Unique couplings identified
- Assignment attempted
 - Rules are followed to prohibit unlikely couplings

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The Automatic Algorithm

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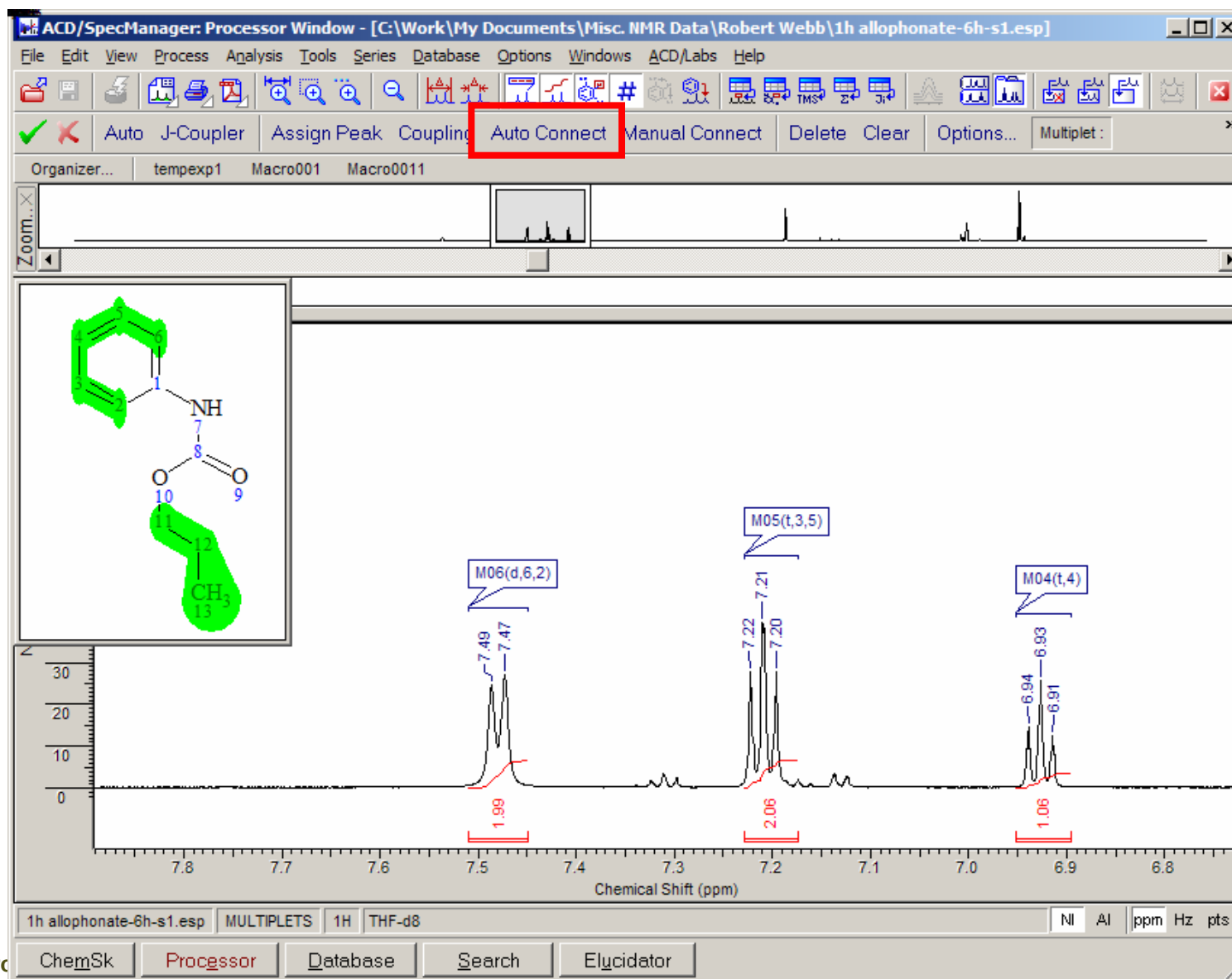
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The Automatic Algorithm

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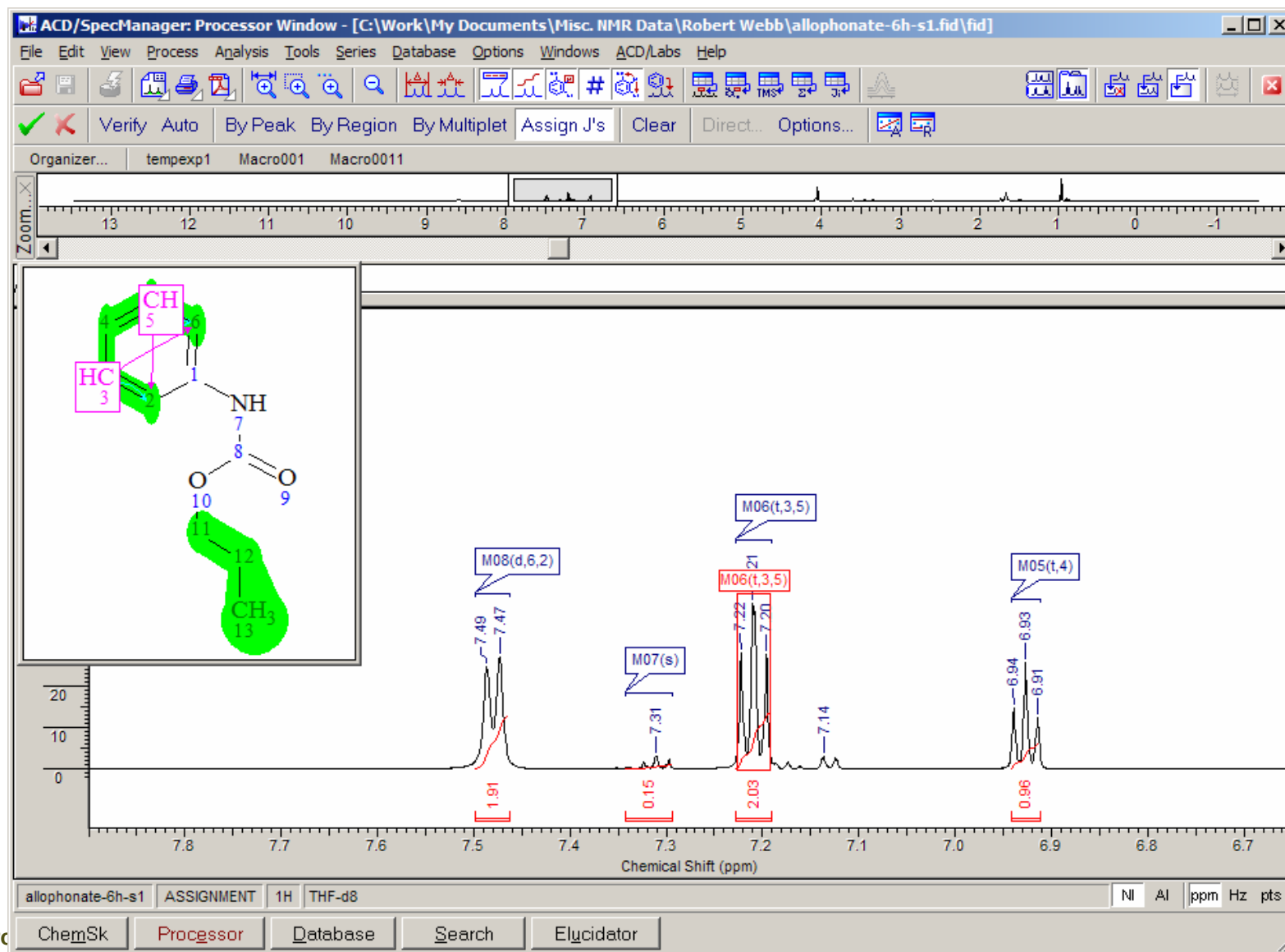
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The Manual Method

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- Coupled multiplets can be associated manually
- Common coupling constant must be present

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Manual Coupling Assignment

Why?

Multiplet Analysis

Coupling Assignment

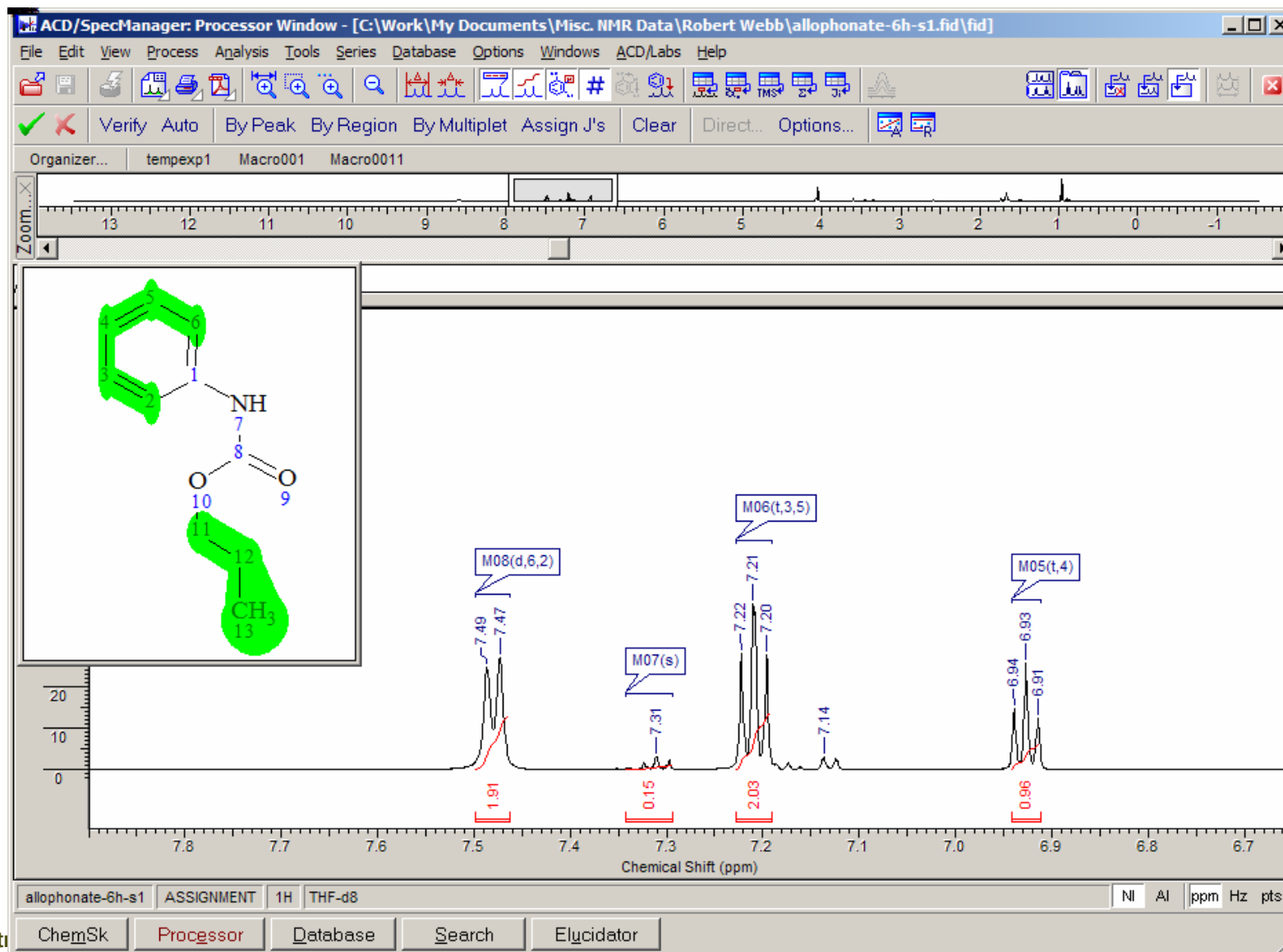
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Spectra



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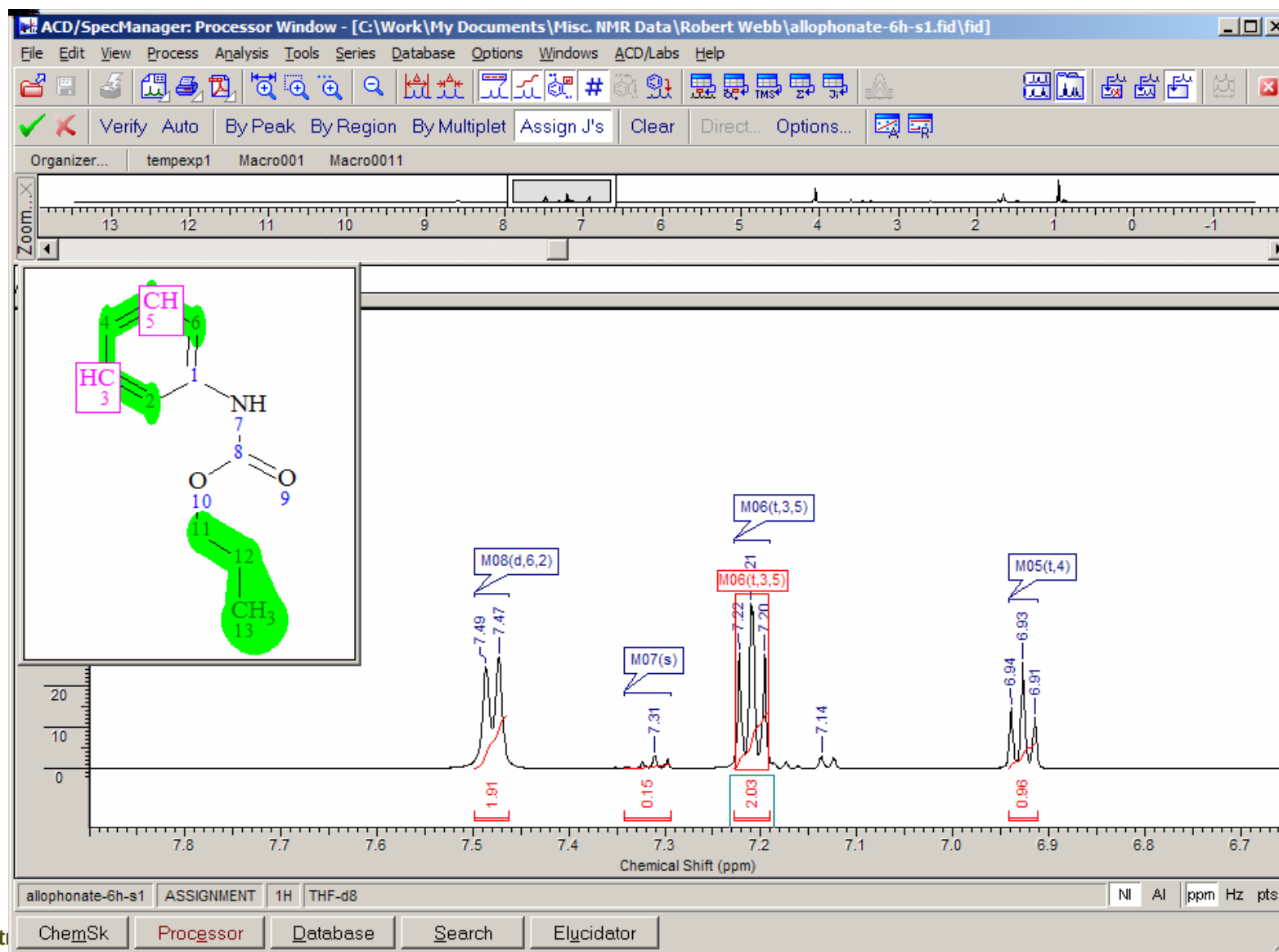
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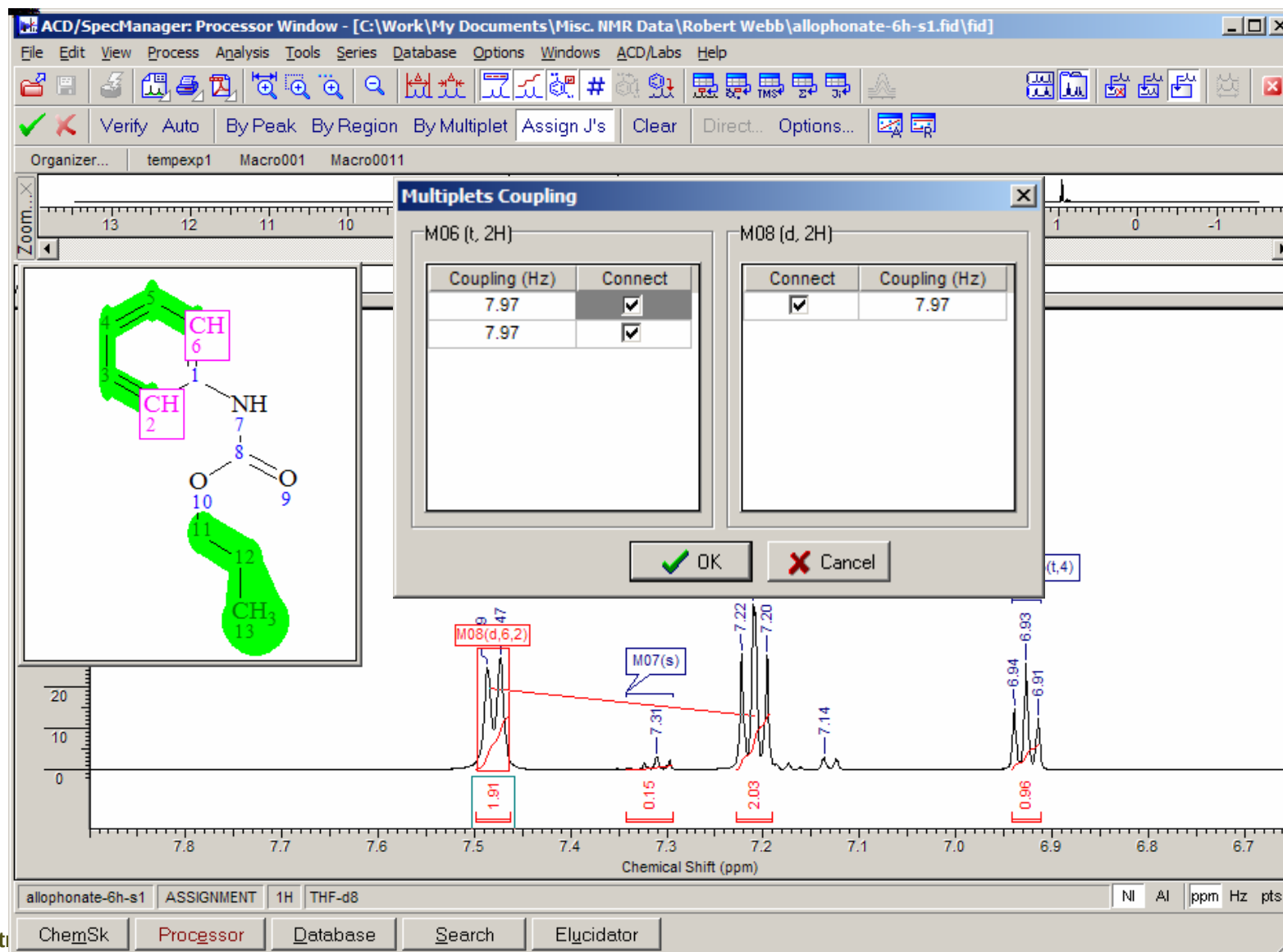
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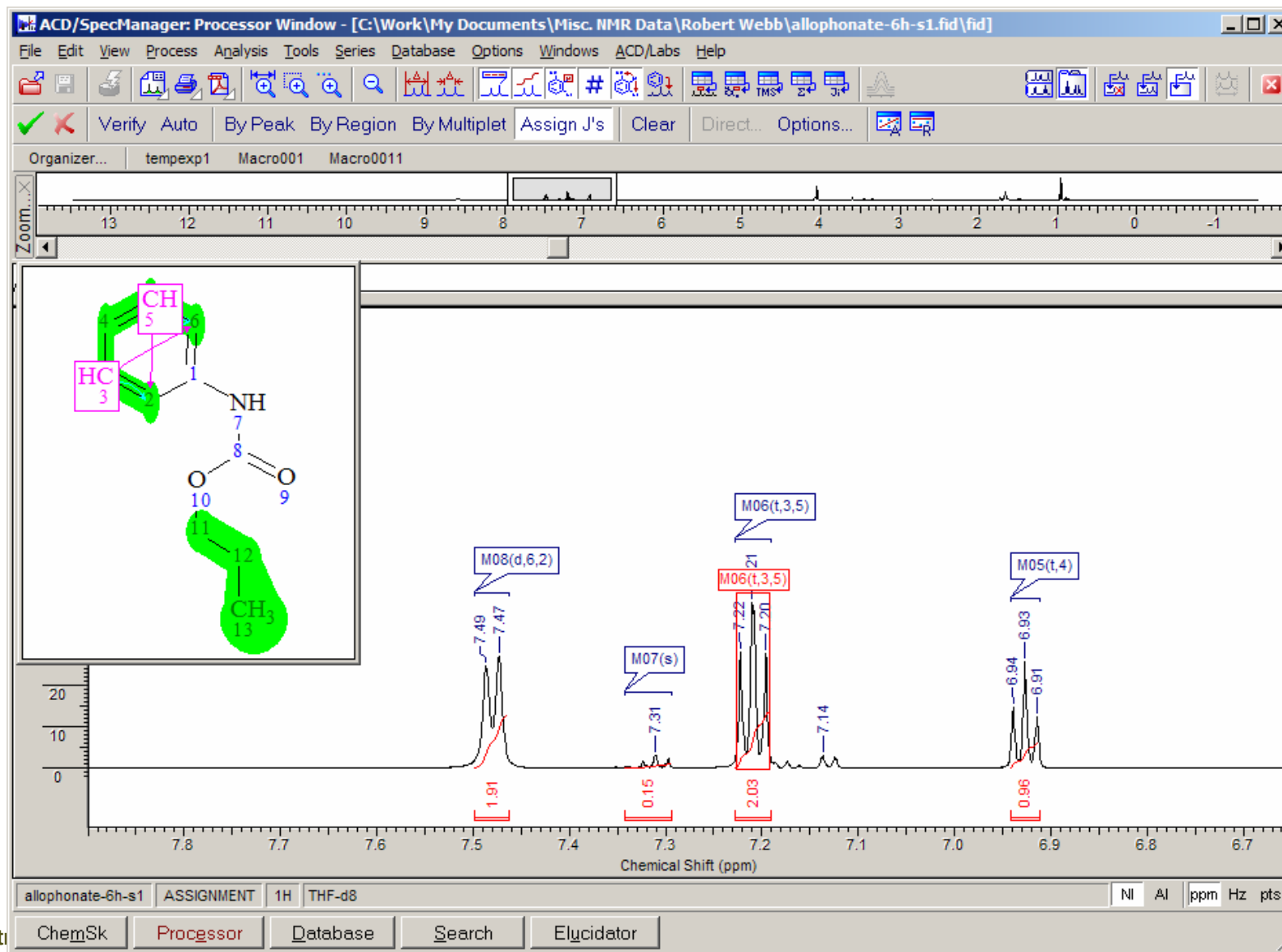
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Compact Multiplet Table

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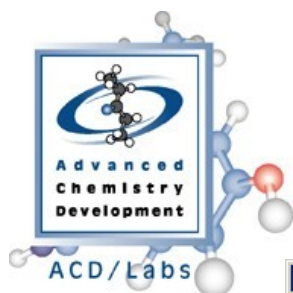
Summary

No.	Shift1...	H's	Type	J (Hz)	▽	Multiplet1	Connectio...	(ppm)
1	0.76	1	m	-		M02	-	[0.75 .. 0.77]
2	7.87	7	s	-		M20	-	[7.86 .. 7.88]
3	7.53	1	s	-		M18	-	[7.52 .. 7.56]
4	0.78	1	s	-		M03	-	[0.78 .. 0.79]
5	7.21	2	m	-		M15	-	[7.18 .. 7.25]
6	4.19	5	s	-		M11	-	[4.14 .. 4.24]
7	0.94	2	m	-		M08	-	[0.91 .. 0.96]
8	0.84	3	m	-		M05	-	[0.80 .. 0.88]
9	12.66	5	s	-		M21	-	[12.61 .. 12.72]
10	7.37	3	m	-		M17	-	[7.34 .. 7.38]
11	7.21	13	tt	2.03		M14	?	[7.18 .. 7.25]
12	7.21	13	tt	2.03		M14	?	[7.18 .. 7.25]
13	7.54	6	dd	2.27		M19	?	[7.52 .. 7.56]
14	7.36	4	d	2.48		M16	?	[7.34 .. 7.38]
15	0.79	2	d	3.07		M04	?	[0.78 .. 0.79]
16	0.75	1	d	3.22		M01	?	[0.75 .. 0.77]
17	0.93	5	dd	3.36		M07	?	[0.91 .. 0.96]
18	7.21	13	tt	4.70		M14	?	[7.18 .. 7.25]
19	7.21	13	tt	4.70		M14	?	[7.18 .. 7.25]
20	0.84	11	ddd	5.26		M06	?	[0.80 .. 0.88]
21	7.54	6	dd	7.09		M19	?	[7.52 .. 7.56]
22	0.84	11	ddd	8.95		M06	?	[0.80 .. 0.88]
23	0.93	5	dd	9.94		M07	?	[0.91 .. 0.96]
24	3.60	7	d	14.03		M10	M09	[3.58 .. 3.62]
25	3.18	7	d	14.03		M09	M10	[3.16 .. 3.20]
26	4.49	7	d	14.47		M12	M13	[4.47 .. 4.51]
27	4.79	7	d	14.62		M13	M12	[4.76 .. 4.81]
28	0.84	11	ddd	16.48		M06	?	[0.80 .. 0.88]

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21	0.84	11	ddd	16.48, 8.95, 5.26		M06	-	[0.80 .. 0.88]

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Visualize the Couplings

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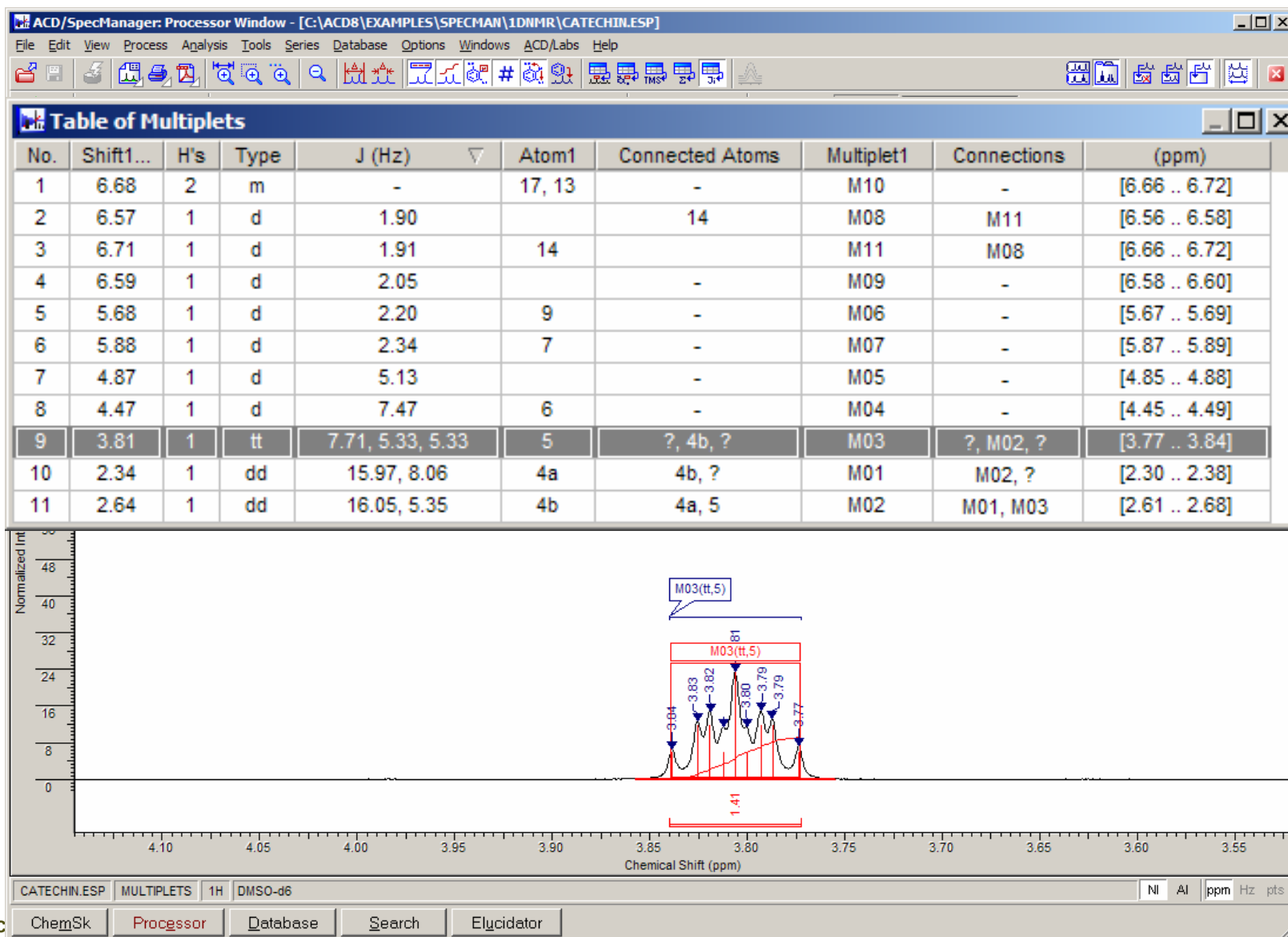
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Visualize the Couplings

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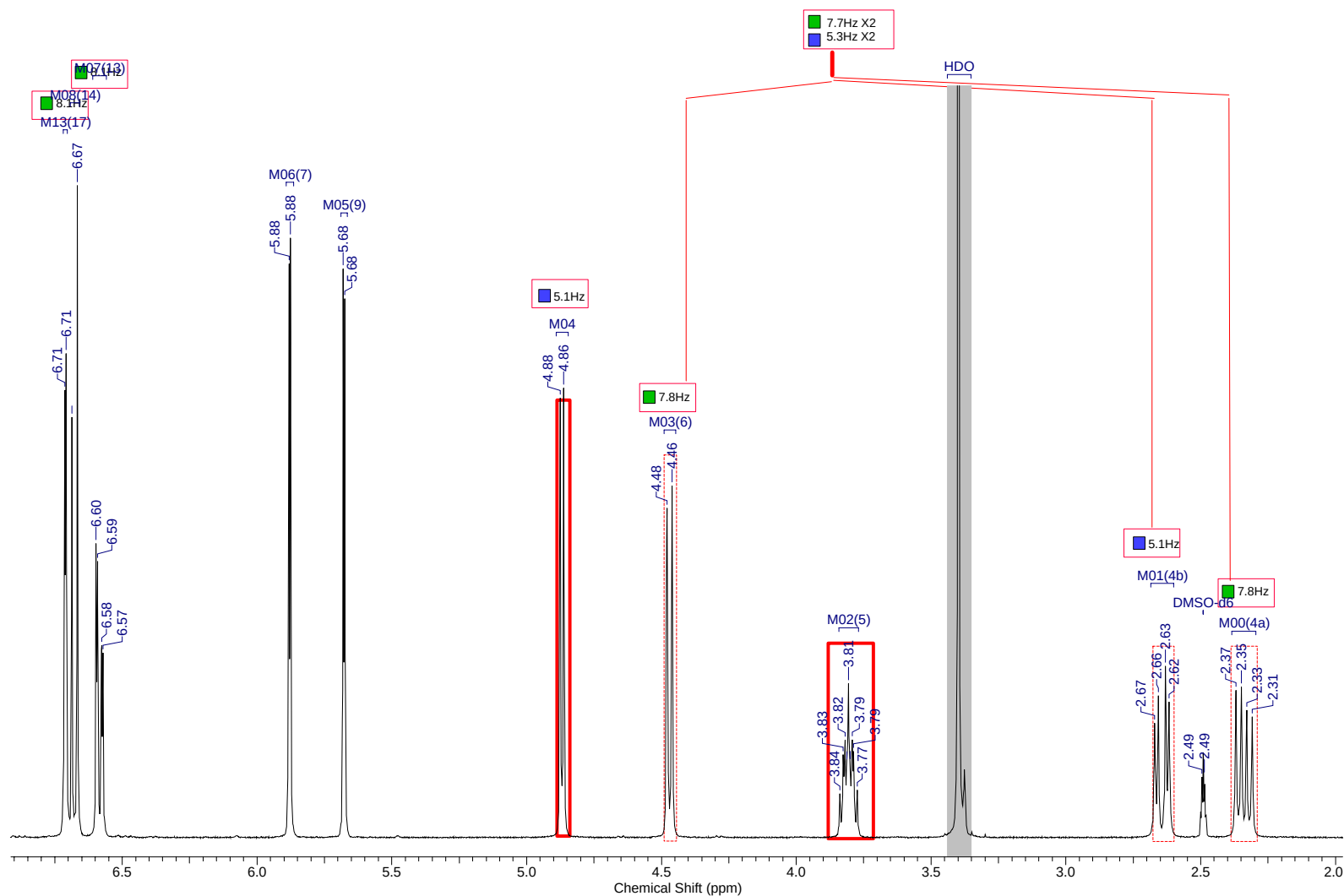
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Spec M02 and M04 are being connected (M02 is current and M04 is selected and user would have to click on it to connect the multiplets)



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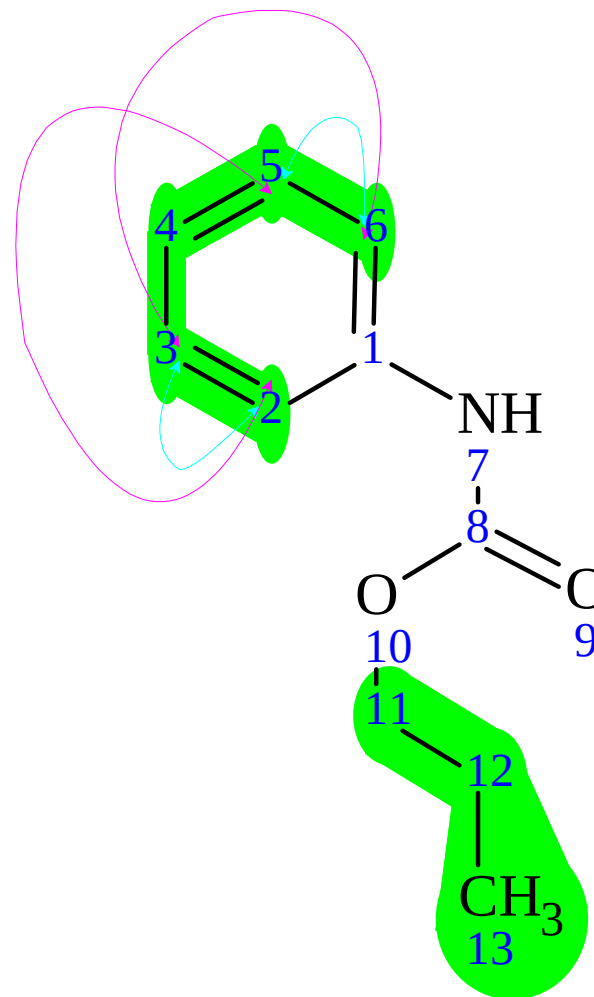
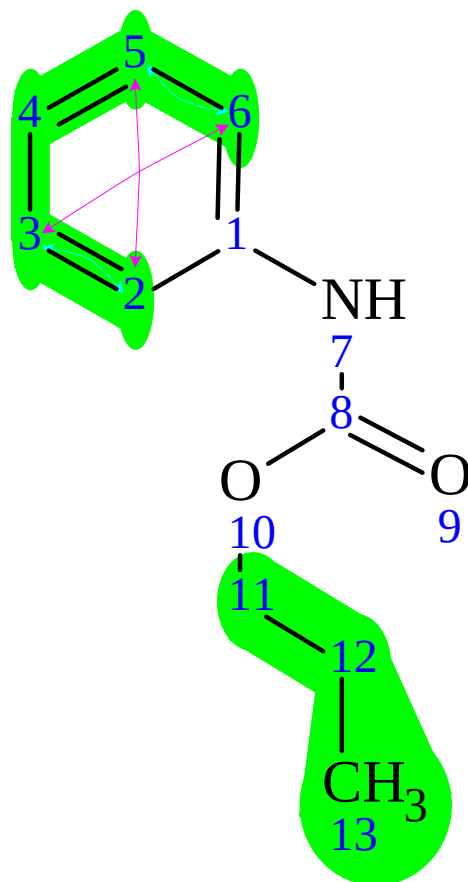
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Guide Your Assignments

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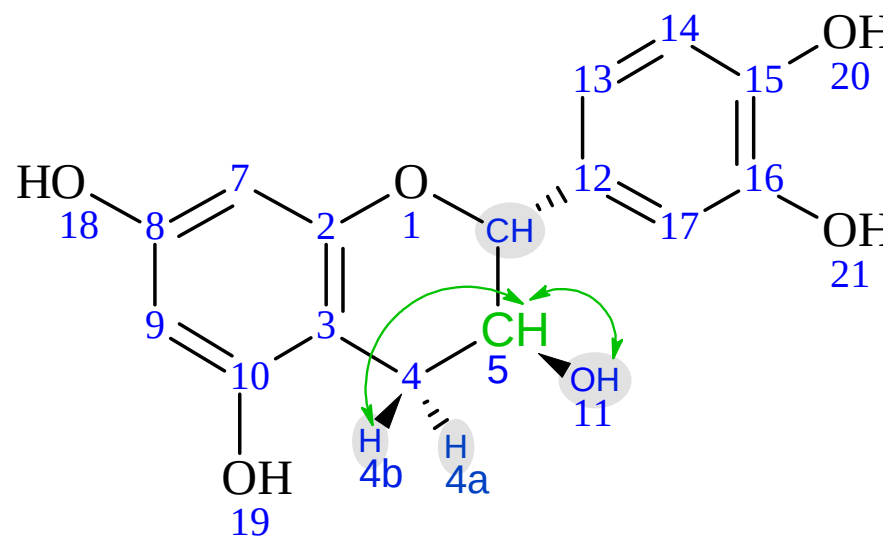
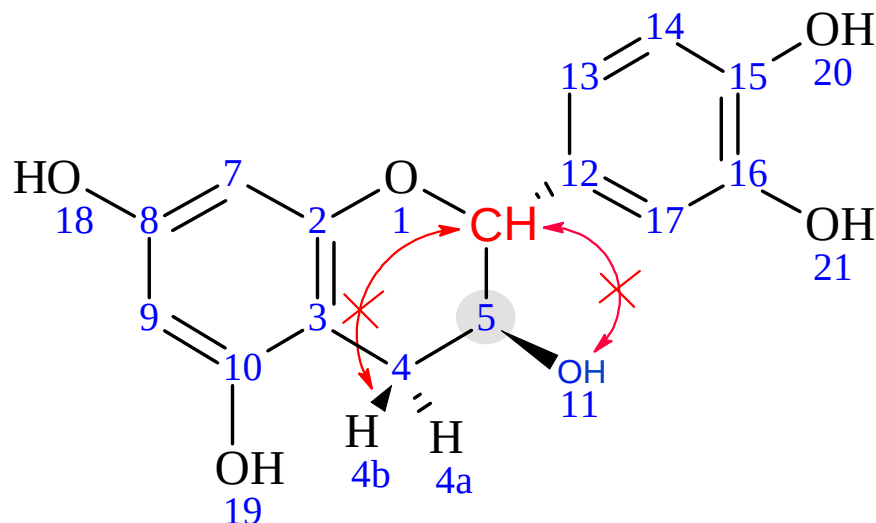
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🌀 What does this mean for the future?

🌀 Better verification results

➤ Use of coupling system
information more often and
more easily

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- 🌀 How will the workflow change?
 - 🌀 Streamlined interaction with spectrum for automatic algorithm
 - 🌀 More work for manual assignment
 - But also more information!
- 🌀 It is all up to the user

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🌀 What are the implications of these features?

- 🌀 More information
- 🌀 Better decision making
- 🌀 Better results

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Version 8 to 9

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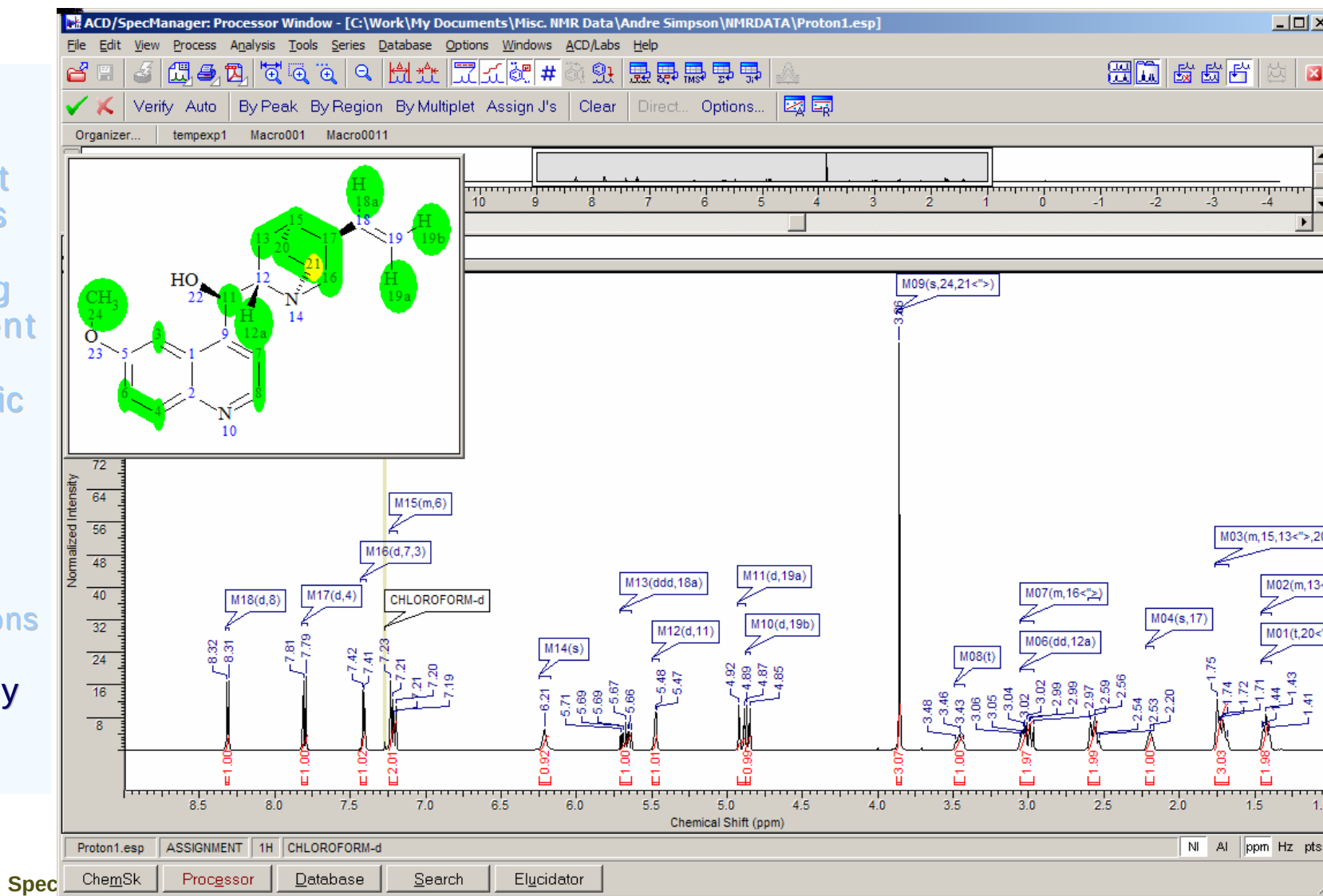
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Acknowledgements

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- 🌀 Sergey Golotvin
 - 🌀 1D NMR Project Leader
- 🌀 Tony Williams
 - 🌀 VP and CSO

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