

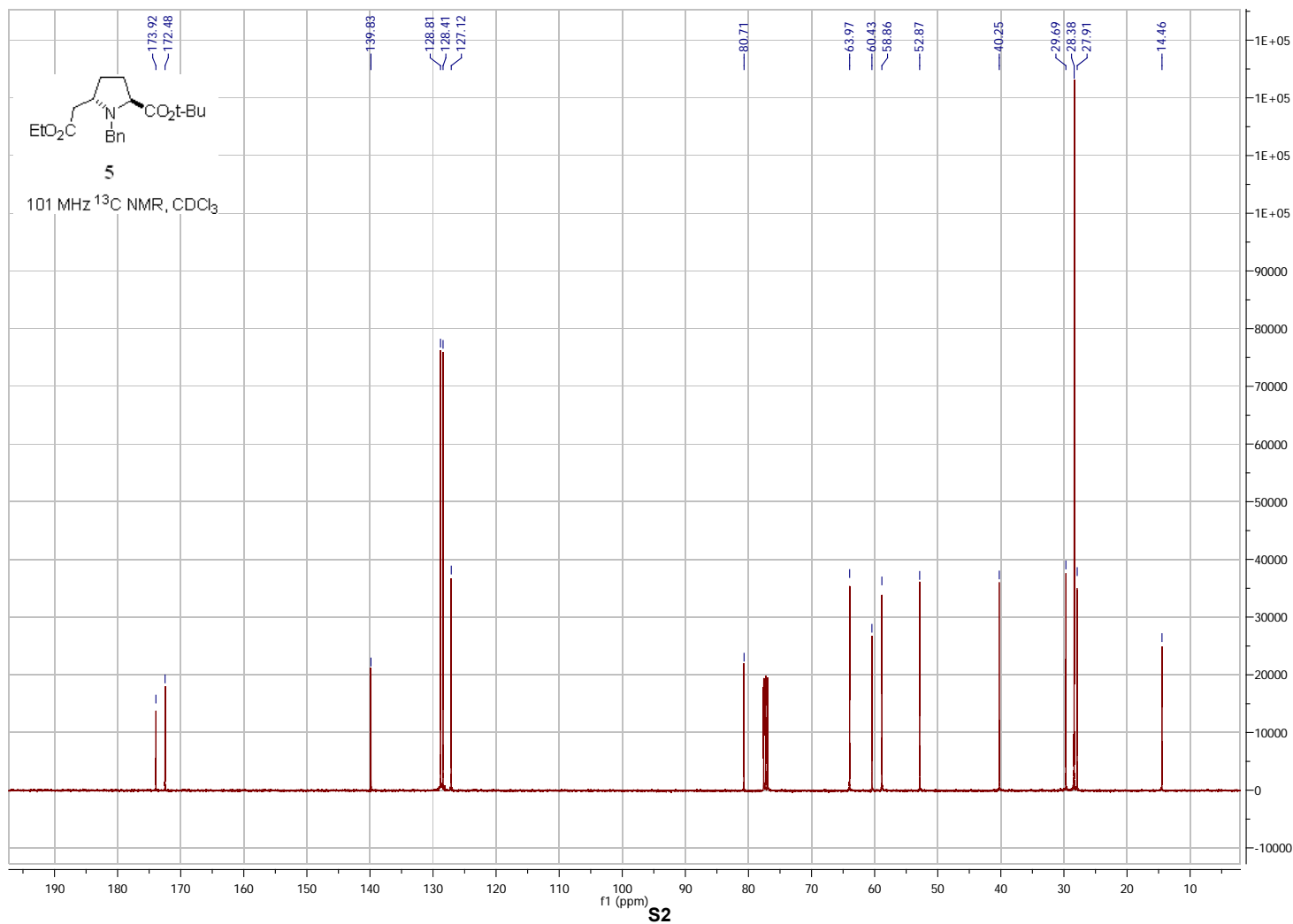
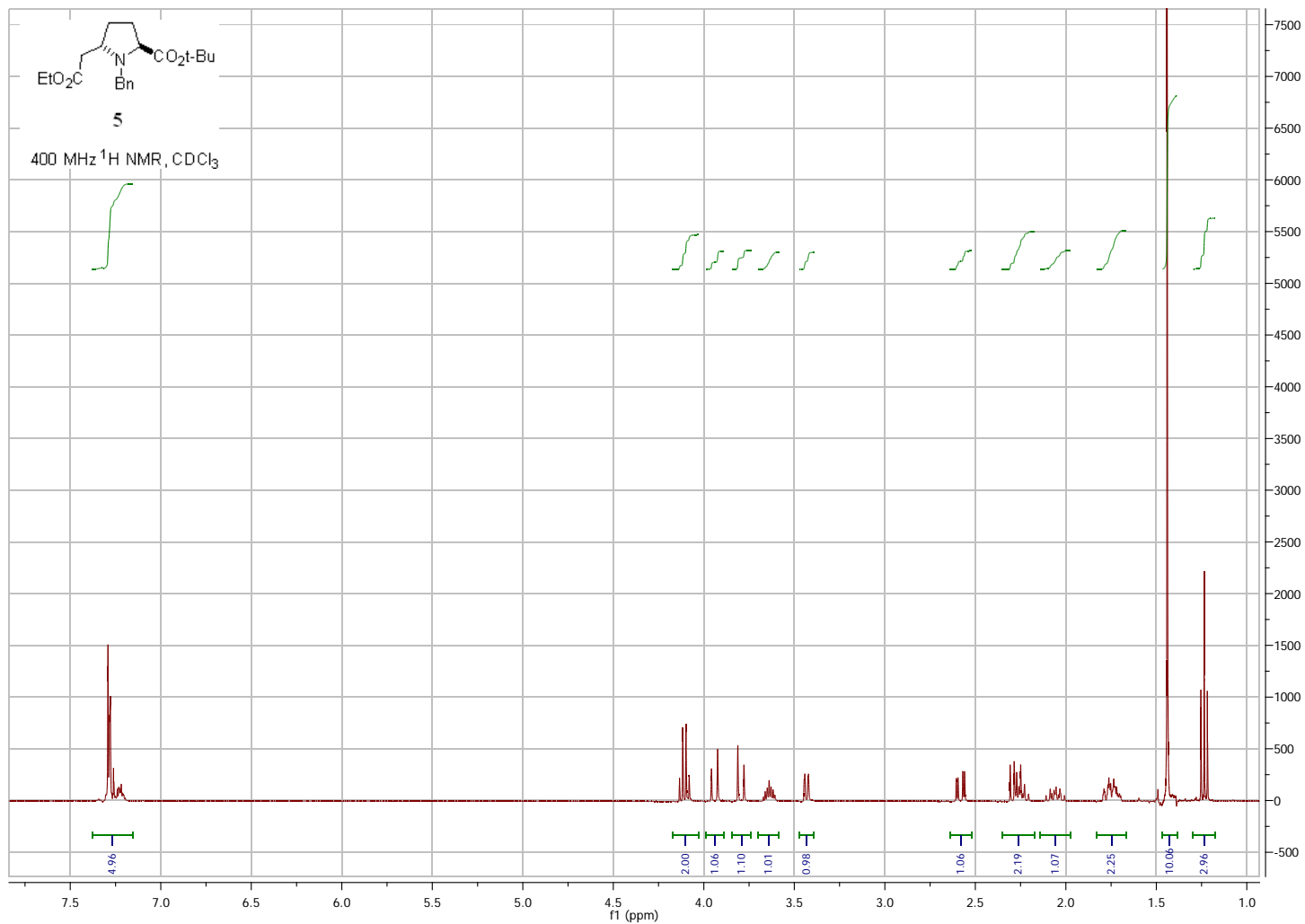
Supporting Information
Journal of Organic Chemistry

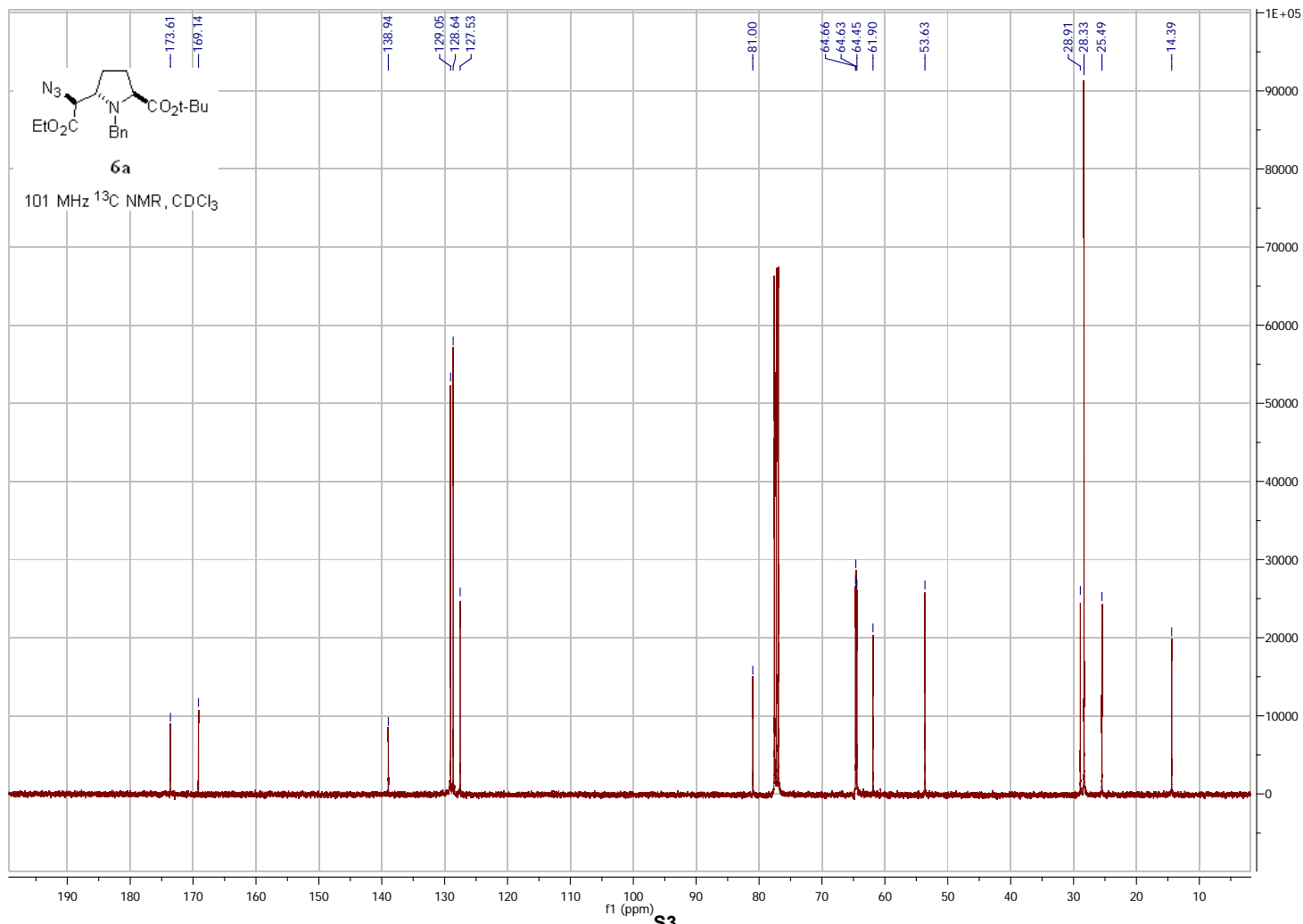
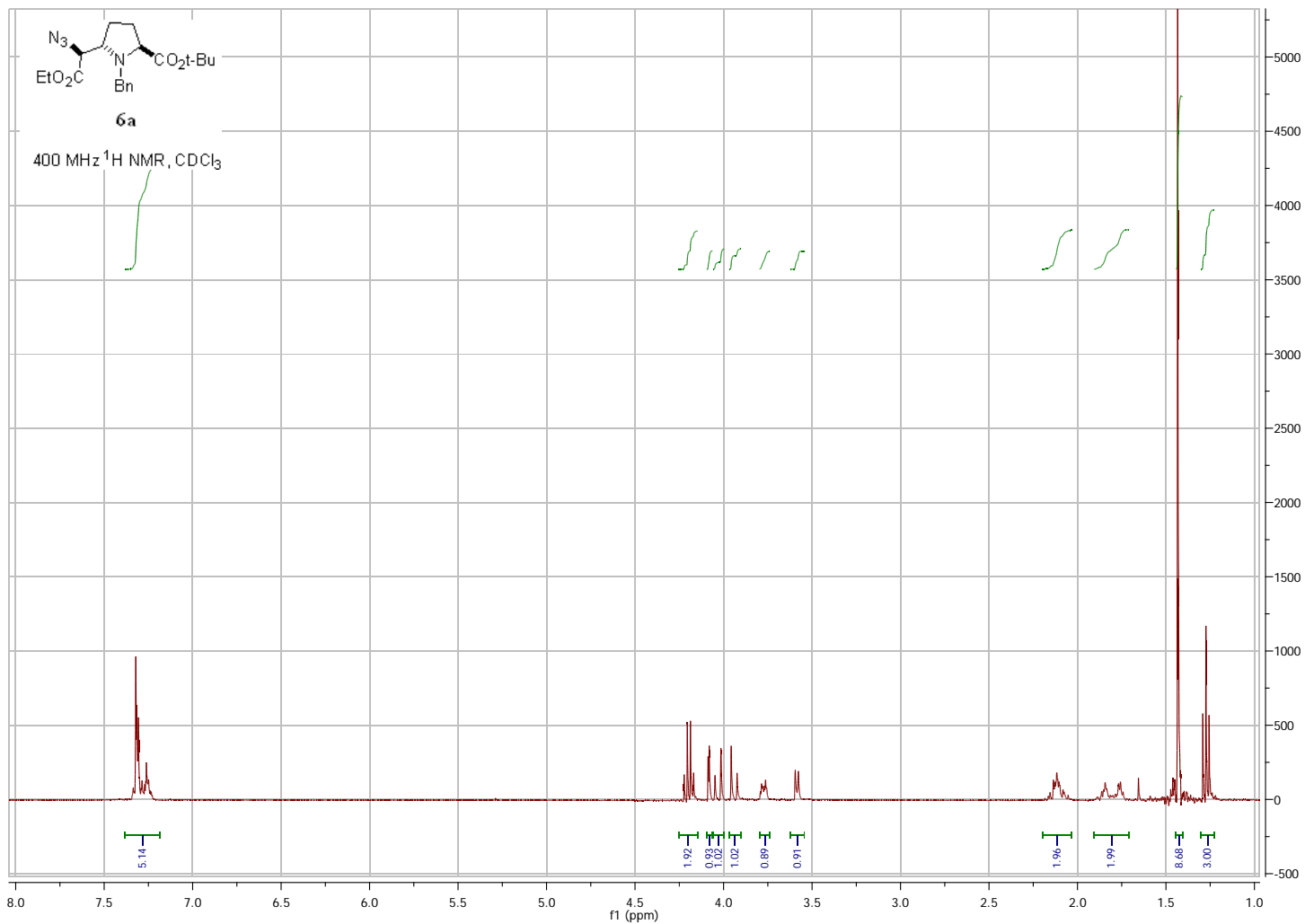
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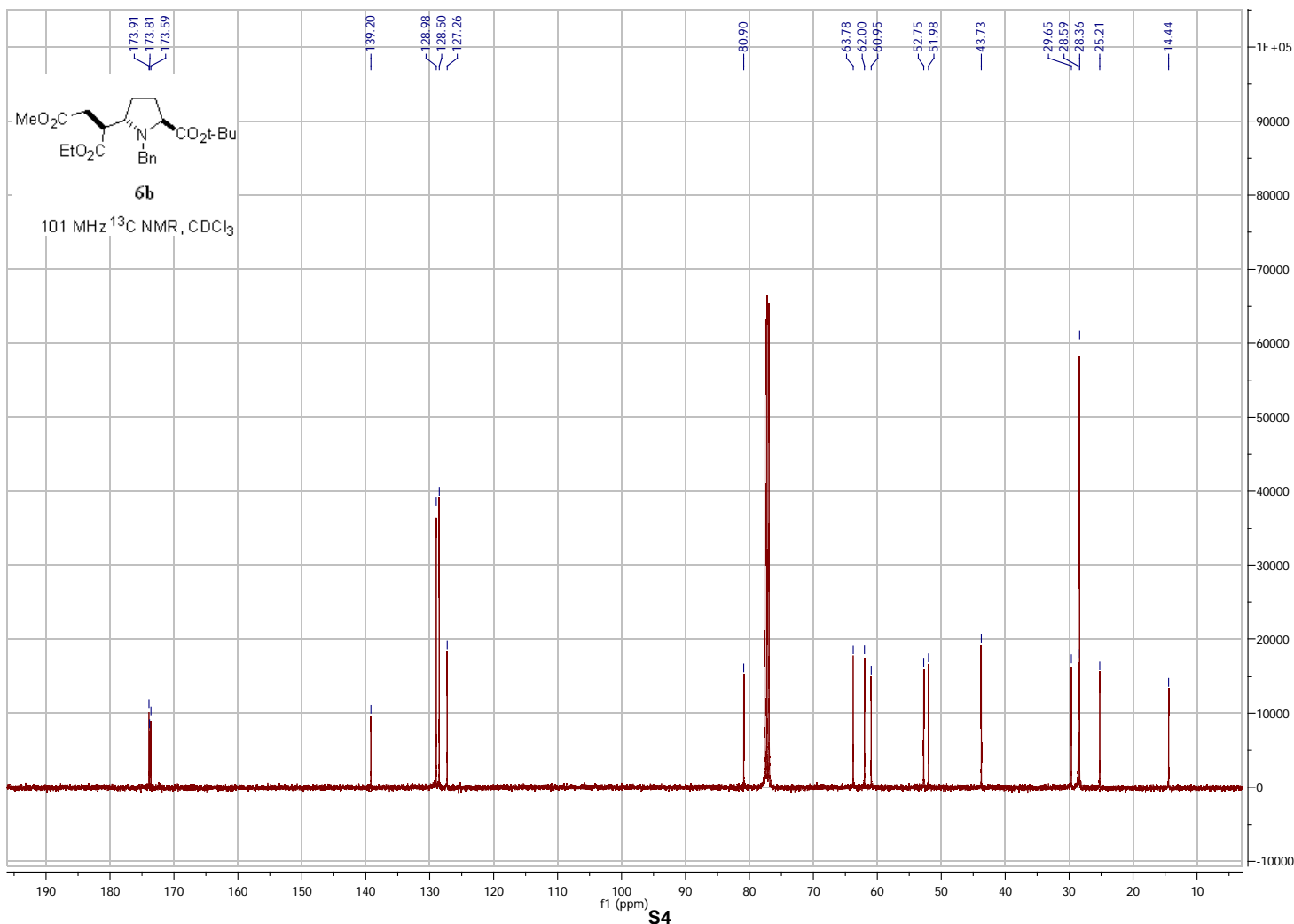
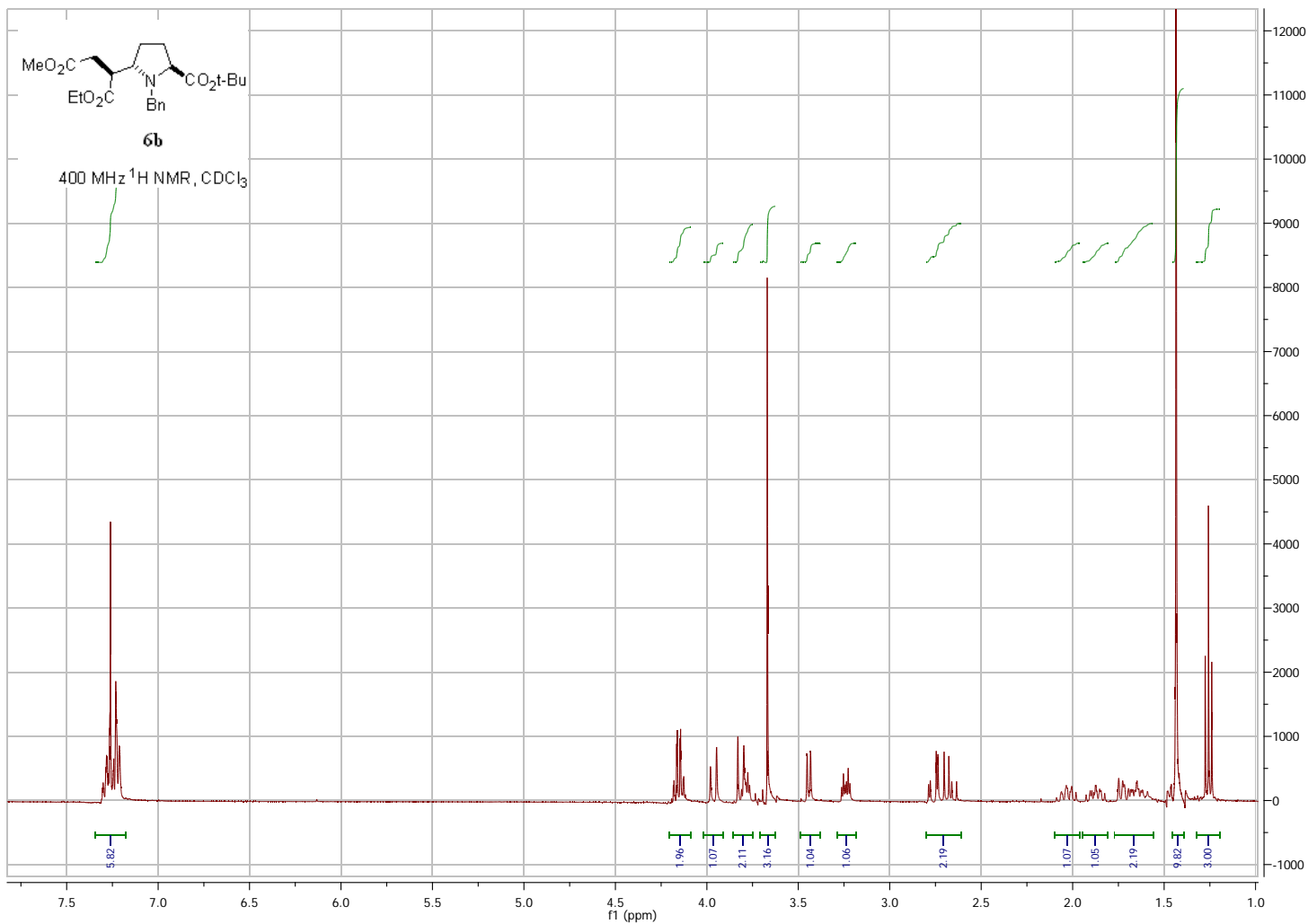
Sujeewa Ranatunga, Wathsala Liyanage, and Juan R. Del Valle*
Drug Discovery Department, H. Lee Moffitt Cancer Center and Research Institute

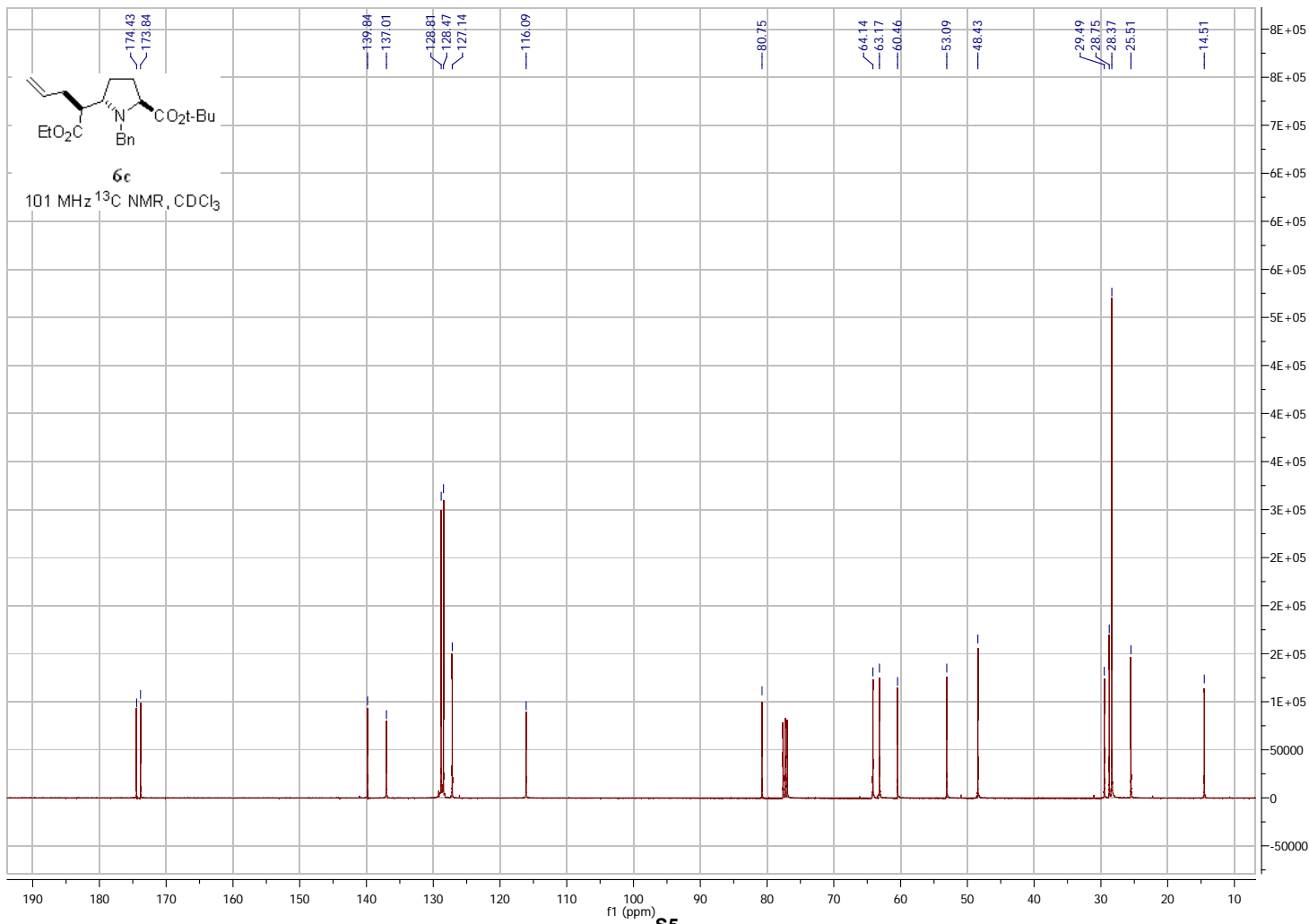
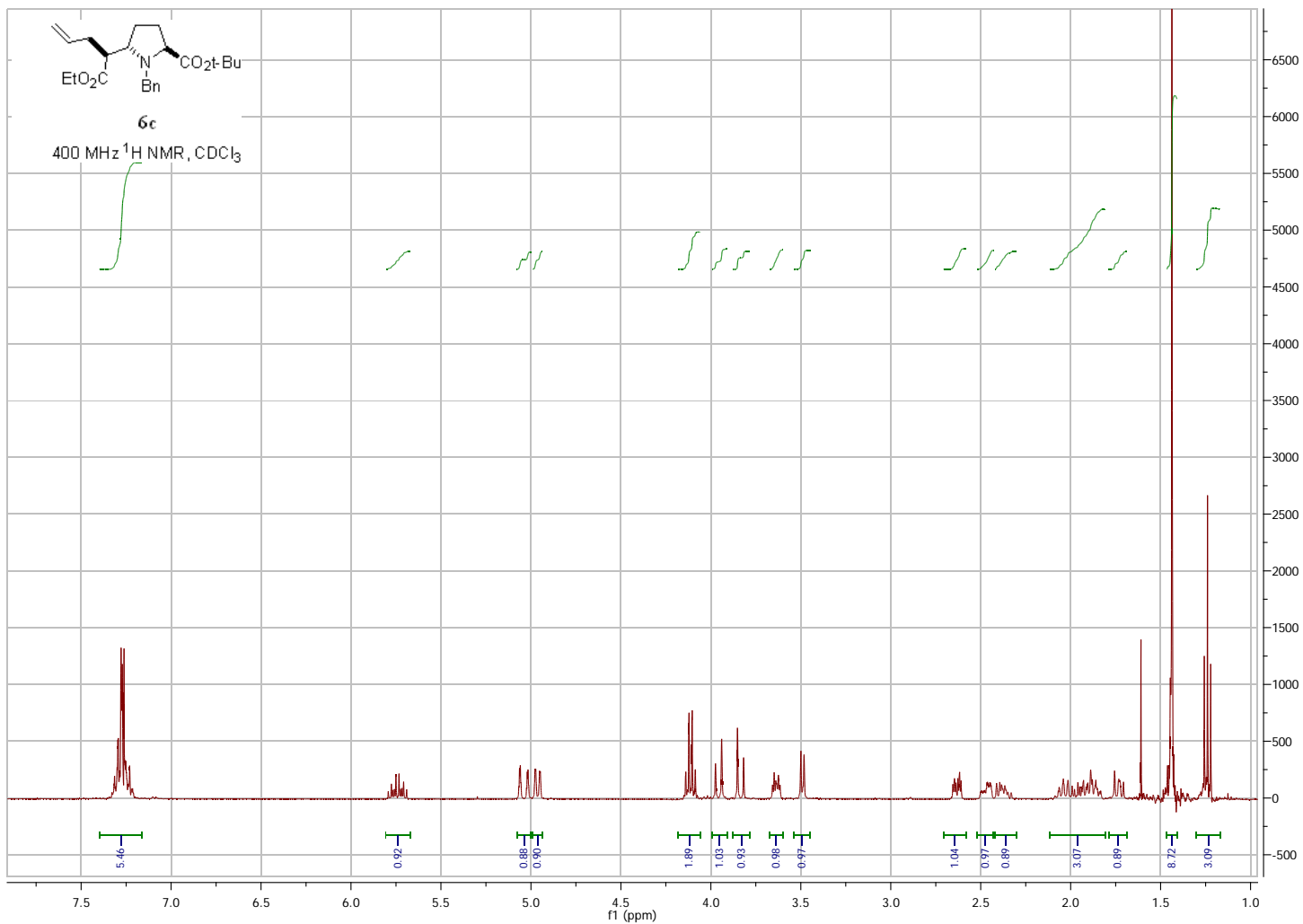
CONTENTS (47 pages)

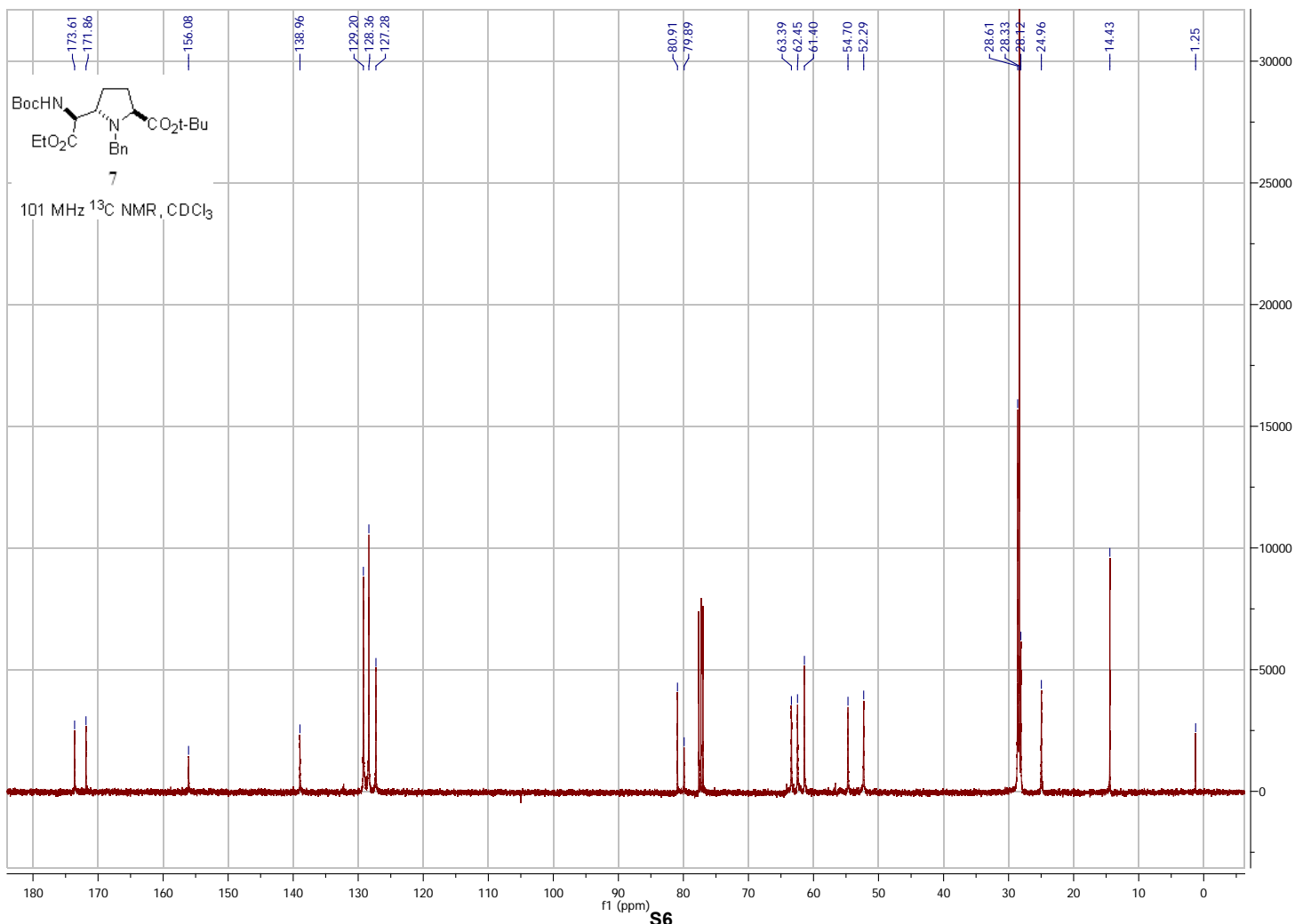
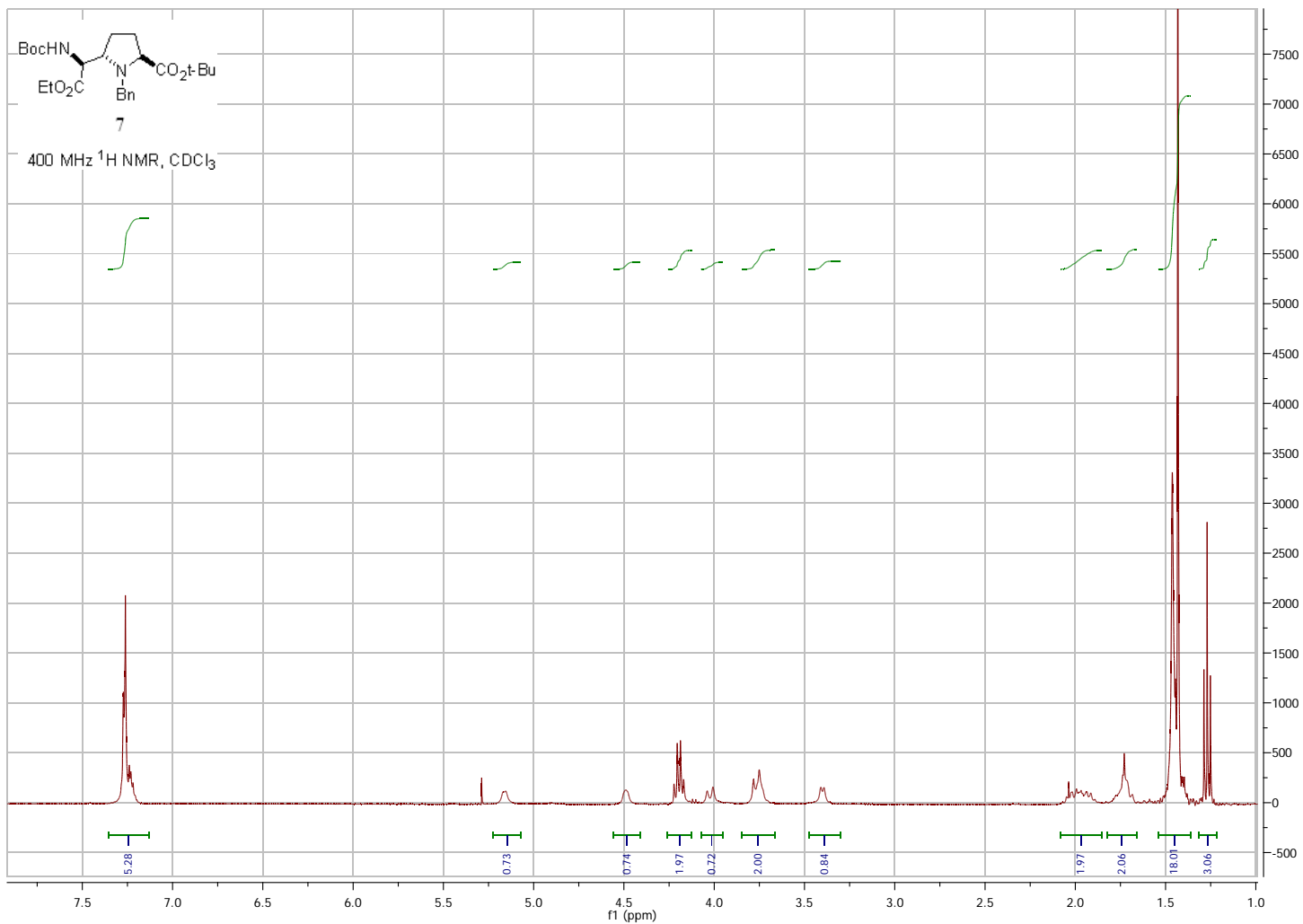
¹ H and ¹³ C NMR spectra for compound 5	S2
¹ H and ¹³ C NMR spectra for compound 6a	S3
¹ H and ¹³ C NMR spectra for compound 6b	S4
¹ H and ¹³ C NMR spectra for compound 6c	S5
¹ H and ¹³ C NMR spectra for compound 7	S6
¹ H and ¹³ C NMR spectra for compound 8	S7
¹ H and ¹³ C NMR spectra for compound 9	S8
¹ H and ¹³ C NMR spectra for product of hydrolysis of 9	S9
¹ H and ¹³ C NMR spectra for compound 10	S10
¹ H and ¹³ C NMR spectra for compound 11	S11
¹ H and ¹³ C NMR spectra for compound 12	S12
¹ H and ¹³ C NMR spectra for compound 13	S13
¹ H and ¹³ C NMR spectra for compound 14a	S14
¹ H and ¹³ C NMR spectra for compound 14b	S15
¹ H and ¹³ C NMR spectra for compound 14c	S16
¹ H and ¹³ C NMR spectra for compound 15	S17
¹ H and ¹³ C NMR spectra for compound 16	S18
¹ H and ¹³ C NMR spectra for product of hydrolysis of 16	S19
¹ H and ¹³ C NMR spectra for compound 17 minor	S20
¹ H and ¹³ C NMR spectra for compound 17 major	S21
¹ H and ¹³ C NMR spectra for compound 18	S22
¹ H and ¹³ C NMR spectra for compound 19	S23
¹ H and ¹³ C NMR spectra for product of oxidation of 19	S24
¹ H and ¹³ C NMR spectra for compound 20	S25
¹ H and ¹³ C NMR spectra for compound 21	S26
¹ H and ¹³ C NMR spectra for compound 22 minor	S27
¹ H and ¹³ C NMR spectra for compound 22 major	S28
¹ H and ¹³ C NMR spectra for compound 23	S29
¹ H and ¹³ C NMR spectra for compound 24	S30
¹ H and ¹³ C NMR spectra for product of oxidation of 24	S31
¹ H and ¹³ C NMR spectra for compound 25	S32
¹ H and ¹³ C NMR spectra for compound 26	S33
¹ H and ¹³ C NMR spectra for compound 28	S34
¹ H and ¹³ C NMR spectra for compound 29	S35
¹ H and ¹³ C NMR spectra for compound 30	S36
¹ H and ¹³ C NMR spectra for compound 31	S37
¹ H and ¹³ C NMR spectra for compound 32major	S38
¹ H and ¹³ C NMR spectra for compound 32 minor	S39
¹ H and ¹³ C NMR spectra for product of oxidation of 31	S40
¹ H and ¹³ C NMR spectra for compound 33	S41
HPLC Trace for 29	S42
HPLC Trace for 30	S43
HPLC Trace for 31	S44
HPLC Trace for 32	S45
HPLC Trace for 33	S46
Procedure for conformational searches	S47

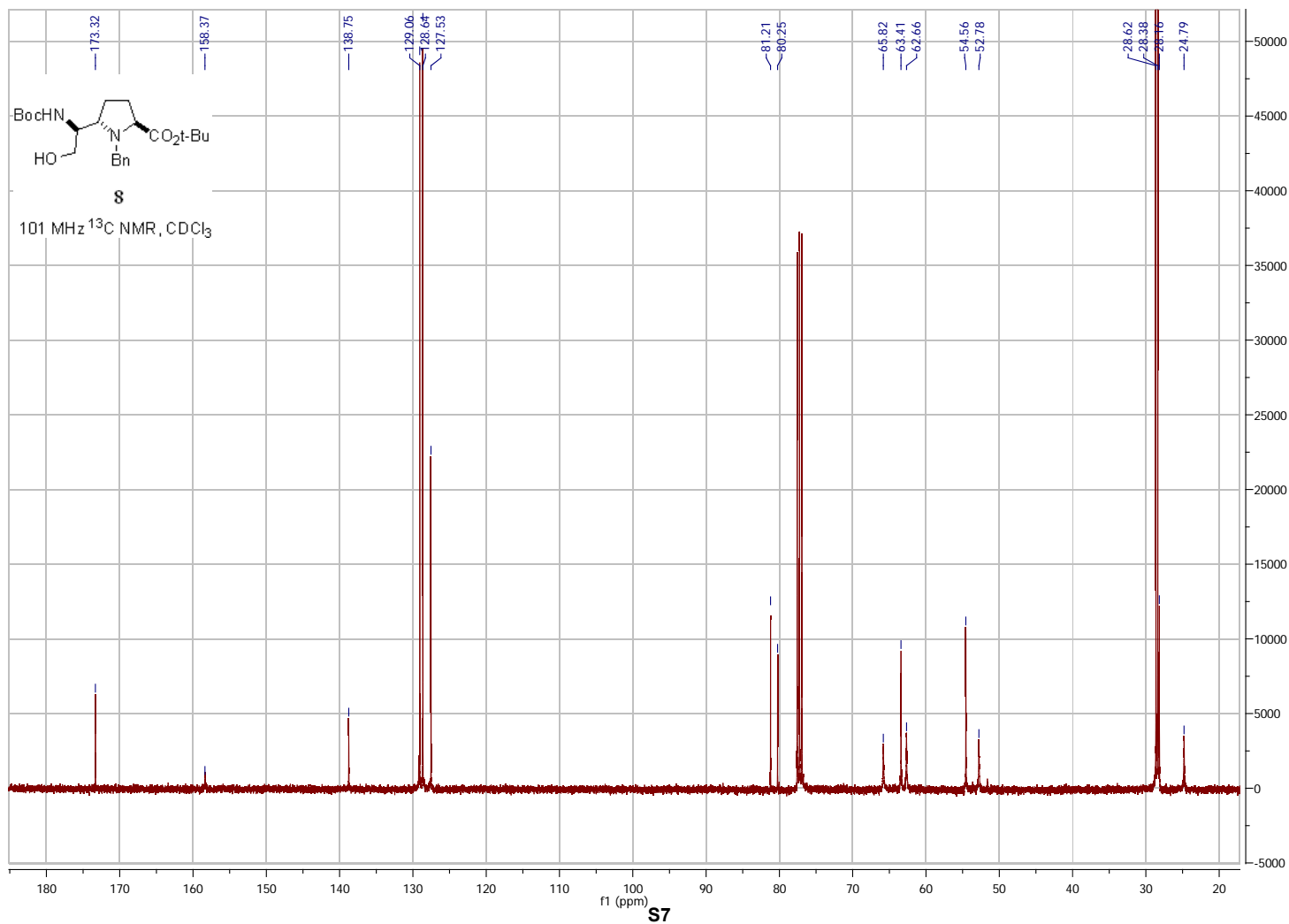
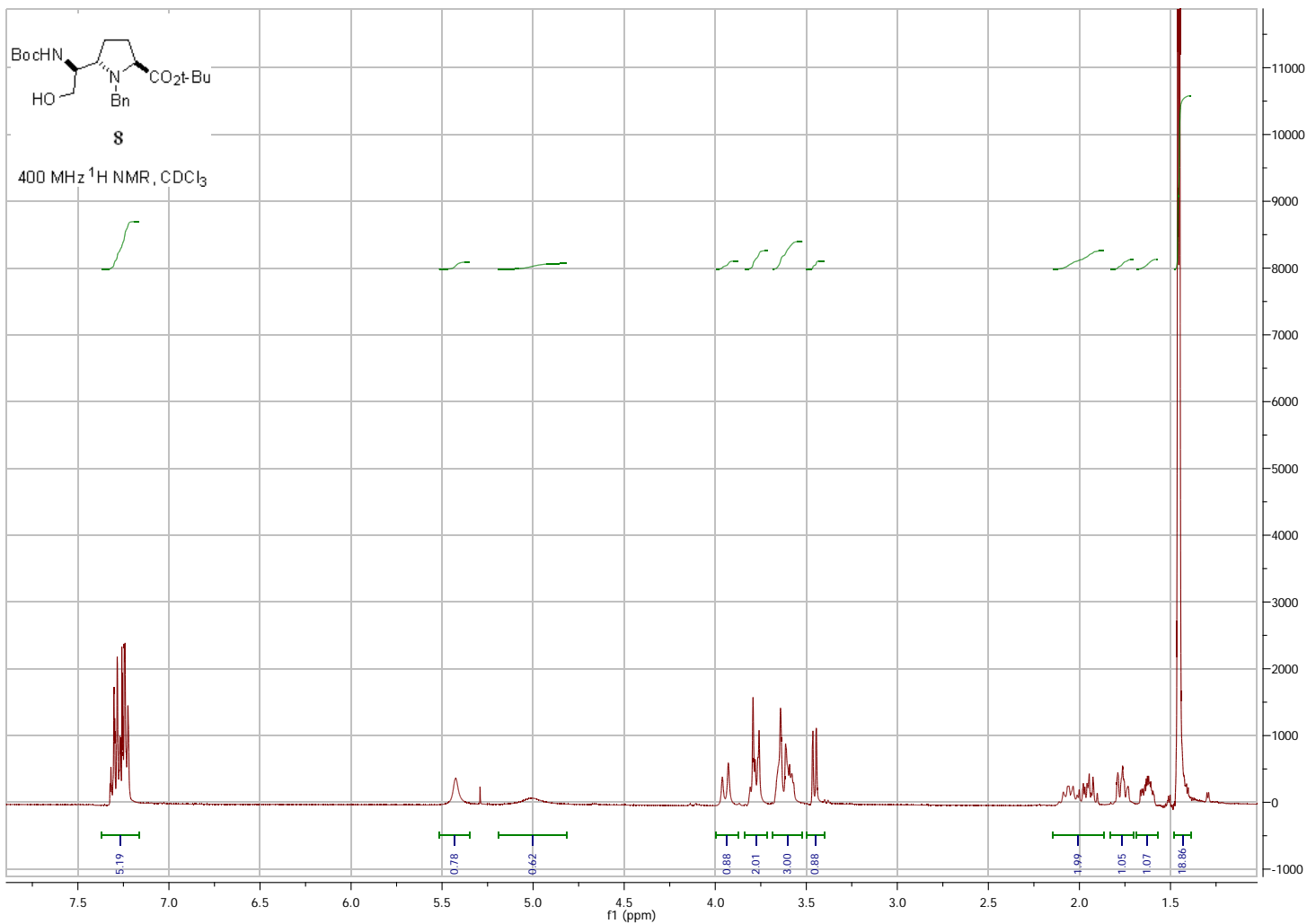


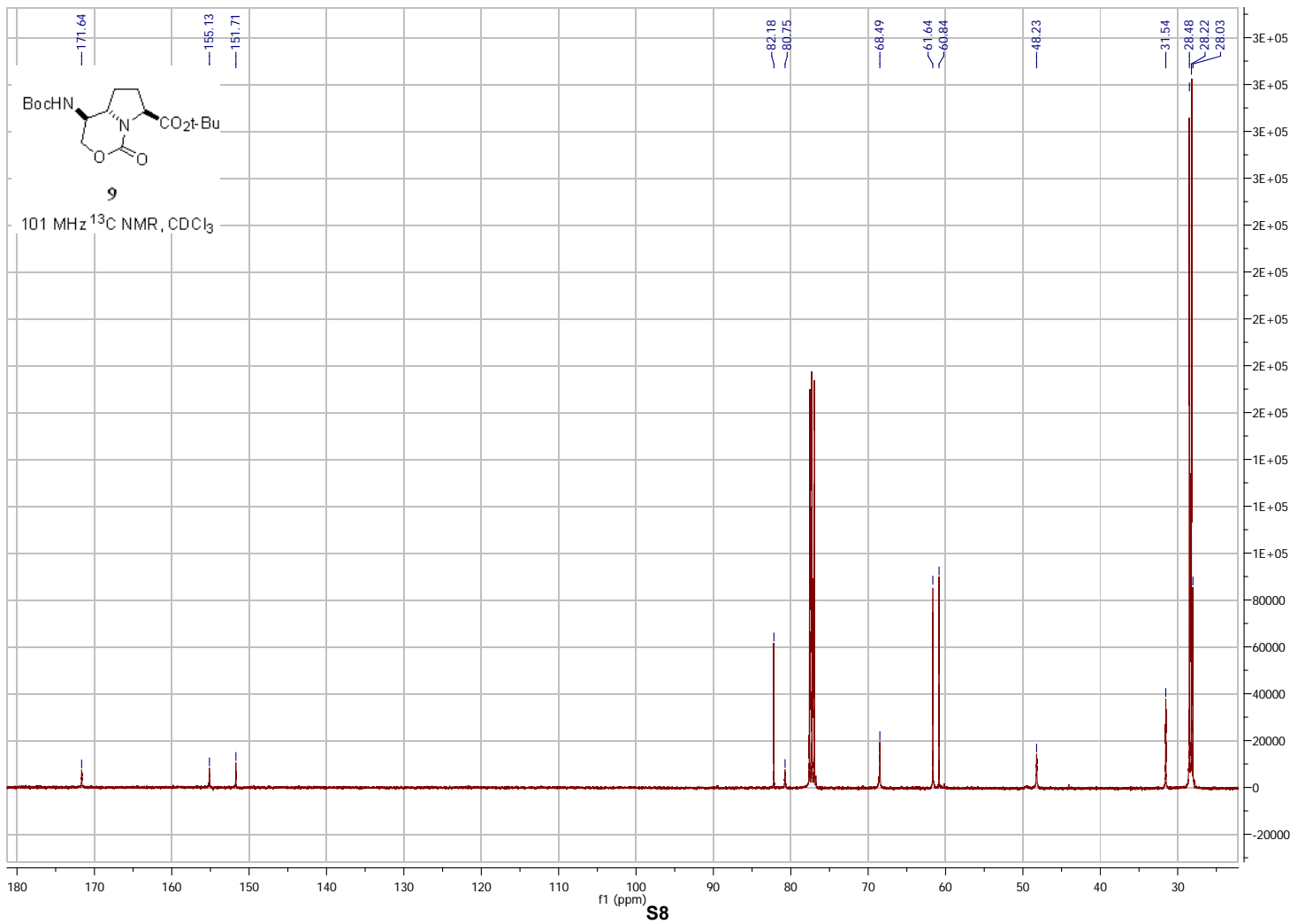
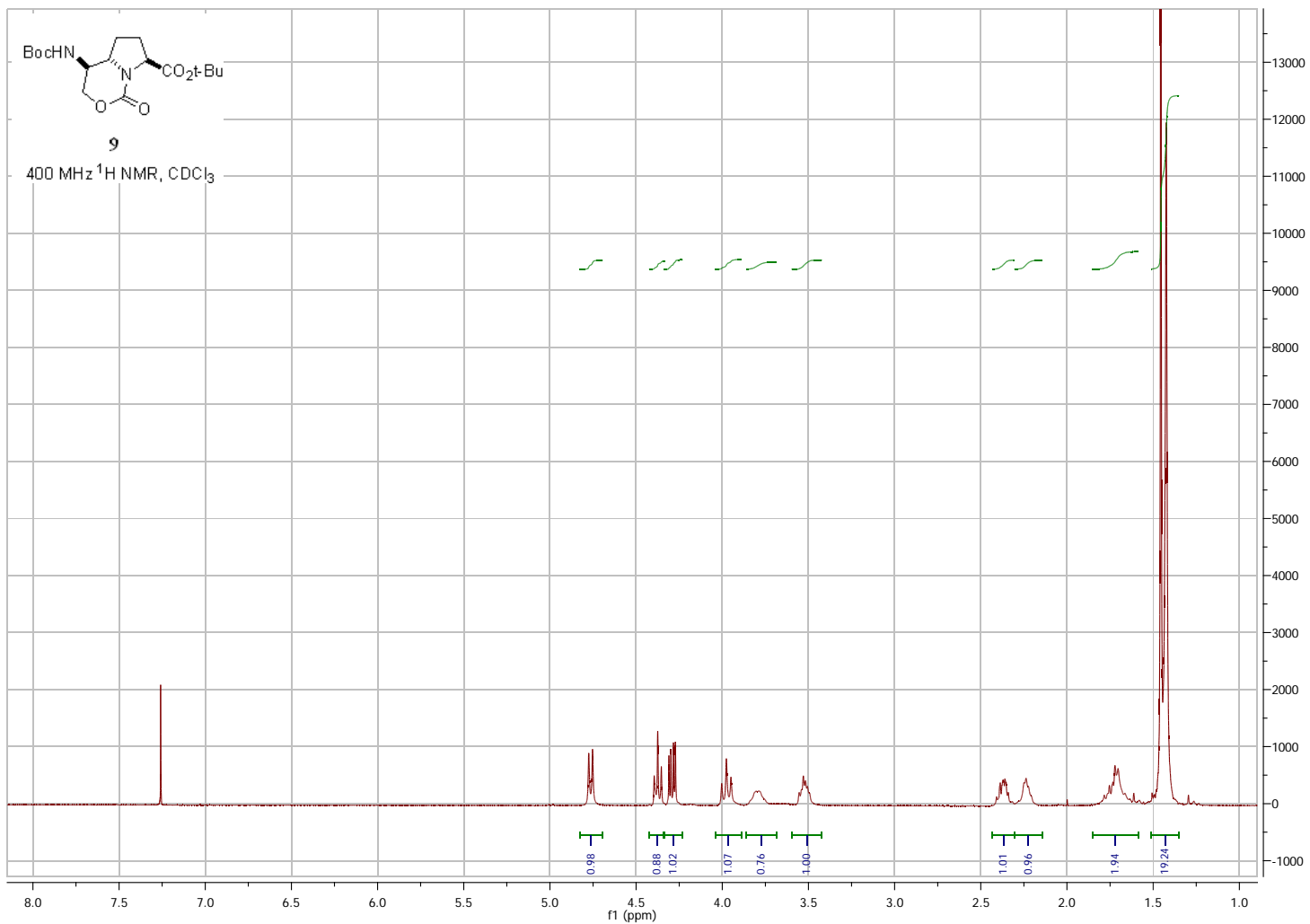


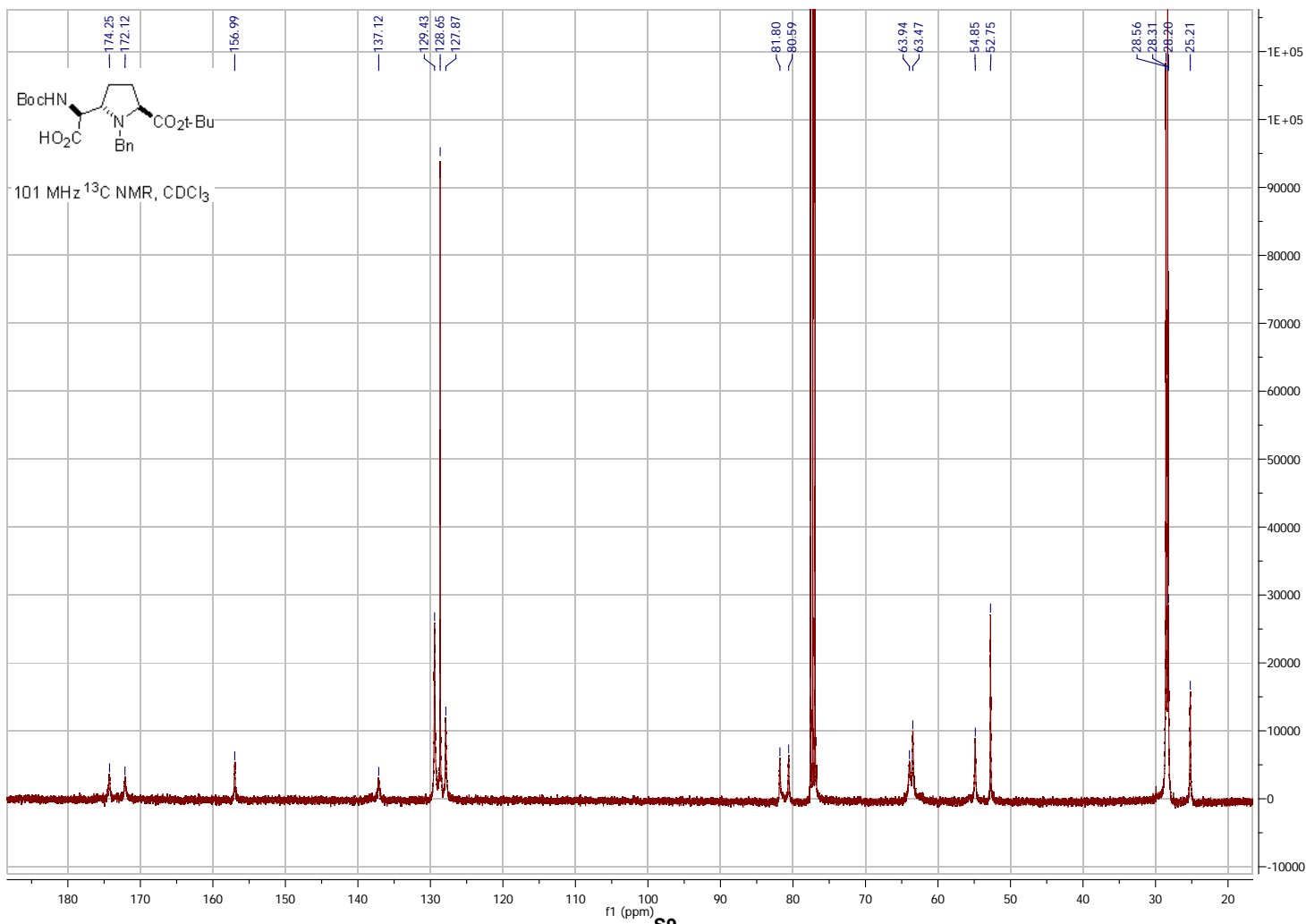
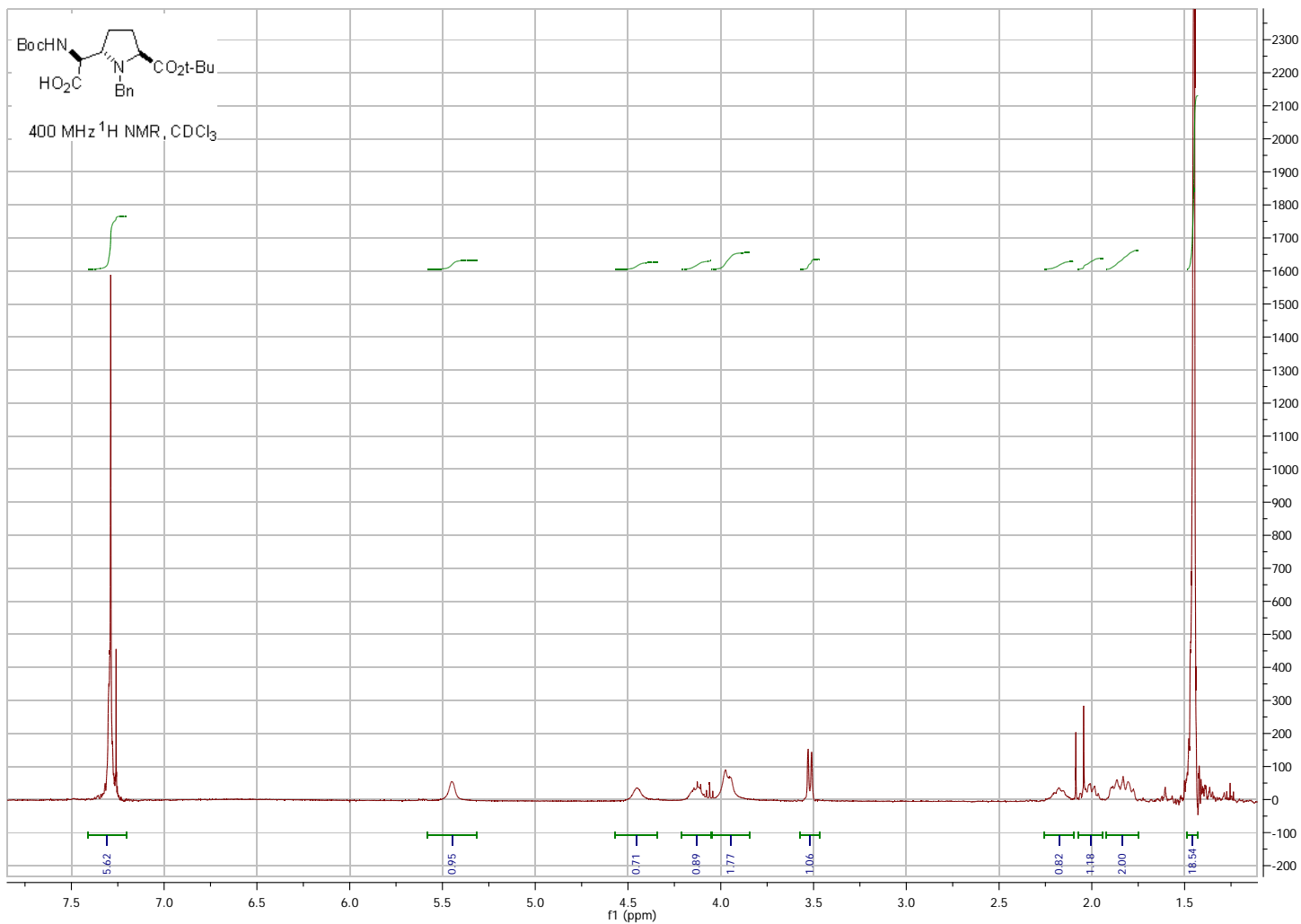


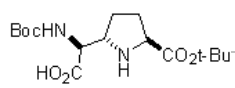






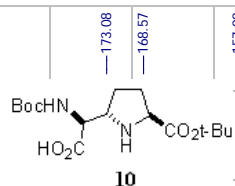
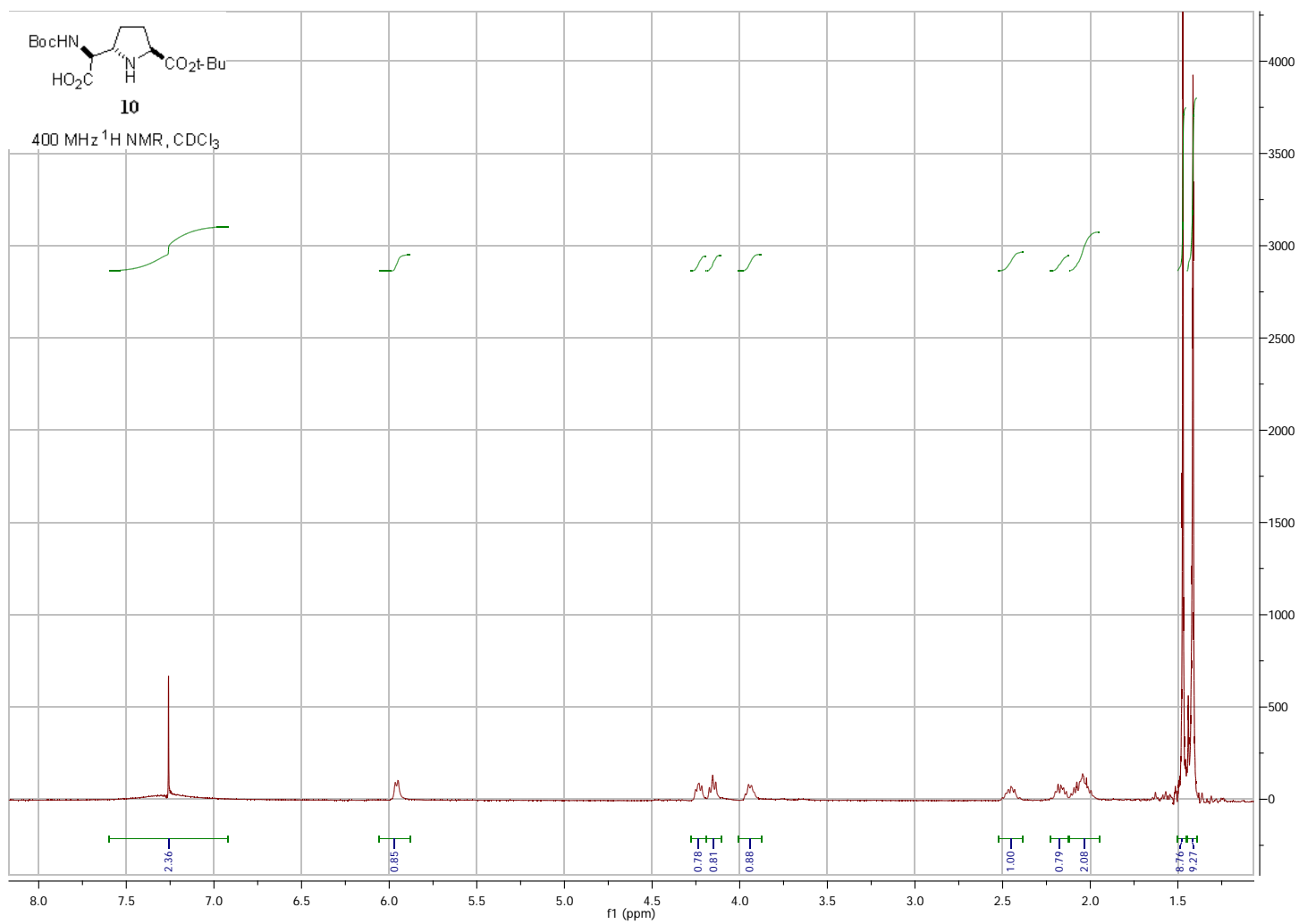






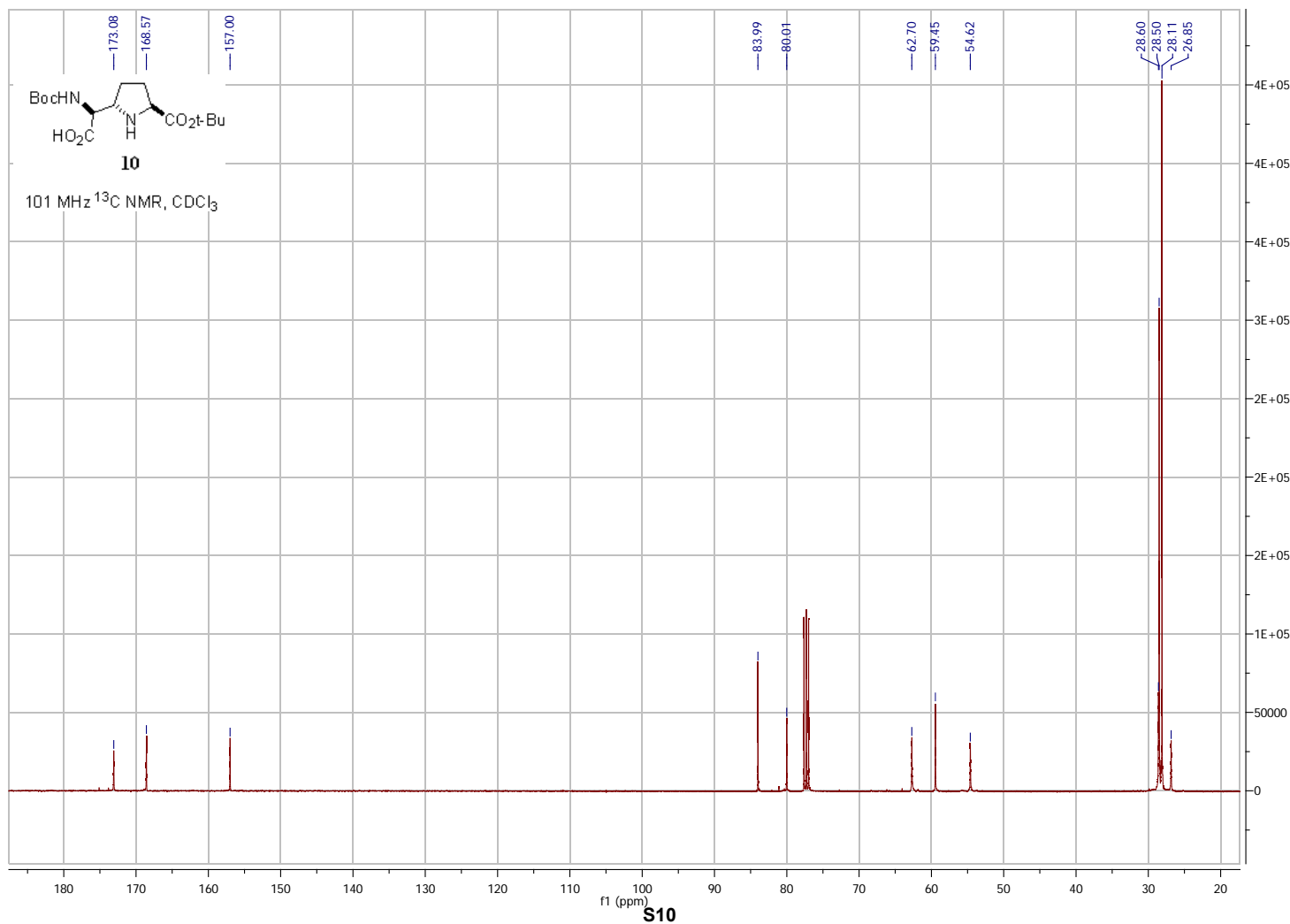
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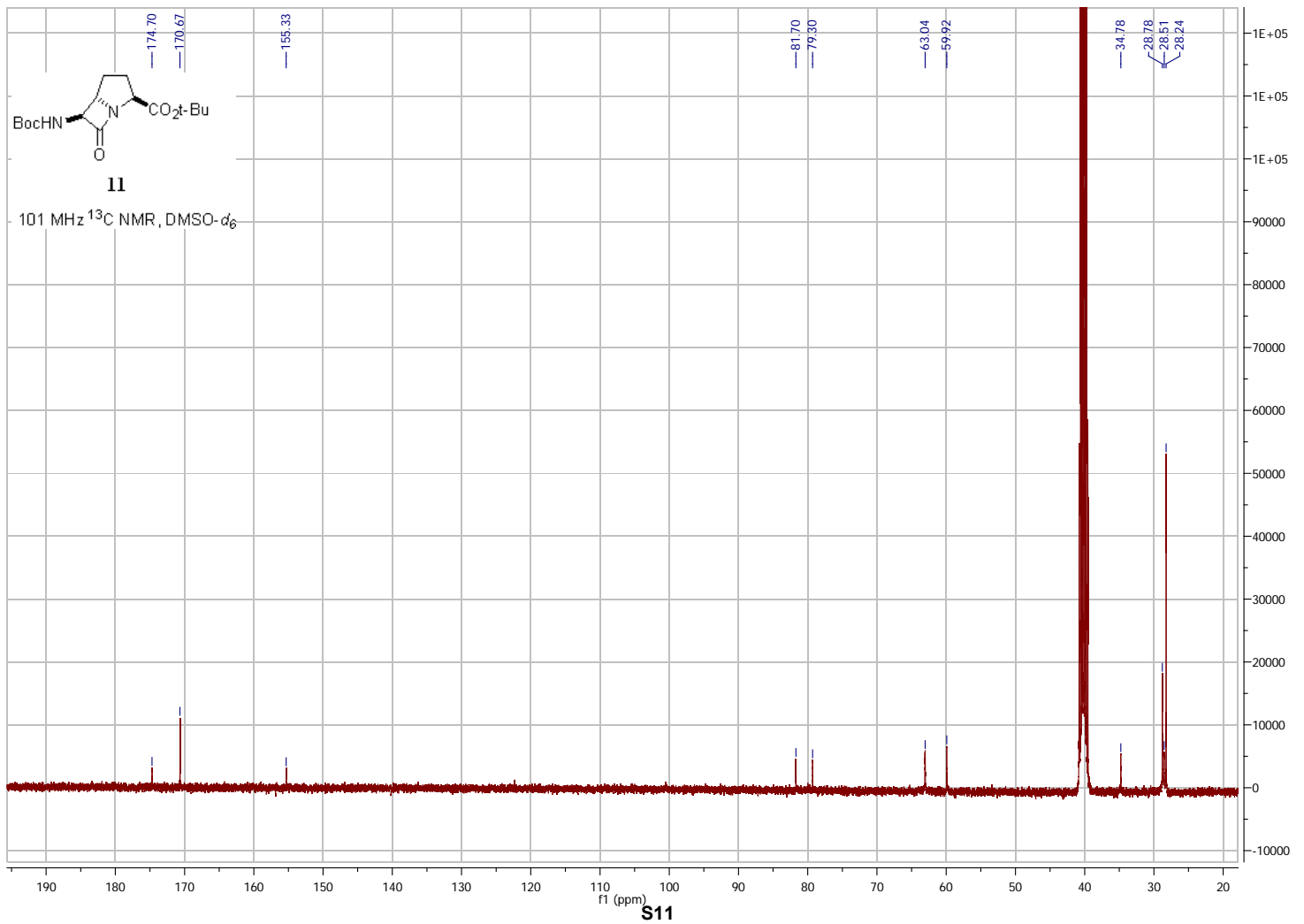
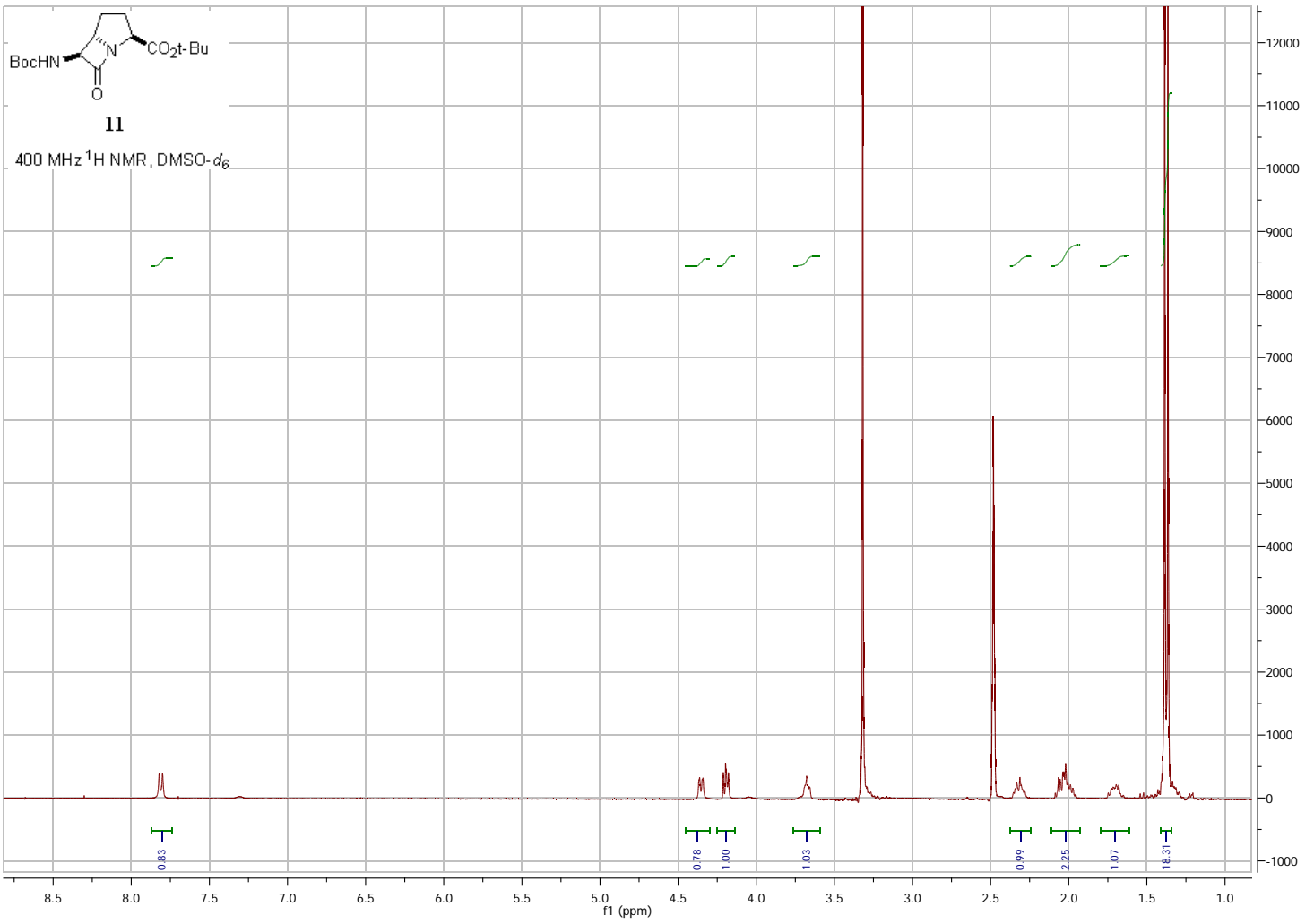
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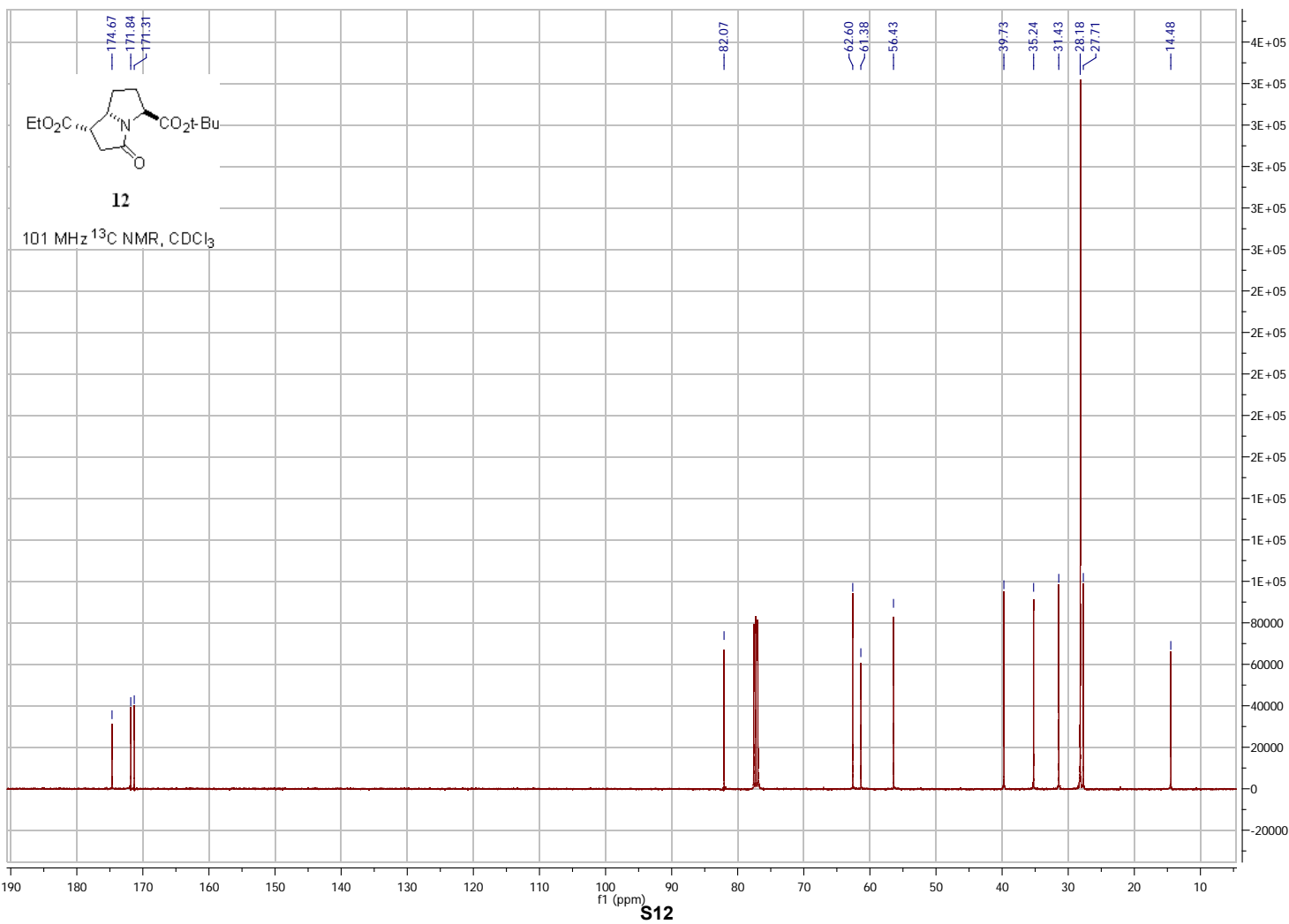
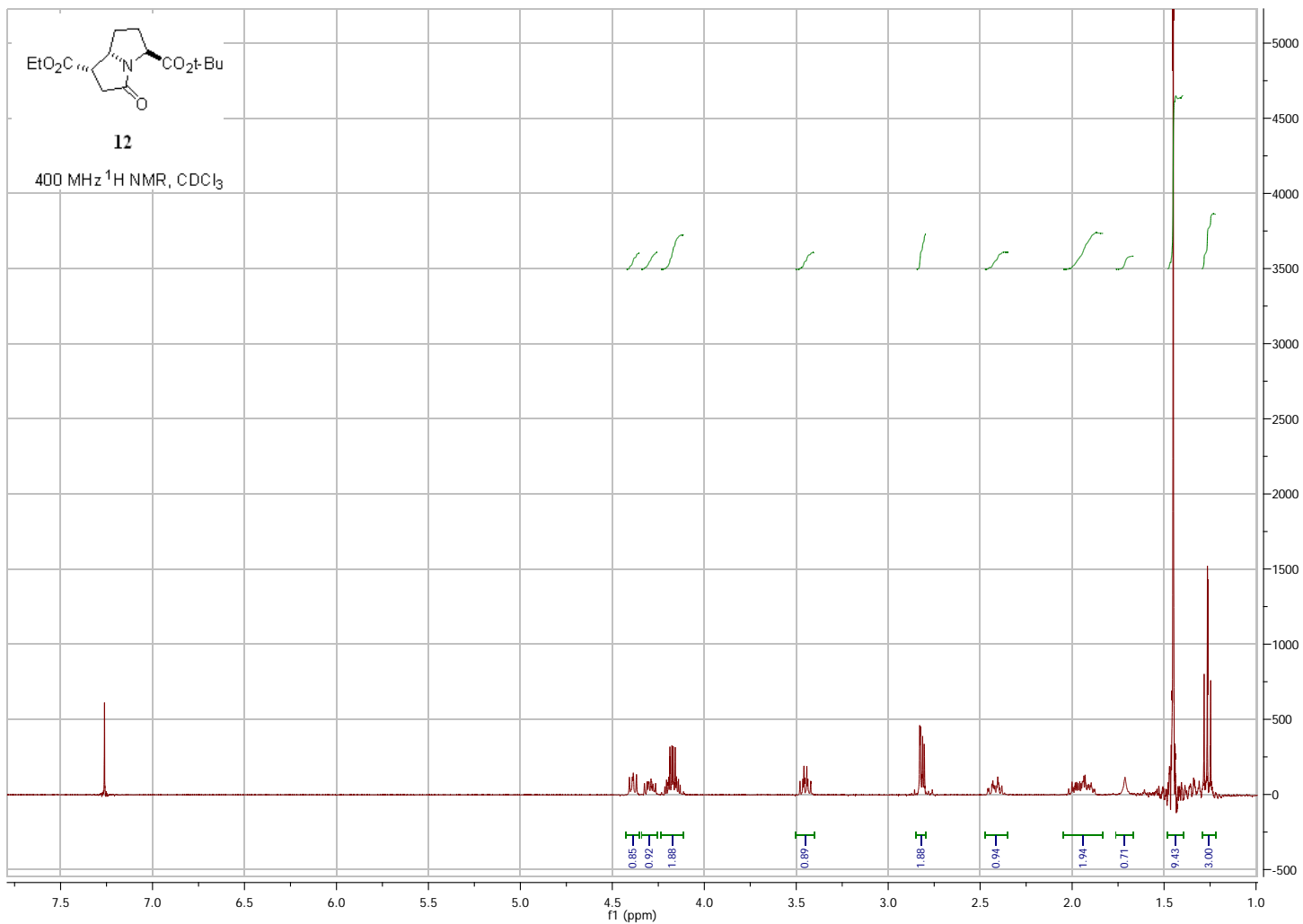


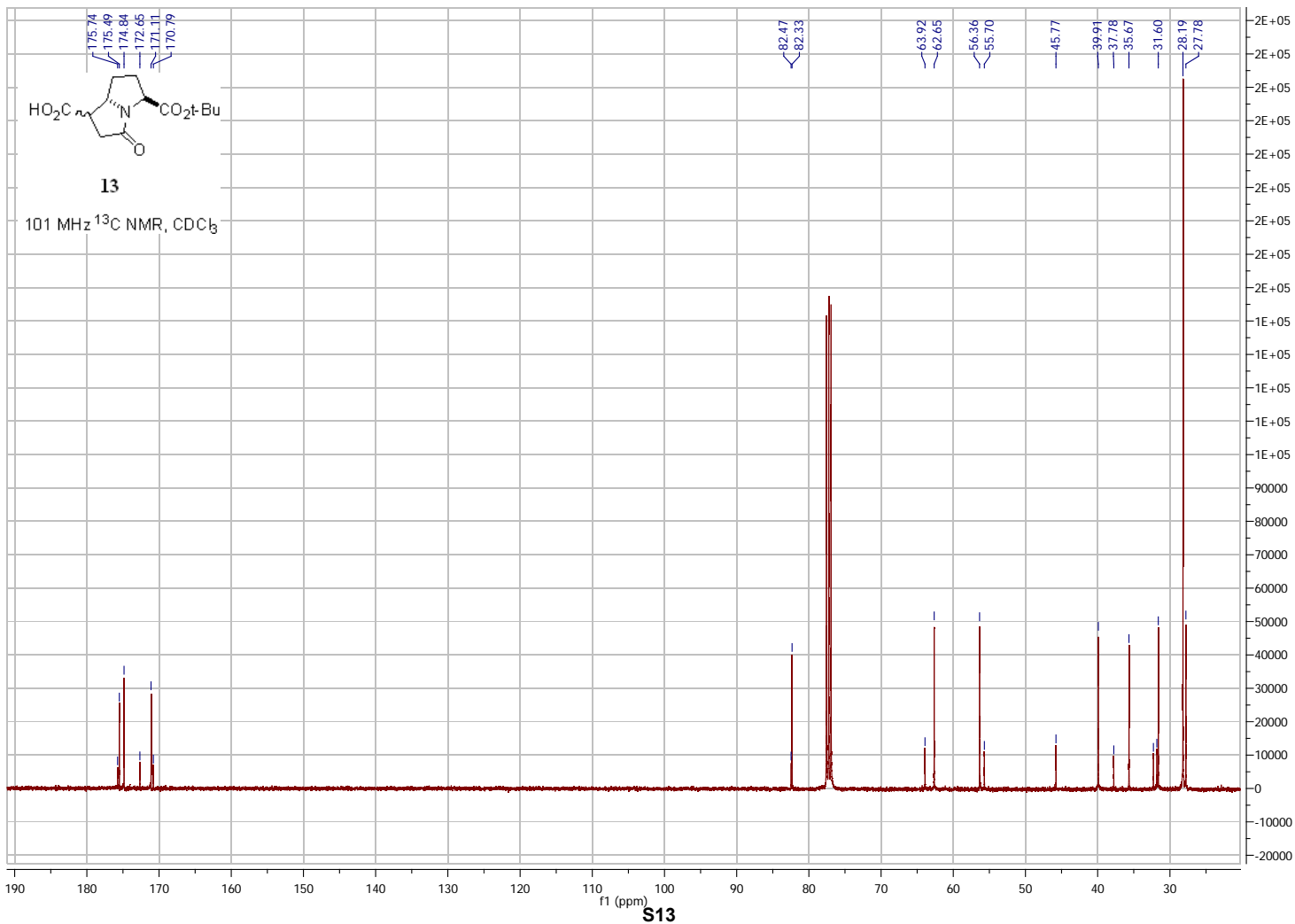
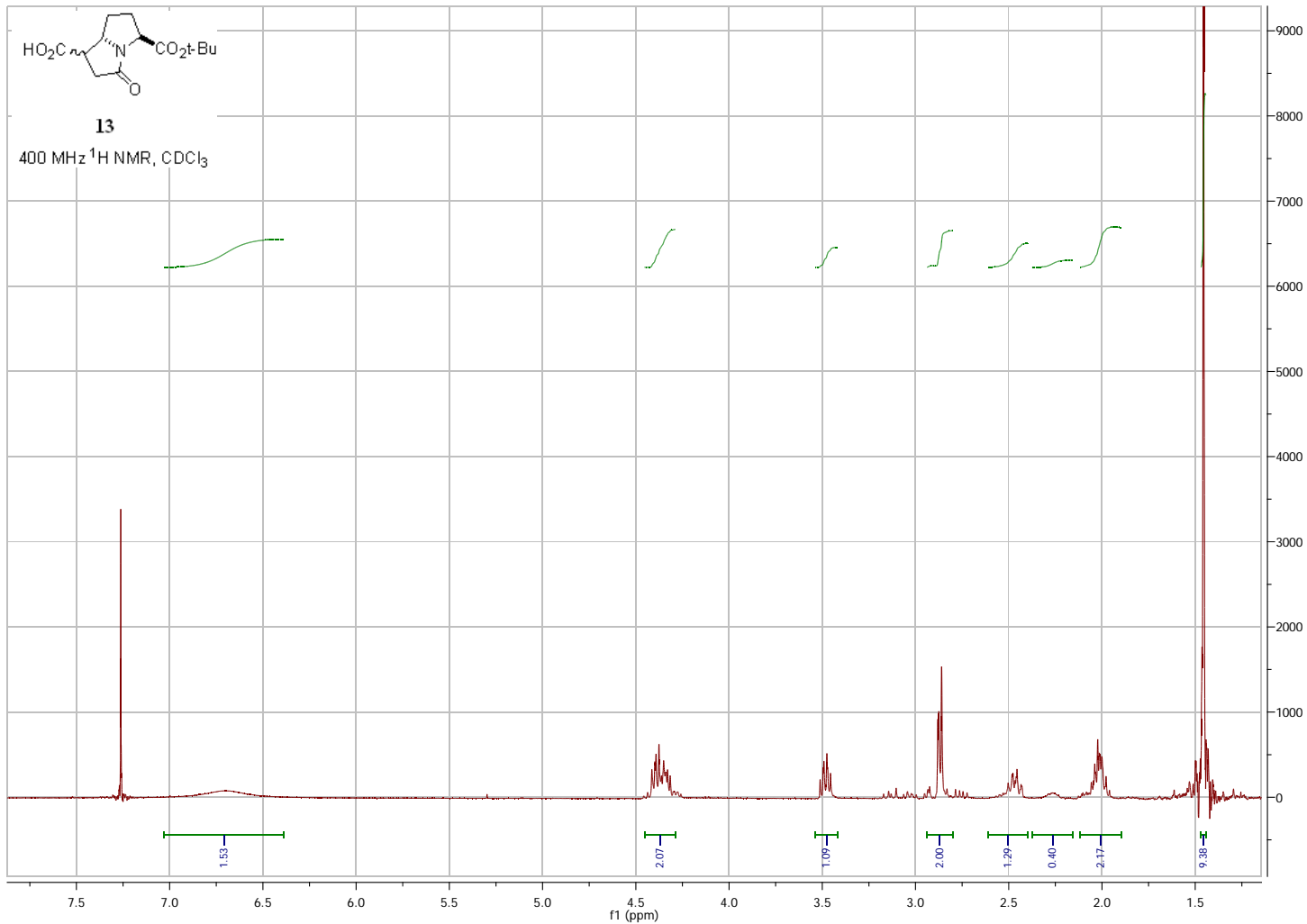
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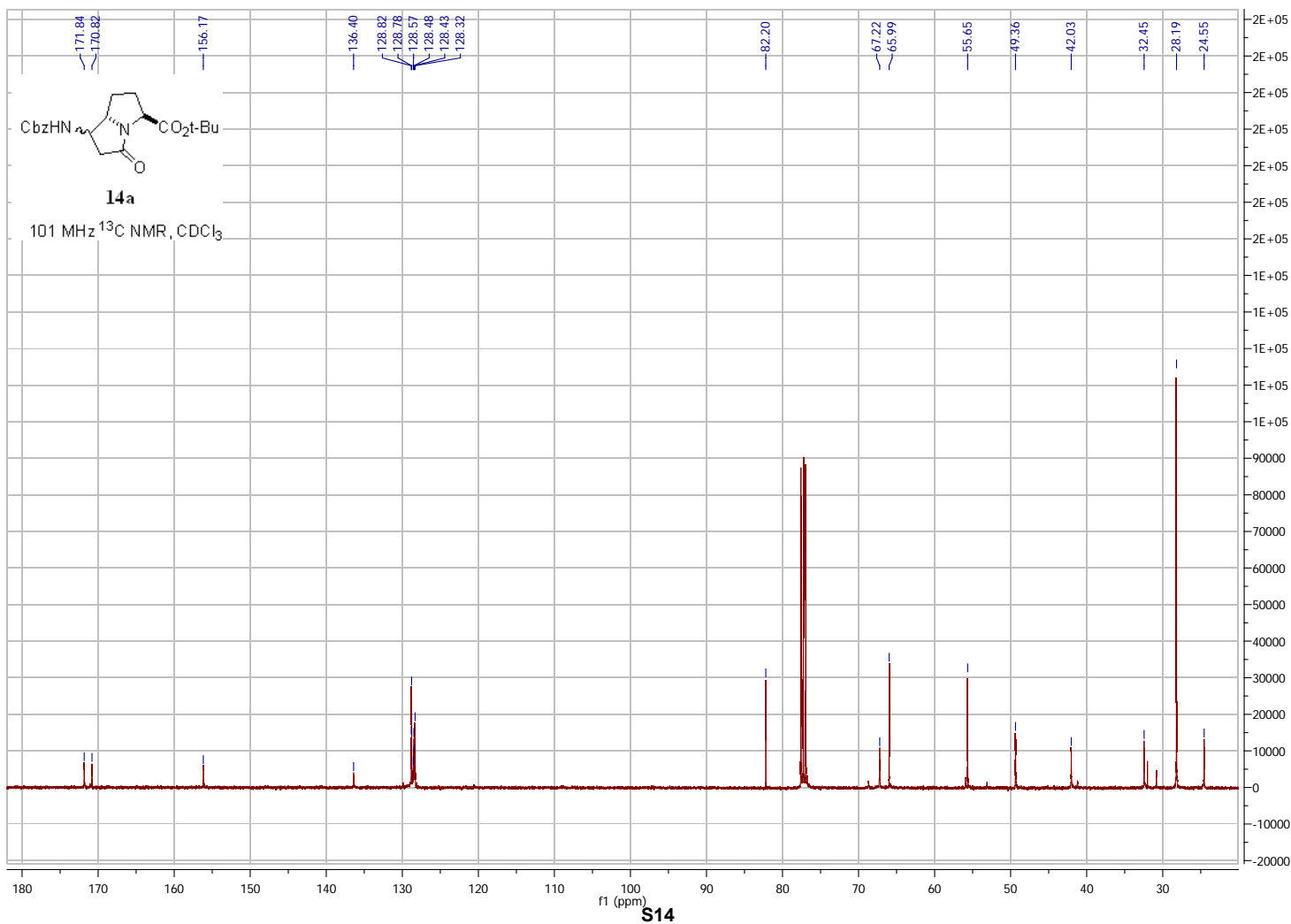
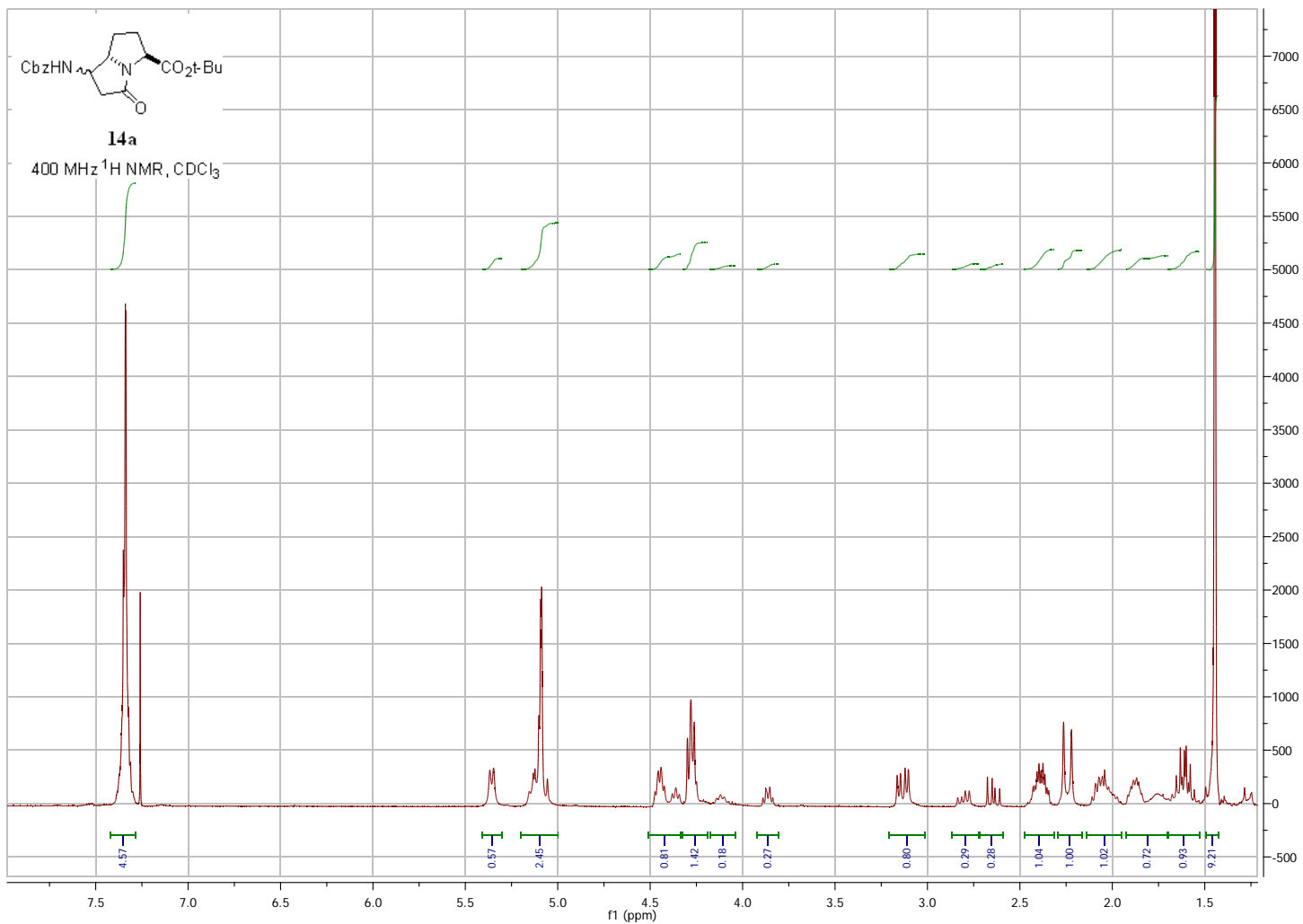
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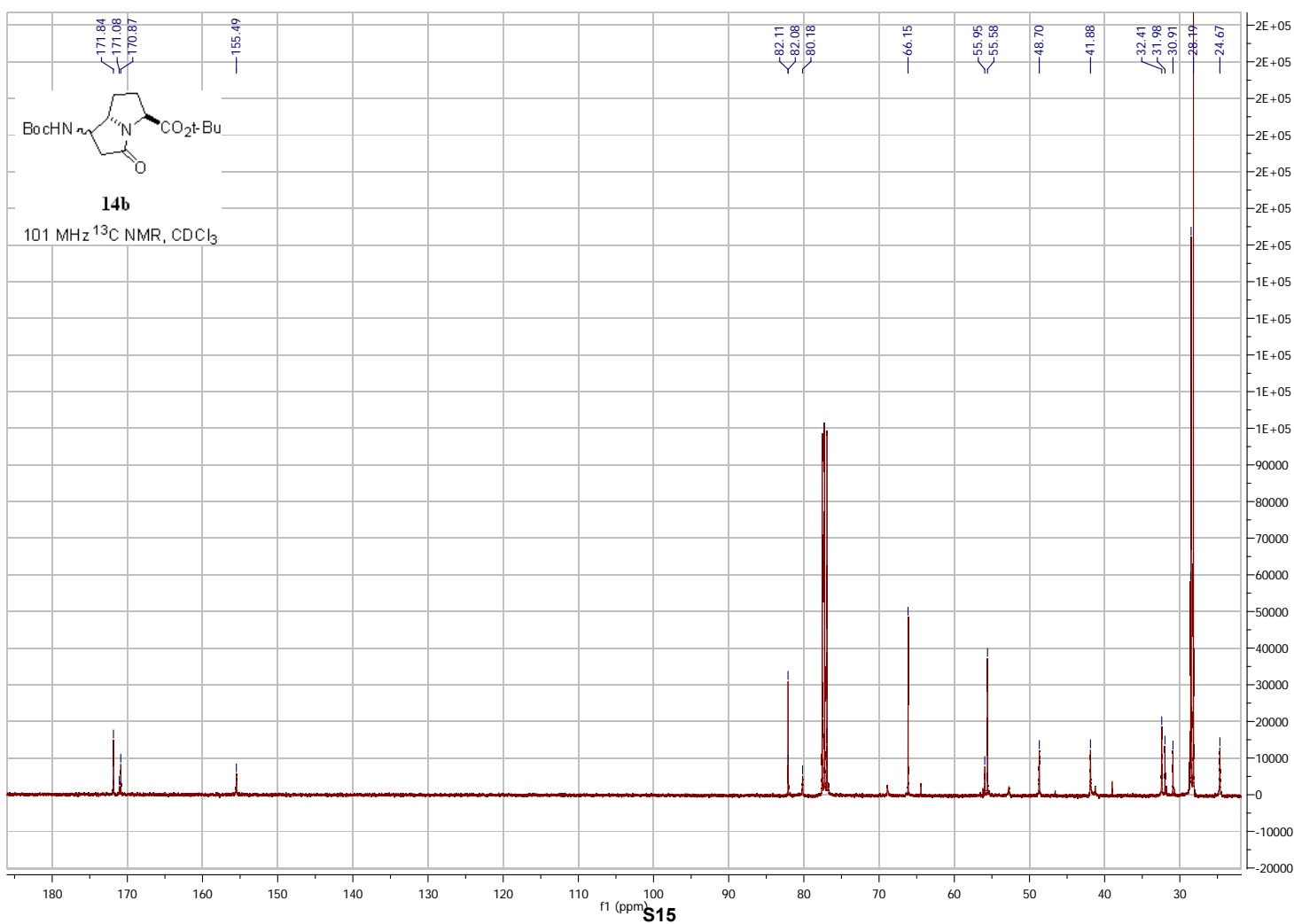
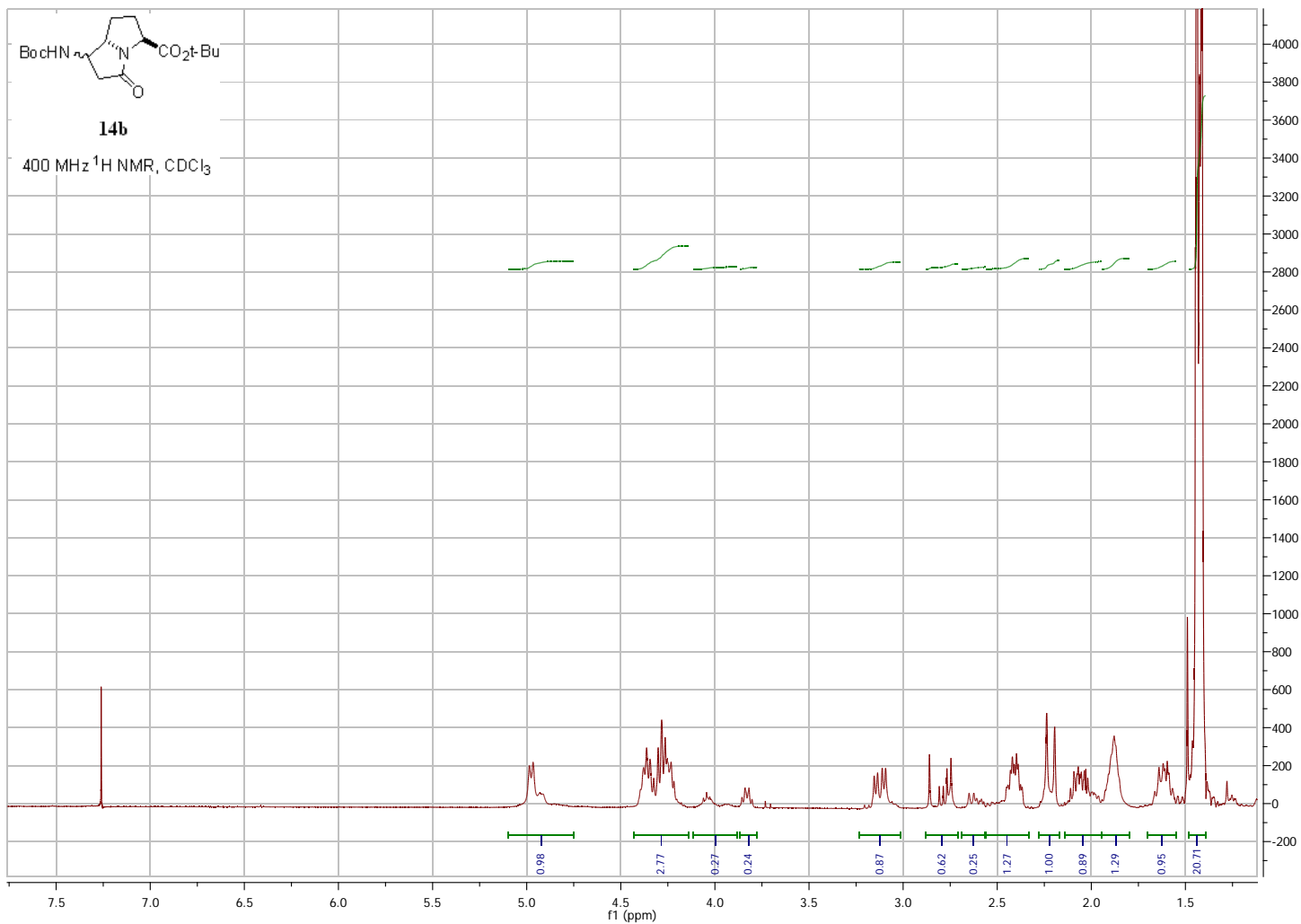


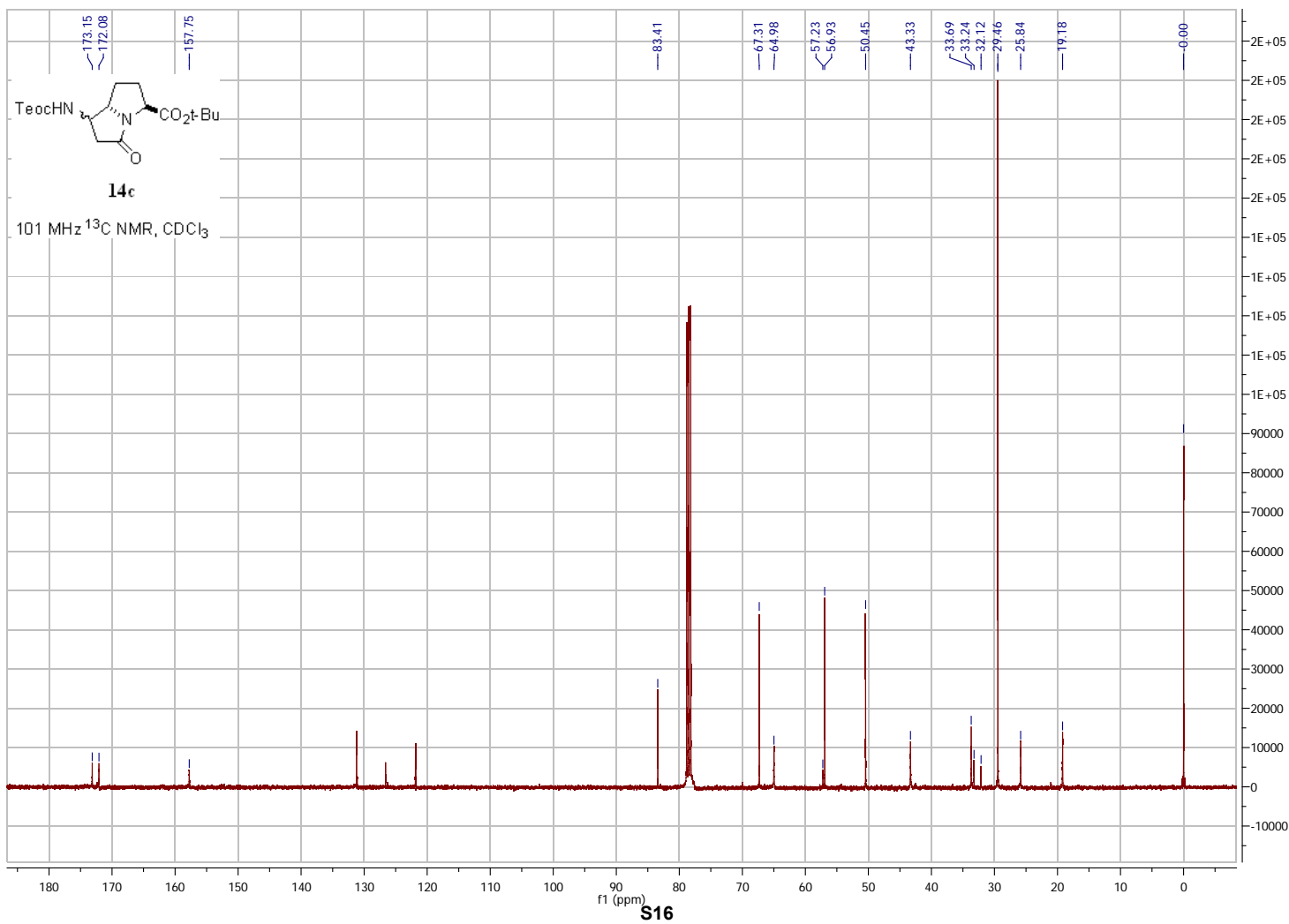
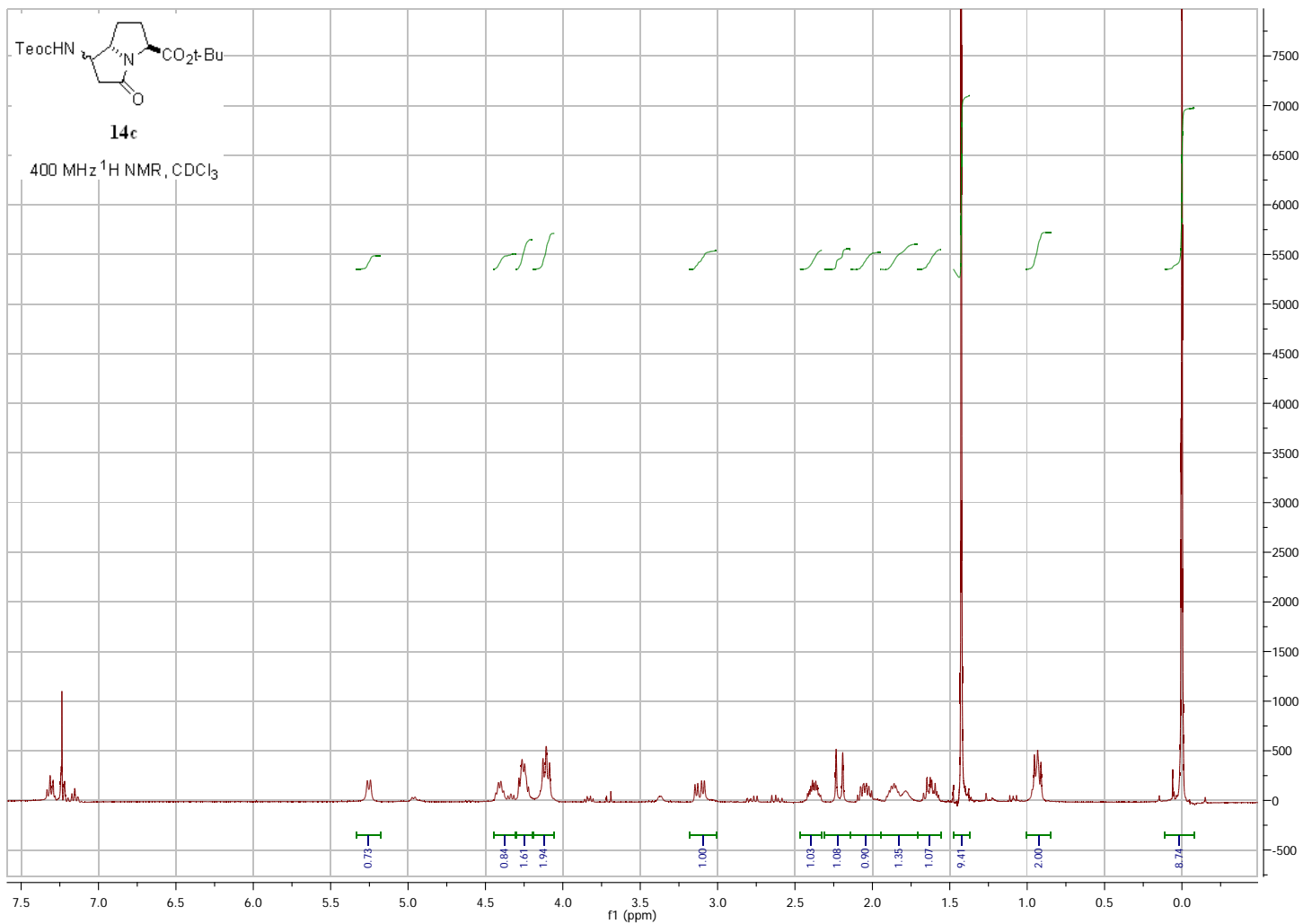


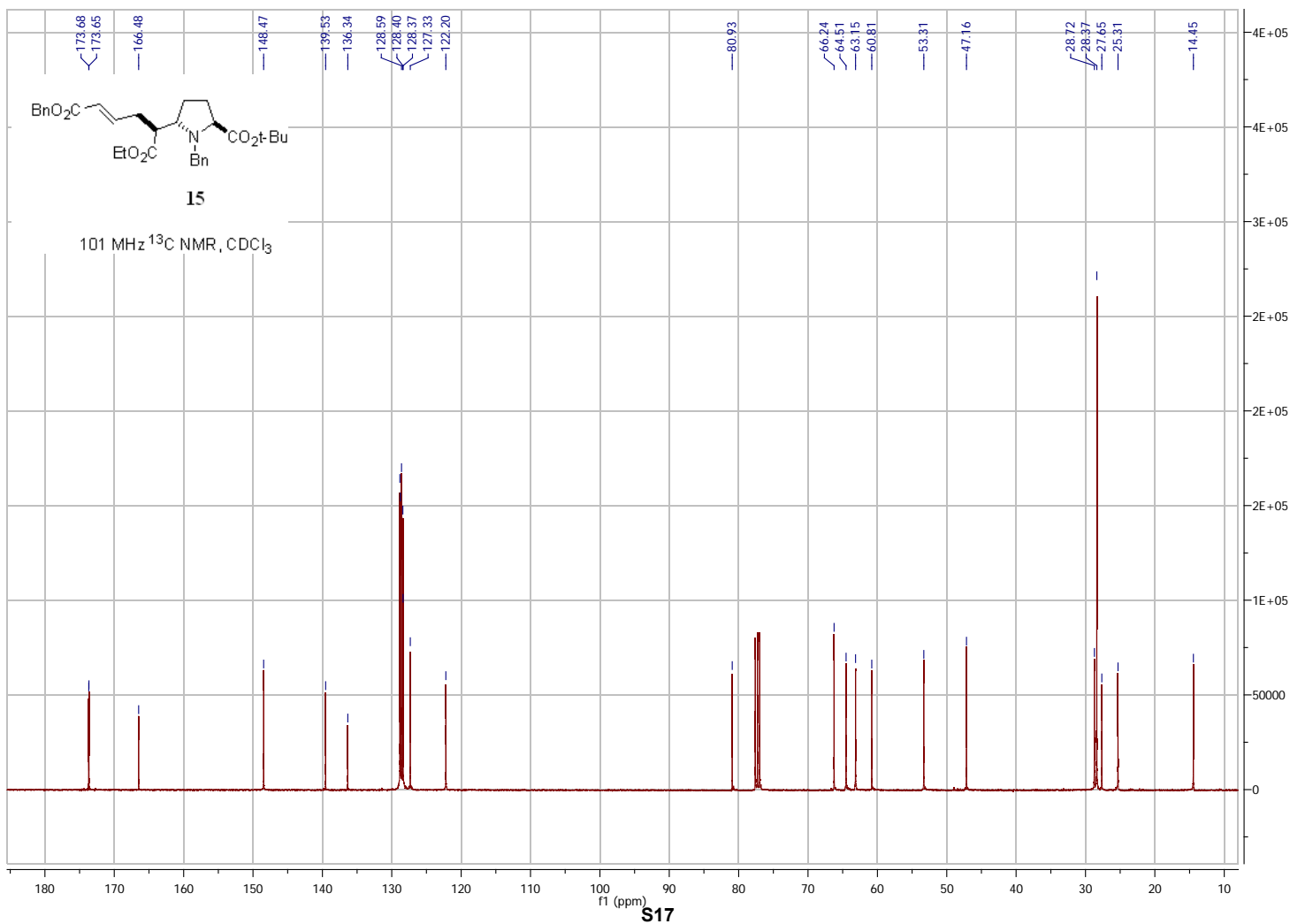
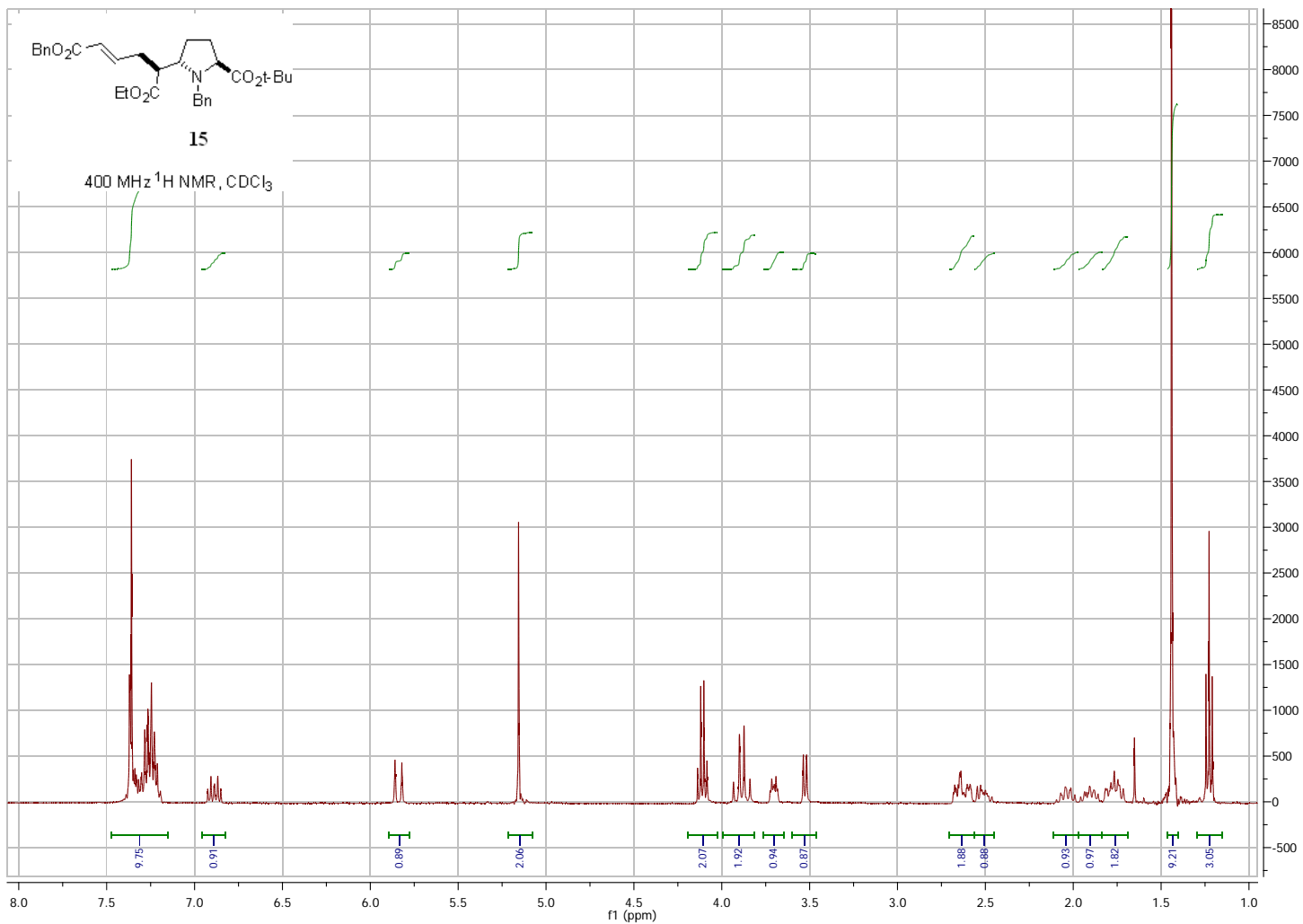


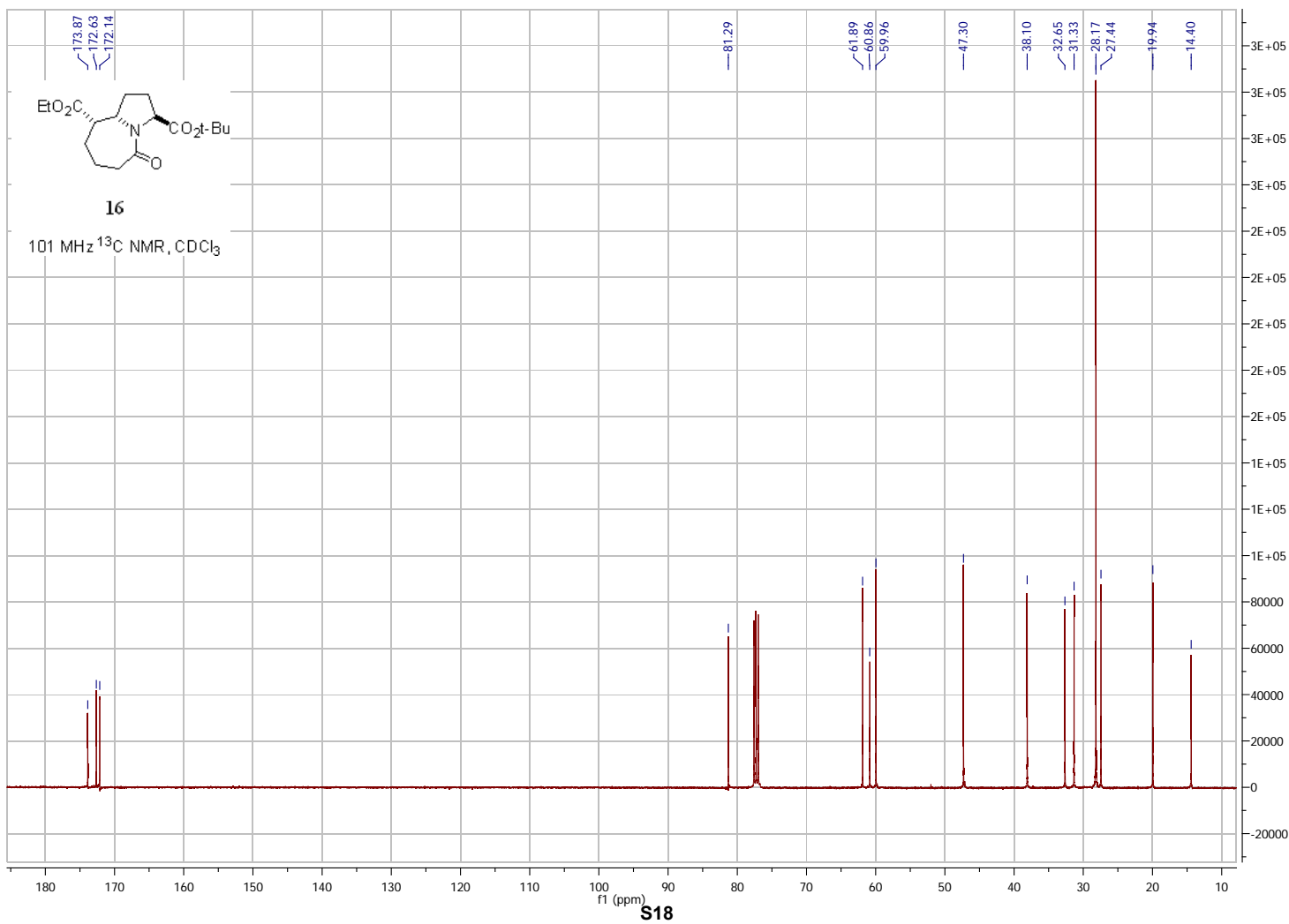
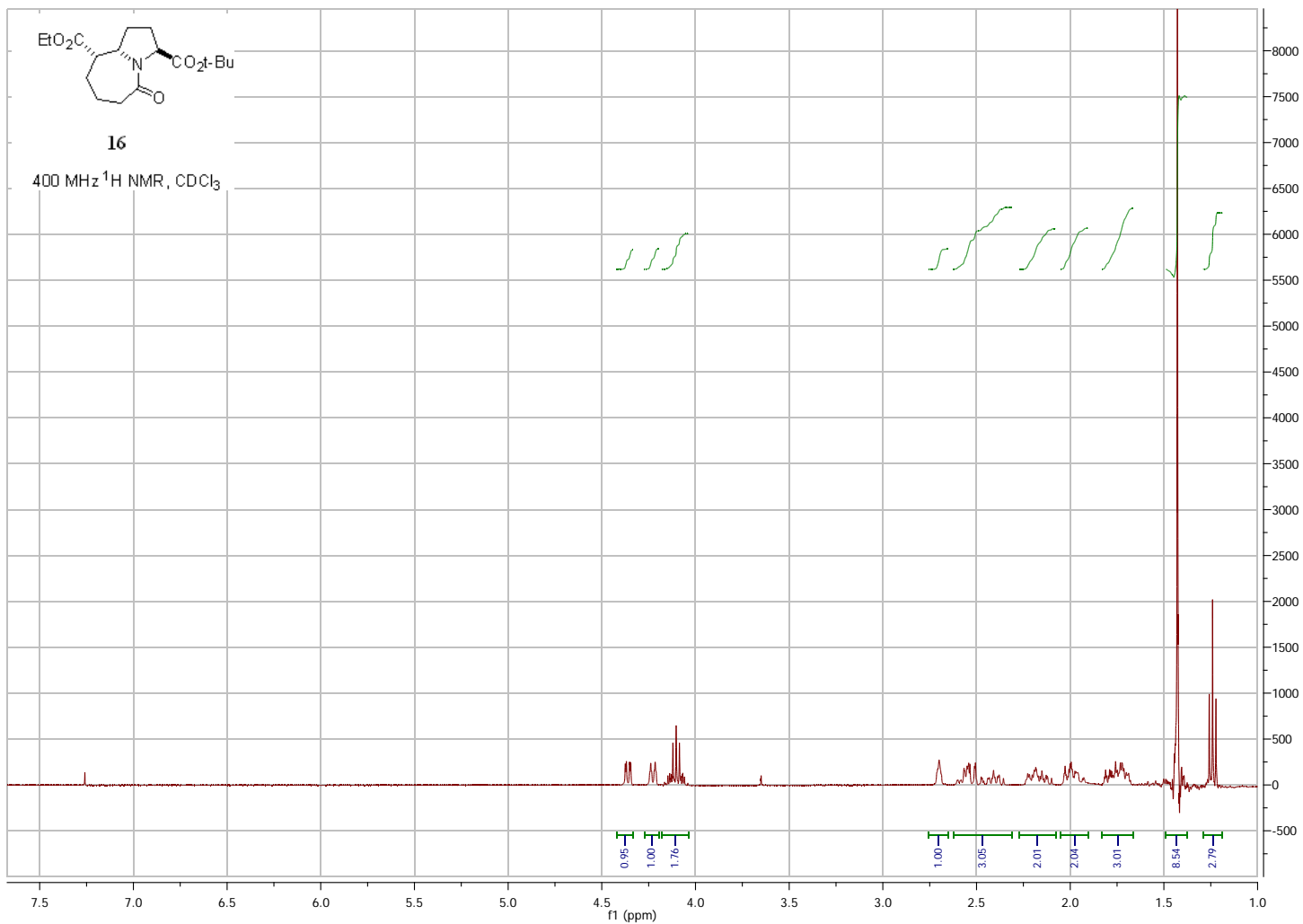


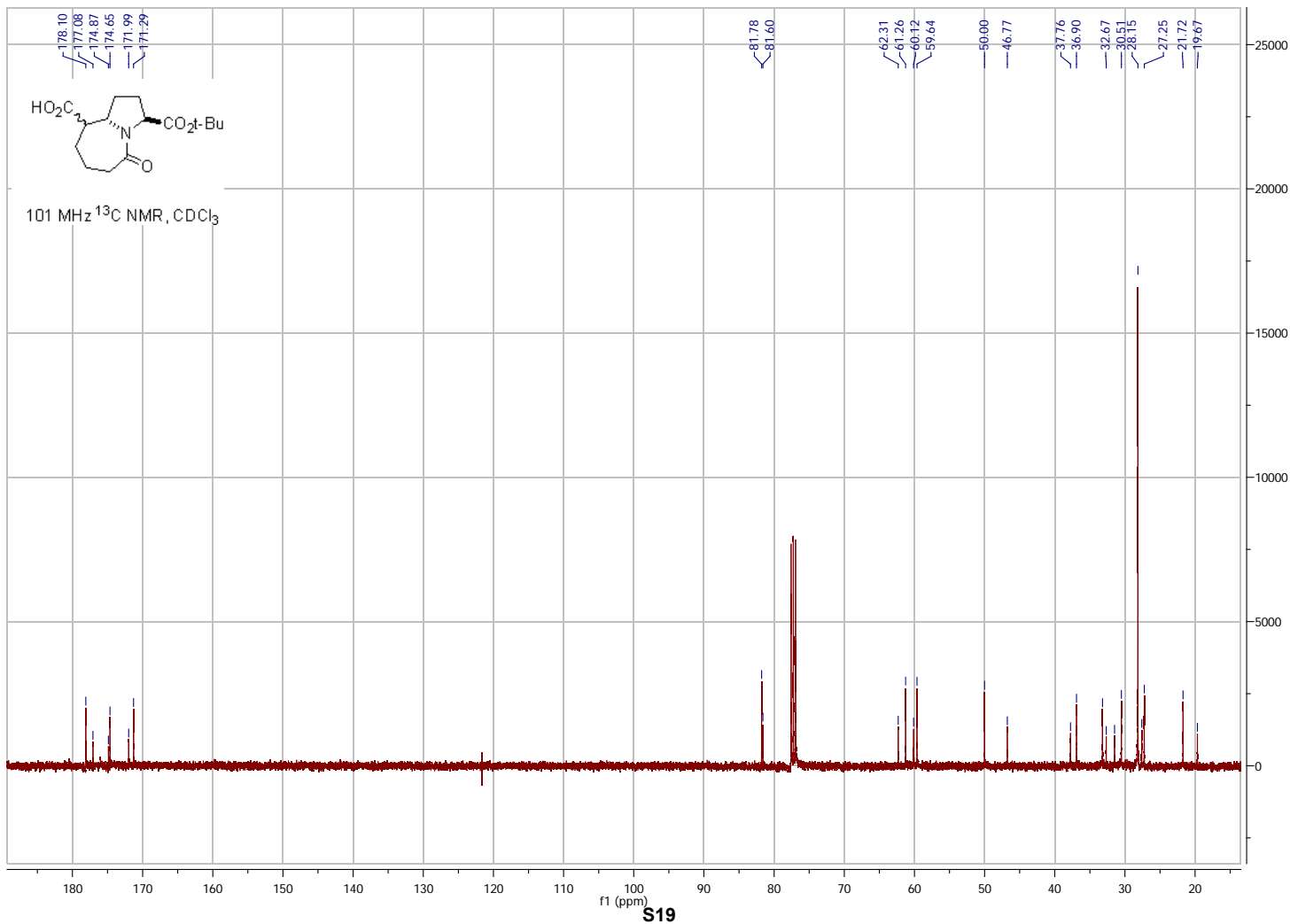
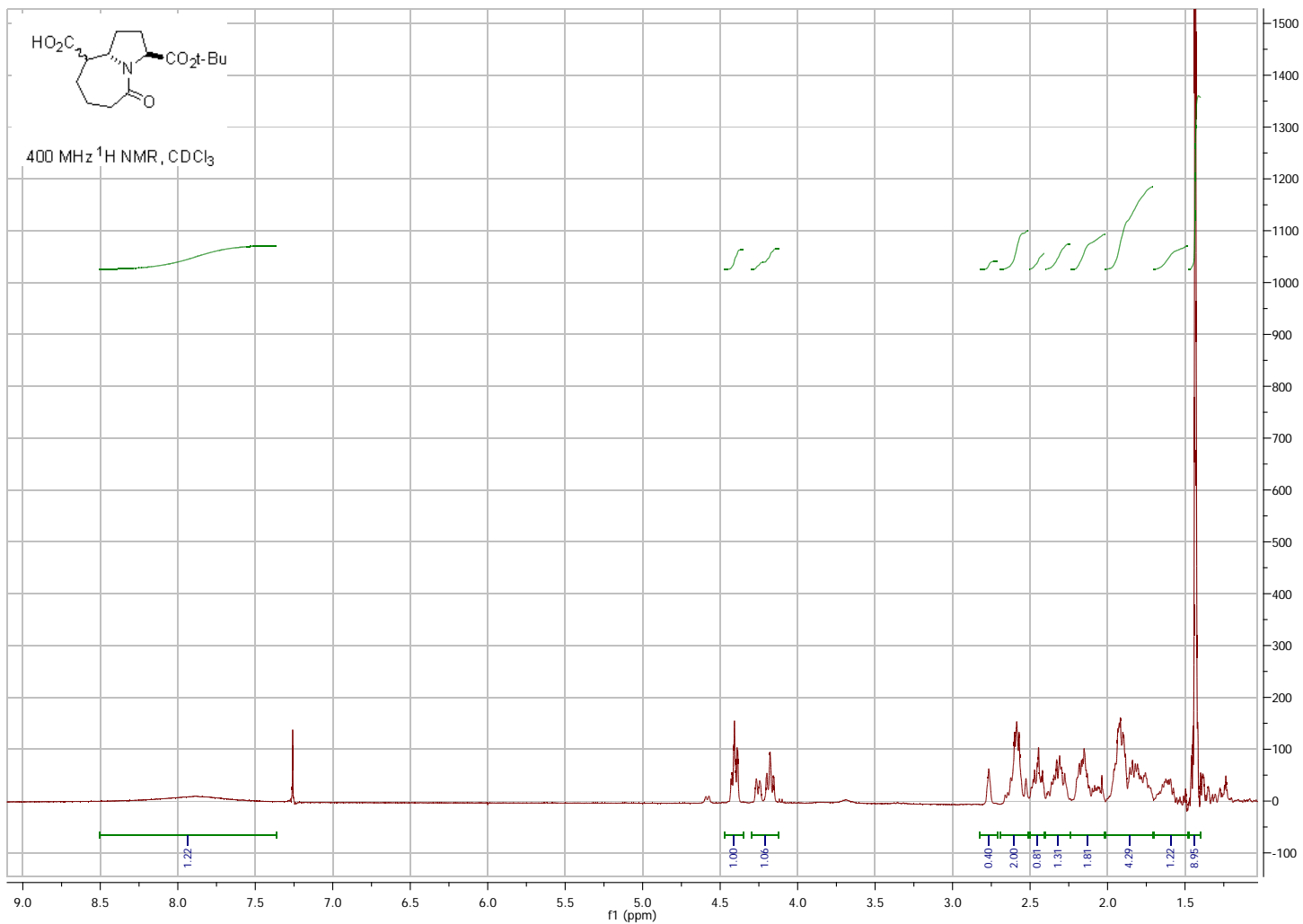


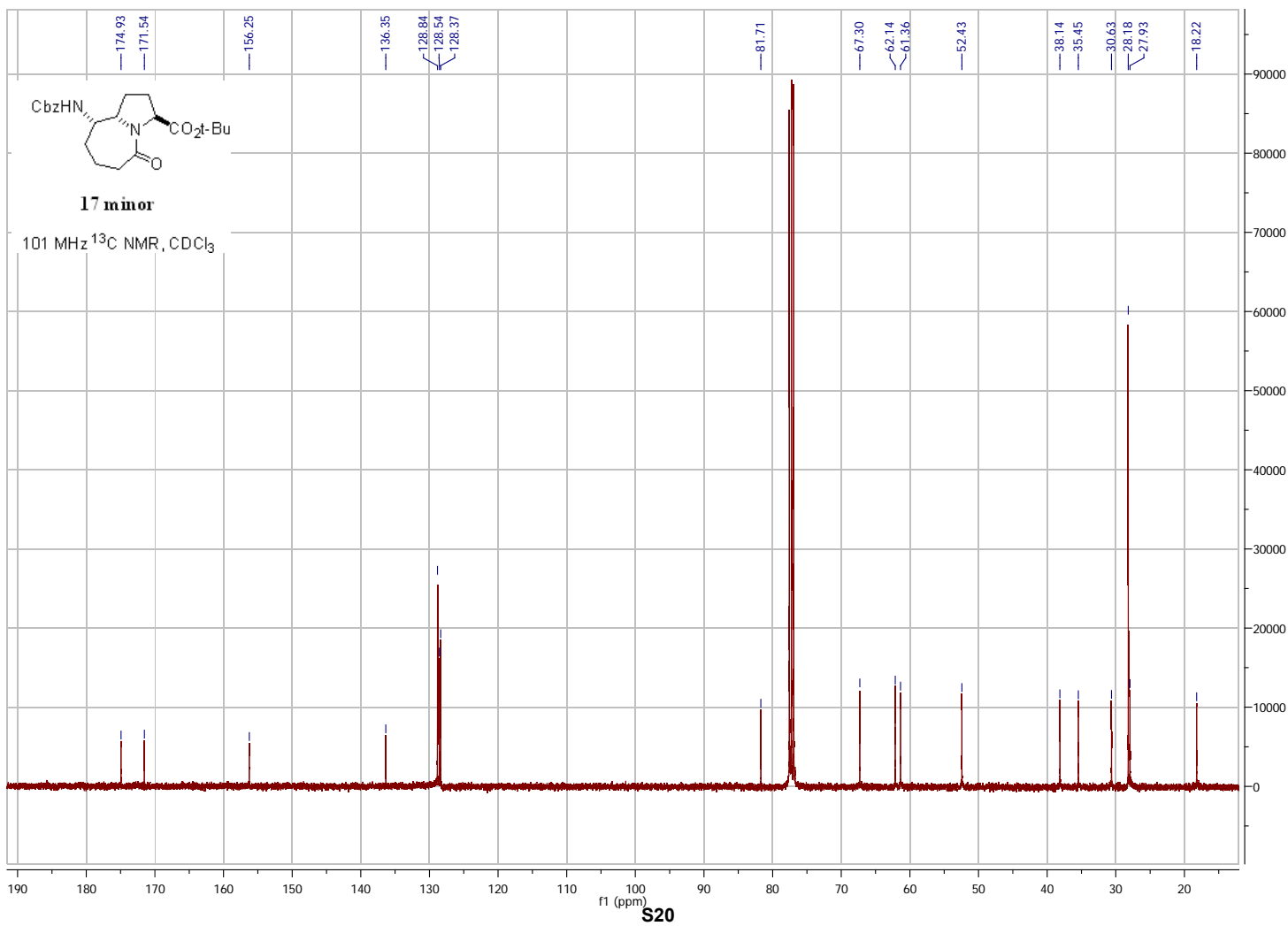
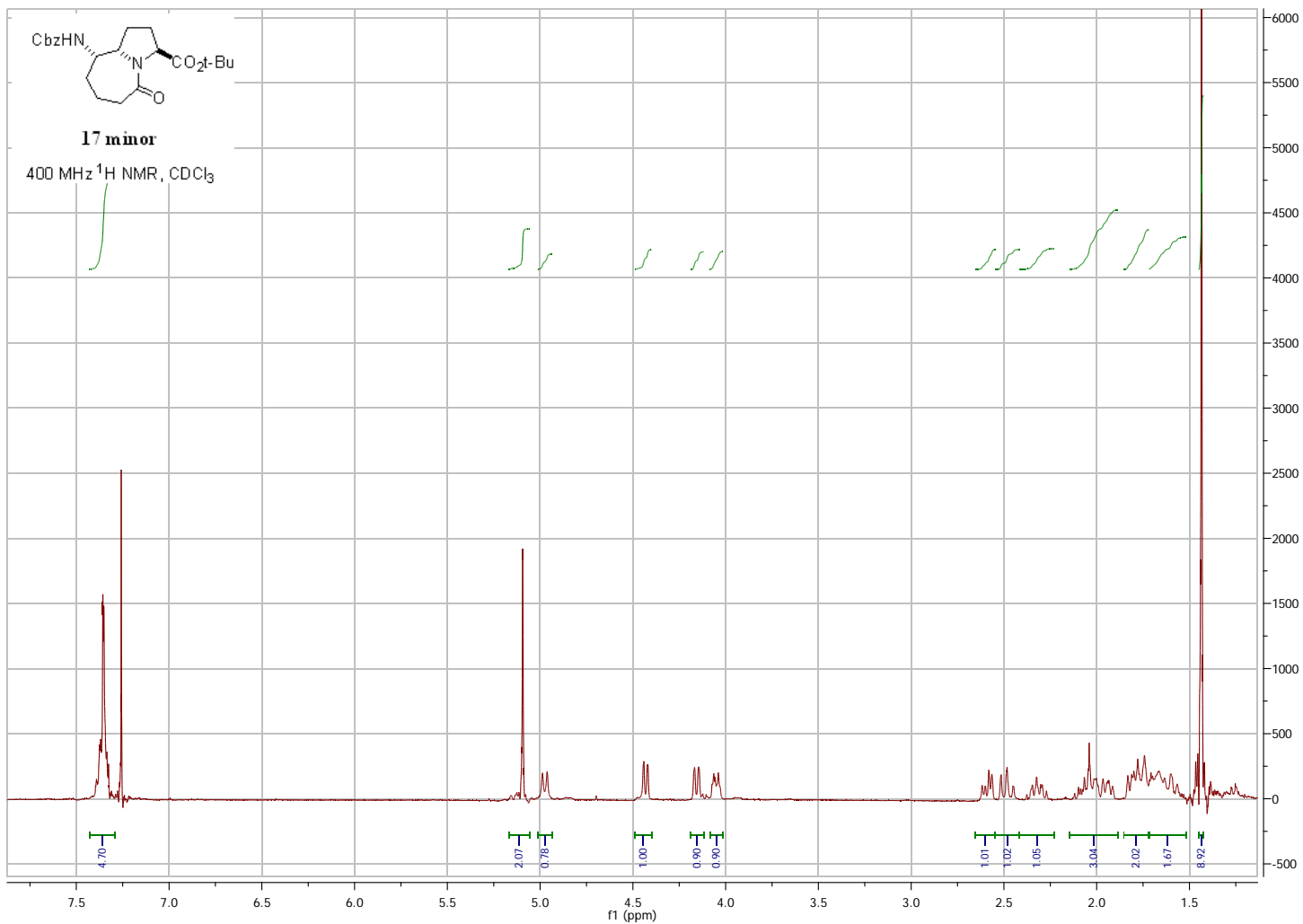


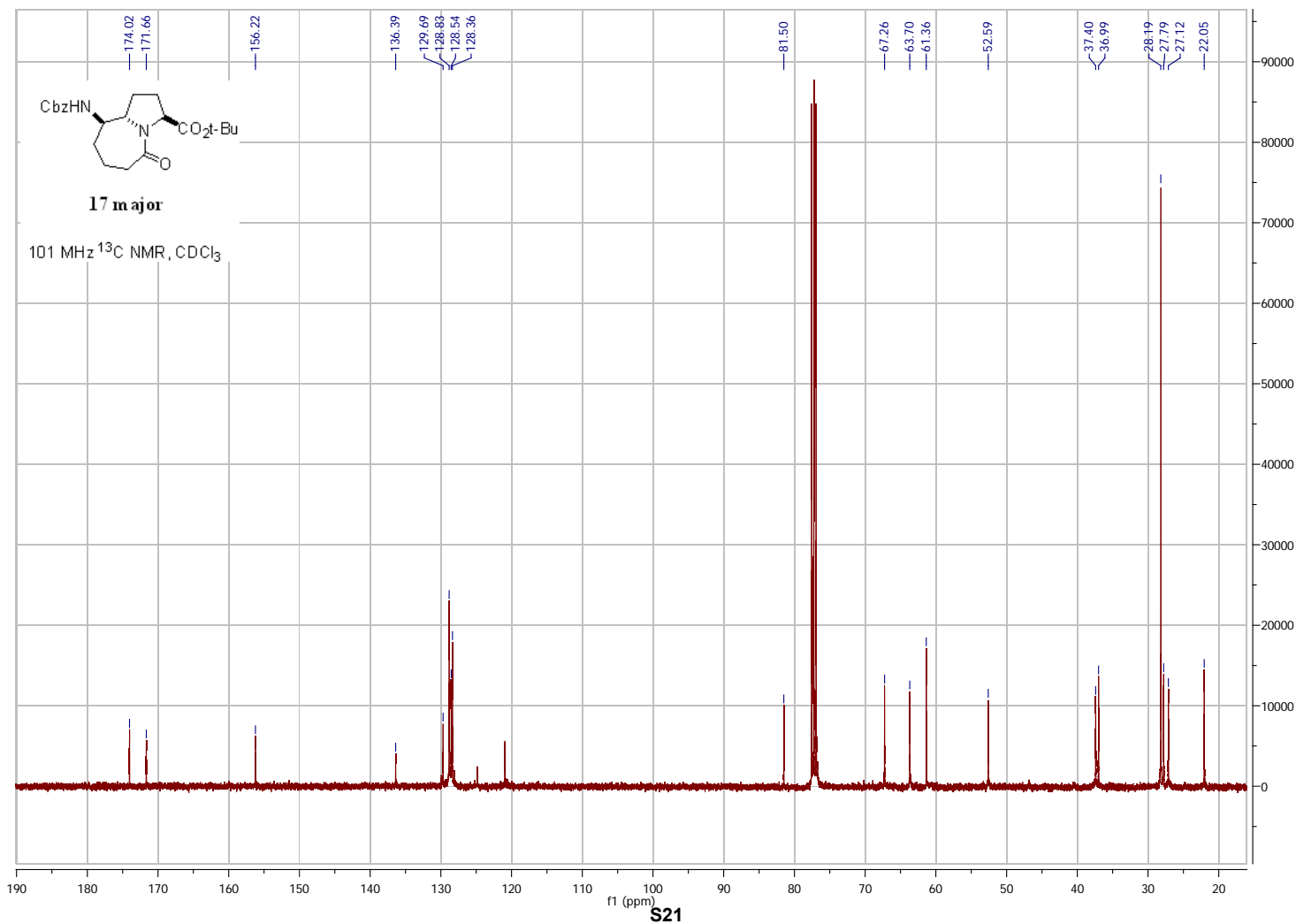
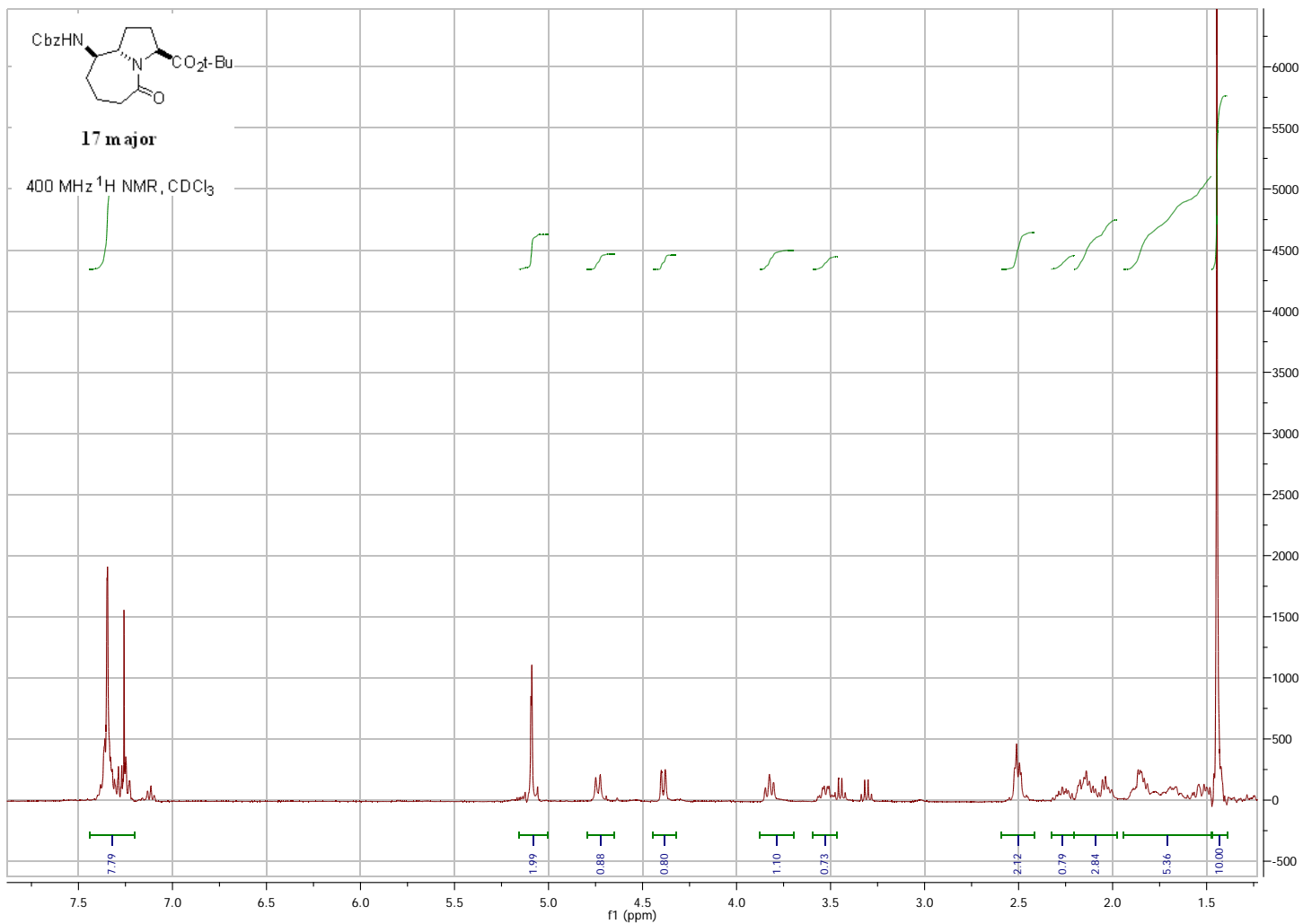


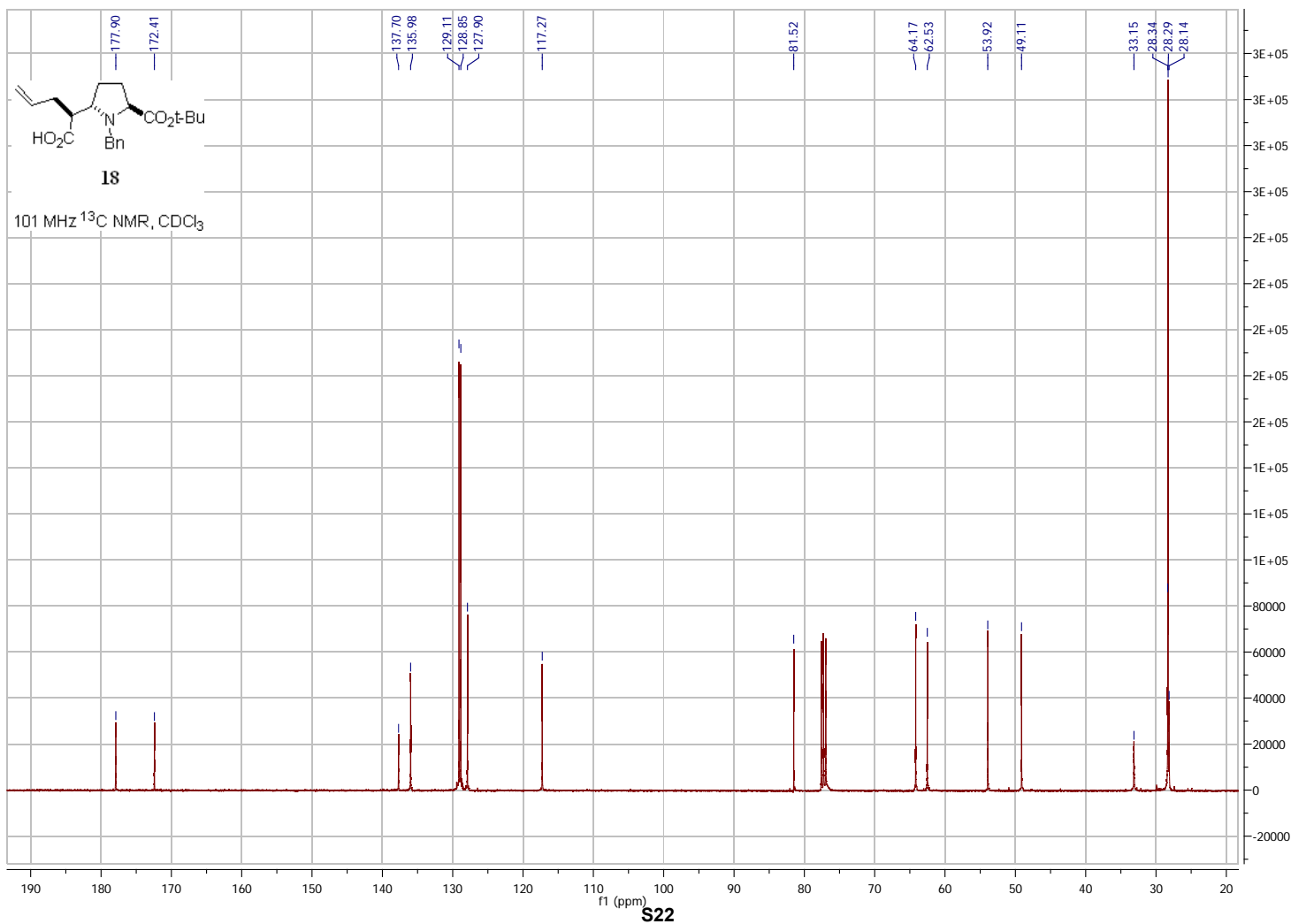
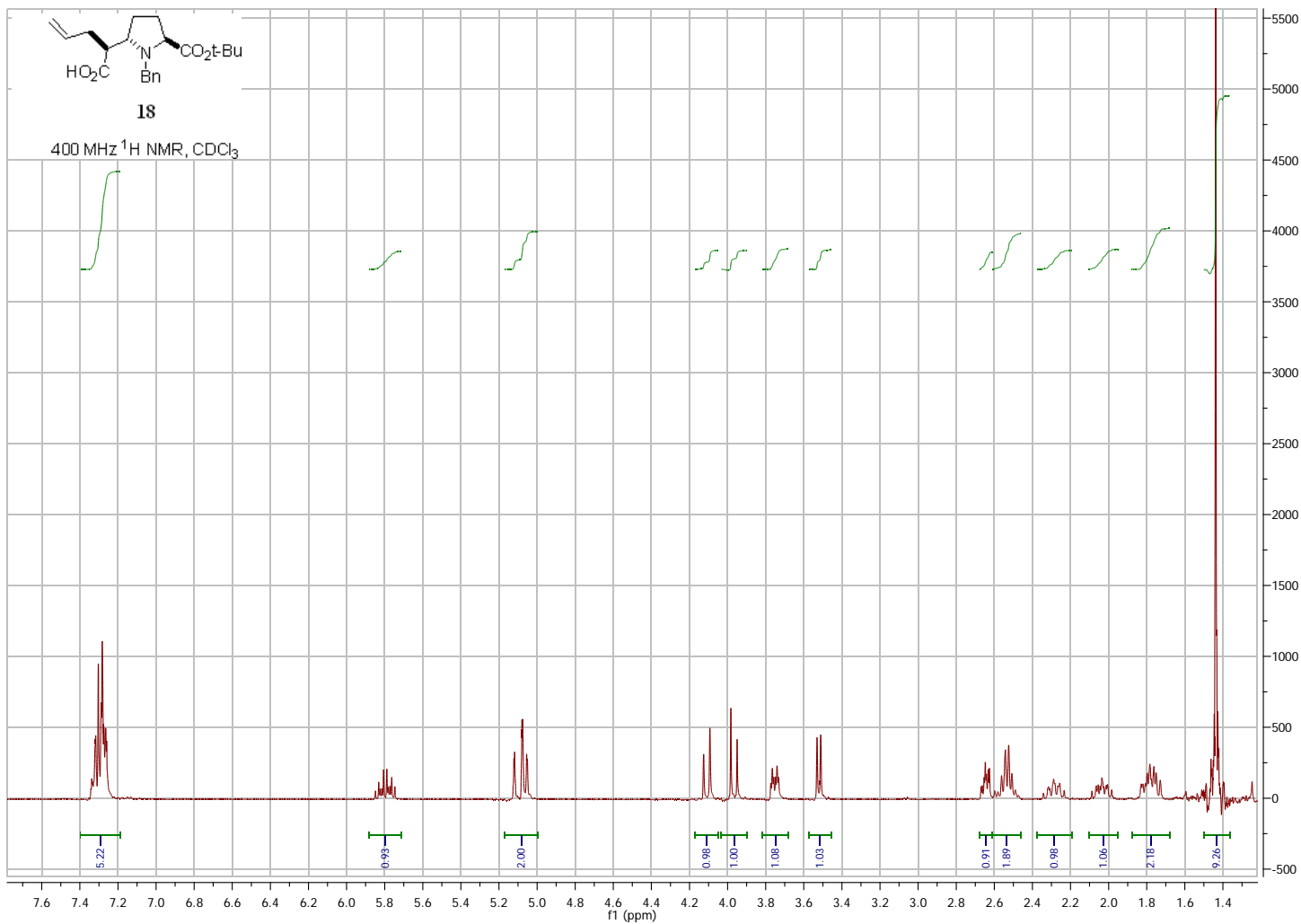


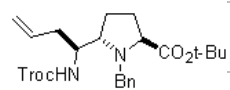






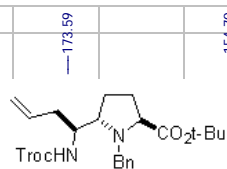
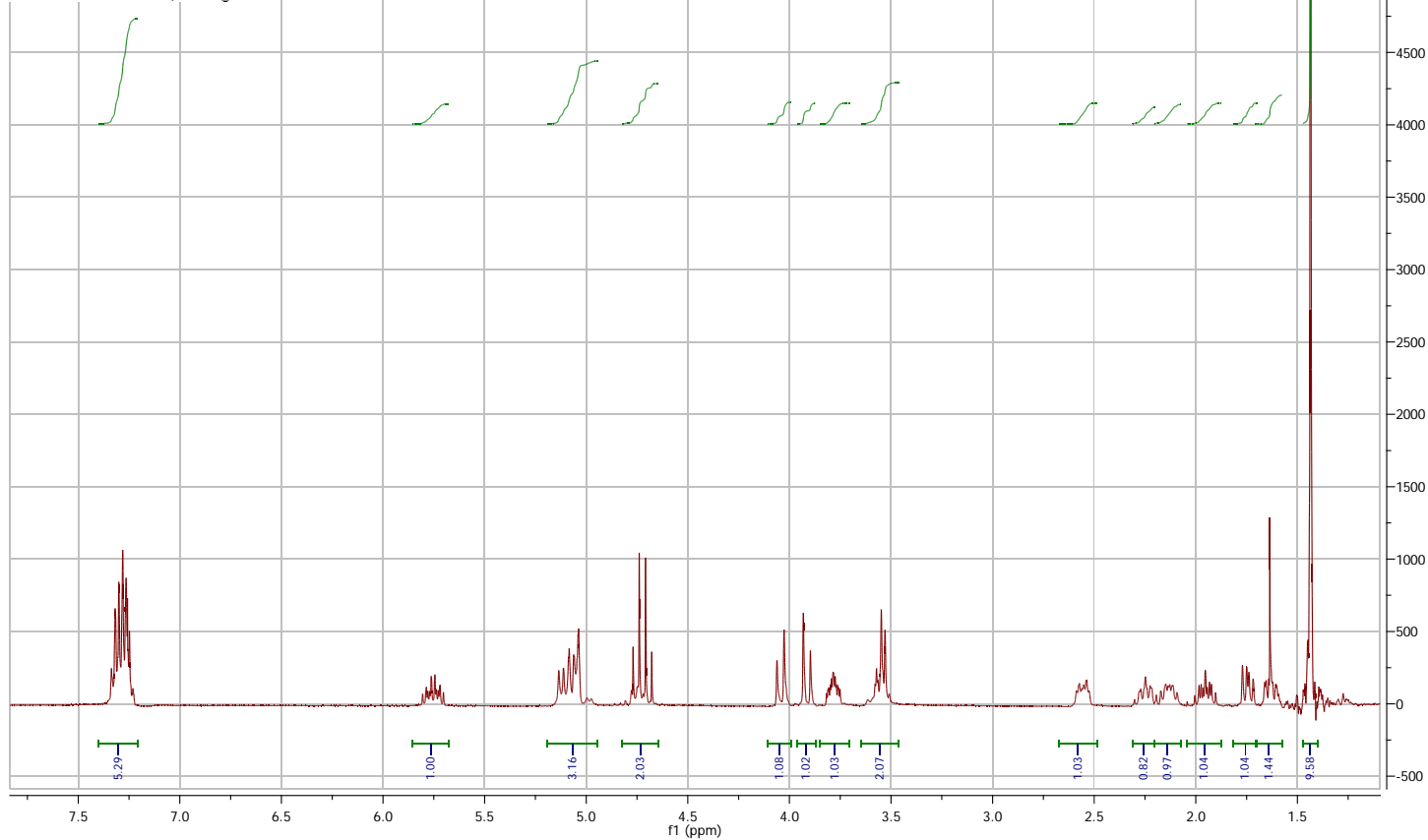






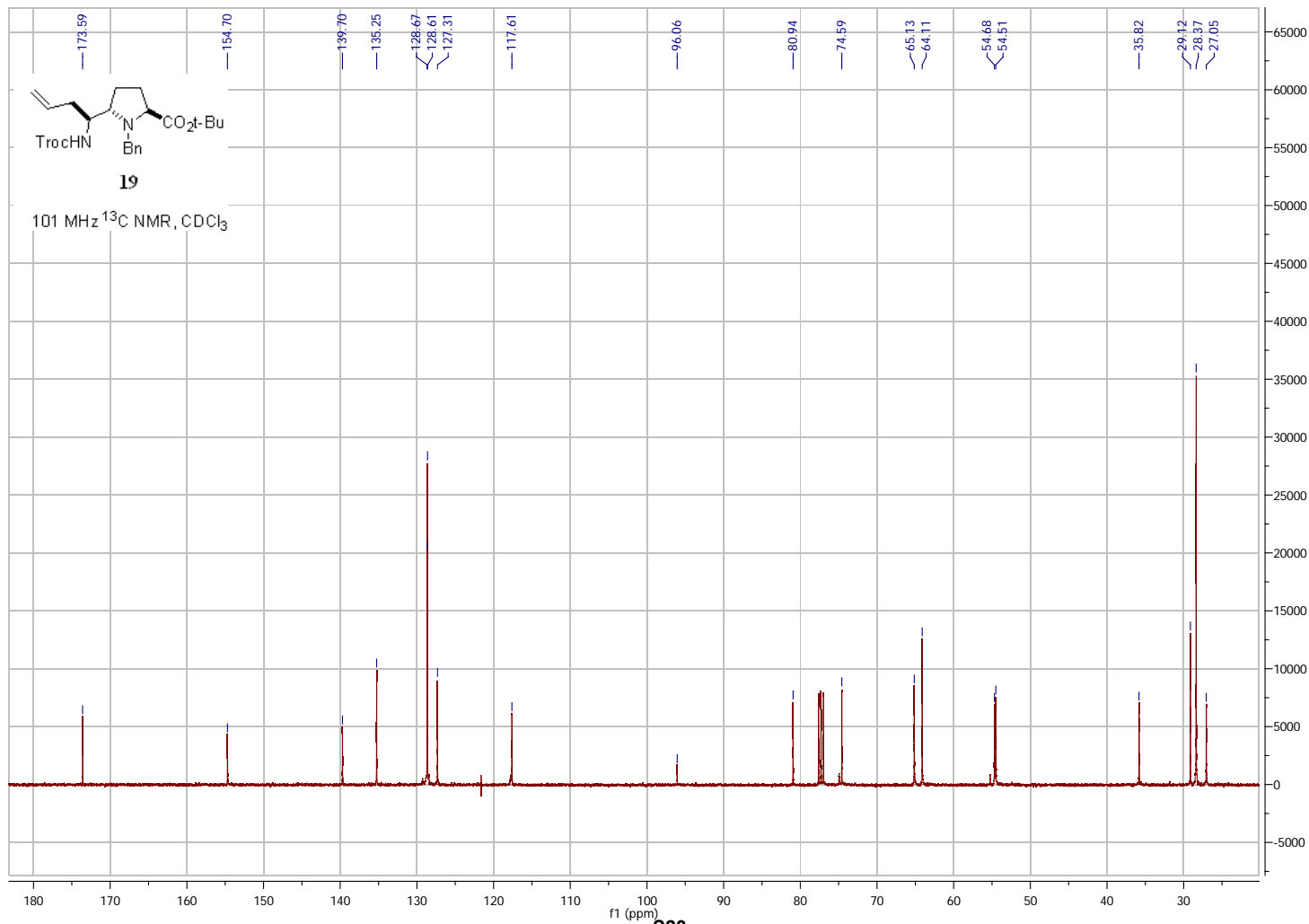
19

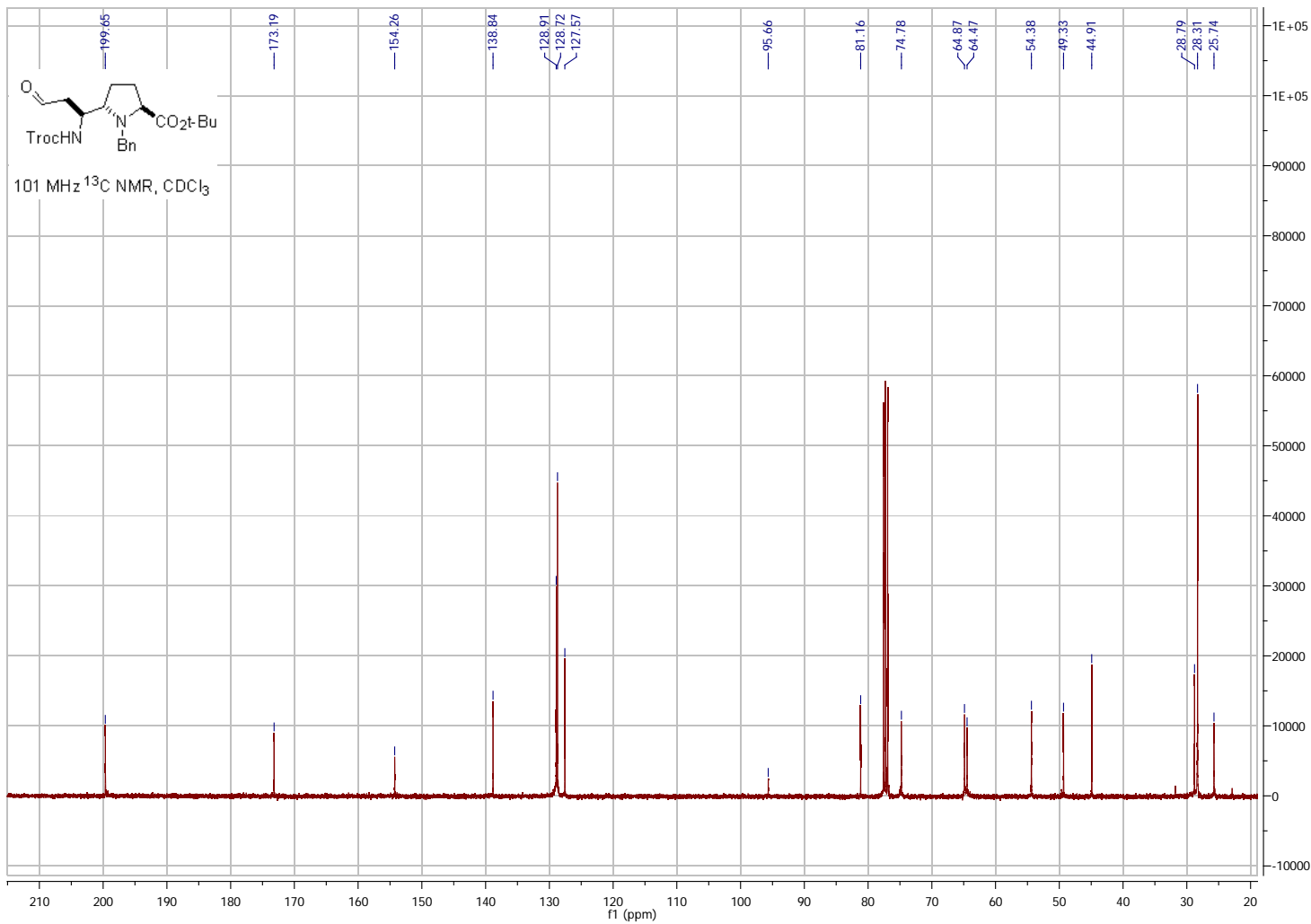
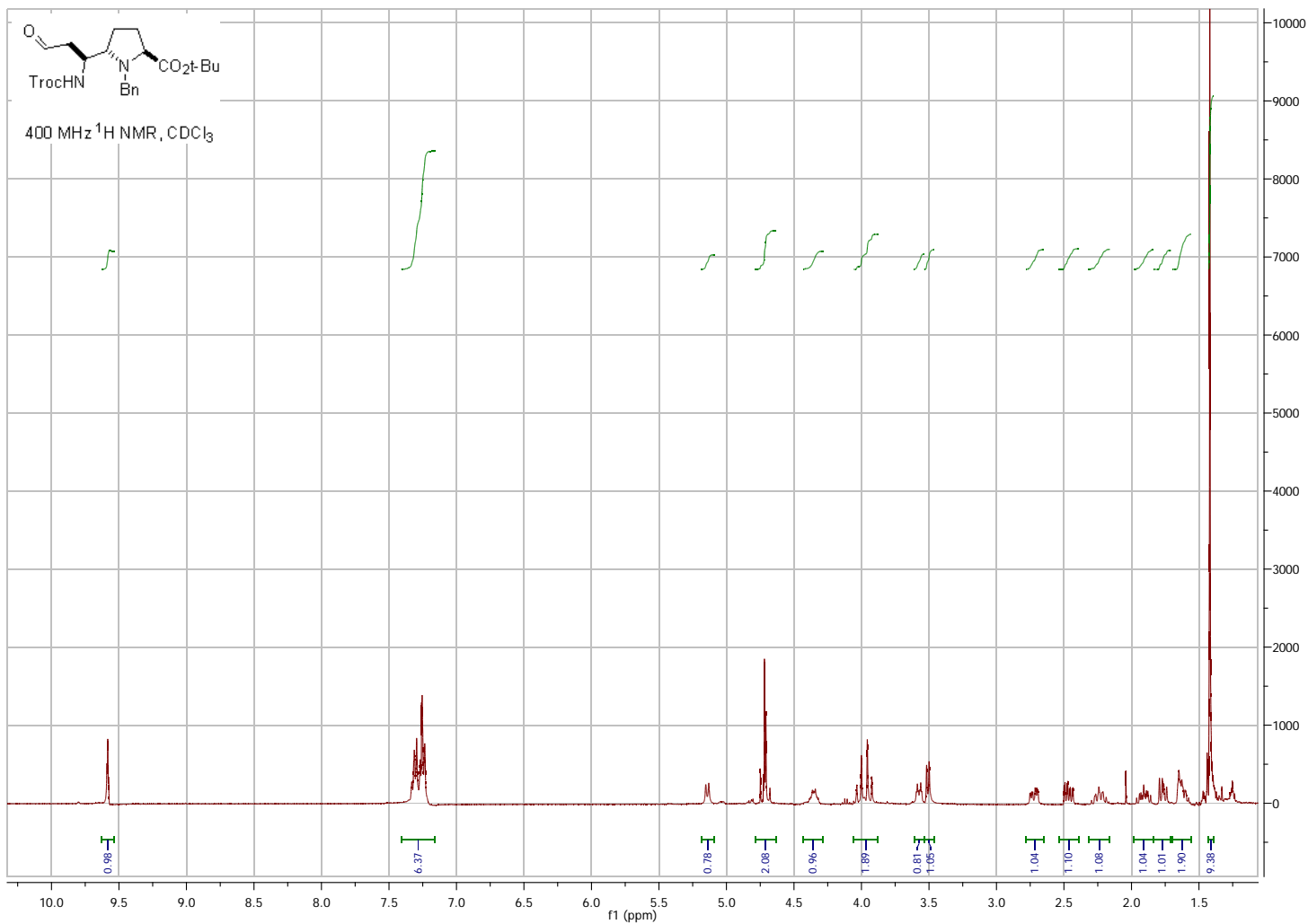
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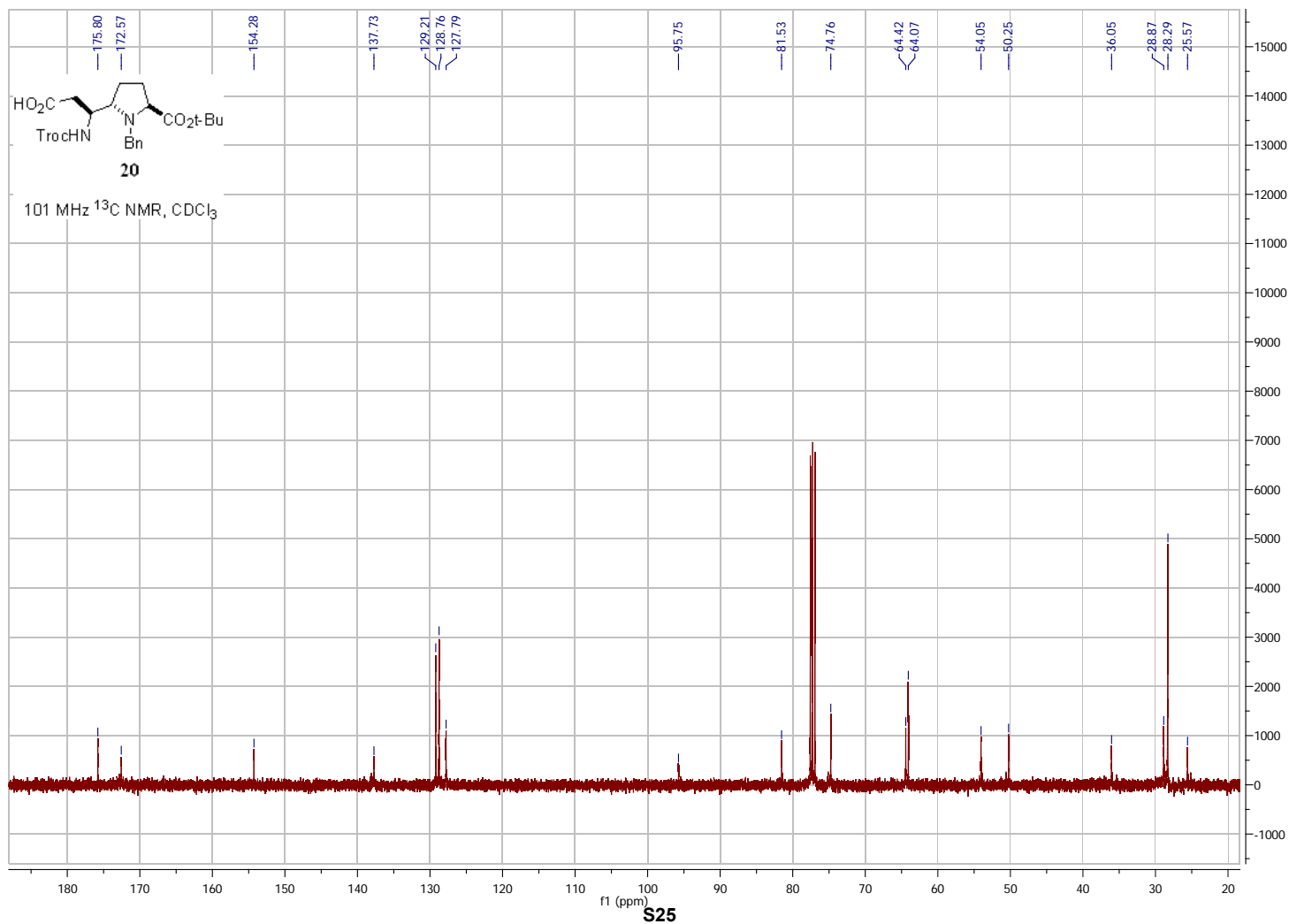
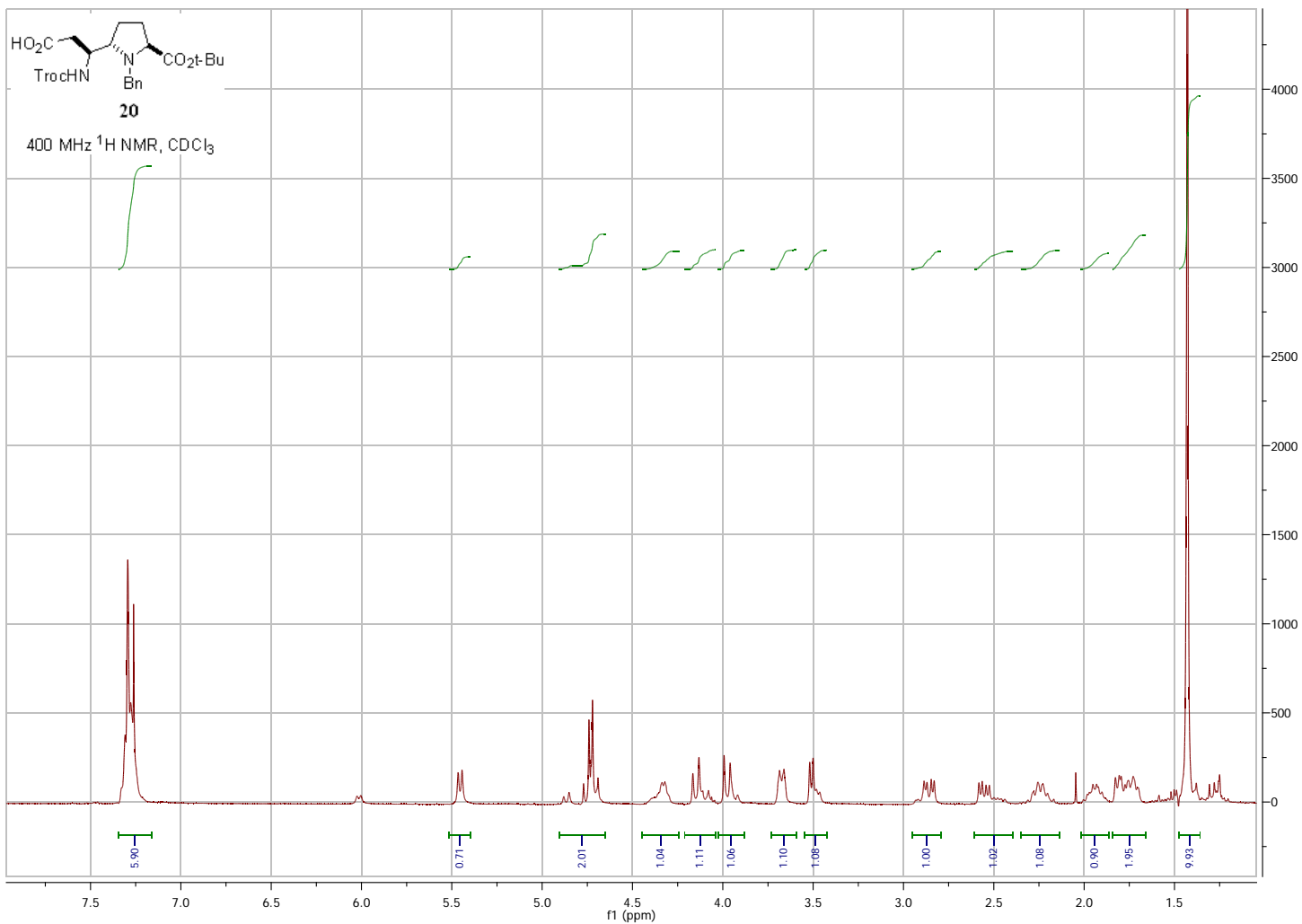


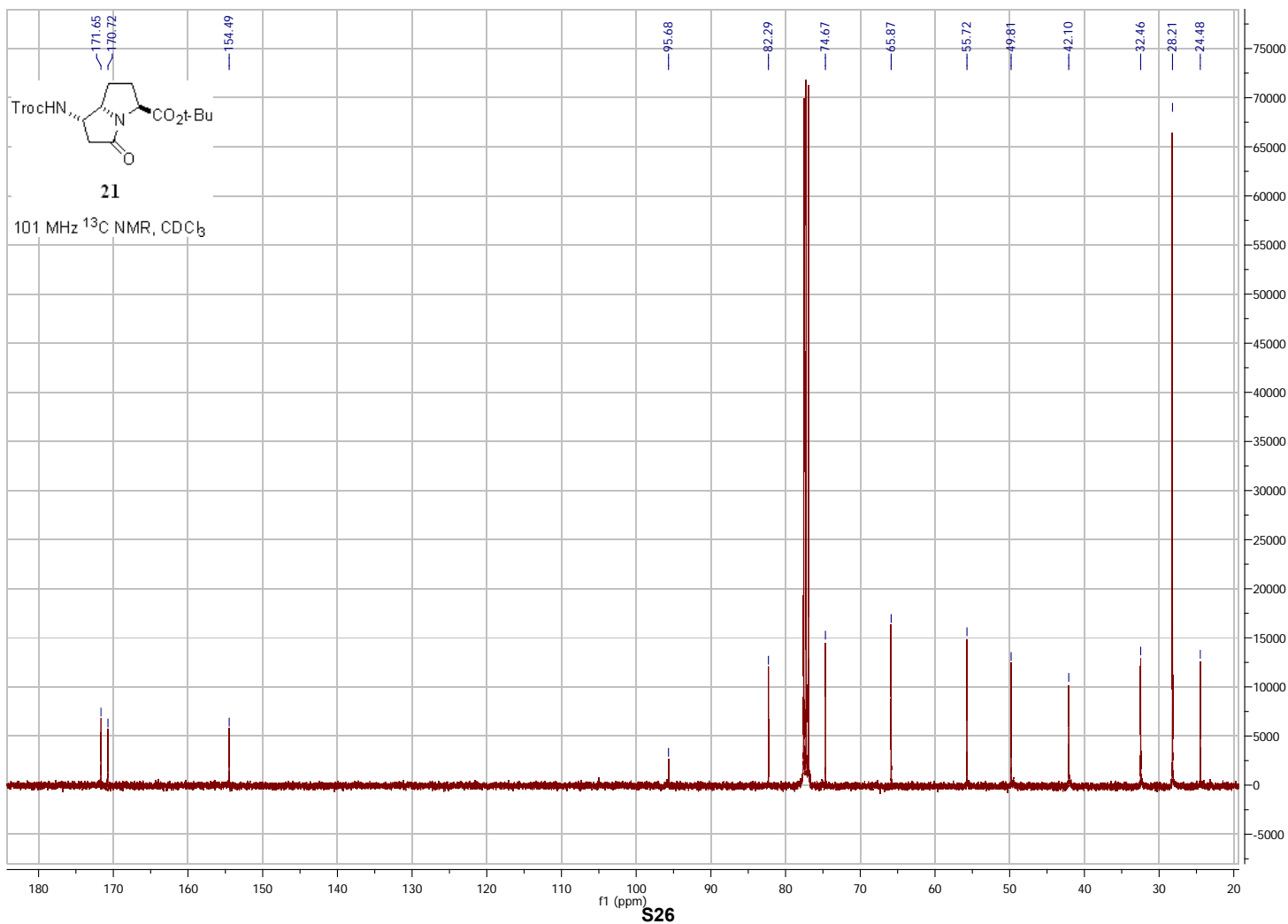
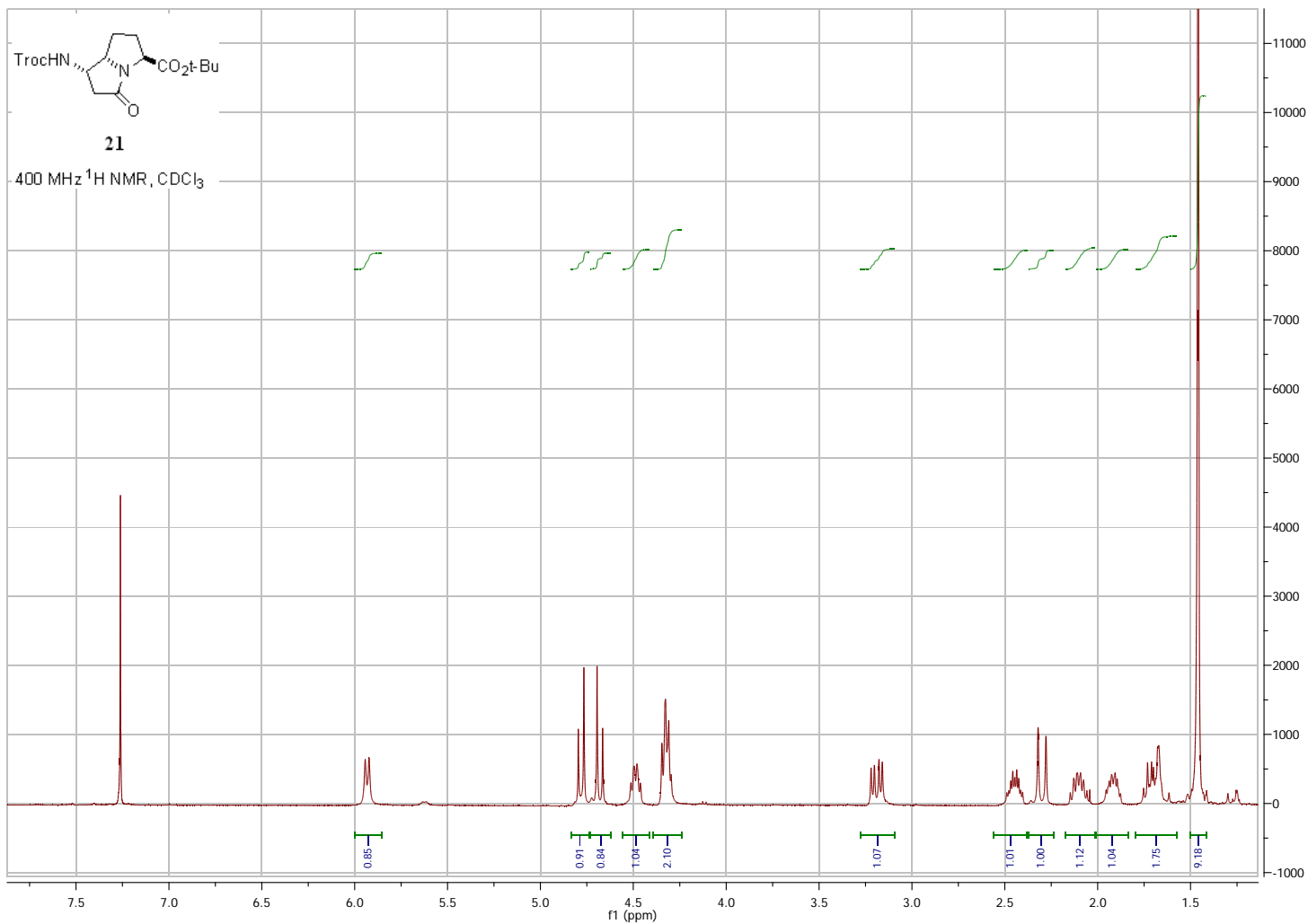
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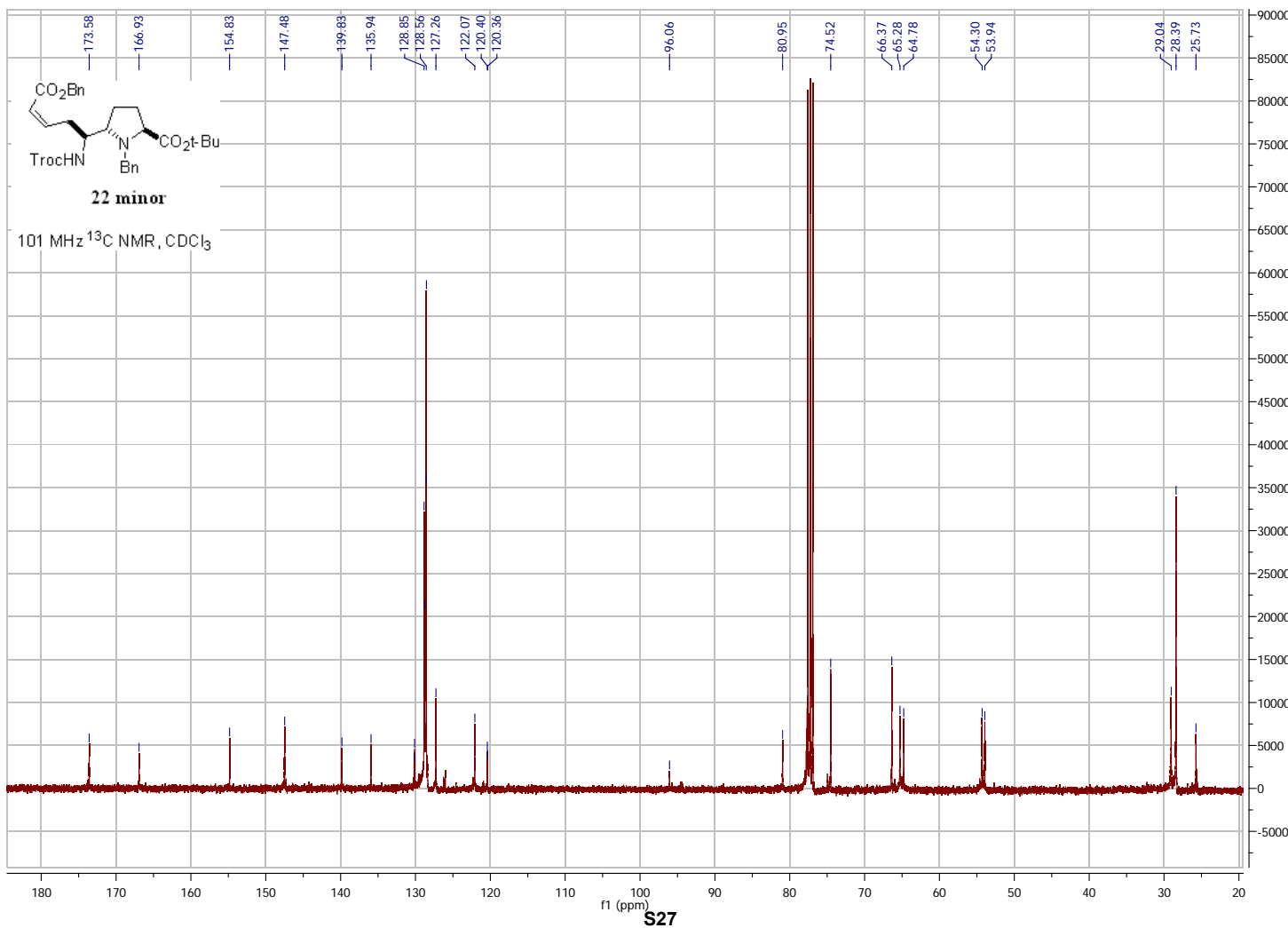
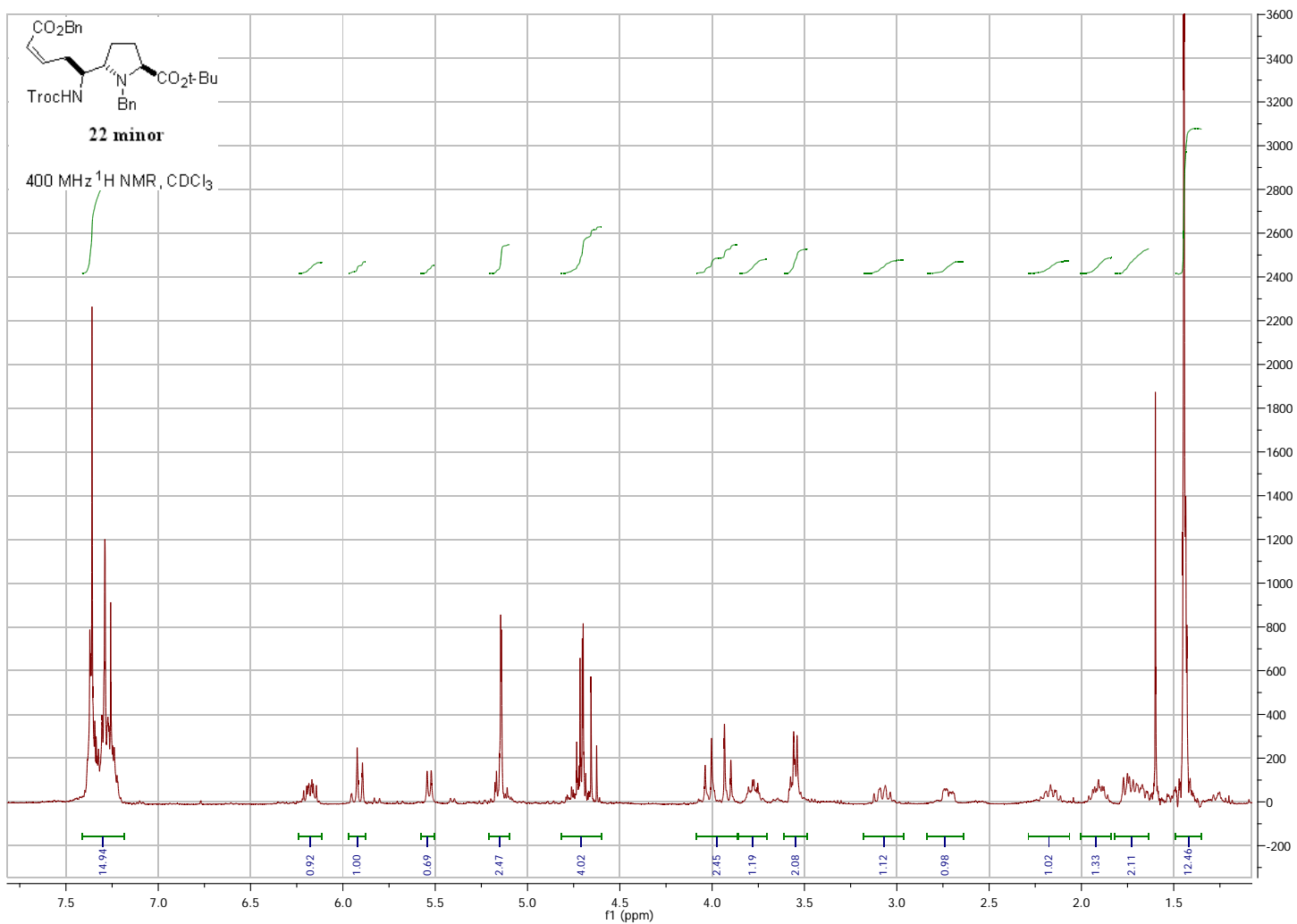
101 MHz ¹³C NMR, CDCl₃

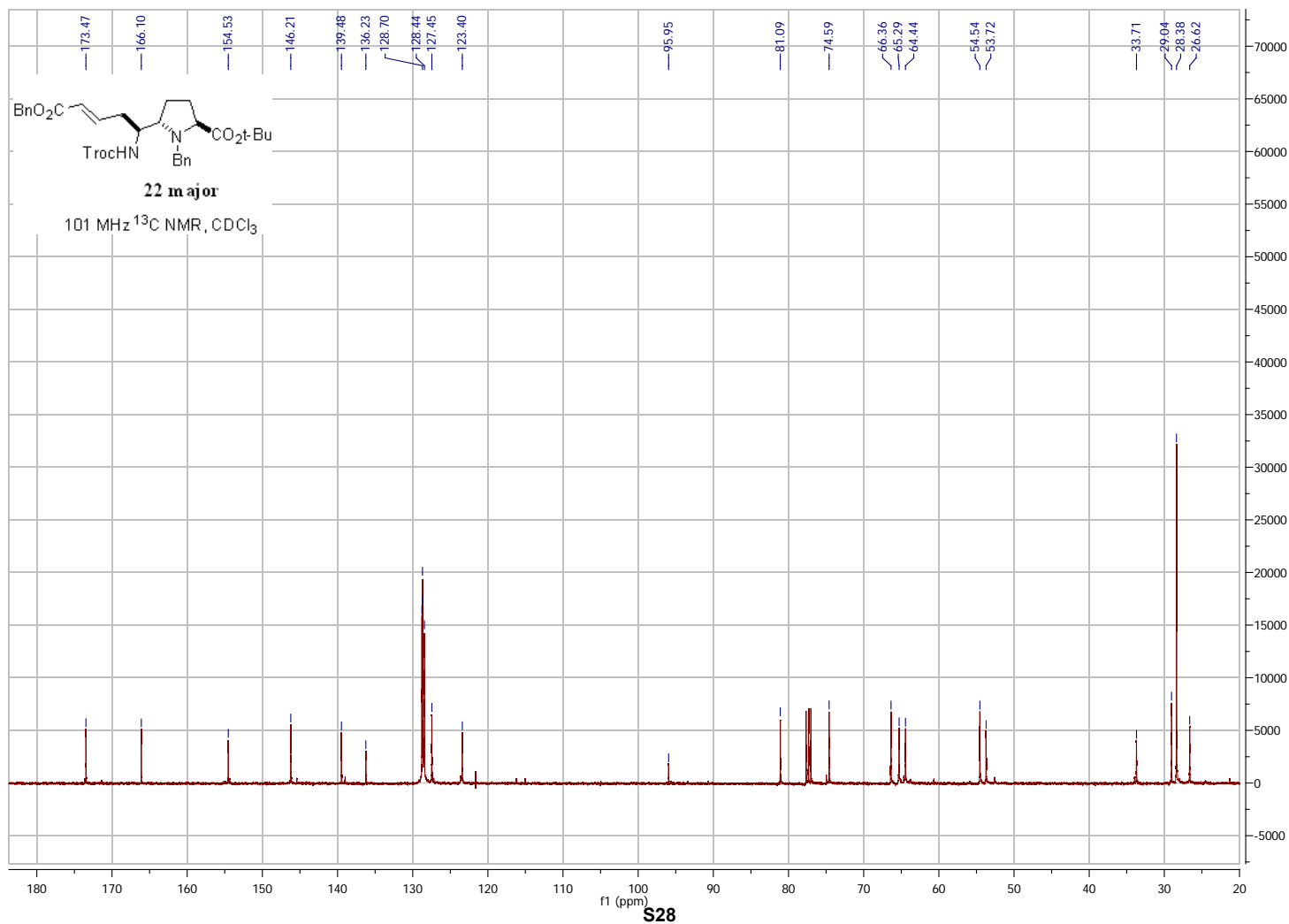
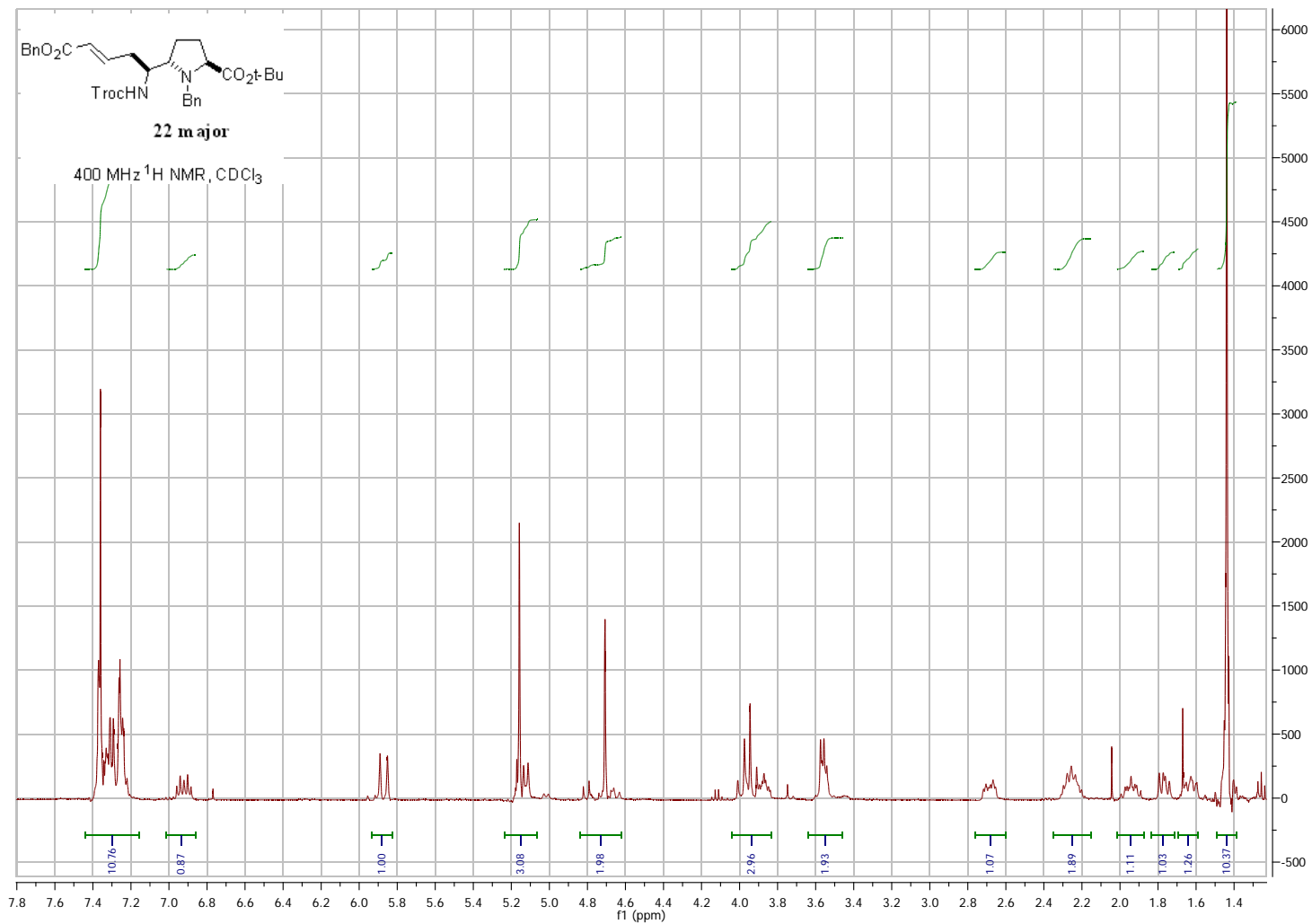


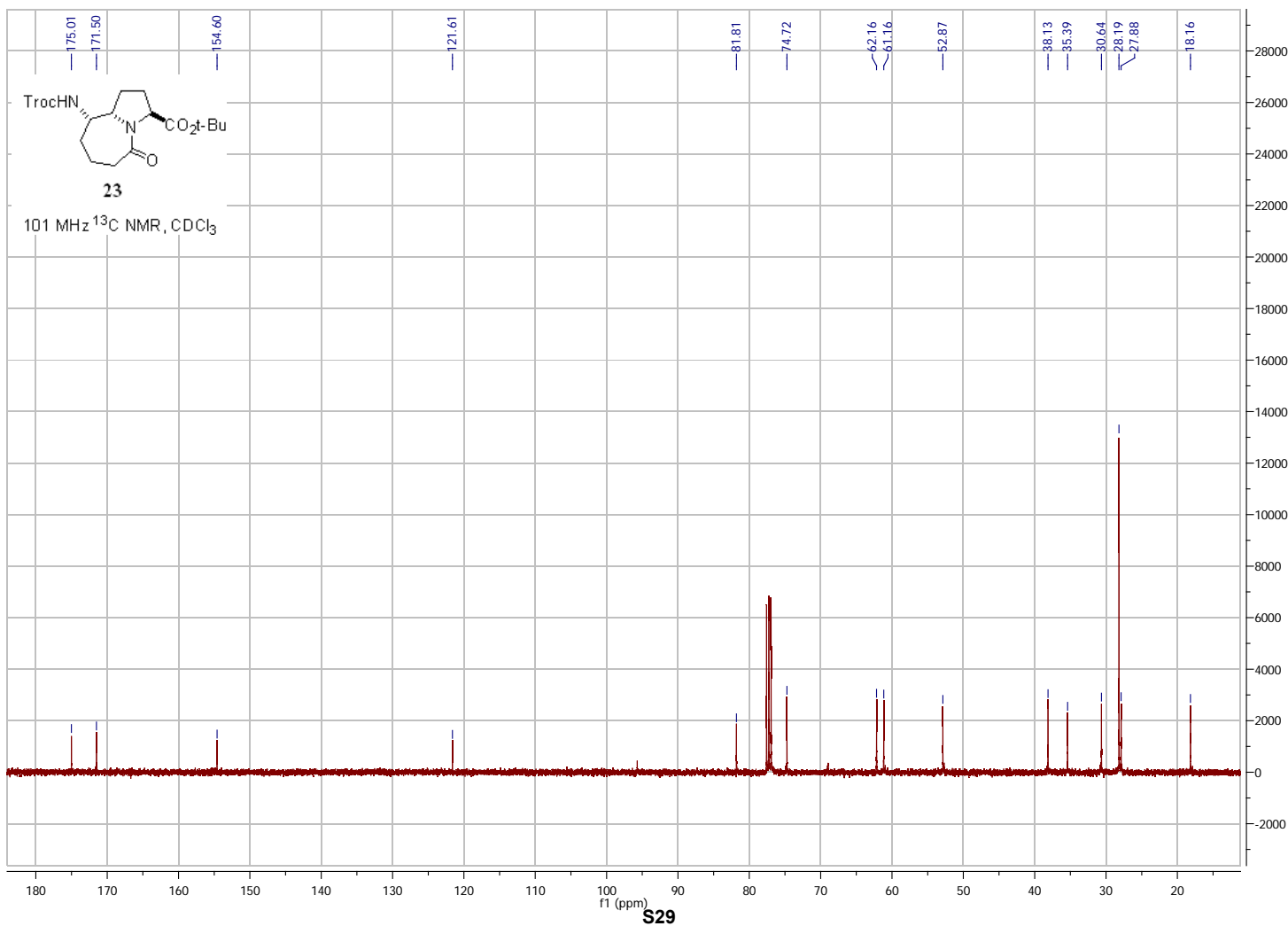
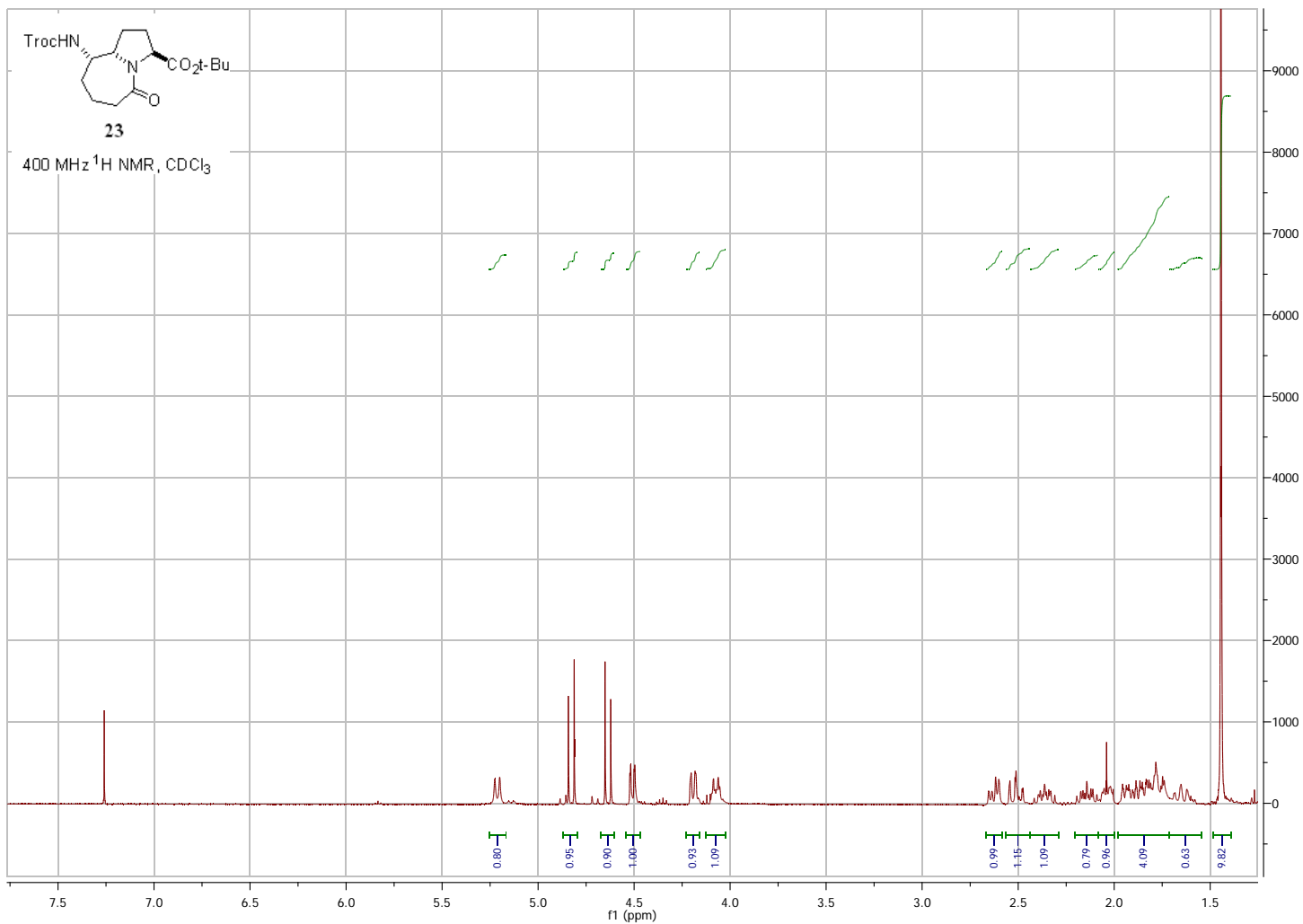


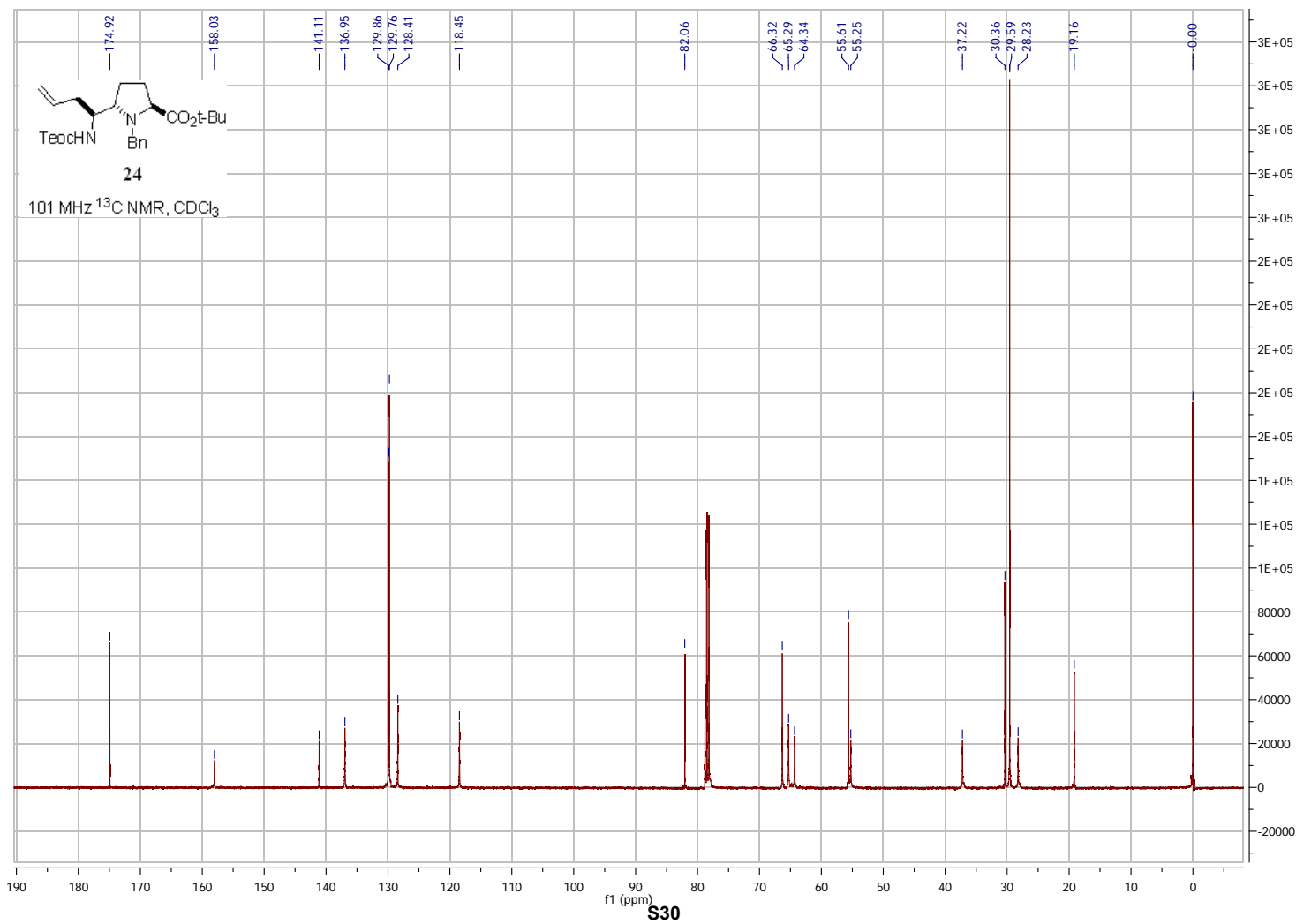
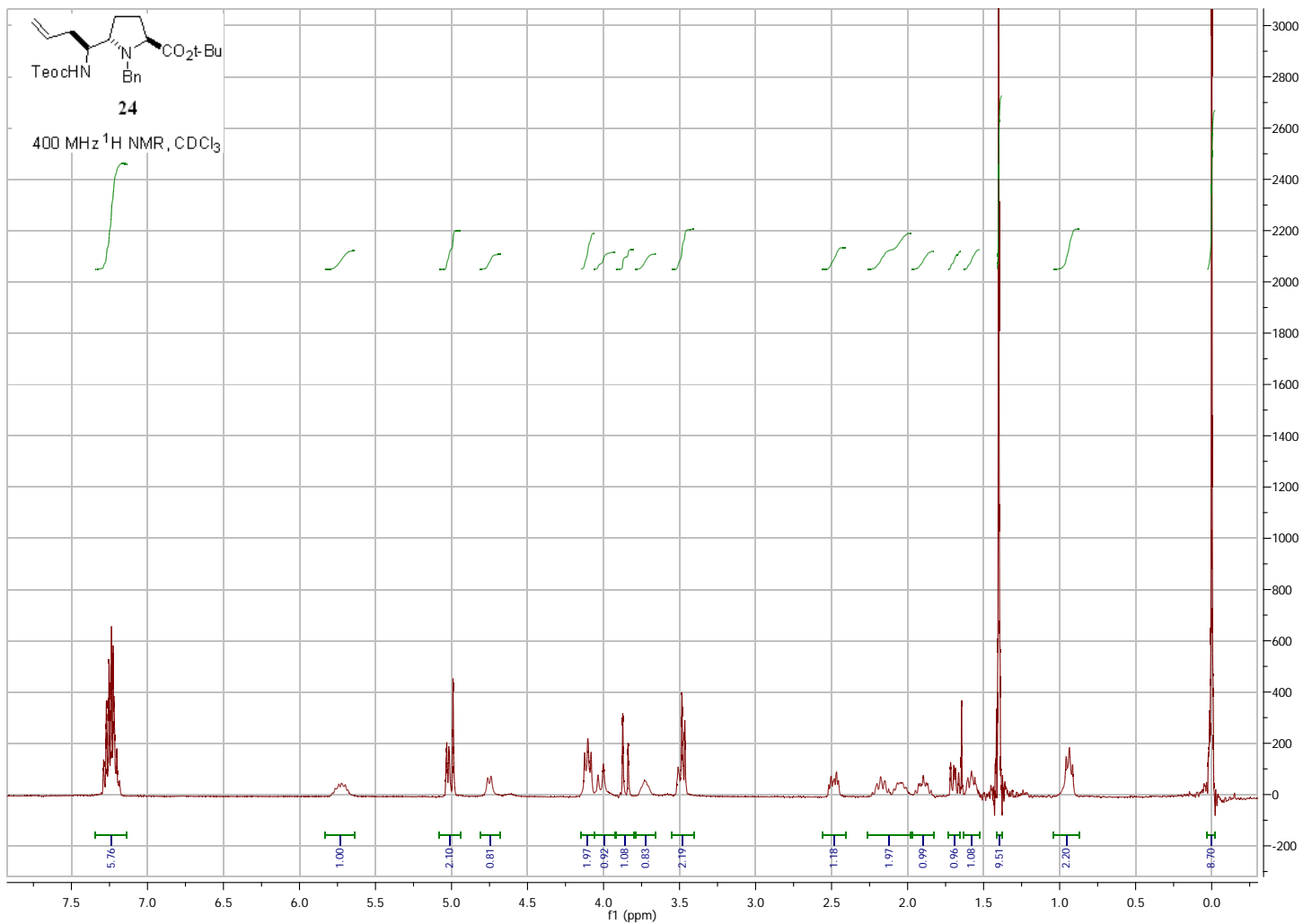


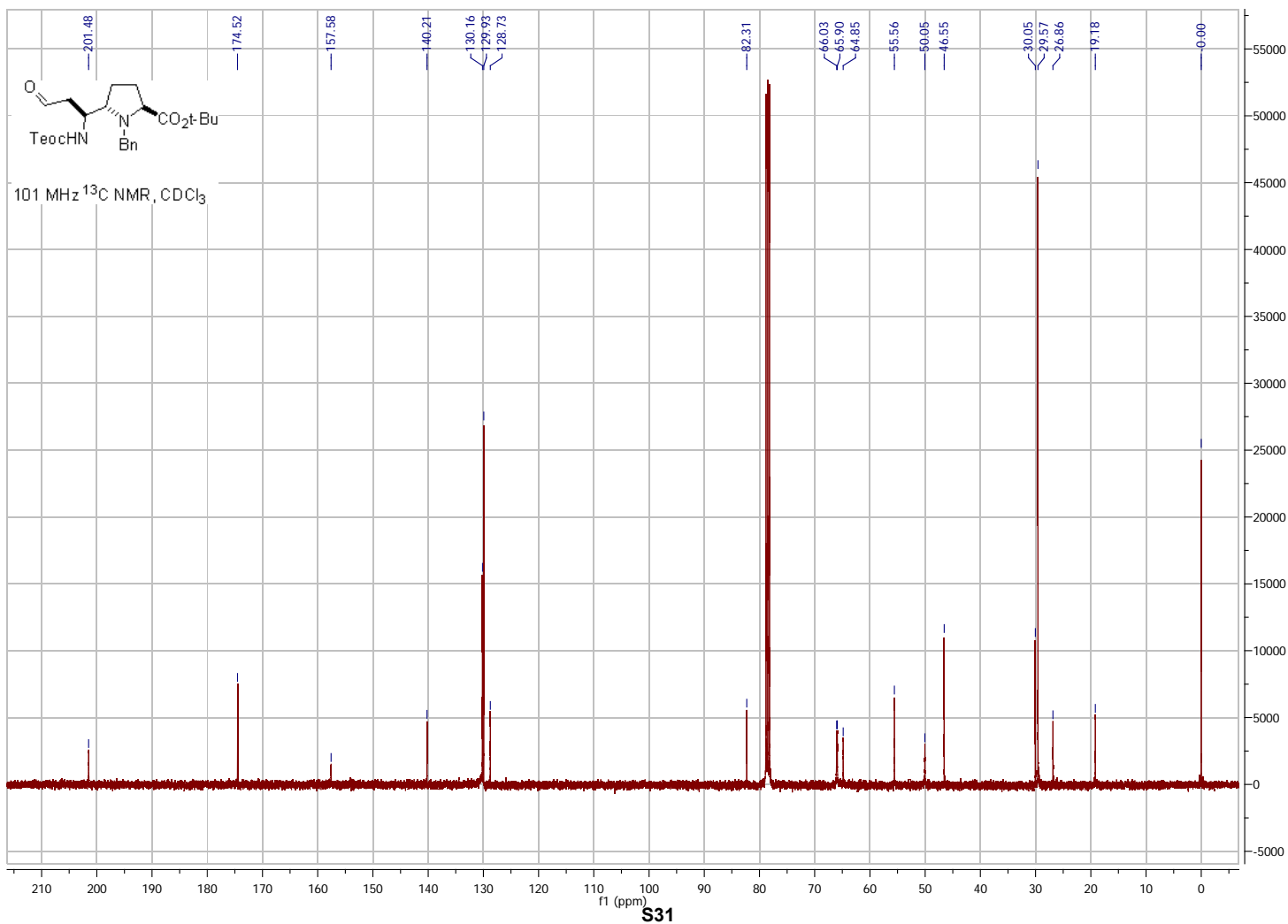
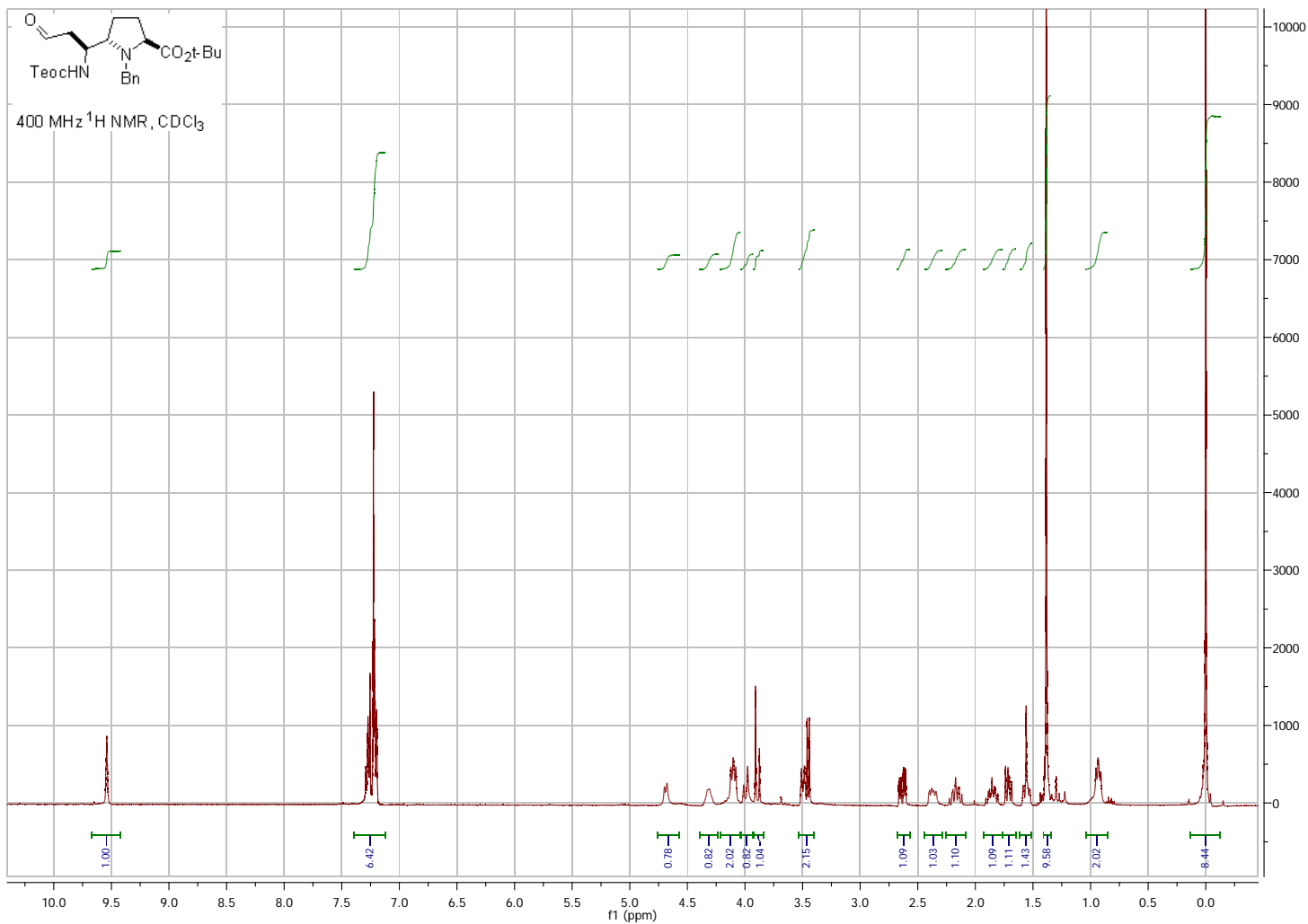


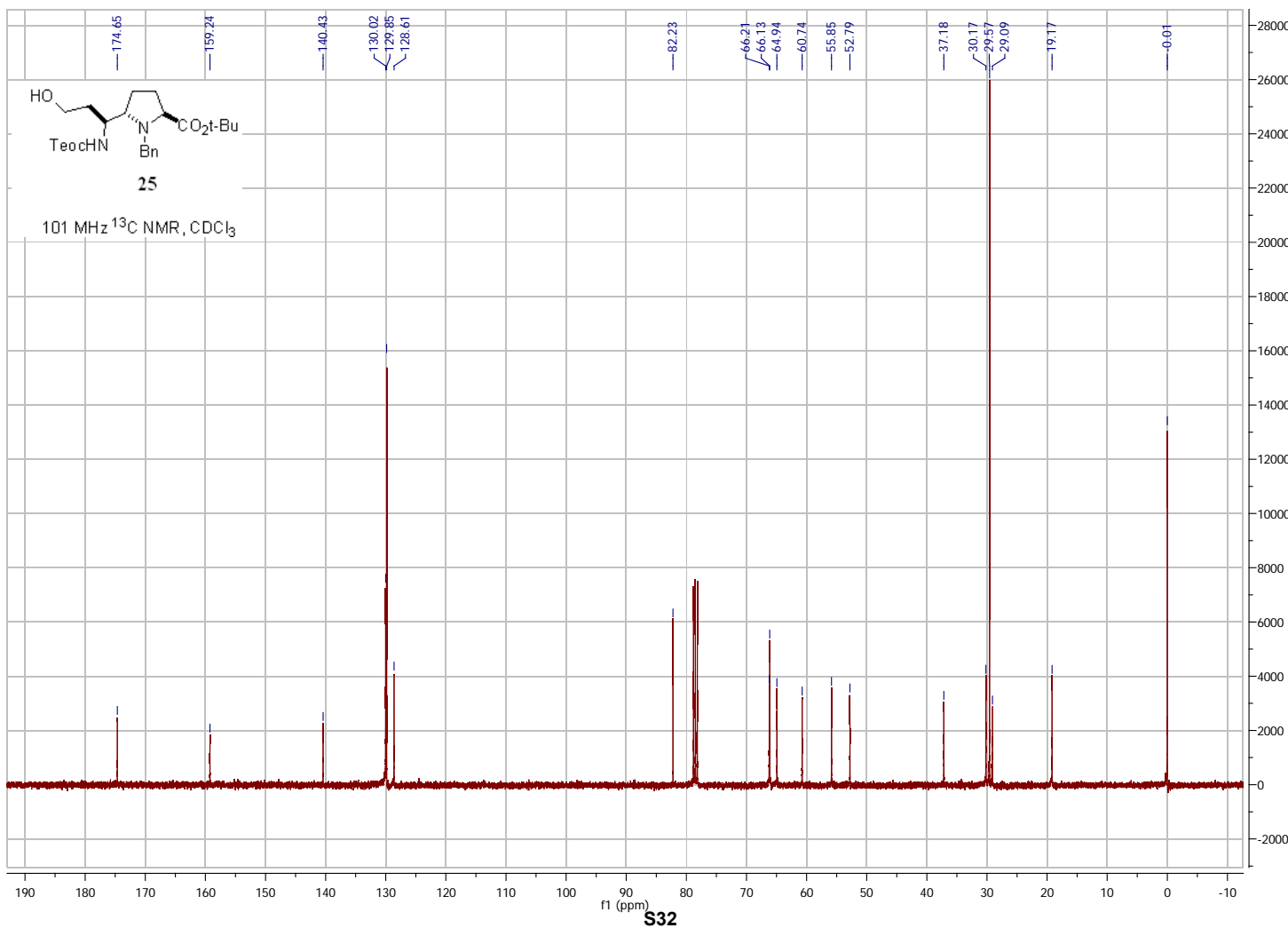
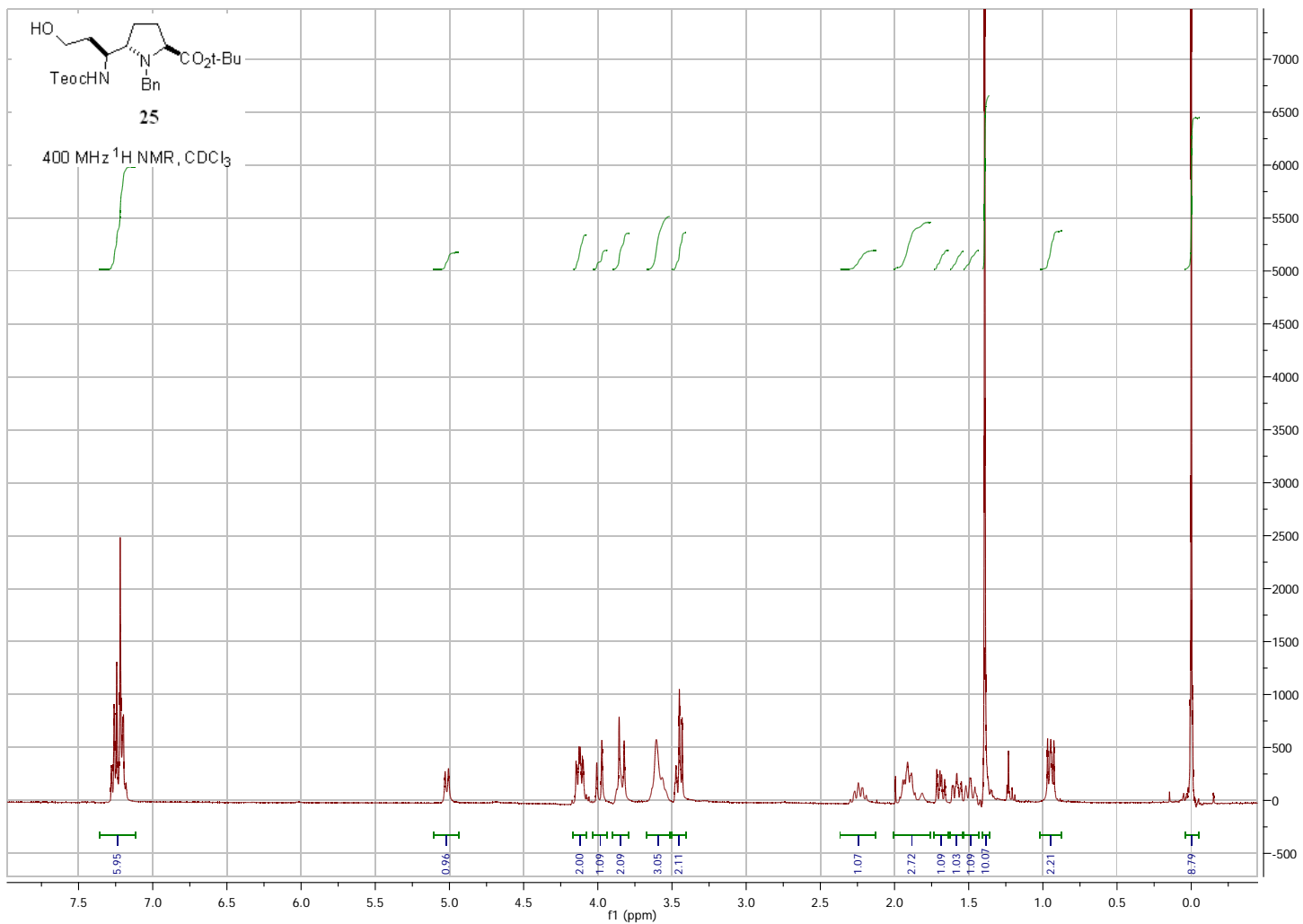


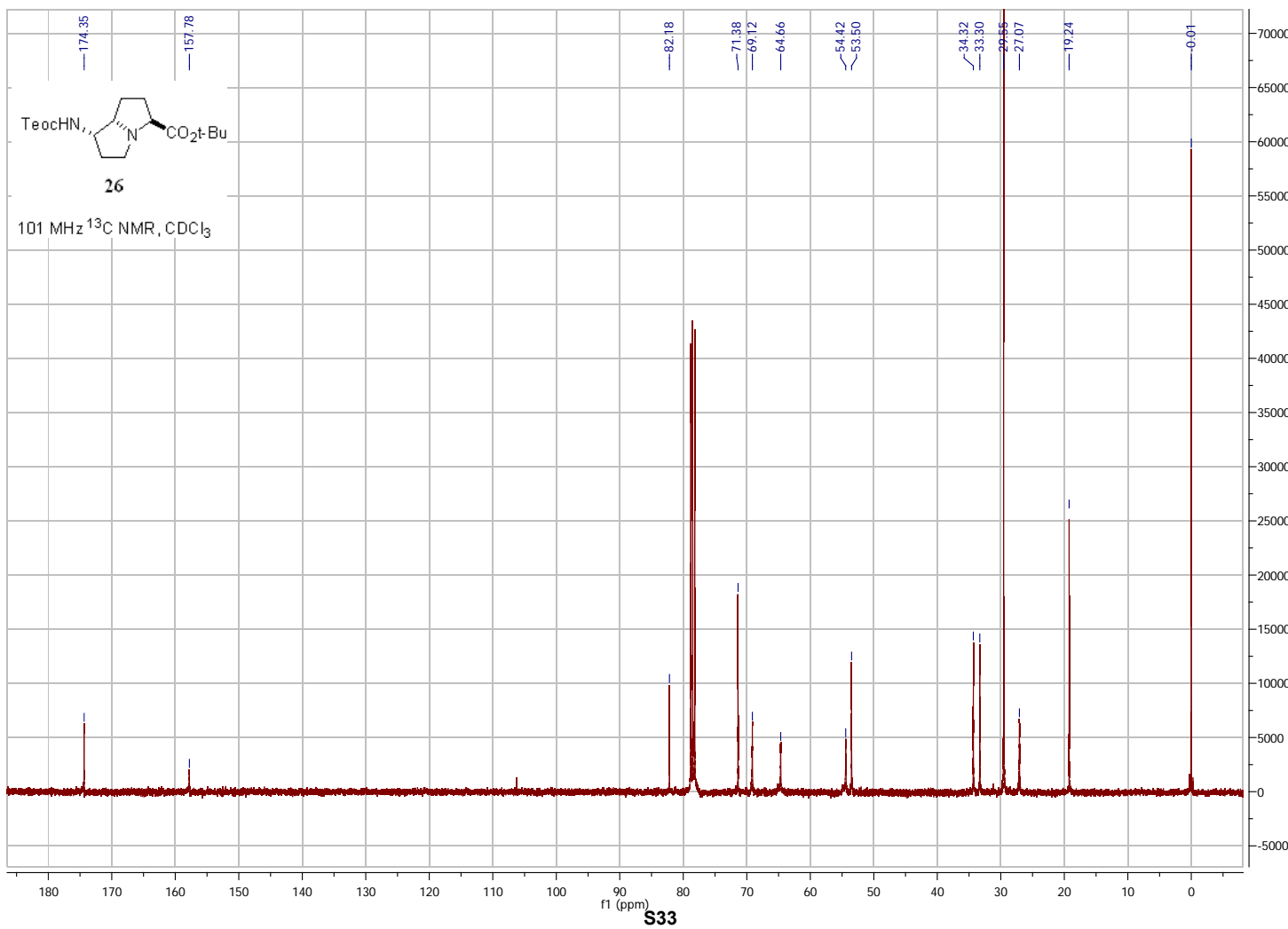
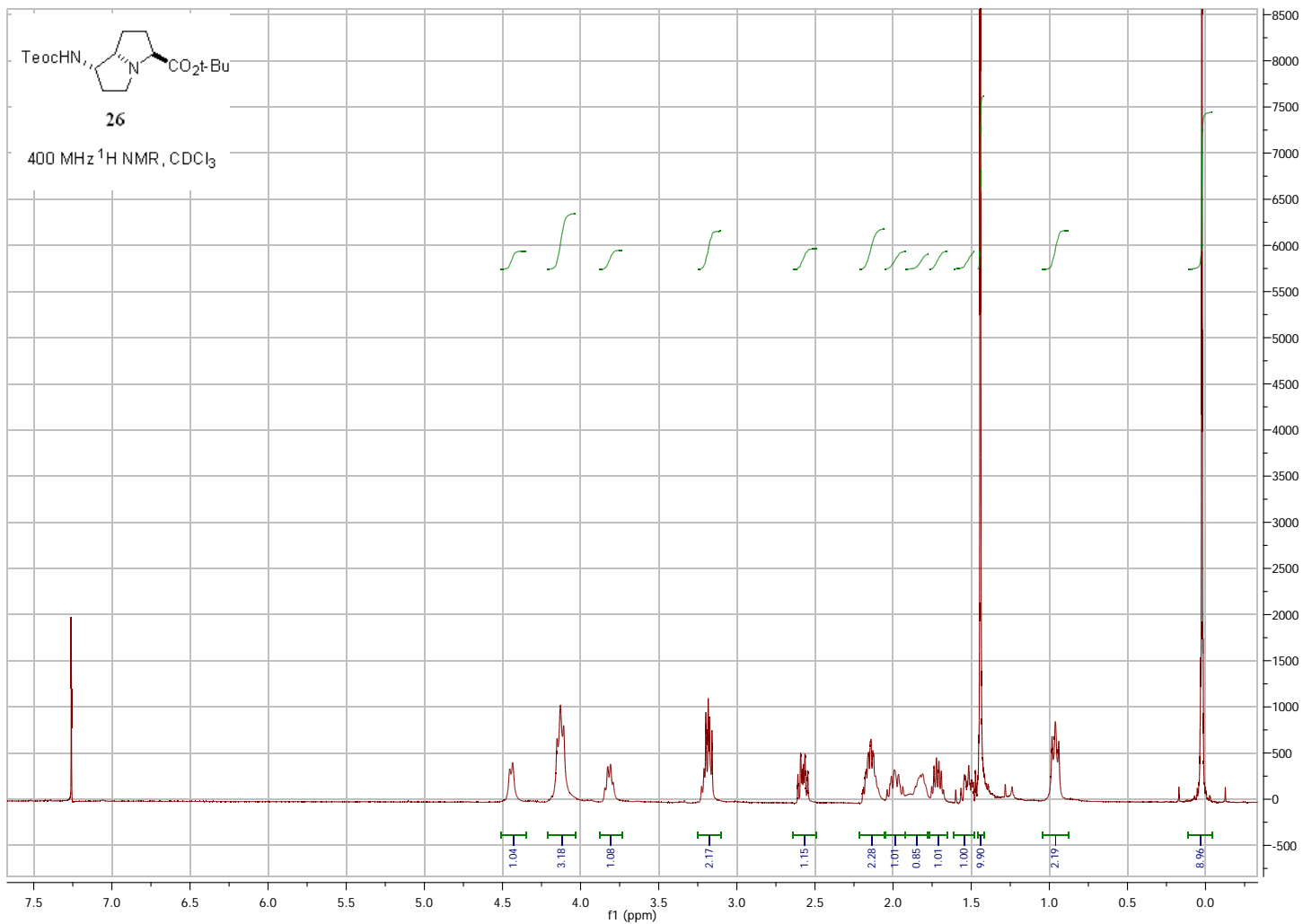


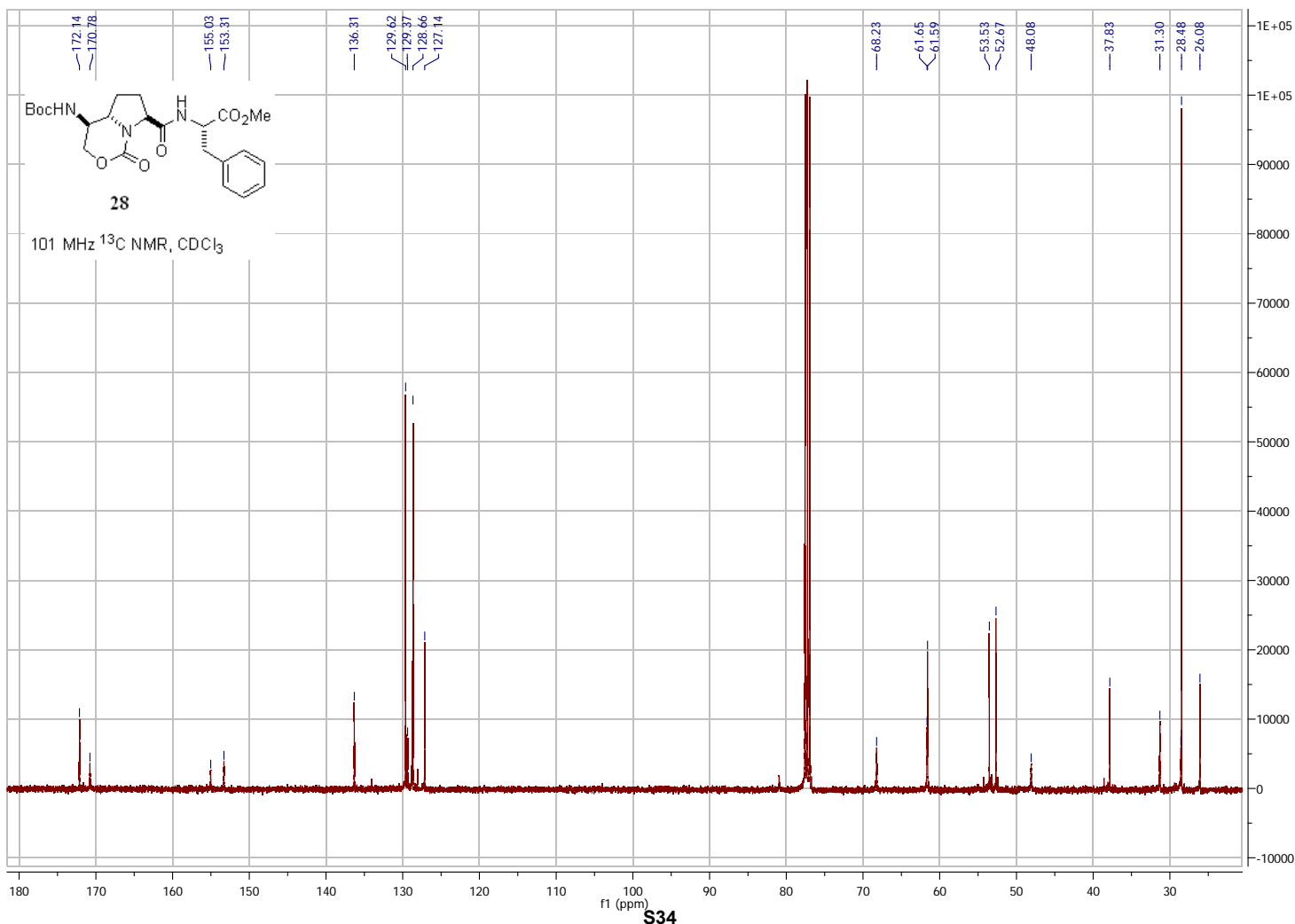
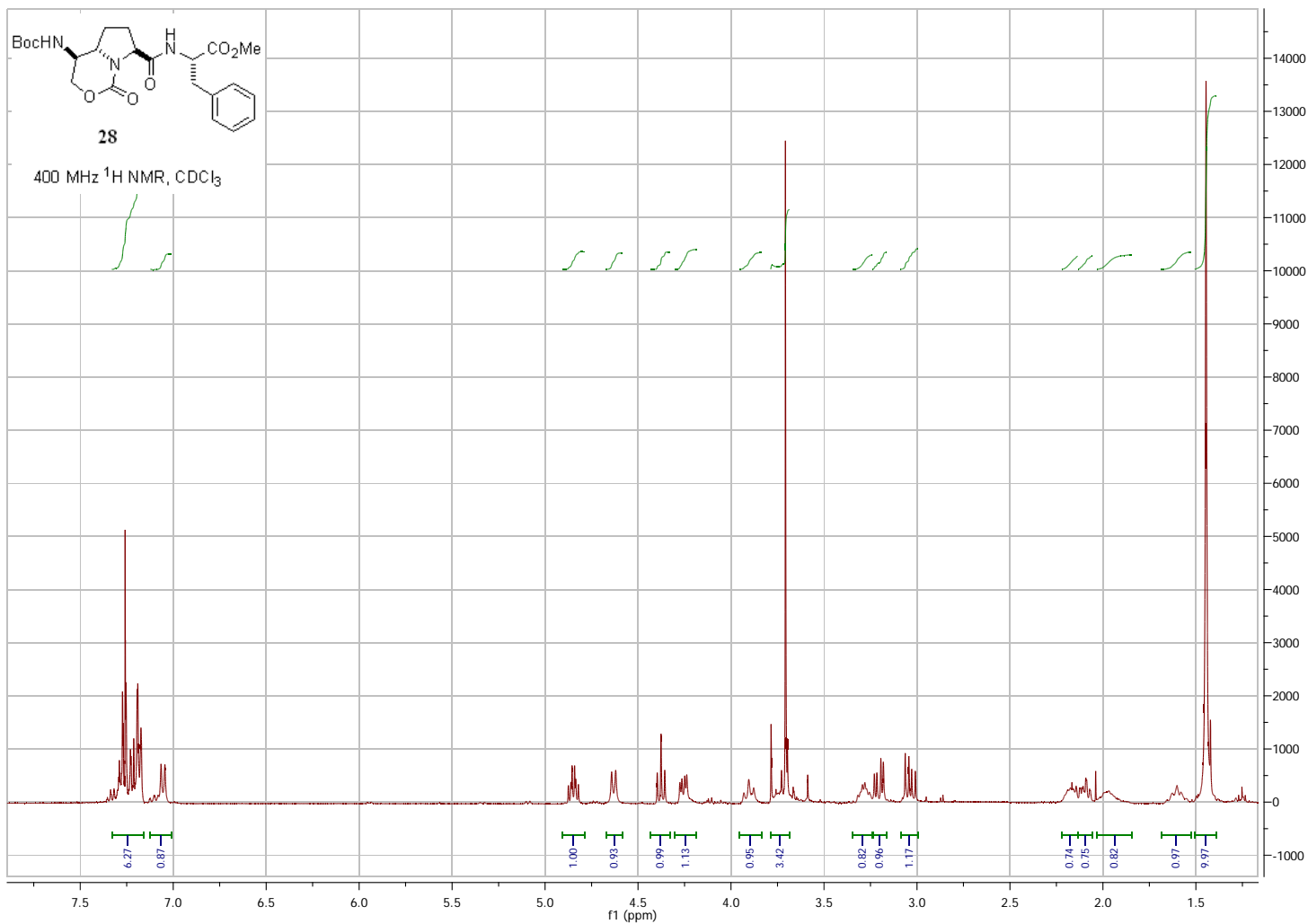


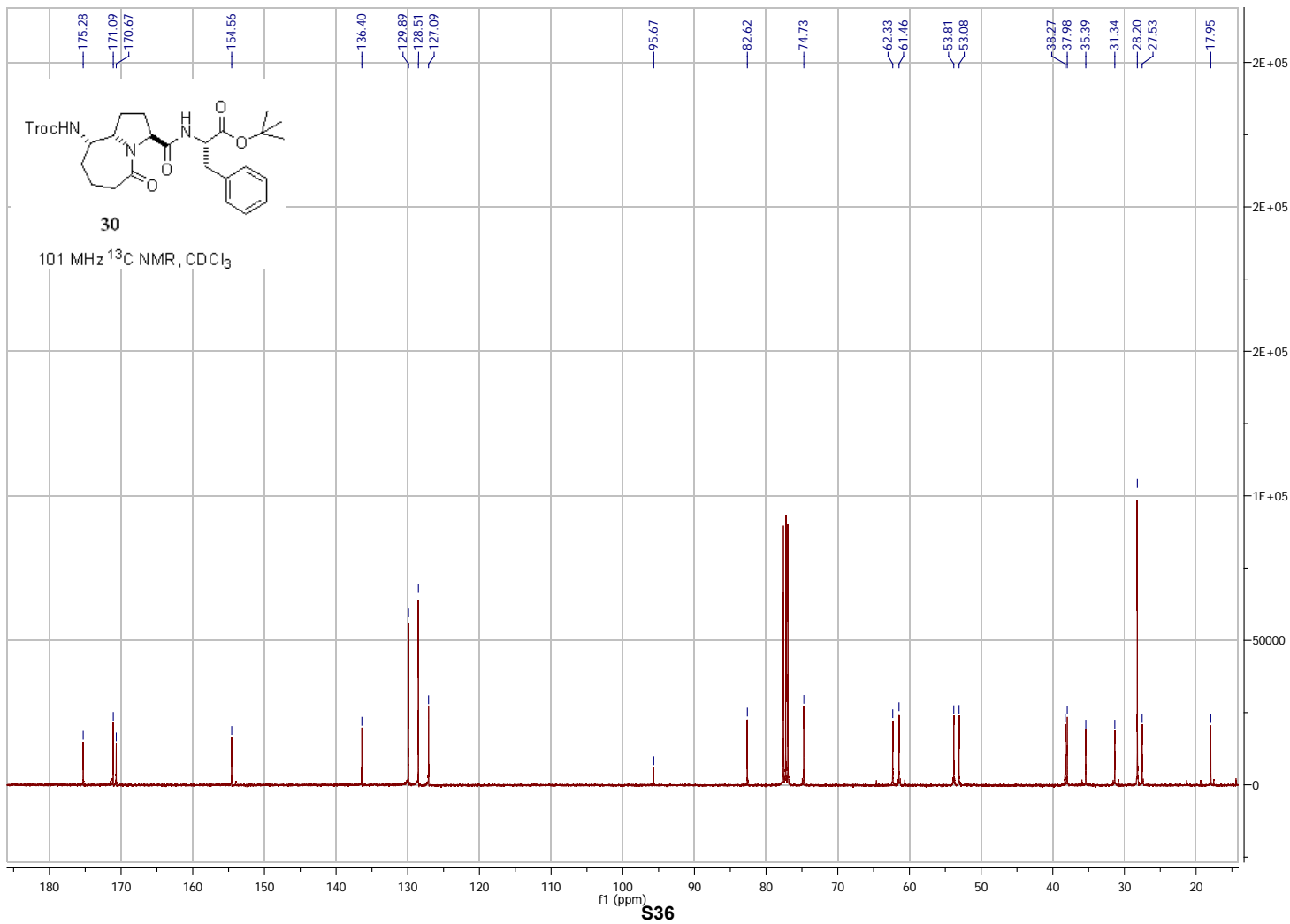
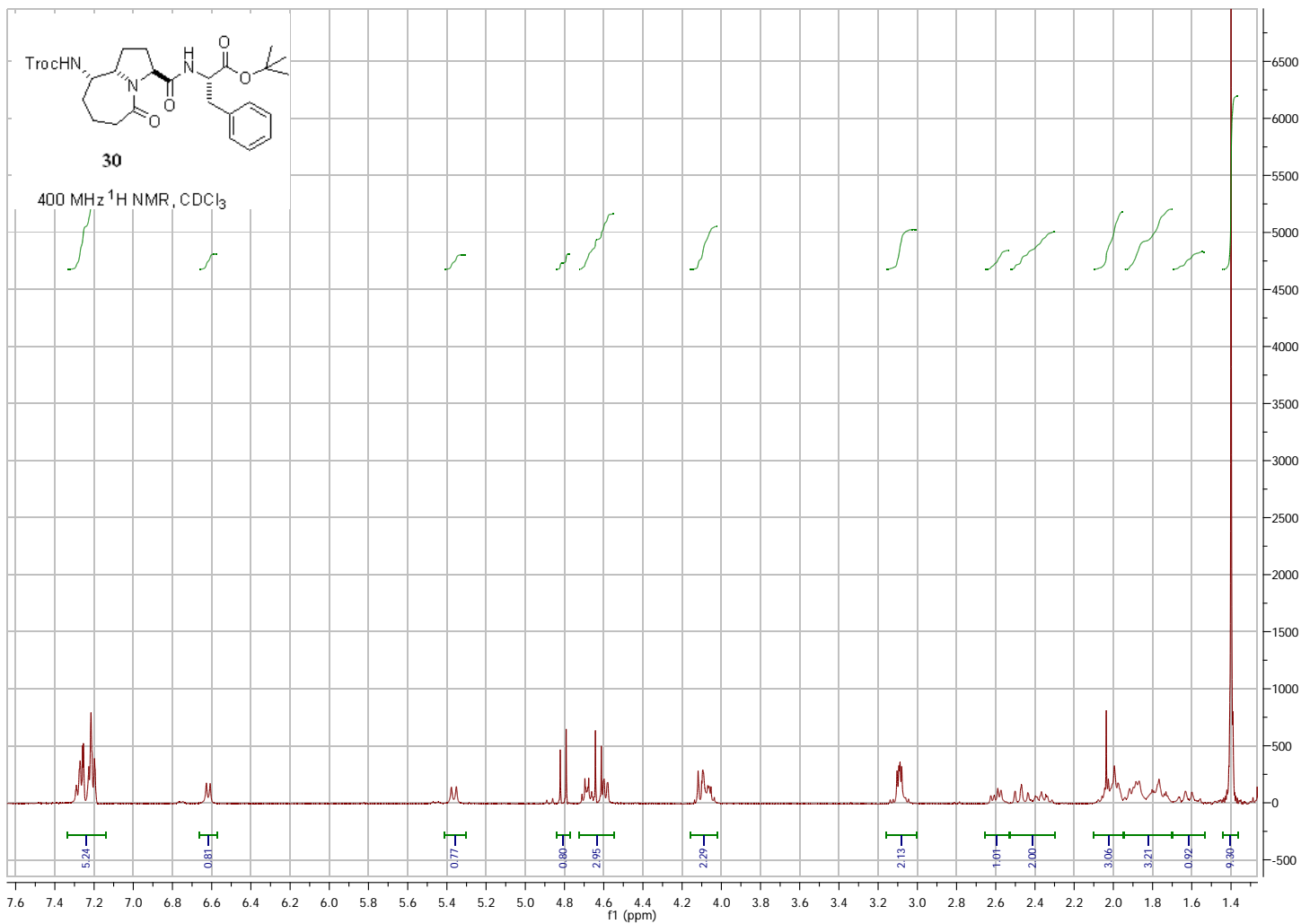


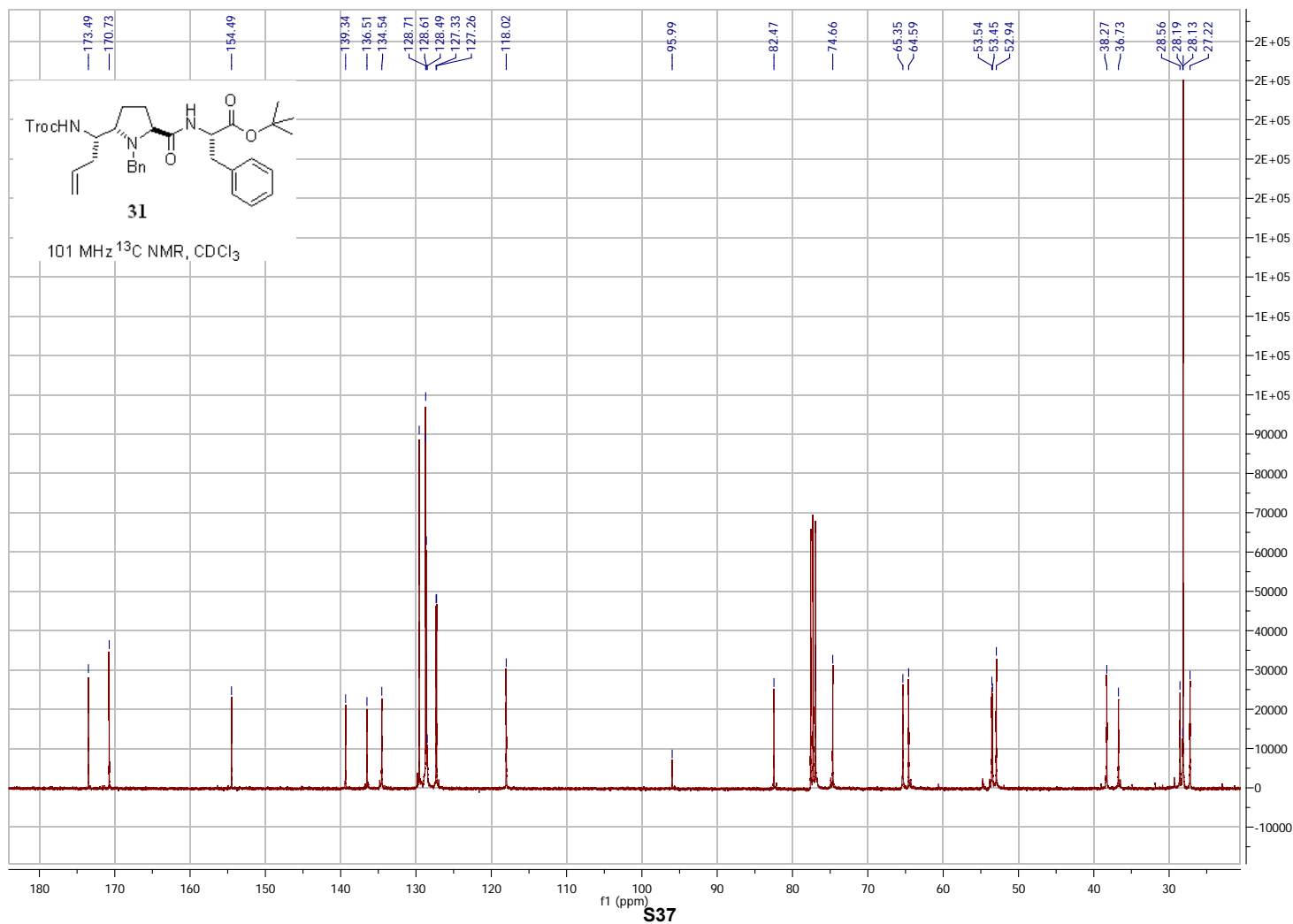
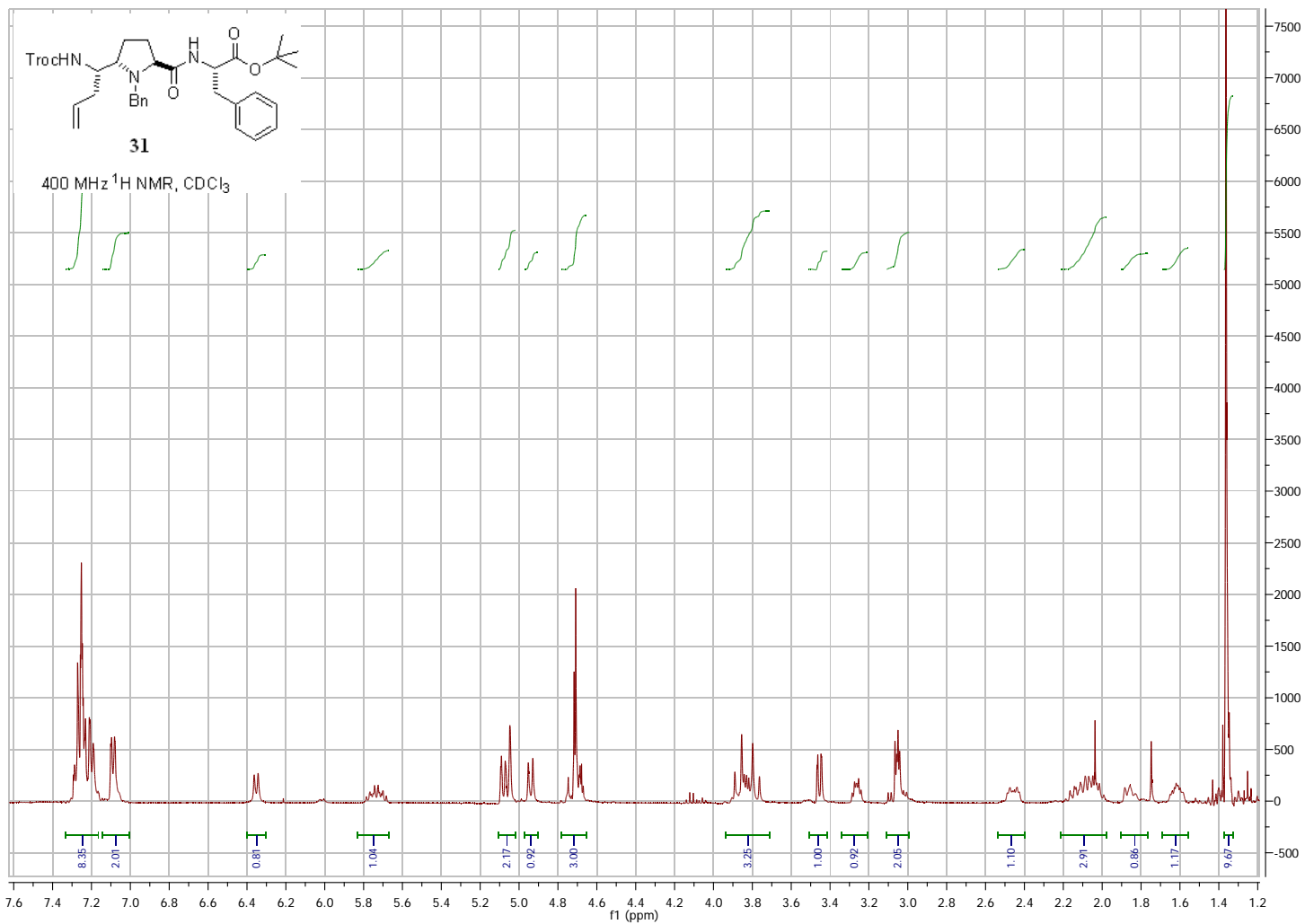


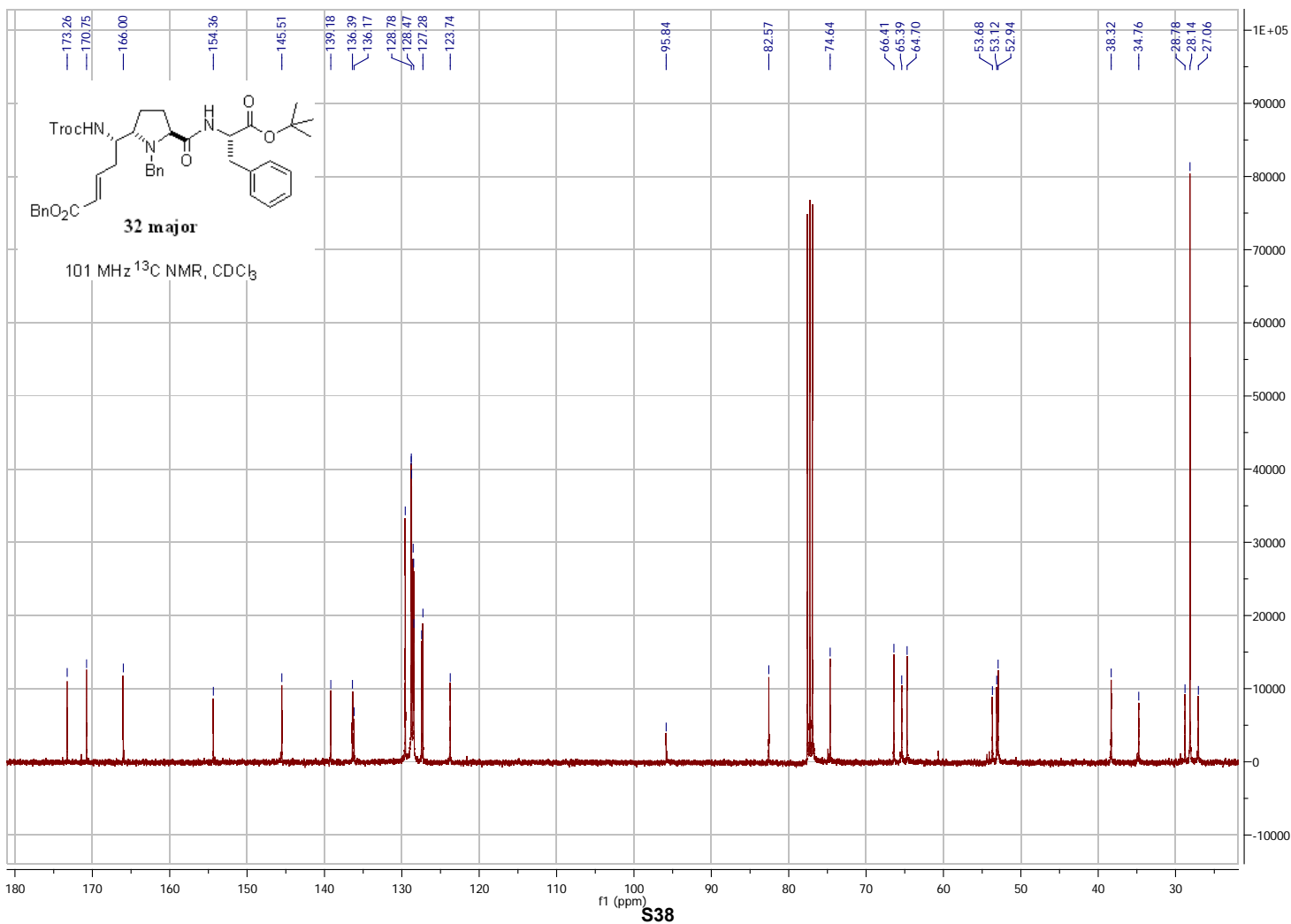
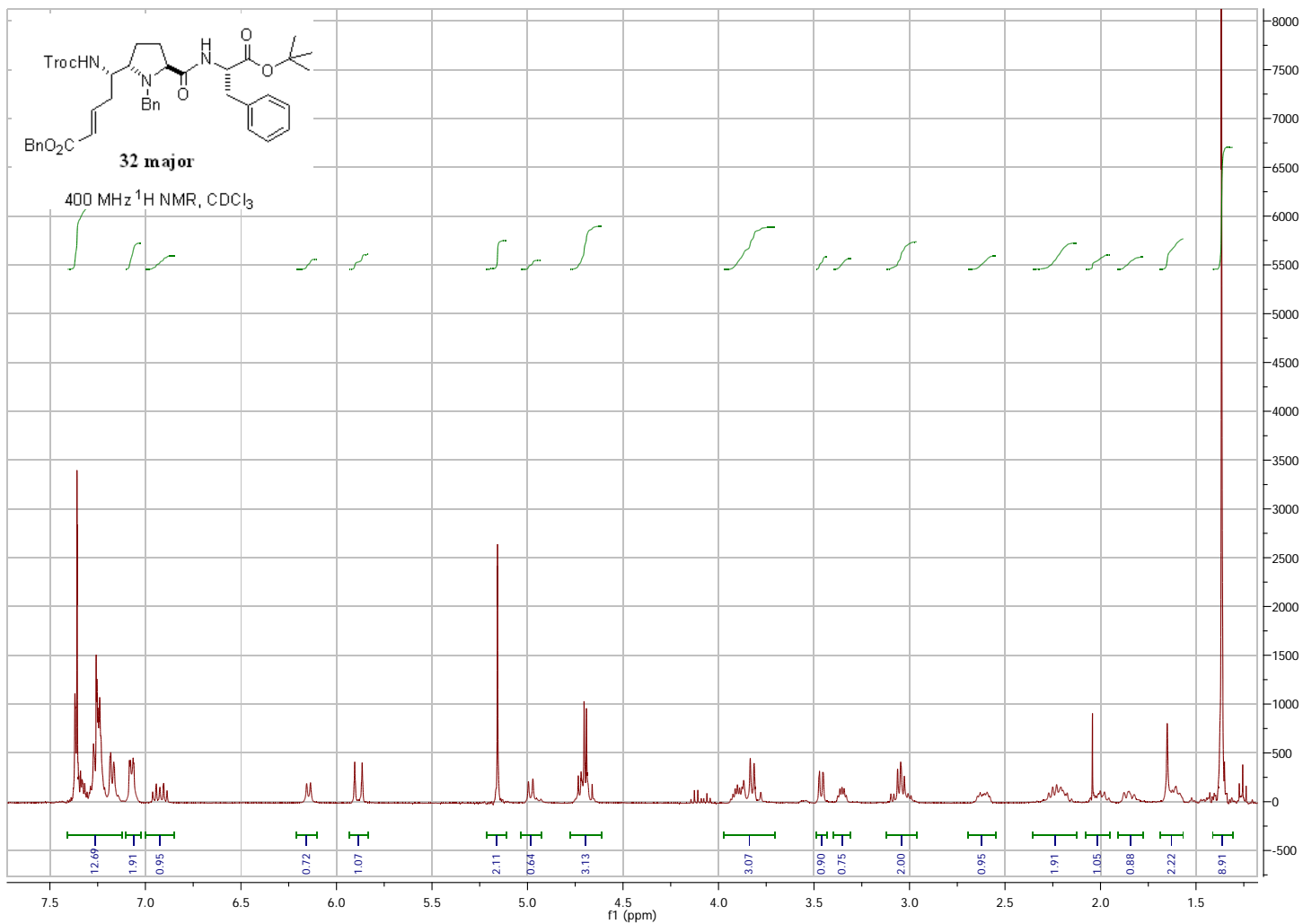


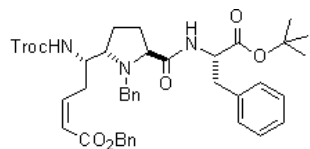






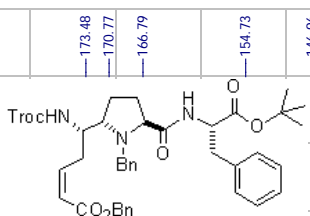
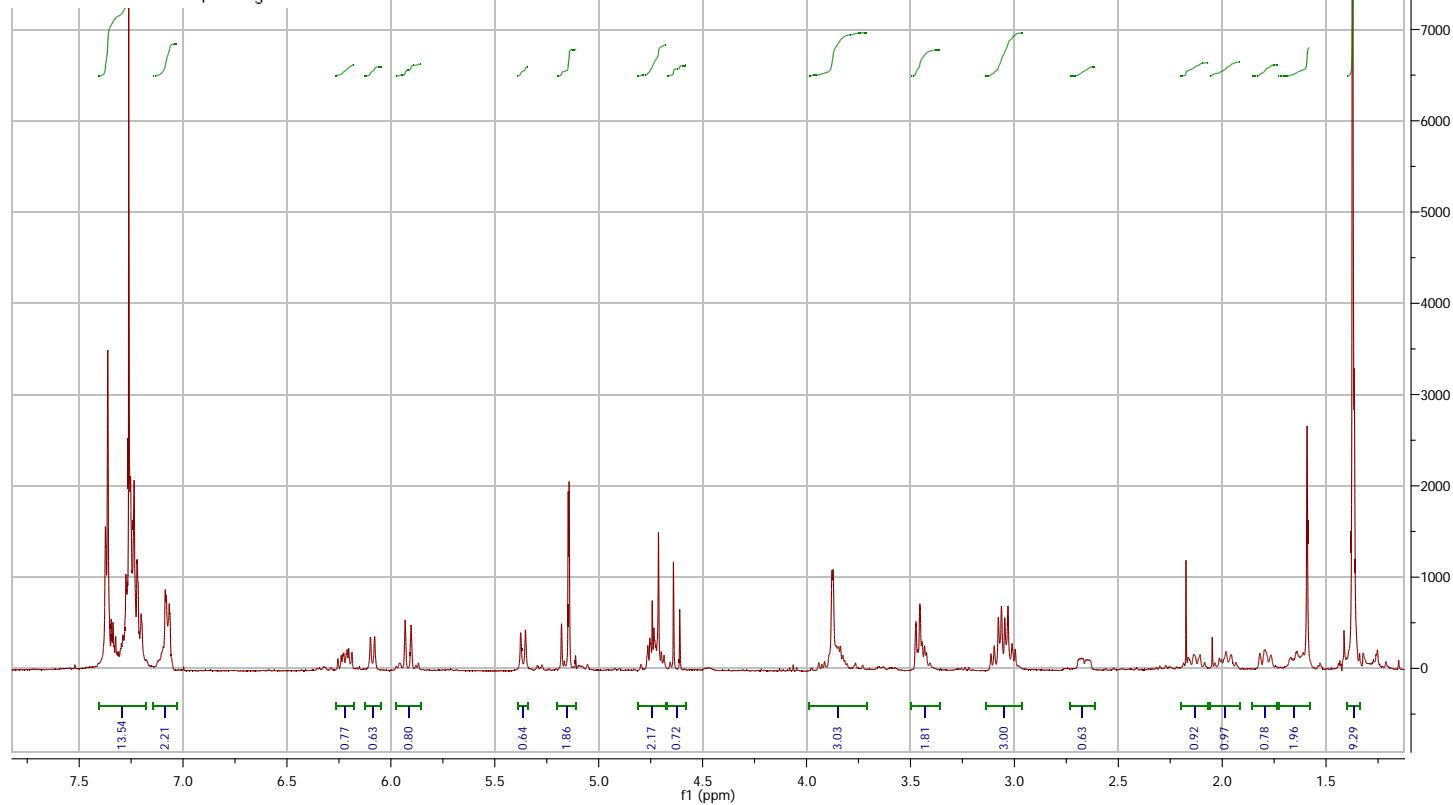






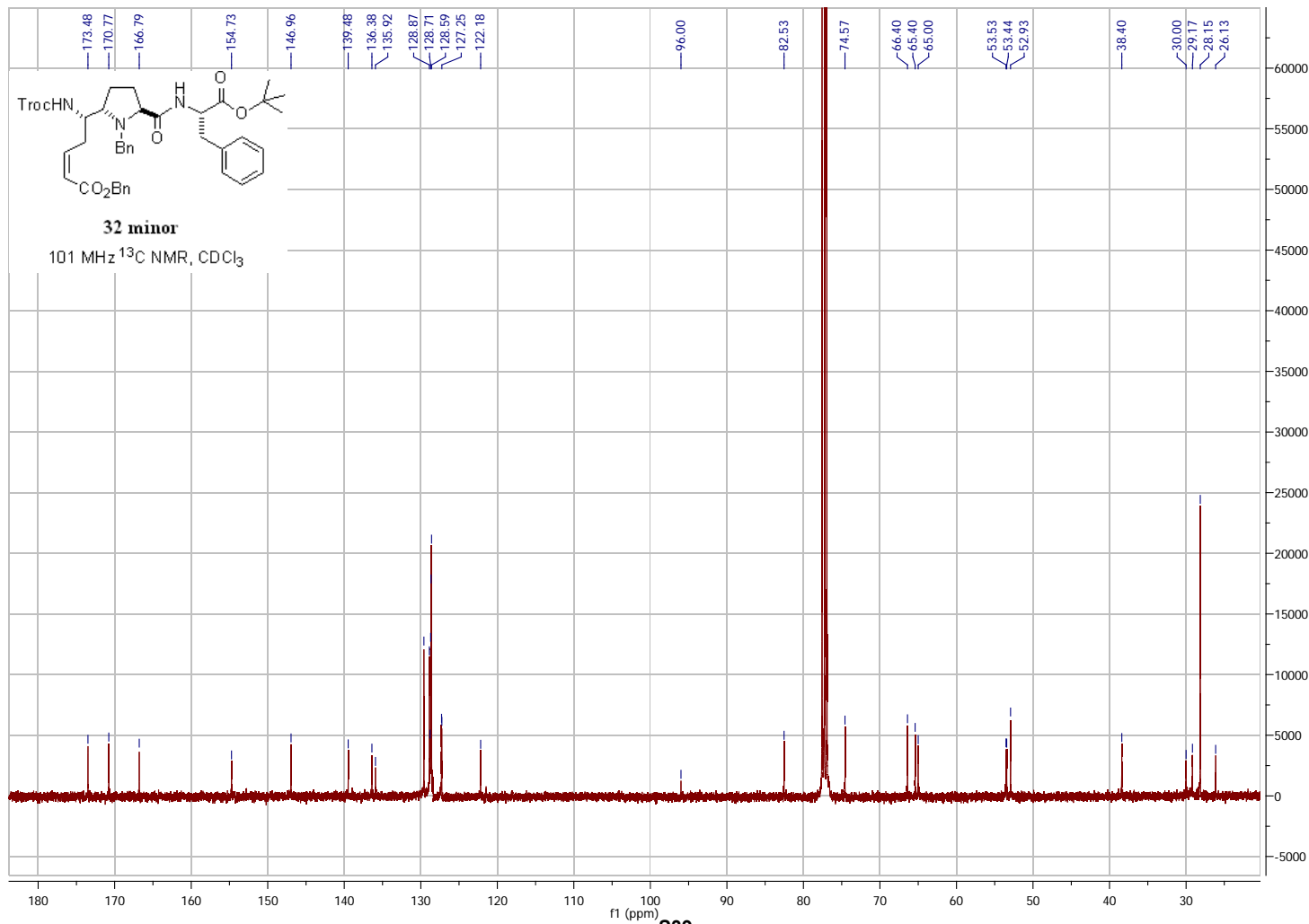
32 minor

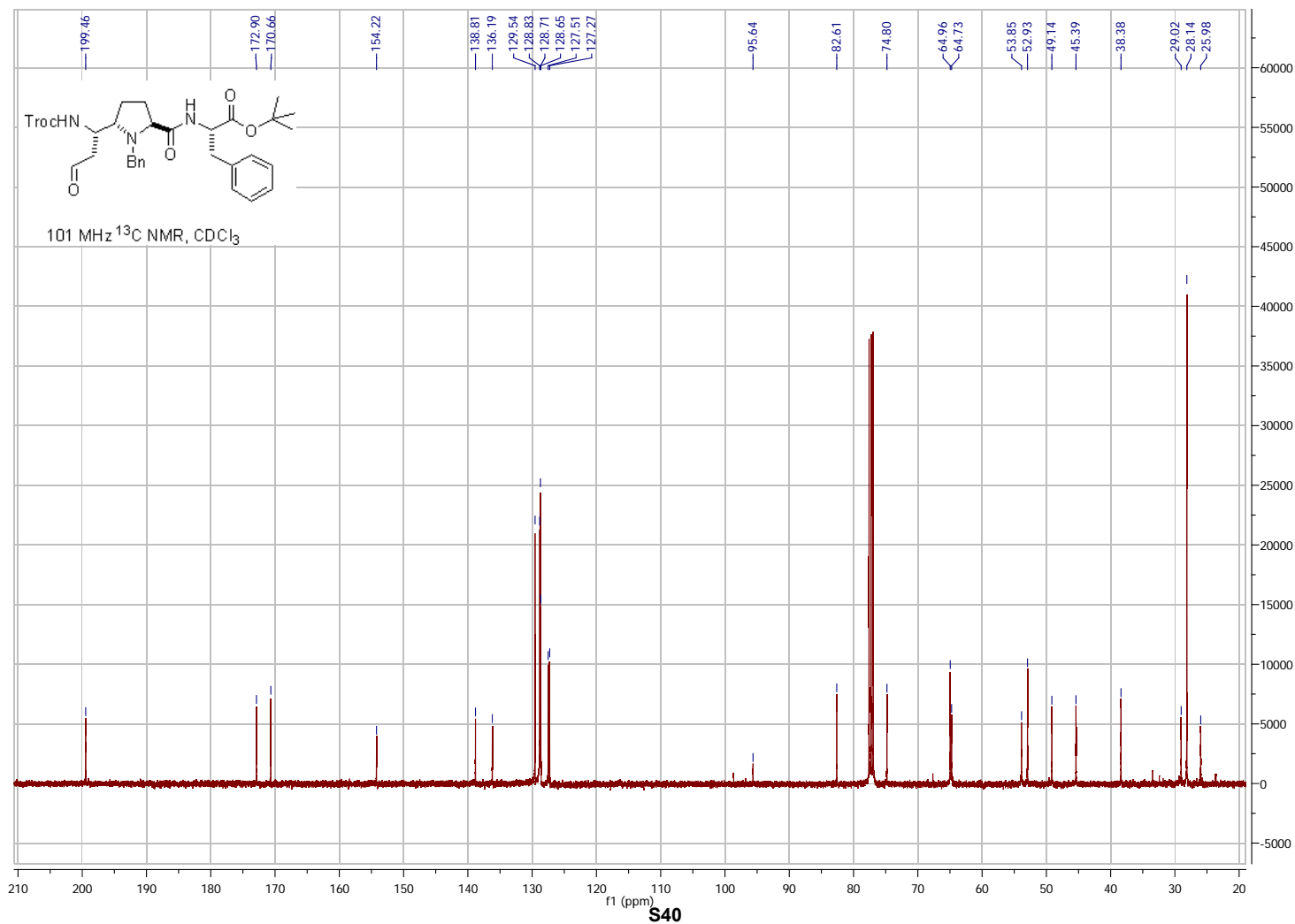
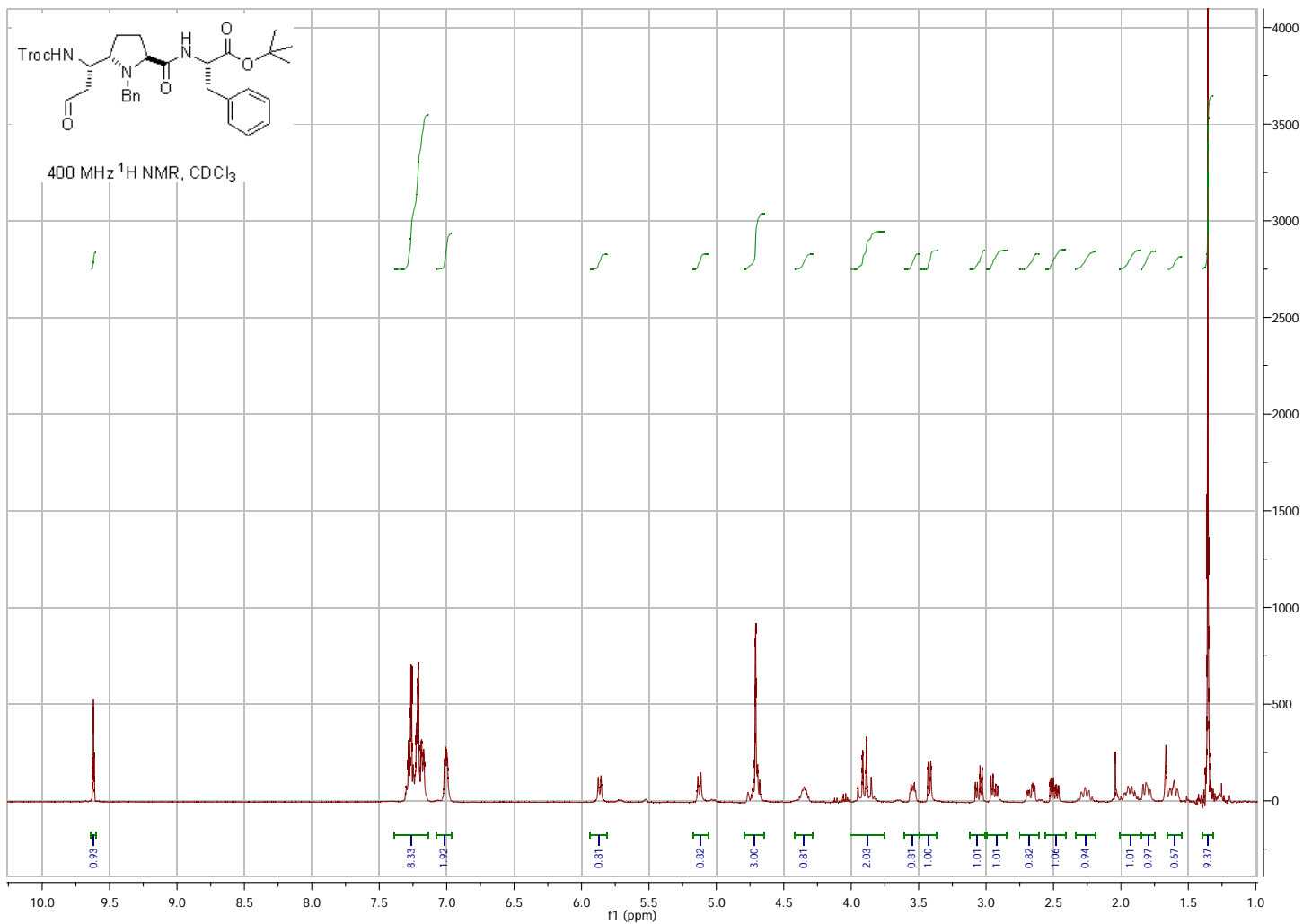
400 MHz ^1H NMR, CDCl_3

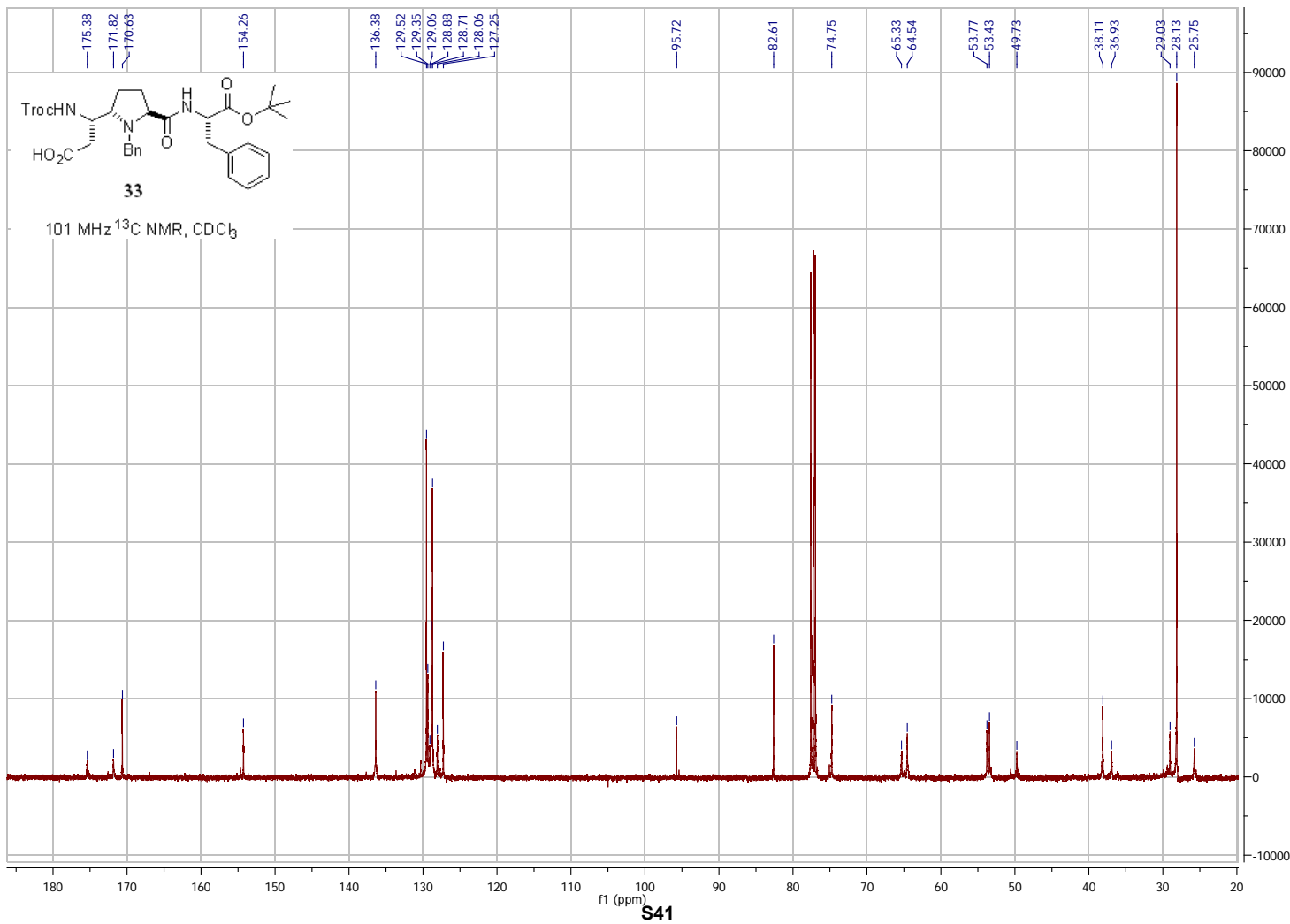
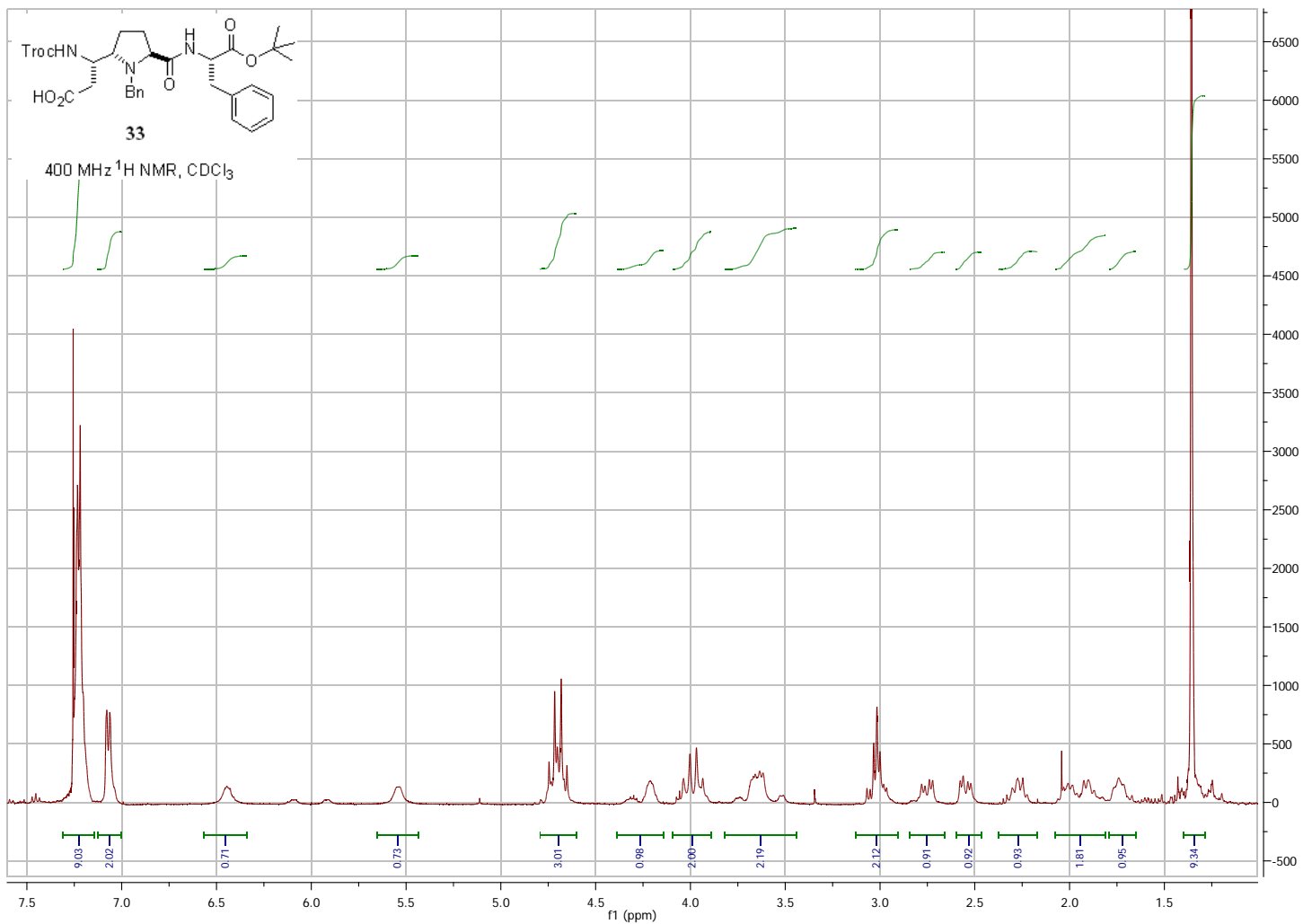


32 minor

101 MHz ^{13}C NMR, CDCl_3

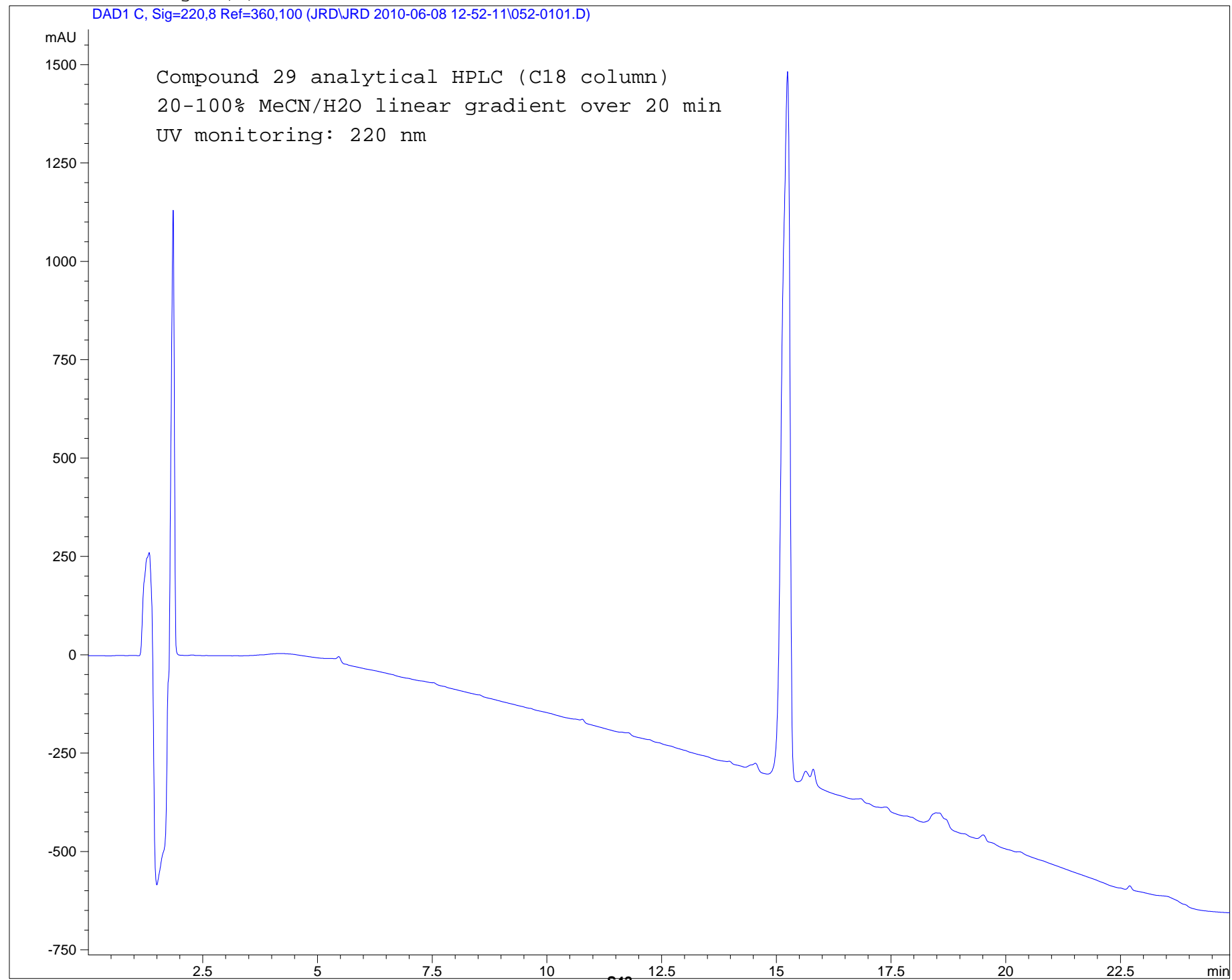






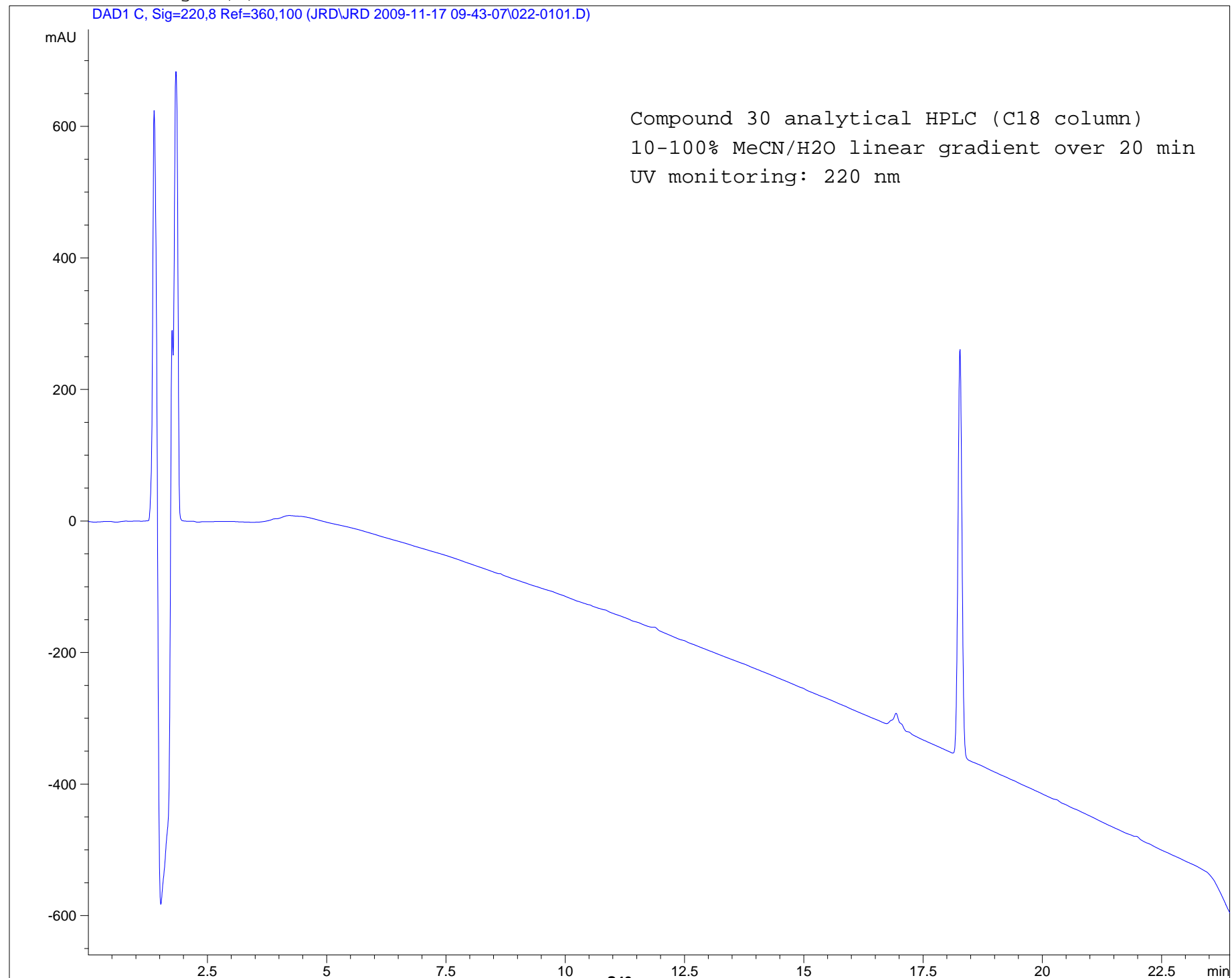
Current Chromatogram(s)

DAD1 C, Sig=220,8 Ref=360,100 (JRD\JRD 2010-06-08 12-52-11\052-0101.D)



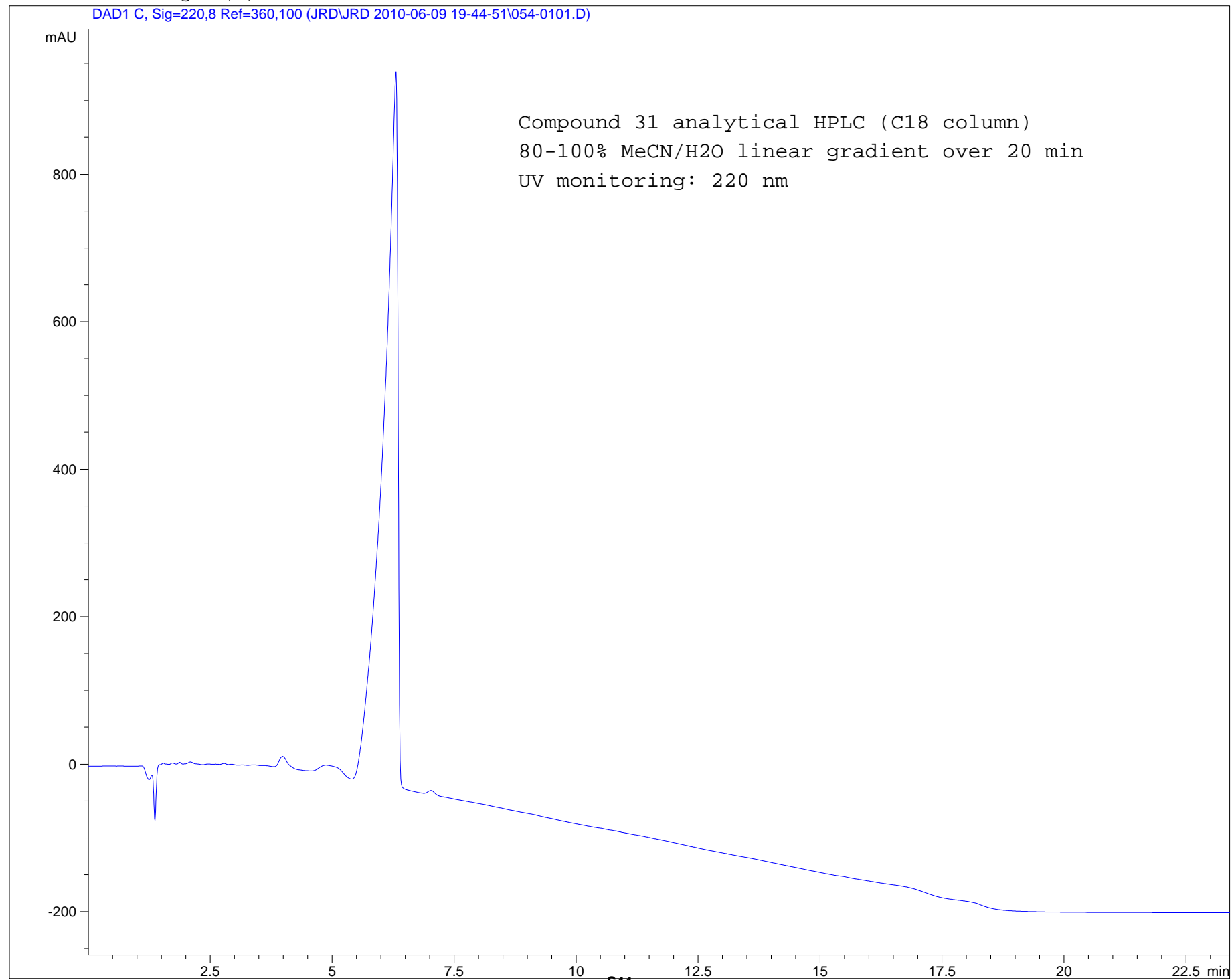
Current Chromatogram(s)

DAD1 C, Sig=220,8 Ref=360,100 (JRD\JRD 2009-11-17 09-43-07\022-0101.D)



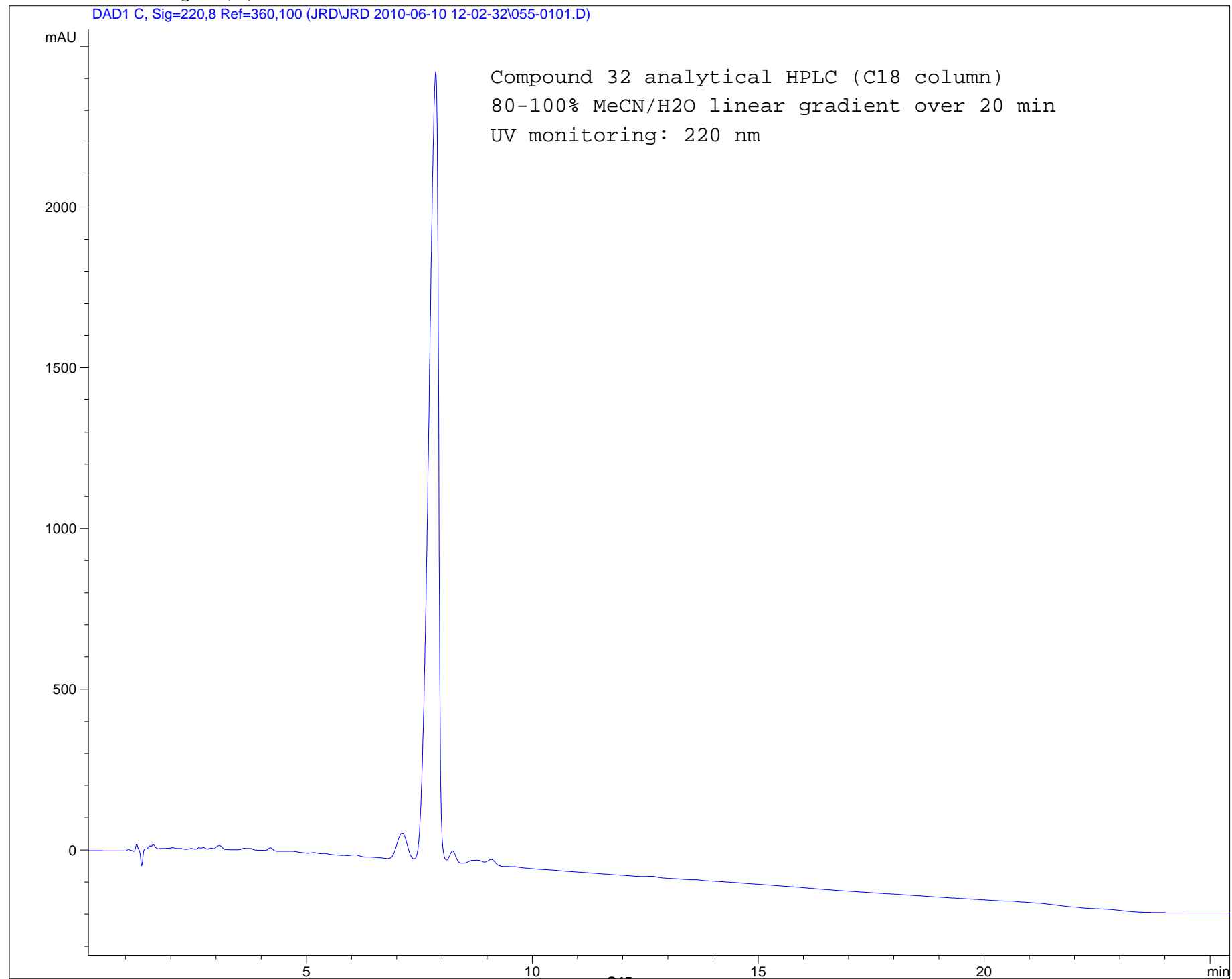
Current Chromatogram(s)

DAD1 C, Sig=220,8 Ref=360,100 (JRD\JRD 2010-06-09 19-44-51\054-0101.D)



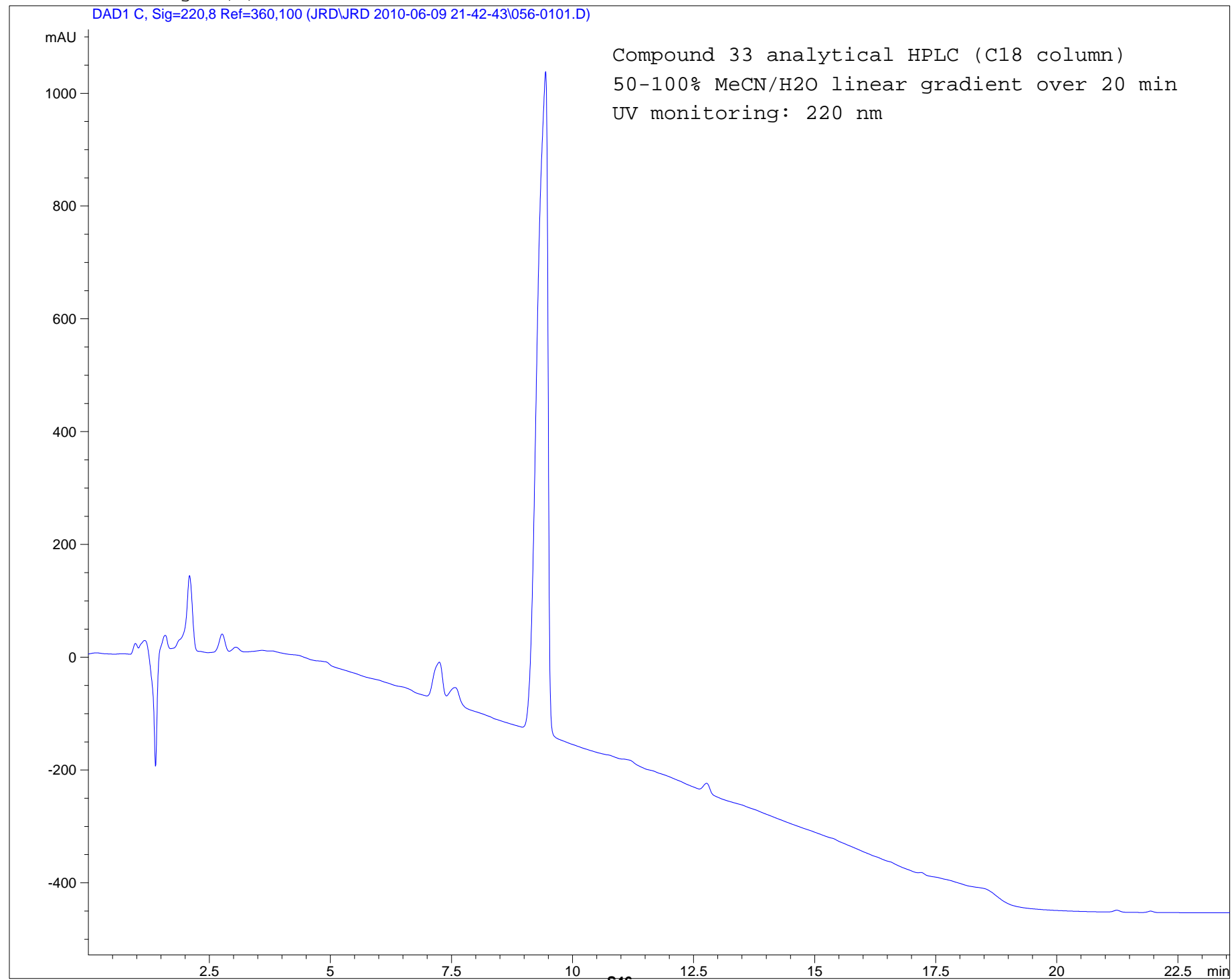
Current Chromatogram(s)

DAD1 C, Sig=220,8 Ref=360,100 (JRD\JRD 2010-06-10 12-02-32\055-0101.D)



Current Chromatogram(s)

DAD1 C, Sig=220,8 Ref=360,100 (JRD\JRD 2010-06-09 21-42-43\056-0101.D)



Procedure for Conformational Searches

Computational modeling was carried out using the Schrodinger 2007 software suite, Maestro version 8.0.308. All structures were prepared with Ligprep (OPLS_2005 force field) using default settings, with the exception of the following: Epik was used to calculate ionization with pH set to 7.0 ± 2.0 . Conformational searching was carried out with Macromodel (MM3* force field¹) using default settings with the exception of the following: solvent was set as CHCl₃, distance-dependant electrostatics were employed, dielectric constant was set to 2.0, atoms were chosen for substructure flexibility, truncated Newtonian conjugate gradient (TNCG) was used as the minimization method, maximum iterations were set to 5000, and Automatic Setup was used for conformational search parameters. The lowest energy conformers for each compound were selected for measurement of indicated dihedral angles and distances.

¹ Allinger, N. L.; Yuh, Y. H.; Lii, J. H. *J. Am. Chem. Soc.* **1989**, *111*, 8551-8566.