Supporting Information

Photoredox Cyanomethylation of Indoles: Catalyst Modification and Mechanism

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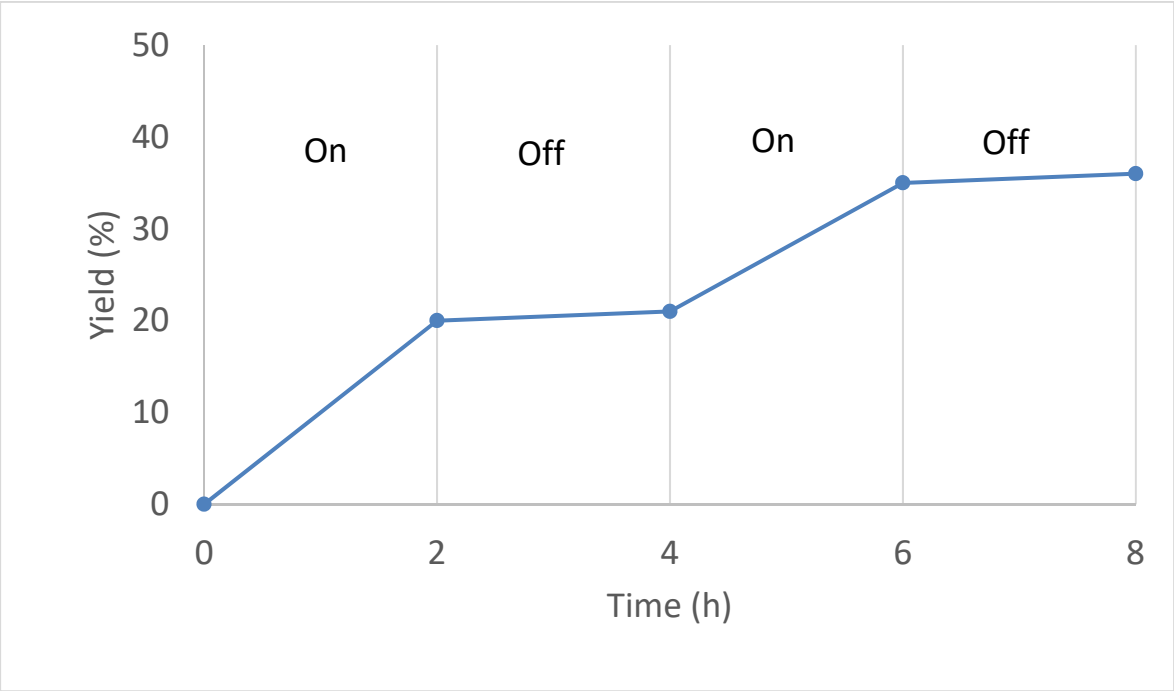


Figure S1. Reaction progress for the conversion of **1** to **3** following Procedure A, with the LED light turned on for 2 h, then off between 2-4 h, turned on between 4-6 h, then turned off from 6-8 h.

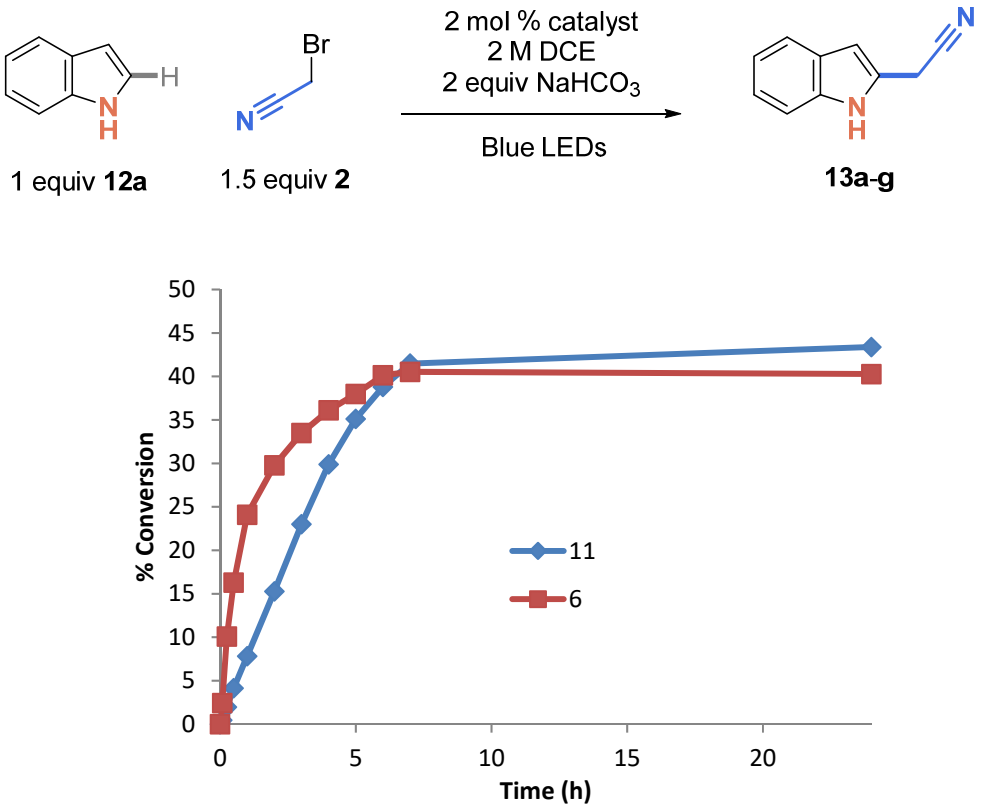


Figure S2. Time course for the reaction of indole and bromoacetonitrile using catalyst **6** or **11**.

Procedure for time course:

Indole (66 mg, 563 µmol), catalyst (0.02 Eq, 11.3 µmol), internal standard ethyl 6-(trifluoromethyl)nicotinate (62 mg, 0.5 equiv, 282 µmol) and sodium hydrogen carbonate (95 mg, 2 Eq, 1.13 mmol) were added to a flame dried vial. The vial was then evacuated, and back-filled with argon three times. Under positive pressure of argon, DCE (0.23 mL) and bromoacetonitrile (101 mg, 58.9 µL, 1.5 equiv, 845 µmol) were added successively. The resulting solution was sparged under argon for 15 min. The vial was then placed in front of the blue light under positive pressure of argon. The reaction was then sampled at set timepoints and the assay yield determined relative to internal standard. Average of two runs +/- 2%.

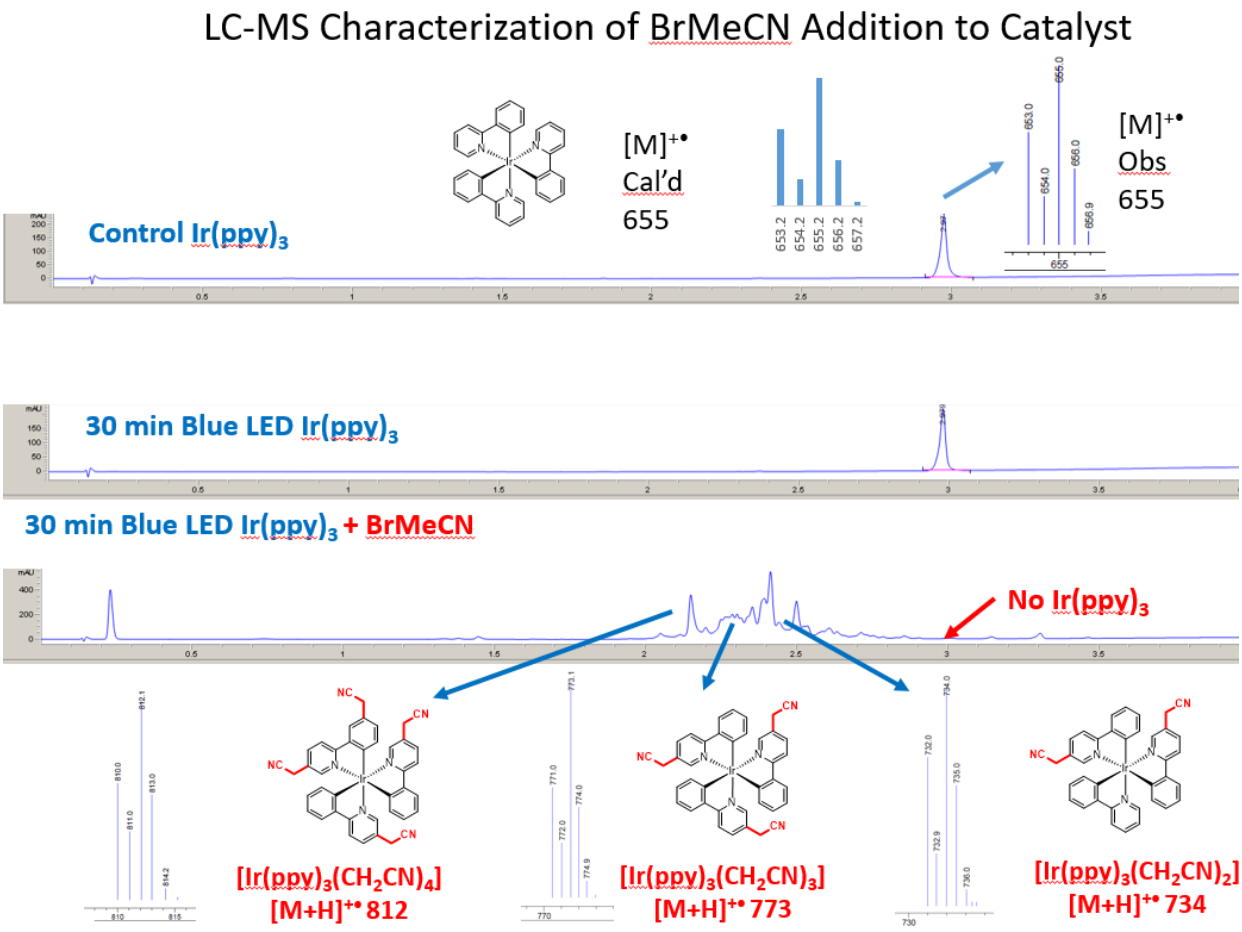


Figure S3. LCMS characterization of $BrCH_2CN$ addition to catalyst **6**.

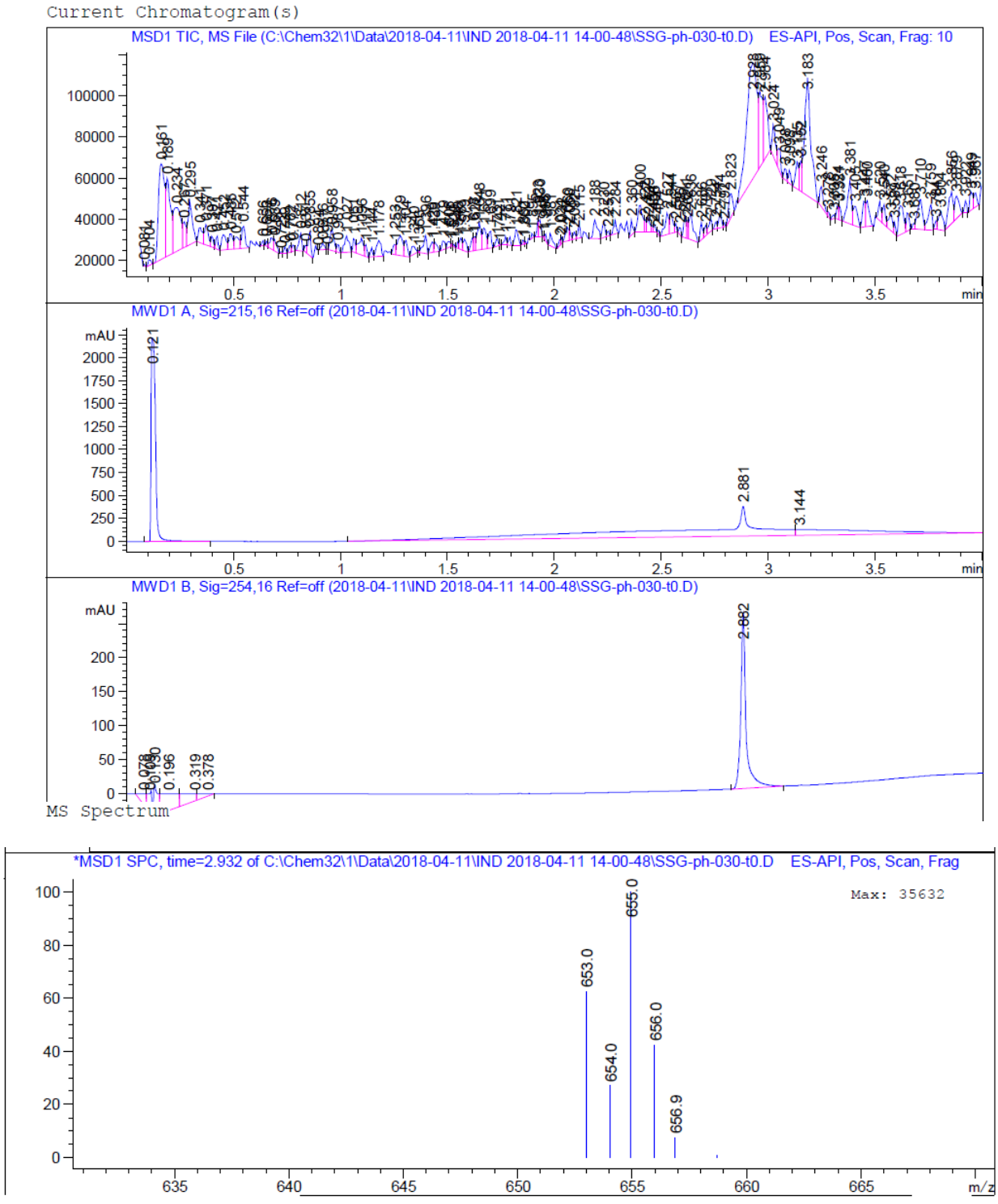
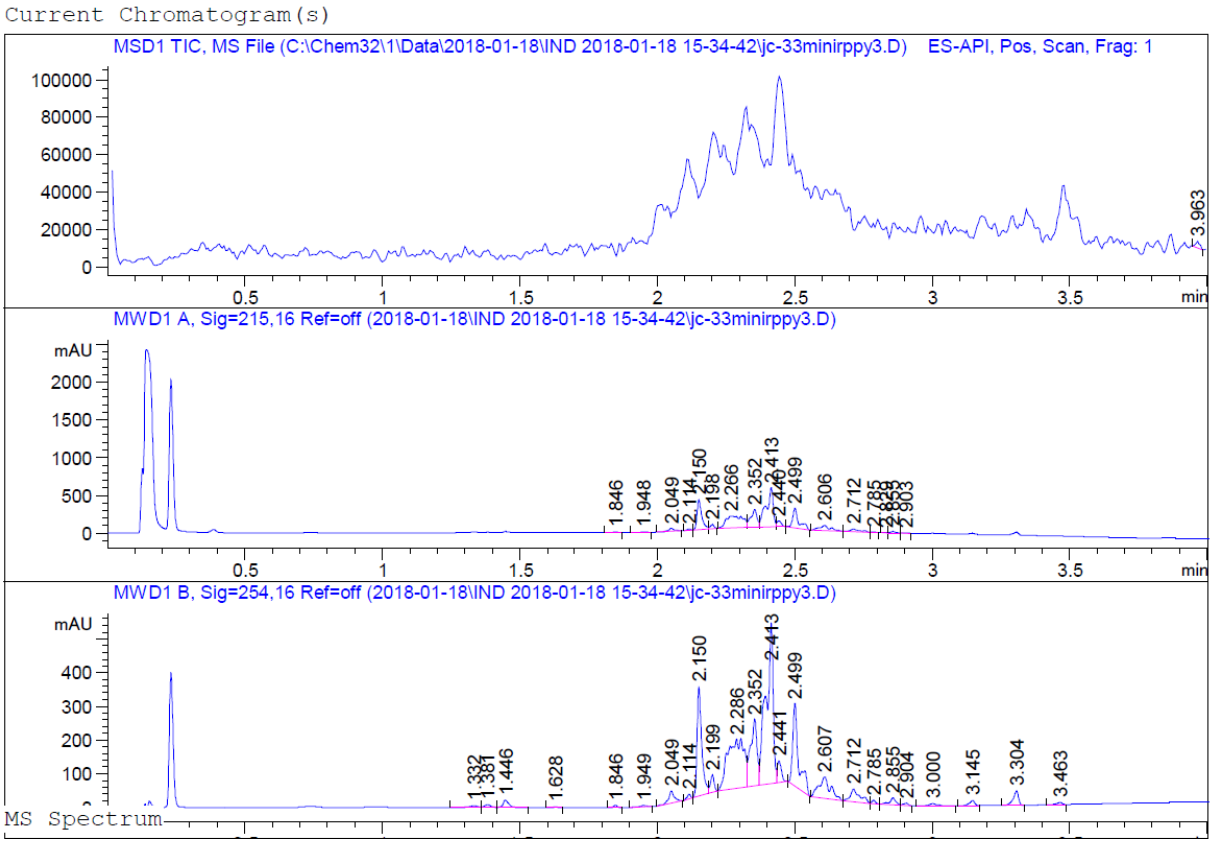


Figure S4. LCMS trace for Catalyst **6**, LCMS, Time 0 with MS spectrum for main peak.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mAU
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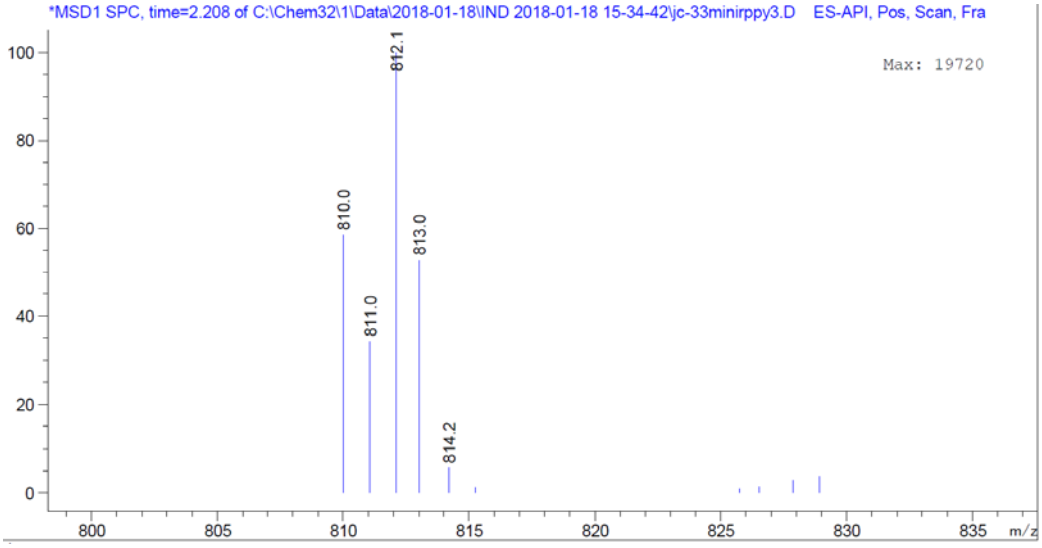
min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*MSD1 SPC, time=2.208 of C:\Chem32\1\Data\2018-01-18\IND 2018-01-18 15-34-42\jc-33minirppy3.D ES-API, Pos, Scan, Fra
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811.0
812.1
813.0
814.2
m/z

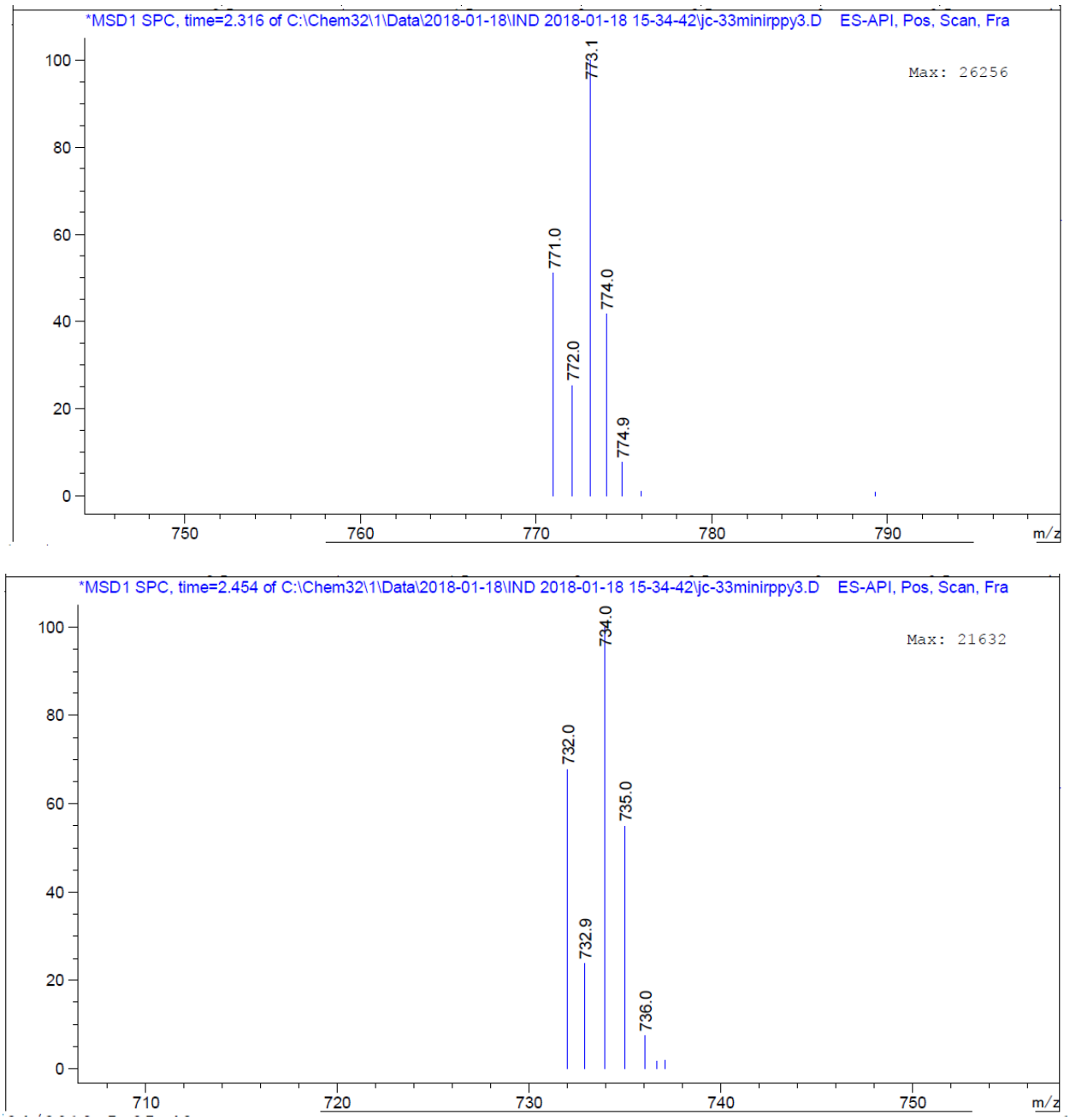


Figure S5. LCMS trace for catalyst **6**, 30 min, 50 equiv BrMeCN, Blue LED with MS spectra for peaks.

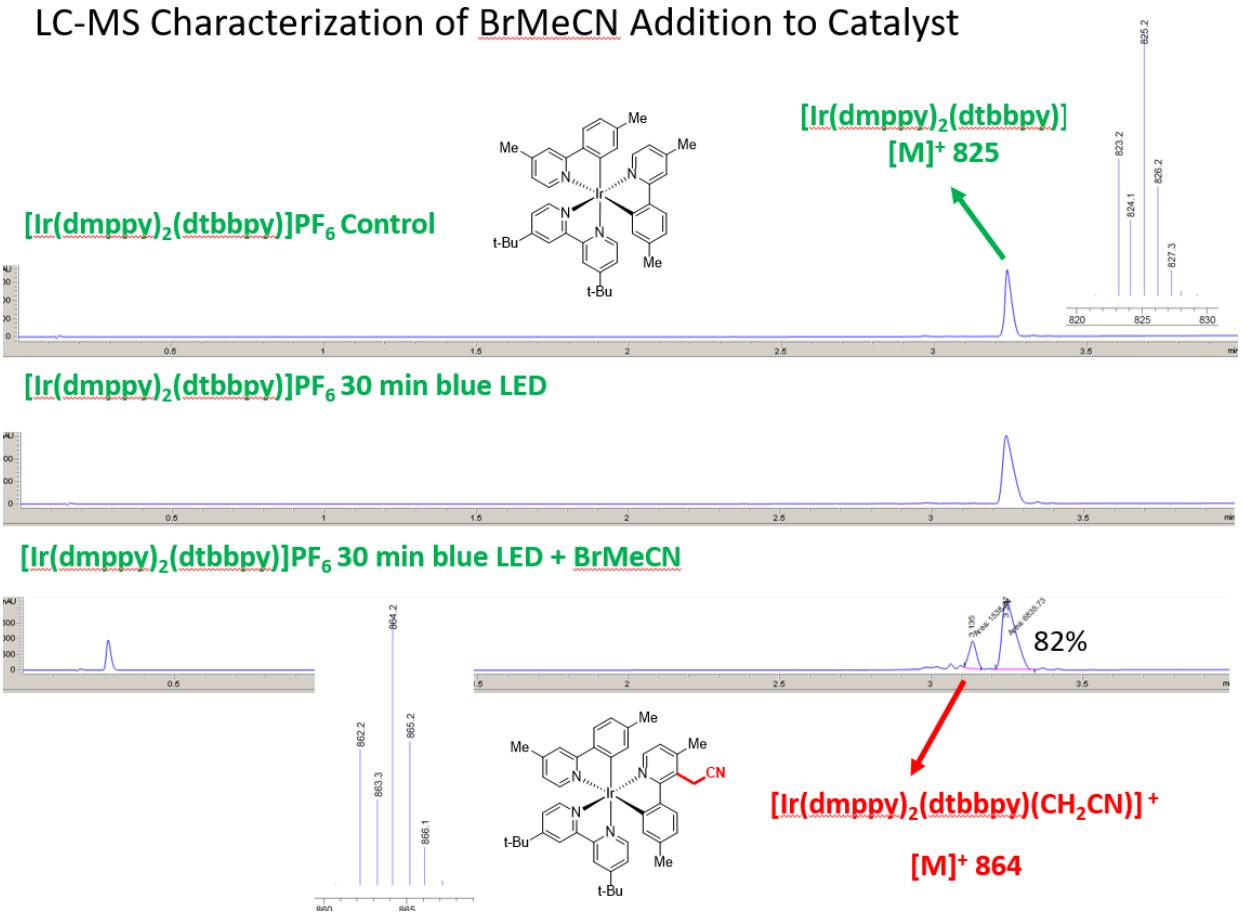


Figure S6. LCMS characterization of $BrCH_2CN$ addition to catalyst **11**.

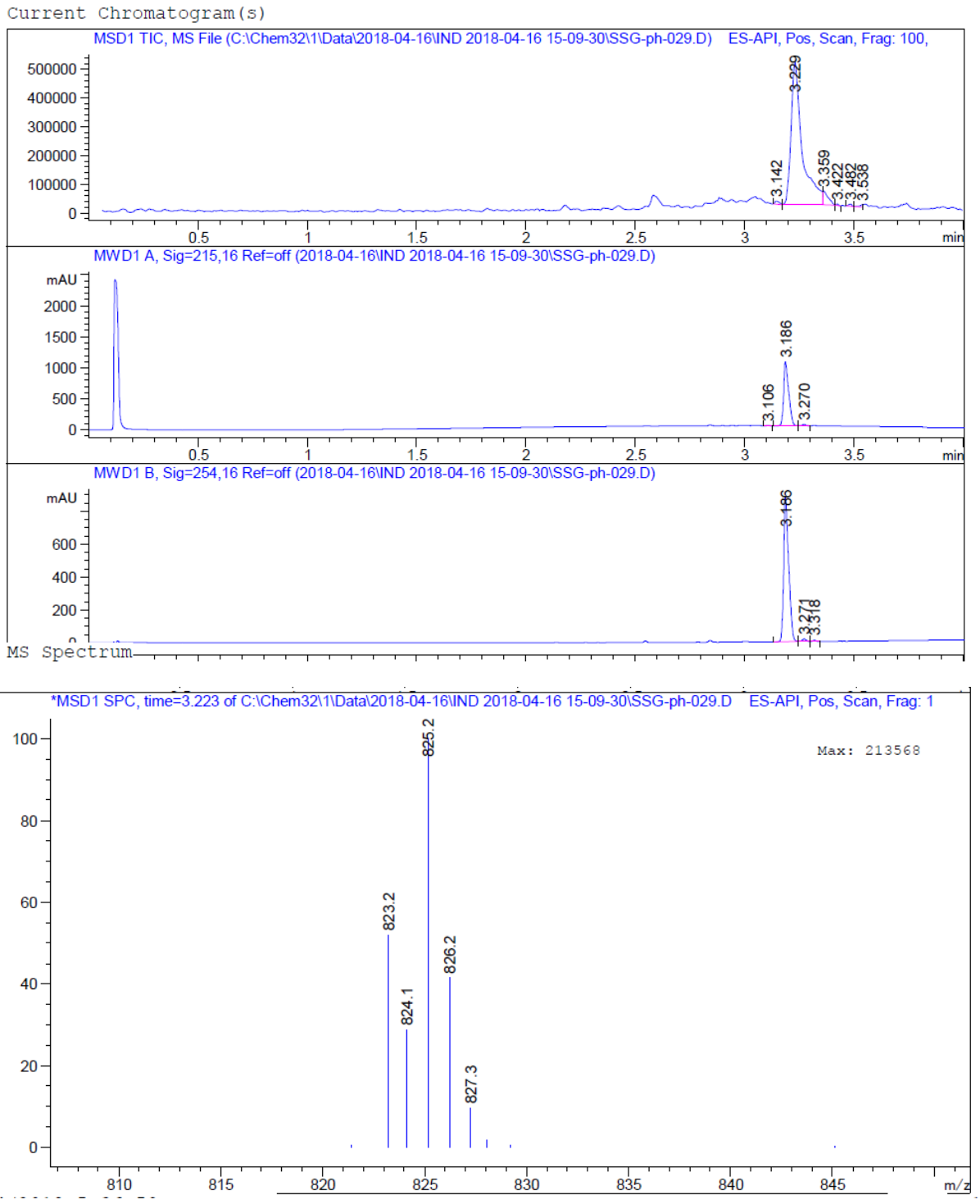
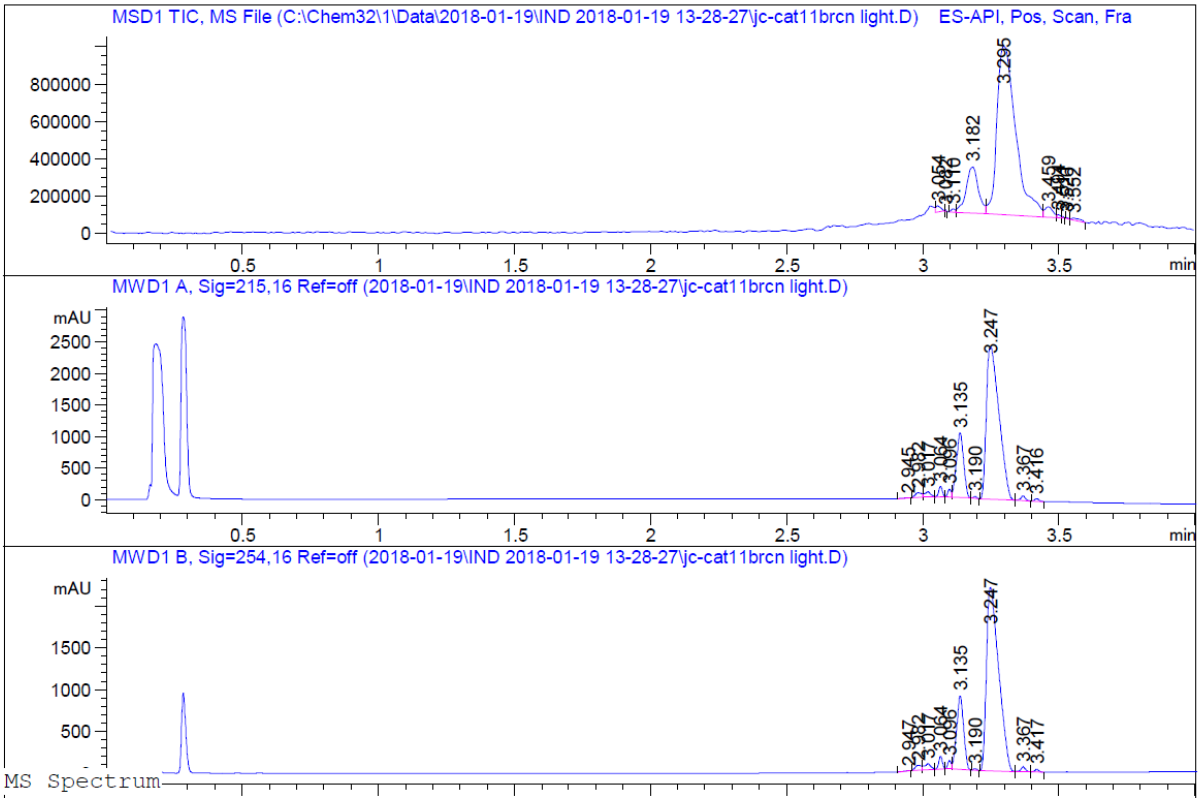
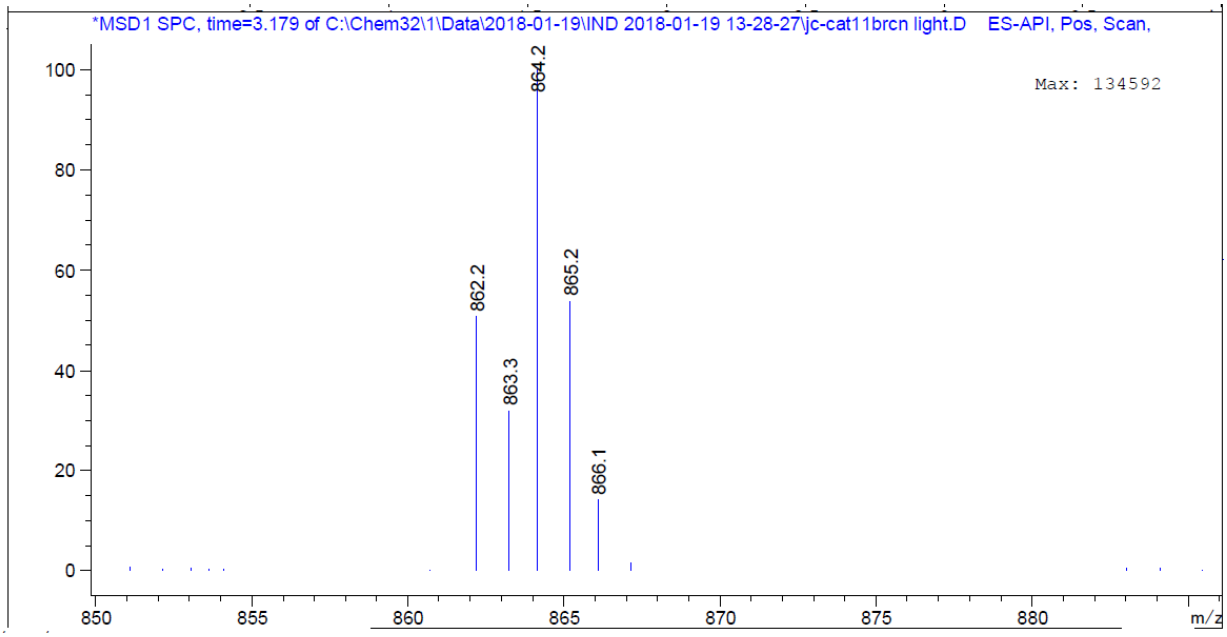


Figure S7. LCMS trace for Catalyst **11**, LCMS, Time 0 with MS spectrum for main peak.

Current Chromatogram(s)



MS Spectrum



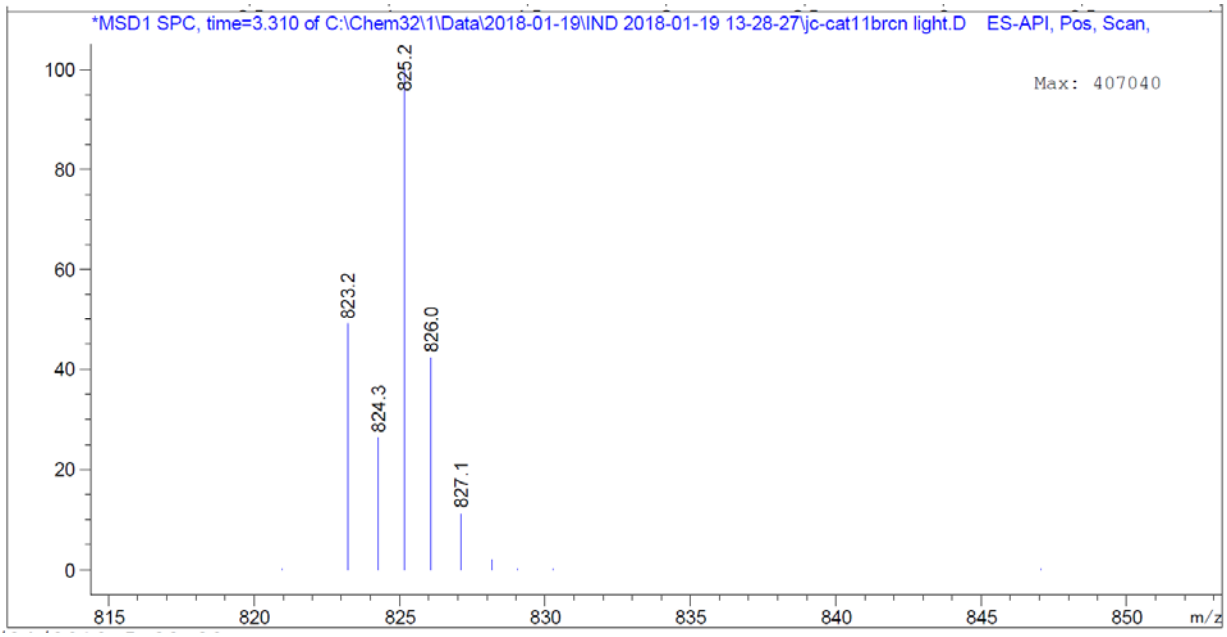


Figure S8. LCMS trace for catalyst **11**, 30 min, 50 equiv BrMeCN, Blue LED with MS spectra for peaks.

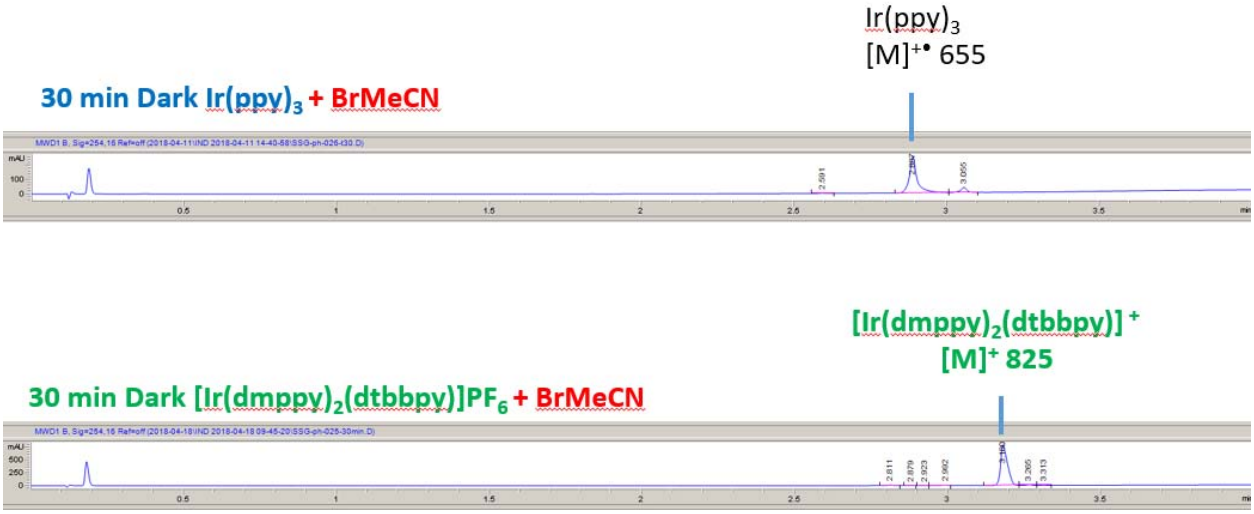


Figure S9. LCMS characterization of catalyst **6** or **11** with $BrCH_2CN$ added and kept in the dark for 30 min.

NMR Spectra

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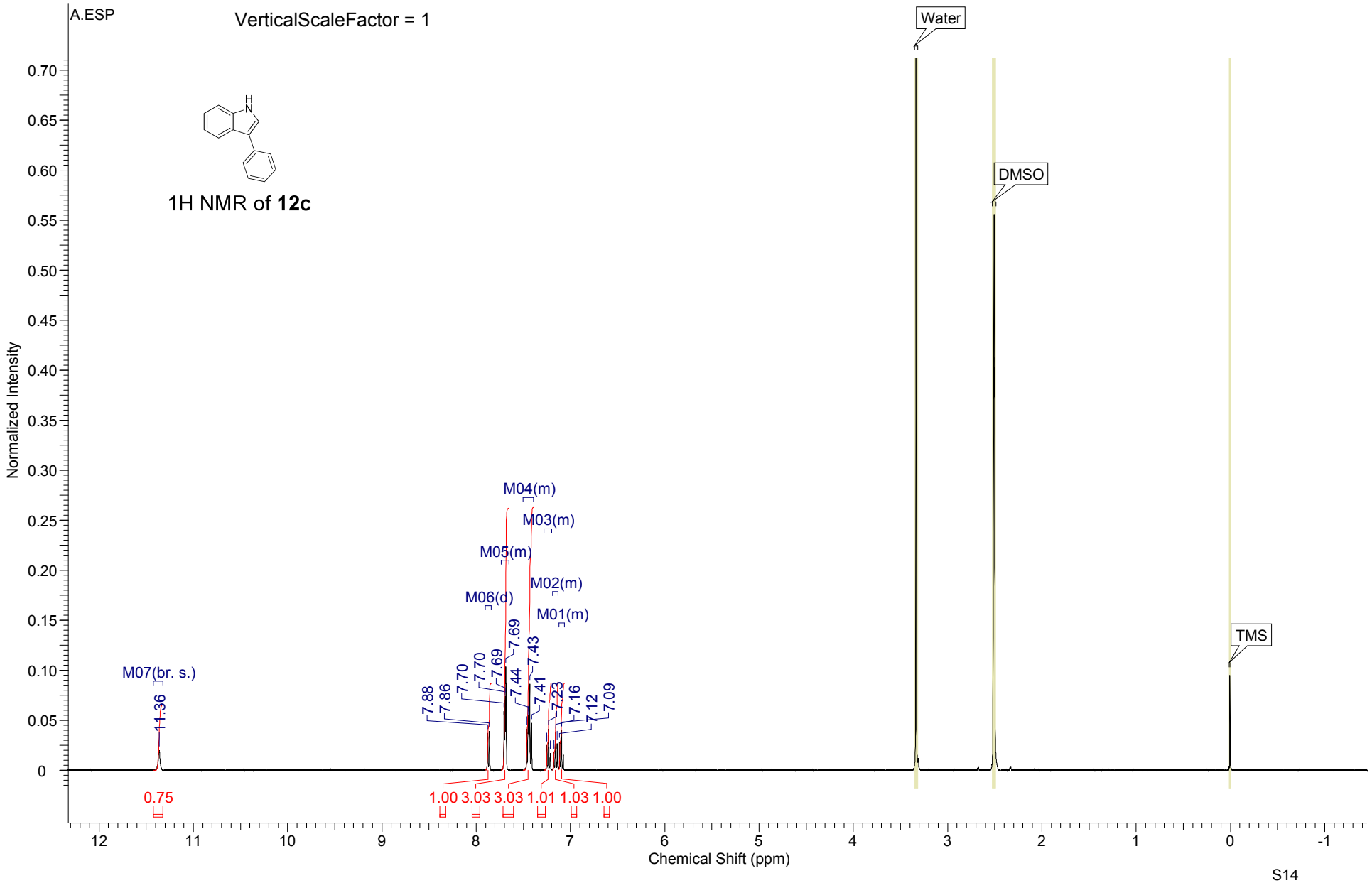

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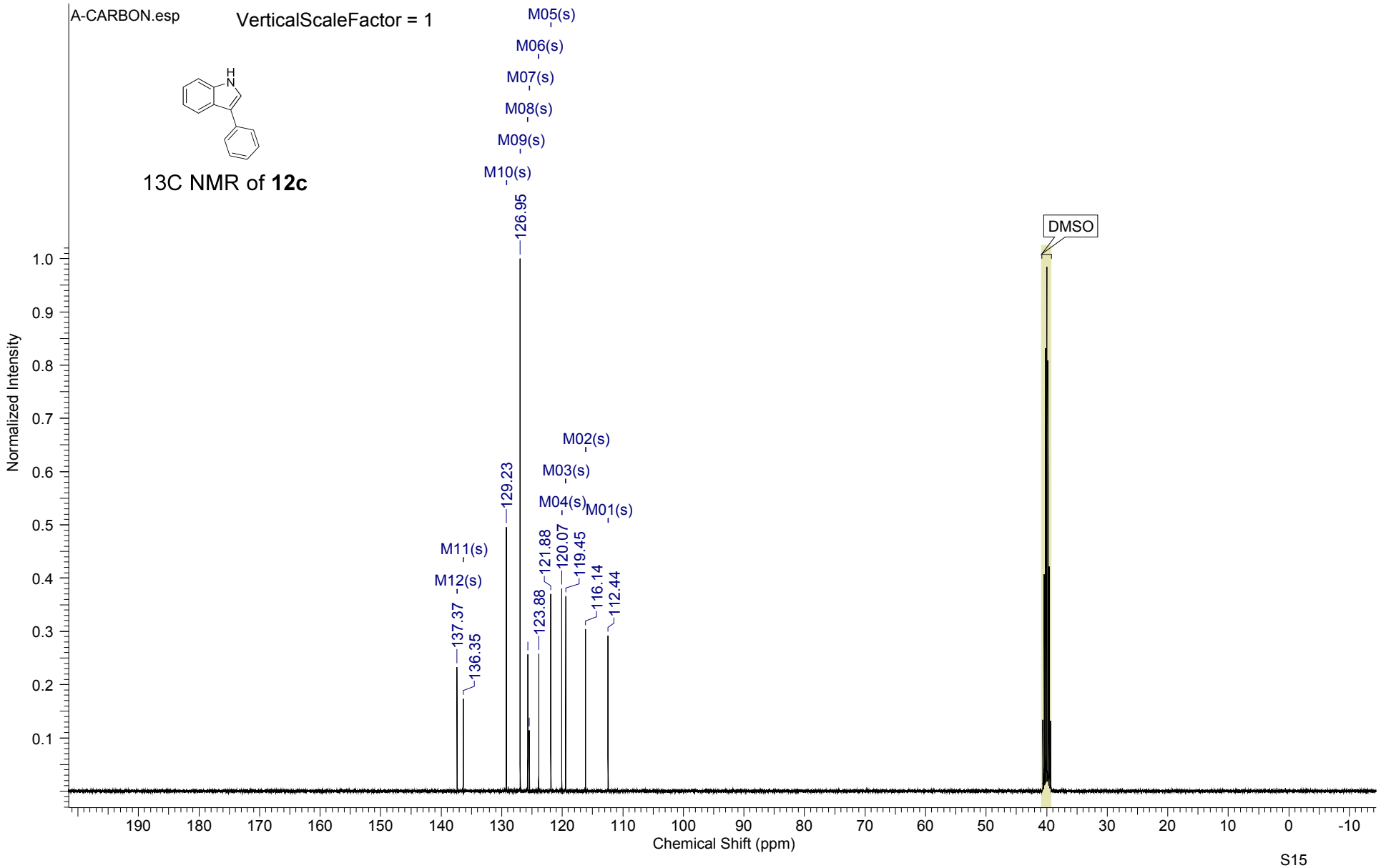

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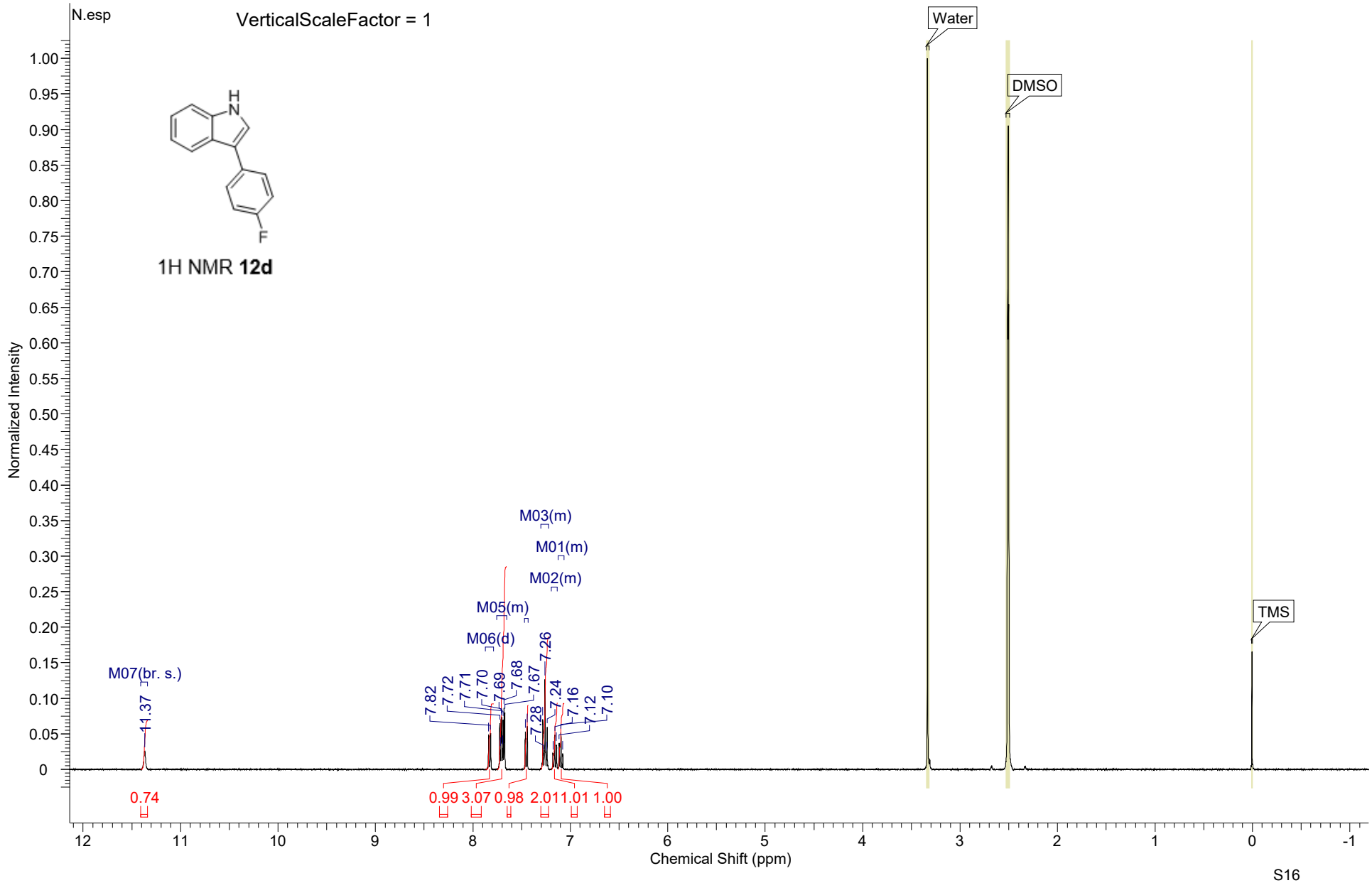

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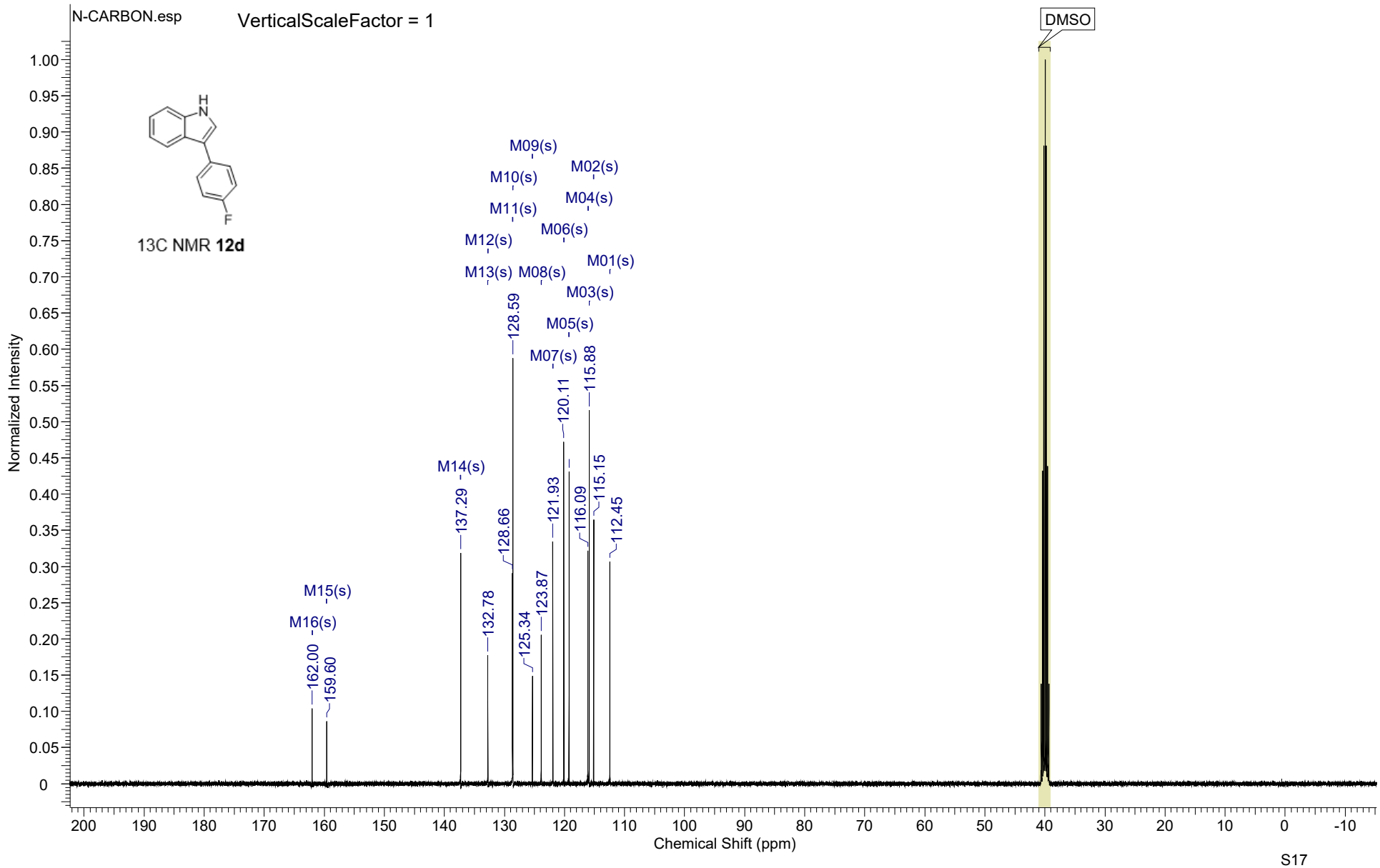

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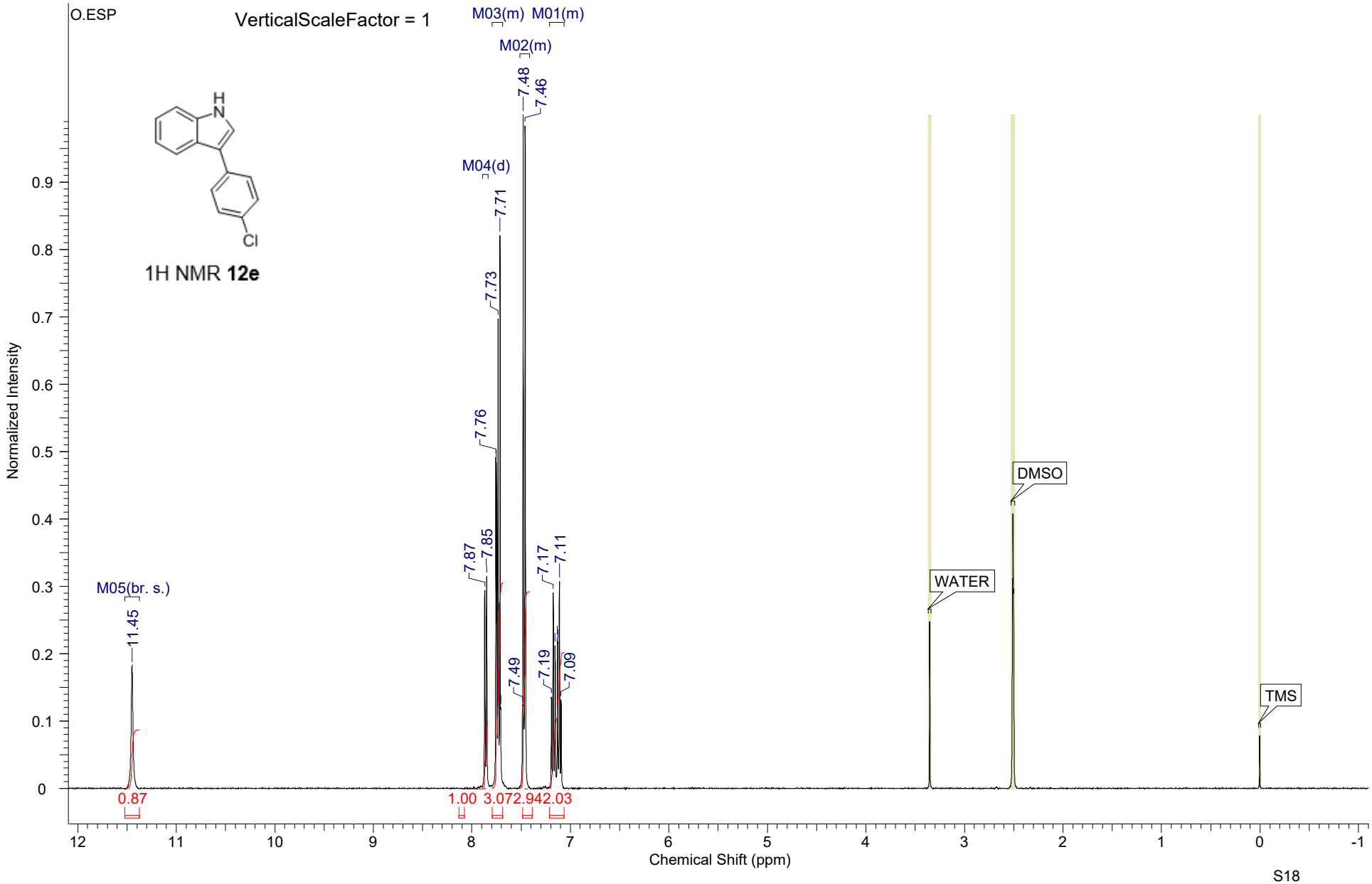

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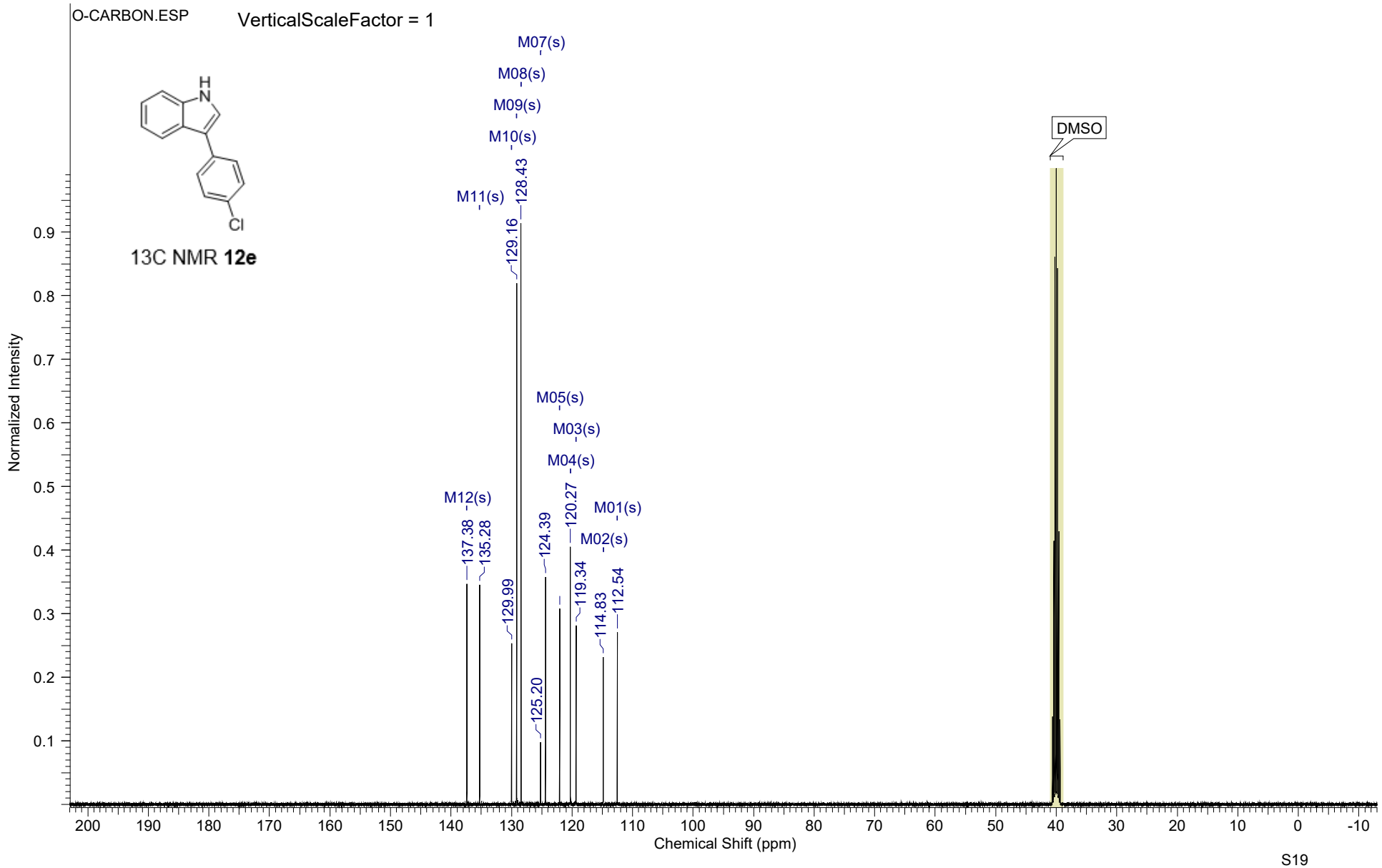

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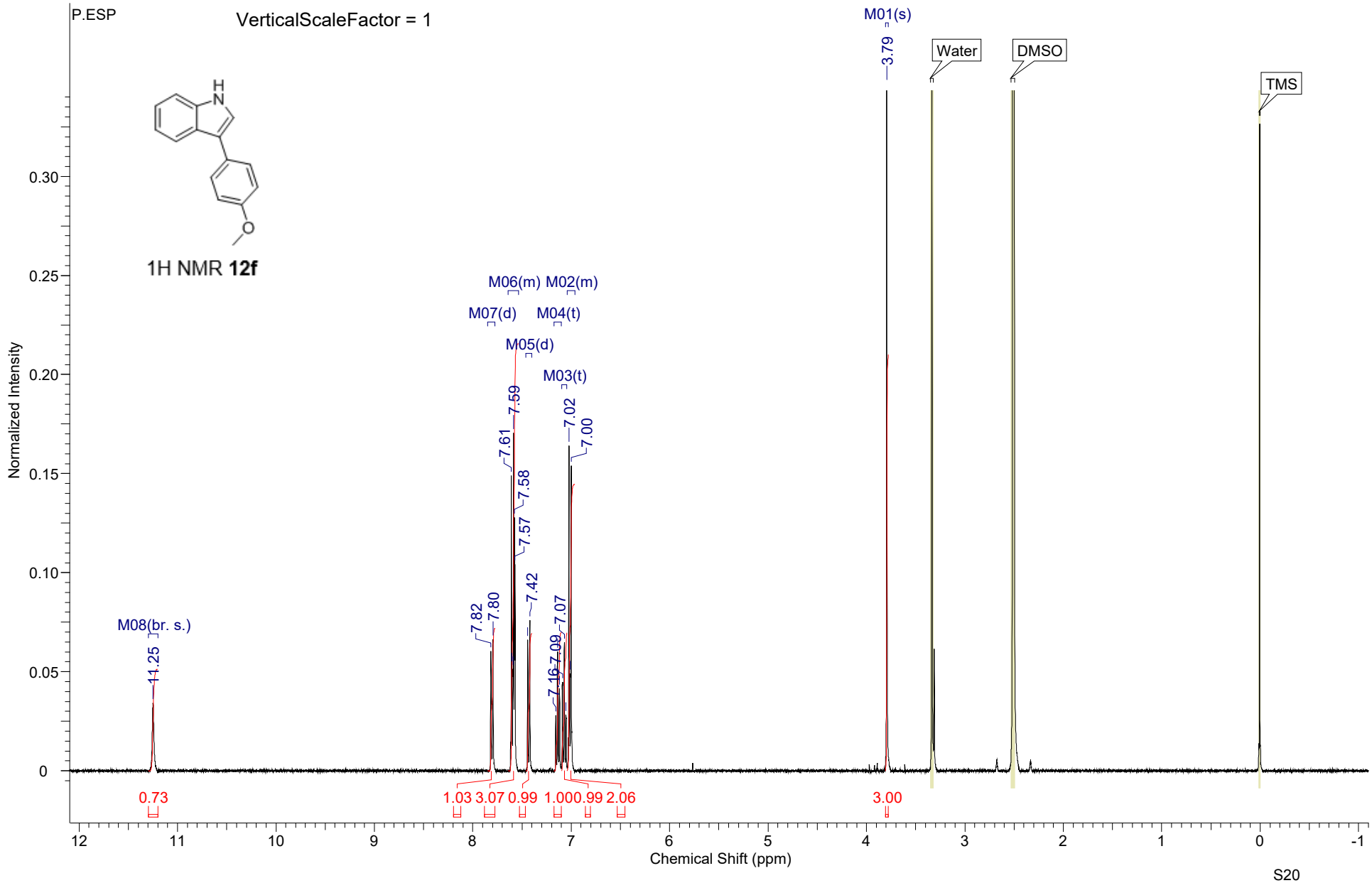

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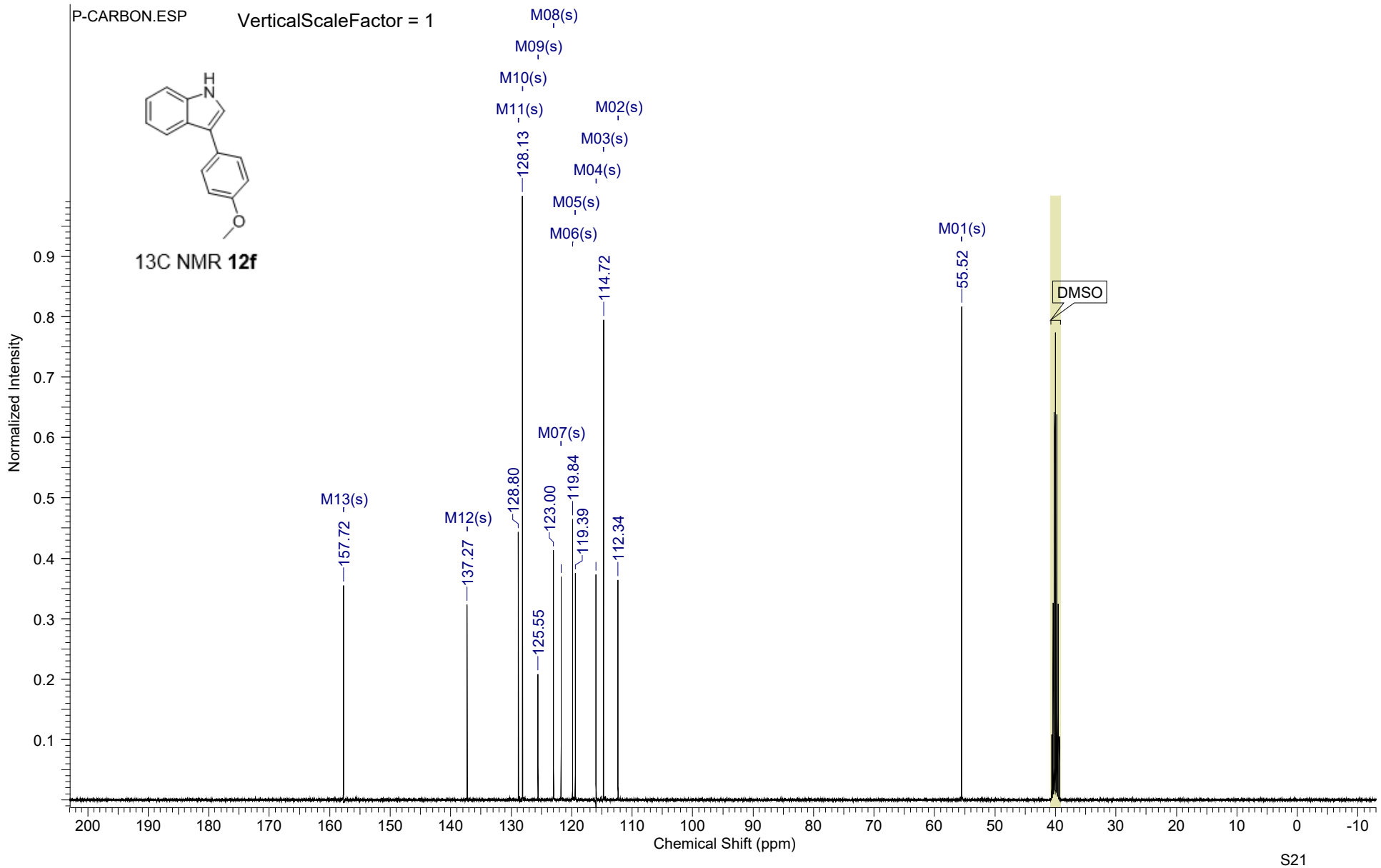

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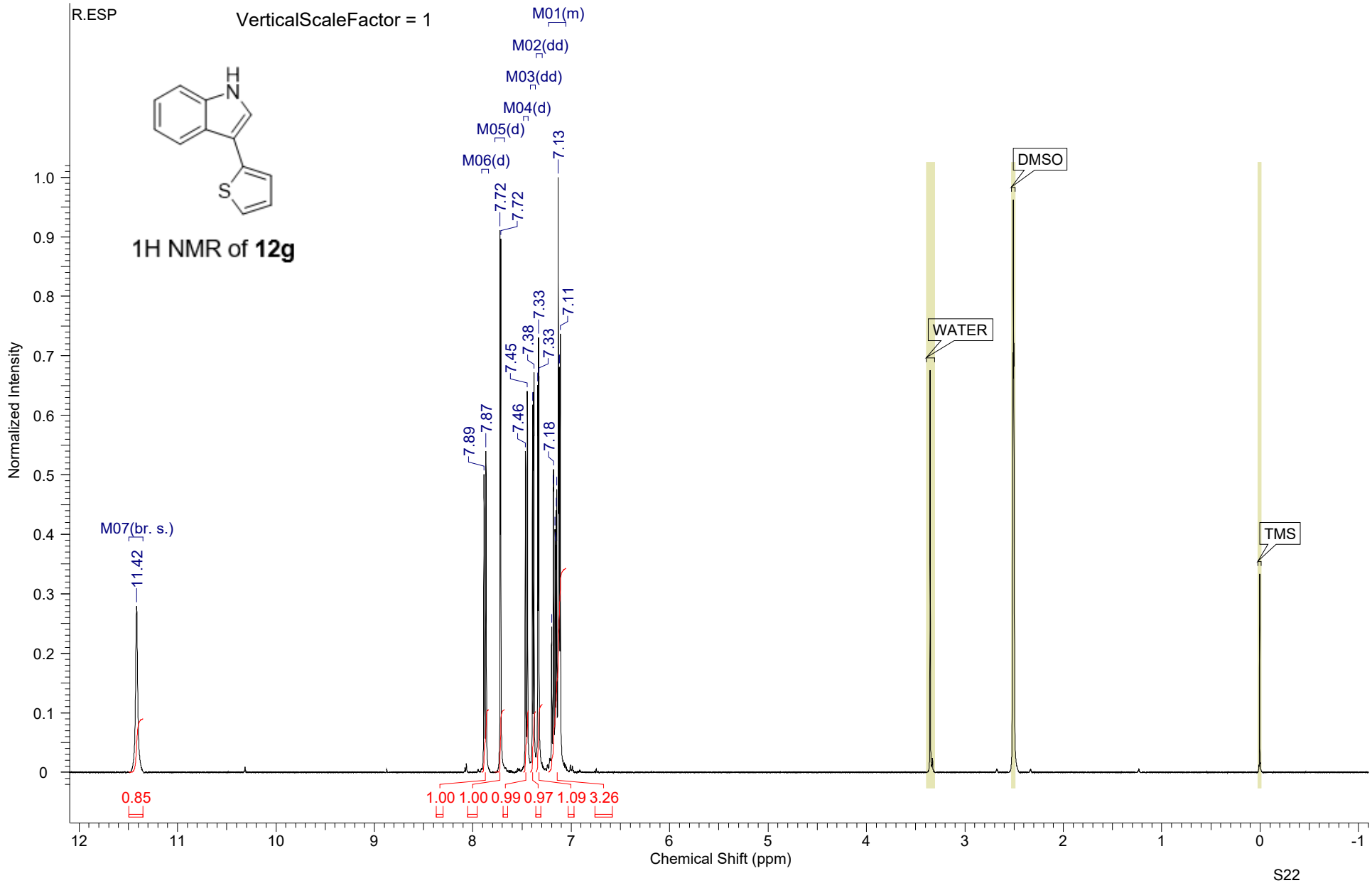

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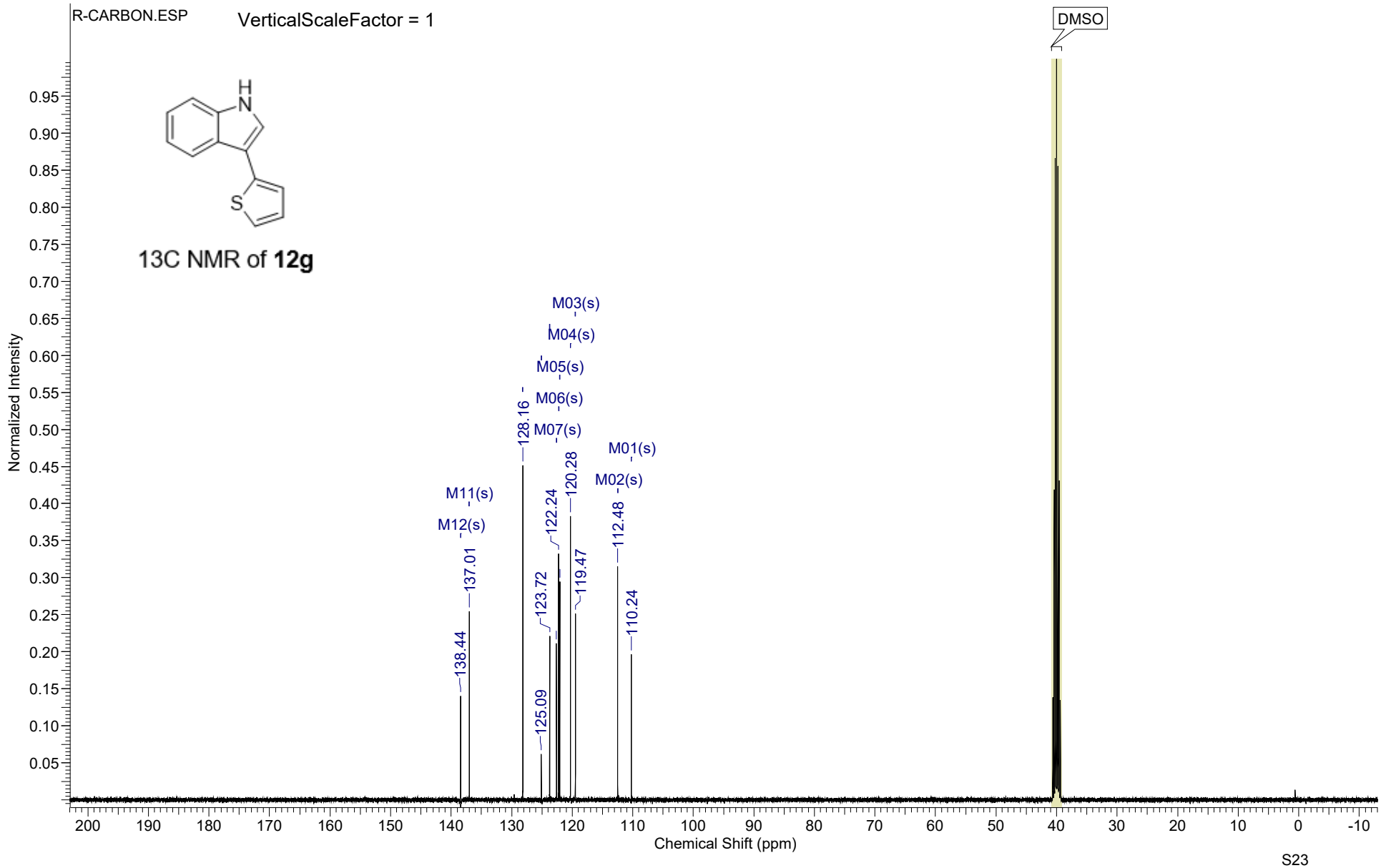

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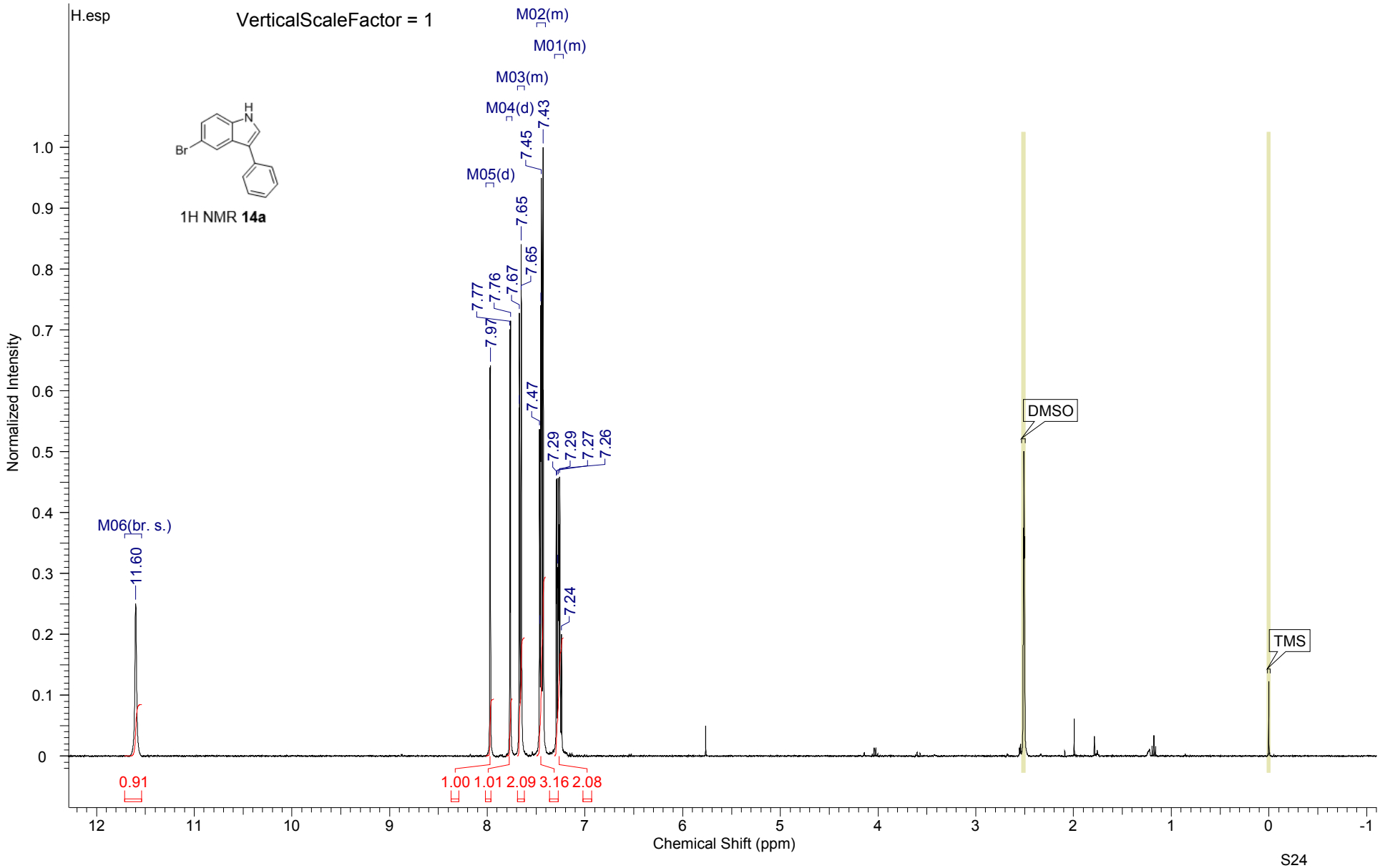

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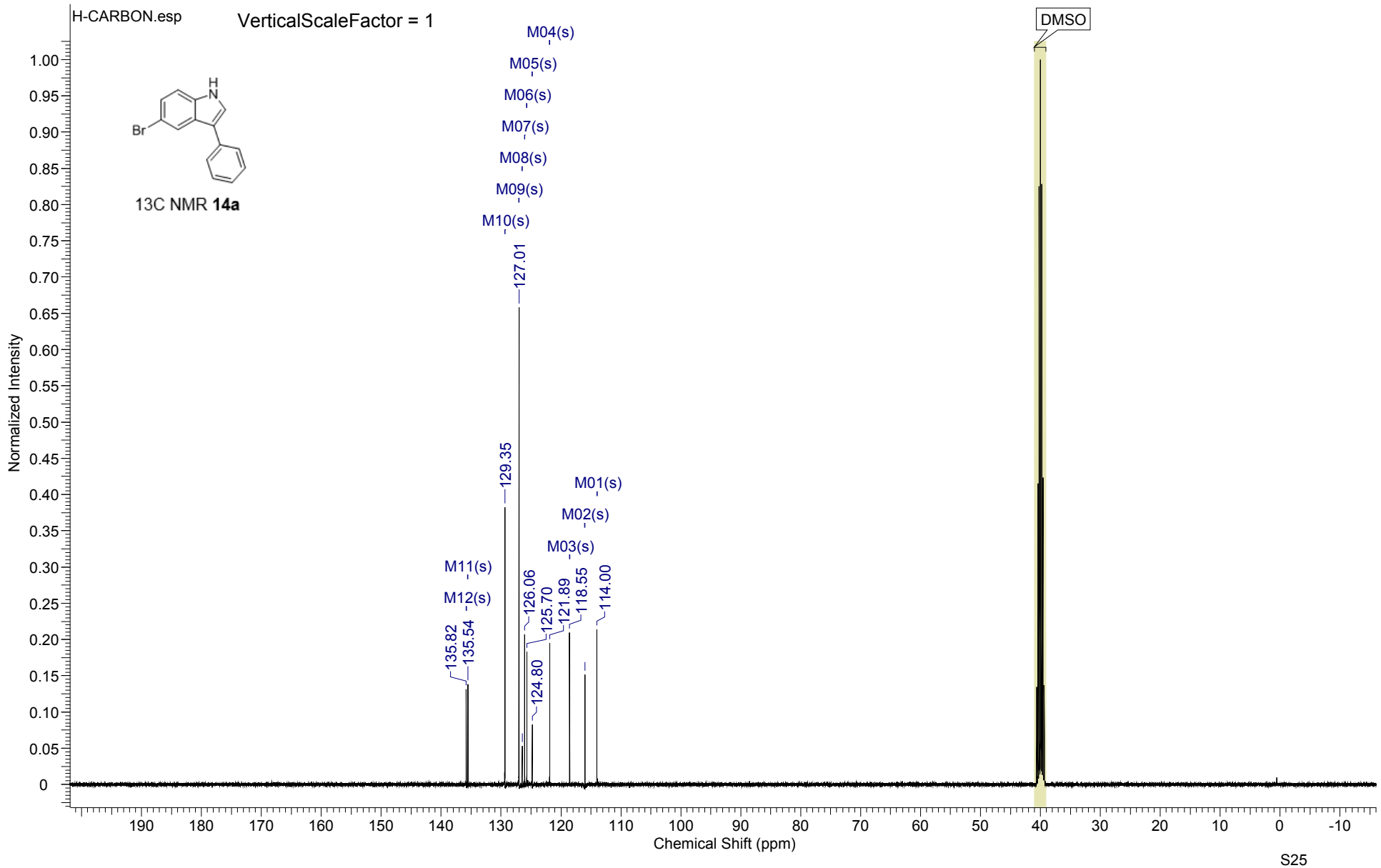

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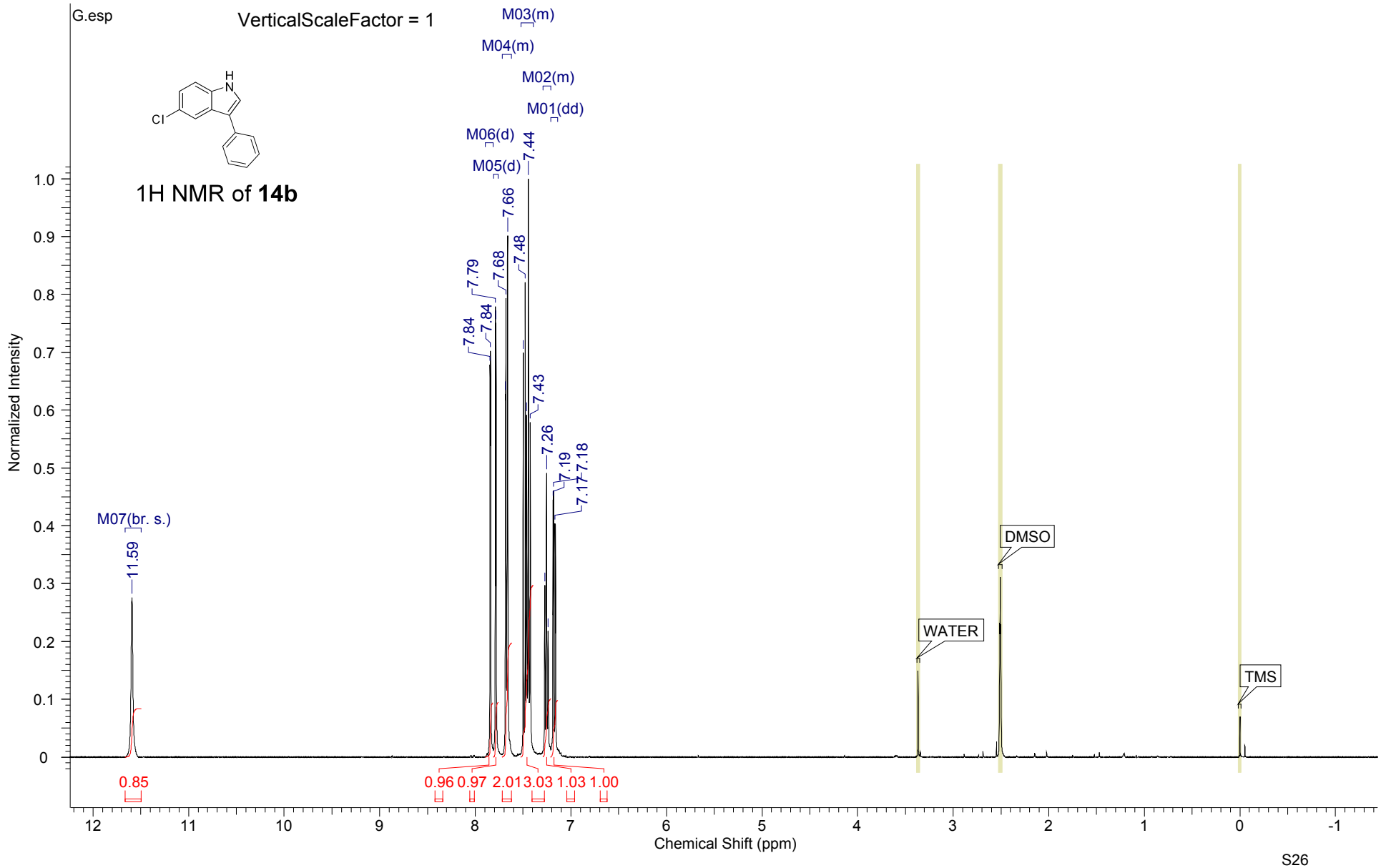

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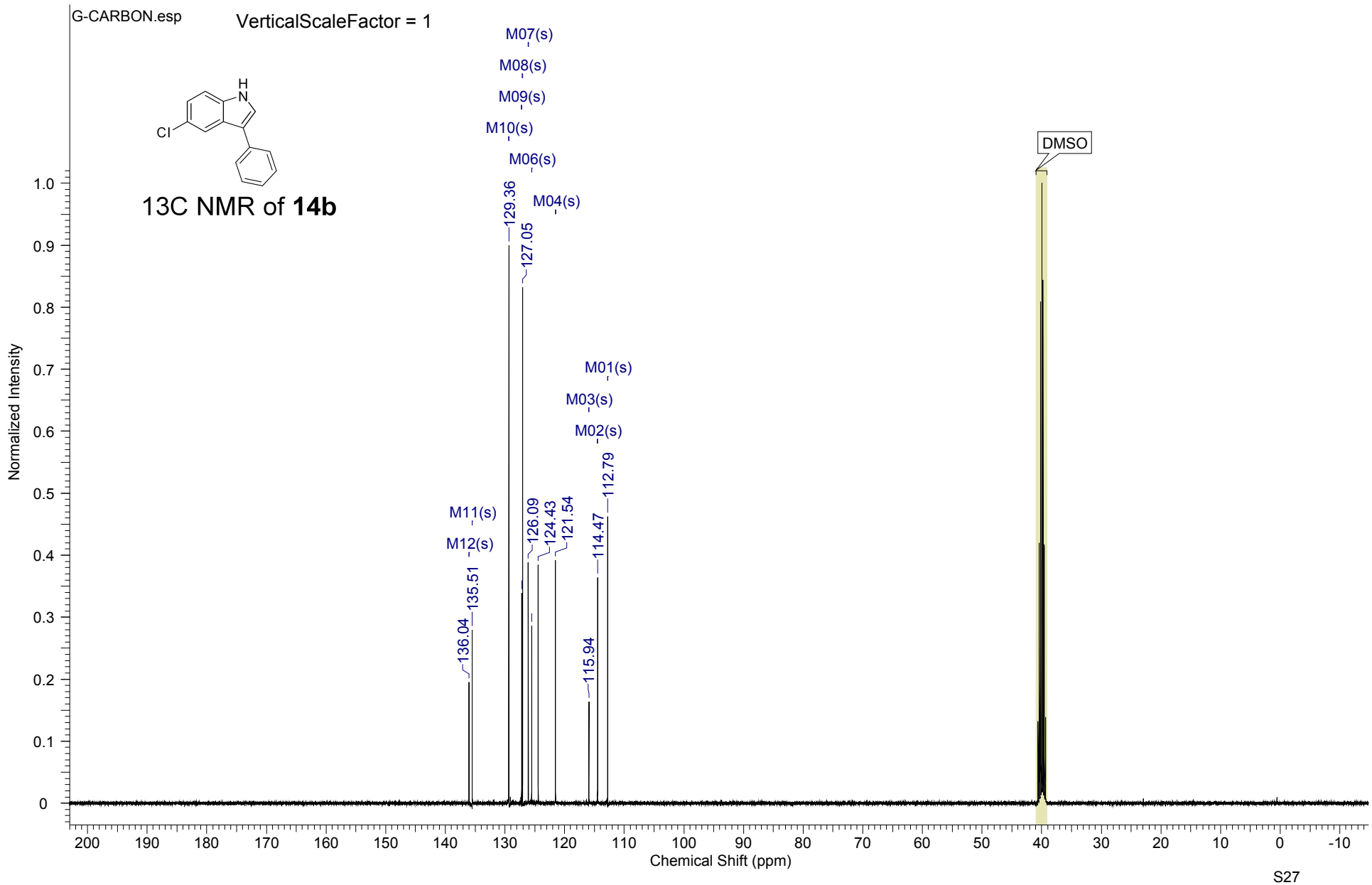

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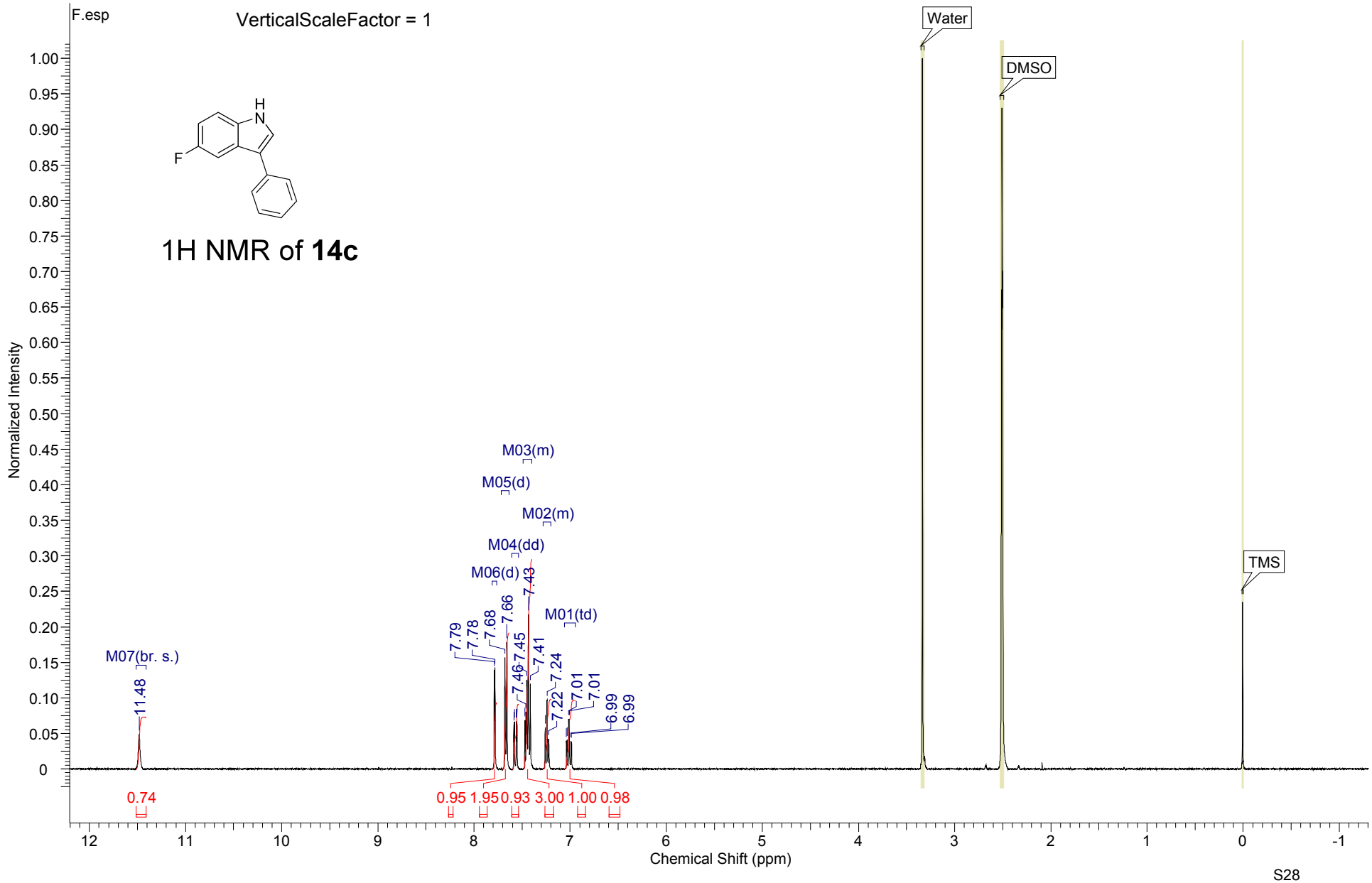
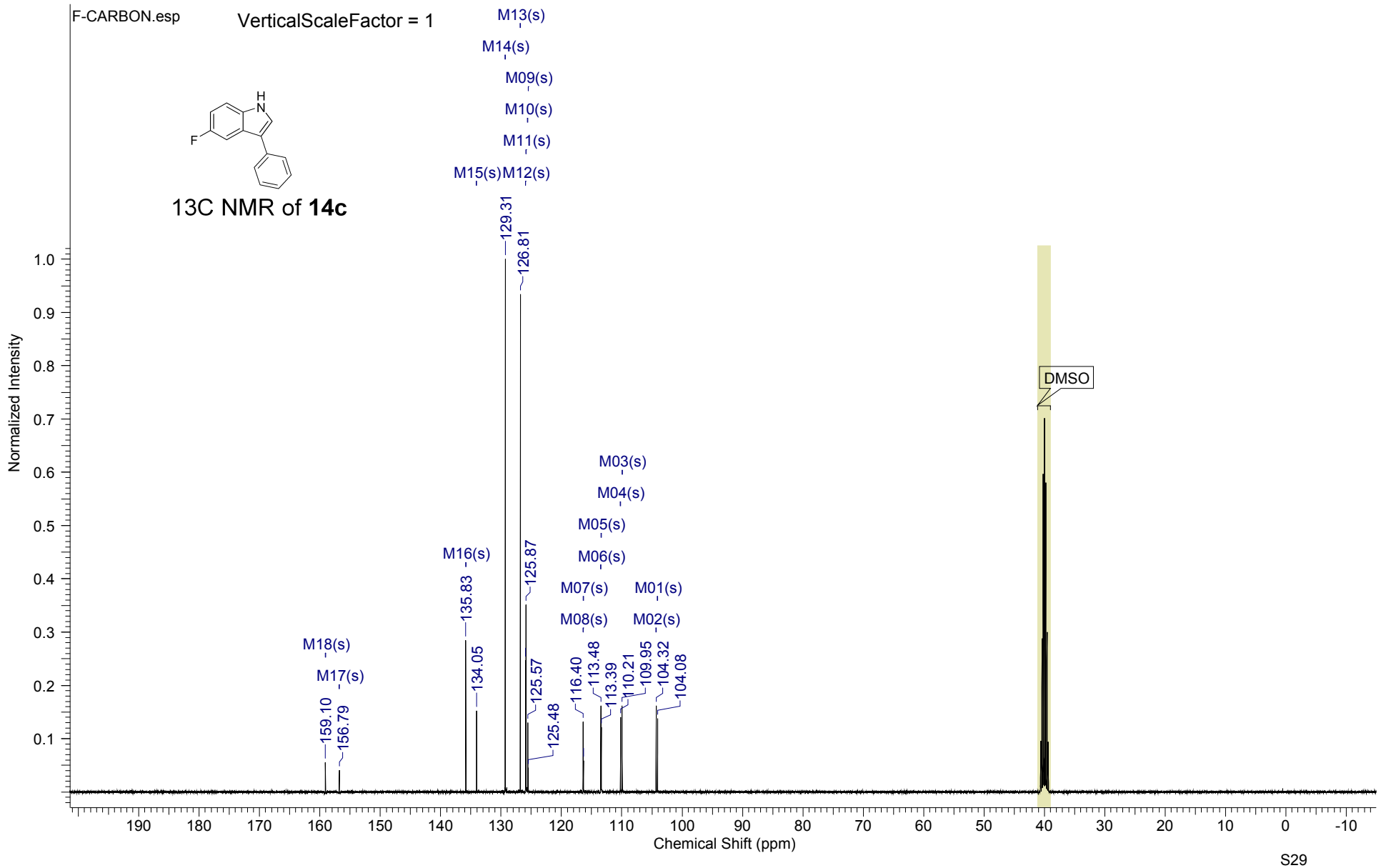
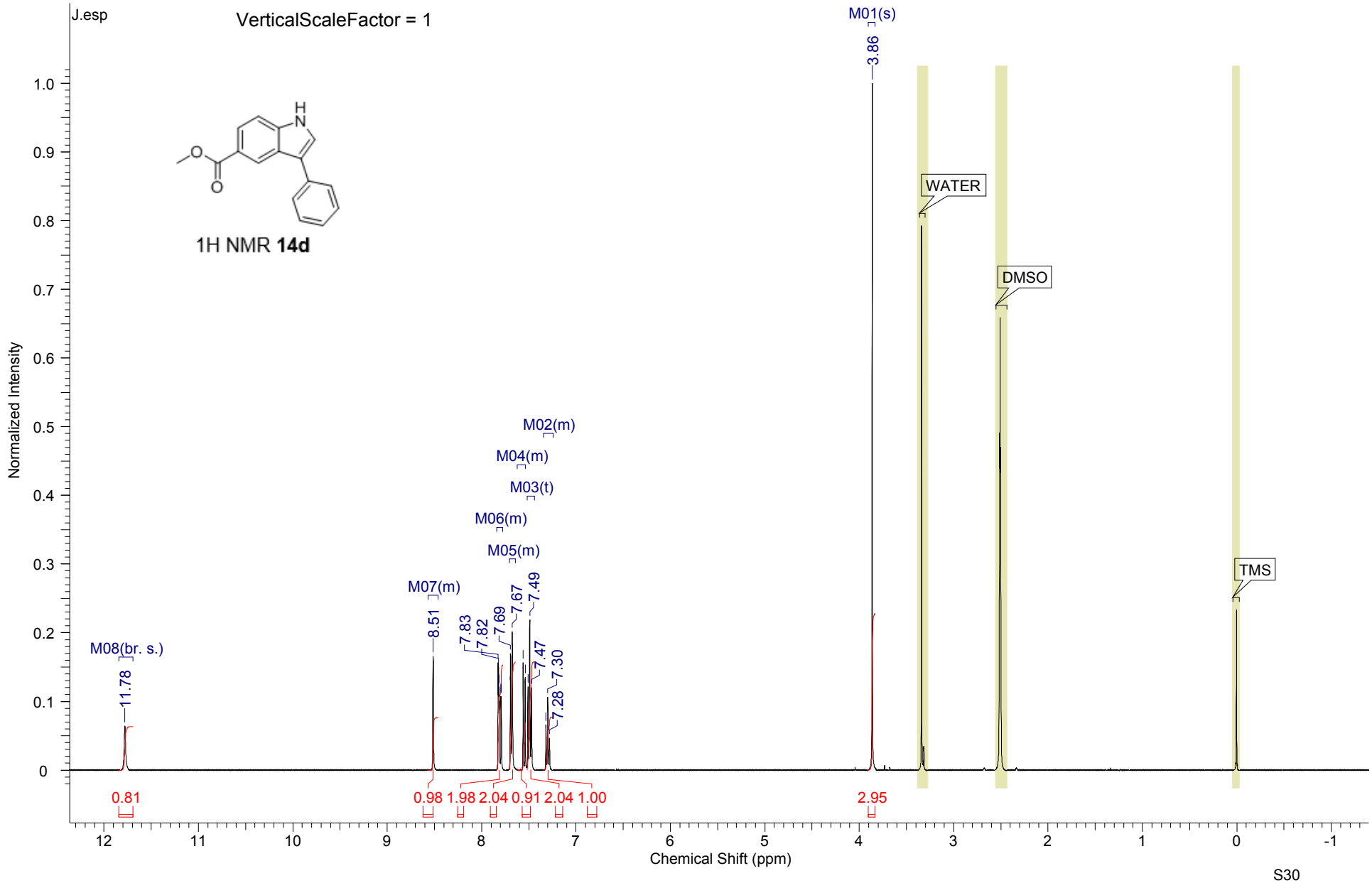
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.659						



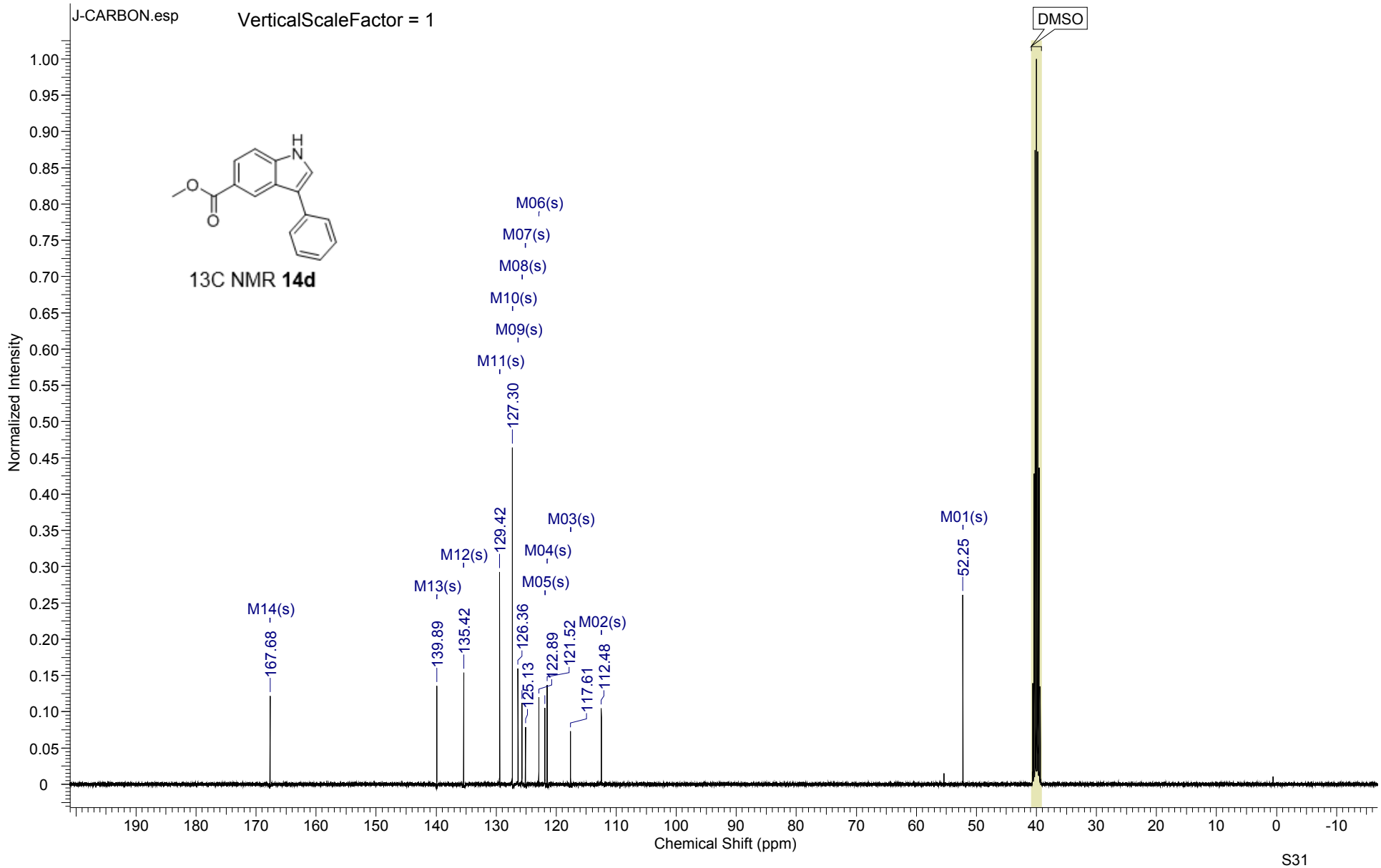
Acquisition Time (sec)	1.3631	***Date***	28 Jul 2017 01:51:12			***Date Stamp***	28 Jul 2017 01:51:12
File Name	D:\NMR\CJO\CJO-F\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	22.973				



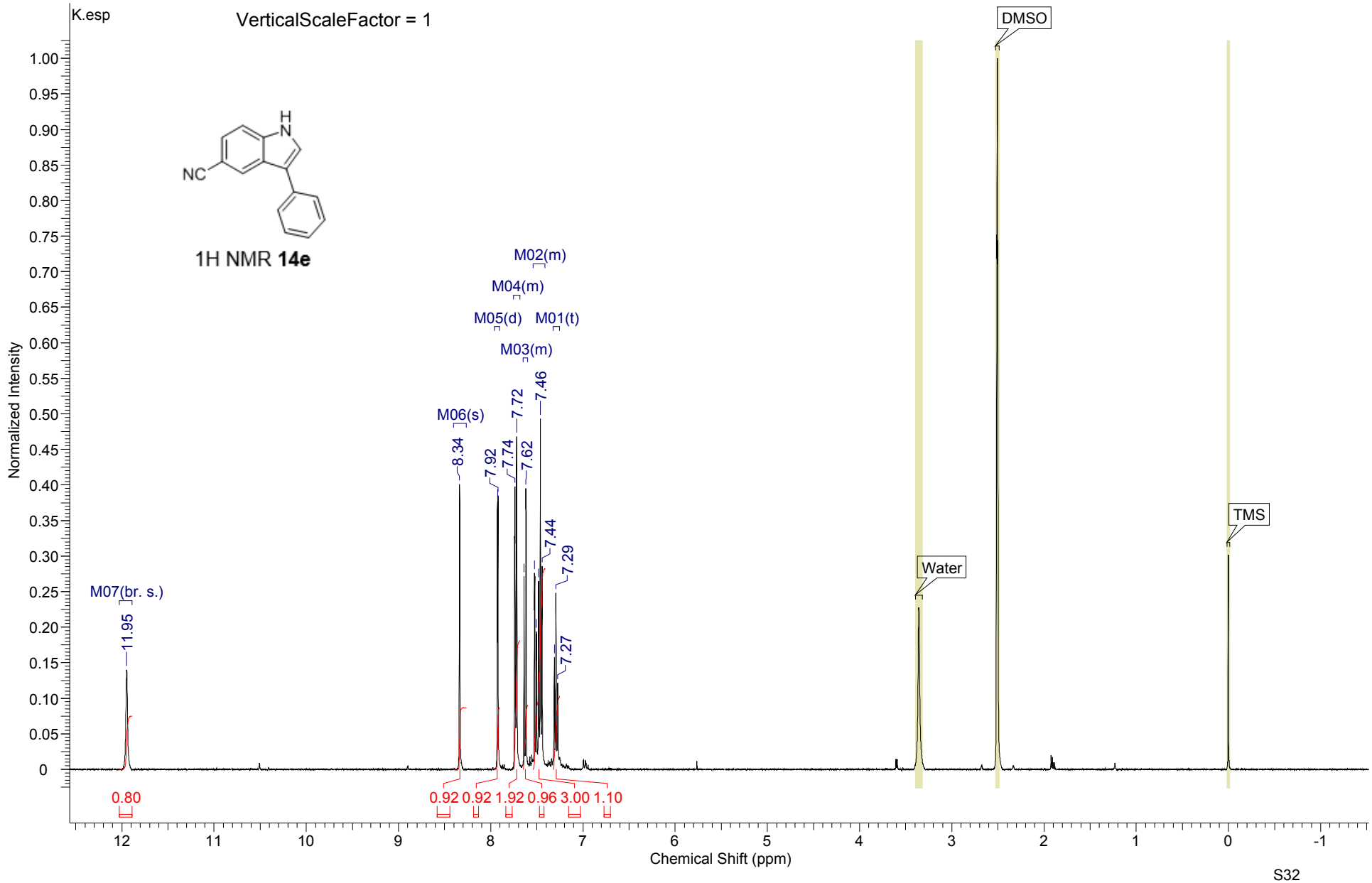
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 09:21:20			***Date Stamp***	03 Aug 2017 09:21:20		
File Name	D:\NMR\CJO\CJO-J\3\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.630						



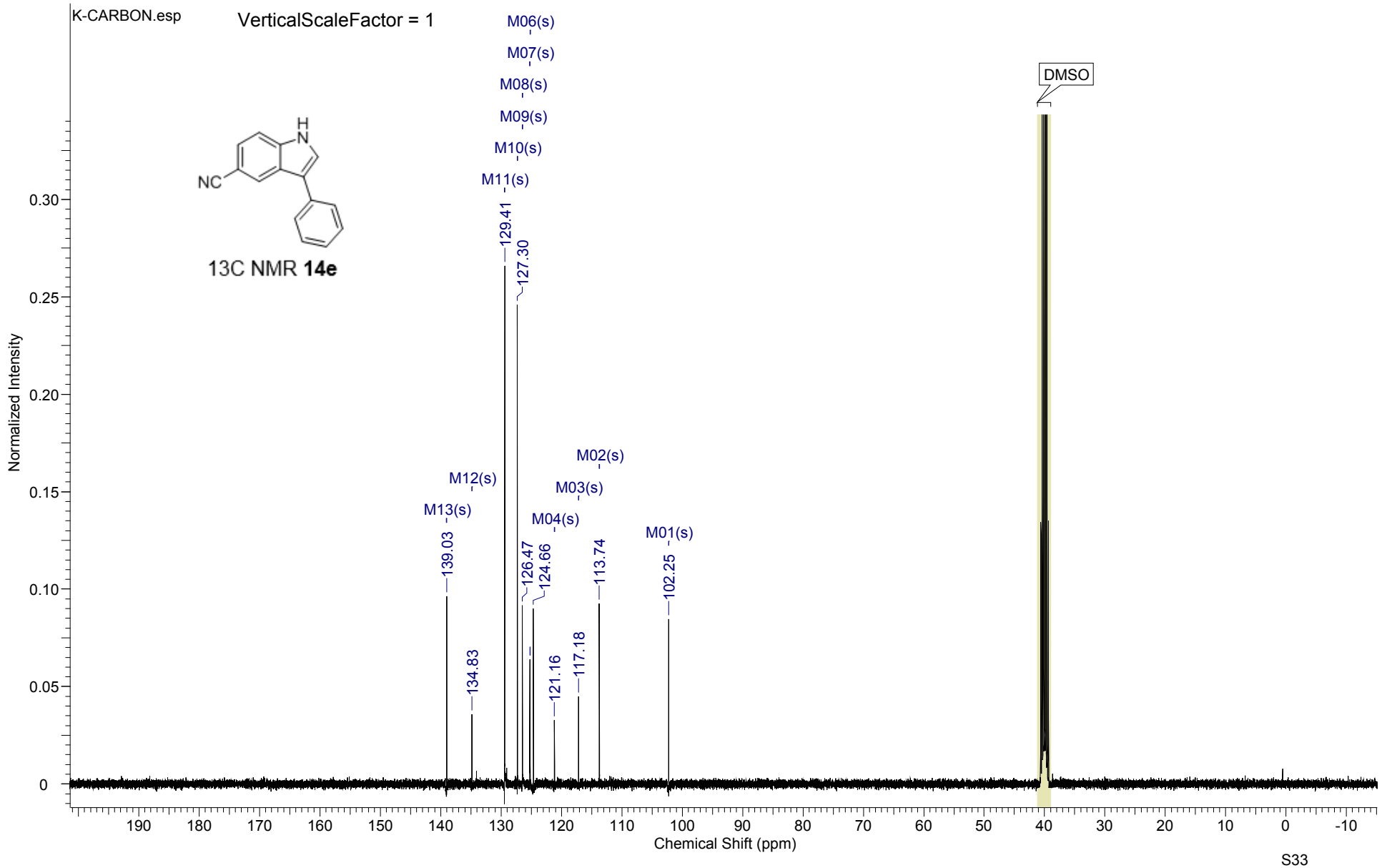
Acquisition Time (sec)	1.3631	***Date***	01 Aug 2017 05:43:44			***Date Stamp***	01 Aug 2017 05:43:44
File Name	D:\NMR\CJO\CJO-J\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.340						



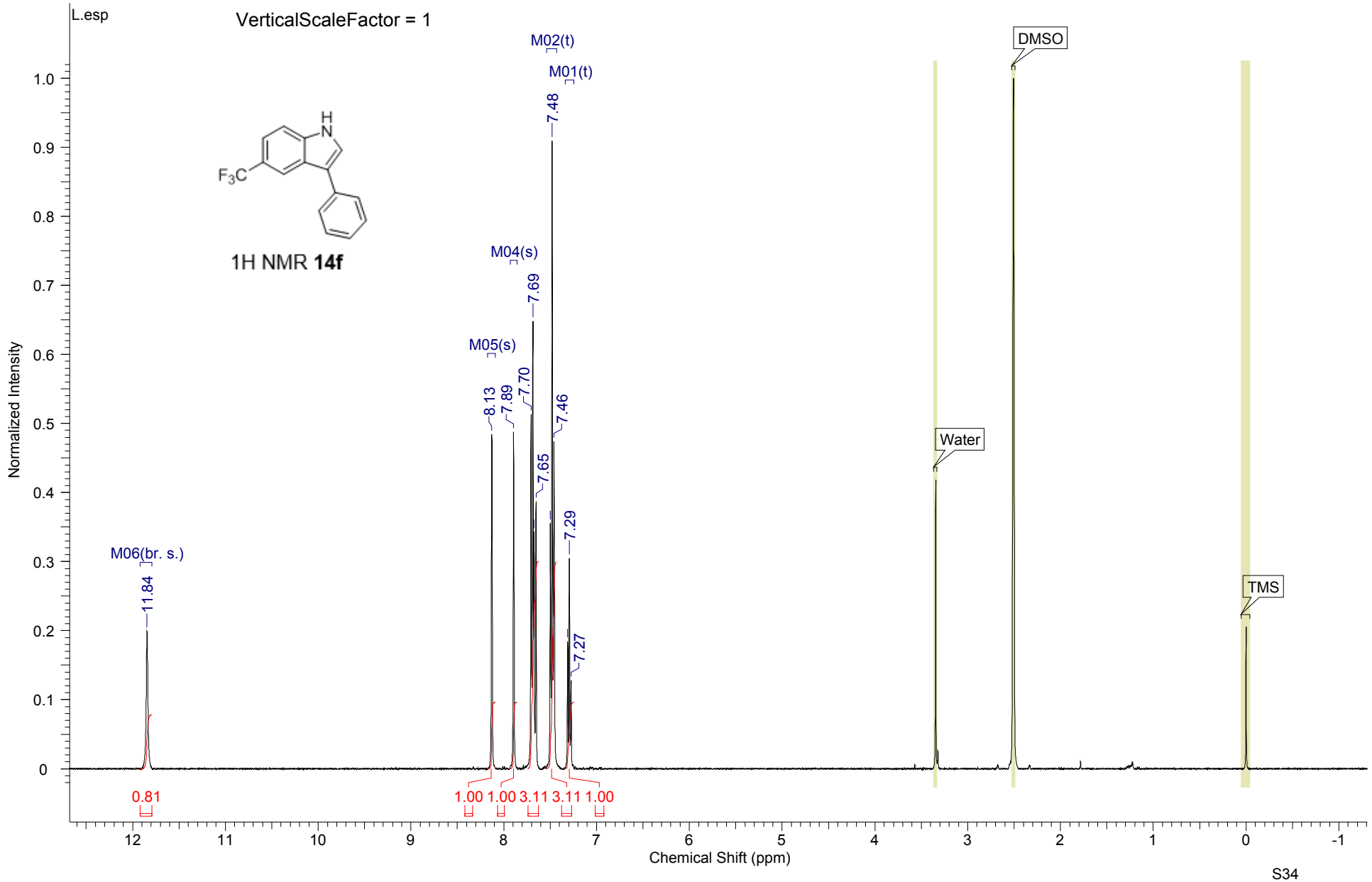
Acquisition Time (sec)	4.0894	***Date***	28 Jul 2017 11:25:04			***Date Stamp***	28 Jul 2017 11:25:04		
File Name	D:\NMR\CJO\CJO-K\2\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.432						



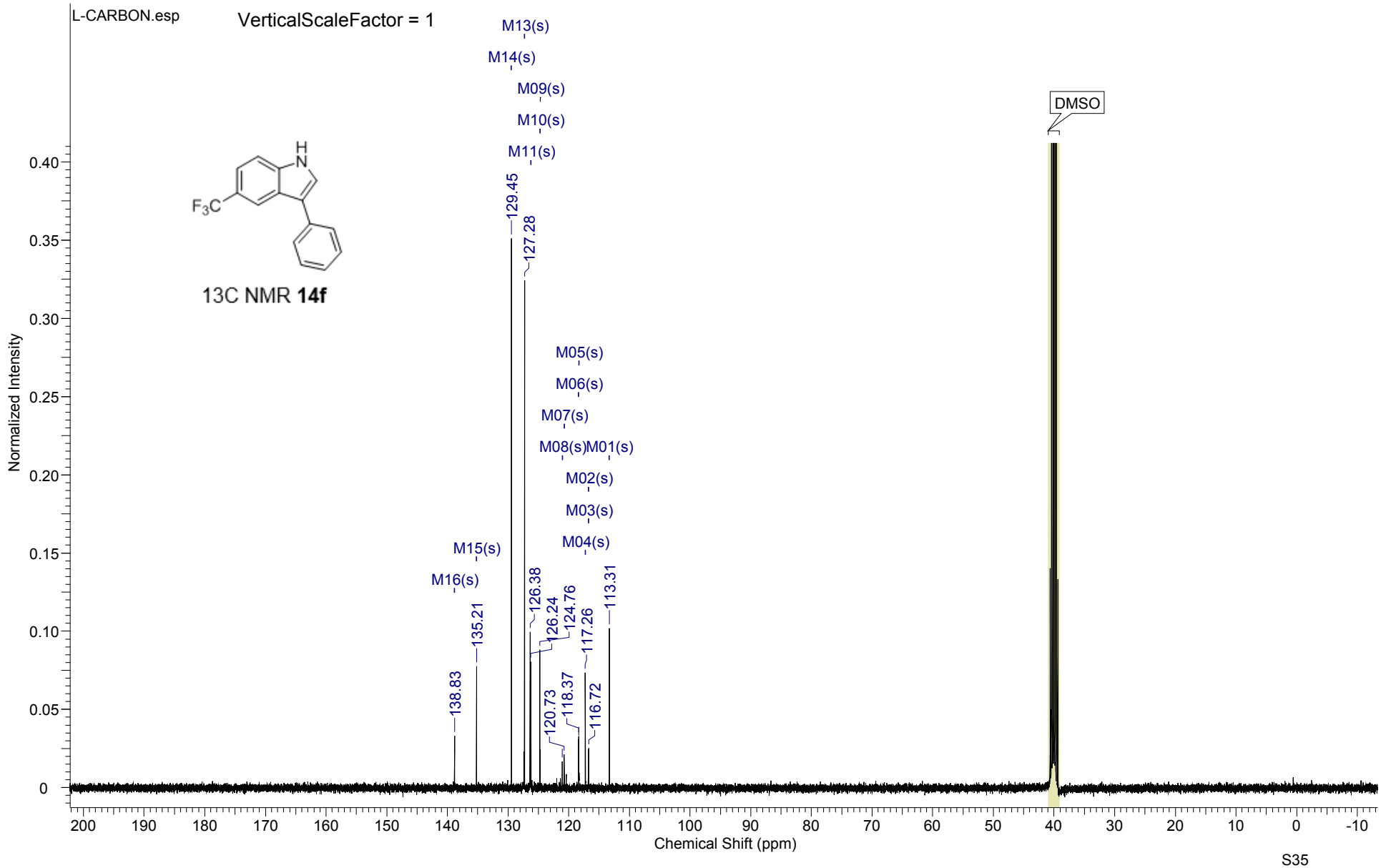
Acquisition Time (sec)	1.3631	***Date***	29 Jul 2017 20:44:00			***Date Stamp***	29 Jul 2017 20:44:00
File Name	D:\NMR\CJO\CJO-K\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.339				



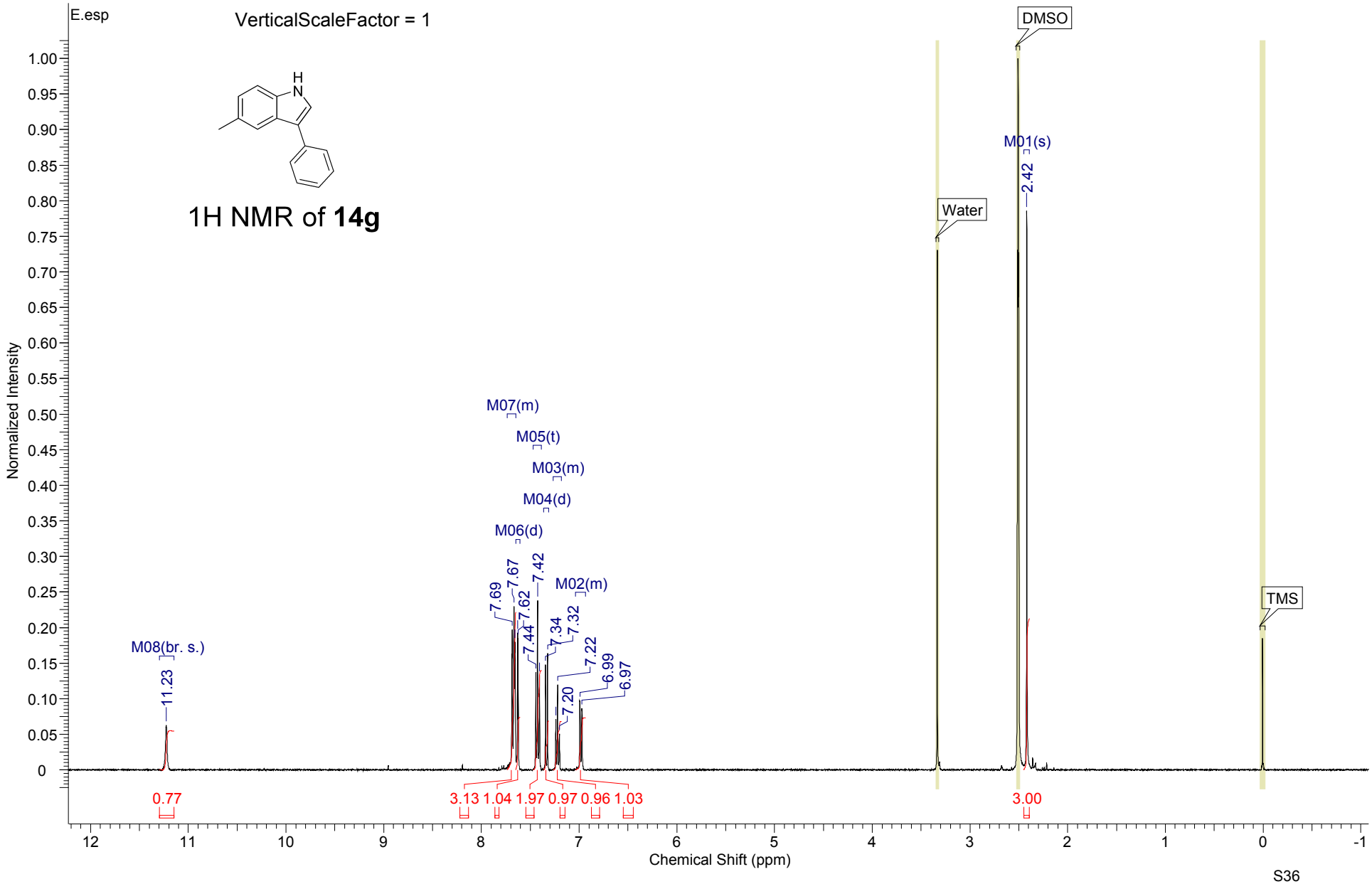
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 08:49:20			***Date Stamp***	03 Aug 2017 08:49:20		
File Name	D:\NMR\CJO\CJO-L\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	110.38	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.559						



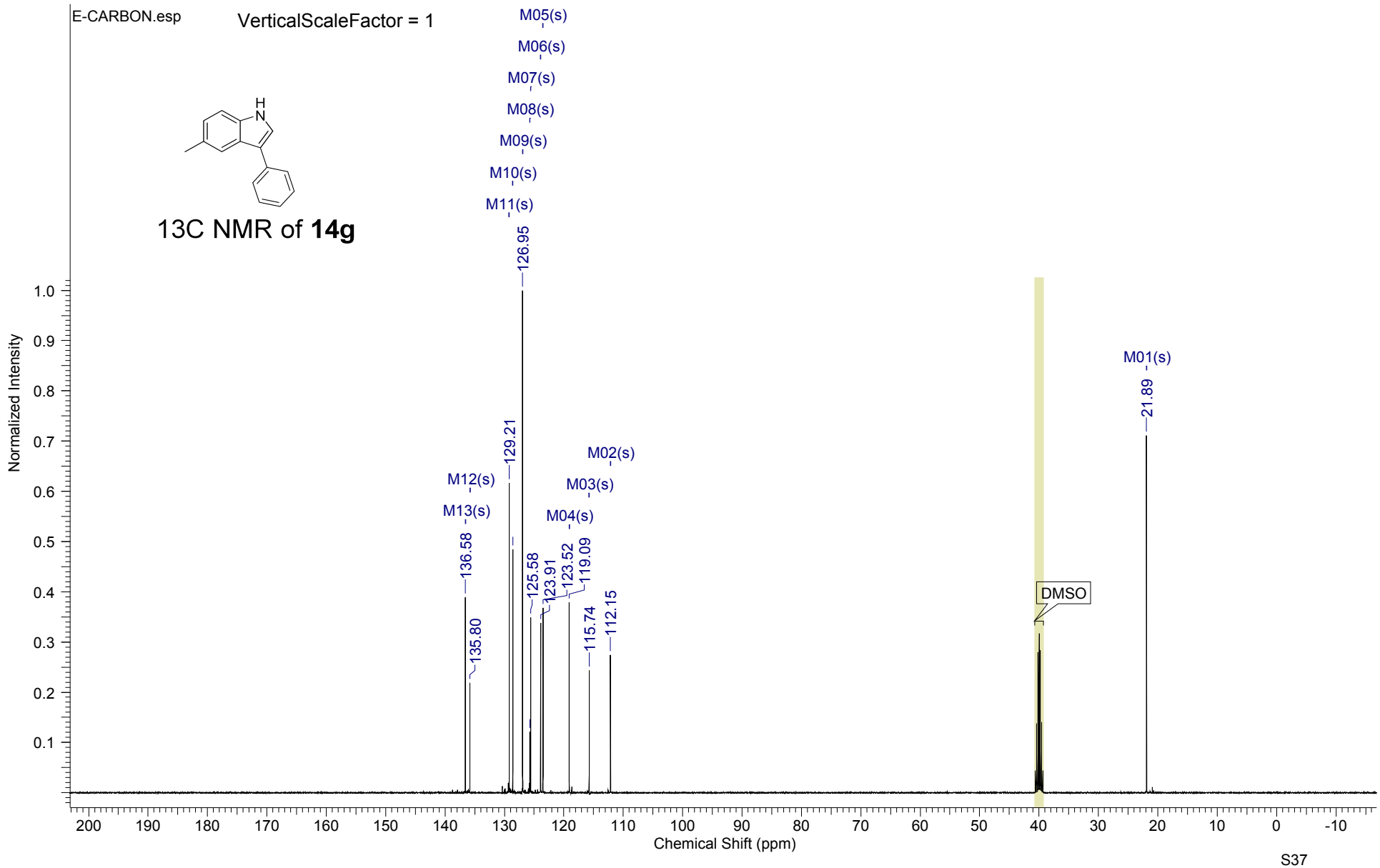
Acquisition Time (sec)	1.3631	***Date***	04 Aug 2017 06:41:20			***Date Stamp***	04 Aug 2017 06:41:20
File Name	D:\NMR\CJO\CJO-L\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.617						



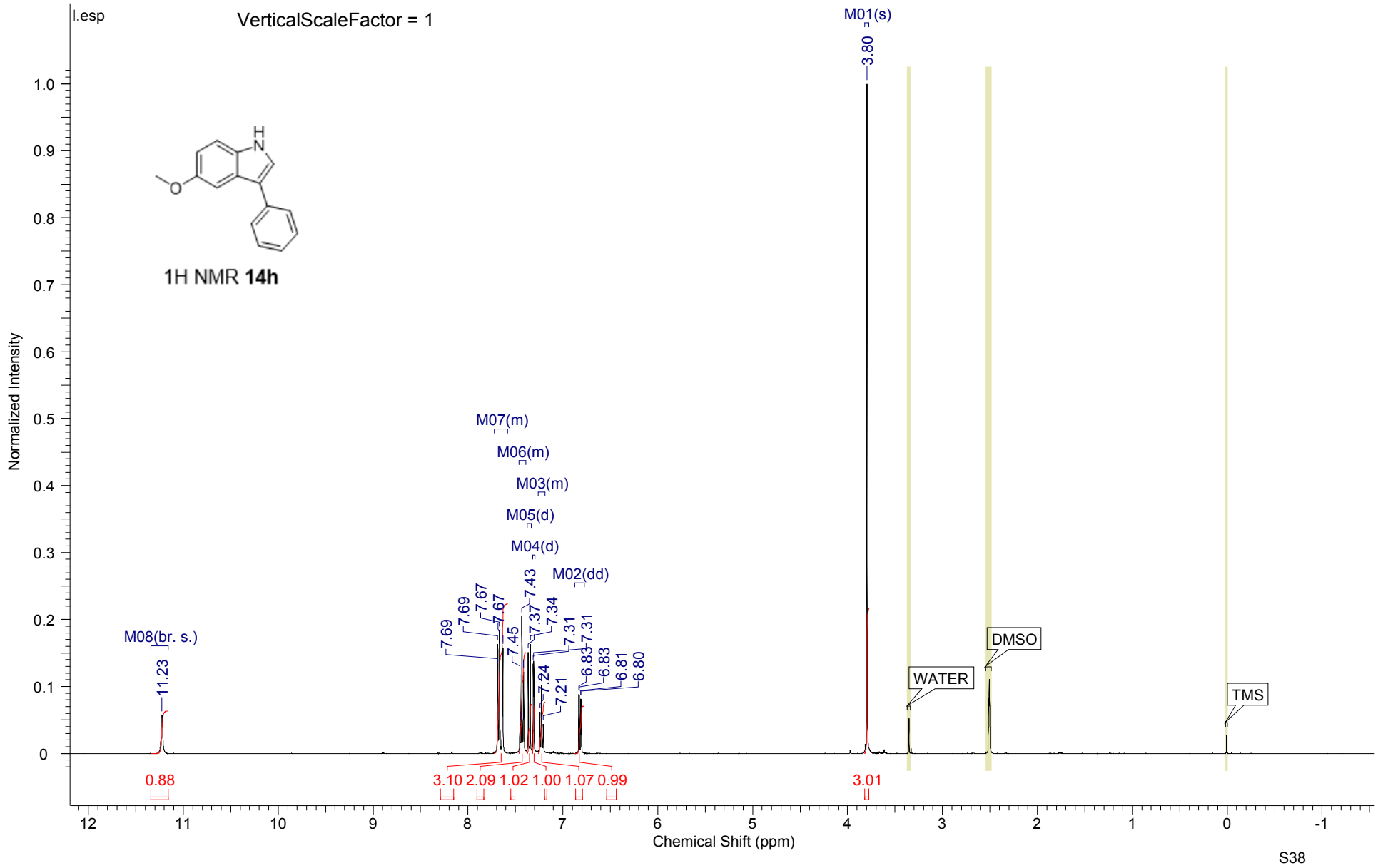
Acquisition Time (sec)	4.0894	***Date***	21 Jul 2017 08:15:12			***Date Stamp***	21 Jul 2017 08:15:12		
File Name	D:\NMR\CJO\CJO-E\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.747						



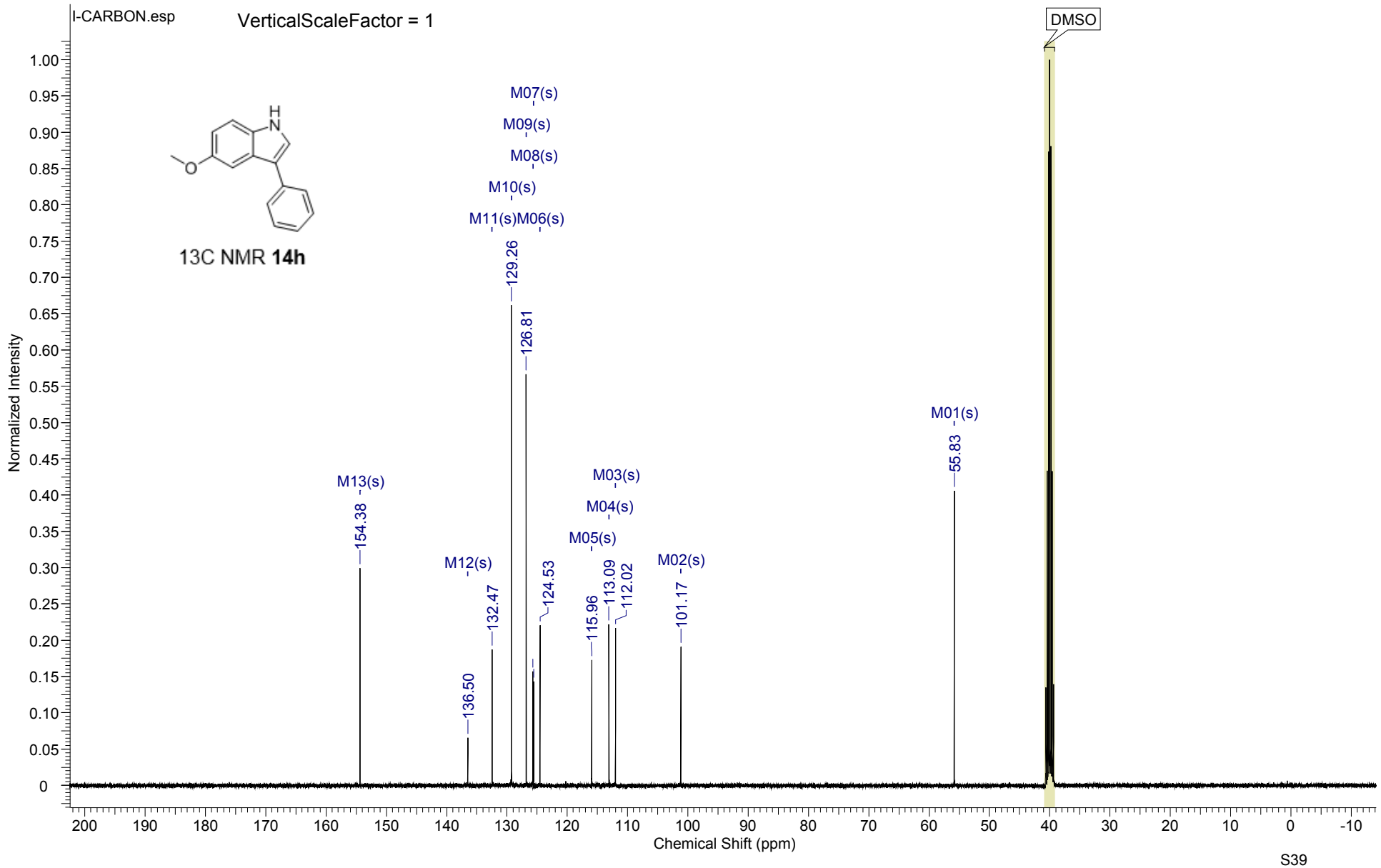
Acquisition Time (sec)	1.3631	***Date***	27 Jul 2017 05:41:36			***Date Stamp***	27 Jul 2017 05:41:36
File Name	D:\NMR\CJO\CJO-E\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.122				



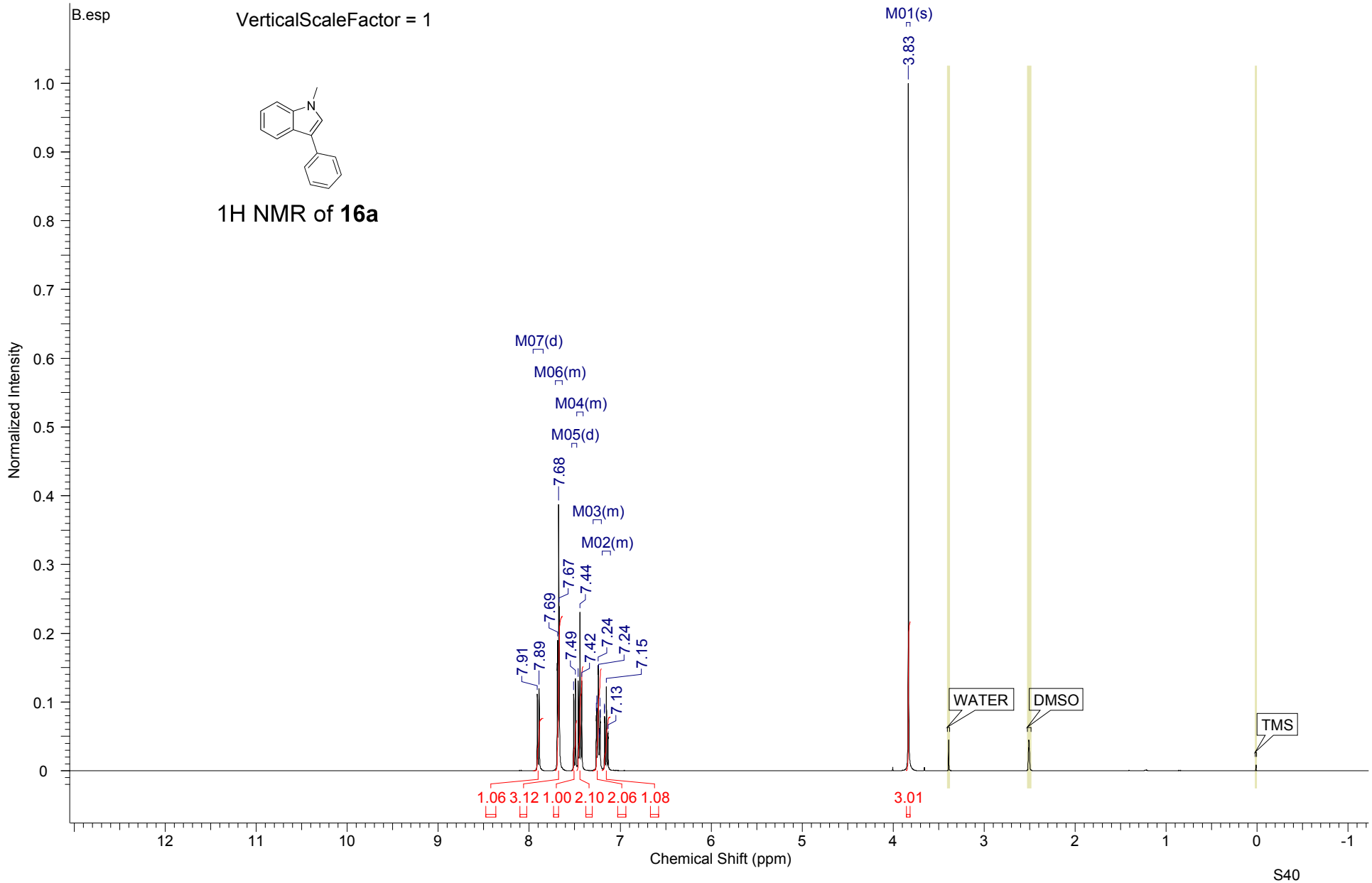
Acquisition Time (sec)	4.0894	***Date***	20 Jul 2017 14:17:52			***Date Stamp***	20 Jul 2017 14:17:52
File Name	D:\NMR\New folder\New folder\015-011(I)\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	86.78	***SW(cyclical) (Hz)***	8012.82
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	2470.9255	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8012.58
Temperature (degree C)	22.609						



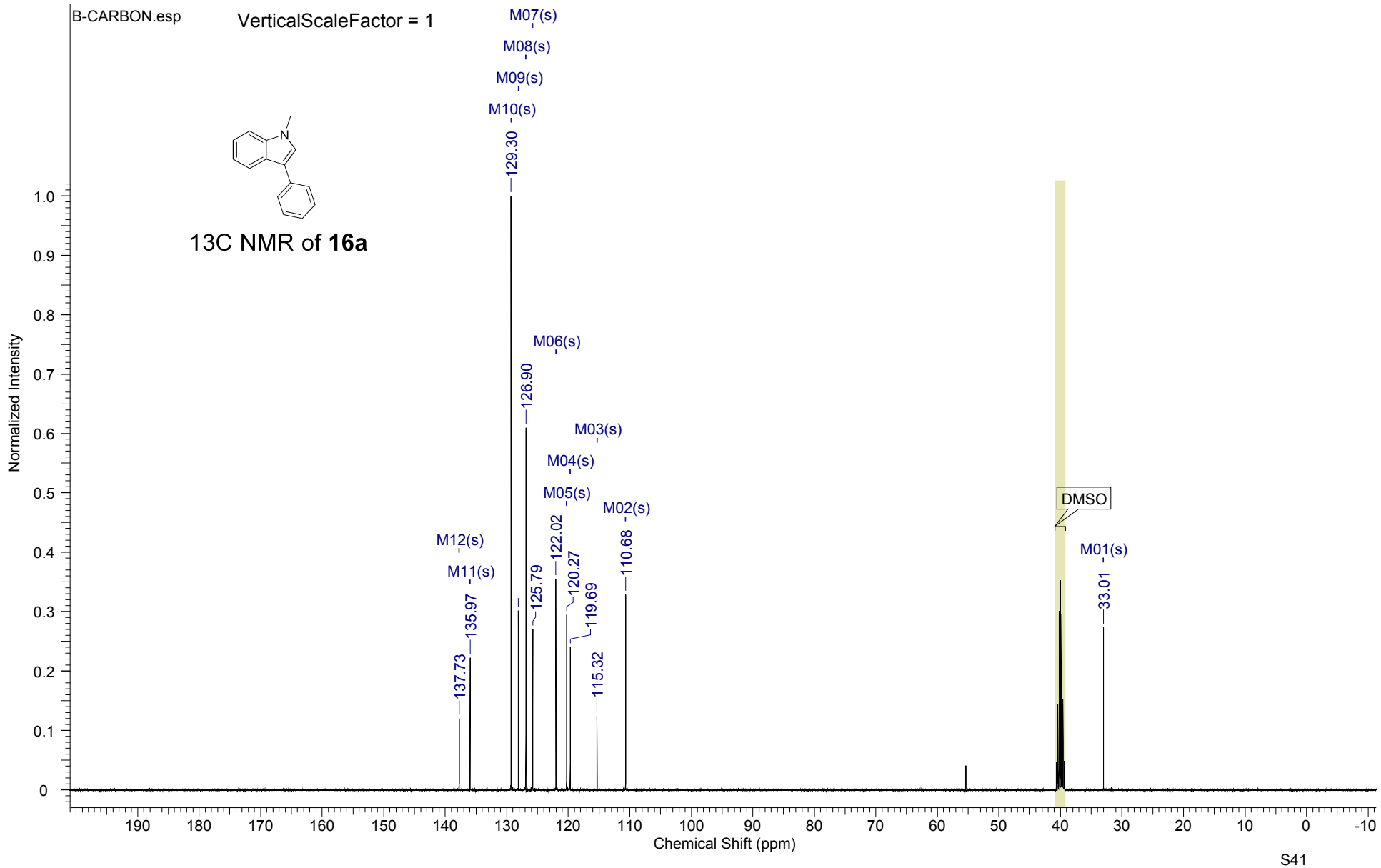
Acquisition Time (sec)	1.3631	***Date***	29 Jul 2017 11:29:20			***Date Stamp***	29 Jul 2017 11:29:20
File Name	D:\NMR\CJO\CJO-I\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.142				



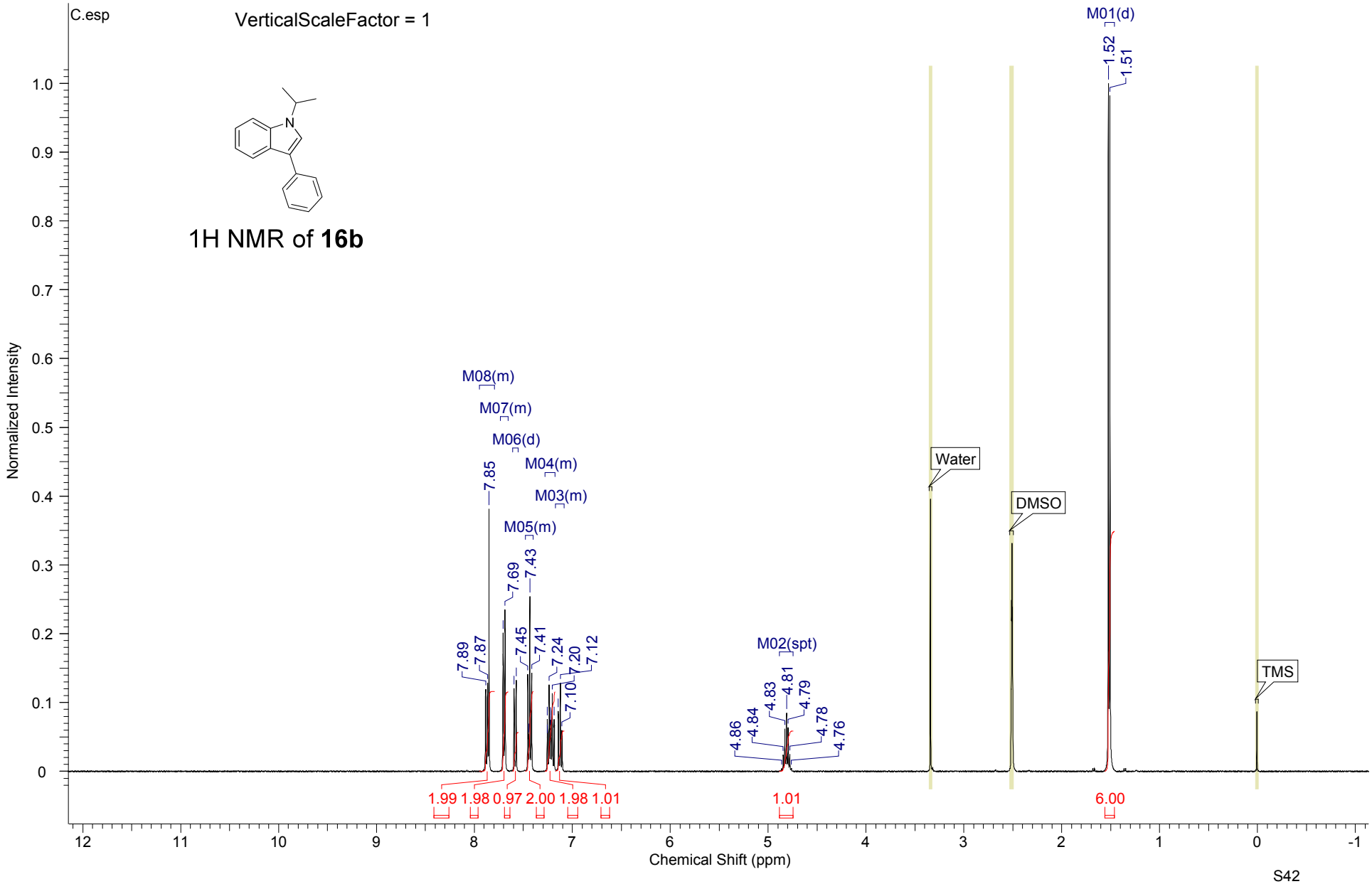
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 08:23:44			***Date Stamp***	03 Aug 2017 08:23:44		
File Name	D:\NMR\CJO\CJO-B\3\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	30.74	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.511						



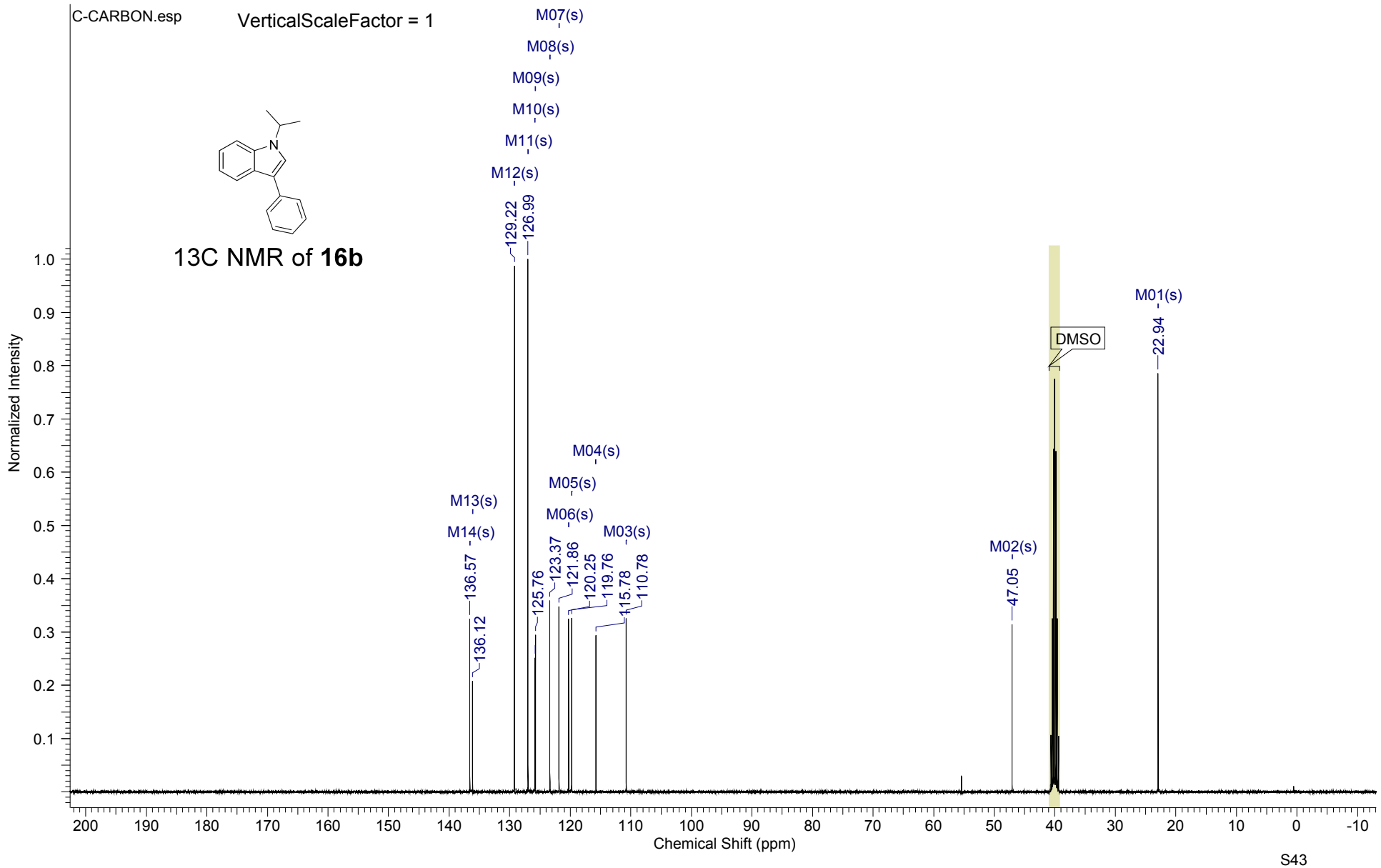
Acquisition Time (sec)	1.3631	***Date***	29 Jul 2017 00:53:36			***Date Stamp***	29 Jul 2017 00:53:36
File Name	D:\NMR\CJO\CJO-B\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.252				



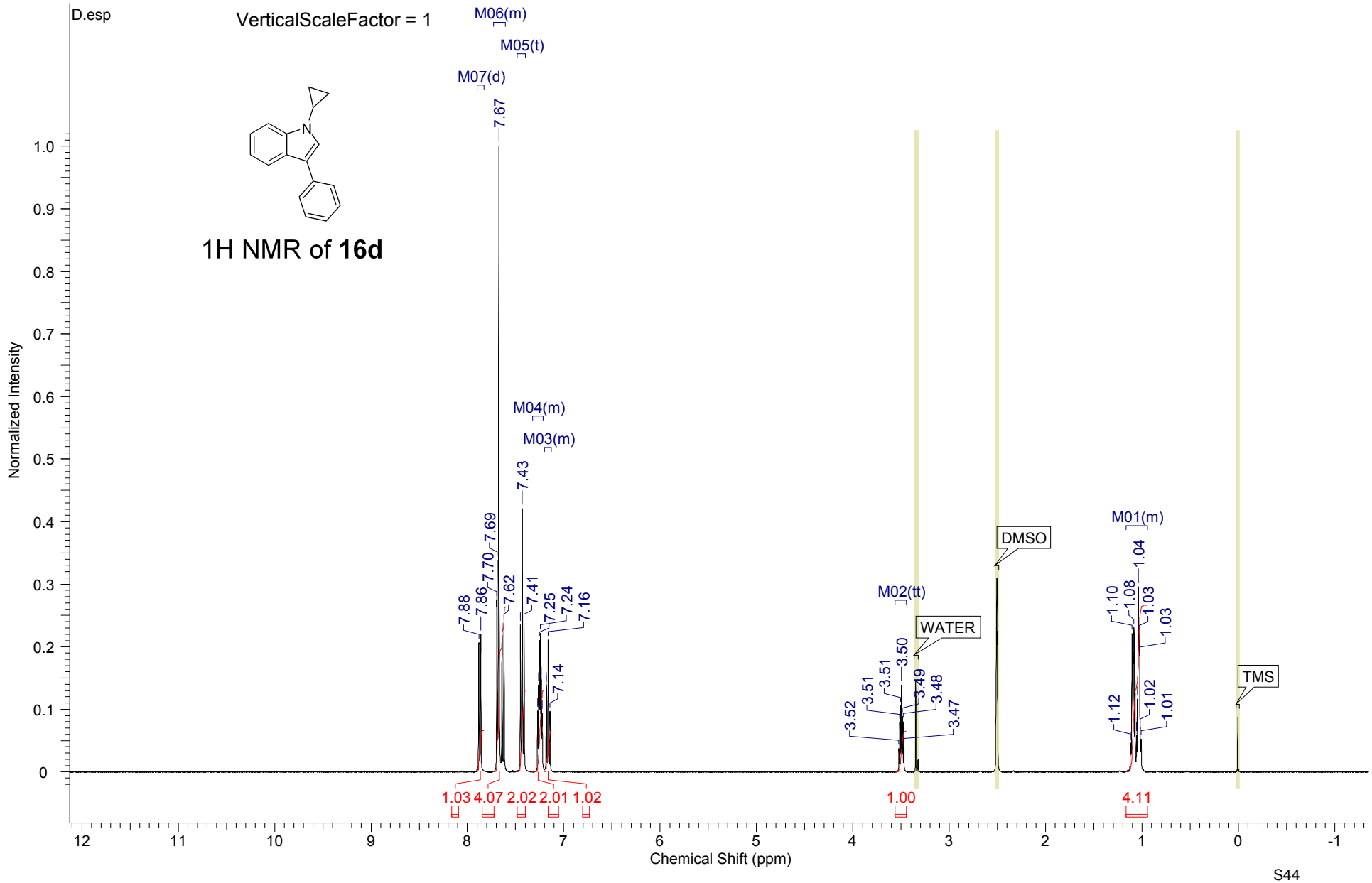
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 08:30:08			***Date Stamp***	03 Aug 2017 08:30:08		
File Name	D:\NMR\CJO\CJO-C\3\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	110.38	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.498						



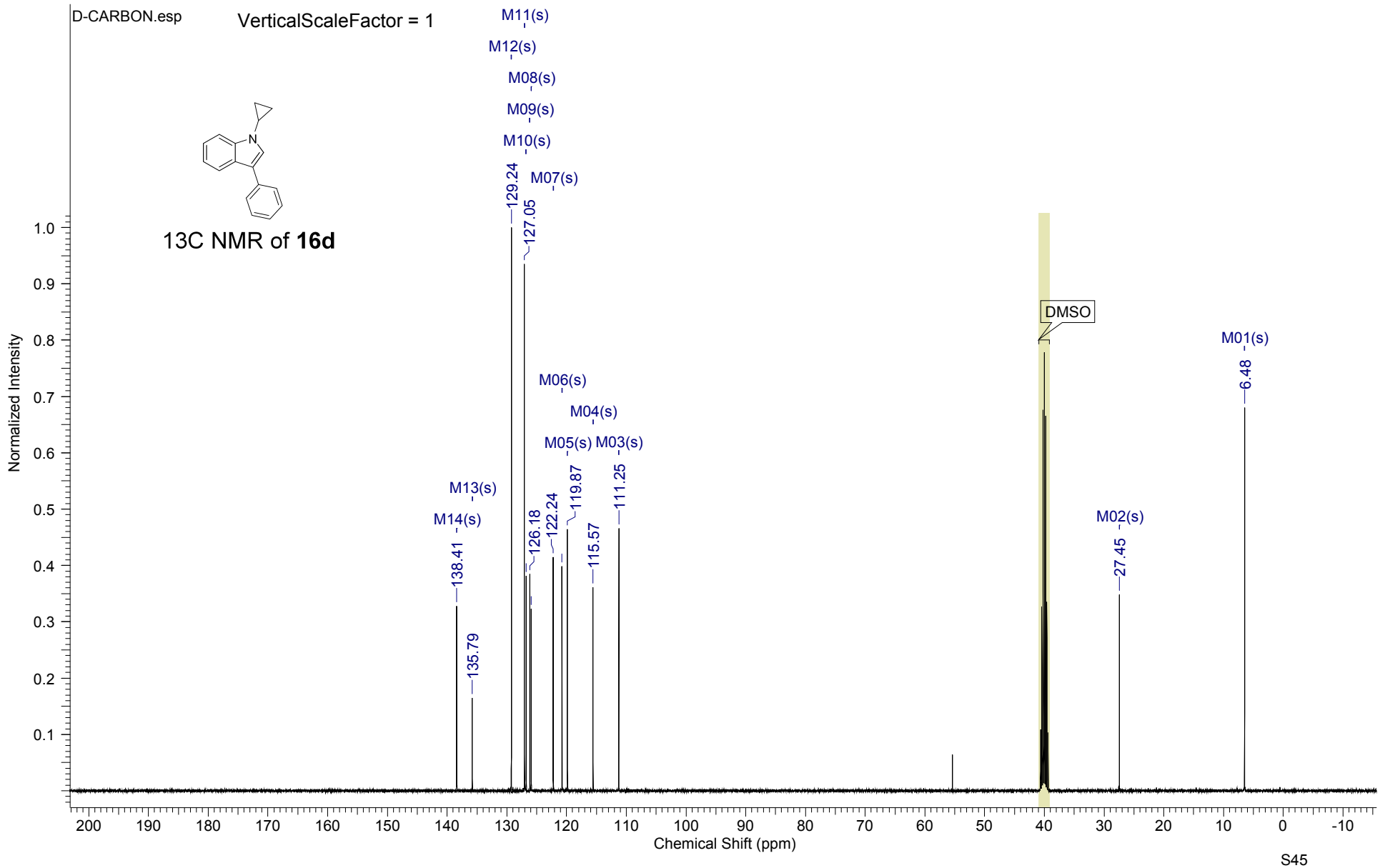
Acquisition Time (sec)	1.3631	***Date***	30 Jul 2017 04:26:56			***Date Stamp***	30 Jul 2017 04:26:56
File Name	D:\NMR\CJO\CJO-C\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.182				



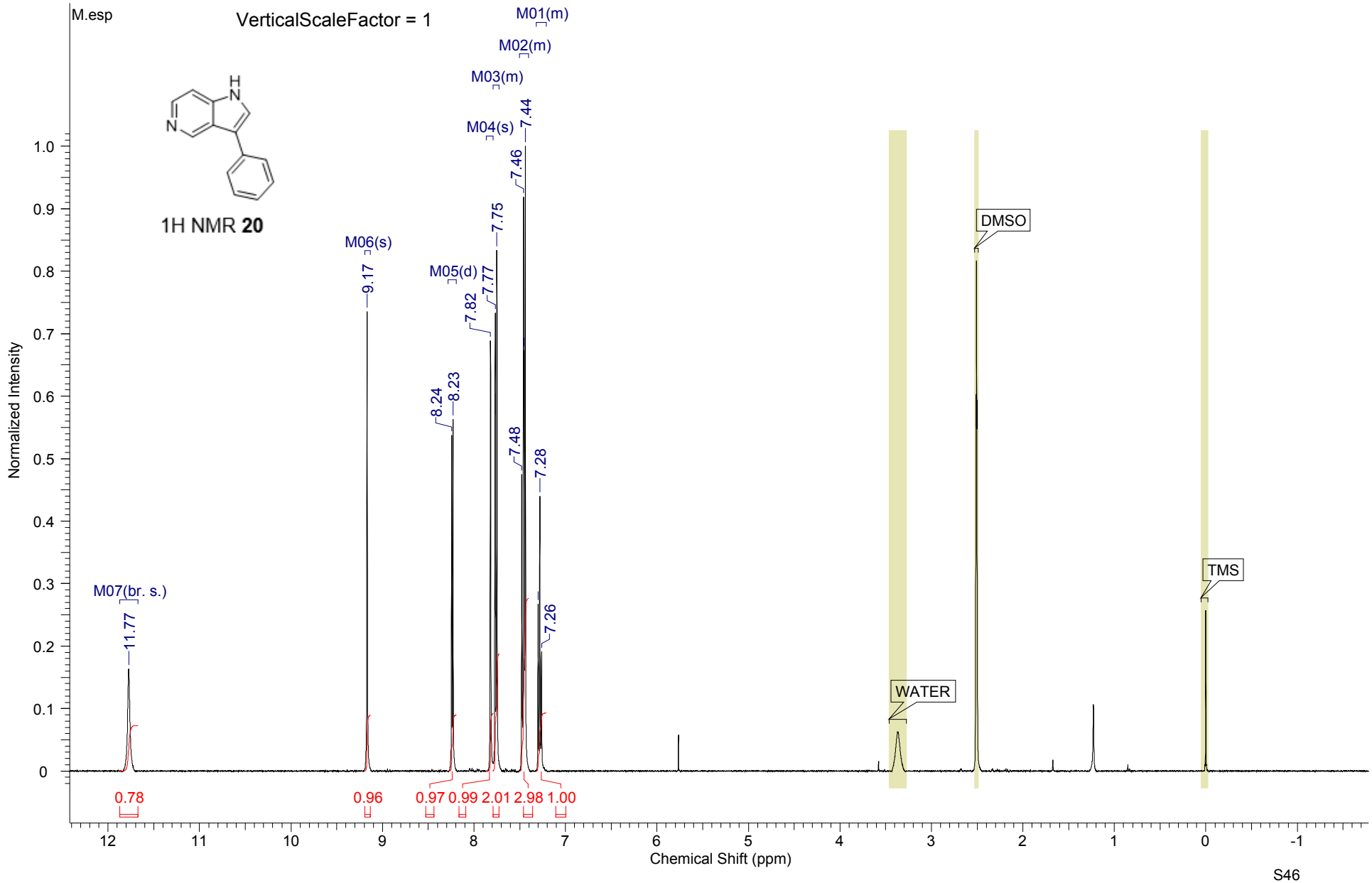
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 08:34:24			***Date Stamp***	03 Aug 2017 08:34:24		
File Name	D:\NMR\CJO\CJO-D\3\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	77.61	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.496						



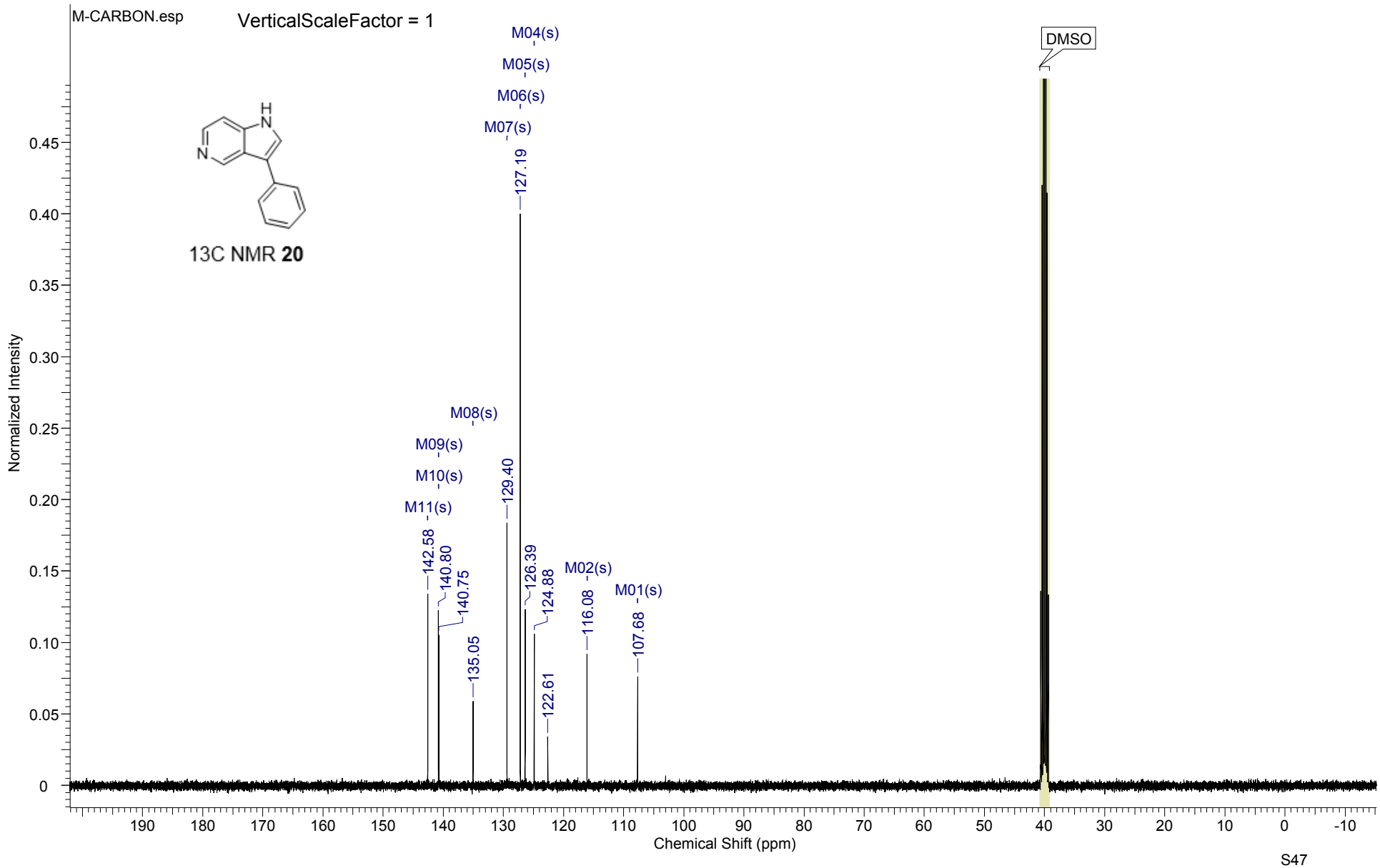
Acquisition Time (sec)	1.3631	***Date***	30 Jul 2017 00:34:24			***Date Stamp***	30 Jul 2017 00:34:24
File Name	D:\NMR\CJO\CJO-D\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD		
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.021				



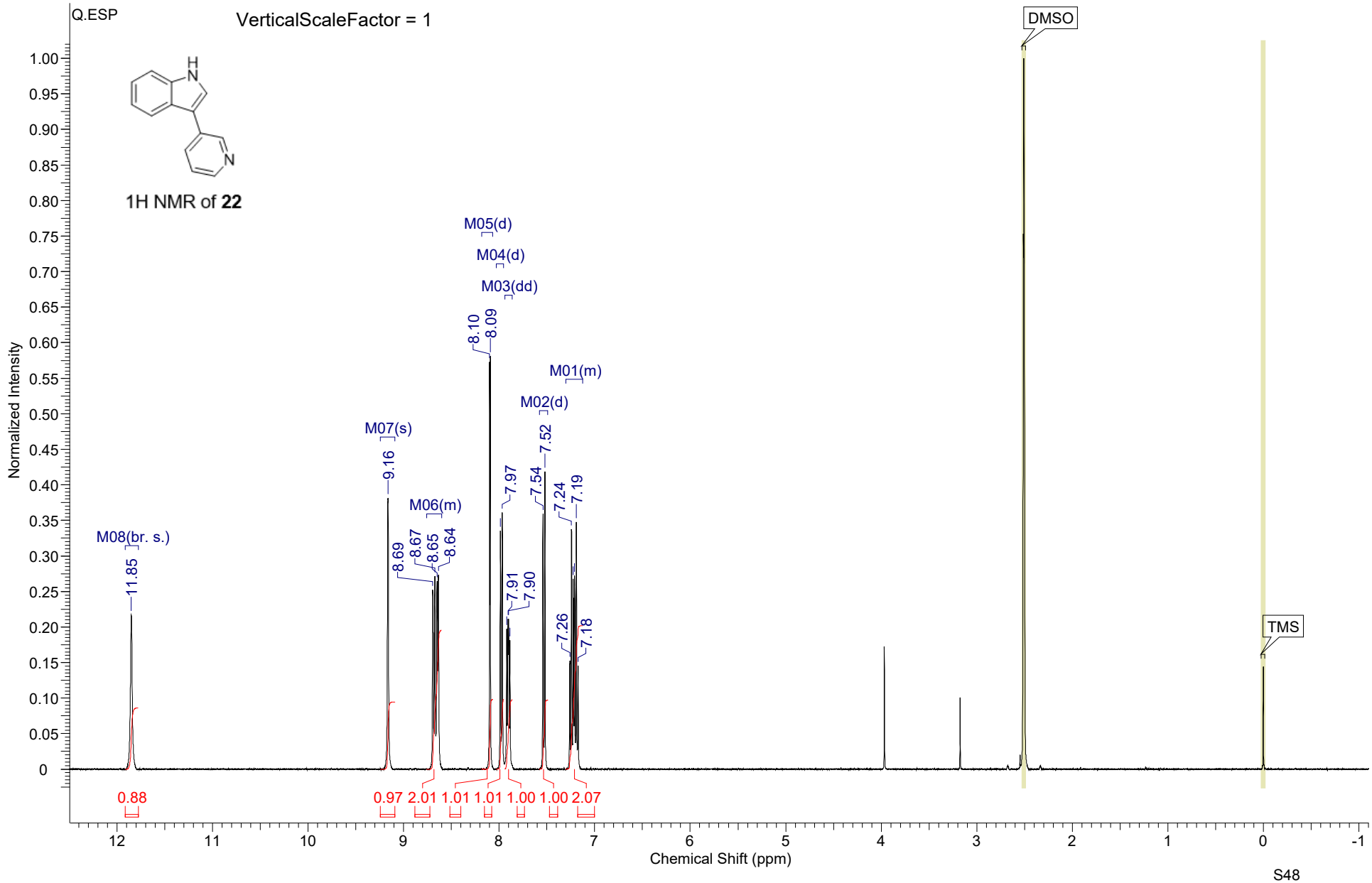
Acquisition Time (sec)	4.0894	***Date***	16 Aug 2017 14:28:32			***Date Stamp***	16 Aug 2017 14:28:32		
File Name	D:\CJO-UCSF\NMR\CJO-M\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	110.38	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.730						



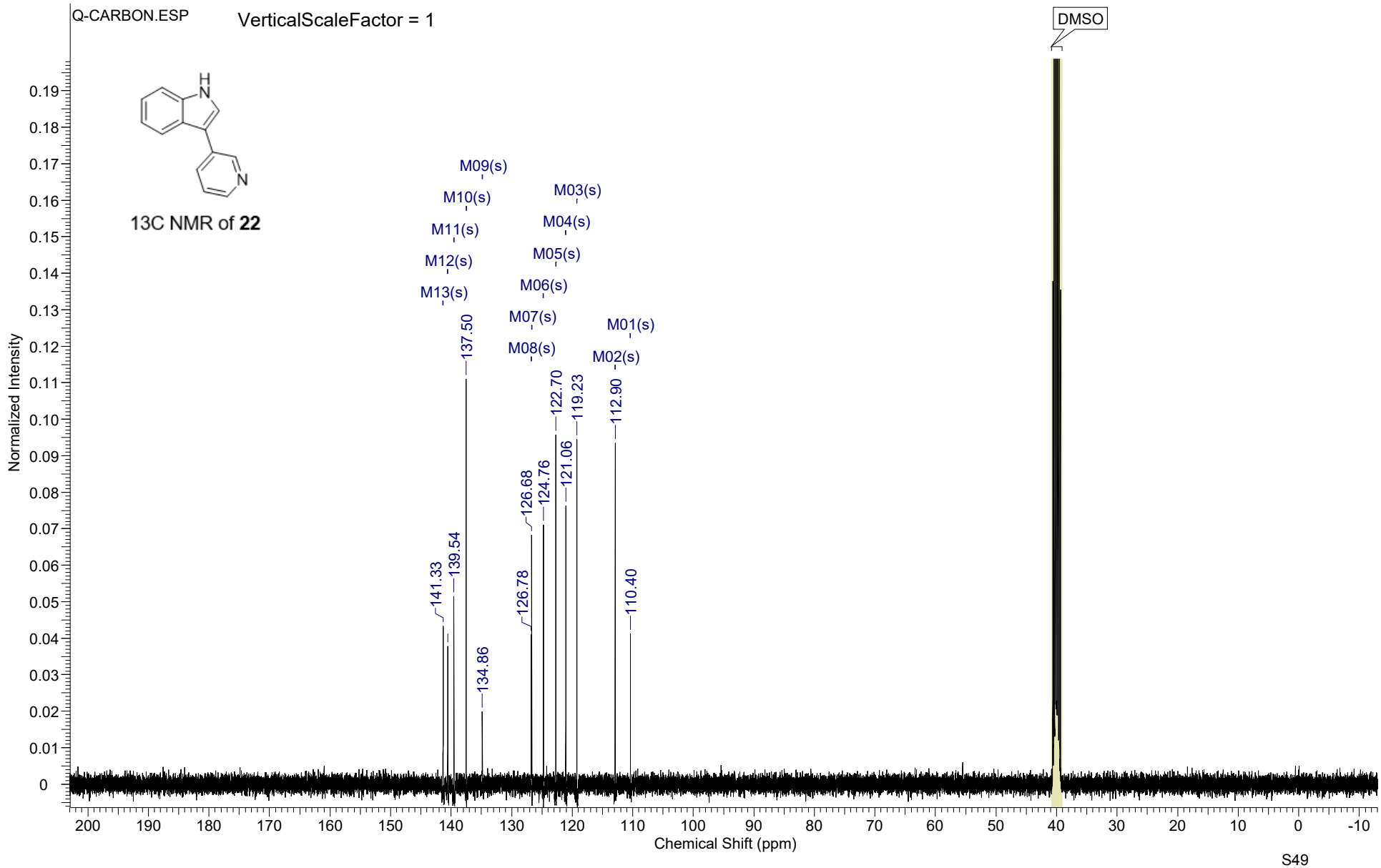
Acquisition Time (sec)	1.3631	***Date***	17 Aug 2017 05:45:52			***Date Stamp***	17 Aug 2017 05:45:52
File Name	D:\CJO-UCSF\NMR\CJO-M\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.262						



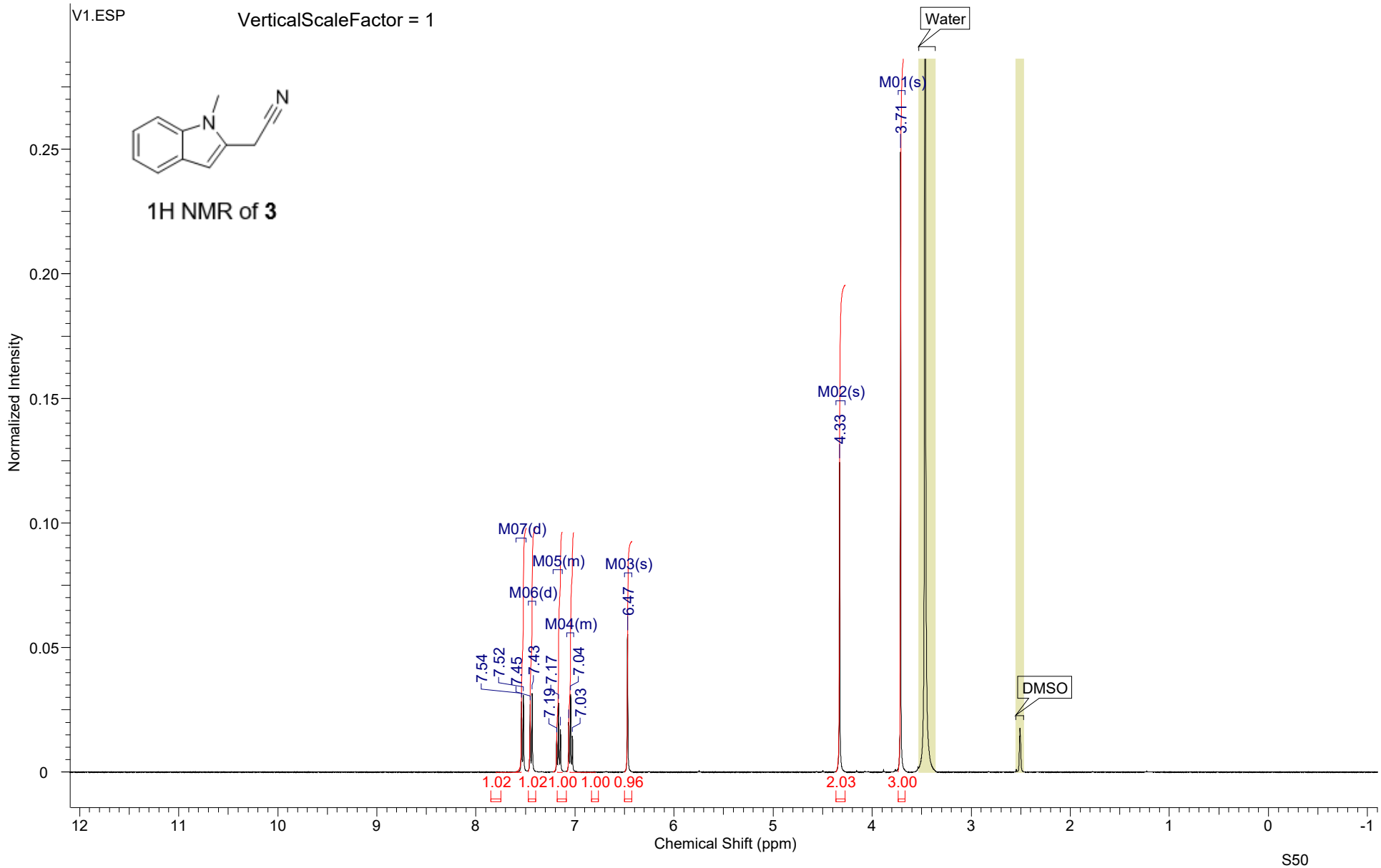
Acquisition Time (sec)	4.0894	***Date***	10 Aug 2017 08:51:28			***Date Stamp***	10 Aug 2017 08:51:28		
File Name	D:\CJO-UCSF\NMR\CJO-Q\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	110.38	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.607						



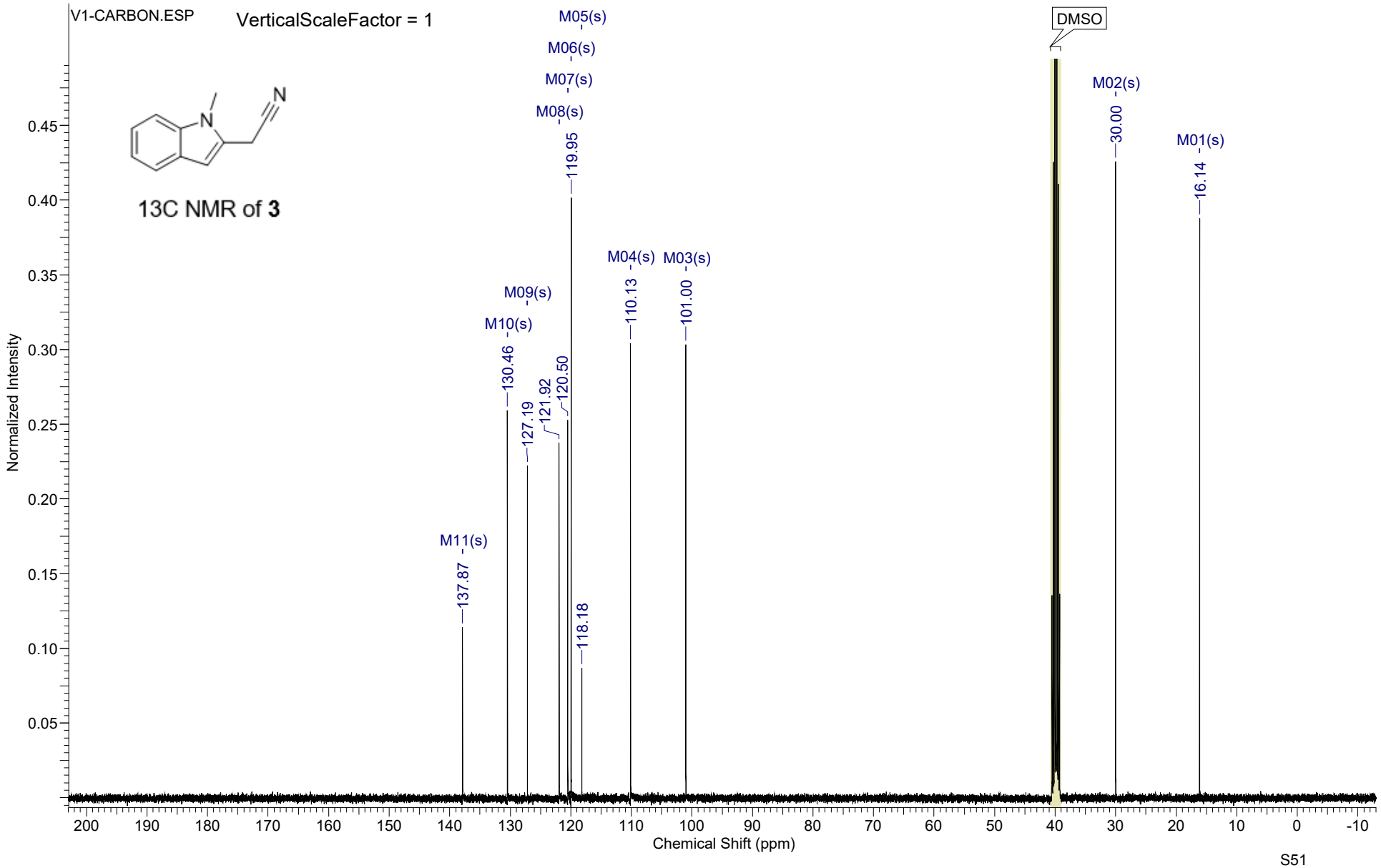
Acquisition Time (sec)	1.3631	***Date***	11 Aug 2017 00:55:44			***Date Stamp***	11 Aug 2017 00:55:44
File Name	D:\CJO-UCSF\NMR\CJO-Q\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.266						



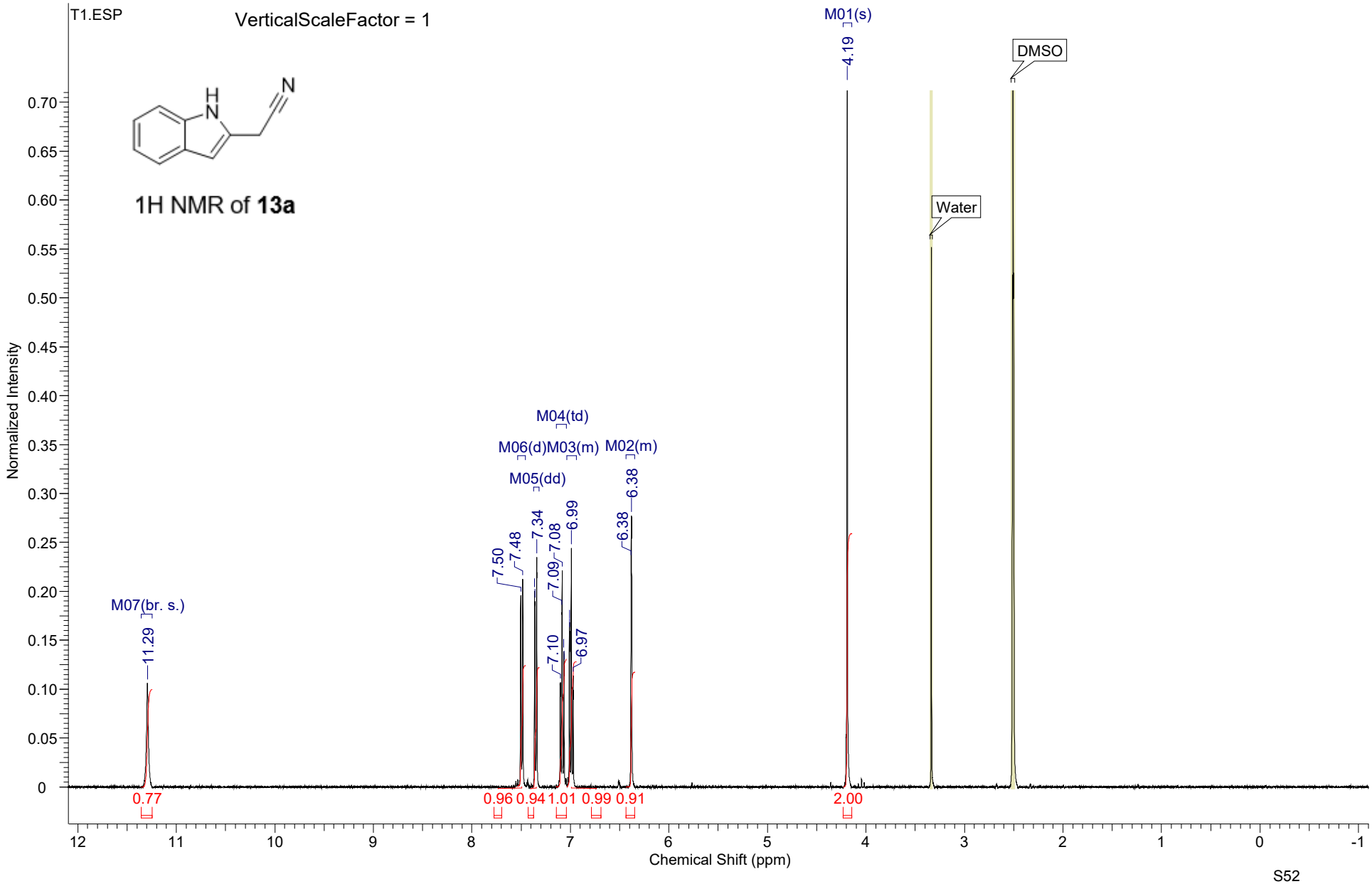
Acquisition Time (sec)	4.0894	***Date***	06 Sep 2017 09:34:08			***Date Stamp***	06 Sep 2017 09:34:08
File Name	D:\CJO-UCSF\NMR\CJO-V1-Alex is cool\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H
Number of Transients	24	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	30.74	***SW(cyclical) (Hz)***	8012.82
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8012.58
Temperature (degree C)	22.400						



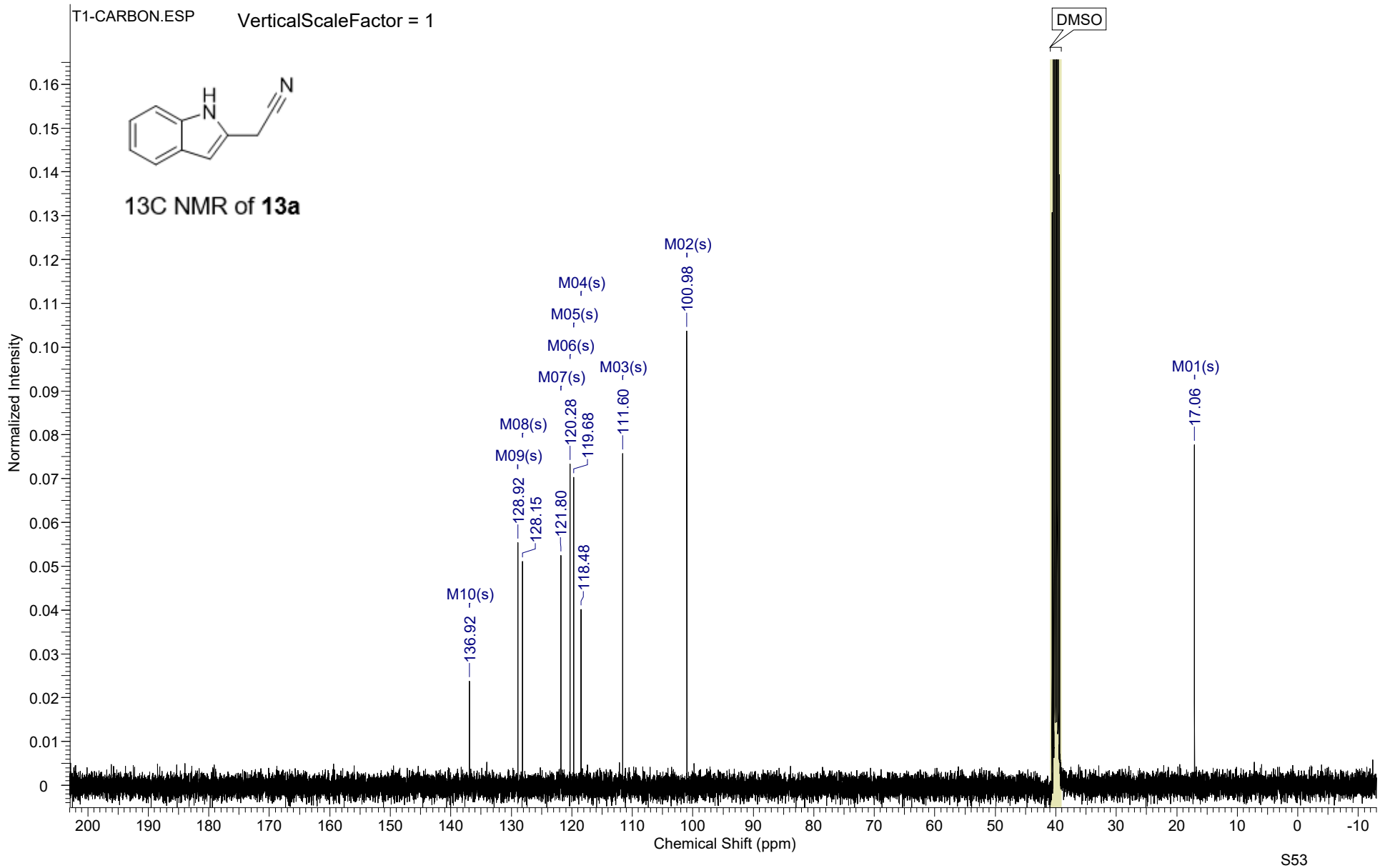
Acquisition Time (sec)	1.3631	***Date***	07 Sep 2017 23:56:00			***Date Stamp***	07 Sep 2017 23:56:00
File Name	D:\CJO-UCSF\NMR\CJO-V1-Alex is cool\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.417						



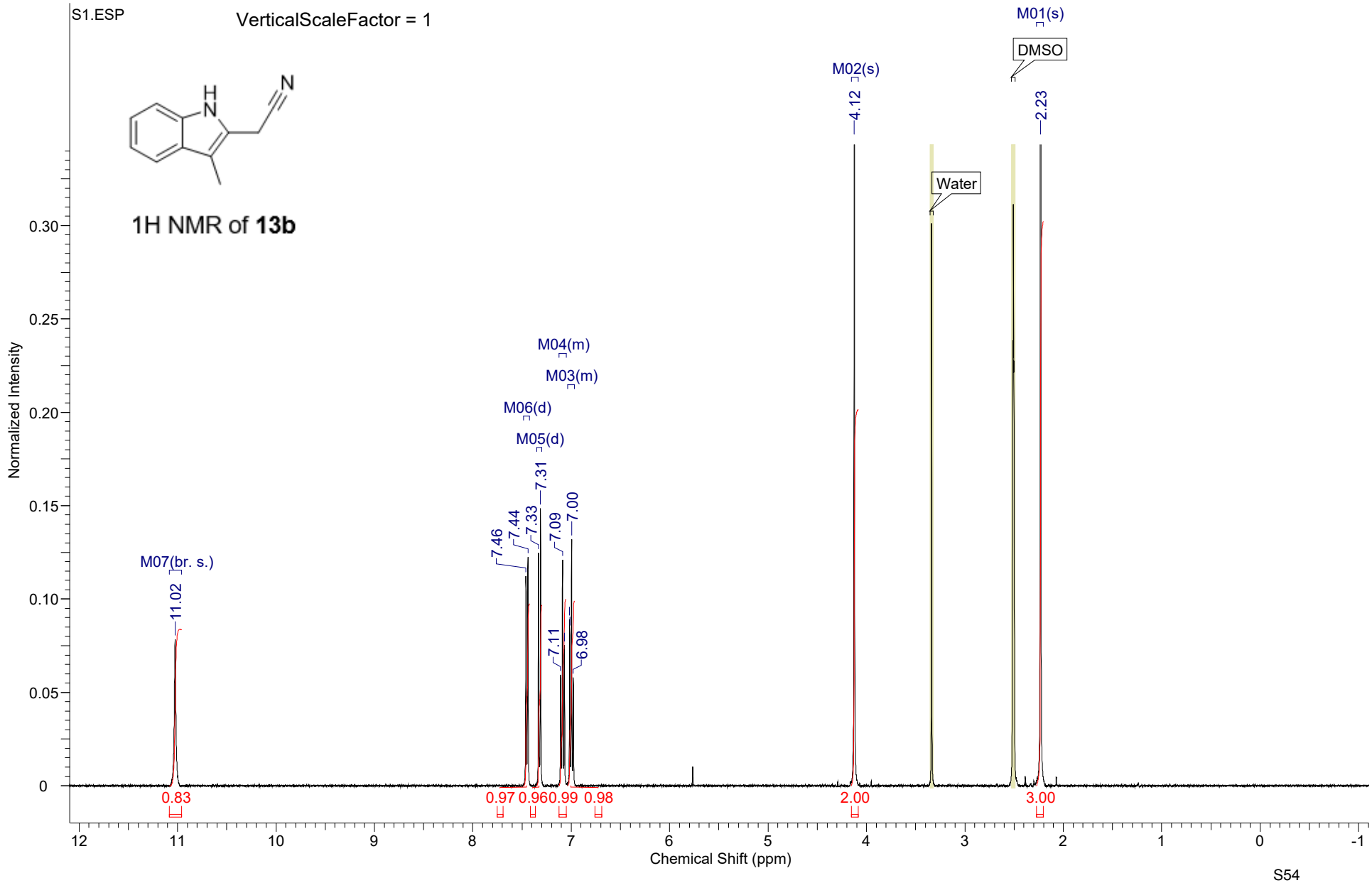
Acquisition Time (sec)	4.0894	***Date***	29 Aug 2017 08:21:36			***Date Stamp***	29 Aug 2017 08:21:36		
File Name	D:\CJO-UCSF\NMR\CJO-T1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.792						



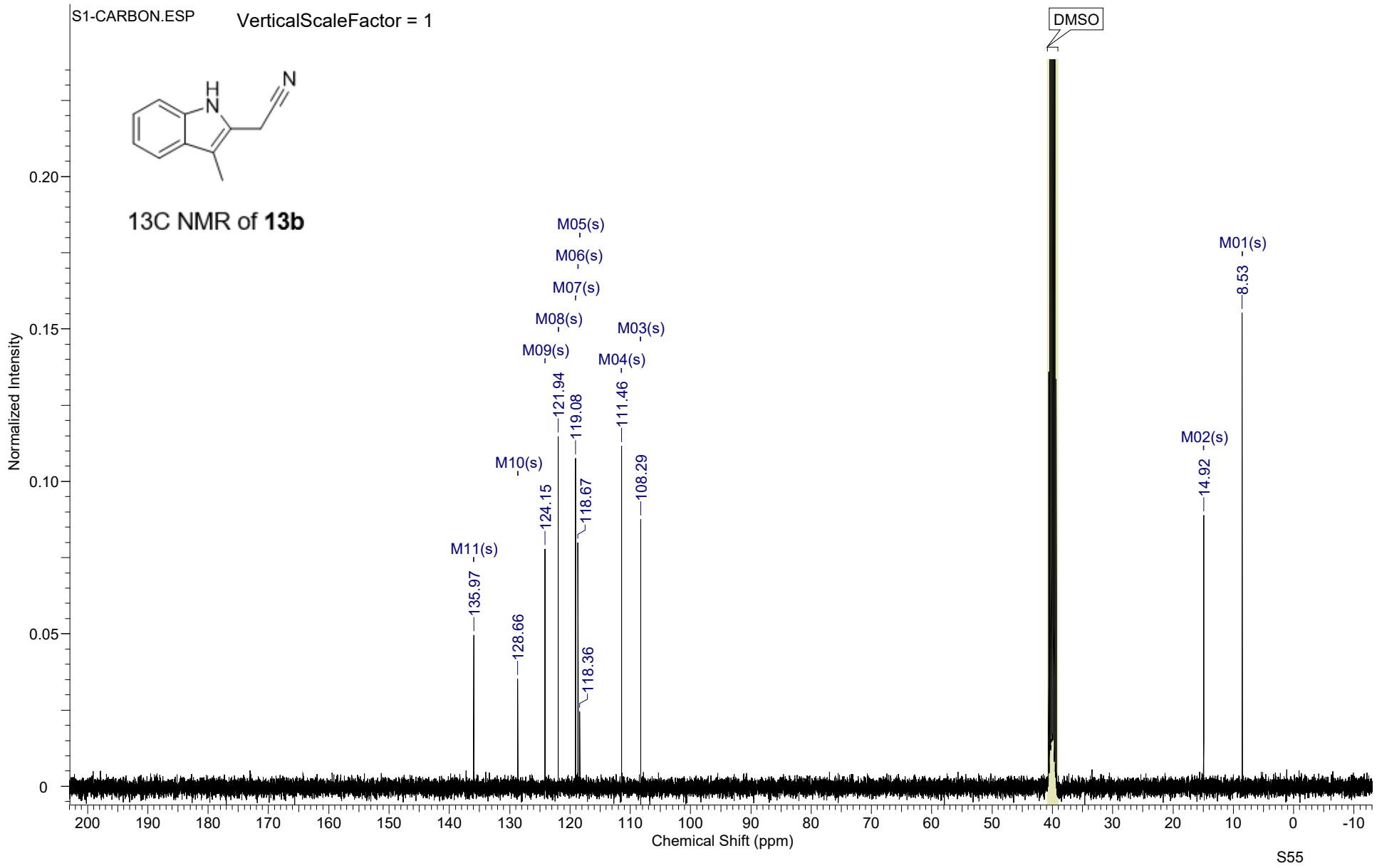
Acquisition Time (sec)	1.3631	***Date***	30 Aug 2017 01:55:28			***Date Stamp***	30 Aug 2017 01:55:28
File Name	D:\CJO-UCSF\NMR\CJO-T1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.051						



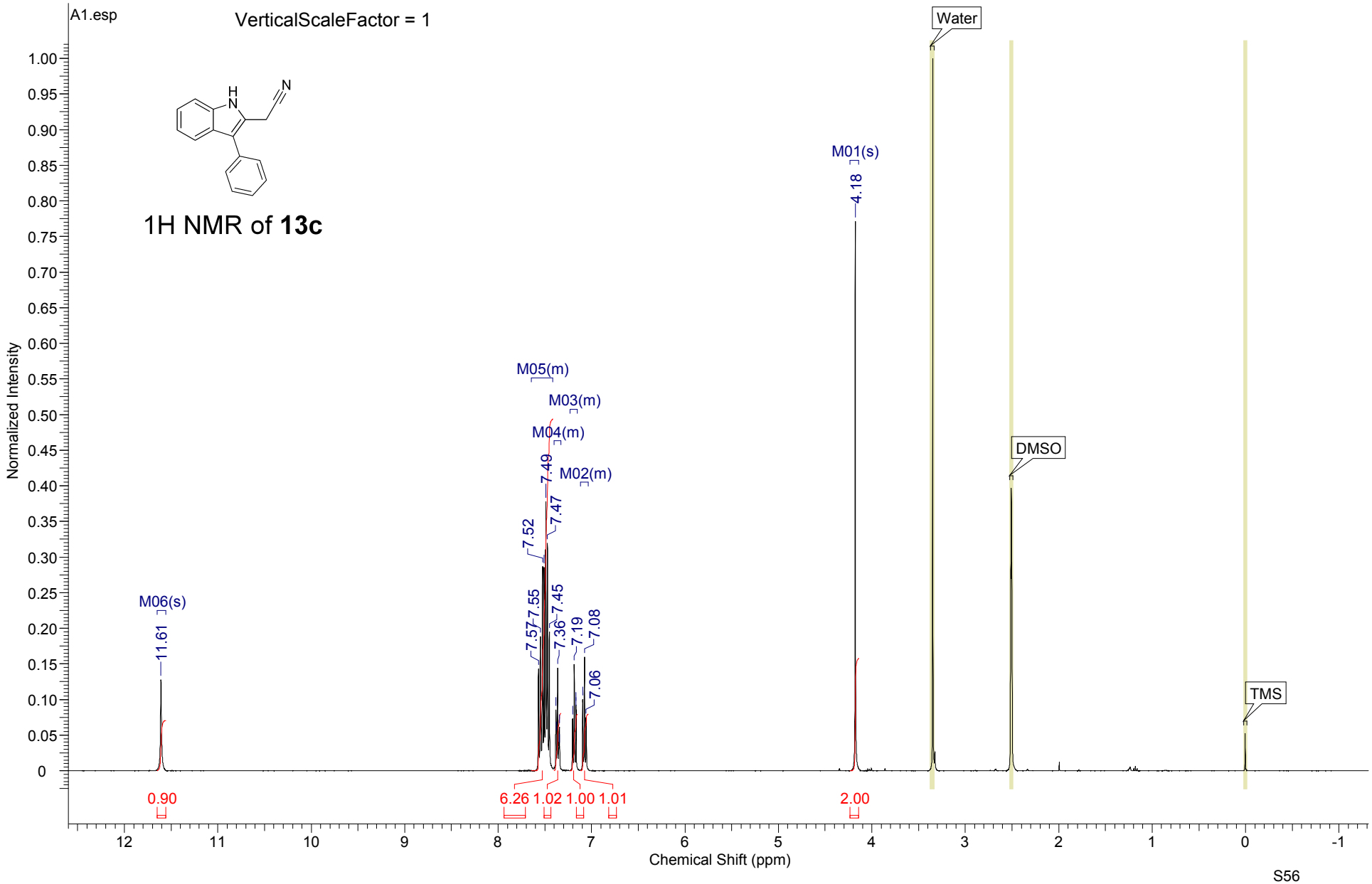
Acquisition Time (sec)	4.0894	***Date***	29 Aug 2017 08:17:20			***Date Stamp***	29 Aug 2017 08:17:20		
File Name	D:\CJO-UCSF\NMR\CJO-S1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.782						



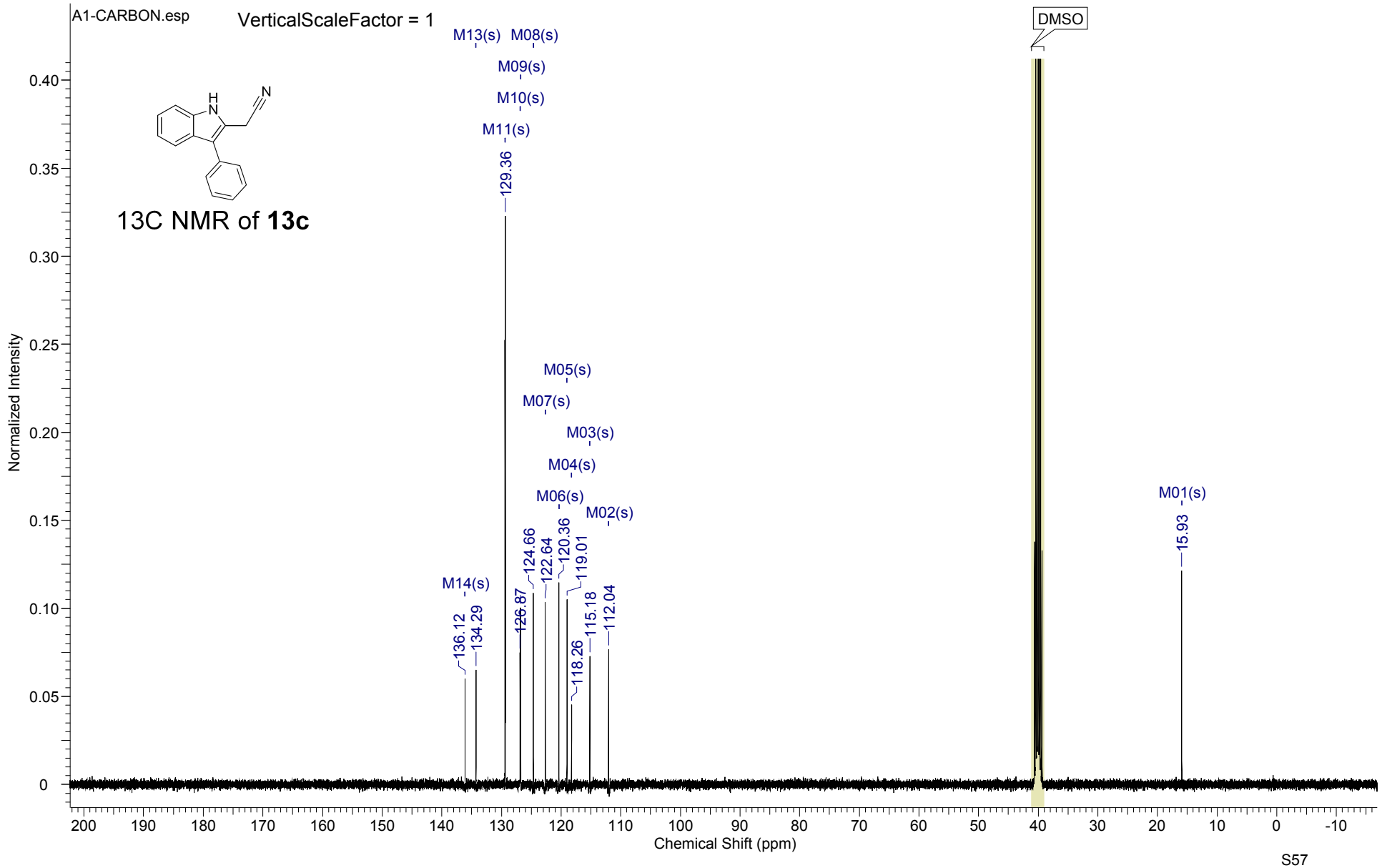
Acquisition Time (sec)	1.3631	***Date***	30 Aug 2017 00:00:16			***Date Stamp***	30 Aug 2017 00:00:16
File Name	D:\CJO-UCSF\NMR\CJO-S1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.154						



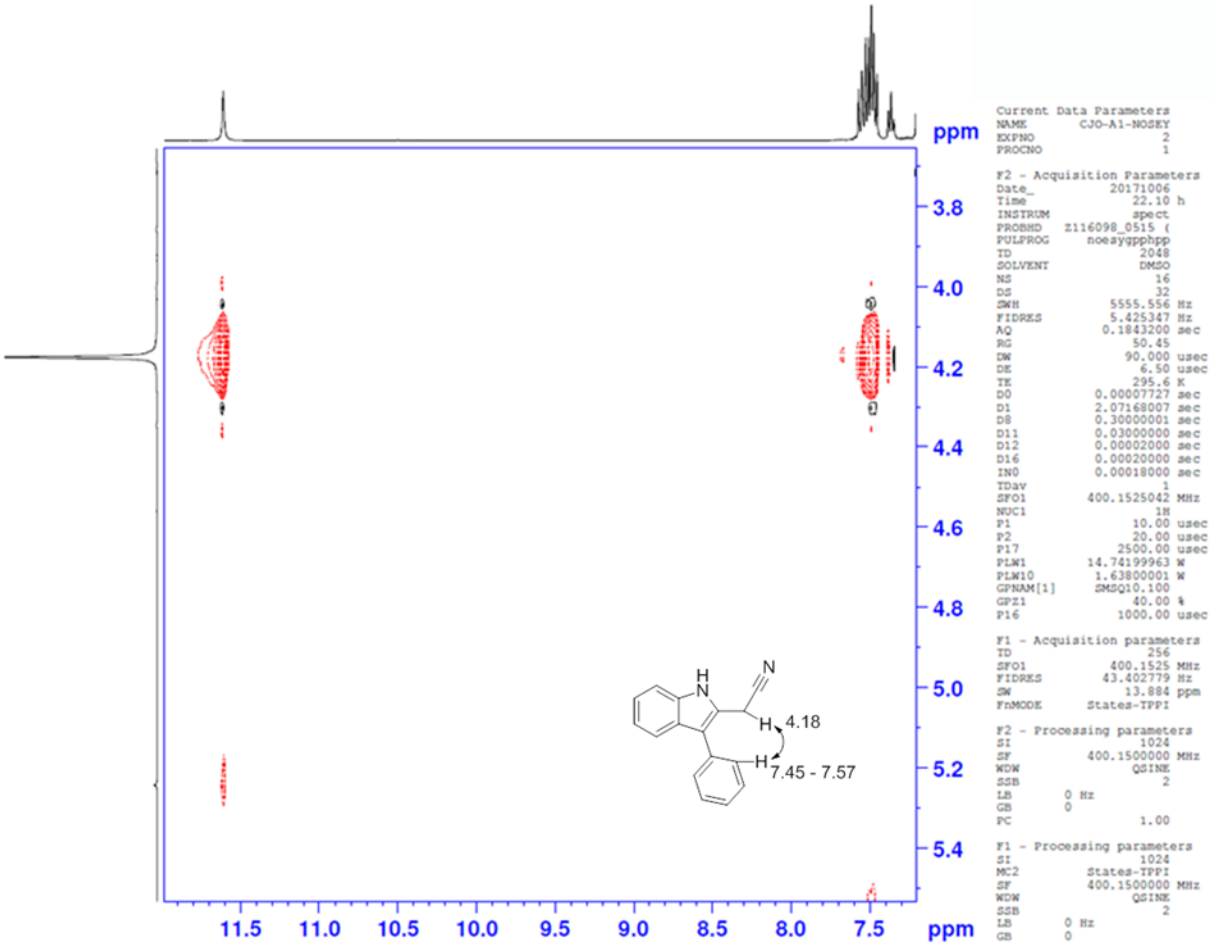
Acquisition Time (sec)	4.0894	***Date***	03 Aug 2017 10:36:00			***Date Stamp***	03 Aug 2017 10:36:00		
File Name	D:\NMR\CJO\CJO-A1\2\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.616						



Acquisition Time (sec)	1.3631	***Date***	04 Aug 2017 00:55:44			***Date Stamp***	04 Aug 2017 00:55:44
File Name	D:\NMR\CJO\CJO-A1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.584						



1H NOSEY NMR spectrum of 13c, in DMSO-d6

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Current Data Parameters
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EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
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Time              22.10 h
INSTRUM             spect
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PULPROG      noesygpphpp
TD                  2048
SOLVENT             DMSO
NS                    16
DS                    32
SWH            5555.556 Hz
FIDRES         5.425347 Hz
AQ             0.1843200 sec
RG                 50.45
DW                 90.000 usec
DE                  6.50 usec
TE                295.6 K
D0             0.00007727 sec
D1             2.07168007 sec
D8             0.30000001 sec
D11            0.03000000 sec
D12            0.00002000 sec
D16            0.00020000 sec
IN0            0.00018000 sec
TDav                   1
SFO1          400.1525042 MHz
NUC1                  1H
P1                 10.00 usec
P2                 20.00 usec
P17              2500.00 usec
PLW1          14.74199963 W
PLW10          1.63800001 W
GPNAM[1]      SMSQ10.100
GPZ1              40.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            400.1525 MHz
FIDRES         43.402779 Hz
SW                13.884 ppm
FnMODE       States-TPPI

F2 - Processing parameters
SI                  1024
SF            400.1500000 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.00

F1 - Processing parameters
SI                  1024
MC2          States-TPPI
SF            400.1500000 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
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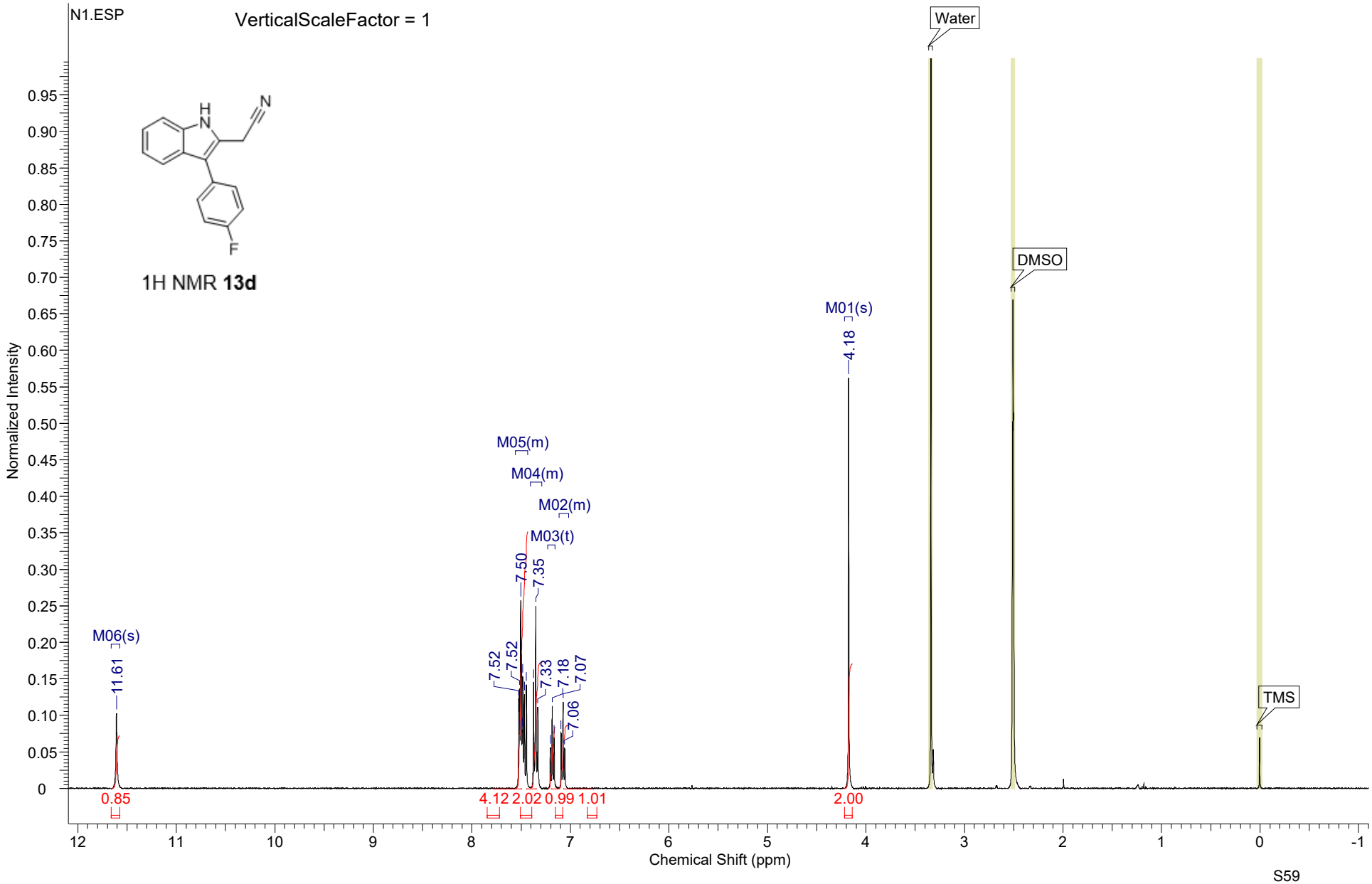
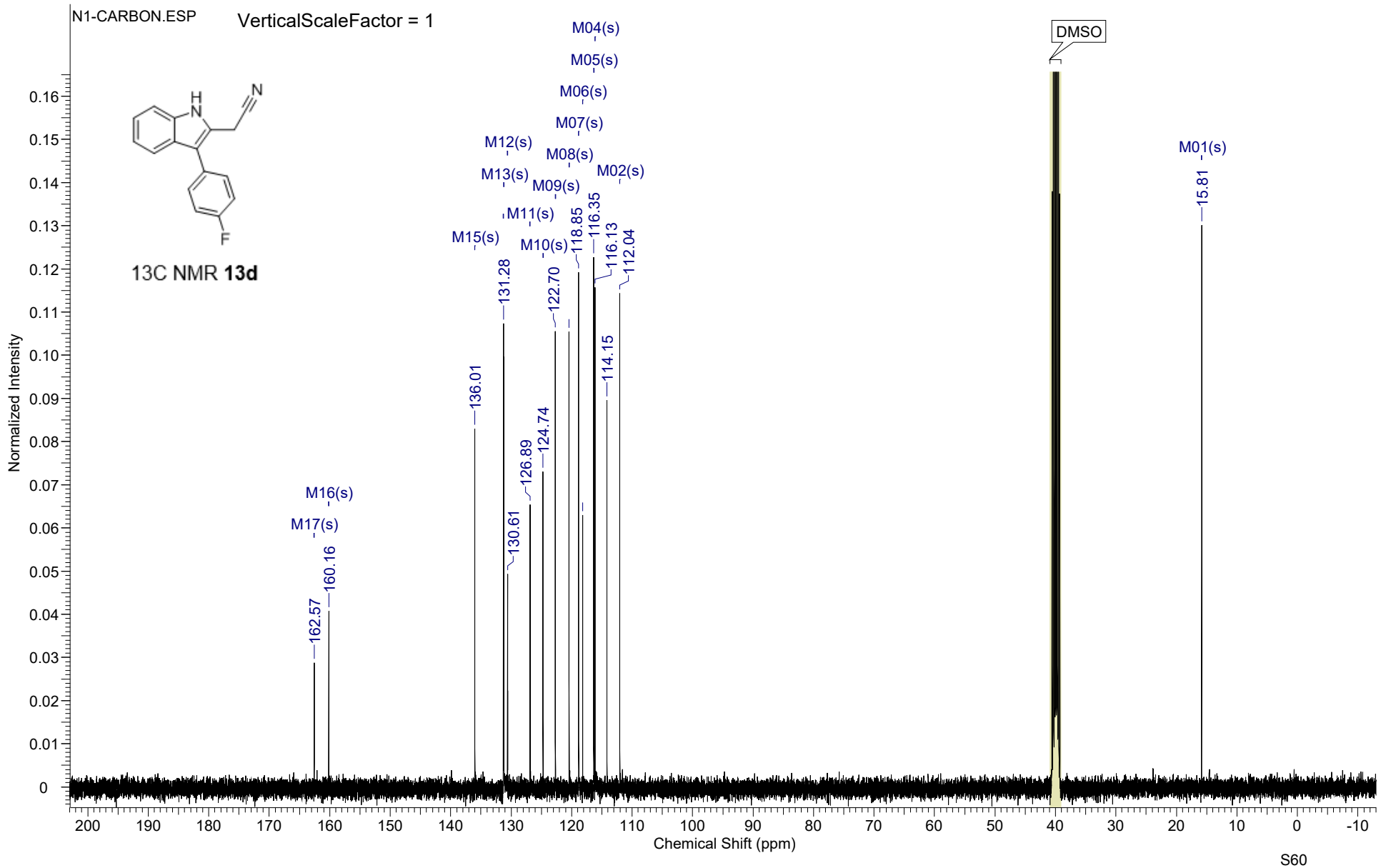
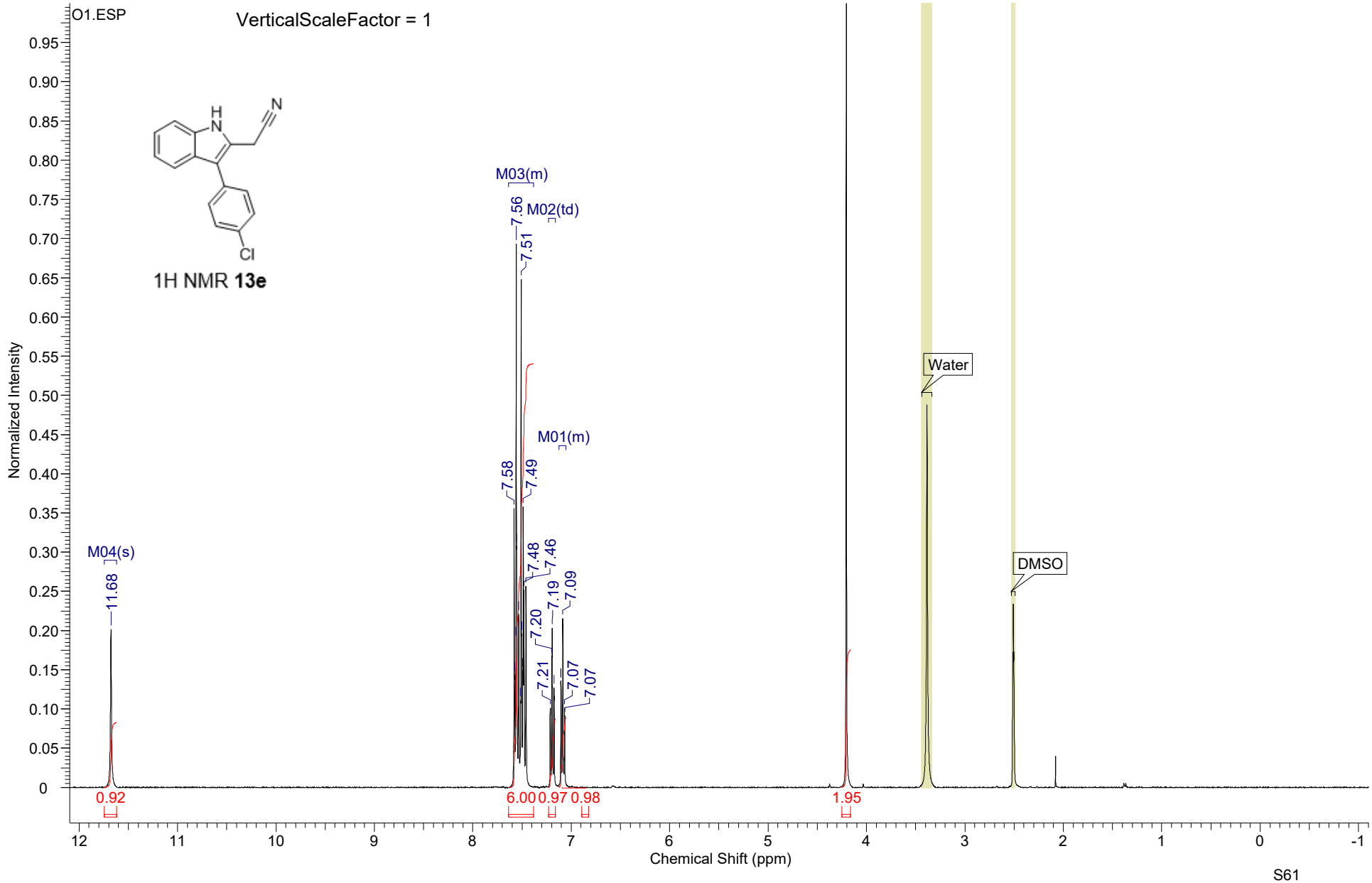
Acquisition Time (sec)	4.0894	***Date***	28 Jul 2017 11:10:08			***Date Stamp***	28 Jul 2017 11:10:08		
File Name	D:\NMR\CJO\CJO-N1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.575						



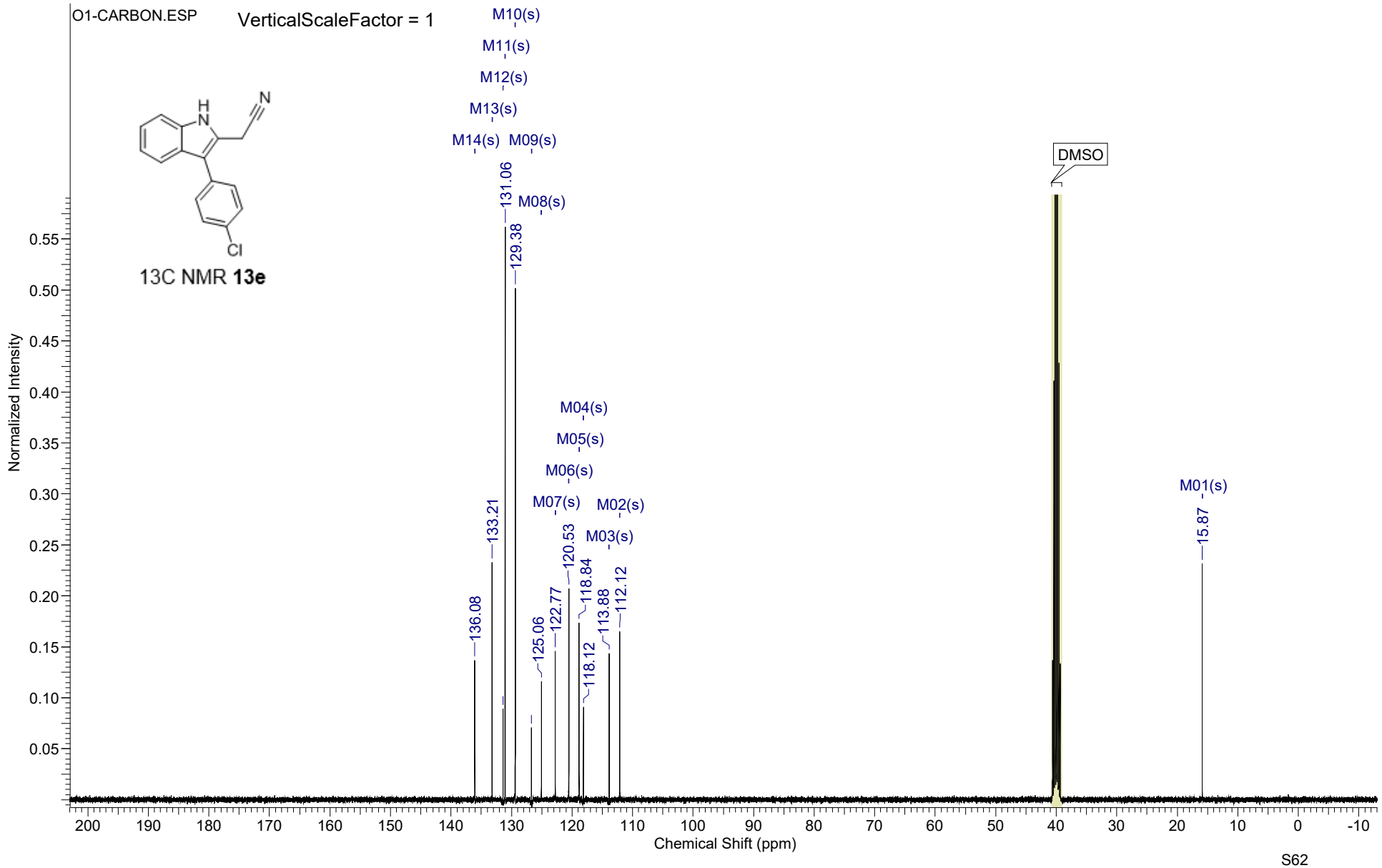
Acquisition Time (sec)	1.3631	***Date***	01 Aug 2017 01:51:12			***Date Stamp***	01 Aug 2017 01:51:12
File Name	D:\NMR\CJO\CJO-N1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.274						



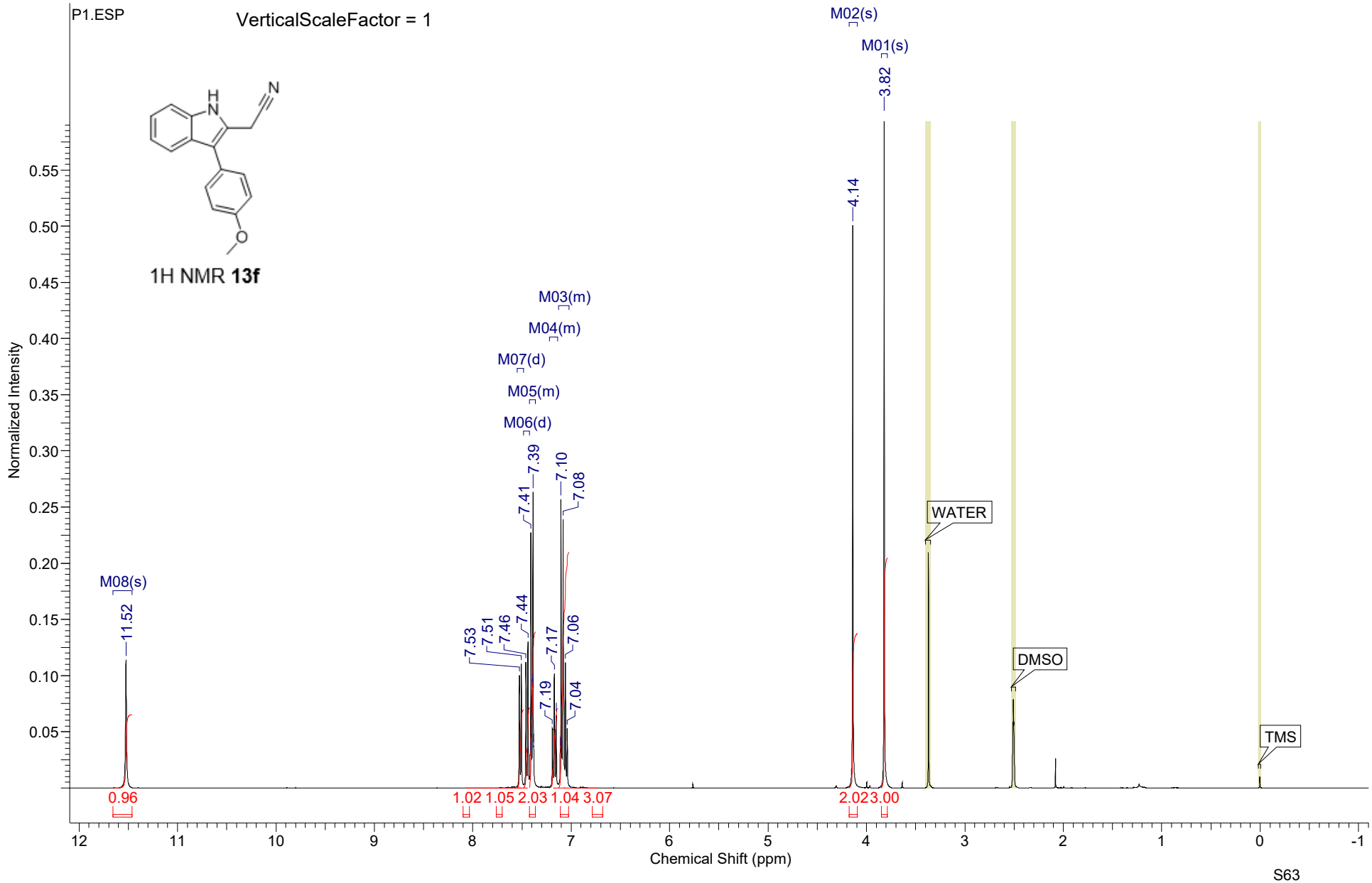
Acquisition Time (sec)	4.0894	***Date***	09 Aug 2017 09:14:56			***Date Stamp***	09 Aug 2017 09:14:56		
File Name	D:\CJO-UCSF\CJO-O1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	77.61	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.859						



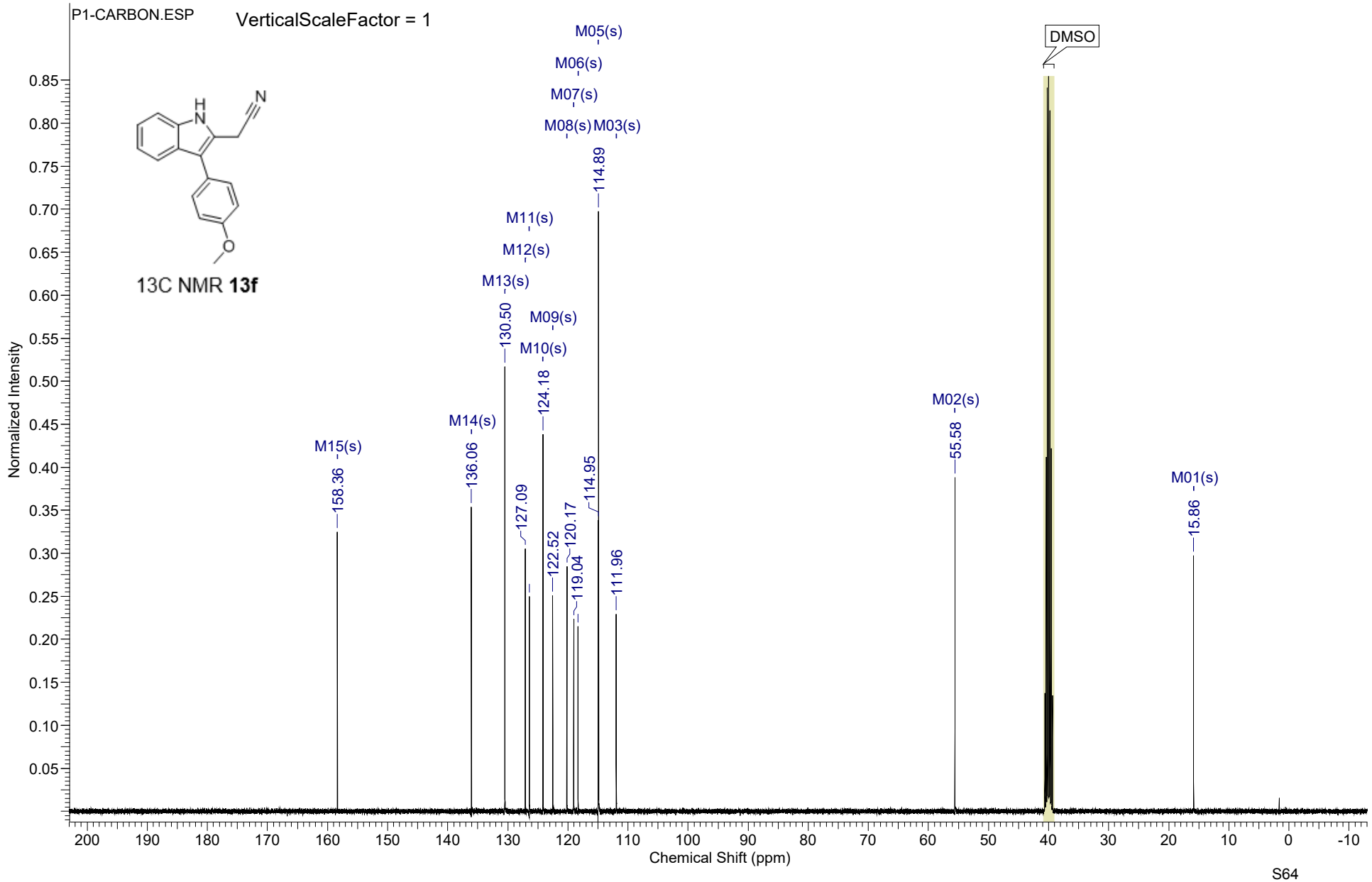
Acquisition Time (sec)	1.3631	***Date***	10 Aug 2017 06:43:28			***Date Stamp***	10 Aug 2017 06:43:28
File Name	D:\CJO-UCSF\NMR\CJO-O1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.387						



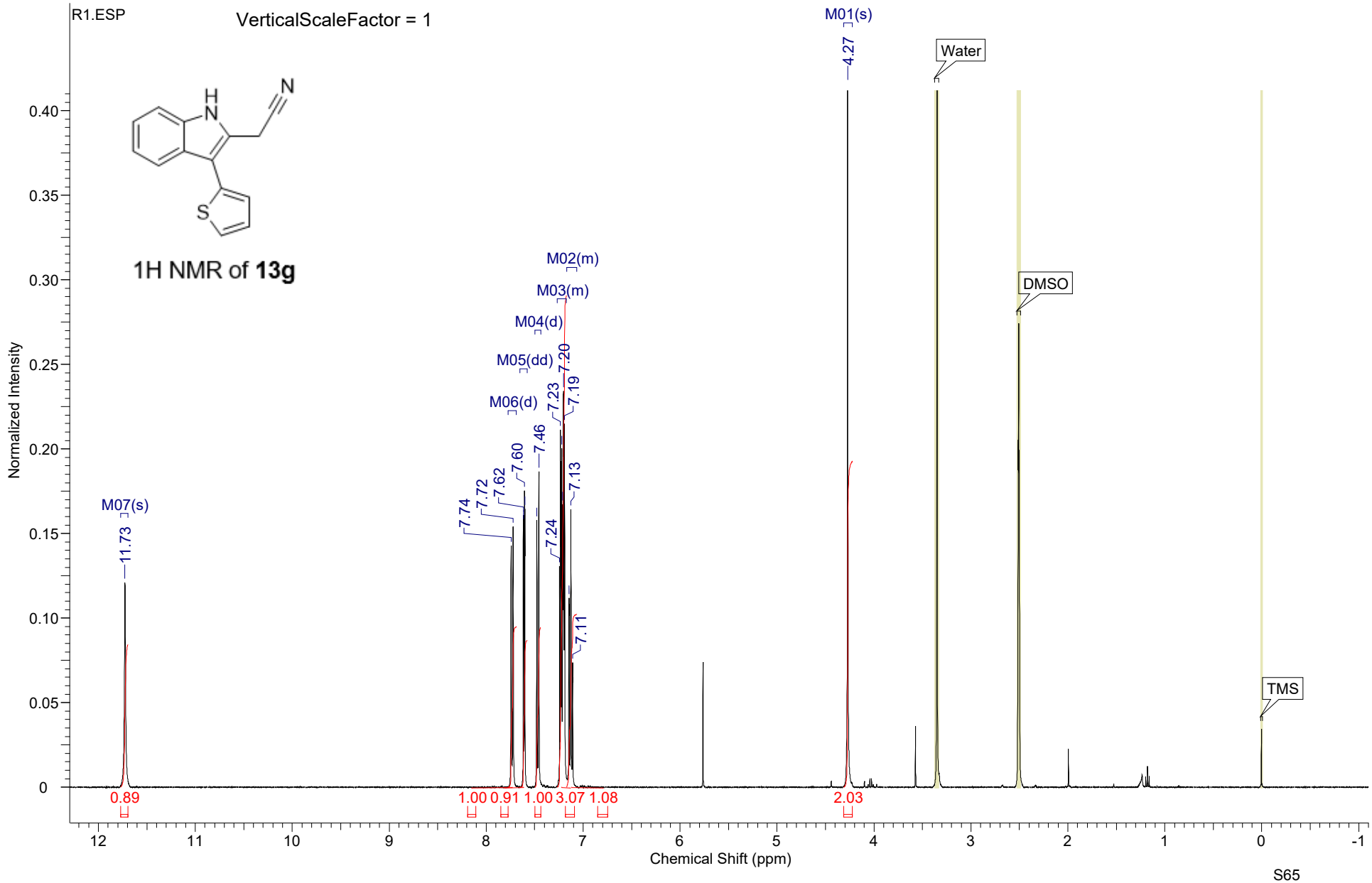
Acquisition Time (sec)	4.0894	***Date***	07 Aug 2017 12:56:48			***Date Stamp***	07 Aug 2017 12:56:48		
File Name	D:\NMR\CJO\CJO-P1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	62.81	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.530						



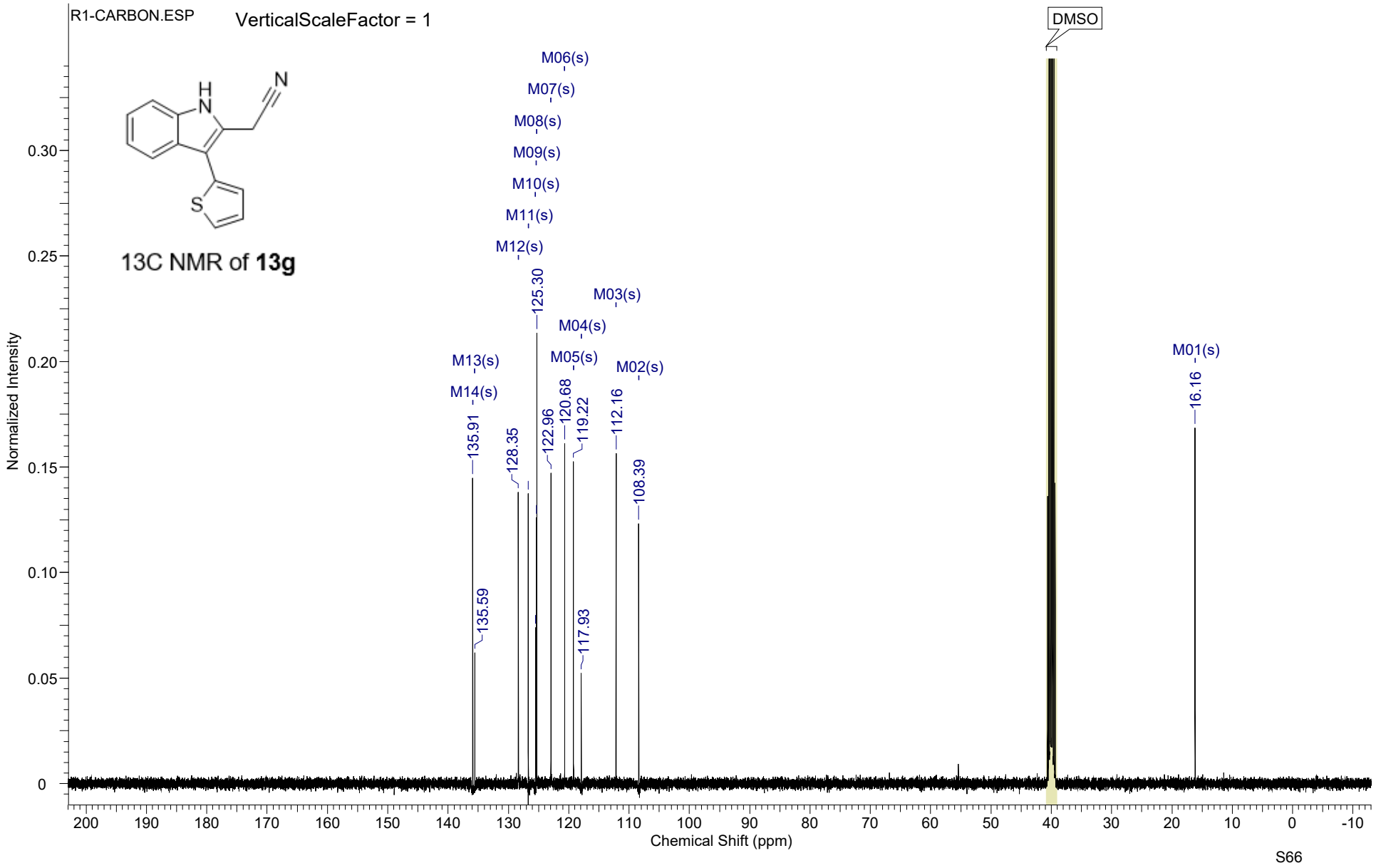
Acquisition Time (sec)	1.3631	***Date***	09 Aug 2017 06:43:28			***Date Stamp***	09 Aug 2017 06:43:28		
File Name	D:\CJO-UCSF\CJO-P1\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C	***Number of Transients***	3000
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	196.40	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.282						



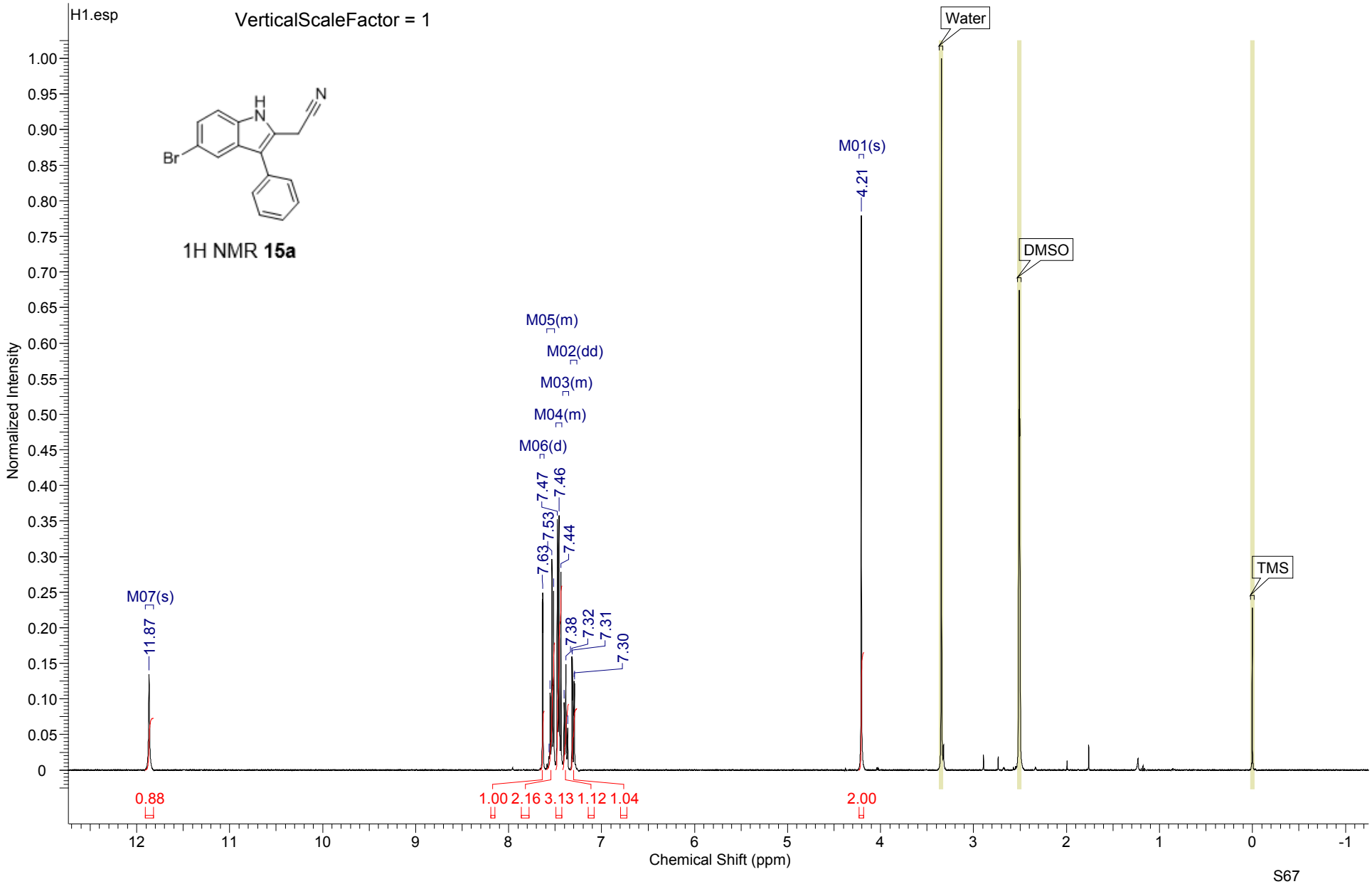
Acquisition Time (sec)	4.0894	***Date***	09 Aug 2017 09:04:16			***Date Stamp***	09 Aug 2017 09:04:16		
File Name	D:\CJO-UCSF\CJO-R1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.839						



Acquisition Time (sec)	1.3631	***Date***	10 Aug 2017 03:48:32			***Date Stamp***	10 Aug 2017 03:48:32
File Name	D:\CJO-UCSF\NMR\CJO-R1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.213						



Acquisition Time (sec)	4.0894	***Date***	04 Aug 2017 11:12:16			***Date Stamp***	04 Aug 2017 11:12:16		
File Name	D:\NMR\CJO\CJO-H1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.760						



Acquisition Time (sec)	1.3631	***Date***	05 Aug 2017 19:20:48			***Date Stamp***	05 Aug 2017 19:20:48
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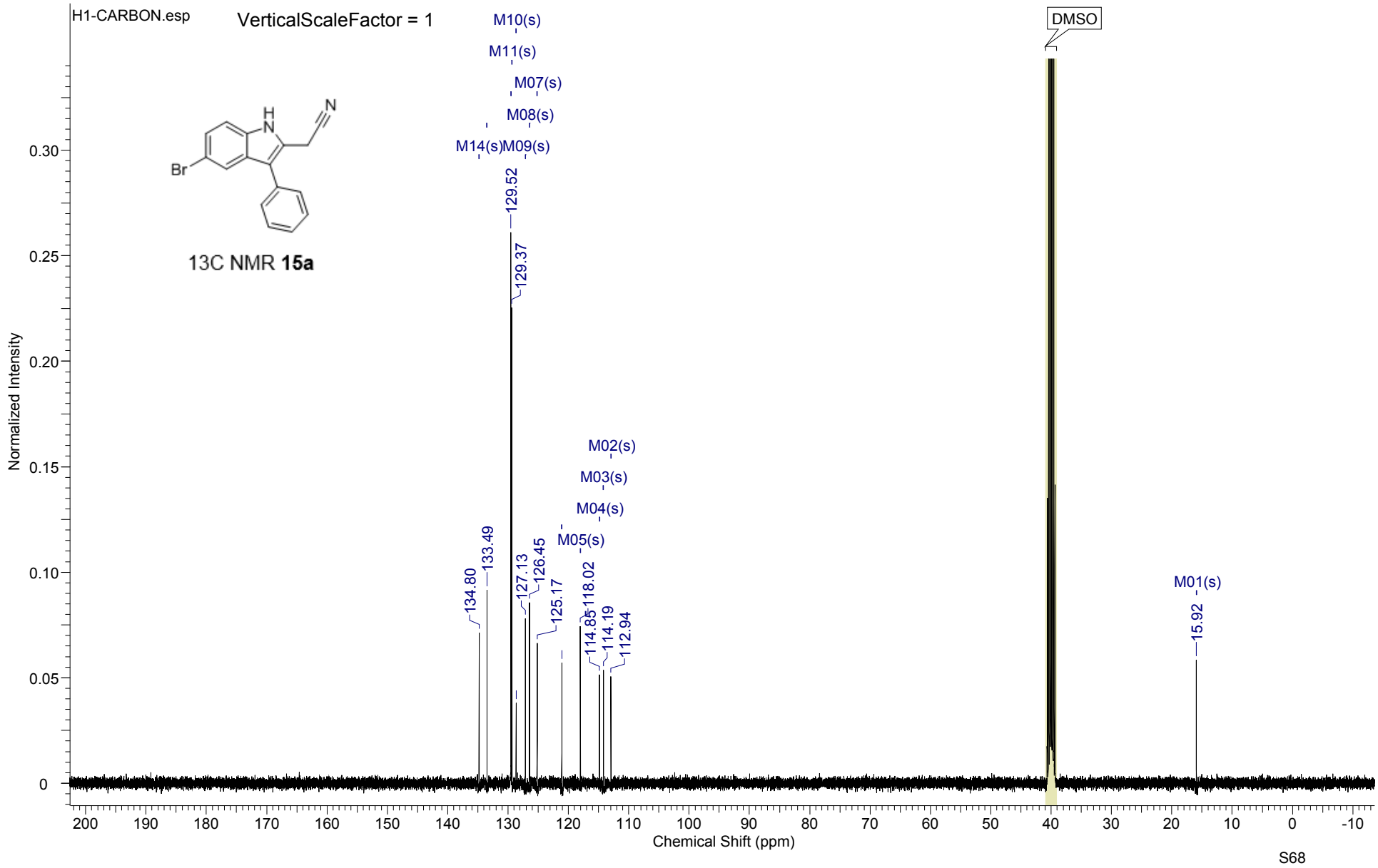
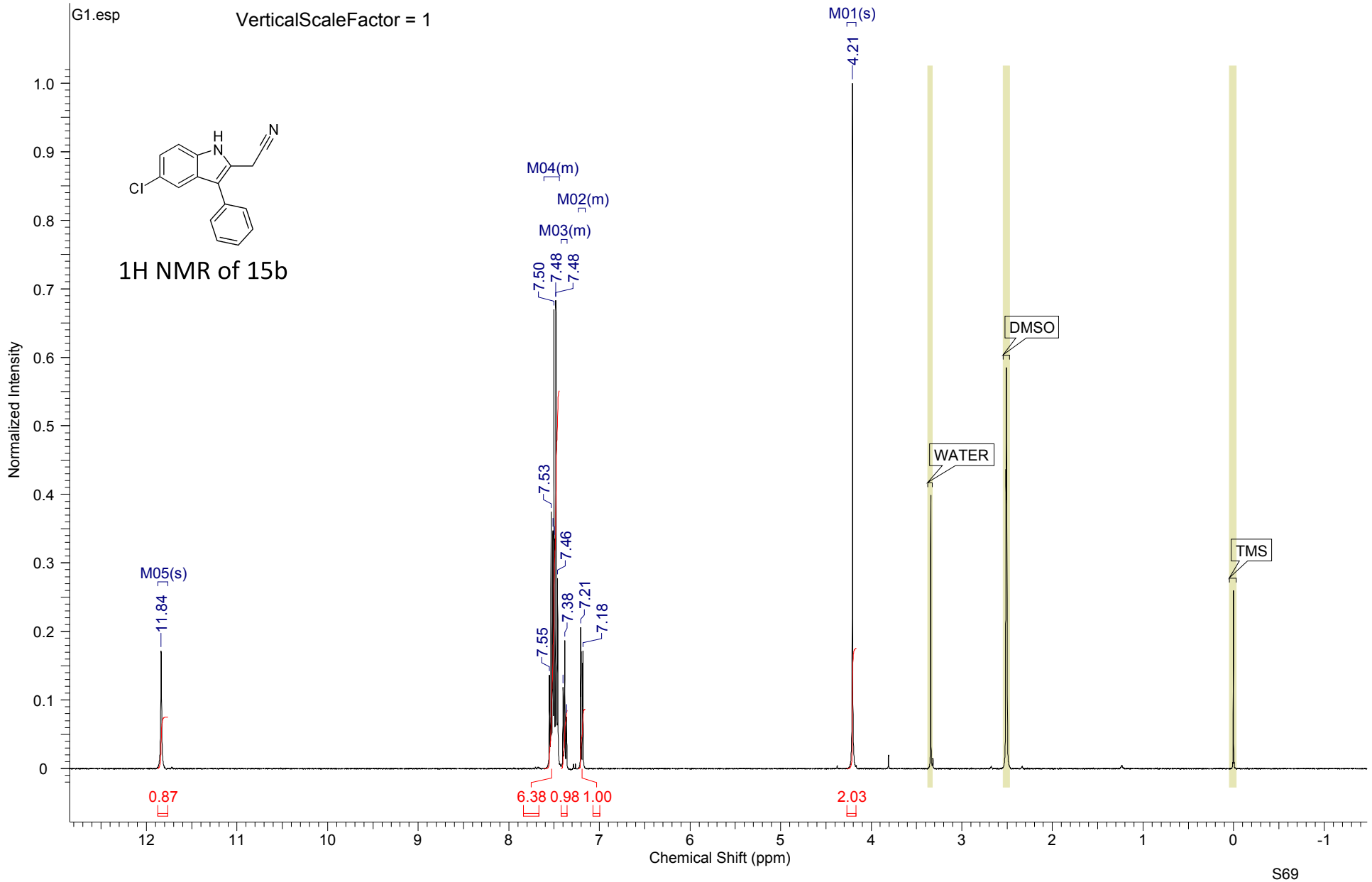
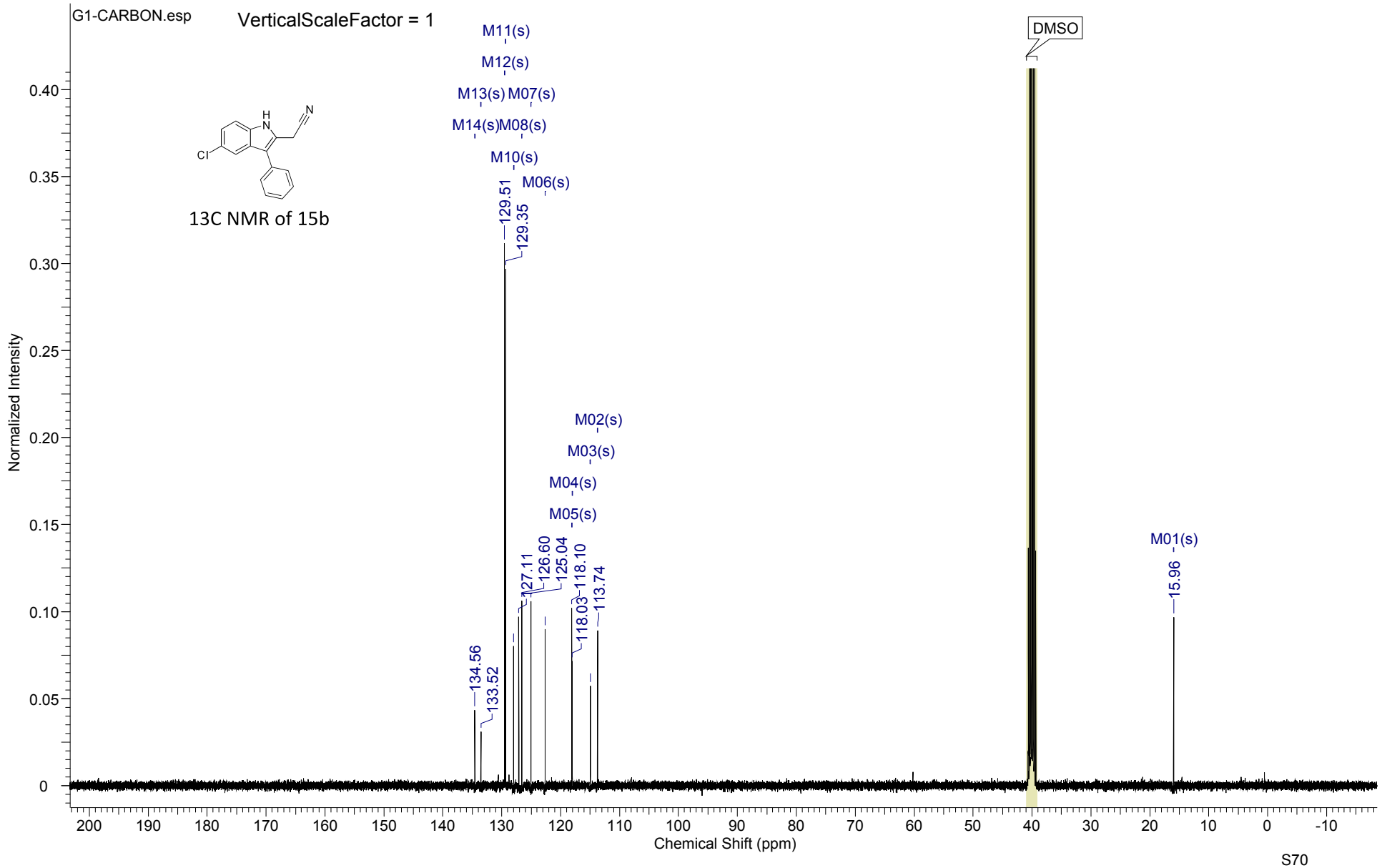
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.208						



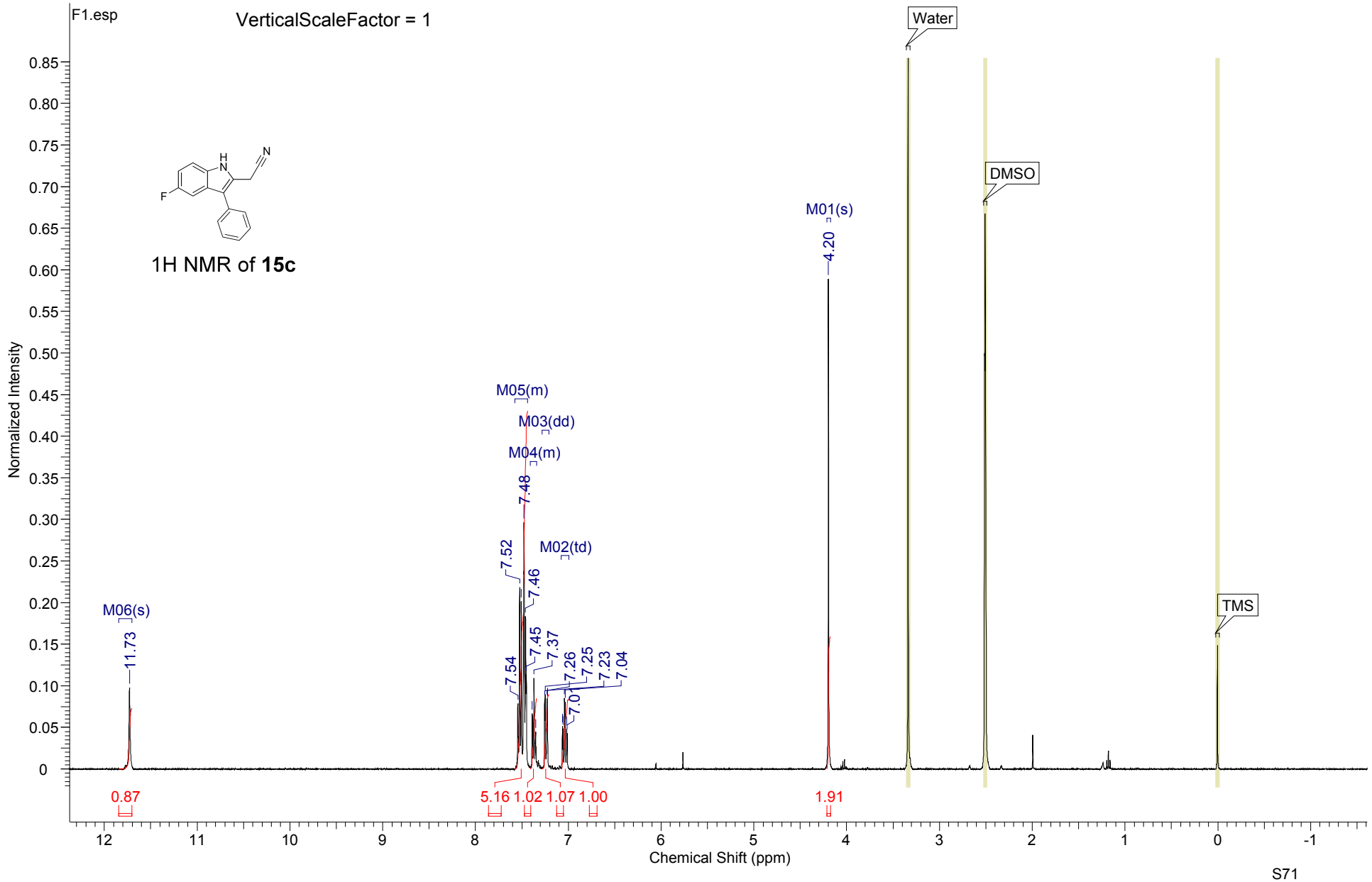
Acquisition Time (sec)	4.0894	***Date***	04 Aug 2017 11:08:00			***Date Stamp***	04 Aug 2017 11:08:00		
File Name	D:\NMR\CJO\CJO-G1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	110.38	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.780						



Acquisition Time (sec)	1.3631	***Date***	05 Aug 2017 16:25:52			***Date Stamp***	05 Aug 2017 16:25:52
File Name	D:\NMR\CJO\CJO-G1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.247						



Acquisition Time (sec)	4.0894	***Date***	01 Aug 2017 08:13:04			***Date Stamp***	01 Aug 2017 08:13:04		
File Name	D:\NMR\CJO\CJO-F1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.666						



Acquisition Time (sec)	1.3631	***Date***	02 Aug 2017 01:51:12			***Date Stamp***	02 Aug 2017 01:51:12
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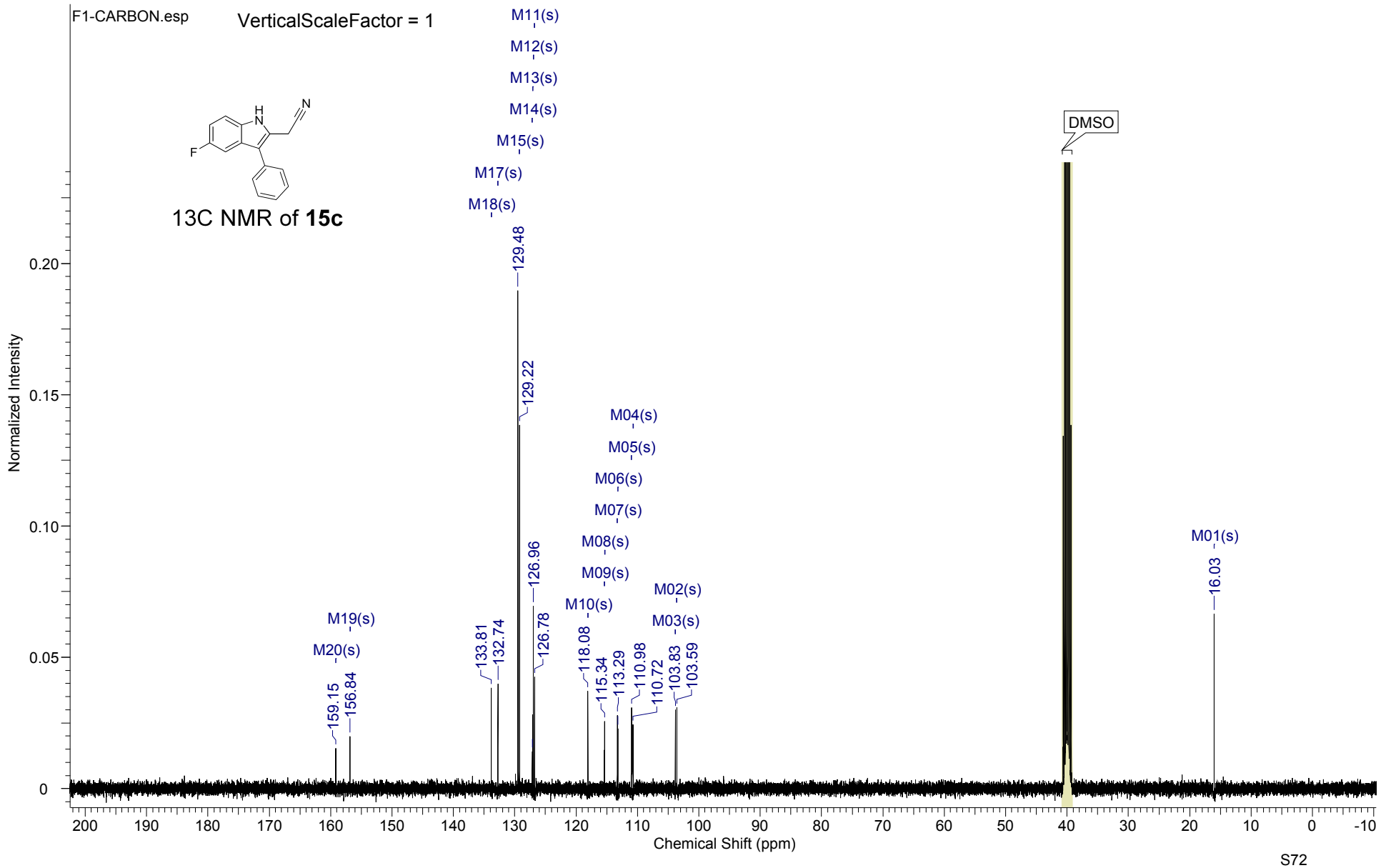
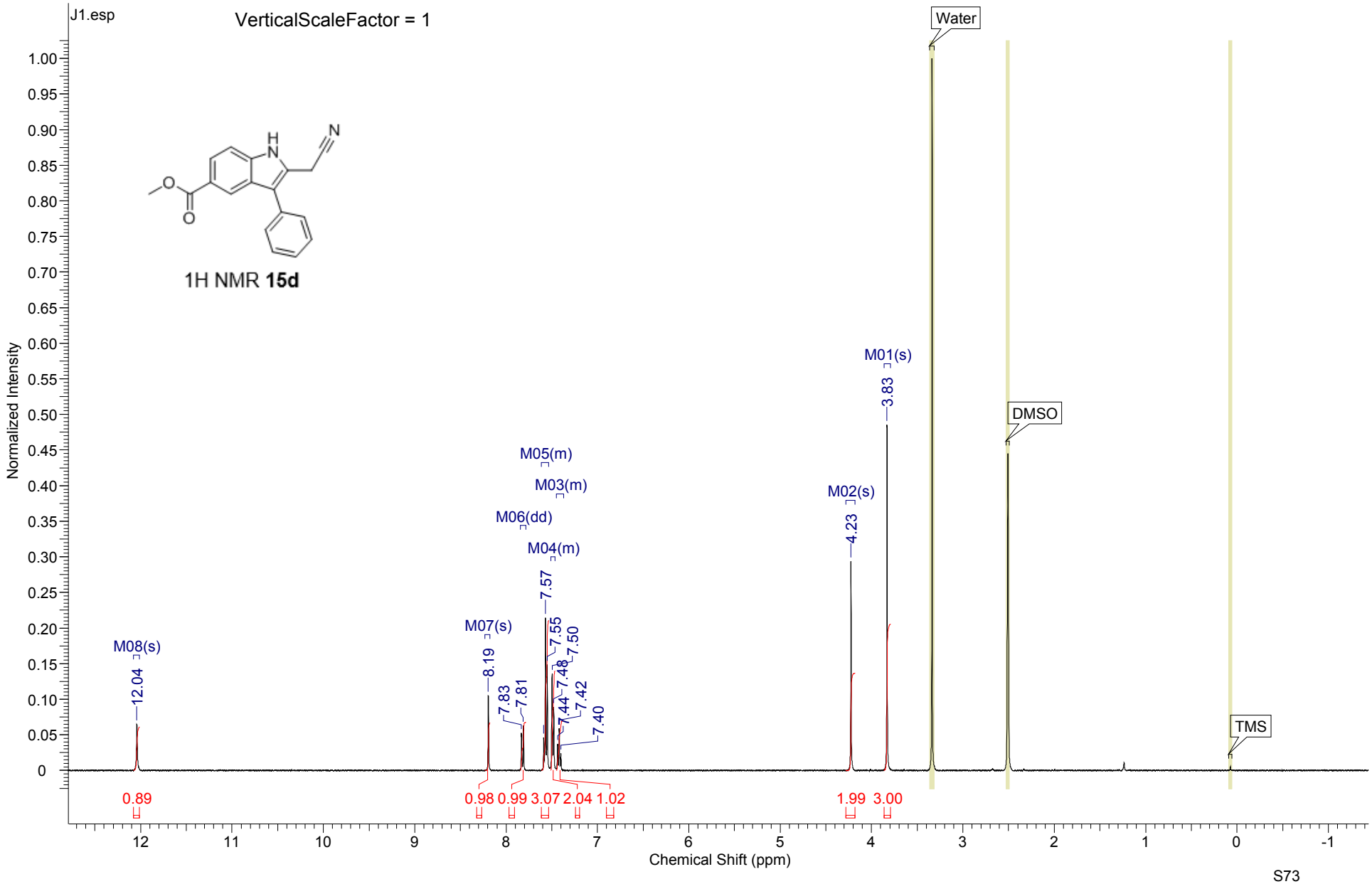
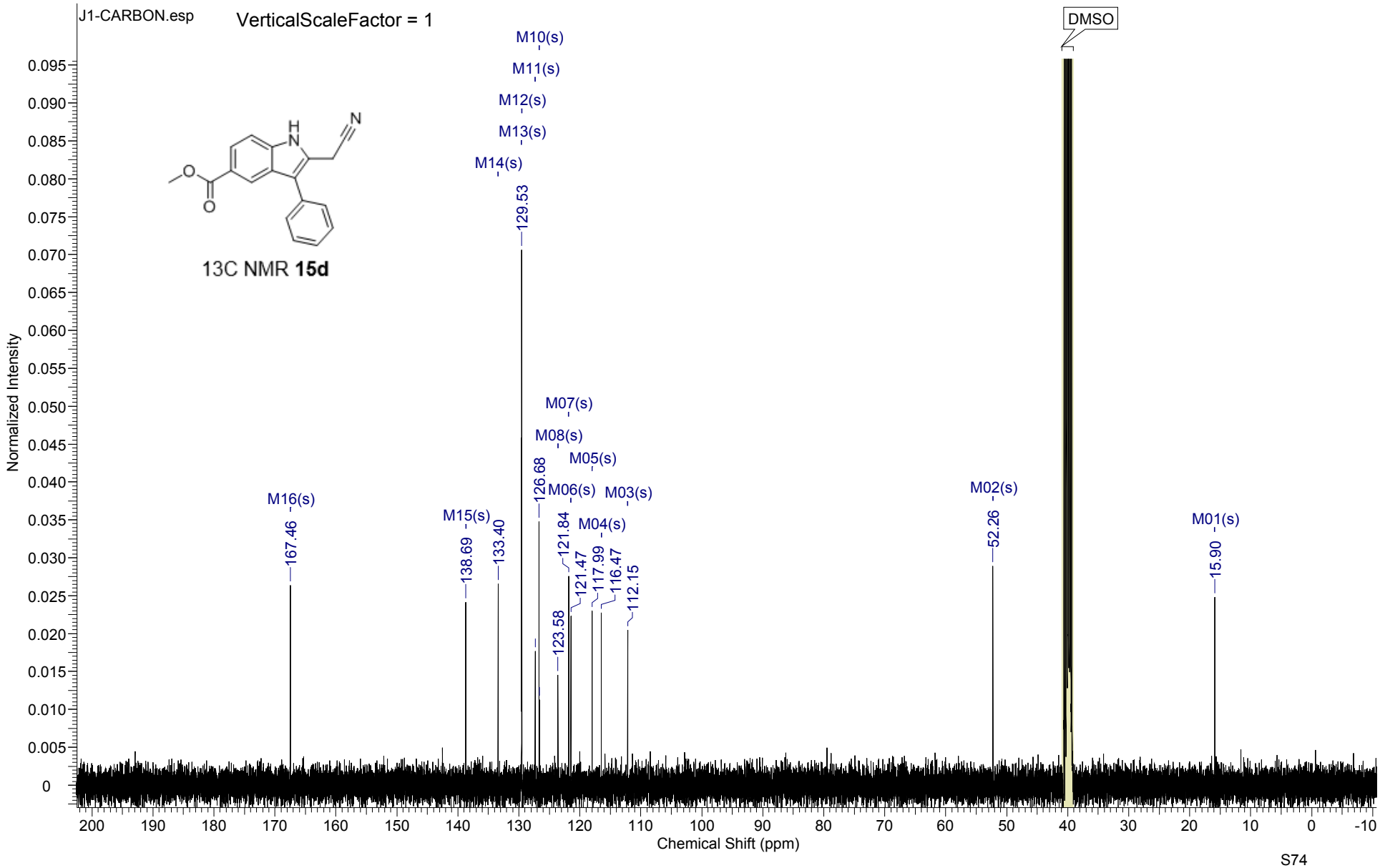
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.437						



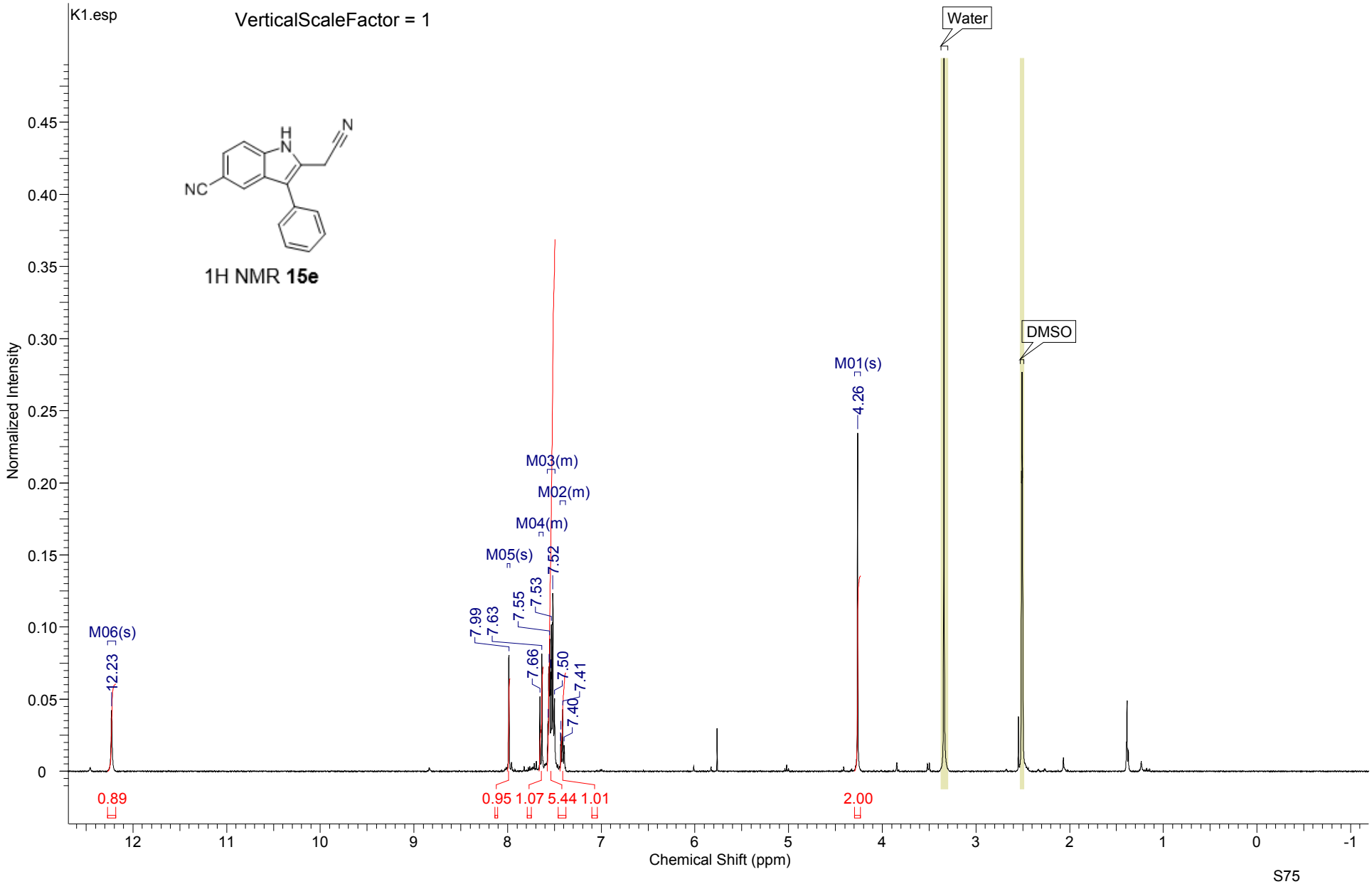
Acquisition Time (sec)	4.0894	***Date***	25 Aug 2017 10:40:16			***Date Stamp***	25 Aug 2017 10:40:16		
File Name	D:\CJO-UCSF\NMR\CJO-J1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.636						



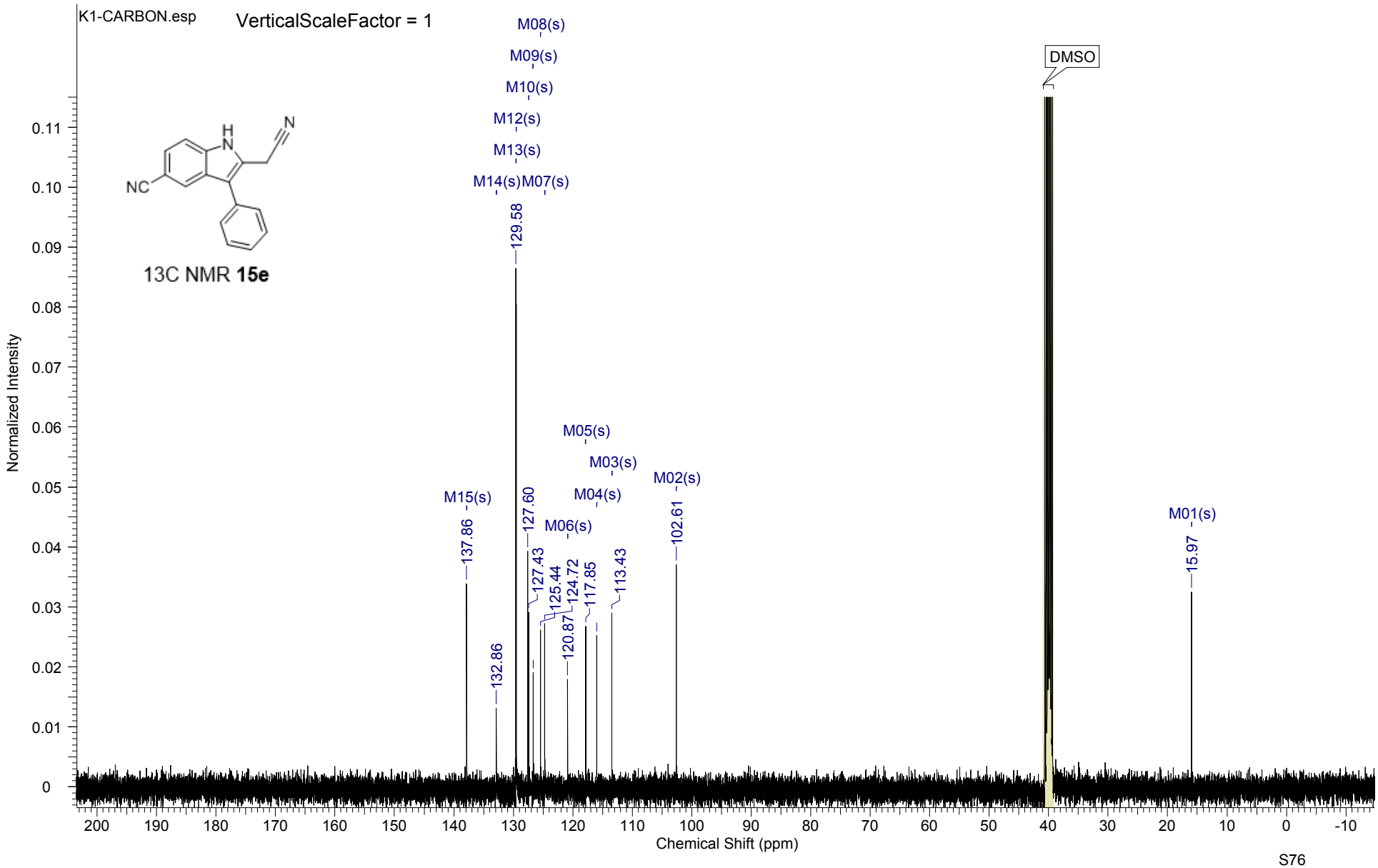
Acquisition Time (sec)	1.3631	***Date***	26 Aug 2017 00:55:44			***Date Stamp***	26 Aug 2017 00:55:44
File Name	D:\CJO-UCSF\NMR\CJO-J1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.395						



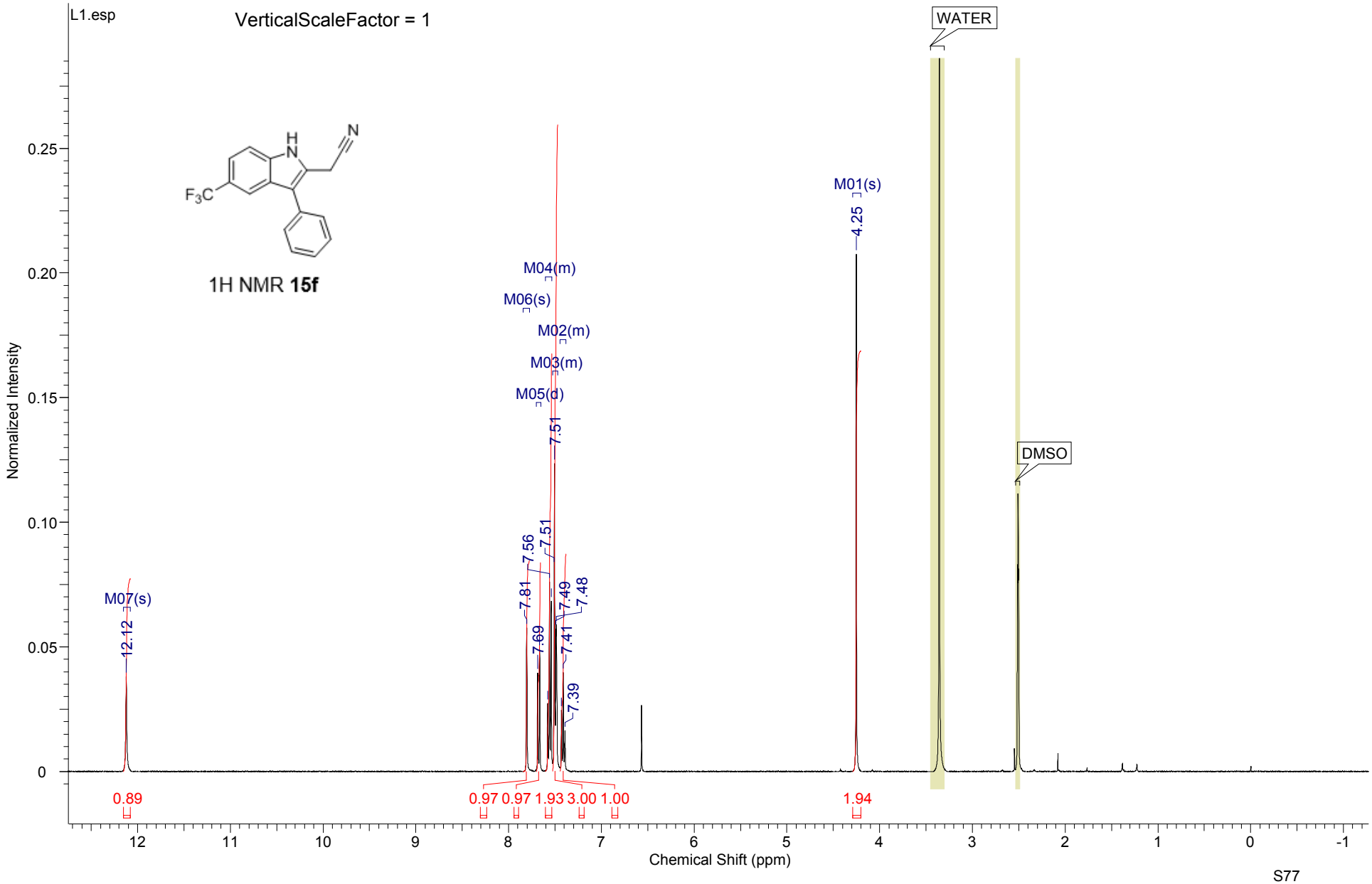
Acquisition Time (sec)	4.0894	***Date***	01 Sep 2017 08:45:04			***Date Stamp***	01 Sep 2017 08:45:04		
File Name	D:\CJO-UCSF\NMR\CJO-K1\2\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.602						



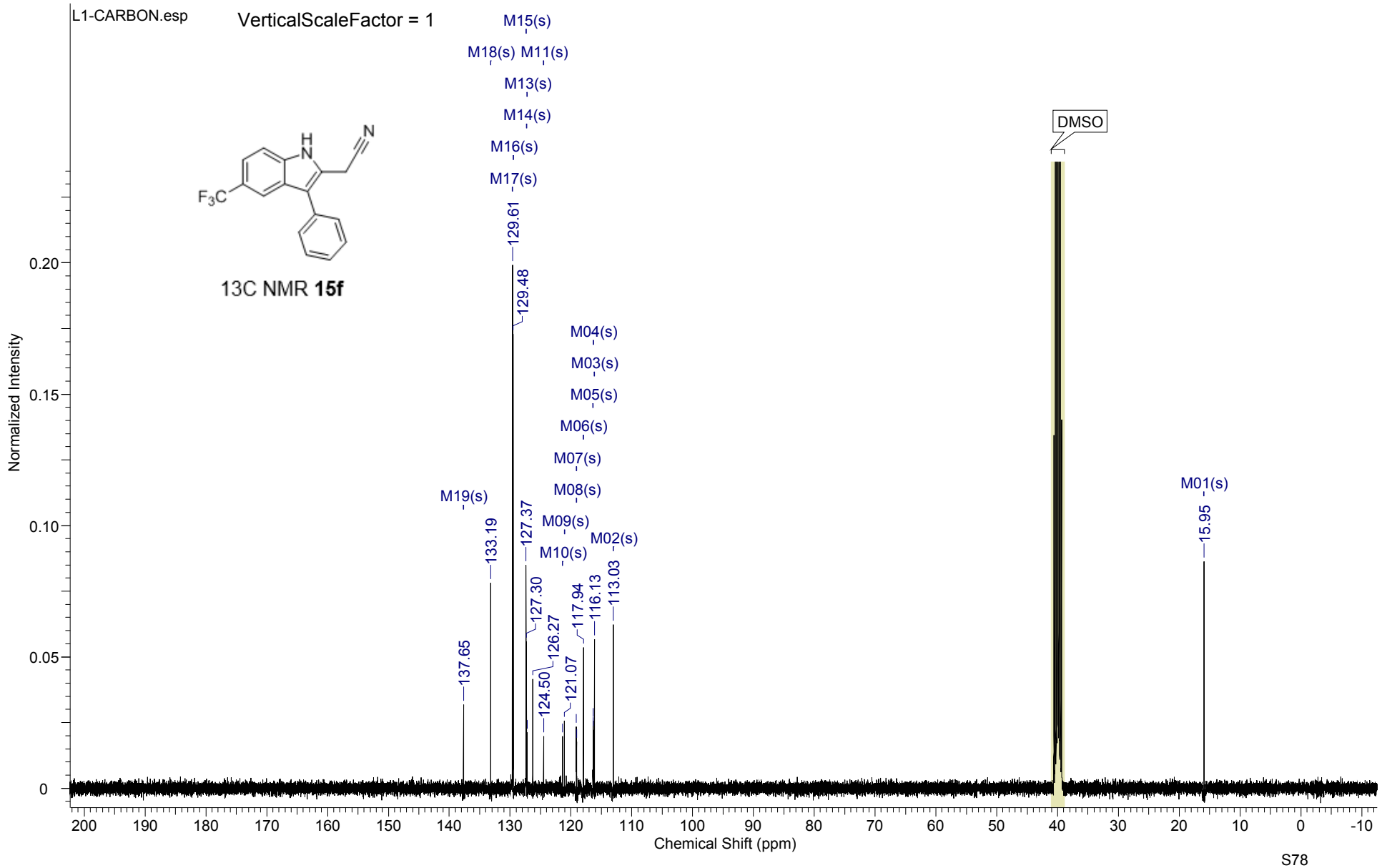
Acquisition Time (sec)	1.3631	***Date***	02 Sep 2017 04:48:16			***Date Stamp***	02 Sep 2017 04:48:16
File Name	E:\CJO-Indole Project\NMR\CJO-K1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.487						



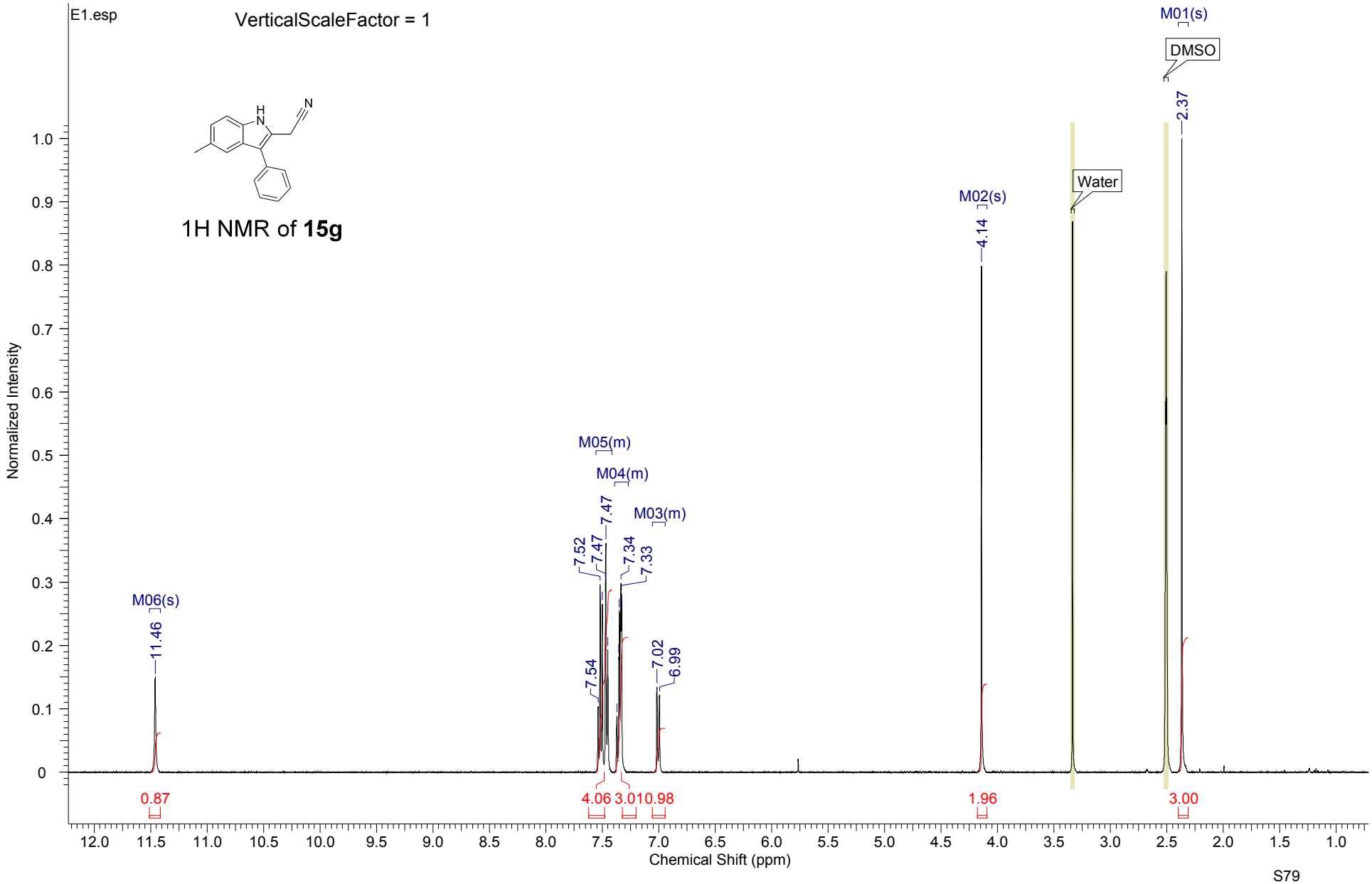
Acquisition Time (sec)	4.0894	***Date***	09 Aug 2017 09:08:32			***Date Stamp***	09 Aug 2017 09:08:32		
File Name	D:\CJO-UCSF\CJO-L1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.855						



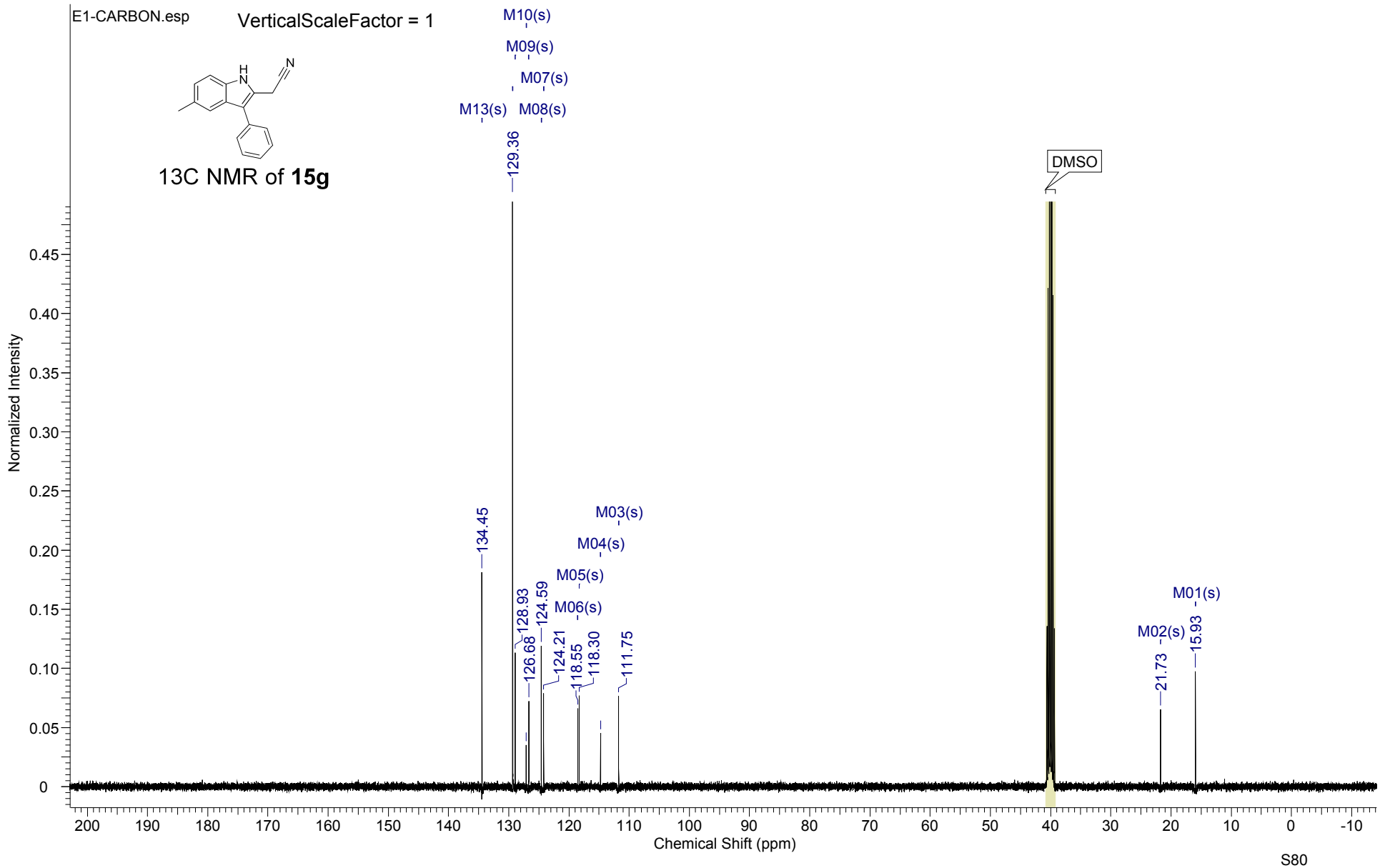
Acquisition Time (sec)	1.3631	***Date***	10 Aug 2017 00:55:44			***Date Stamp***	10 Aug 2017 00:55:44
File Name	D:\CJO-UCSF\NMR\CJO-L1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.169						



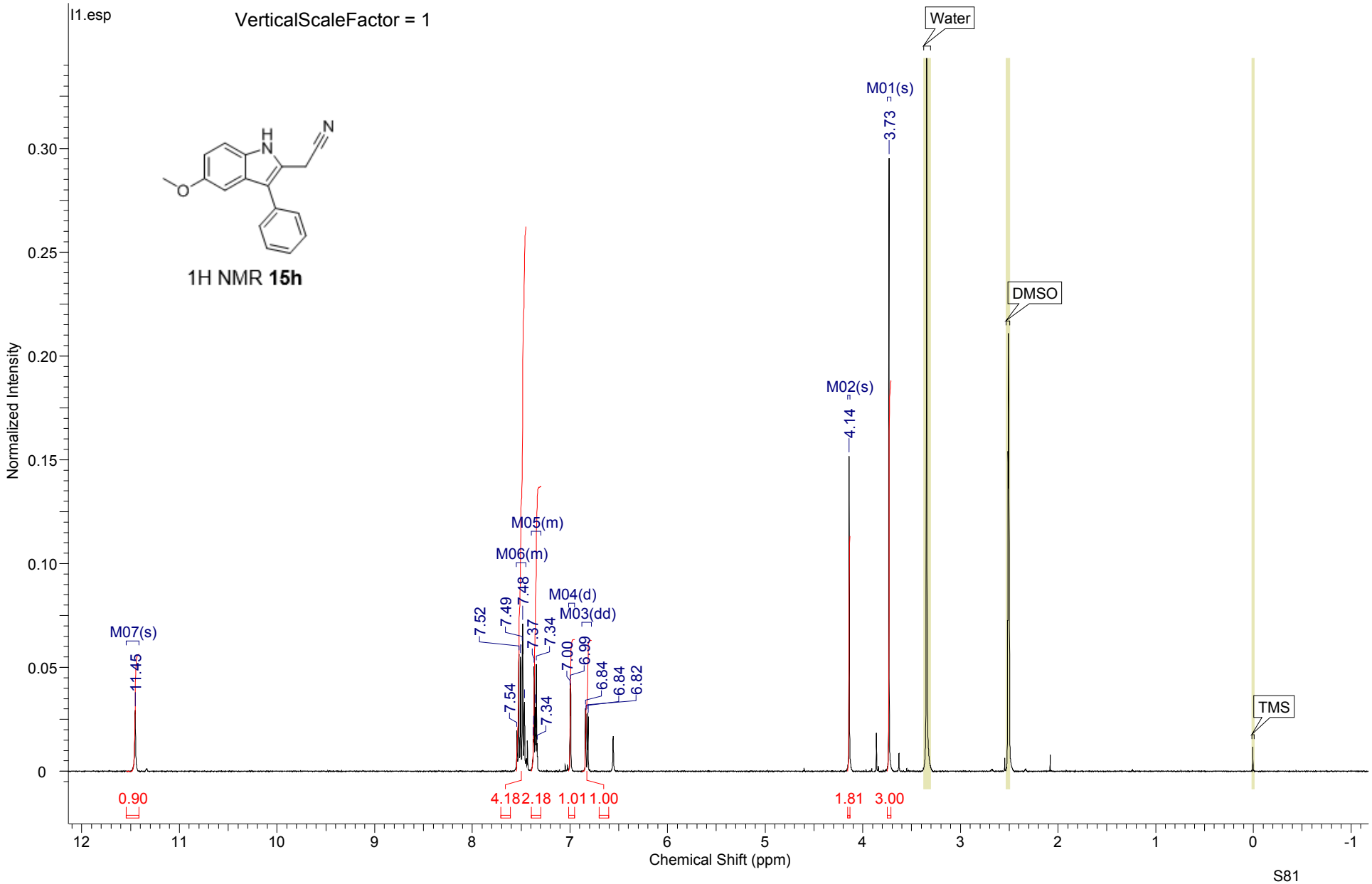
Acquisition Time (sec)	4.0894	***Date***	29 Aug 2017 08:25:52			***Date Stamp***	29 Aug 2017 08:25:52		
File Name	D:\CJO-UCSF\NMR\CJO-E1\6\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.786						



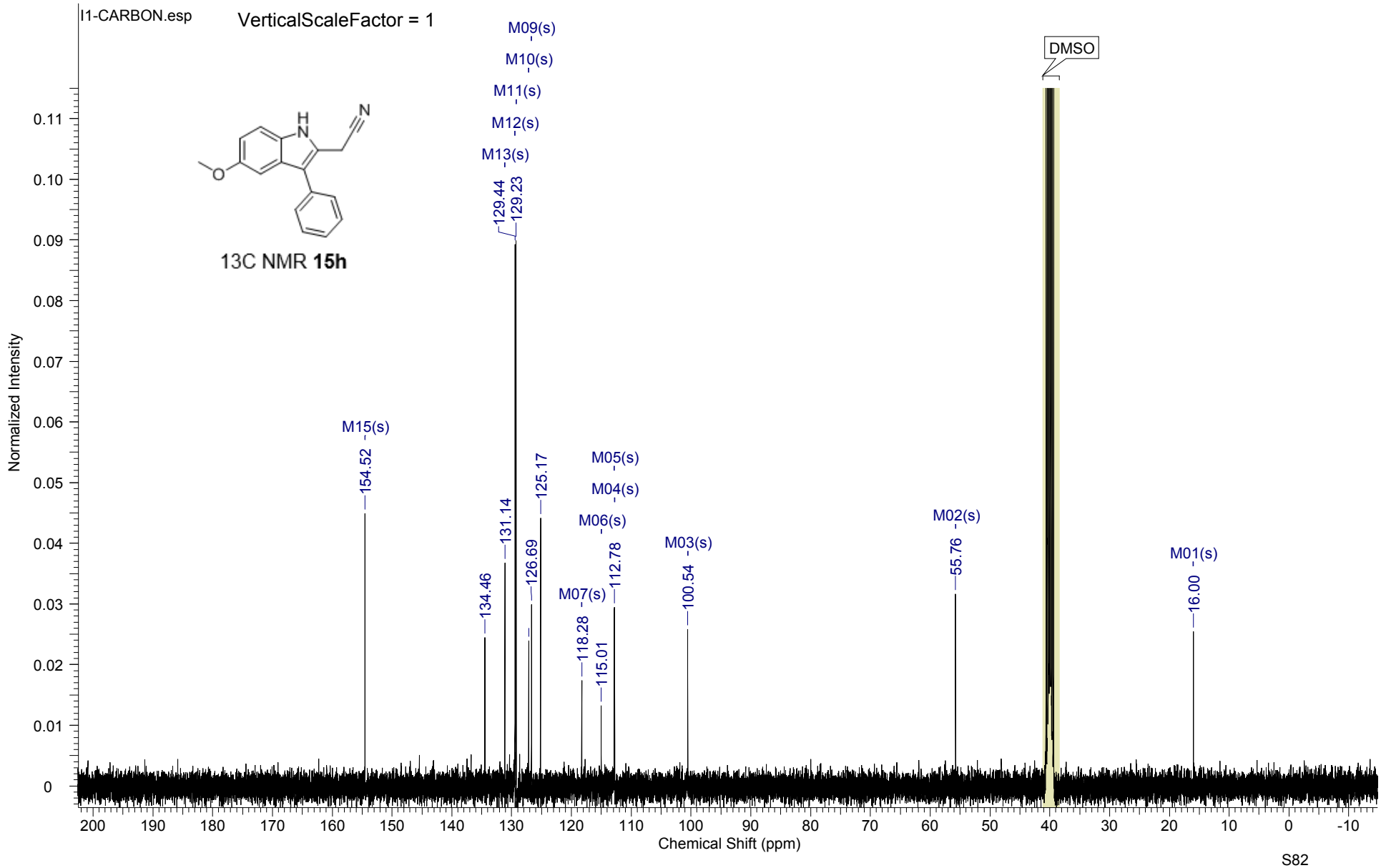
Acquisition Time (sec)	1.3631	***Date***	01 Sep 2017 06:13:36			***Date Stamp***	01 Sep 2017 06:13:36
File Name	D:\CJO-UCSF\NMR\CJO-E1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.511						



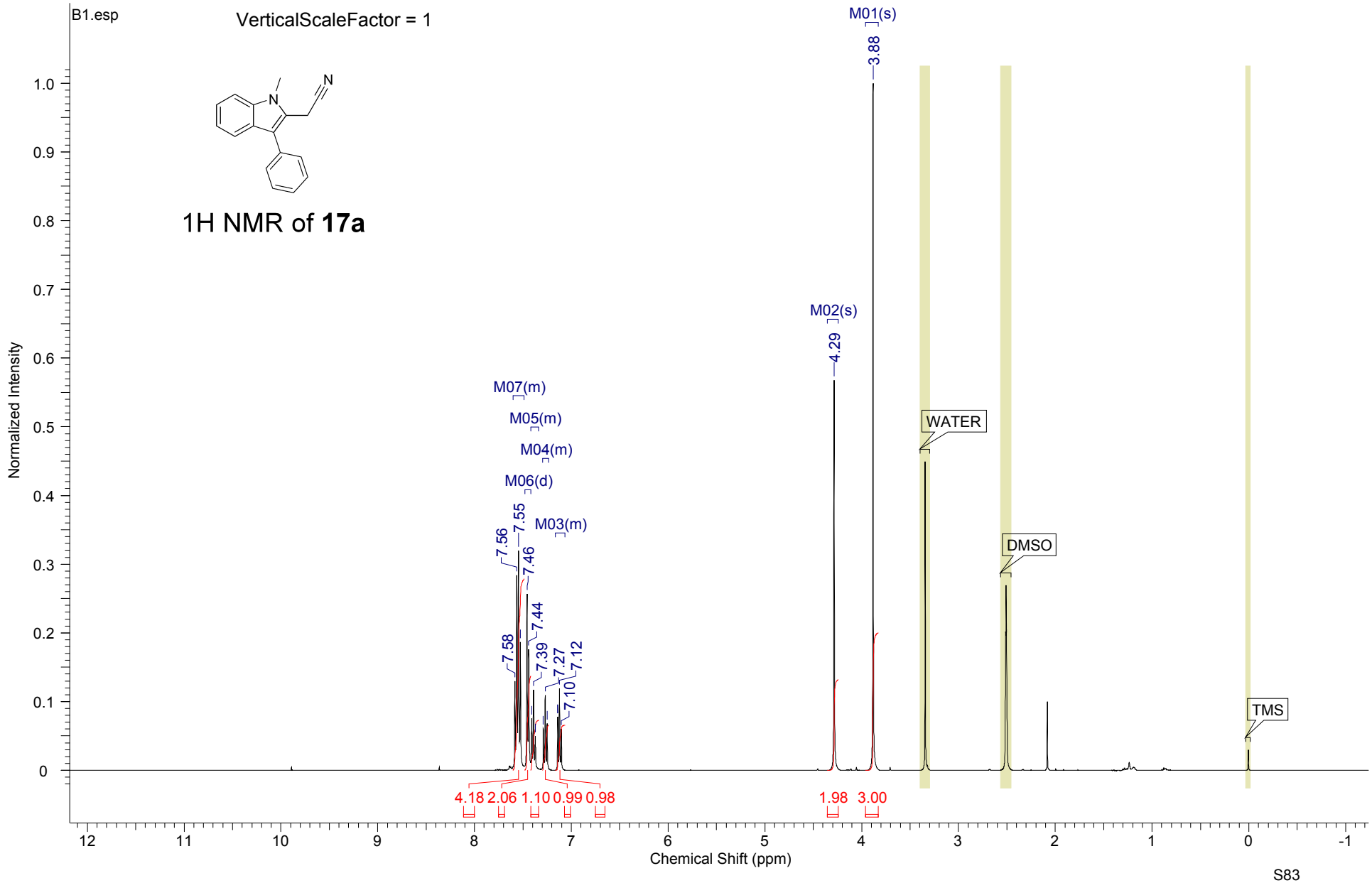
Acquisition Time (sec)	4.0894	***Date***	11 Aug 2017 09:08:32			***Date Stamp***	11 Aug 2017 09:08:32		
File Name	D:\CJO-UCSF\NMR\CJO-I1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.667						



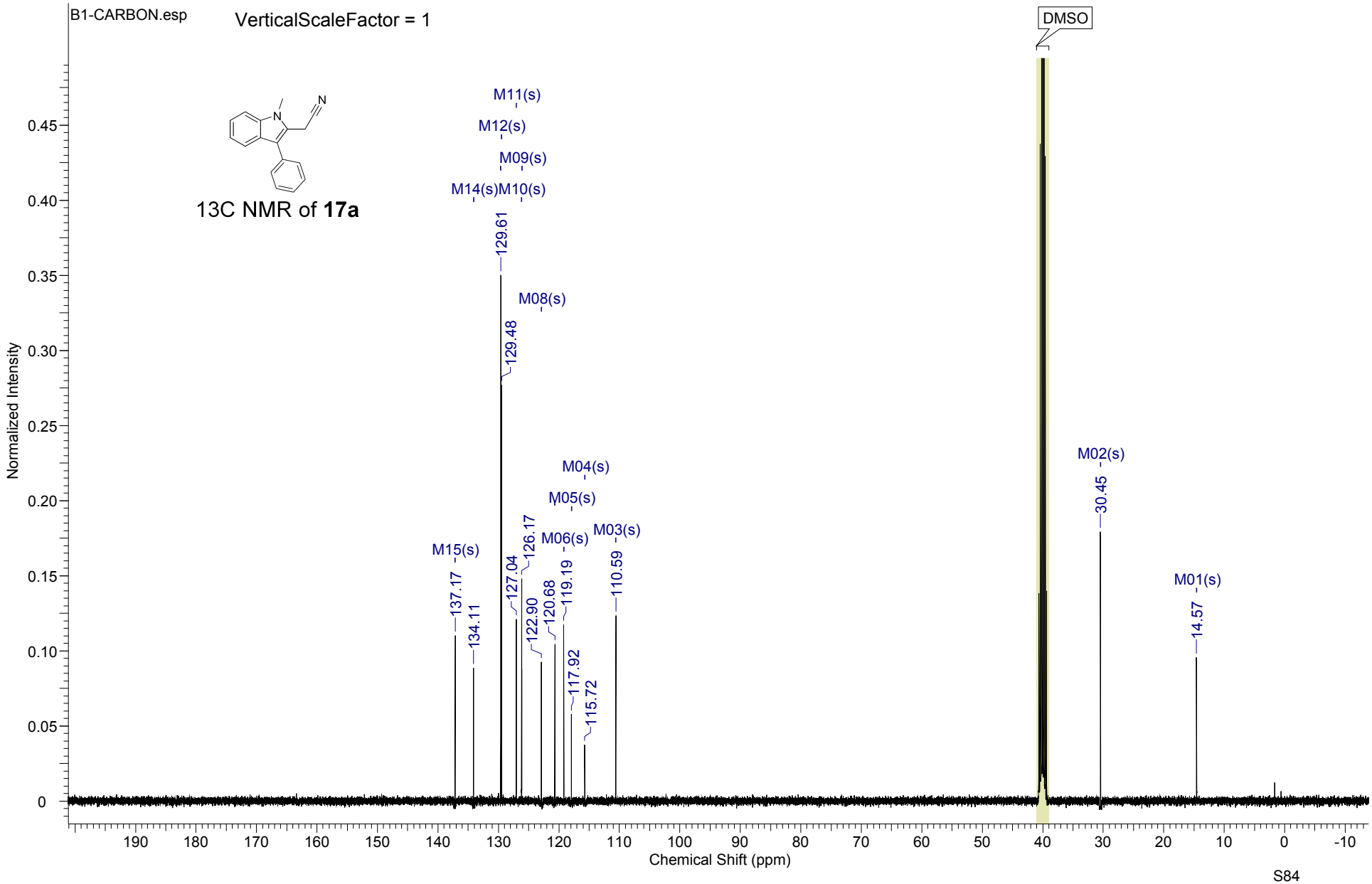
Acquisition Time (sec)	1.3631	***Date***	12 Aug 2017 03:48:32			***Date Stamp***	12 Aug 2017 03:48:32
File Name	D:\CJO-UCSF\NMR\CJO-I1\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.313						



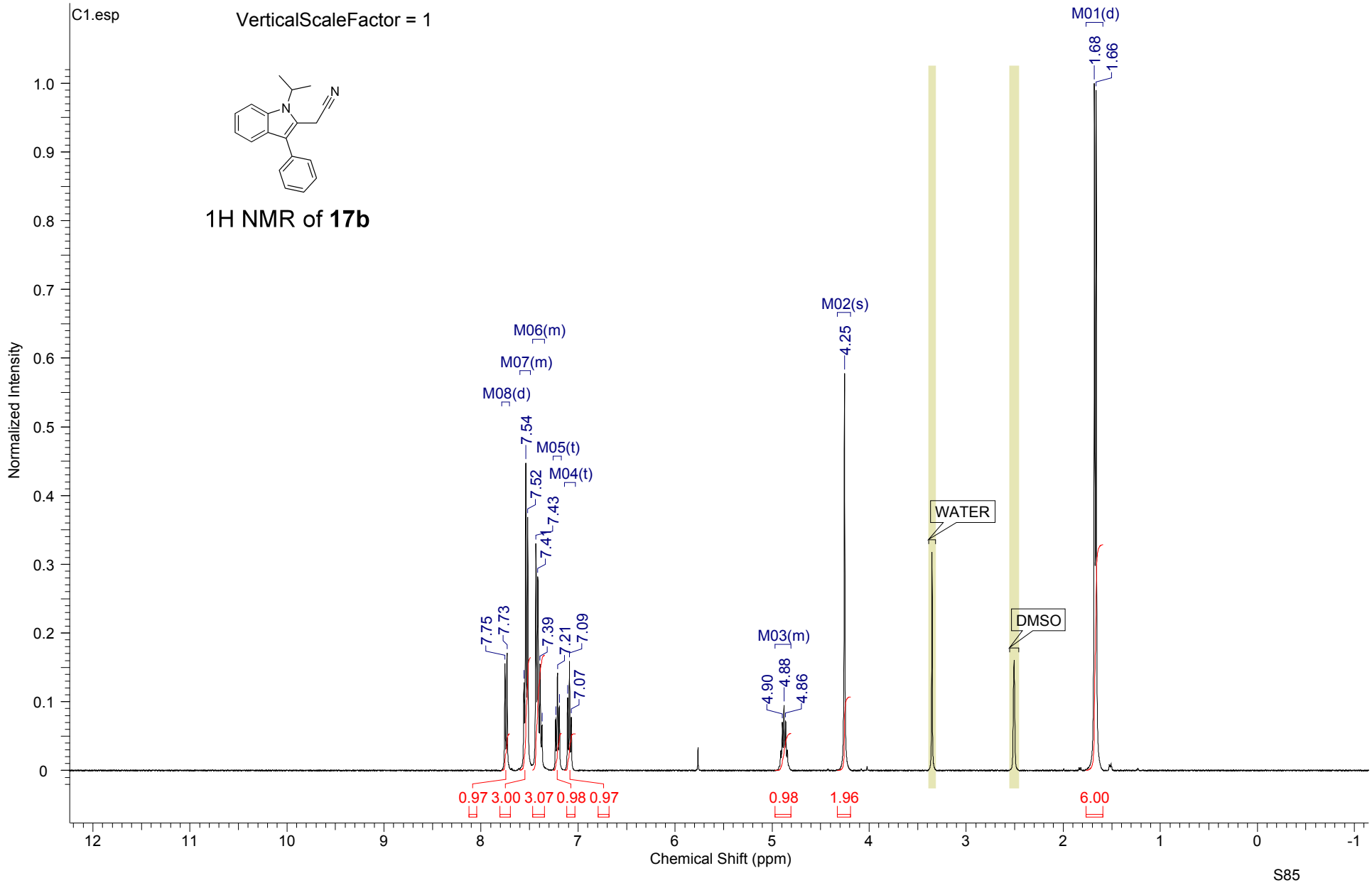
Acquisition Time (sec)	4.0894	***Date***	08 Aug 2017 09:23:28			***Date Stamp***	08 Aug 2017 09:23:28		
File Name	D:\CJO-B1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.592						



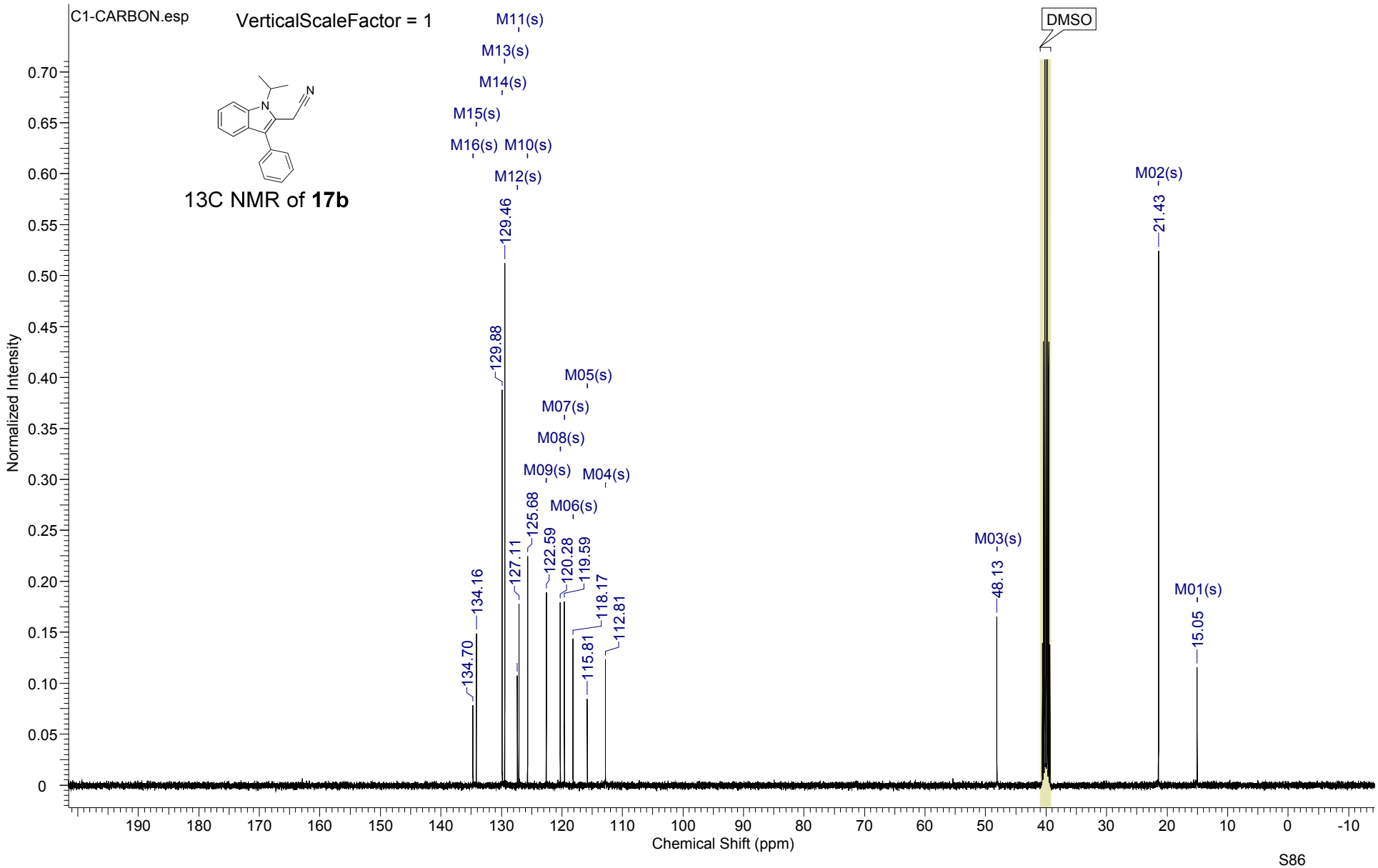
Acquisition Time (sec)	1.3631	***Date***	09 Aug 2017 03:48:32			***Date Stamp***	09 Aug 2017 03:48:32		
File Name	D:\CJO-UCSF\CJO-B1\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C	***Number of Transients***	3000
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	196.40	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.384						



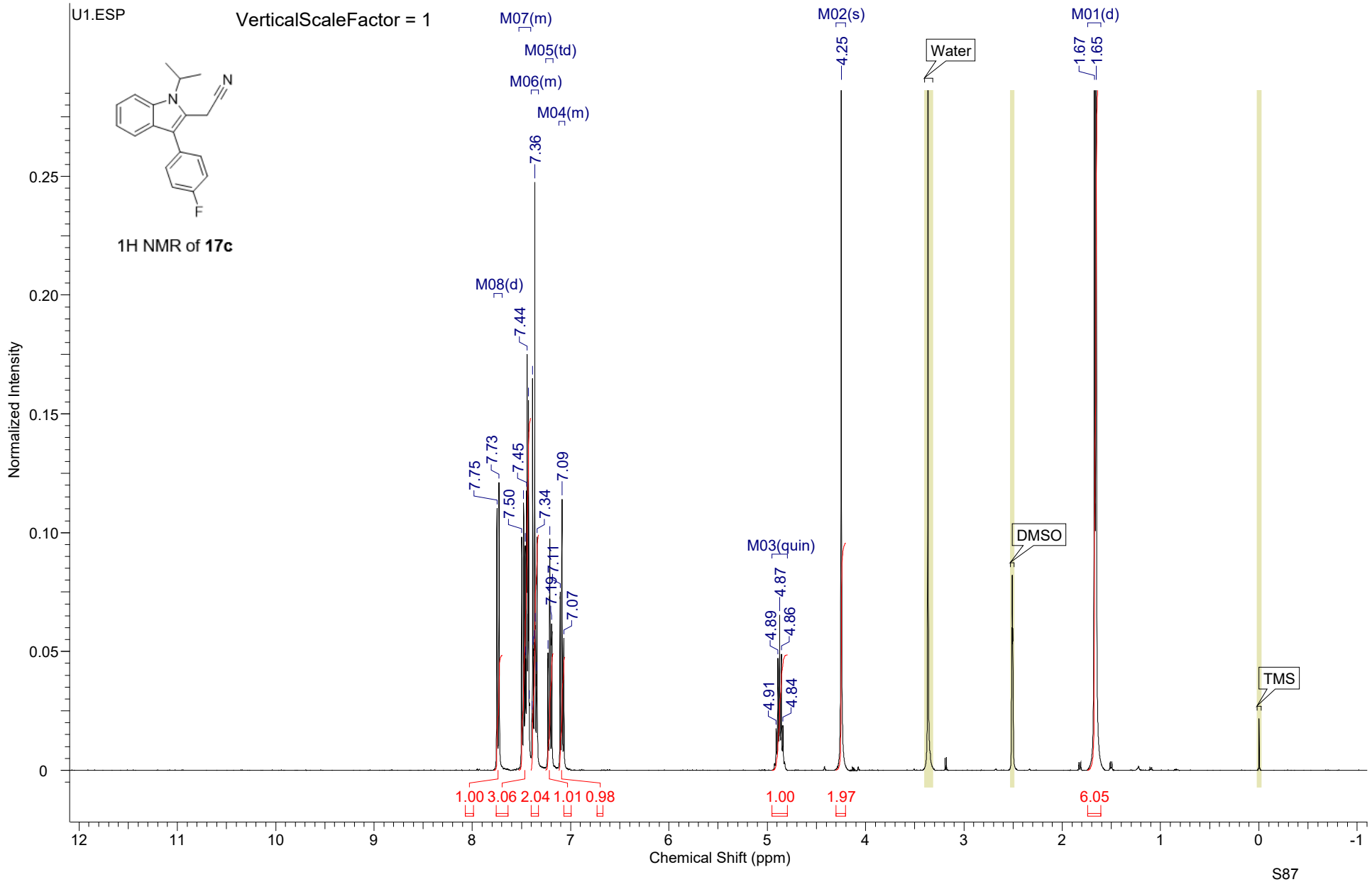
Acquisition Time (sec)	4.0894	***Date***	12 Sep 2017 10:23:12			***Date Stamp***	12 Sep 2017 10:23:12		
File Name	D:\CJO-UCSF\NMR\CJO-C1\3\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	70.44	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9255	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.468						



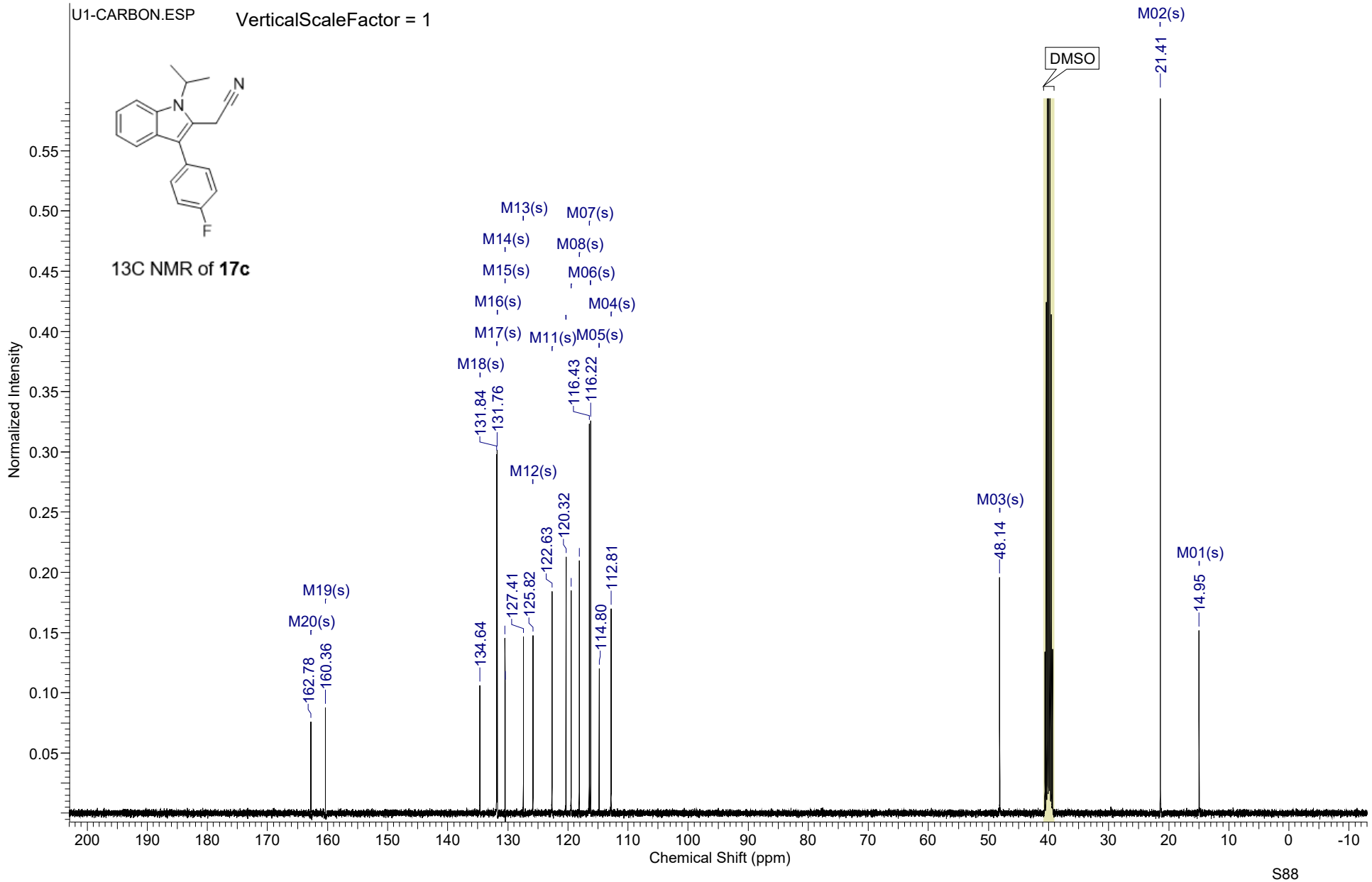
Acquisition Time (sec)	1.3631	***Date***	12 Sep 2017 23:58:08			***Date Stamp***	12 Sep 2017 23:58:08
File Name	D:\CJO-UCSF\NMR\CJO-C1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.224						



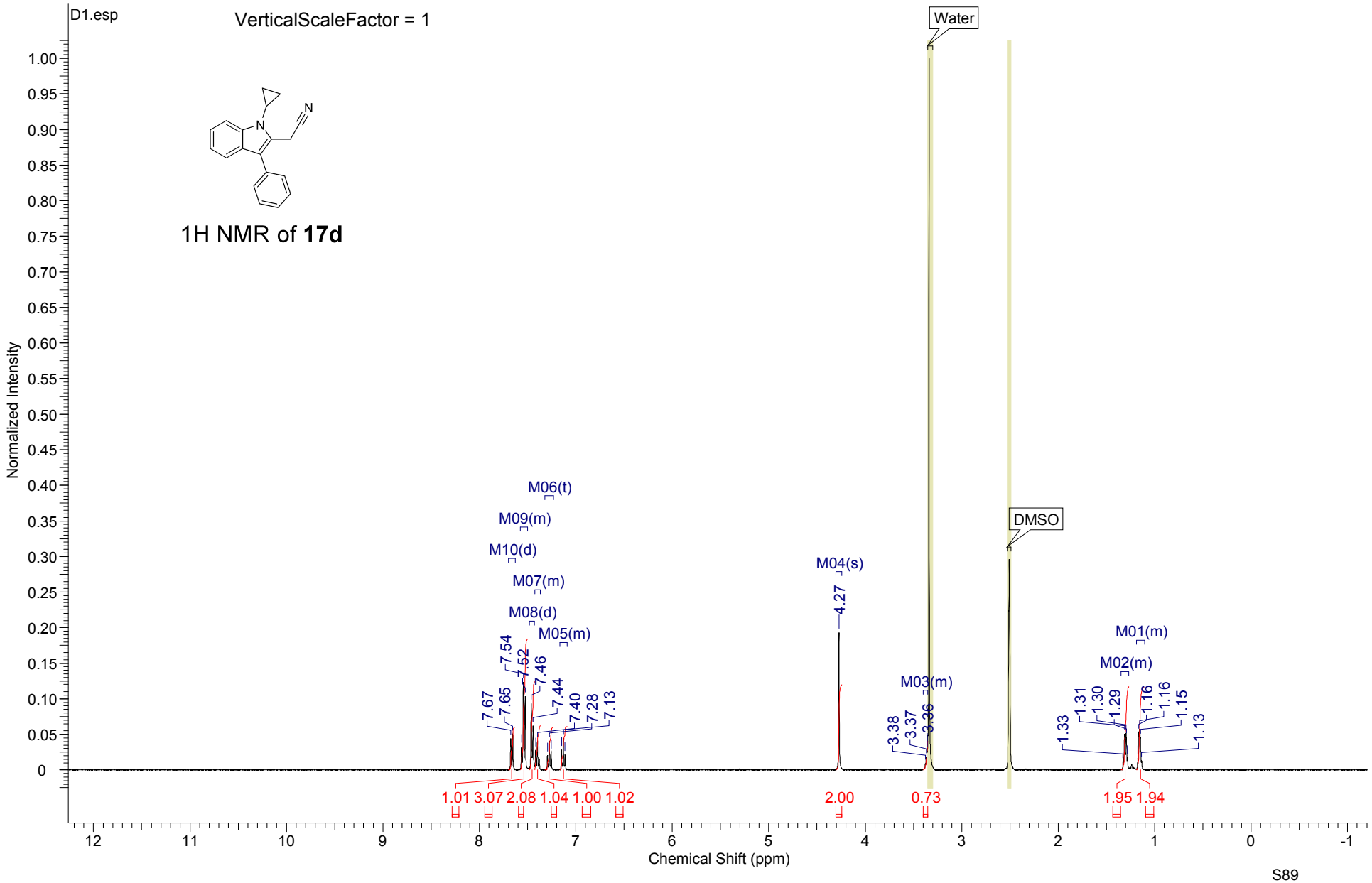
Acquisition Time (sec)	4.0894	***Date***	05 Aug 2017 13:28:48			***Date Stamp***	05 Aug 2017 13:28:48		
File Name	D:\NMR\CJO\CJO-U1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	56.60	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.742						



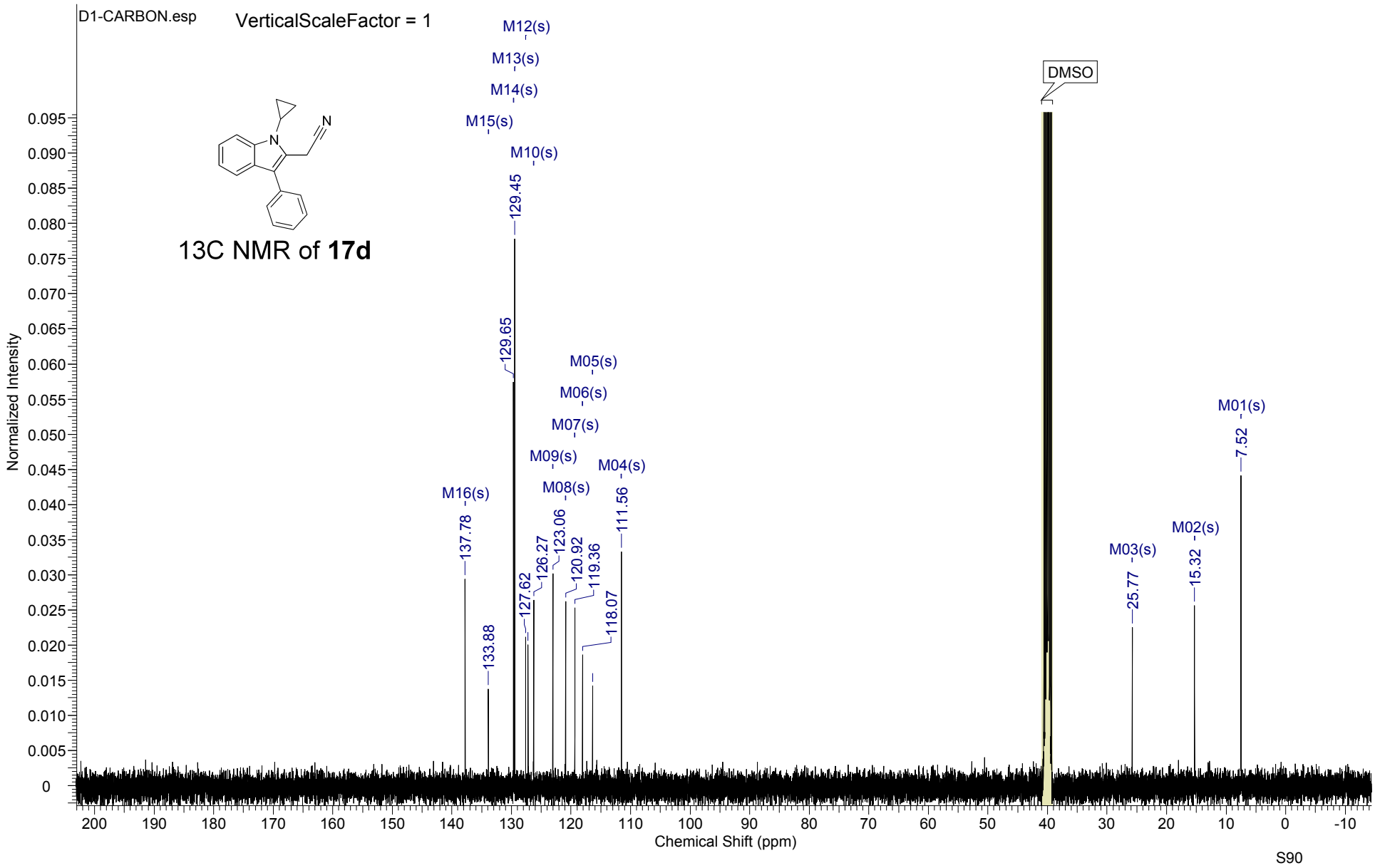
Acquisition Time (sec)	1.3631	***Date***	05 Aug 2017 22:13:36			***Date Stamp***	05 Aug 2017 22:13:36		
File Name	D:\NMR\CJO\CJO-U1\2\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C	***Number of Transients***	3000
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	196.40	***SW(cyclical) (Hz)***	24038.46	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD
Sweep Width (Hz)	24037.73	***Temperature (degree C)***	23.286						



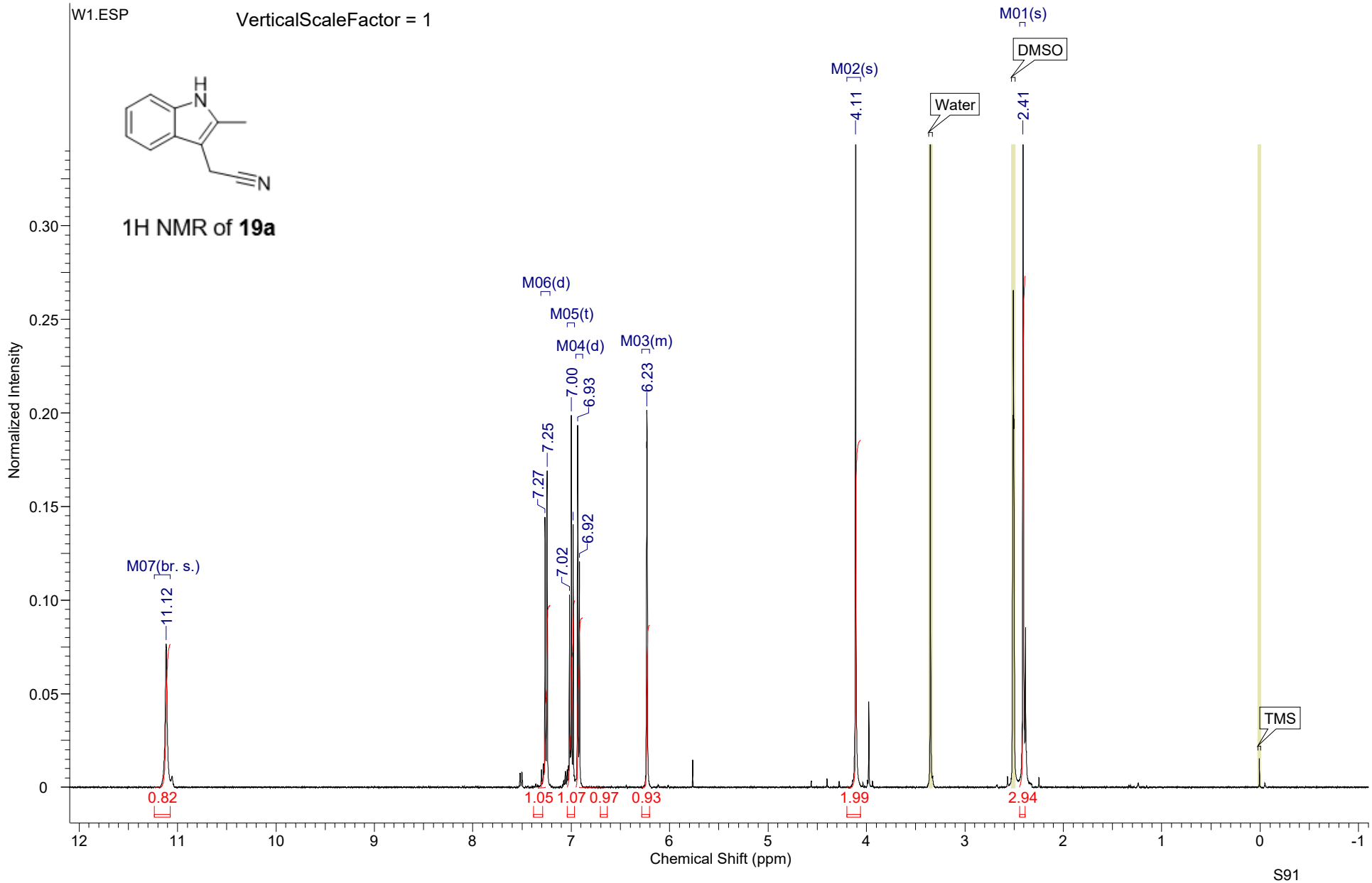
Acquisition Time (sec)	4.0894	***Date***	31 Aug 2017 11:25:04			***Date Stamp***	31 Aug 2017 11:25:04		
File Name	D:\CJO-UCSF\NMR\CJO-D1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	125.72	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.748						



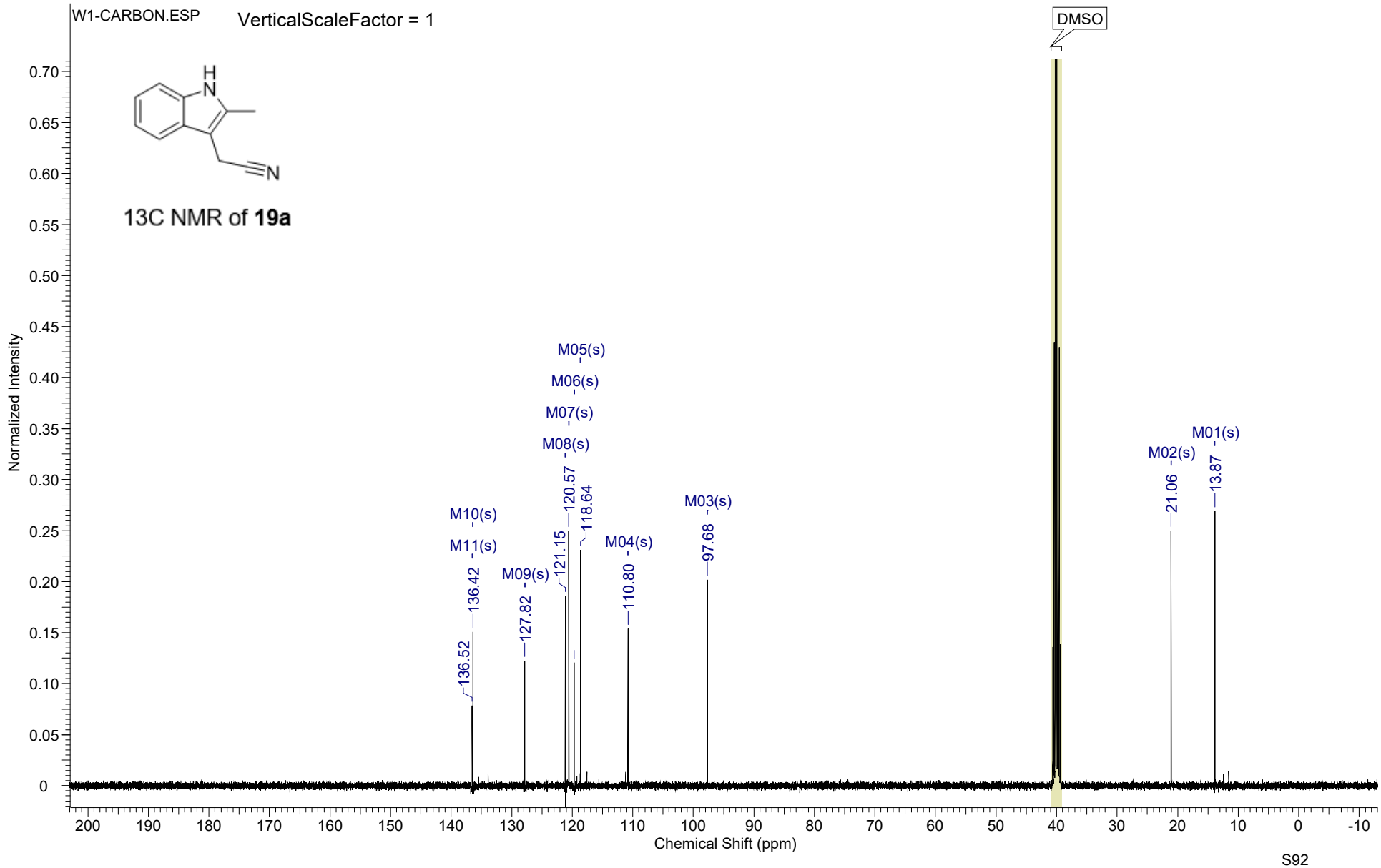
Acquisition Time (sec)	1.3631	***Date***	02 Sep 2017 01:53:20			***Date Stamp***	02 Sep 2017 01:53:20
File Name	E:\CJO-Indole Project\NMR\CJO-D1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	4000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.352						



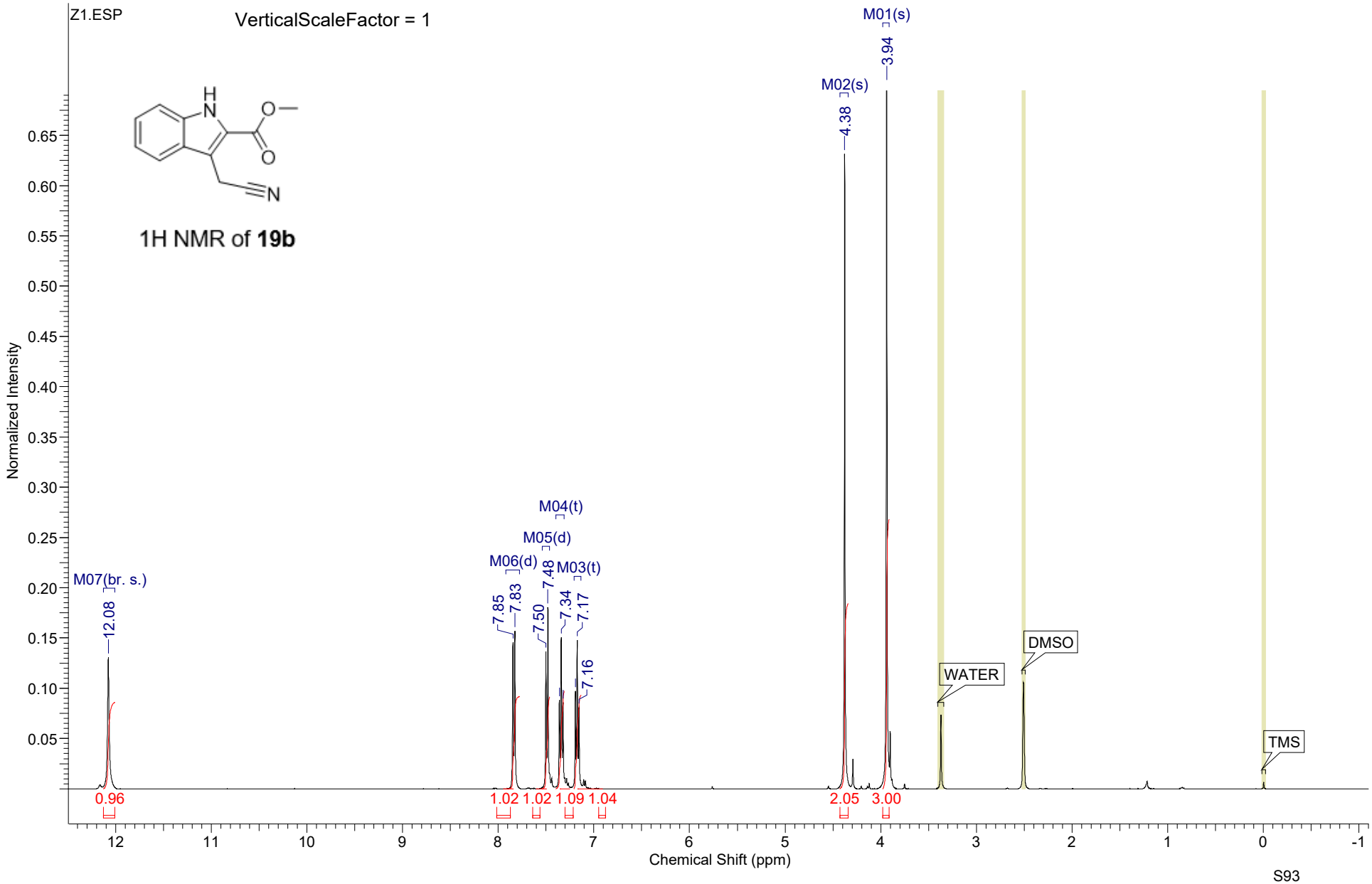
Acquisition Time (sec)	4.0894	***Date***	19 Sep 2017 08:32:16			***Date Stamp***	19 Sep 2017 08:32:16		
File Name	D:\CJO-UCSF\NMR\CJO-W1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.650						



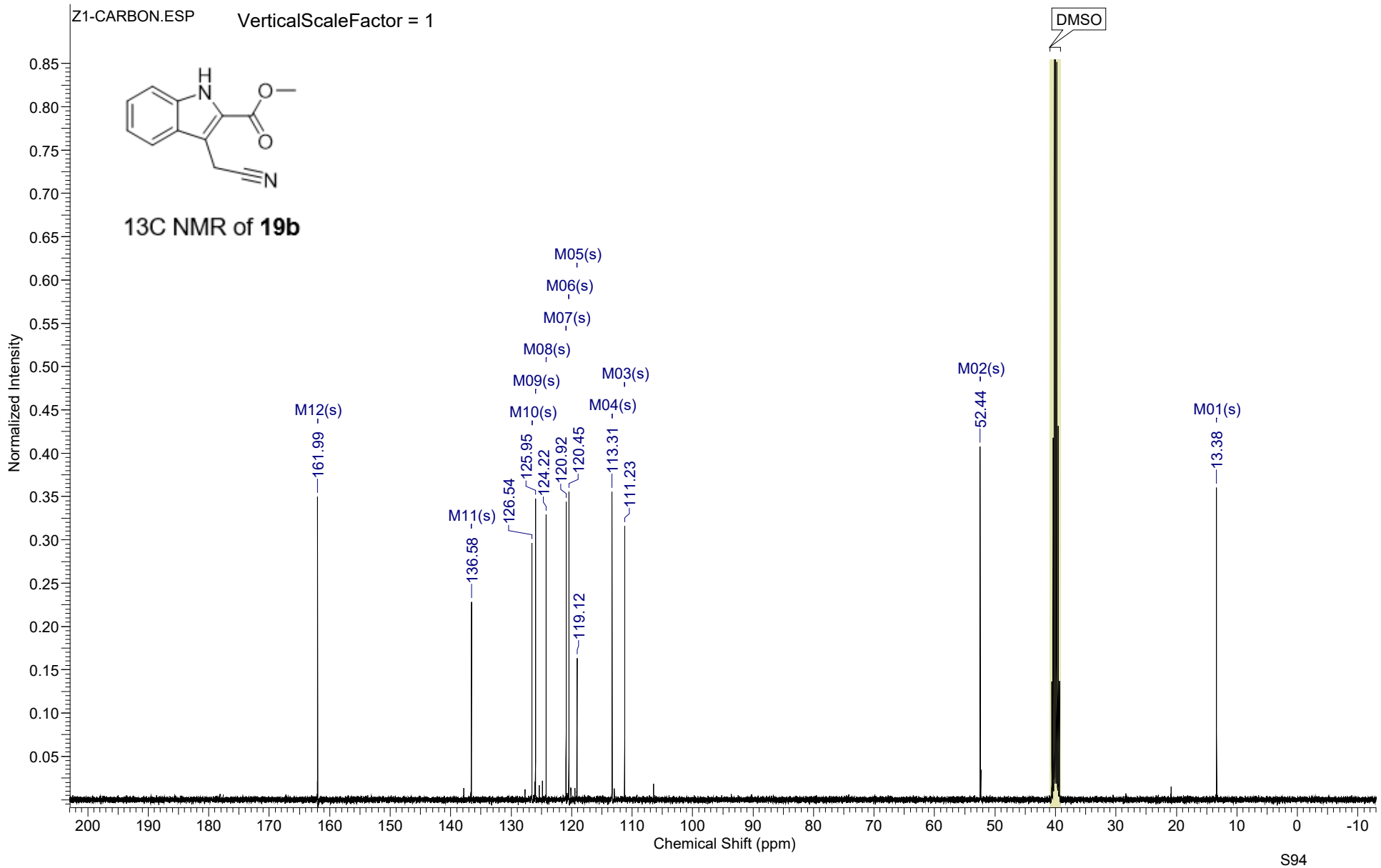
Acquisition Time (sec)	1.3631	***Date***	19 Sep 2017 23:58:08			***Date Stamp***	19 Sep 2017 23:58:08
File Name	D:\CJO-UCSF\NMR\CJO-W1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.164						



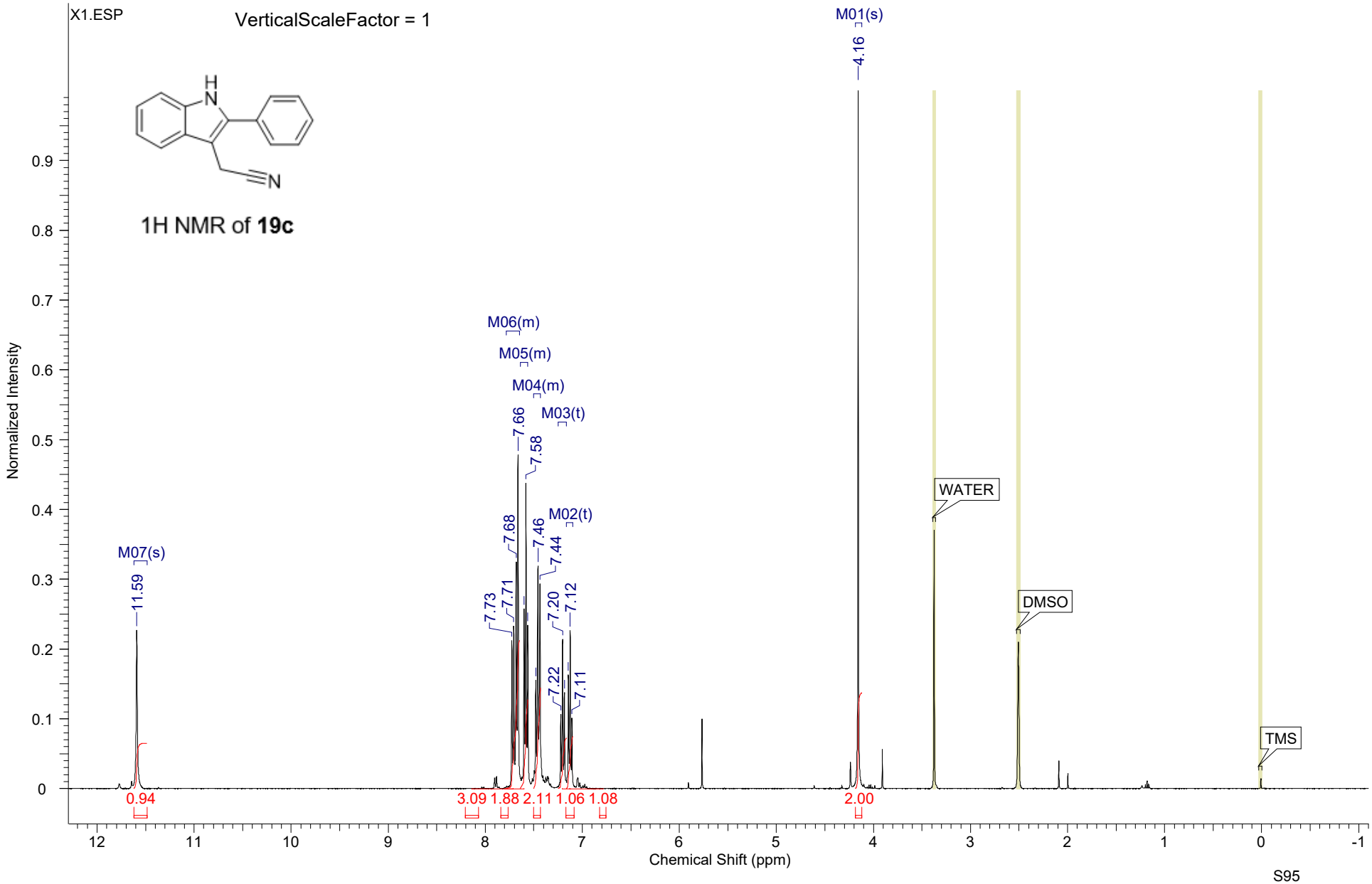
Acquisition Time (sec)	4.0894	***Date***	23 Sep 2017 10:36:00			***Date Stamp***	23 Sep 2017 10:36:00		
File Name	D:\CJO-UCSF\NMR\CJO-Z1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	62.81	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.674						



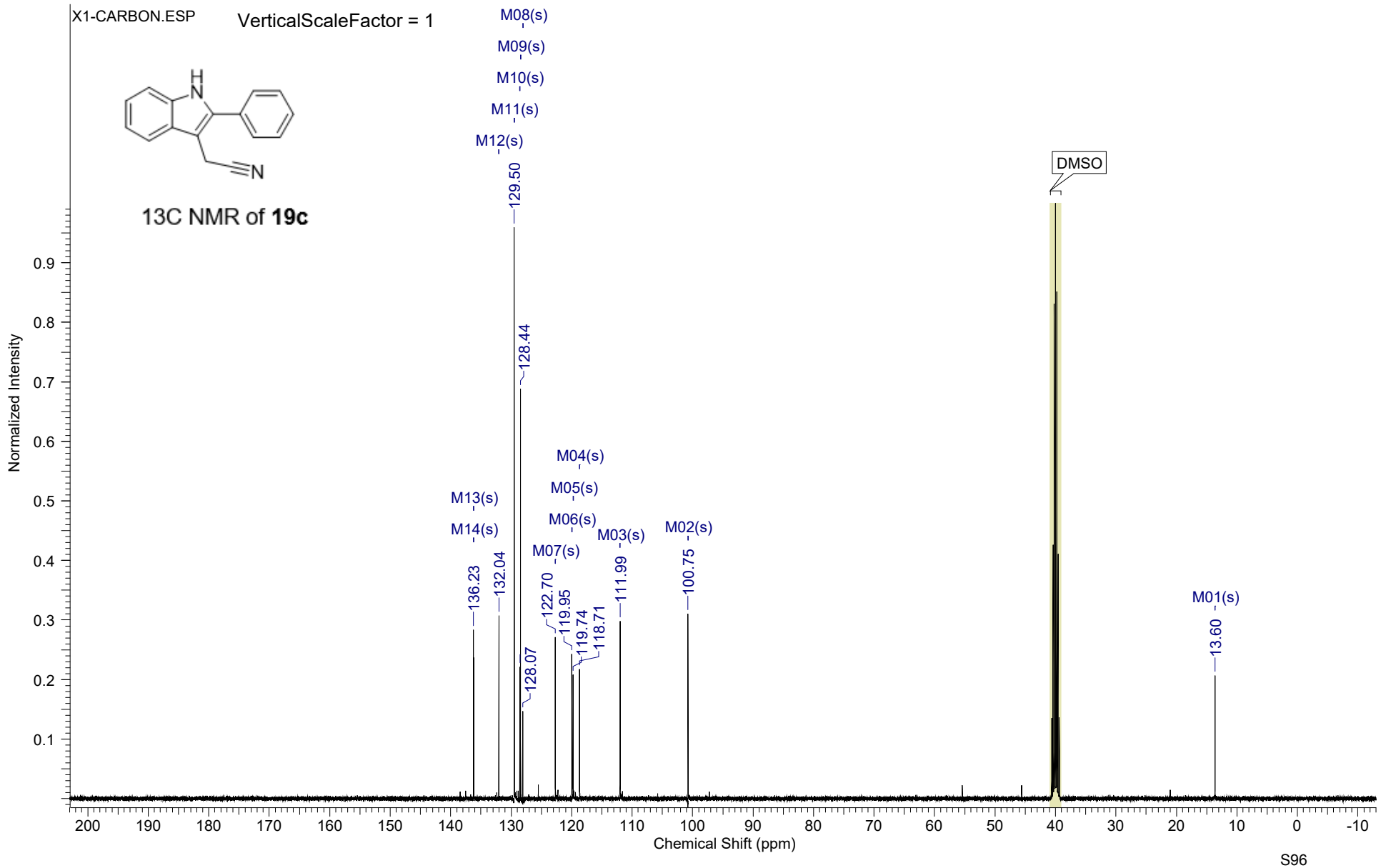
Acquisition Time (sec)	1.3631	***Date***	23 Sep 2017 12:31:12			***Date Stamp***	23 Sep 2017 12:31:12
File Name	D:\CJO-UCSF\NMR\CJO-Z1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.130						



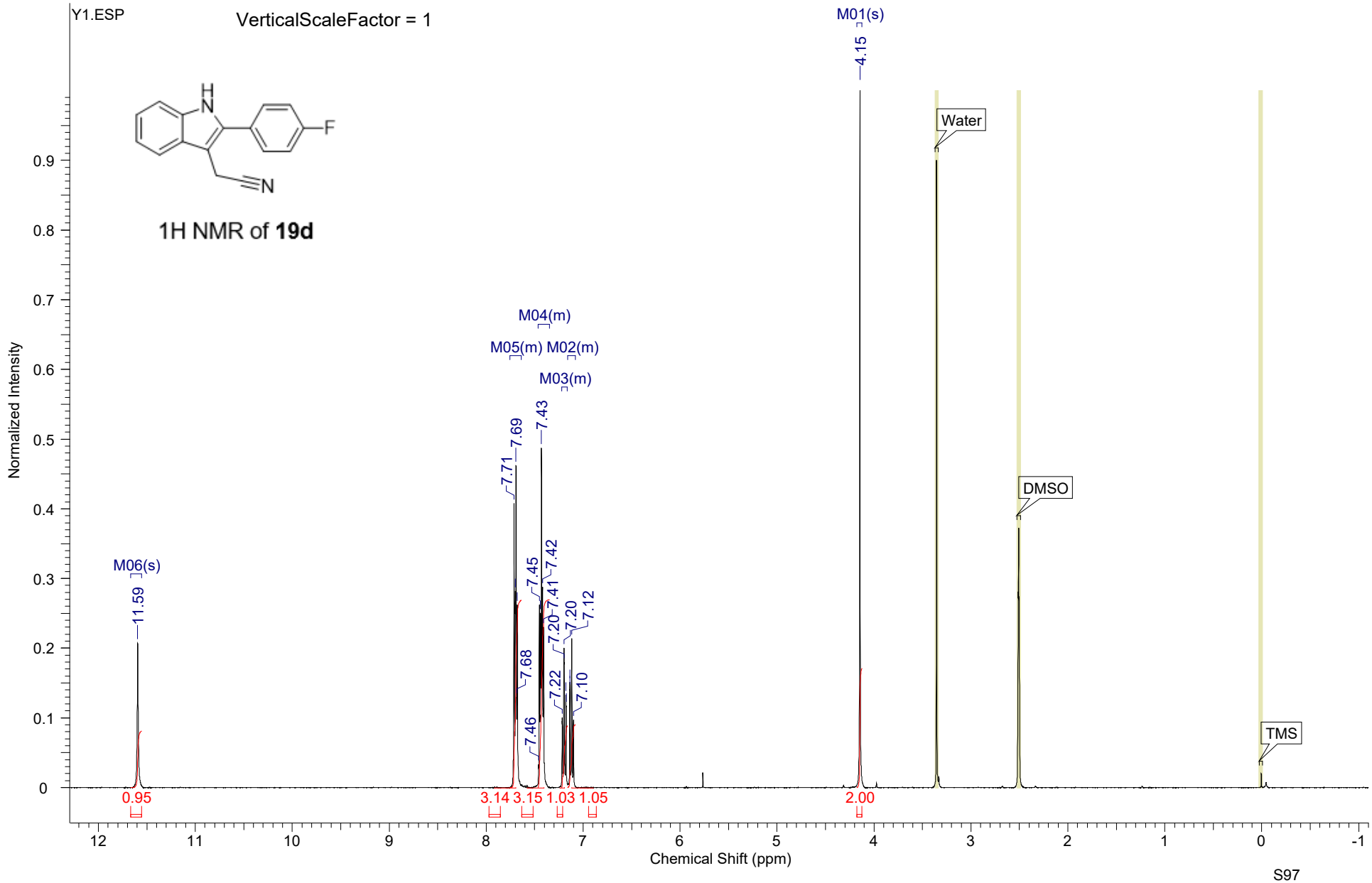
Acquisition Time (sec)	4.0894	***Date***	19 Sep 2017 08:34:24			***Date Stamp***	19 Sep 2017 08:34:24		
File Name	D:\CJO-UCSF\NMR\CJO-X1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	70.44	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.639						



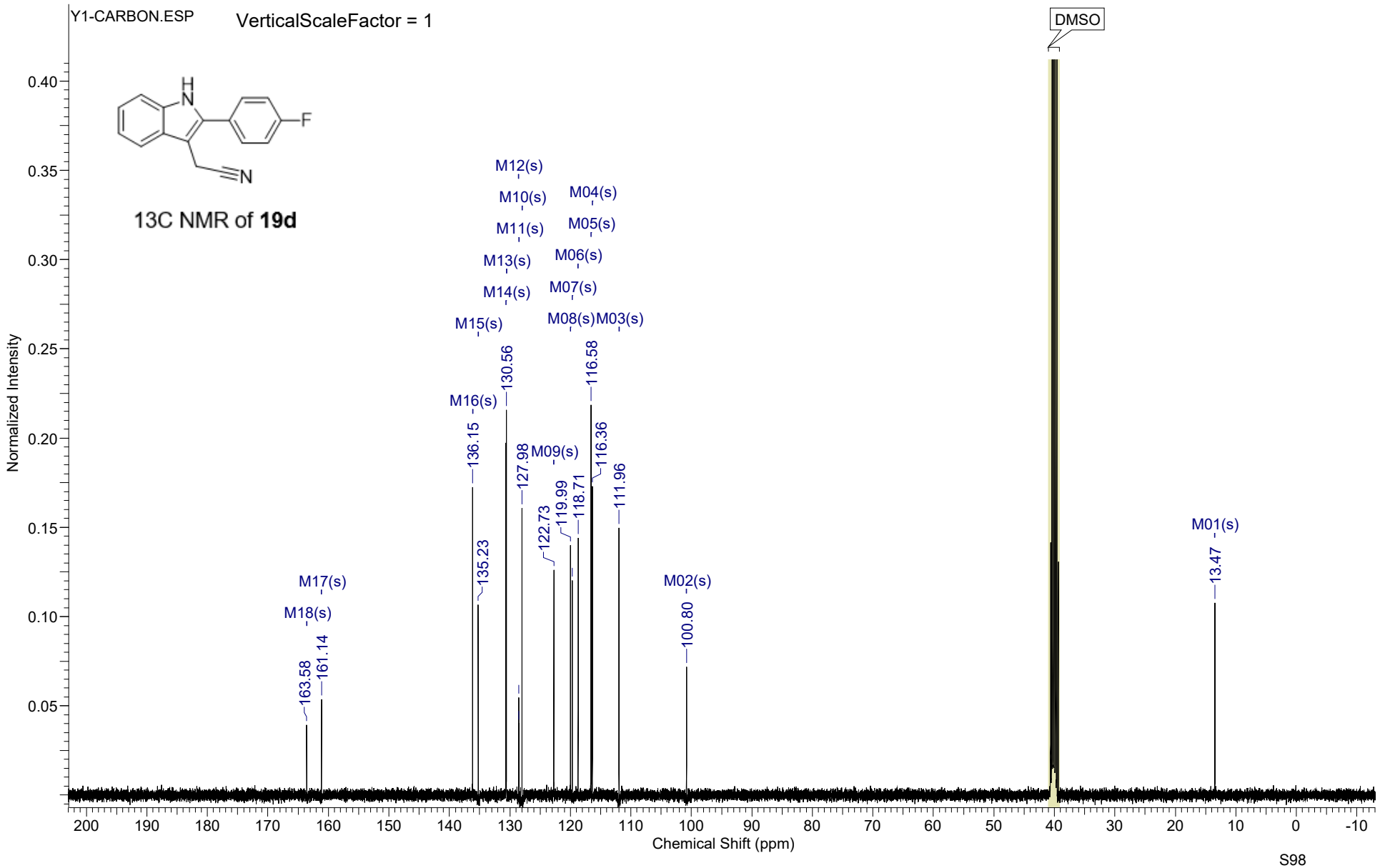
Acquisition Time (sec)	1.3631	***Date***	20 Sep 2017 01:55:28			***Date Stamp***	20 Sep 2017 01:55:28
File Name	D:\CJO-UCSF\NMR\CJO-X1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	22.973						



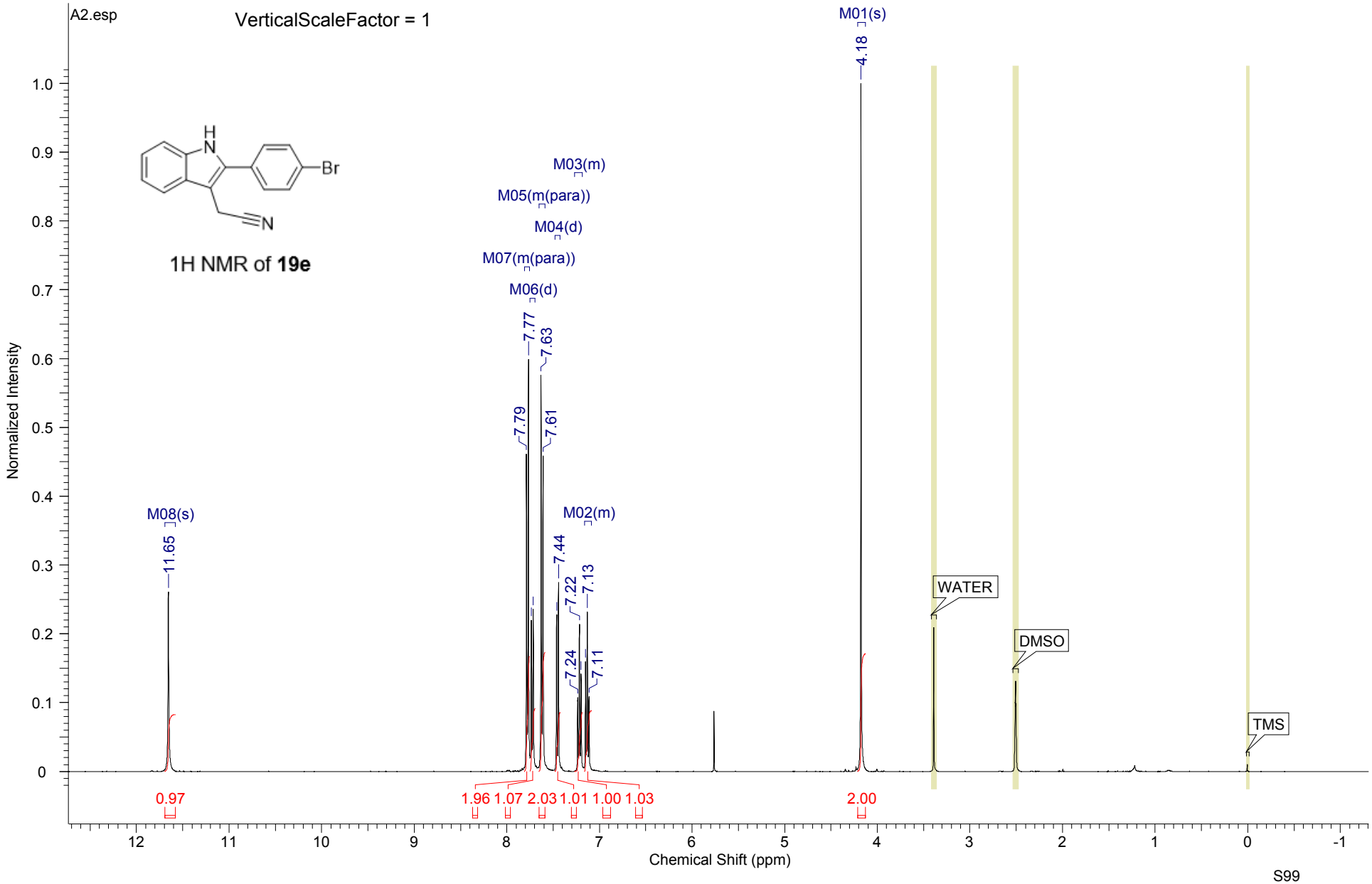
Acquisition Time (sec)	4.0894	***Date***	19 Sep 2017 08:38:40			***Date Stamp***	19 Sep 2017 08:38:40		
File Name	D:\CJO-UCSF\NMR\CJO-Y1\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	97.12	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.630						



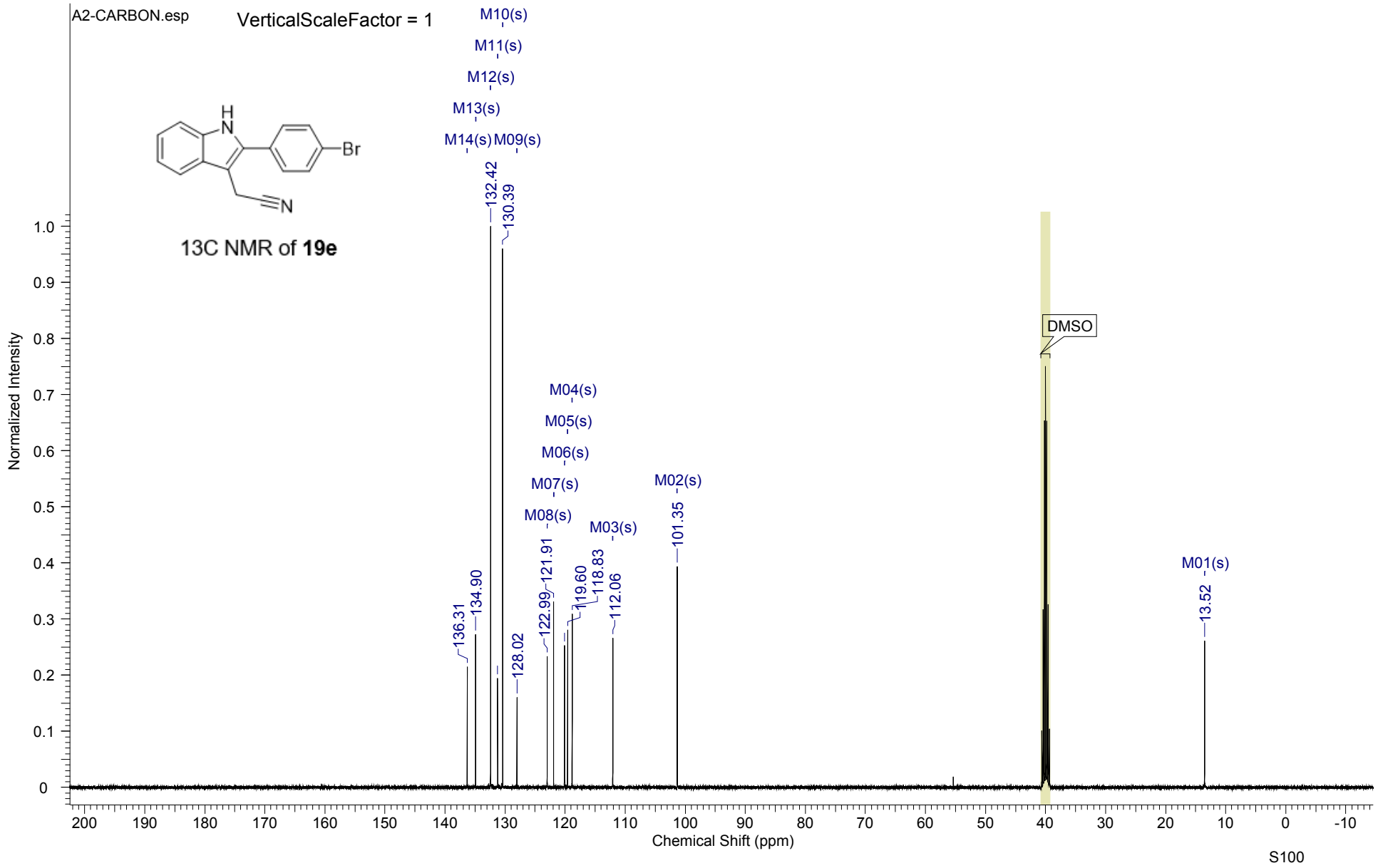
Acquisition Time (sec)	1.3631	***Date***	20 Sep 2017 03:50:40			***Date Stamp***	20 Sep 2017 03:50:40
File Name	D:\CJO-UCSF\NMR\CJO-Y1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.037						



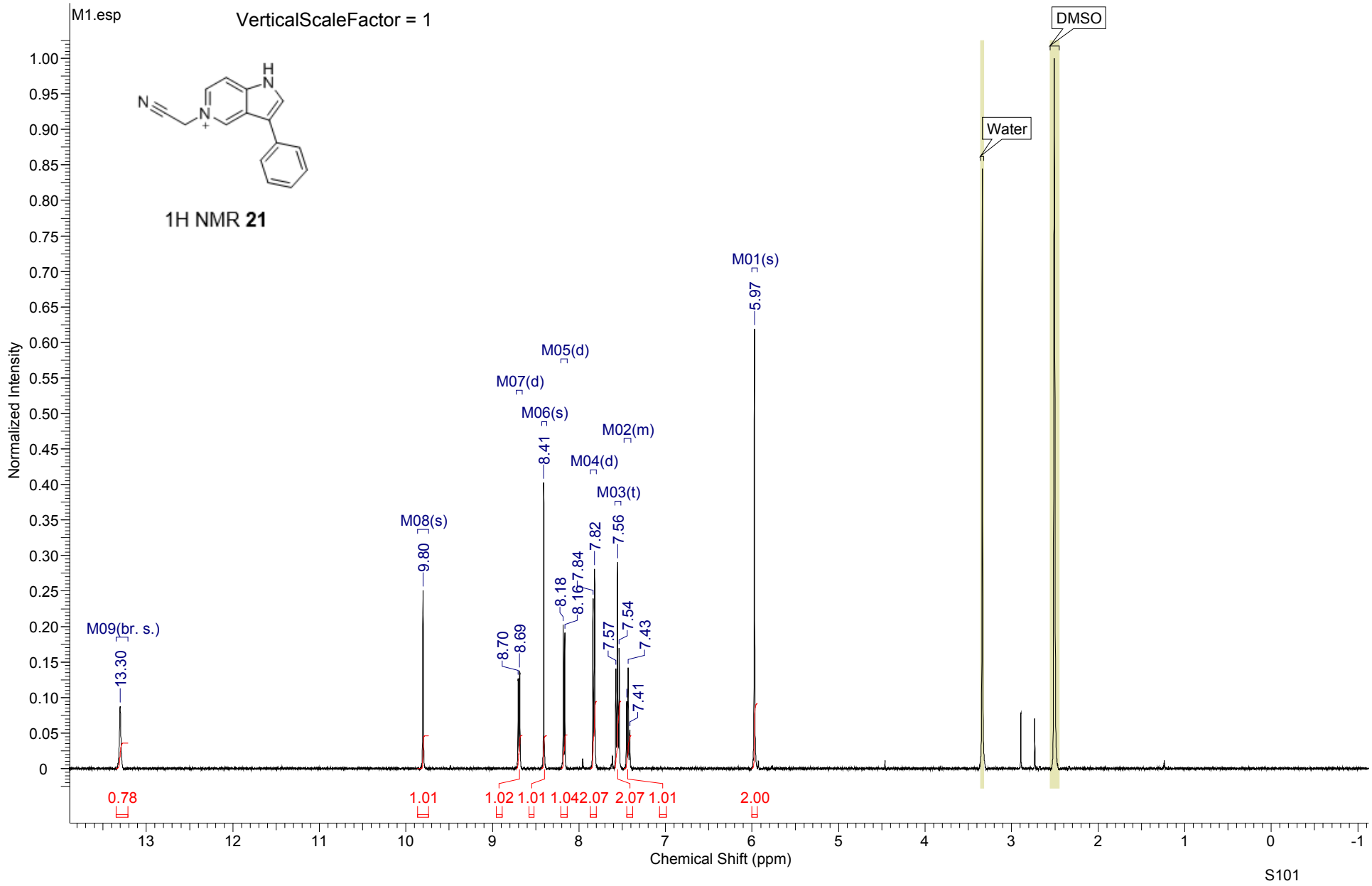
Acquisition Time (sec)	4.0894	***Date***	23 Sep 2017 12:35:28			***Date Stamp***	23 Sep 2017 12:35:28		
File Name	D:\CJO-UCSF\NMR\CJO-A2\1\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	32
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	56.60	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.636						



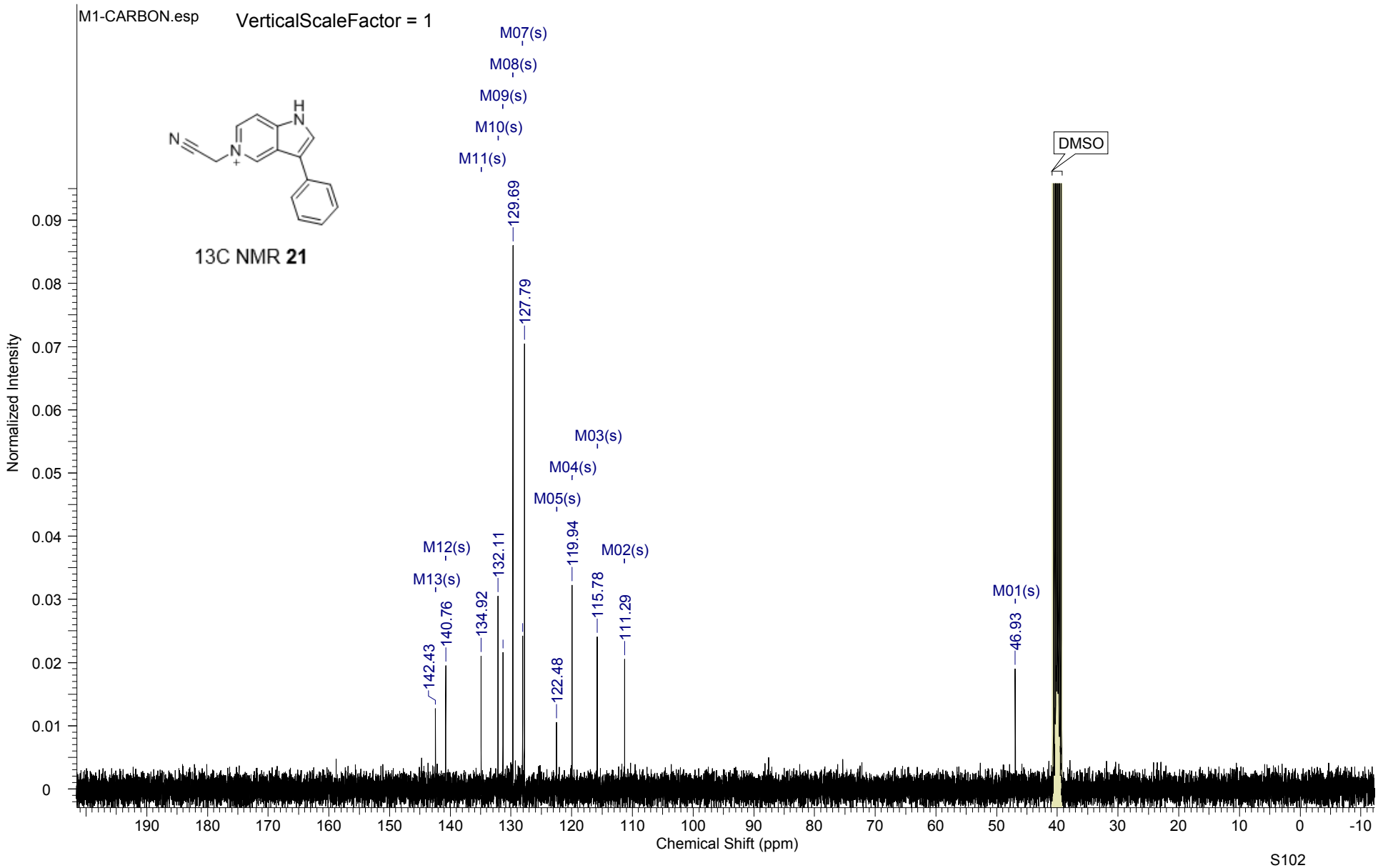
Acquisition Time (sec)	1.3631	***Date***	23 Sep 2017 14:30:40			***Date Stamp***	23 Sep 2017 14:30:40
File Name	D:\CJO-UCSF\NMR\CJO-A2\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.354						



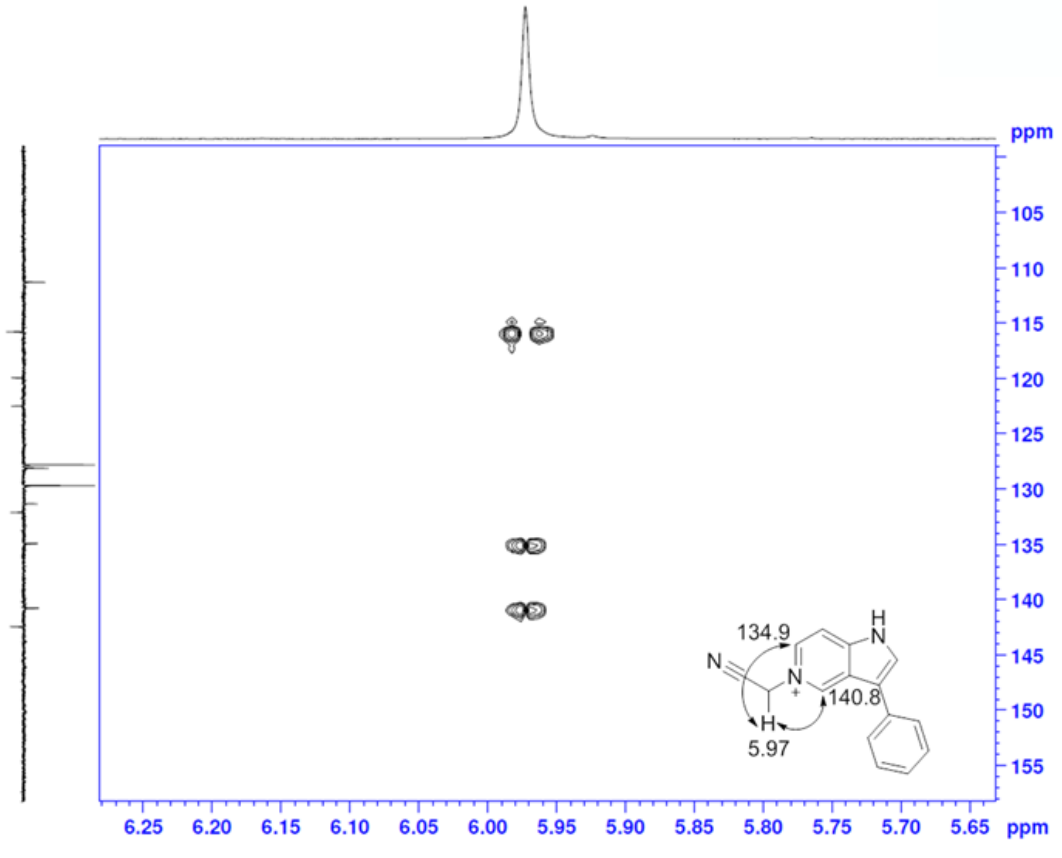
Acquisition Time (sec)	4.0894	***Date***	29 Aug 2017 08:40:48			***Date Stamp***	29 Aug 2017 08:40:48		
File Name	D:\CJO-UCSF\NMR\CJO-M1\5\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9260	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.583						



Acquisition Time (sec)	1.3631	***Date***	06 Sep 2017 00:57:52			***Date Stamp***	06 Sep 2017 00:57:52
File Name	D:\CJO-UCSF\NMR\CJO-M1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	3000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.364						



HMBC (1H-13C) NMR spectrum of 21, peak of interest, in DMSO-d6



Current Data Parameters
NAME q-1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
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Time 22.06 h
INSTRUM spect
PROBHD Z114098_0515 (
PULPROG hmbcetgpl3nd
TD 4096
SOLVENT DMSO
NS 16
DS 16
SWH 5197.505 Hz
FIDRES 2.537844 Hz
AQ 0.3940352 sec
RG 196.4
DW 96.200 usec
DE 6.50 usec
TE 295.6 K
CNST6 120.0000000
CNST7 170.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.04210000 sec
D16 0.00020000 sec
IN0 0.00002240 sec
TDav 1
SFO1 400.1522008 MHz
NUC1 1H
P1 10.00 usec
P2 20.00 usec
PLW1 14.74199963 W
SFO2 100.6278193 MHz
NUC2 13C
P3 10.00 usec
P24 2000.00 usec
PLW2 72.86900330 W
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SPOFFS7 0 Hz
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GPZ1 80.00 %
GPNAM[3] SMSQ10.100
GPZ3 14.00 %
GPNAM[4] SMSQ10.100
GPZ4 -8.00 %
GPNAM[5] SMSQ10.100
GPZ5 -4.00 %
GPNAM[6] SMSQ10.100
GPZ6 -2.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6279 MHz
FIDRES 172.842926 Hz
SW 219.859 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 2048
SF 400.1500000 MHz
WDW SINE
SSB 4
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
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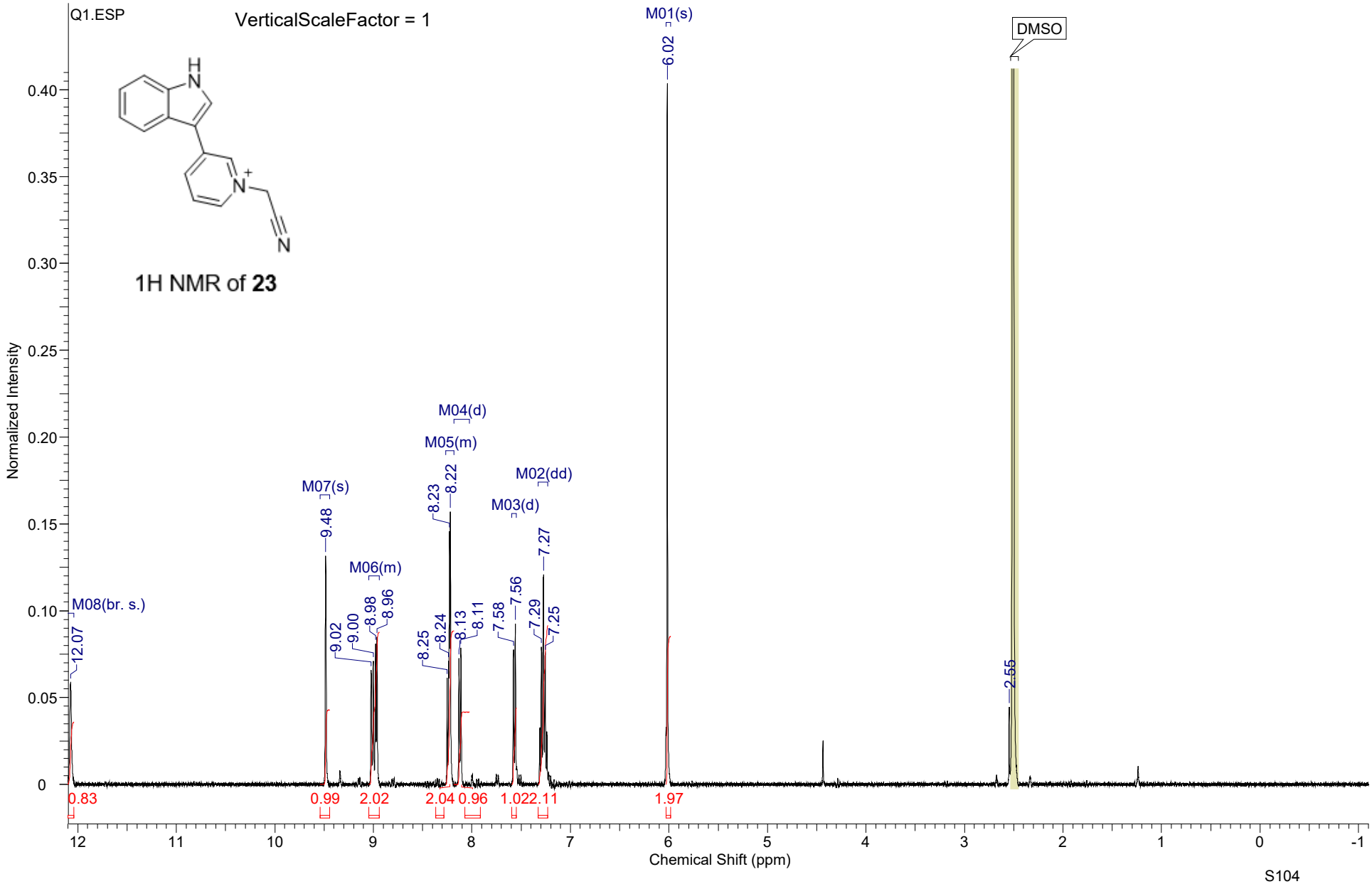
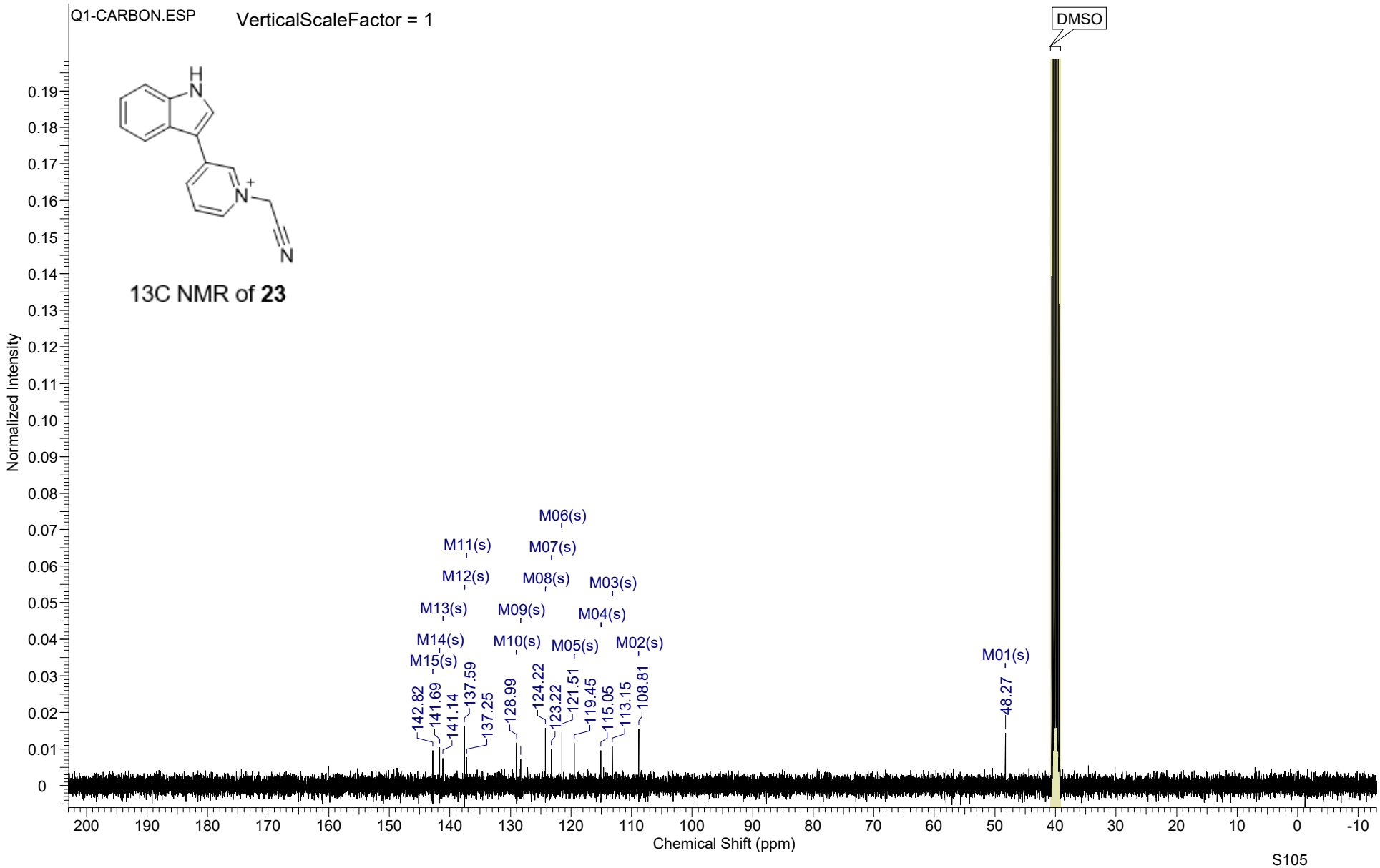
MC2 echo-antiecho
SF 100.6177975 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Acquisition Time (sec)	4.0894	***Date***	06 Sep 2017 10:14:40			***Date Stamp***	06 Sep 2017 10:14:40		
File Name	D:\CJO-UCSF\NMR\CJO-Q1\5\fid			***Frequency (MHz)***	400.15	***Nucleus***	1H	***Number of Transients***	30
Origin	spect	***Original Points Count***	32768	***Owner***	IND-NMR	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	141.25	***SW(cyclical) (Hz)***	8012.82	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	2470.9255	***Spectrum Type***	STANDARD
Sweep Width (Hz)	8012.58	***Temperature (degree C)***	22.624						



Acquisition Time (sec)	1.3631	***Date***	04 Oct 2017 23:56:00			***Date Stamp***	04 Oct 2017 23:56:00
File Name	D:\CJO-UCSF\NMR\CJO-Q1\CARBON\fid			***Frequency (MHz)***	100.63	***Nucleus***	13C
Number of Transients	2000	***Origin***	spect	***Original Points Count***	32768	***Owner***	IND-NMR
Points Count	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	196.40	***SW(cyclical) (Hz)***	24038.46
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	10061.7803	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73
Temperature (degree C)	23.313						



Organic LETTERS

	ol-
Corresponding Author	Dr. Jay Conrad
Title	Rapid Access to Cyanomethyl Indoles via Photoredox Catalysis

RECOMMENDED COMPOUND CHARACTERIZATION CHECKLIST

NOTE: CHECKLIST IS RECOMMENDED BUT NOT REQUIRED

TO DISPLAY INSTRUCTIONS: Double-click HERE (Formula Bar must be visible: Select View>Formula Bar) TO CLOSE: Enter/Return

COMPOUND	IDENTITY													PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	___ NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	<>	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	<>	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	* SI = Supporting Information
3	X					X	X			X					X								
13a		X				X	X			X					X								
13b		X				X	X			X					X								
13c	X					X	X			X					X								
13d	X					X	X			X					X								
13e	X					X	X			X					X								
13f	X					X	X			X					X								
13g	X					X	X			X					X								
15a	X					X	X			X					X								
15b	X					X	X			X					X								
15c	X					X	X			X					X								
15d	X					X	X			X					X								
15e	X					X	X			X					X								

COMPOUND	IDENTITY													PURITY					COMPUTATIONAL DATA in SI*			
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	___ NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	<>	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	<>	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy	* SI = Supporting Information
15f	X					X	X			X					X								
15g	X					X	X			X					X								
15h	X					X	X			X					X								
17a	X					X	X			X					X								
17b	X					X	X			X					X								
17c	X					X	X			X					X								
17d	X					X	X			X					X								
19a		X				X	X			X					X								
19b	X					X	X			X					X								
19c		X				X	X			X					X								
19d	X					X	X			X					X								
19e	X					X	X			X					X								
21		X				X	X								X								
23	X					X	X								X								

COMPOUND	IDENTITY														PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	___ NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	<>	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	<>	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy

* SI = Supporting Information

COMPOUND	IDENTITY														PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	___ NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	<>	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	<>	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy

* SI = Supporting Information

COMPOUND			IDENTITY												PURITY					COMPUTATIONAL DATA in SI*		
Compound, structure, or table-entry number	New	Known	Melting point range	IR	UV-Vis	1H NMR	13C NMR	___ NMR	MS	HRMS	Optical rotation/ORD/CD	Enantiomeric/Diastereomeric ratio	X-ray [ORTEP and CIF in SI*]	<>	Copy of 1H/13C NMR spectrum in SI*	Copy of chromatogram in SI*	Quant. GC, HPLC, or electrophoresis	Elemental analysis	<>	Cartesian coordinates or Z-matrix	# of imaginary frequencies	Total energy

* SI = Supporting Information