

Supporting Information

Design, Synthesis and Biological Evaluation of Theranostic Vitamin-Linker-Taxoid Conjugates

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Figure S1. Assessment of non-specific internalization in L1210FR, MX-1, ID8, and L1210 cell lines based on the extent of internalization of fluorescent taxoid probe **6** (5 μ M) by flow cytometry and confocal fluorescence microscopy (CFM) at 3 h, 37 $^{\circ}$ C.

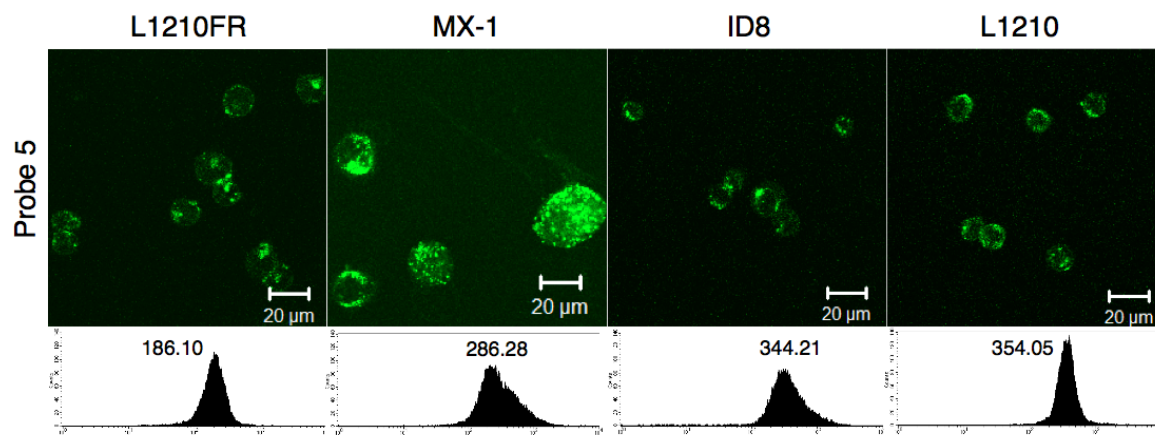


Figure S2. Assessment of the time-dependent internalization of theranostic conjugate **2** (5 μ M) by RME in murine leukemia L1210FR (BR+) cell line based on the flow cytometry and confocal fluorescence microscopy analysis in the time period from 15 min to 24 h at 37 $^{\circ}$ C.

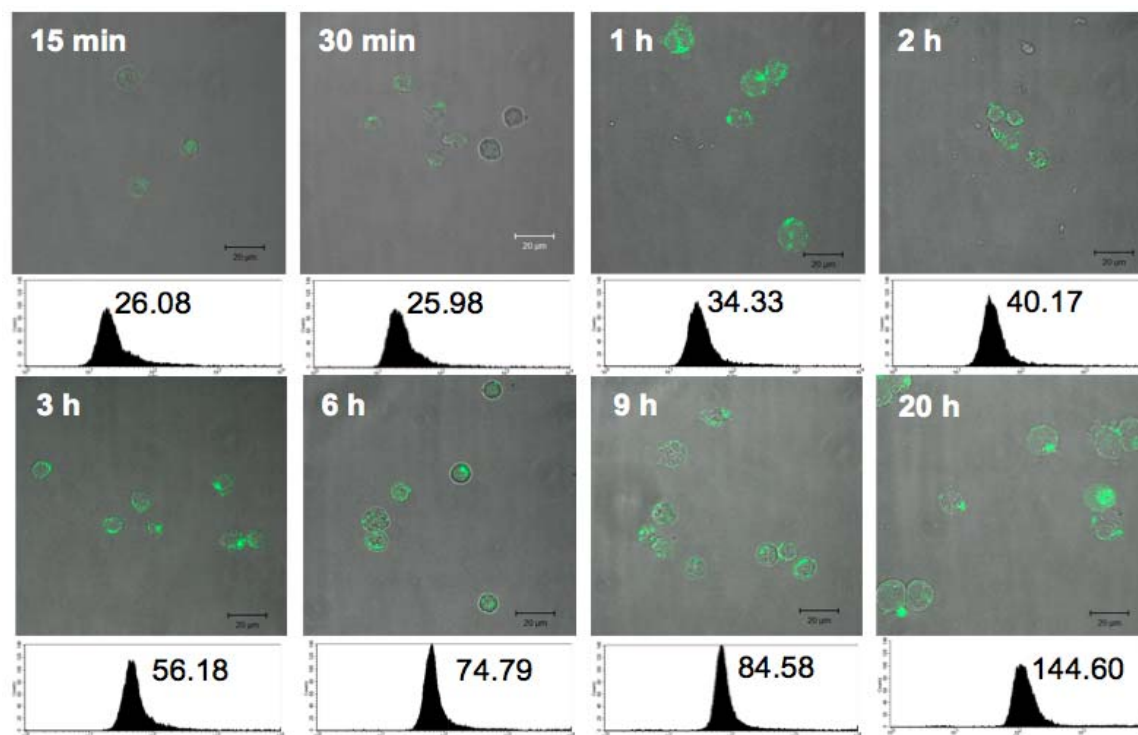
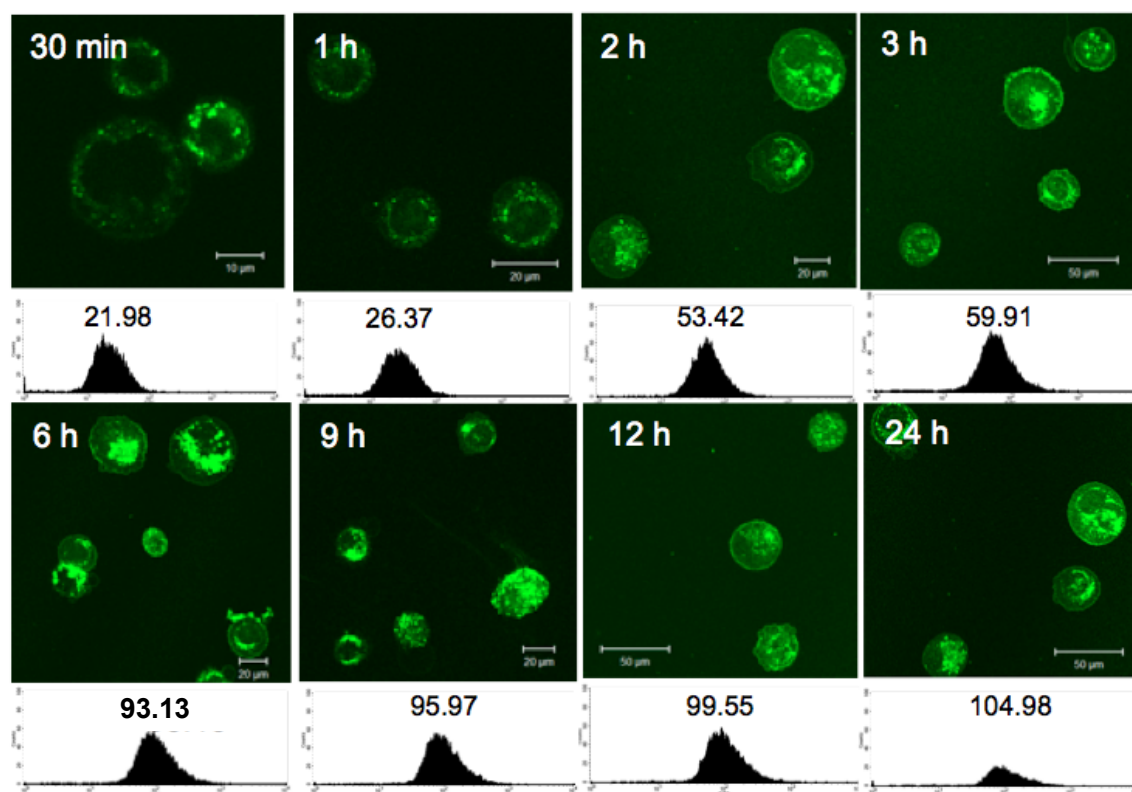
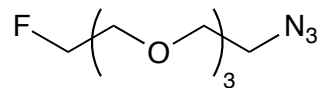


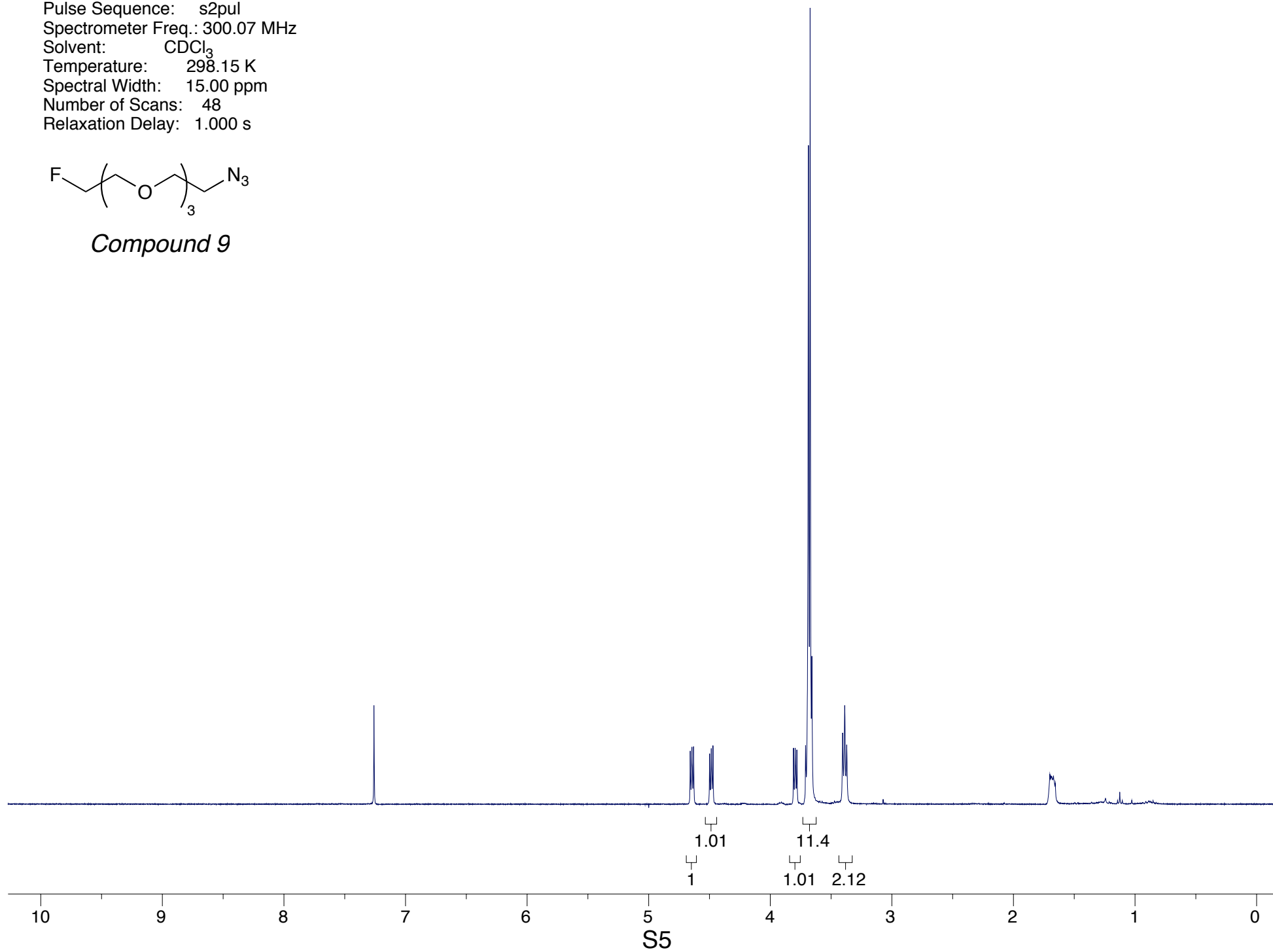
Figure S3. Assessment of the time-dependent internalization of 5 μ M theranostic conjugate **2** by RME in human breast carcinoma MX-1 (BR+) cell line based on the flow cytometry and confocal fluorescence microscopy analysis in the time period from 30 min to 24 h at 37 $^{\circ}$ C.



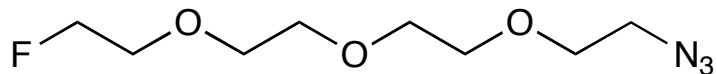
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Processed by: Jacob Vineberg
Pulse Sequence: s2pul
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Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 15.00 ppm
Number of Scans: 48
Relaxation Delay: 1.000 s



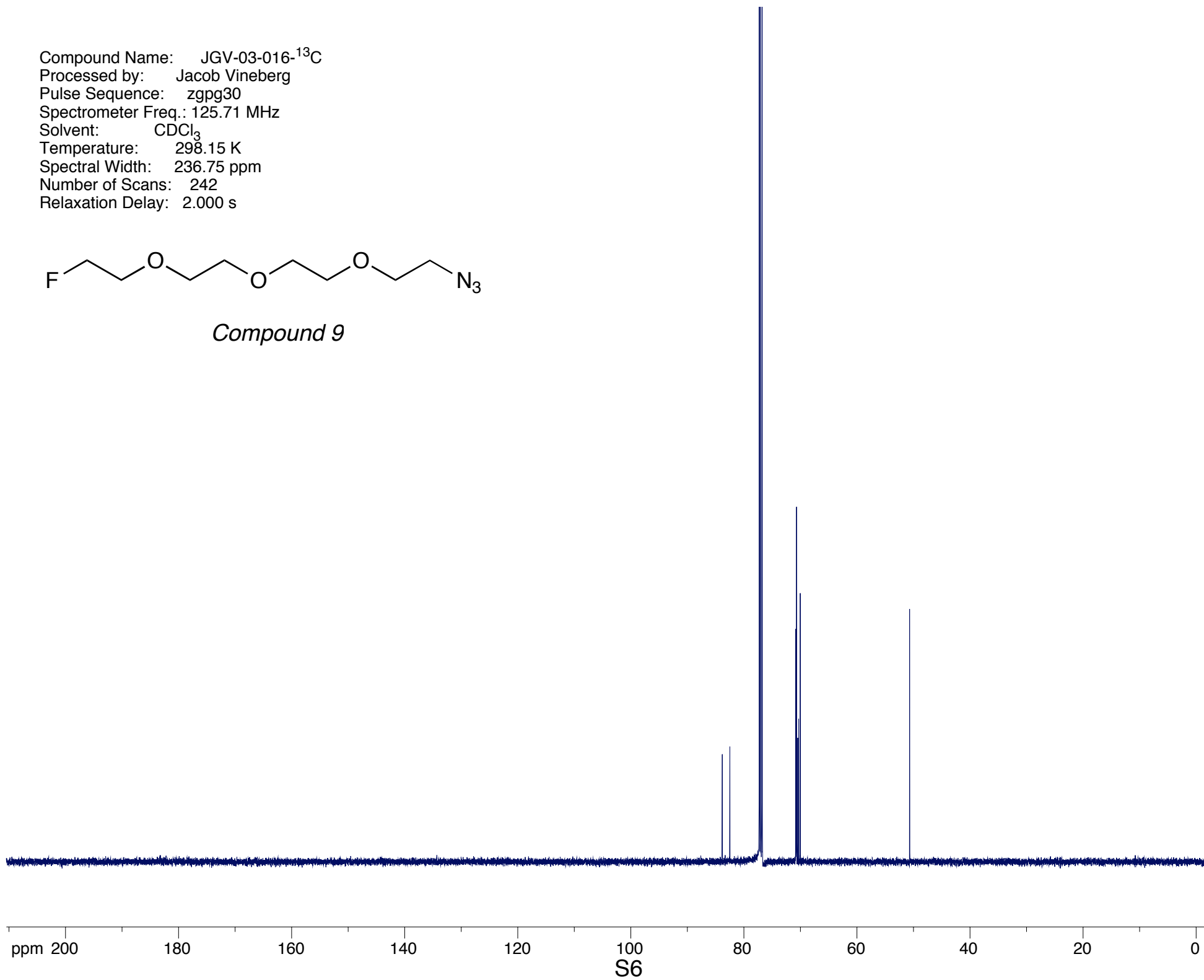
Compound 9



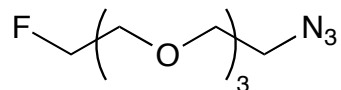
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Processed by: Jacob Vineberg
Pulse Sequence: zgpg30
Spectrometer Freq.: 125.71 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 242
Relaxation Delay: 2.000 s



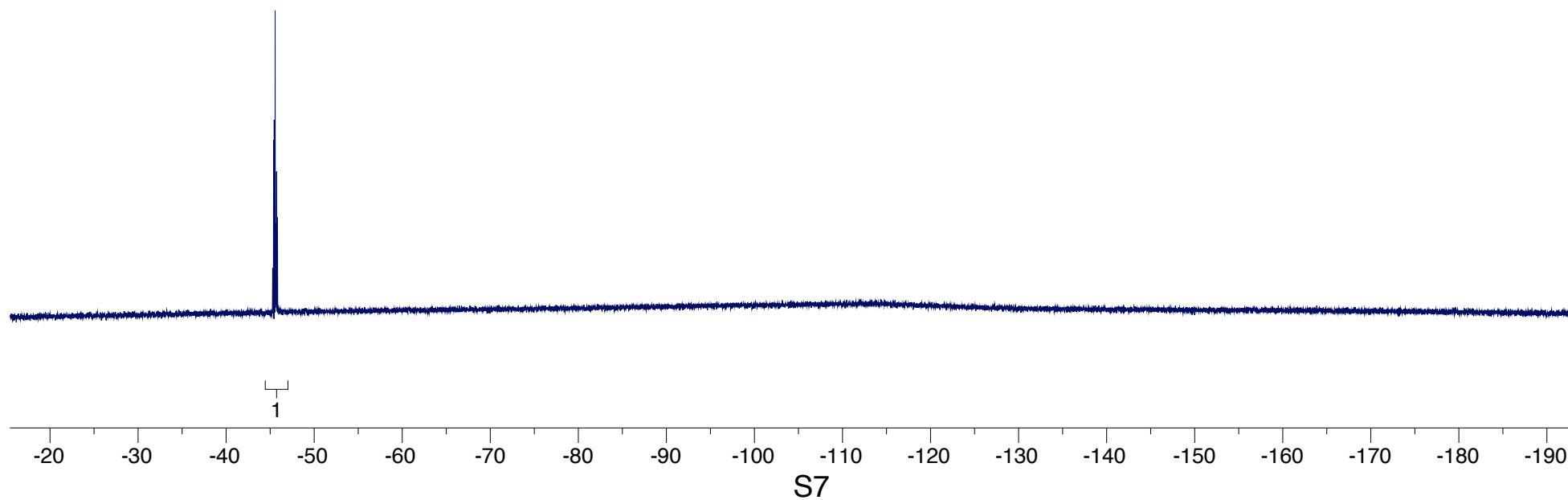
Compound 9



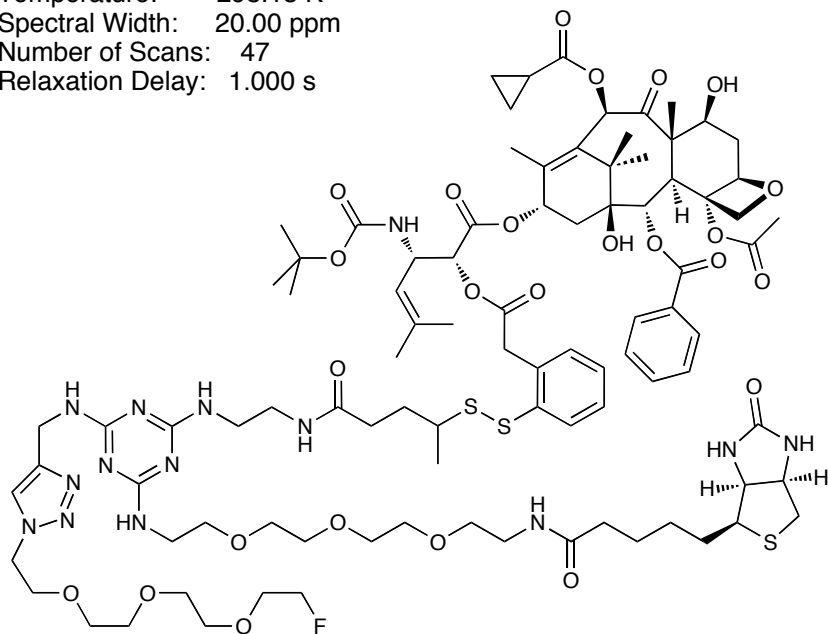
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Number of Scans: 200
Relaxation Delay: 4.000 s



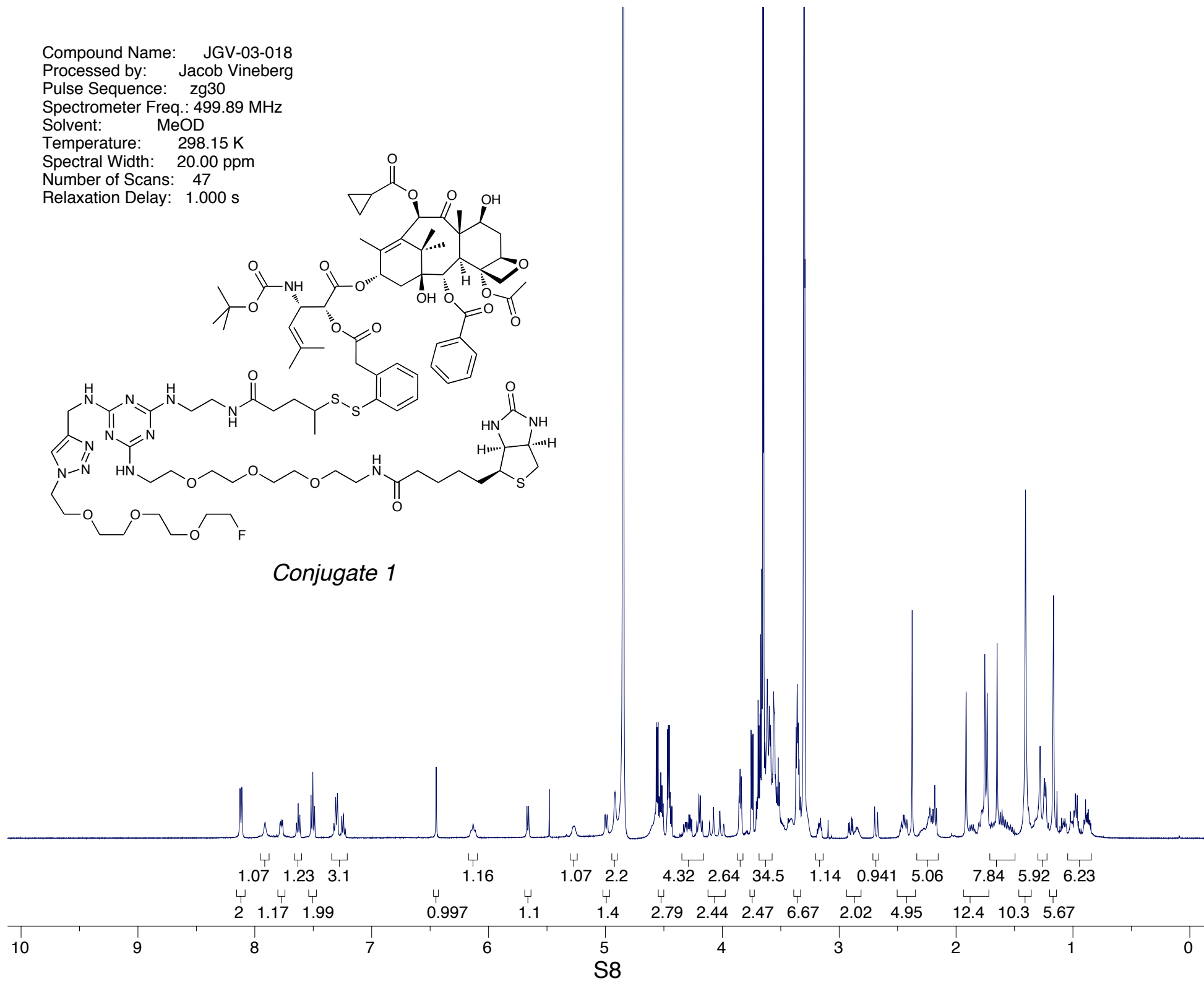
Compound 9



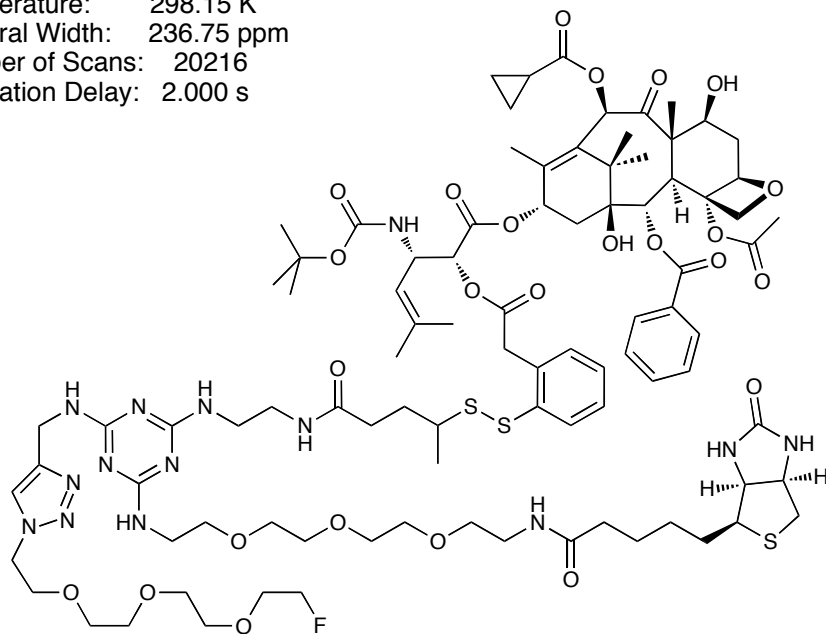
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 Solvent: MeOD
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 Number of Scans: 47
 Relaxation Delay: 1.000 s



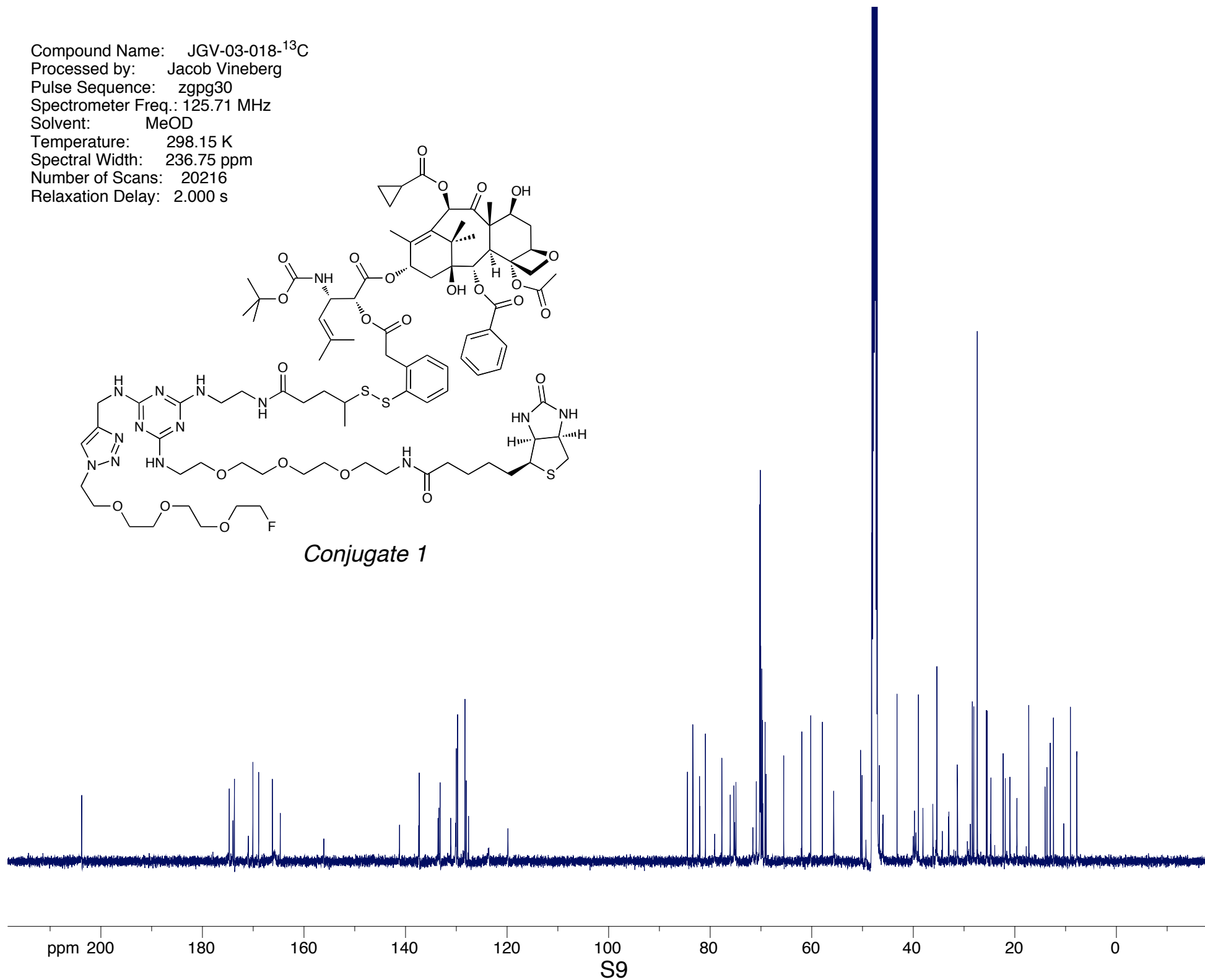
Conjugate 1



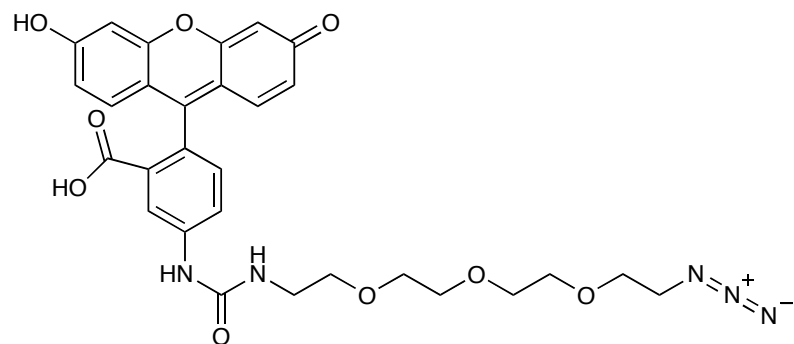
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Processed by: Jacob Vineberg
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Solvent: MeOD
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 20216
Relaxation Delay: 2.000 s



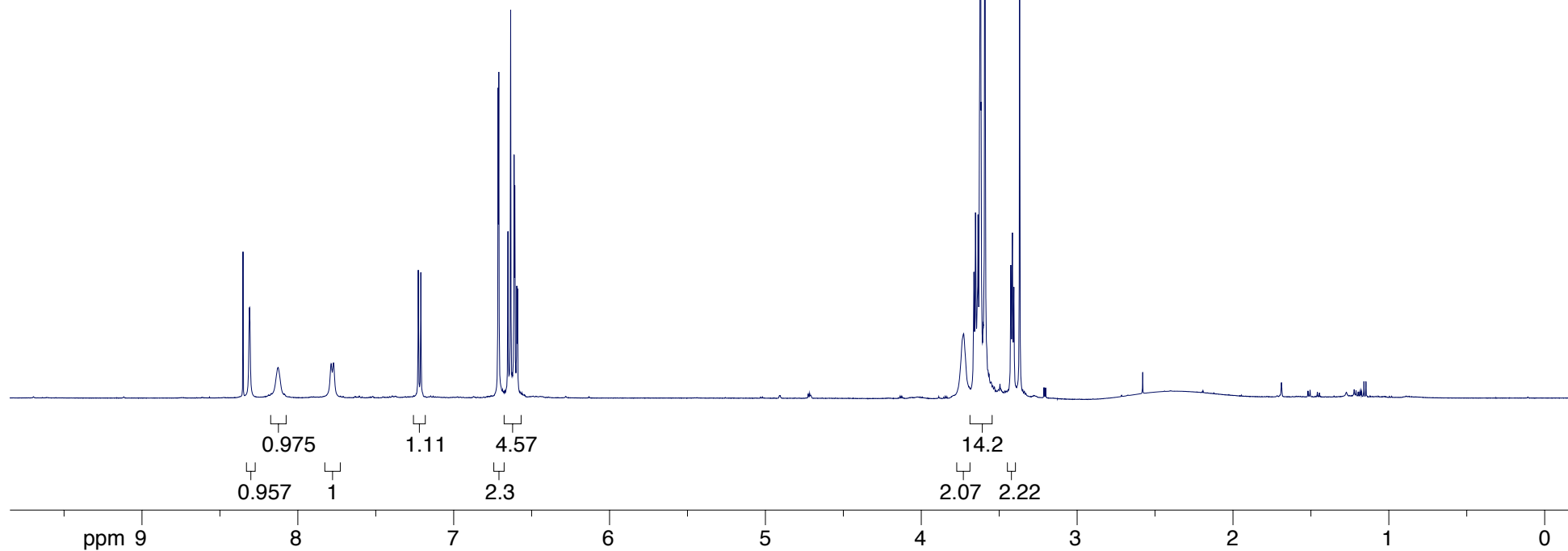
Conjugate 1



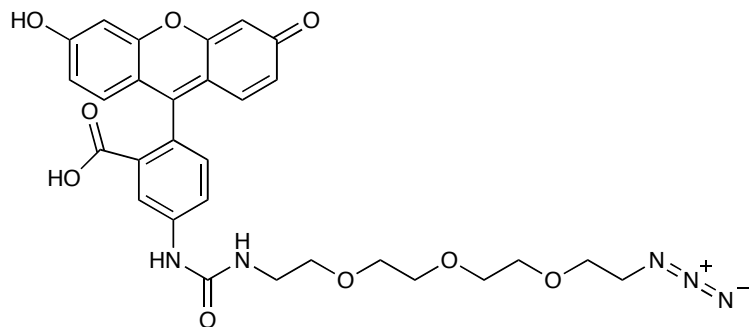
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Pulse Sequence: zg30
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Solvent: DMSO
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Spectral Width: 20.00 ppm
Number of Scans: 43
Relaxation Delay: 1.000 s



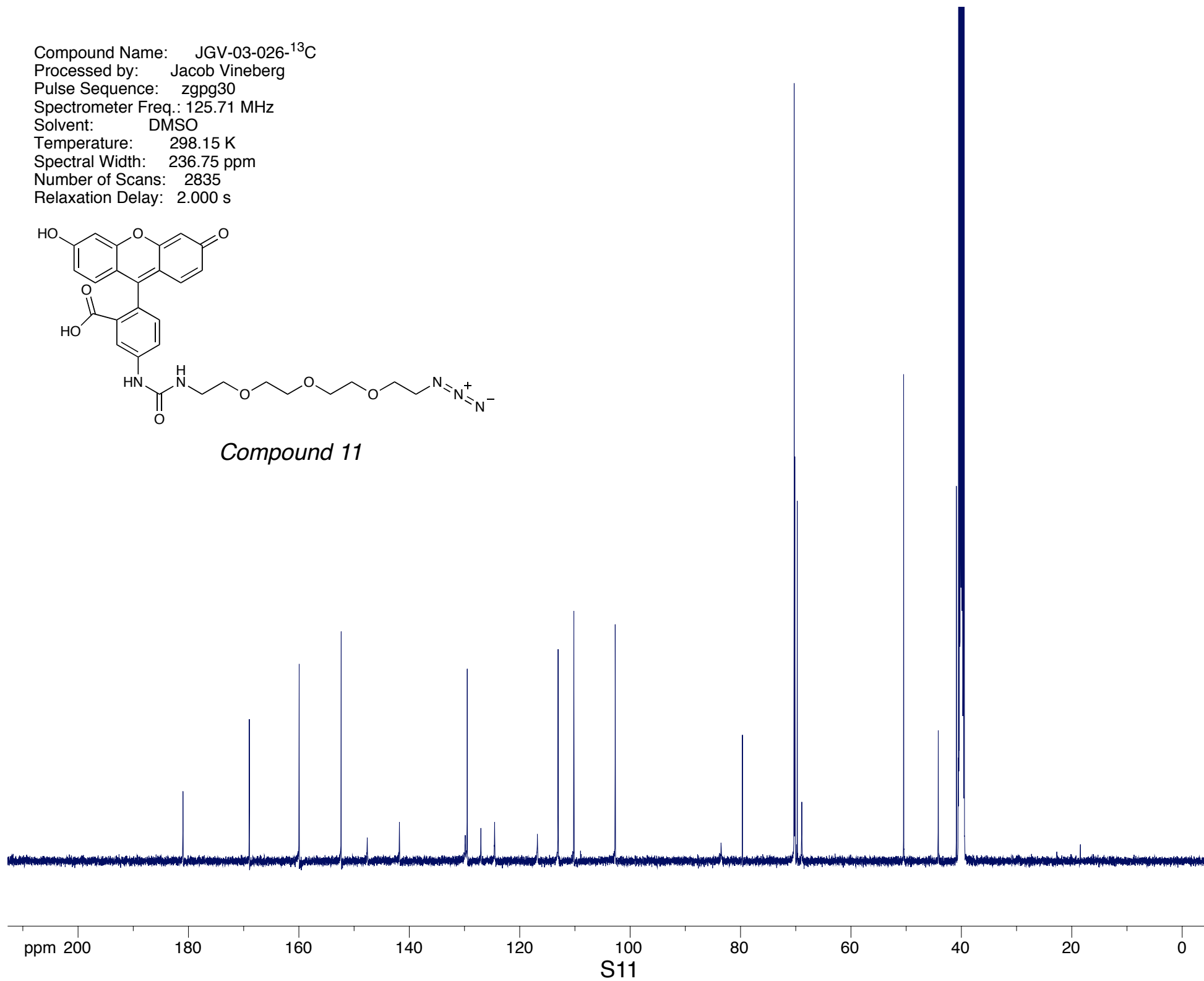
Compound 11



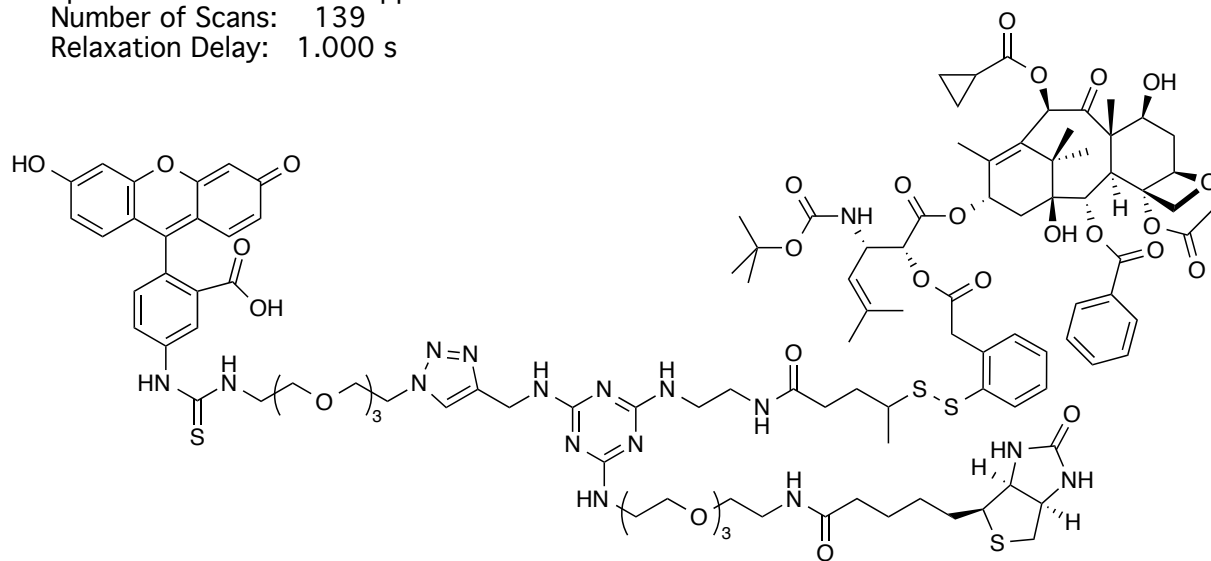
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Processed by: Jacob Vineberg
Pulse Sequence: zgpg30
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Solvent: DMSO
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 2835
Relaxation Delay: 2.000 s



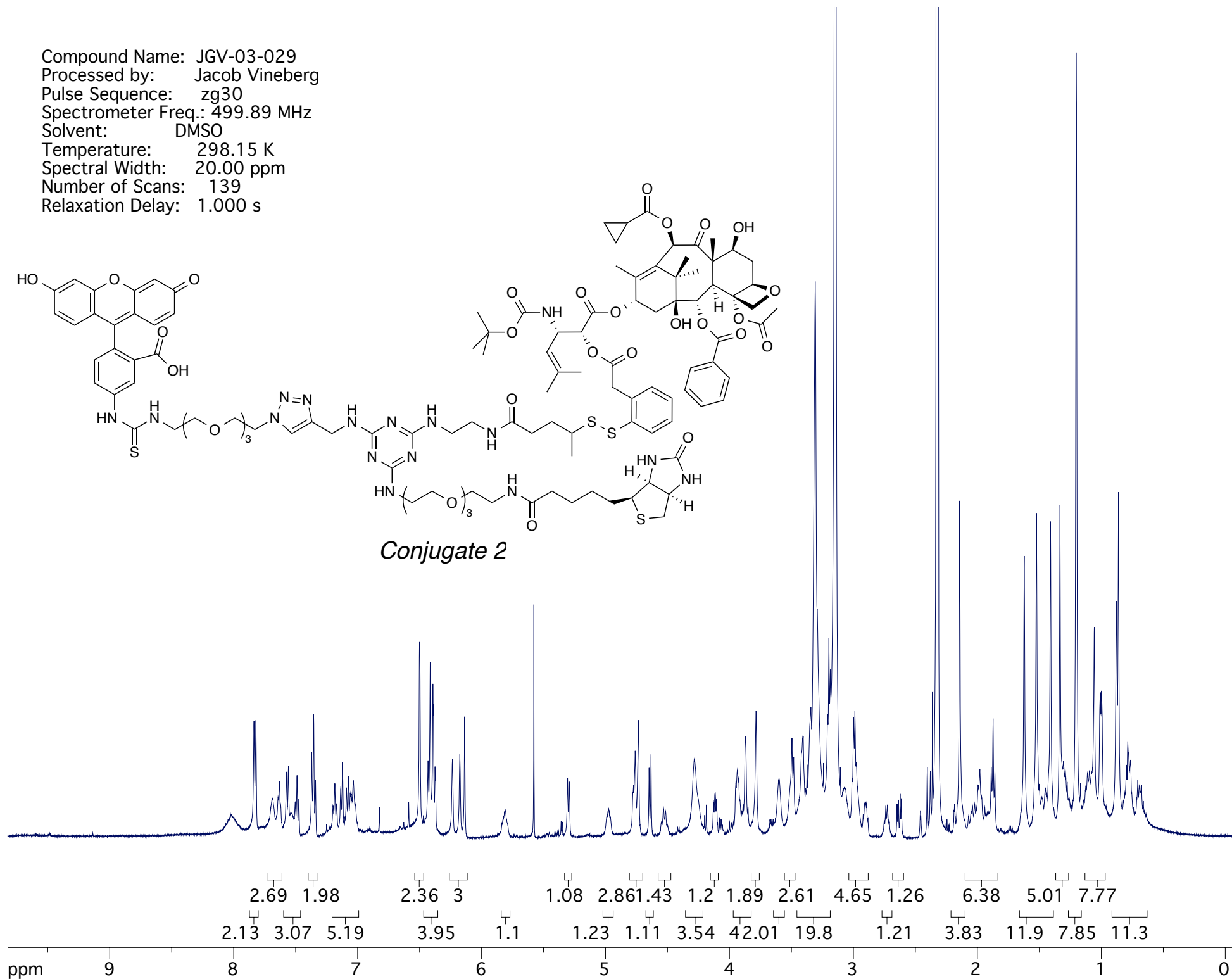
Compound 11



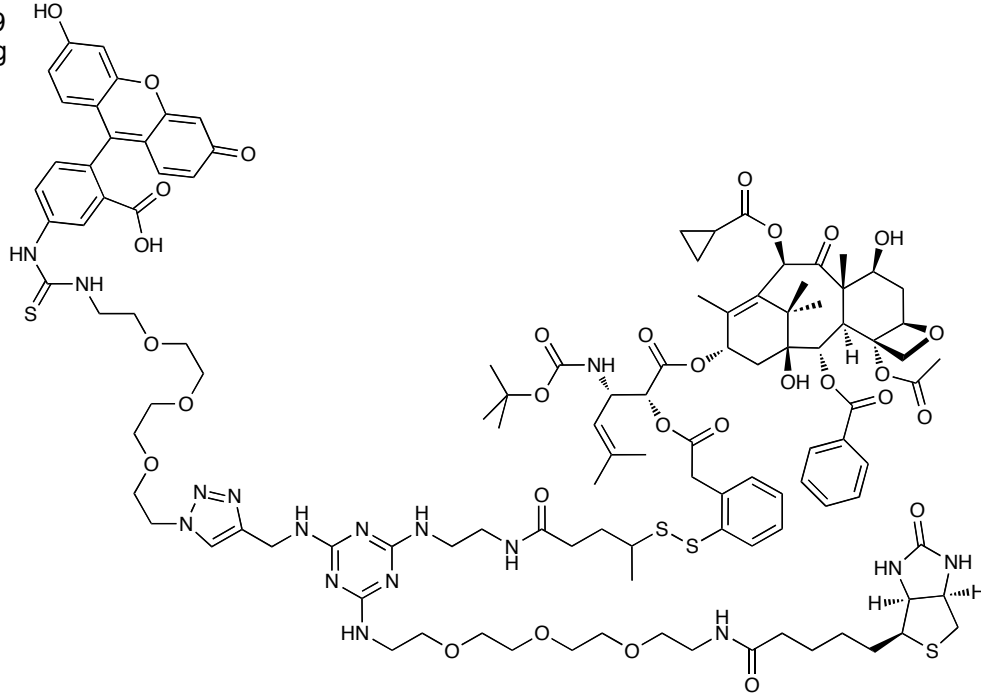
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 Processed by: Jacob Vineberg
 Pulse Sequence: zg30
 Spectrometer Freq.: 499.89 MHz
 Solvent: DMSO
 Temperature: 298.15 K
 Spectral Width: 20.00 ppm
 Number of Scans: 139
 Relaxation Delay: 1.000 s



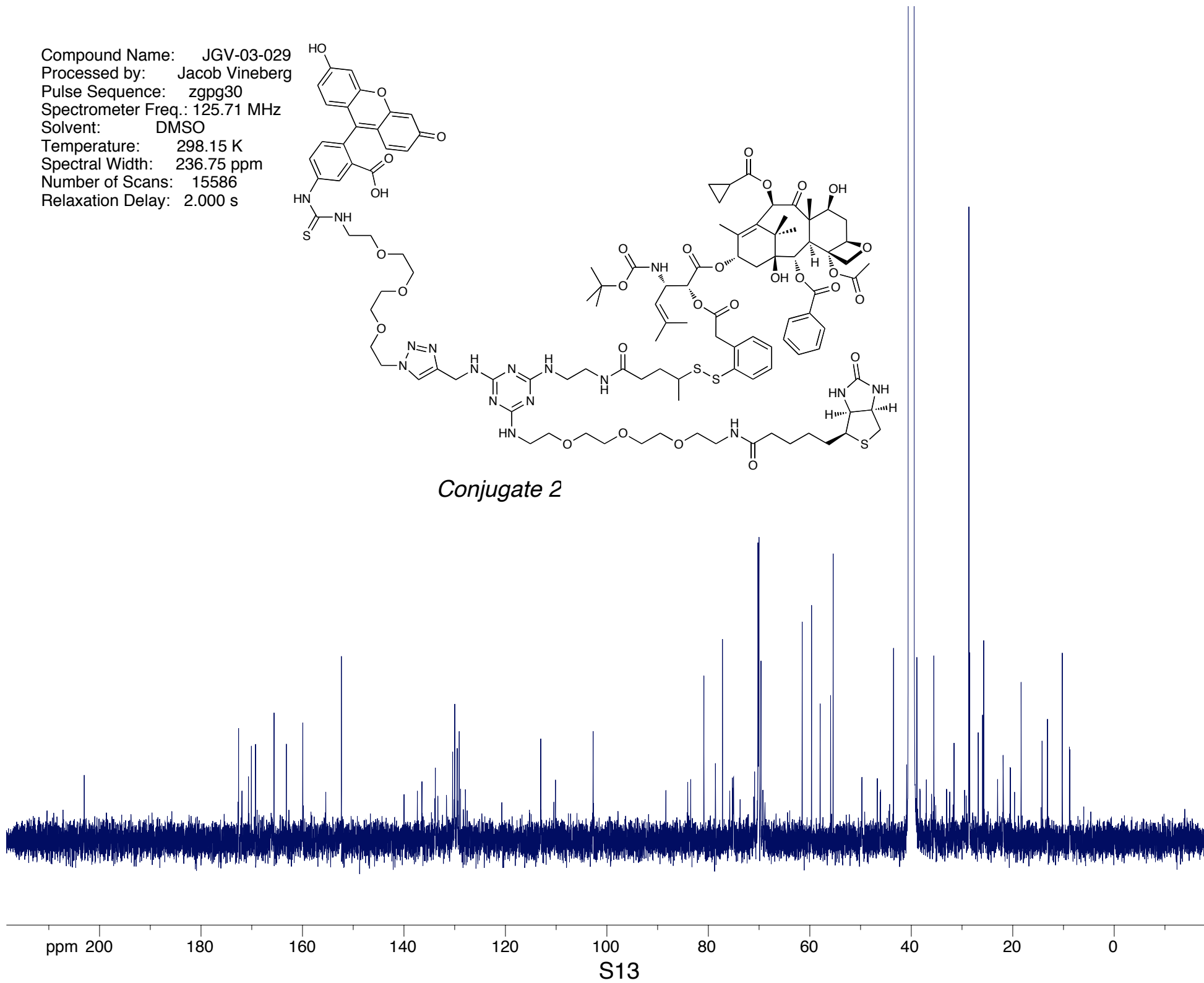
Conjugate 2



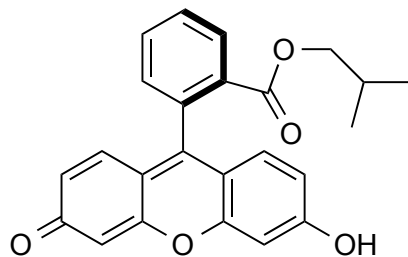
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Processed by: Jacob Vineberg
Pulse Sequence: zgpg30
Spectrometer Freq.: 125.71 MHz
Solvent: DMSO
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 15586
Relaxation Delay: 2.000 s



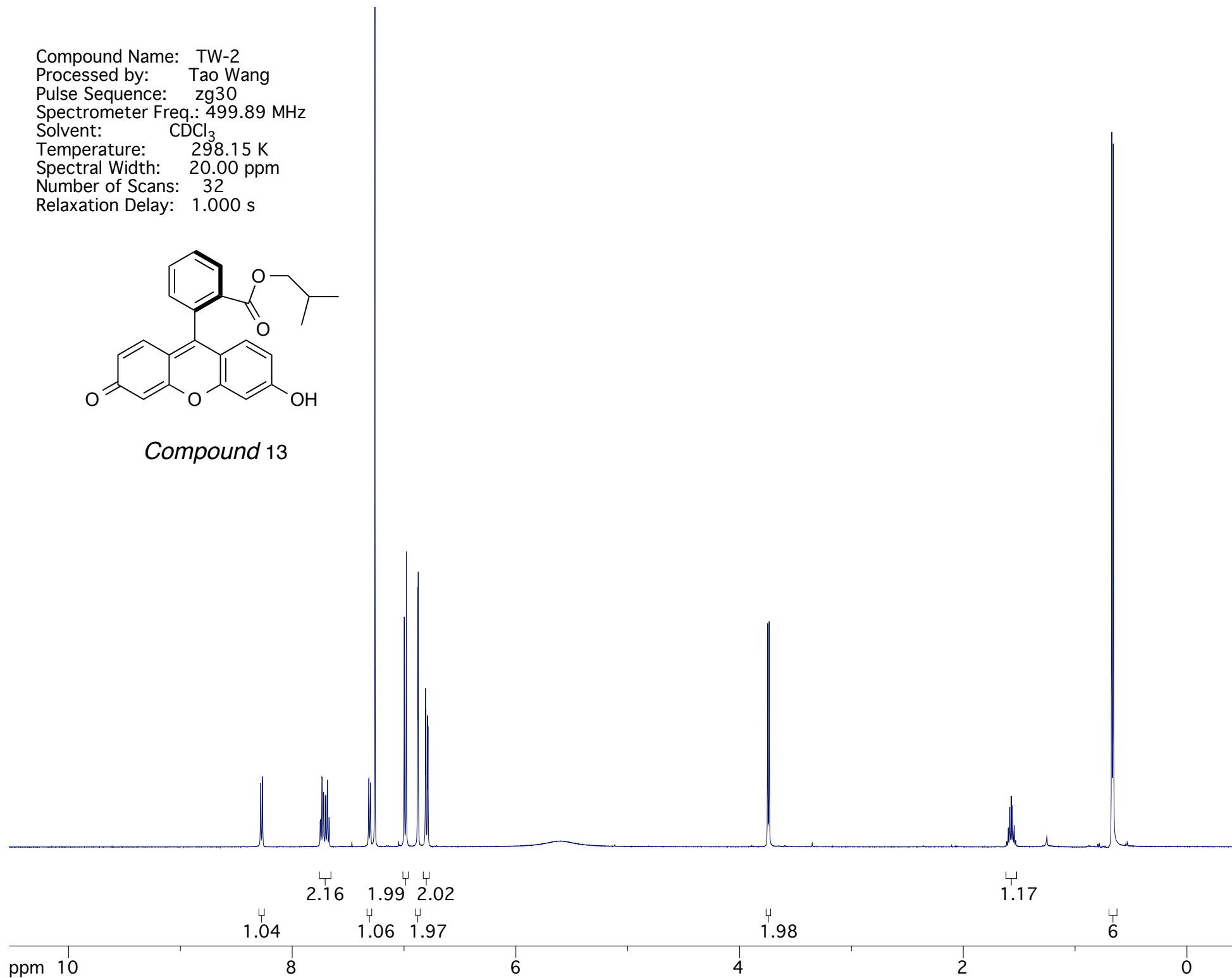
Conjugate 2



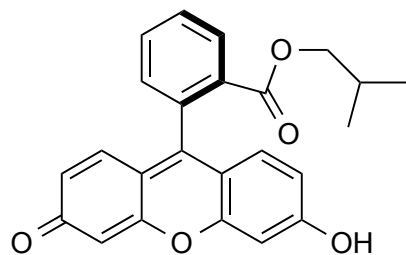
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Processed by: Tao Wang
Pulse Sequence: zg30
Spectrometer Freq.: 499.89 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 20.00 ppm
Number of Scans: 32
Relaxation Delay: 1.000 s



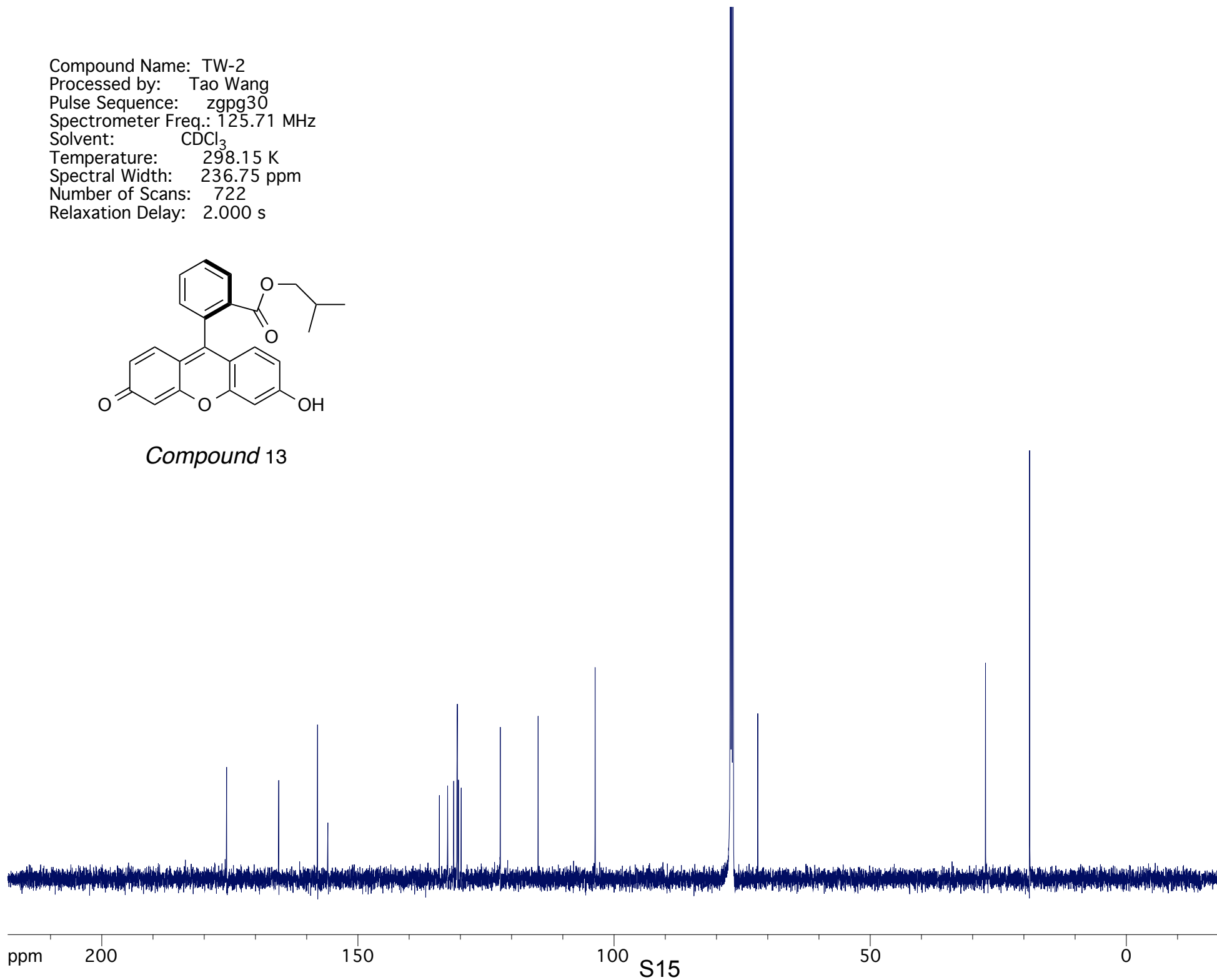
Compound 13



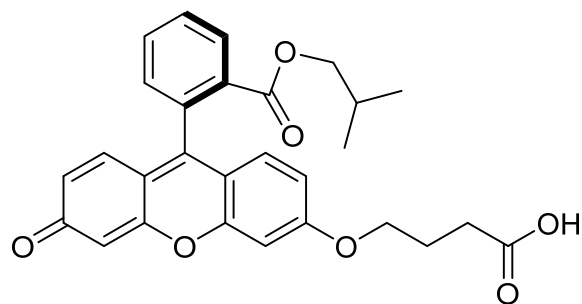
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Pulse Sequence: zgpg30
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Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 722
Relaxation Delay: 2.000 s



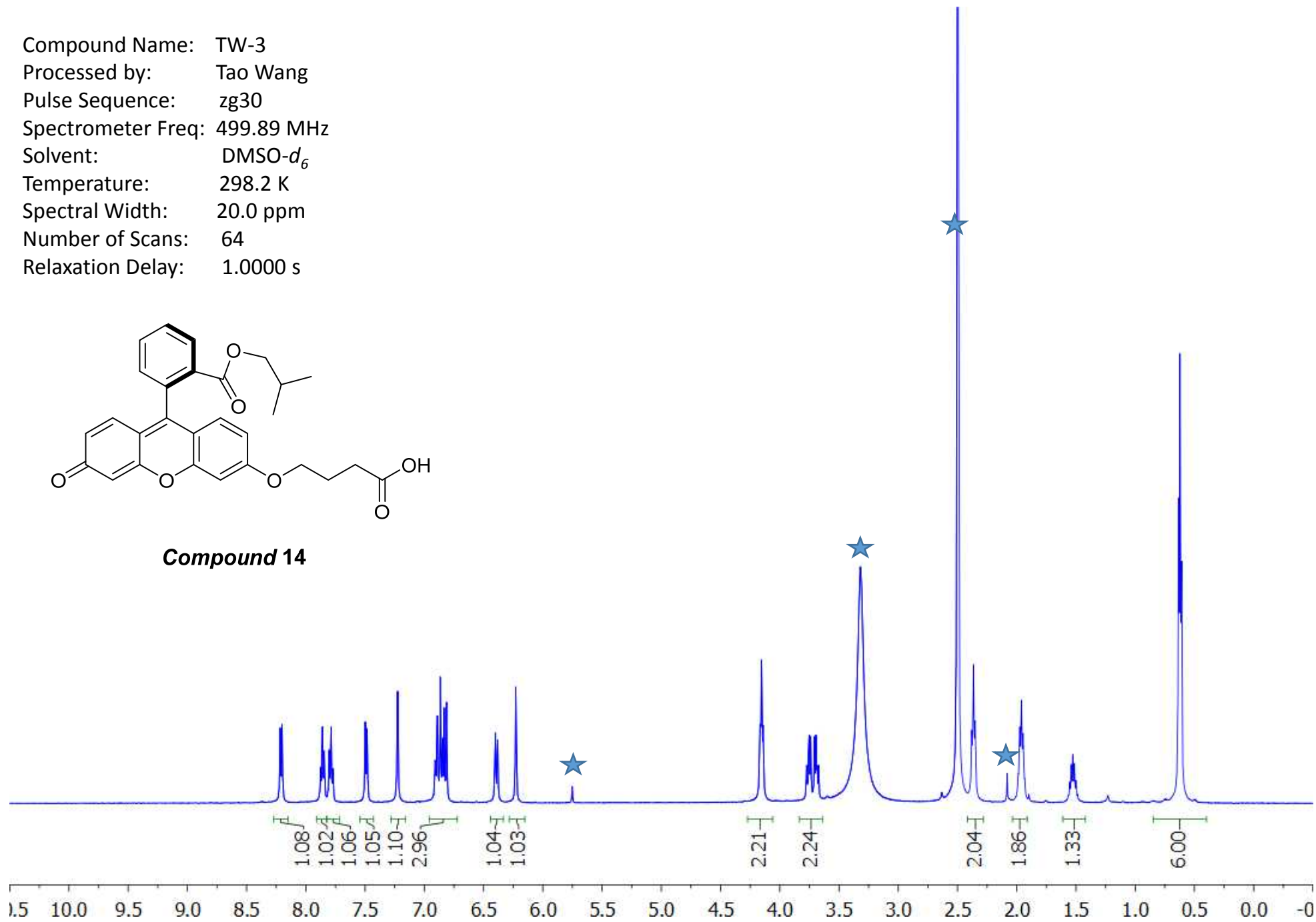
Compound 13



Compound Name: TW-3
Processed by: Tao Wang
Pulse Sequence: zg30
Spectrometer Freq: 499.89 MHz
Solvent: DMSO- d_6
Temperature: 298.2 K
Spectral Width: 20.0 ppm
Number of Scans: 64
Relaxation Delay: 1.0000 s

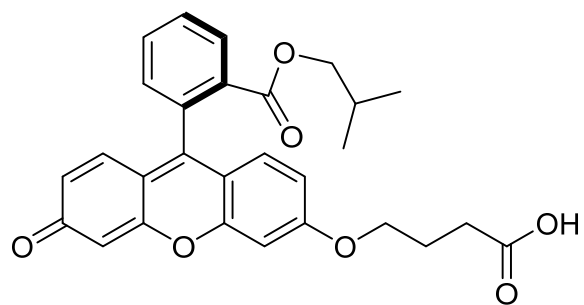


Compound 14

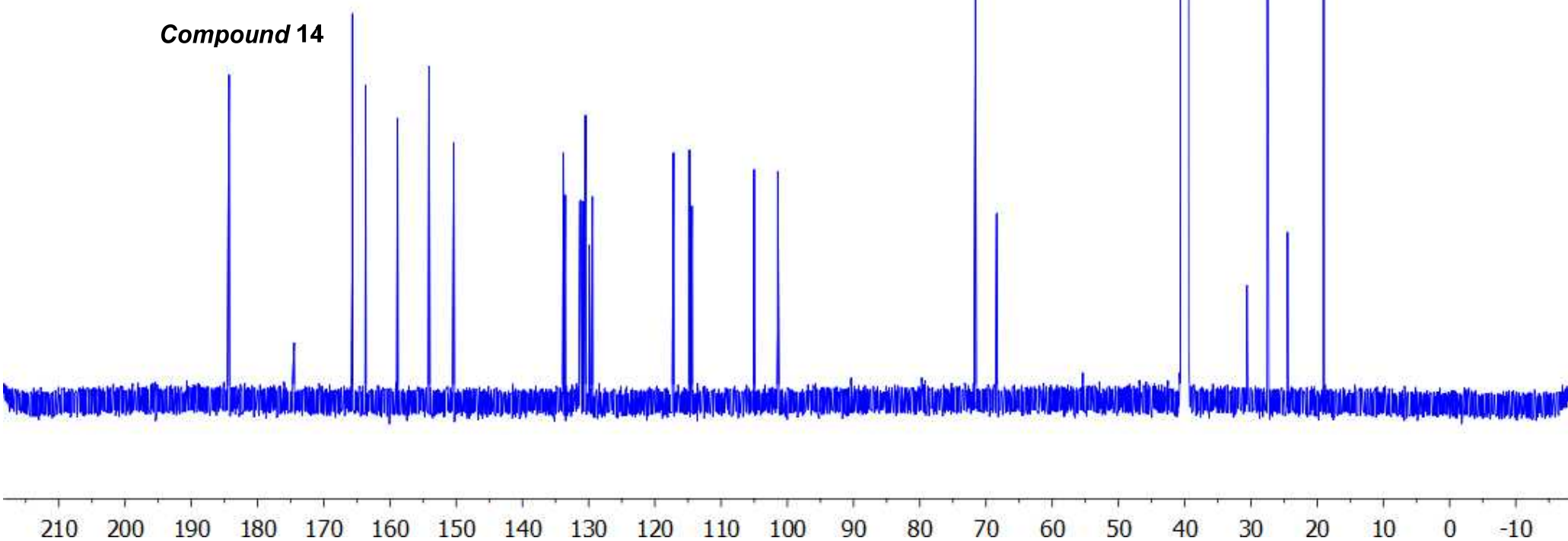


★ Peaks arising from the solvent used: DMSO- d_6 (wet)

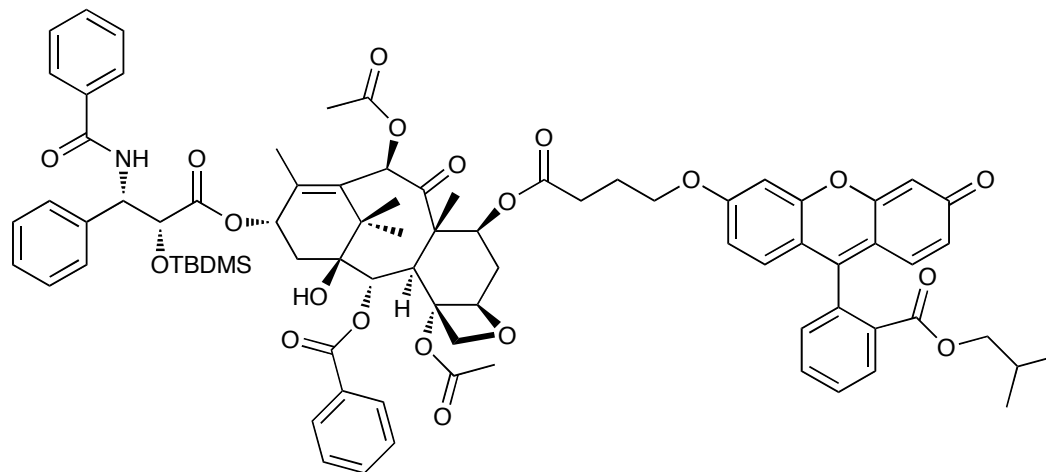
Compound Name: TW-3
Processed by: Tao Wang
Pulse Sequence: zgpg30
Spectrometer Freq: 125.71 MHz
Solvent: DMSO- d_6
Temperature: 298.1 K
Spectral Width: 236.75 ppm
Number of Scans: 19324
Relaxation Delay: 2.0000 s



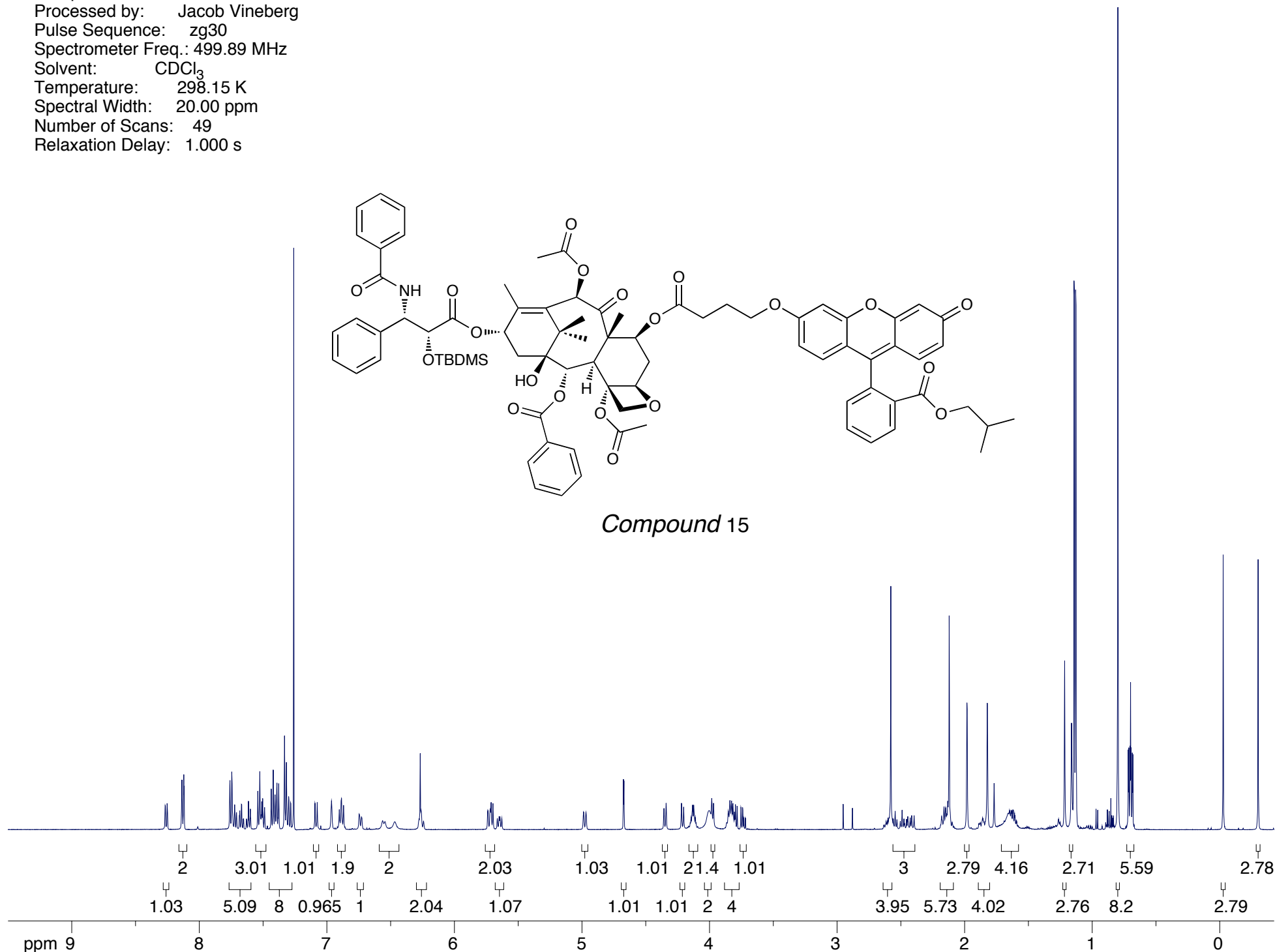
Compound 14



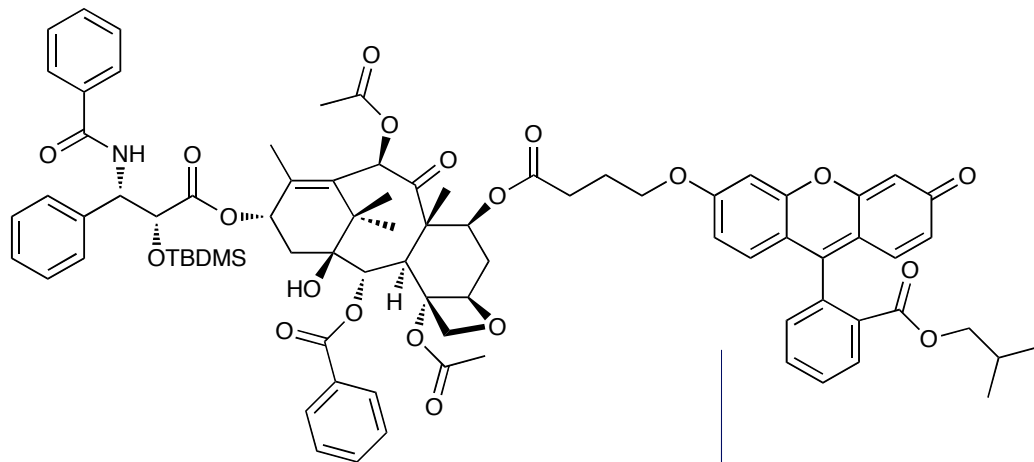
Compound Name: JGV-03-002
Processed by: Jacob Vineberg
Pulse Sequence: zg30
Spectrometer Freq.: 499.89 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 20.00 ppm
Number of Scans: 49
Relaxation Delay: 1.000 s



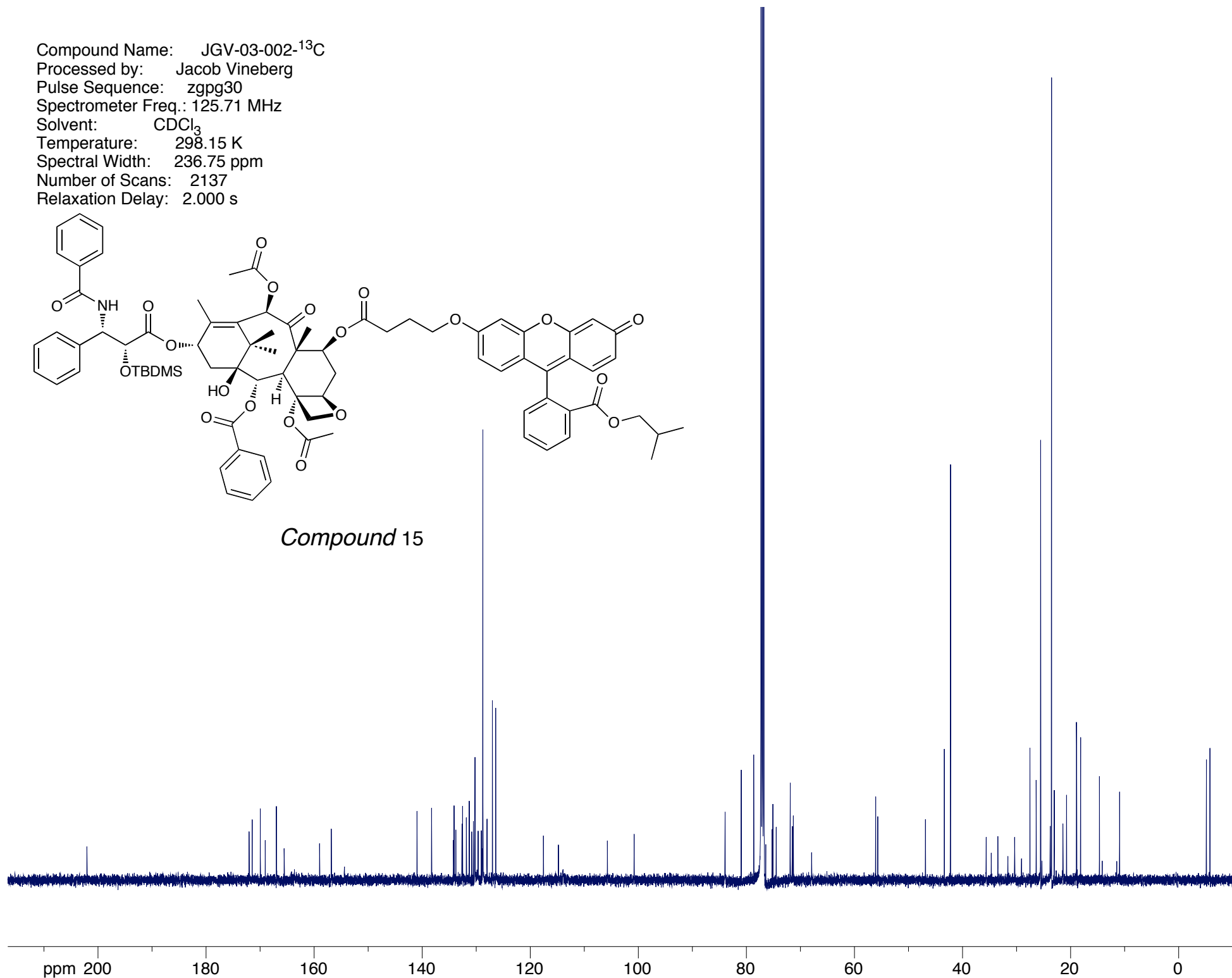
Compound 15



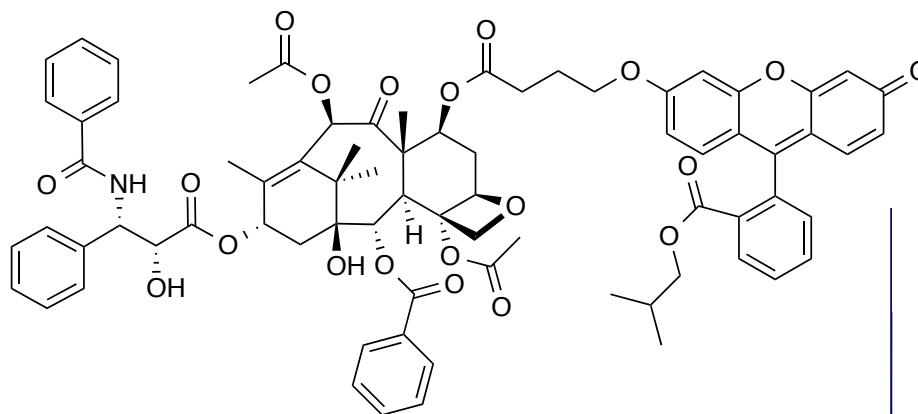
Compound Name: JGV-03-002-¹³C
Processed by: Jacob Vineberg
Pulse Sequence: zgpg30
Spectrometer Freq.: 125.71 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 2137
Relaxation Delay: 2.000 s



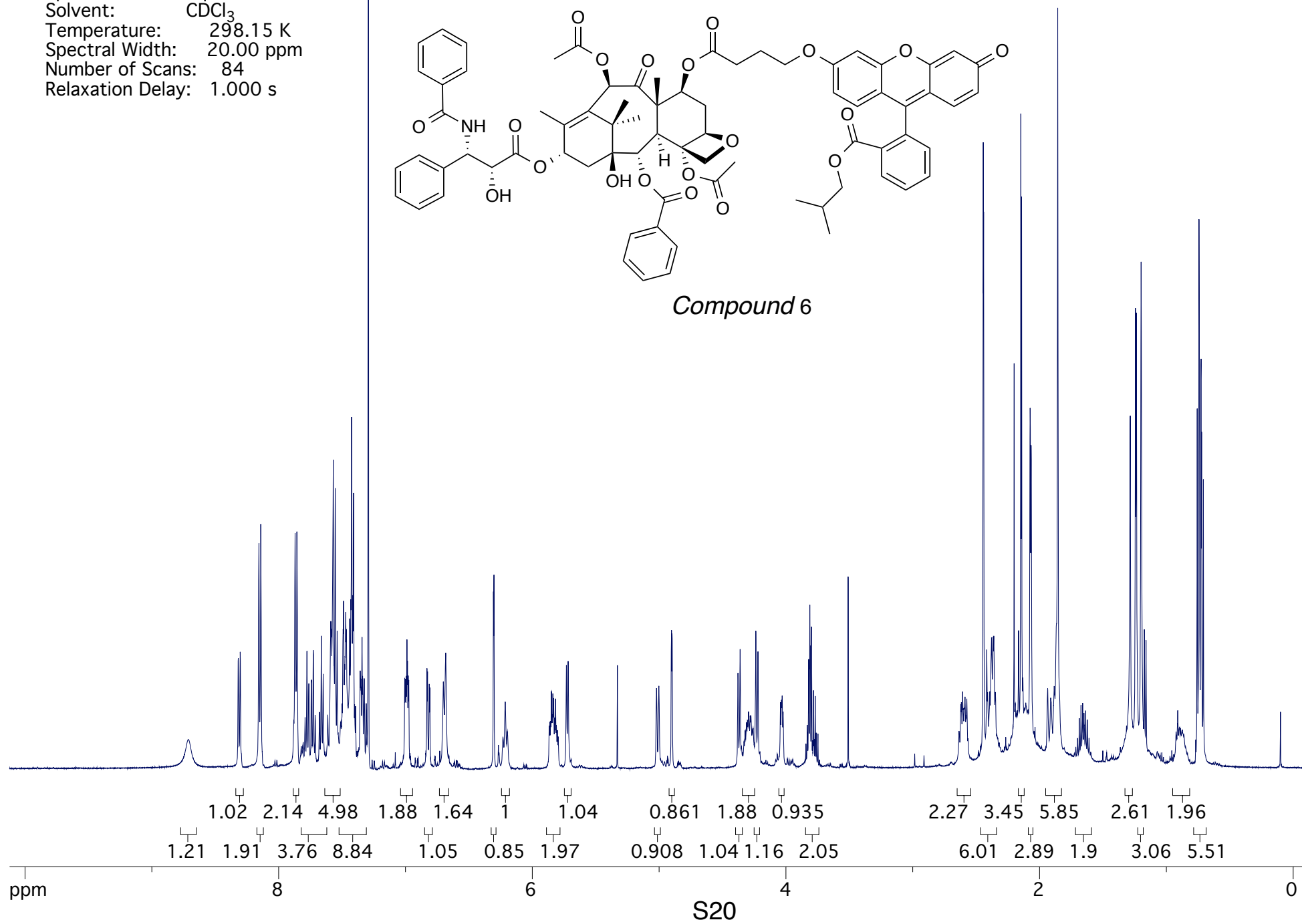
Compound 15



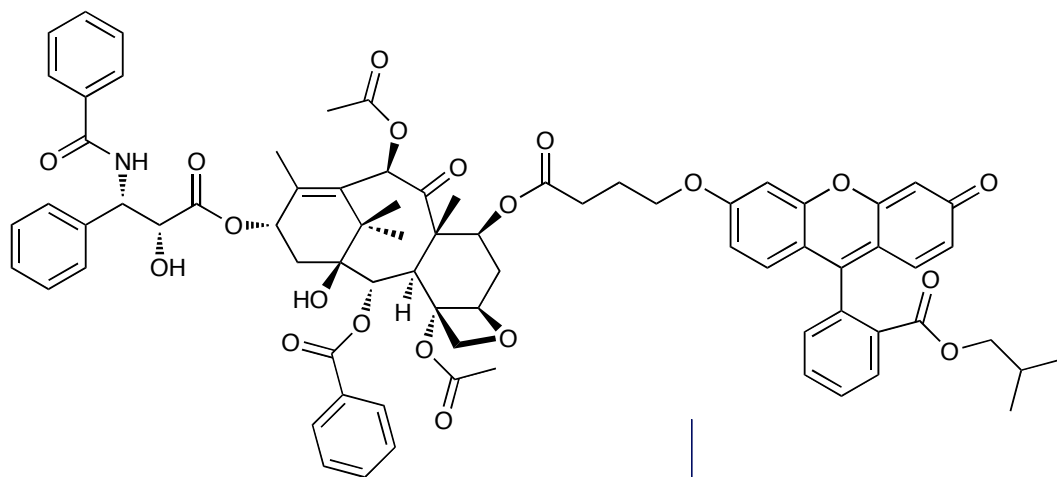
Compound Name: JGV-03-003
Processed by: Jacob Vineberg
Pulse Sequence: zg30
Spectrometer Freq.: 499.89 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 20.00 ppm
Number of Scans: 84
Relaxation Delay: 1.000 s



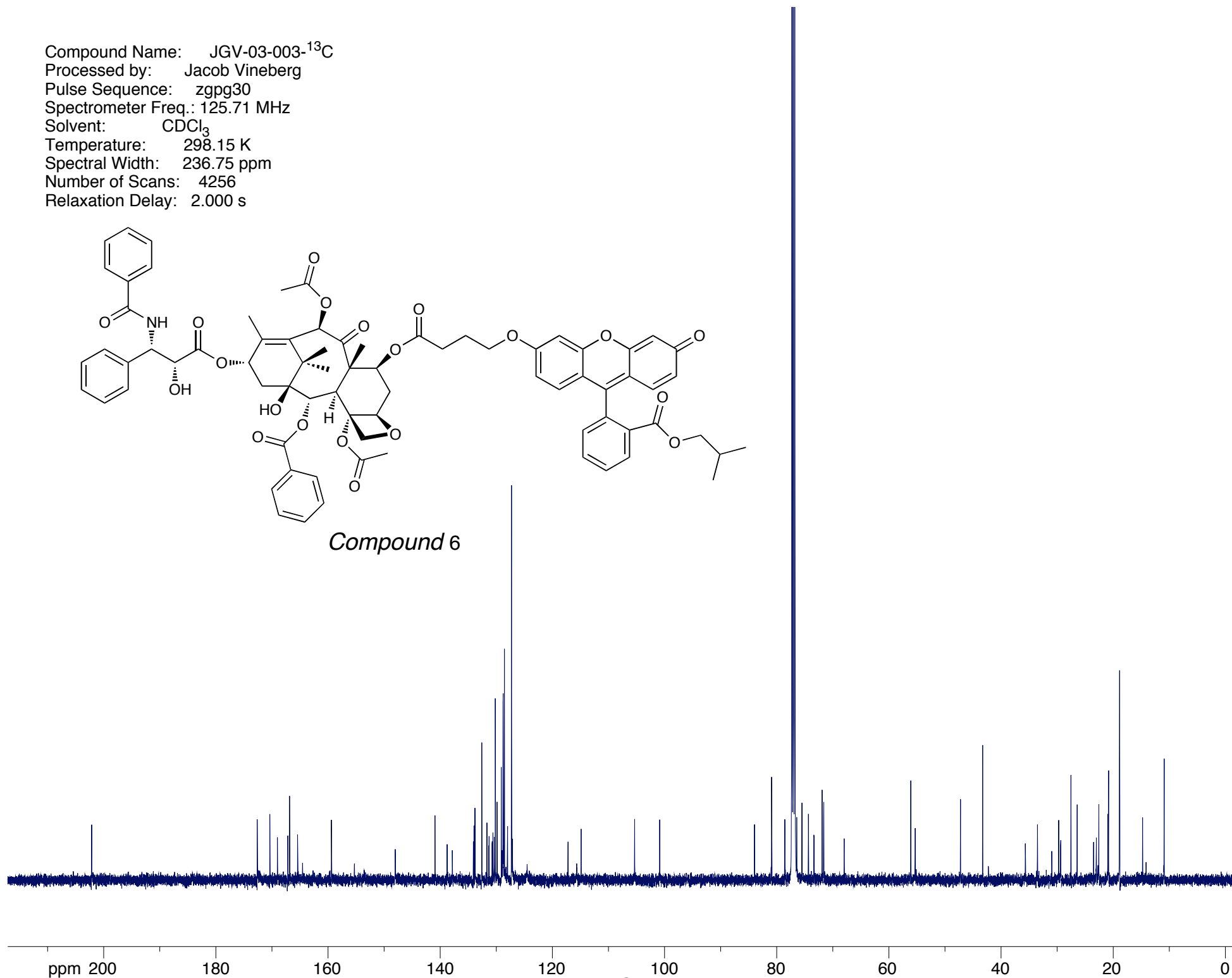
Compound 6



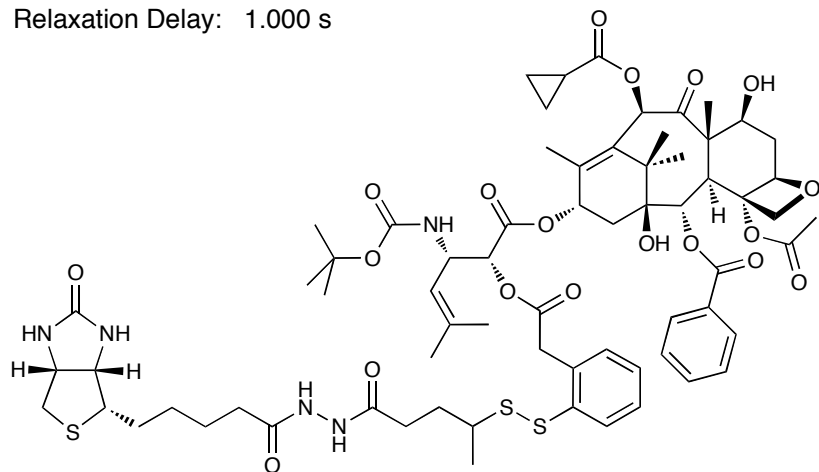
Compound Name: JGV-03-003-¹³C
Processed by: Jacob Vineberg
Pulse Sequence: zgpg30
Spectrometer Freq.: 125.71 MHz
Solvent: CDCl₃
Temperature: 298.15 K
Spectral Width: 236.75 ppm
Number of Scans: 4256
Relaxation Delay: 2.000 s



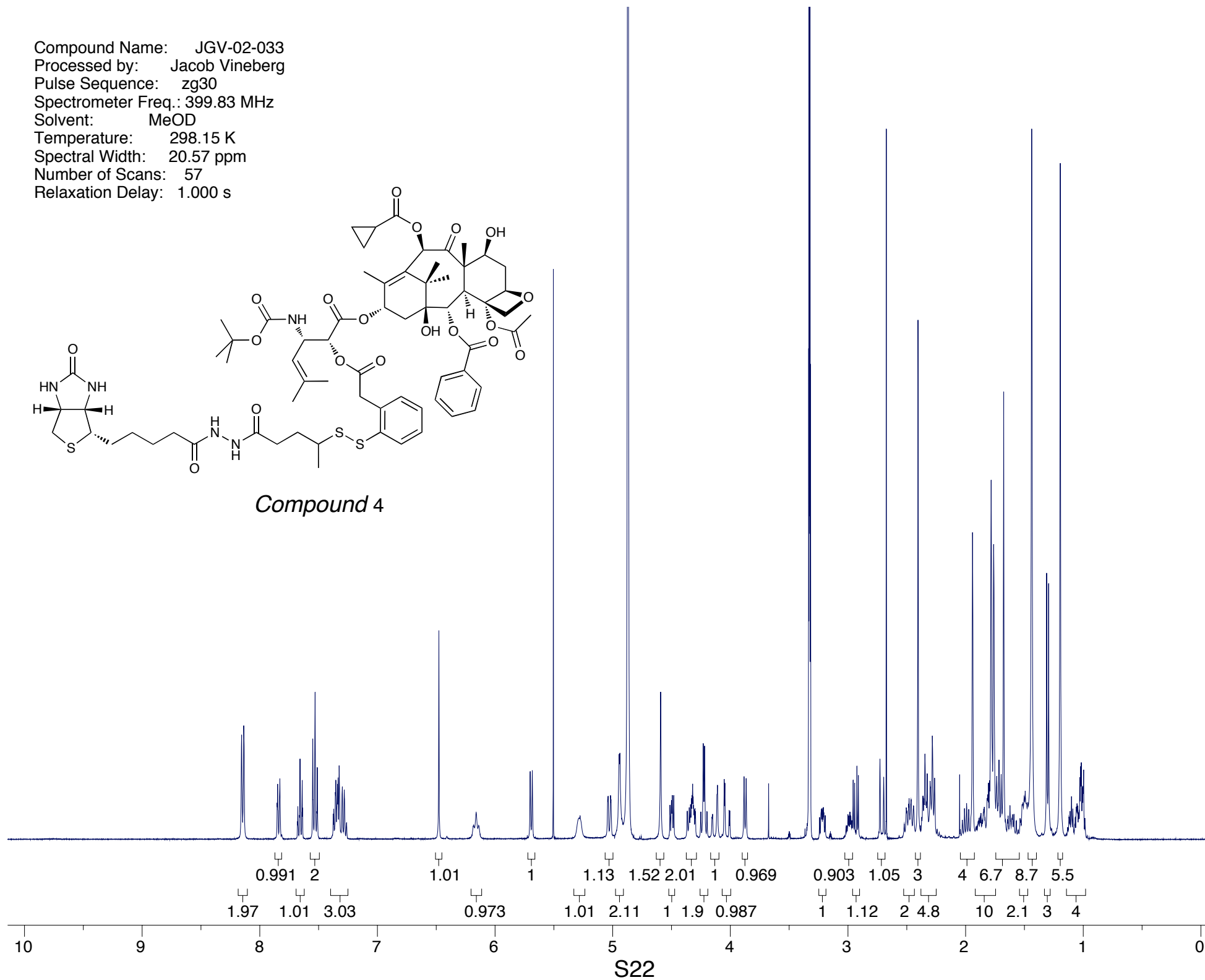
Compound 6



Compound Name: JGV-02-033
Processed by: Jacob Vineberg
Pulse Sequence: zg30
Spectrometer Freq.: 399.83 MHz
Solvent: MeOD
Temperature: 298.15 K
Spectral Width: 20.57 ppm
Number of Scans: 57
Relaxation Delay: 1.000 s



Compound 4



Compound Name: JGV-02-033-¹³C

Processed by: Jacob Vineberg

Pulse Sequence: zgpg30

Spectrometer Freq.: 125.71 MHz

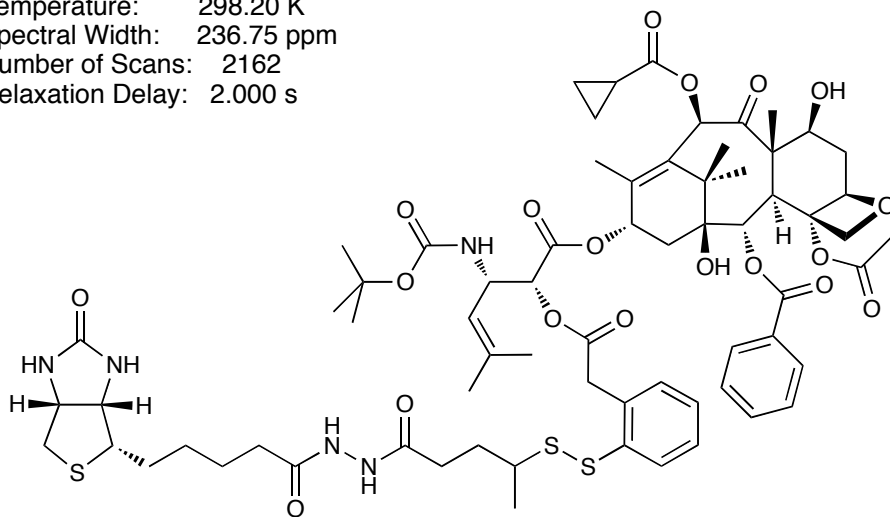
Solvent: MeOD

Temperature: 298.20 K

Spectral Width: 236.75 ppm

Number of Scans: 2162

Relaxation Delay: 2.000 s



Compound 4

