

## Supplementary Information

# Phosphine-Catalyzed [4 + 2] Annulation and Vinylogous Addition Reactions between 1,4-Dien-3-ones and 1,1-Dicyanoalkenes

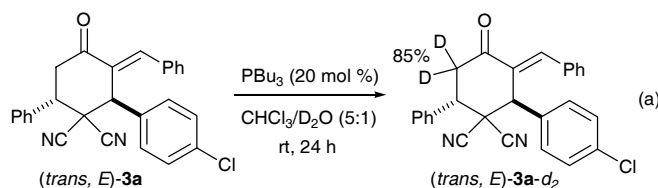
Rong Zhou, Jianfang Wang, Junjun Tian, and Zhengjie He\*

The State Key Laboratory of Elemento-Organic Chemistry and Department of Chemistry, Nankai University, 94 Weijin Road, Tianjin 300071, P. R. China

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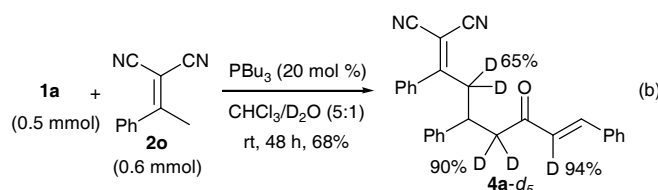
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## I. Experiments for Mechanistic Investigations



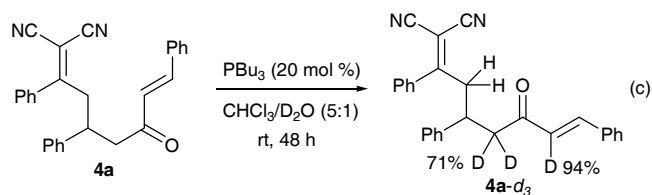
**Experiment (a):** under a  $N_2$  atmosphere, to a solution of (*trans, E*)-**3a** (126 mg, 0.3 mmol) in  $CHCl_3/D_2O$  (3.6 mL, 5:1, V/V) was added  $PBu_3$  (15  $\mu$ L, 0.06 mmol) through a microsyringe. The resulting mixture was stirred at room temperature for 24 h. The reaction mixture was concentrated on a rotary evaporator under reduced pressure and the residue was subjected to column chromatography isolation on silica gel (eluant, petroleum ether–ethyl acetate 10:1) to give a partially deuterated product (*trans, E*)-**3a-d<sub>2</sub>** (Scheme 4, a).

For (*trans, E*)-**3a-d<sub>2</sub>**,  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.91 (s, 1H), 7.51 (d,  $J = 8.4$  Hz, 2H), 7.43–7.29 (m, 10H), 7.13 (d,  $J = 7.2$  Hz, 2H), 4.94 (s, 1H), 3.56 (s, 1H), 3.30 (d,  $J = 13.6$  Hz, 0.15 H), 3.13 (d,  $J = 4.9$  Hz, 0.15 H).



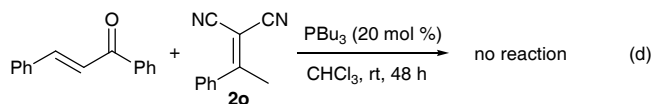
**Experiment (b):** under a  $N_2$  atmosphere, to a solution of styryl ketone **1a** (117 mg, 0.5 mmol) and activated alkenes **2o** (101 mg, 0.6 mmol) in  $CHCl_3/D_2O$  (6 mL, 5:1) was added  $PBu_3$  (25  $\mu$ L, 0.1 mmol). The resulting mixture was stirred at room temperature until **1a** was completely consumed (monitored by TLC). The mixture was concentrated on a rotary evaporator under reduced pressure, and the residue was subjected to column chromatography isolation on silica gel (gradient eluant, petroleum ether–ethyl acetate 20:1–10:1) to give a partially deuterated vinylogous Michael adduct **4a-d<sub>5</sub>** in 68% yield.

For **4a-d<sub>5</sub>**,  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.61–7.45 (m, 6H), 7.44–7.34 (m, 5H), 7.33–7.21 (m, 3H), 6.99 (d,  $J = 6.7$  Hz, 2H), 6.65 (d,  $J = 16.2$  Hz, 0.06 H), 3.54 (d,  $J = 4.4$  Hz, 0.1H), 3.31 (d,  $J = 10.2$  Hz, 0.1H), 3.23 (d,  $J = 6.2$  Hz, 1H), 3.11–2.98 (m, 0.70 H).

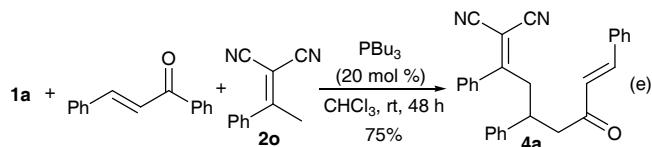


**Experiment (c):** under the same conditions as above, the normal vinylogous Michael adduct **4a** (132 mg, 0.33 mmol) was treated with  $\text{PBu}_3$  (16  $\mu\text{L}$ , 0.066 mmol) in  $\text{CHCl}_3/\text{D}_2\text{O}$  (3 mL, 5:1) at room temperature for 48 h. After the same work-up and chromatographic isolation as that of experiment (b), a partially deuterated product **4a-d<sub>3</sub>** was obtained in almost quantitative yield.

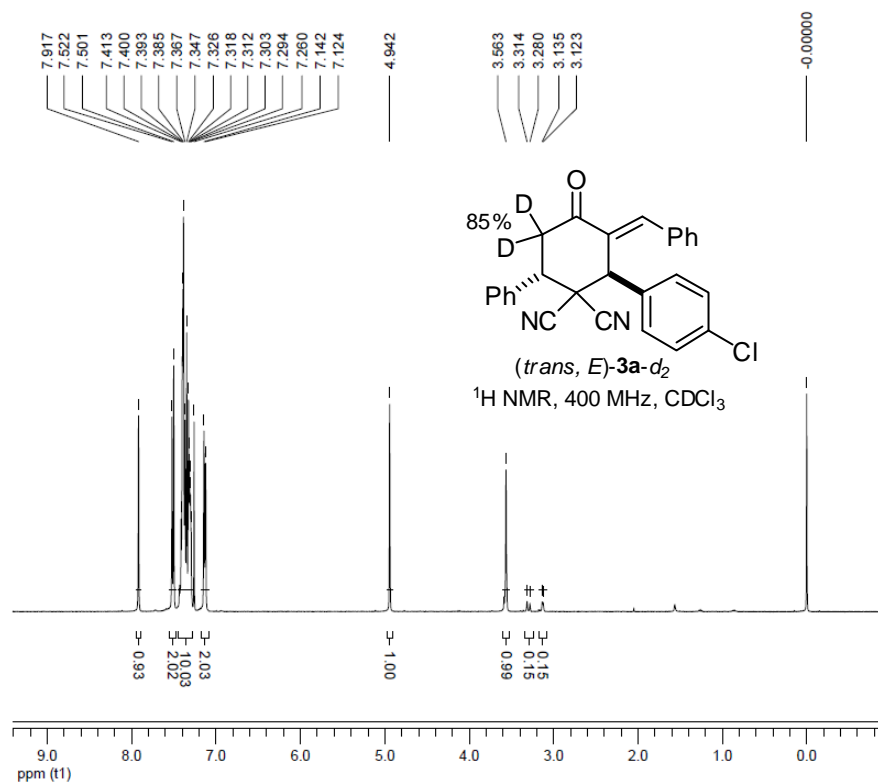
For **4a-d<sub>3</sub>**,  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.61–7.45 (m, 6H), 7.44–7.34 (m, 5H), 7.33–7.21 (m, 3H), 6.99 (d,  $J = 7.1$  Hz, 2H), 6.65 (d,  $J = 16.2$  Hz, 0.06 H), 3.54 (d,  $J = 4.4$  Hz, 0.29H), 3.31 (d,  $J = 10.5$  Hz, 0.29H), 3.26–3.21 (m, 1H), 3.10–2.96 (m, 2H).



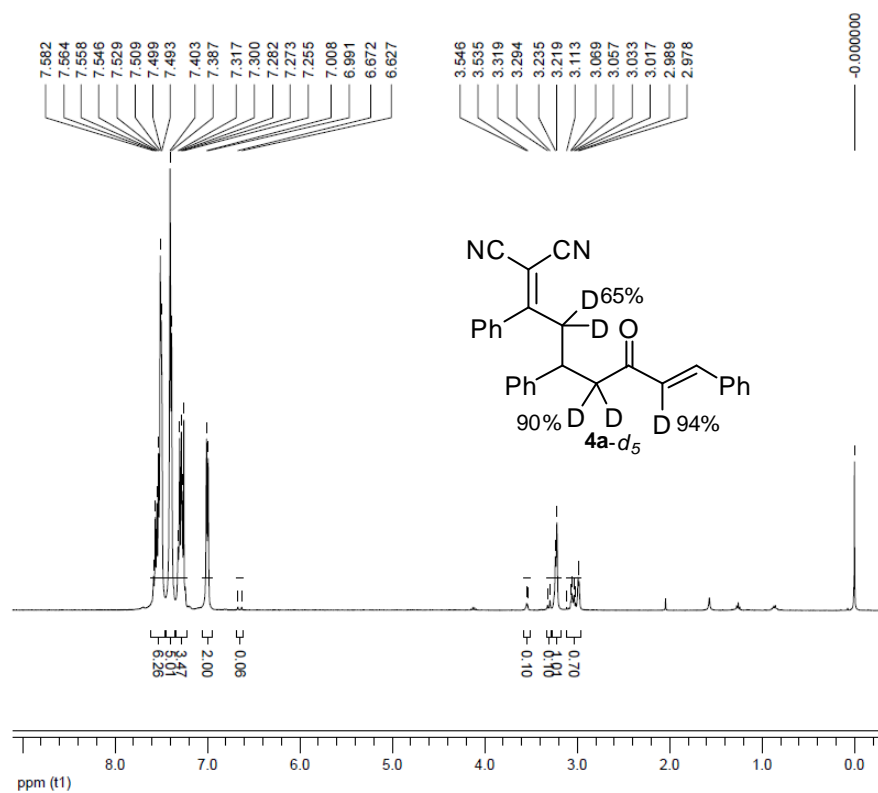
**Experiment (d):** under a  $\text{N}_2$  atmosphere, to a solution of chalcone (104 mg, 0.5 mmol) and activated alkene **2o** (101 mg, 0.6 mmol) in  $\text{CHCl}_3$  (5 mL) was added  $\text{PBu}_3$  (25  $\mu\text{L}$ , 0.1 mmol). The resulting mixture was stirred at room temperature for 48 h. Except starting materials, no vinylogous Michael adduct was detected by TLC during the entire process.



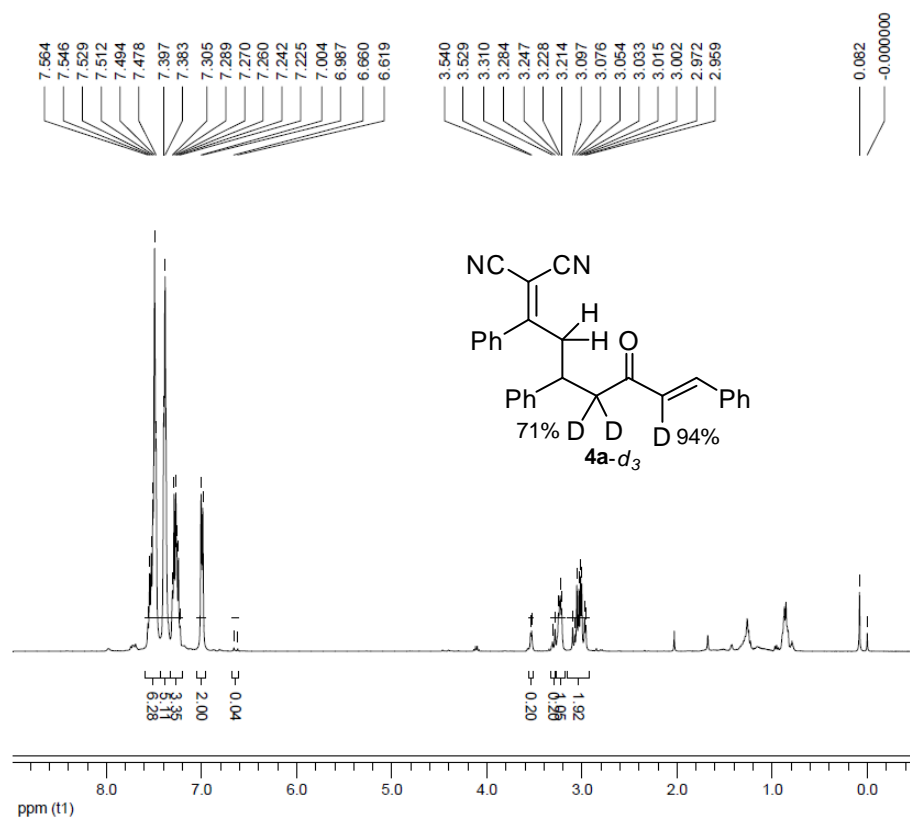
**Experiment (e):** under a  $\text{N}_2$  atmosphere, to a solution of **1a** (117 mg, 0.5 mmol), chalcone (104 mg, 0.5 mmol), and activated alkene **2o** (101 mg, 0.6 mmol) in  $\text{CHCl}_3$  (5 mL) was added  $\text{PBu}_3$  (25  $\mu\text{L}$ , 0.1 mmol). The resulting mixture was stirred at room temperature for 48 h. The reaction mixture was concentrated on a rotary evaporator under reduced pressure, and the residue was subjected to column chromatography isolation on silica gel (gradient eluant, petroleum ether–ethyl acetate 20:1–10:1) to give vinylogous Michael adduct **4a** in 75% yield and a complete recovery of chalcone.



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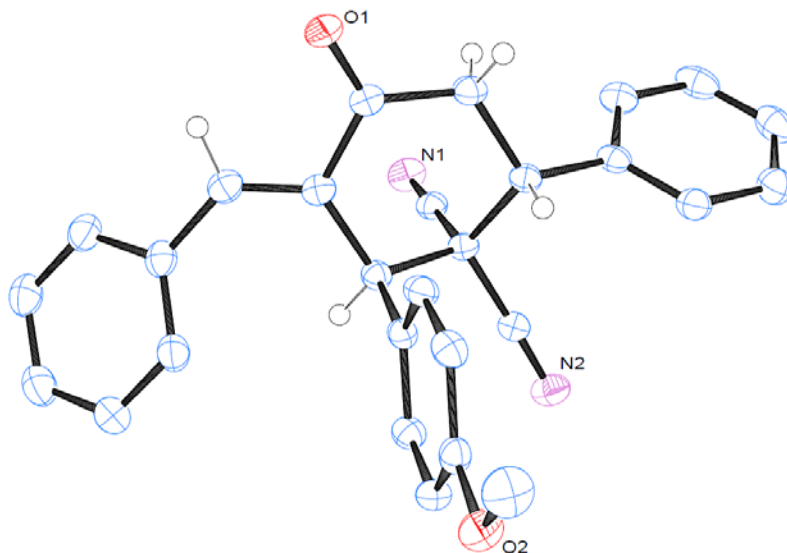
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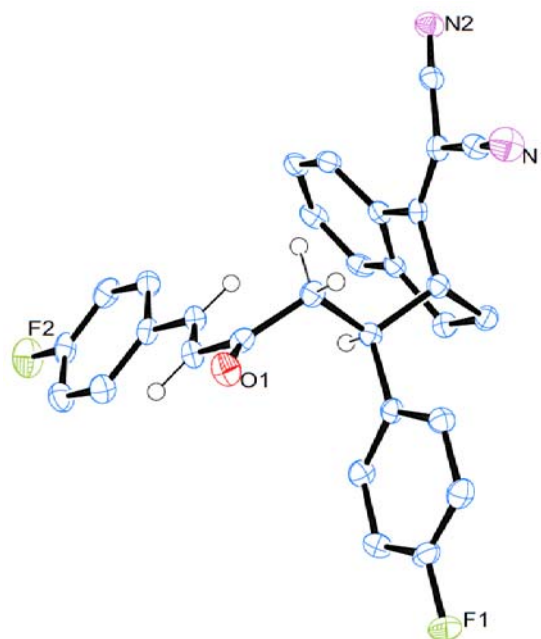
## II. ORTEP Drawings of (*trans, E*)-**3b** and **4b**

**Table 1. Crystal data and structure refinement for (*trans, E*)-**3b**.**



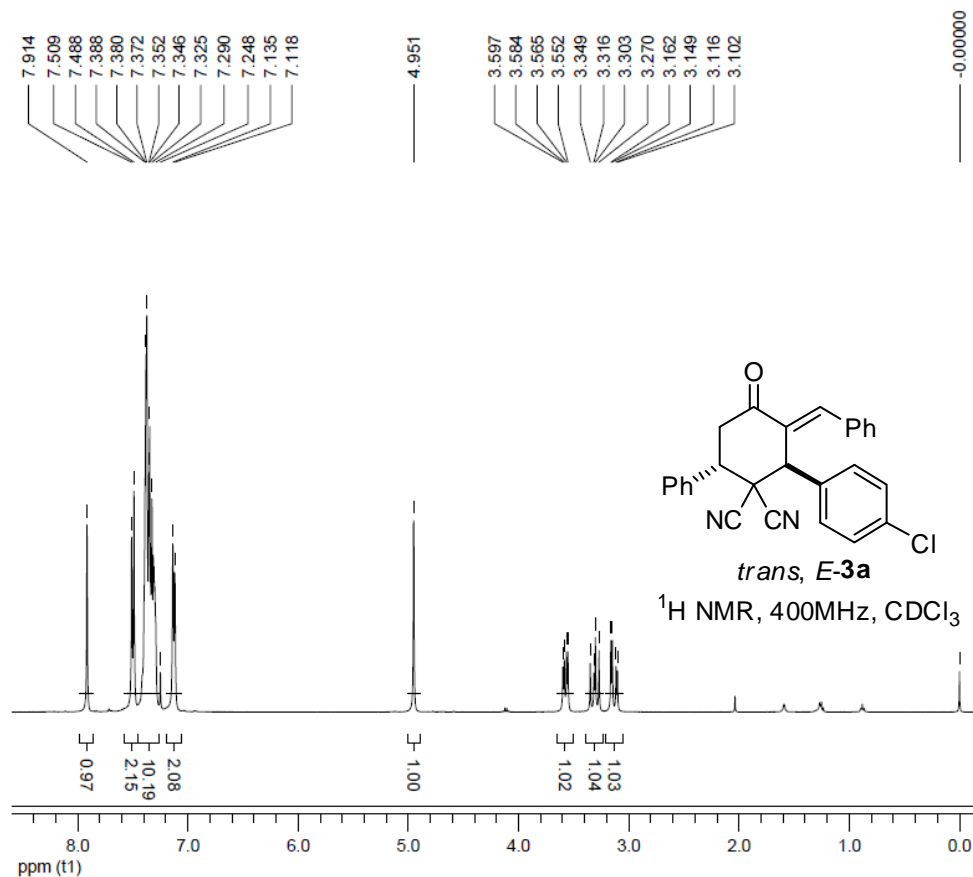
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Empirical formula	C <sub>28</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>
Formula weight	418.48
Temperature	113(2) K
Wavelength	0.71075 Å
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 11.0620(10) Å    α = 90°. b = 16.7680(16) Å    β = 105.781(4)°. c = 12.3210(13) Å    γ = 90°.
Volume	2199.3(4) Å <sup>3</sup>
Z, Calculated density	4, 1.264 Mg/m <sup>3</sup>
Absorption coefficient	0.080 mm <sup>-1</sup>
F(000)	880
Crystal size	0.22 x 0.20 x 0.18 mm <sup>3</sup>
Theta range for data collection	1.91 to 27.90°
Limiting indices	-14 ≤ h ≤ 14, -21 ≤ k ≤ 22, -15 ≤ l ≤ 16
Reflections collected / unique	20943 / 5255 [R(int) = 0.0322]
Completeness to the θ = 27.90°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9857 and 0.9826
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5255 / 0 / 290
Goodness-of-fit on F <sup>2</sup>	0.995
Final R indices [I > 2σ(I)]	R1 = 0.0381, wR2 = 0.0889
R indices (all data)	R1 = 0.0524, wR2 = 0.0958
Largest diff. peak and hole	0.254 and -0.145 e. Å <sup>-3</sup>

**Table 2. Crystal data and structure refinement for 4b.**



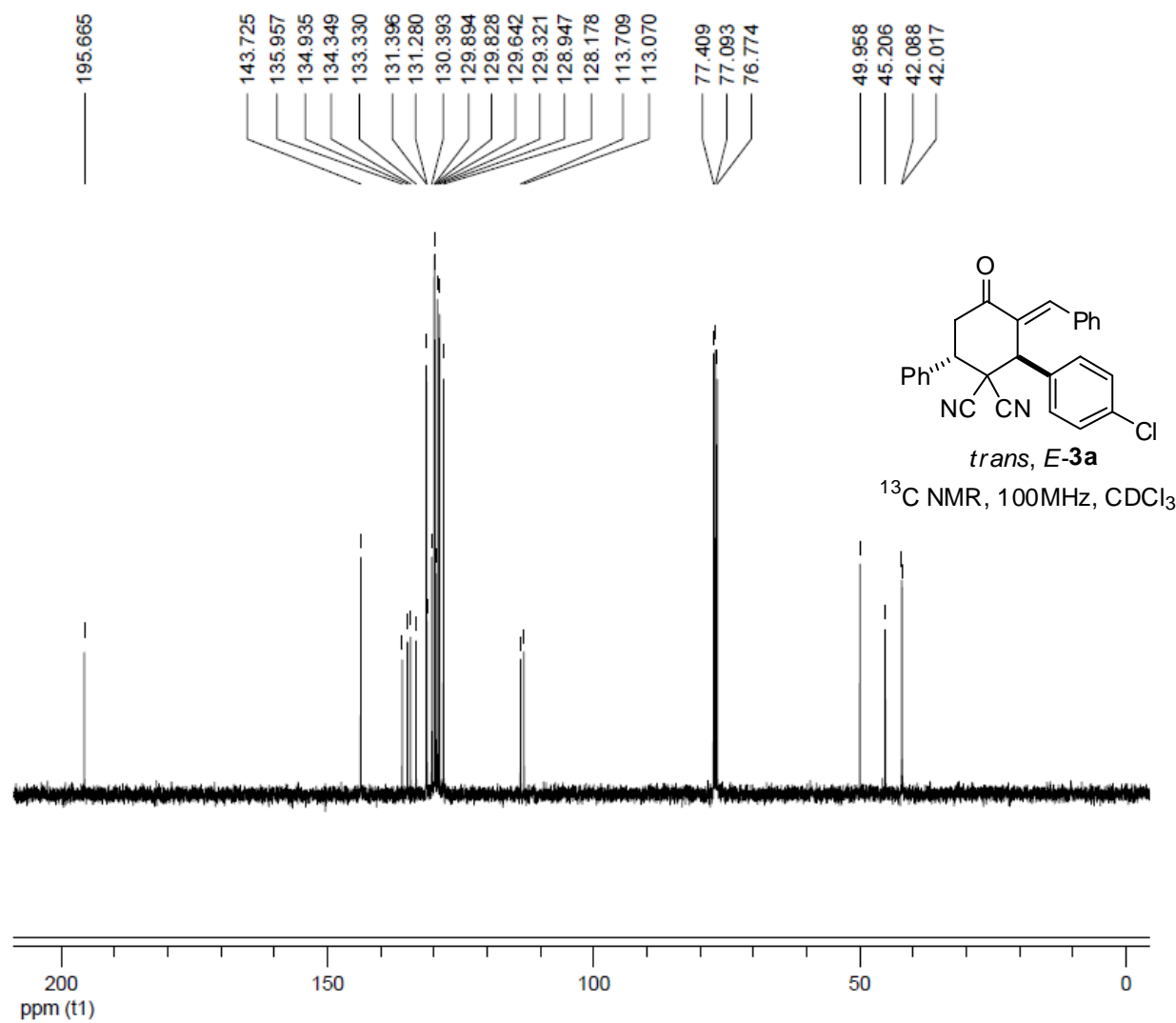
Identification code	<b>4b</b>
Empirical formula	C <sub>30</sub> H <sub>22</sub> F <sub>2</sub> N <sub>2</sub> O
Formula weight	464.50
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 12.828(2) Å    α = 90°. b = 11.141(2) Å    β = 103.208(10) (4)°. c = 16.665(3) Å    γ = 90°.
Volume	2318.7(7) Å <sup>3</sup>
Z, Calculated density	4, 1.331 Mg/m <sup>3</sup>
Absorption coefficient	0.092 mm <sup>-1</sup>
F(000)	968
Crystal size	0.20 x 0.18 x 0.12 mm <sup>3</sup>
Theta range for data collection	2.45 to 27.87°
Limiting indices	-13 ≤ h ≤ 16, -14 ≤ k ≤ 13, -21 ≤ l ≤ 21
Reflections collected / unique	11067 / 4433 [R(int) = 0.0302]
Completeness to the θ = 27.87°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9890 and 0.9818
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4433 / 2 / 316
Goodness-of-fit on F <sup>2</sup>	1.043
Final R indices [I > 2σ(I)]	R1 = 0.0285, wR2 = 0.0599
R indices (all data)	R1 = 0.0332, wR2 = 0.0606
Largest diff. peak and hole	0.221 and -0.127 e. Å <sup>-3</sup>

### III. $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra of 3, 4, 5 and 6



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Document's Title:

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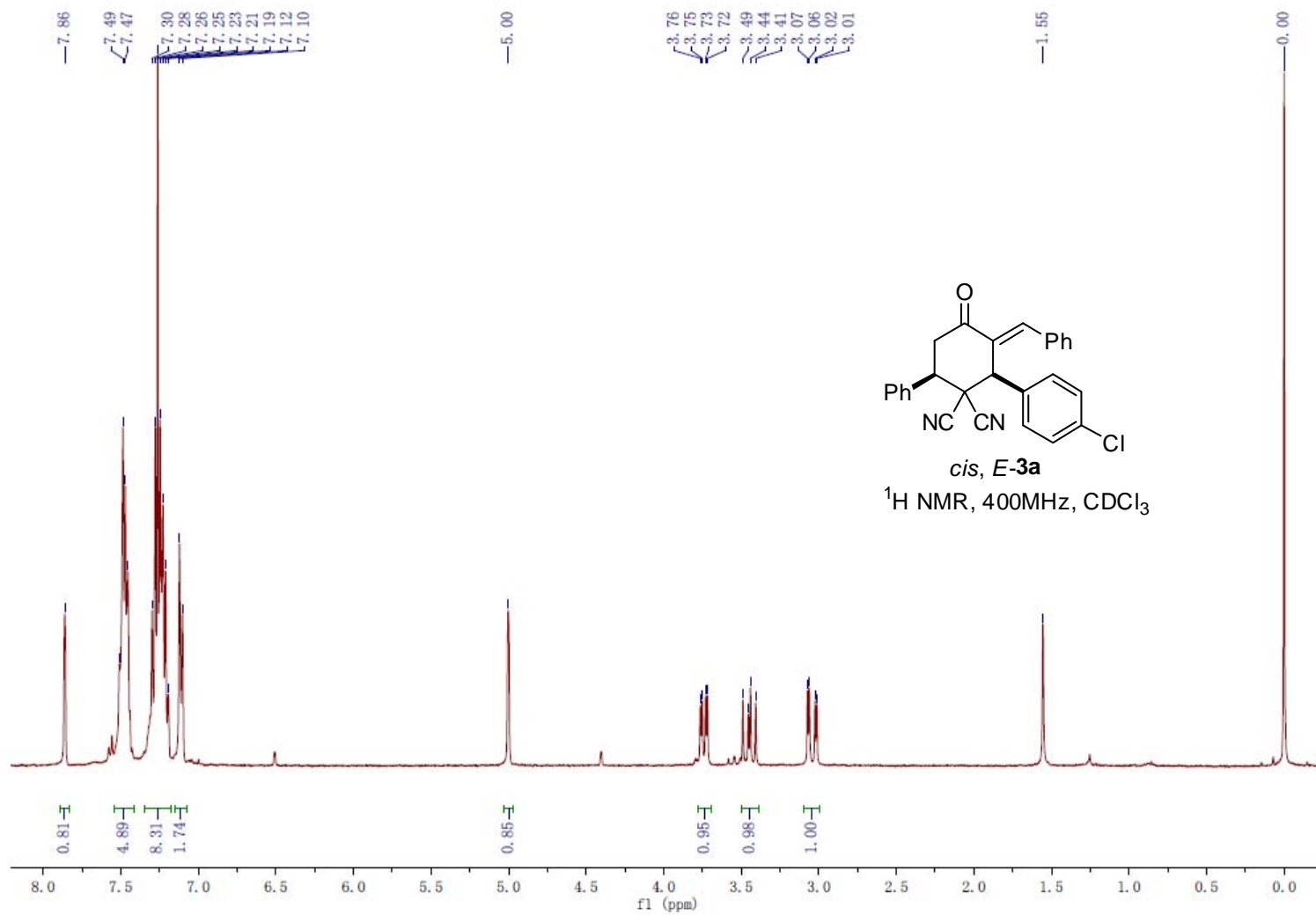
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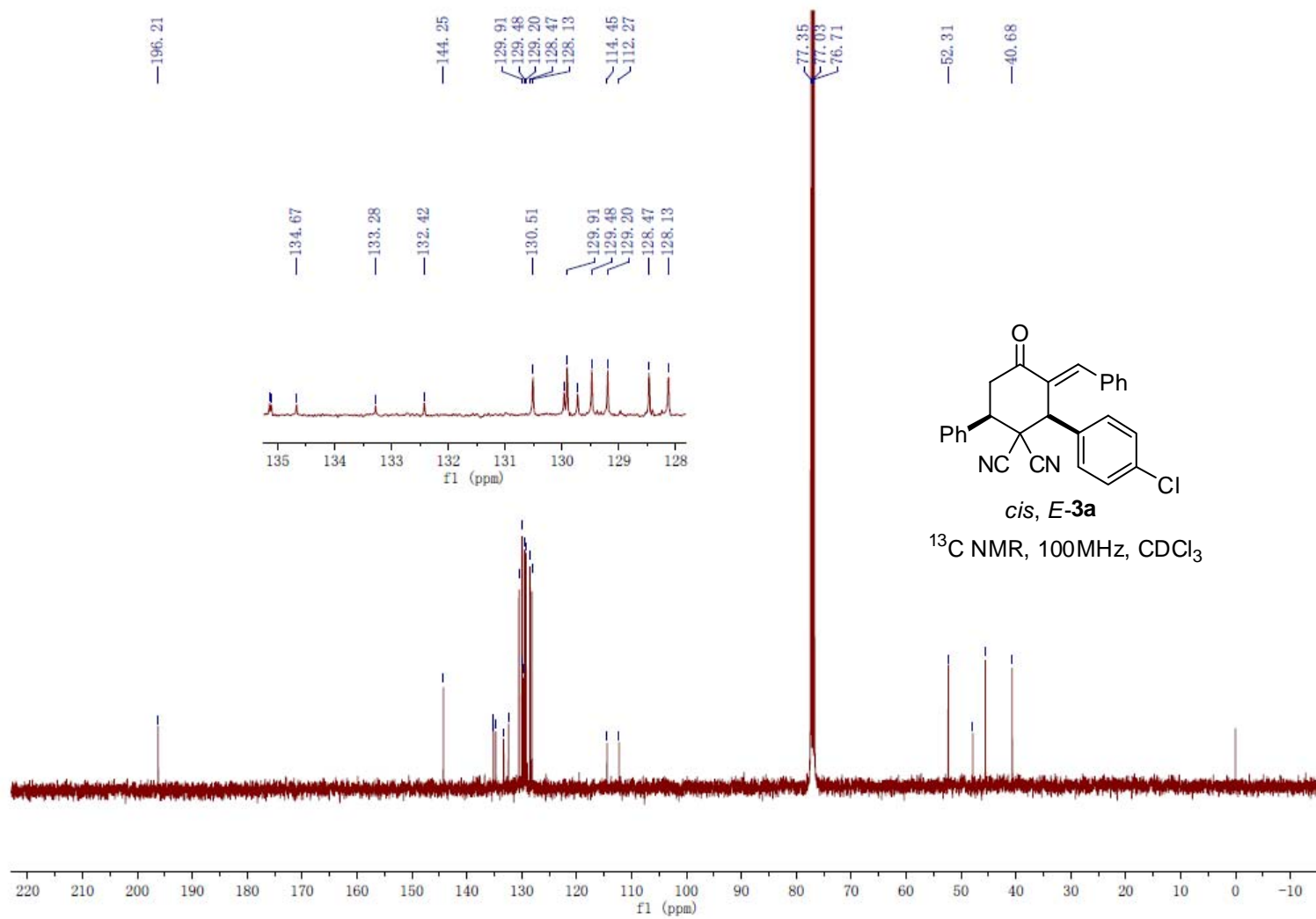
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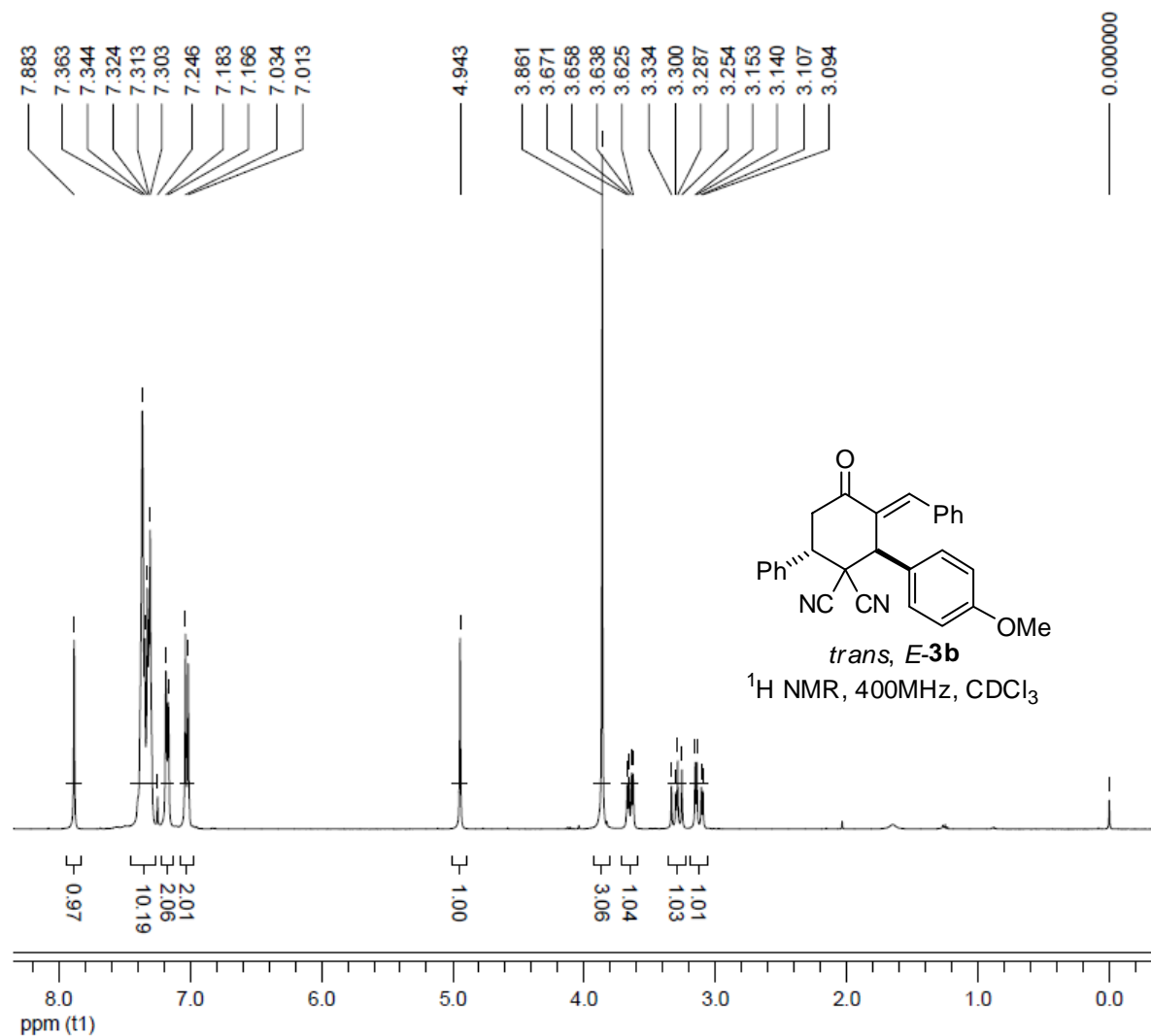
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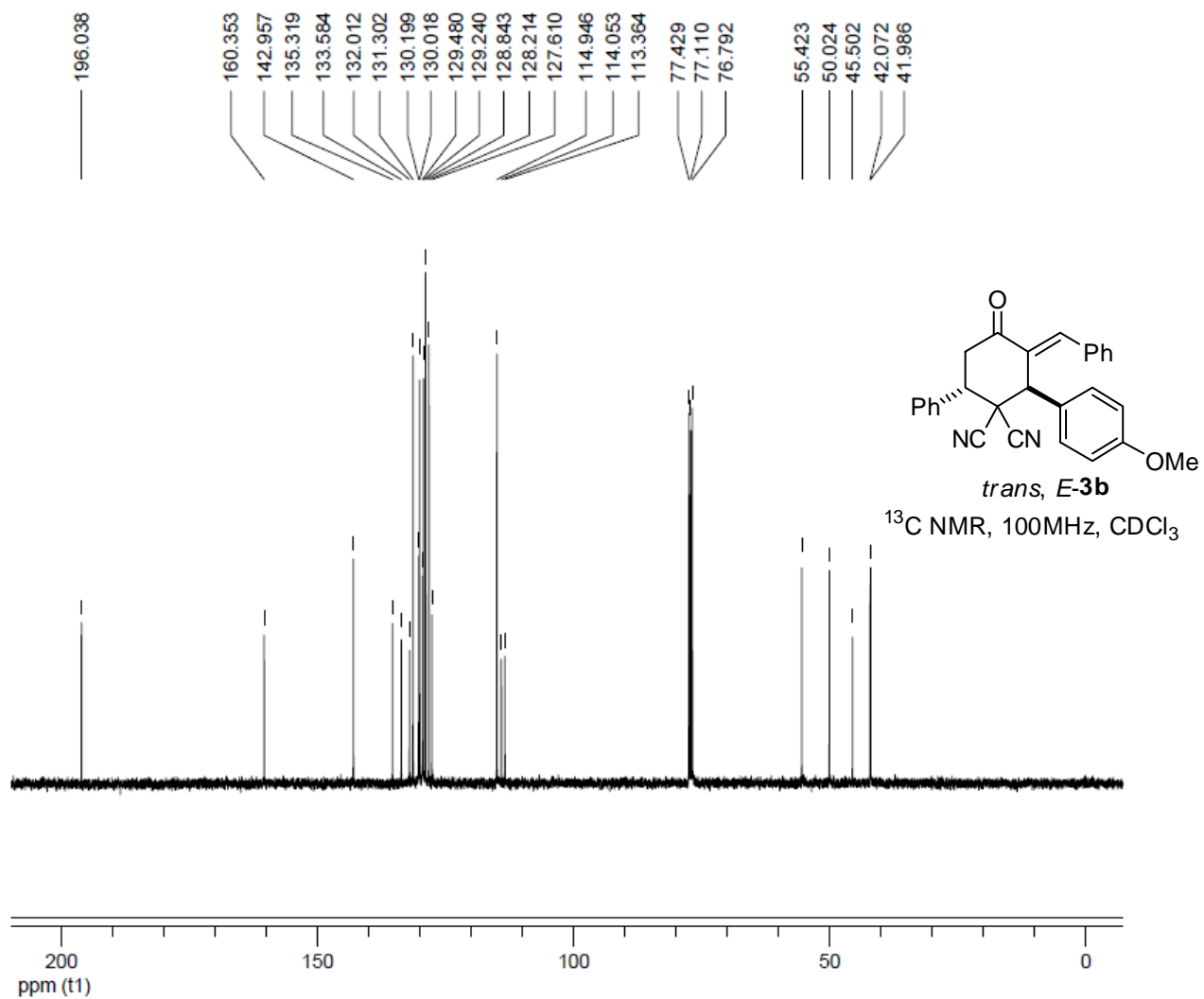
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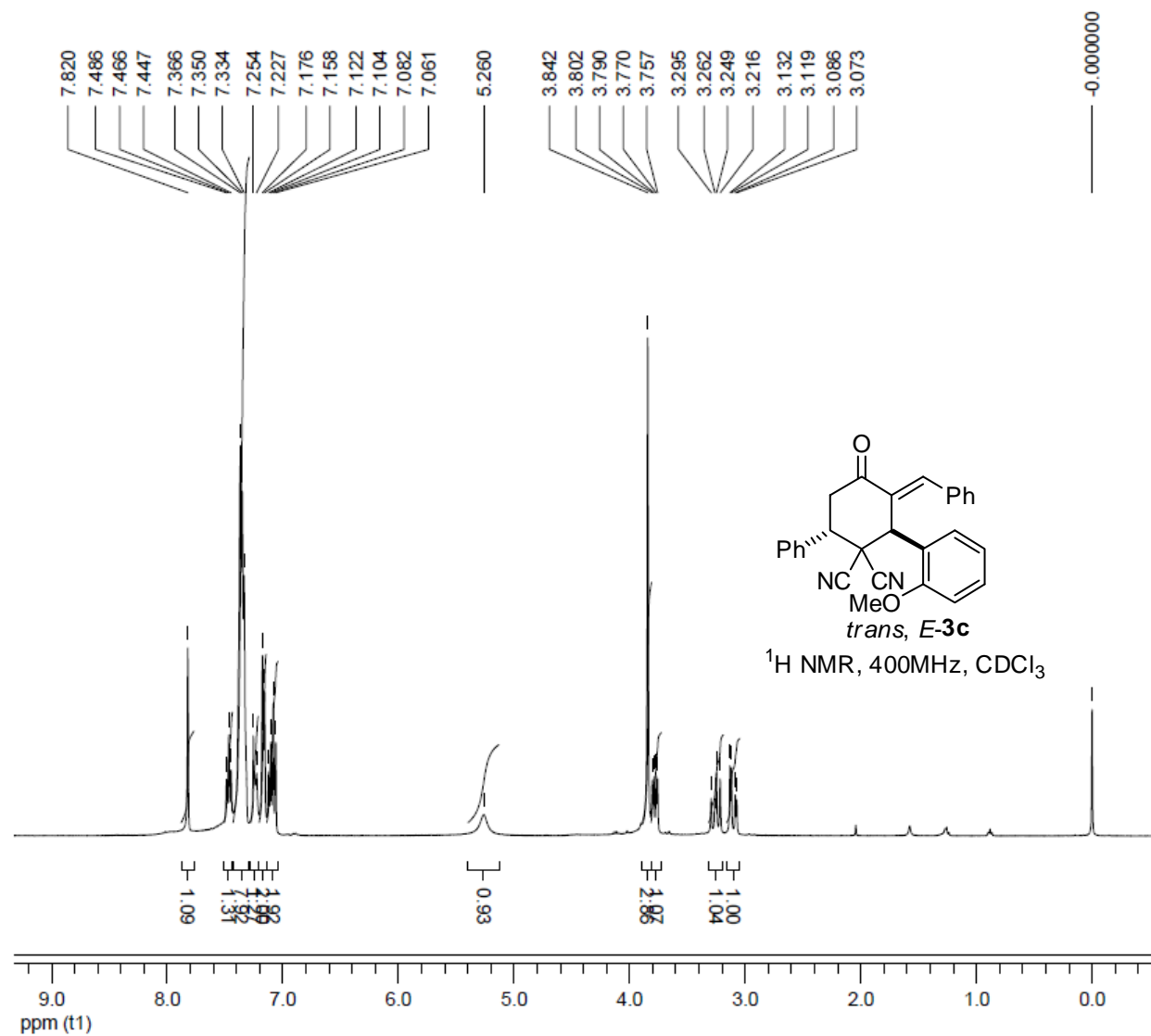
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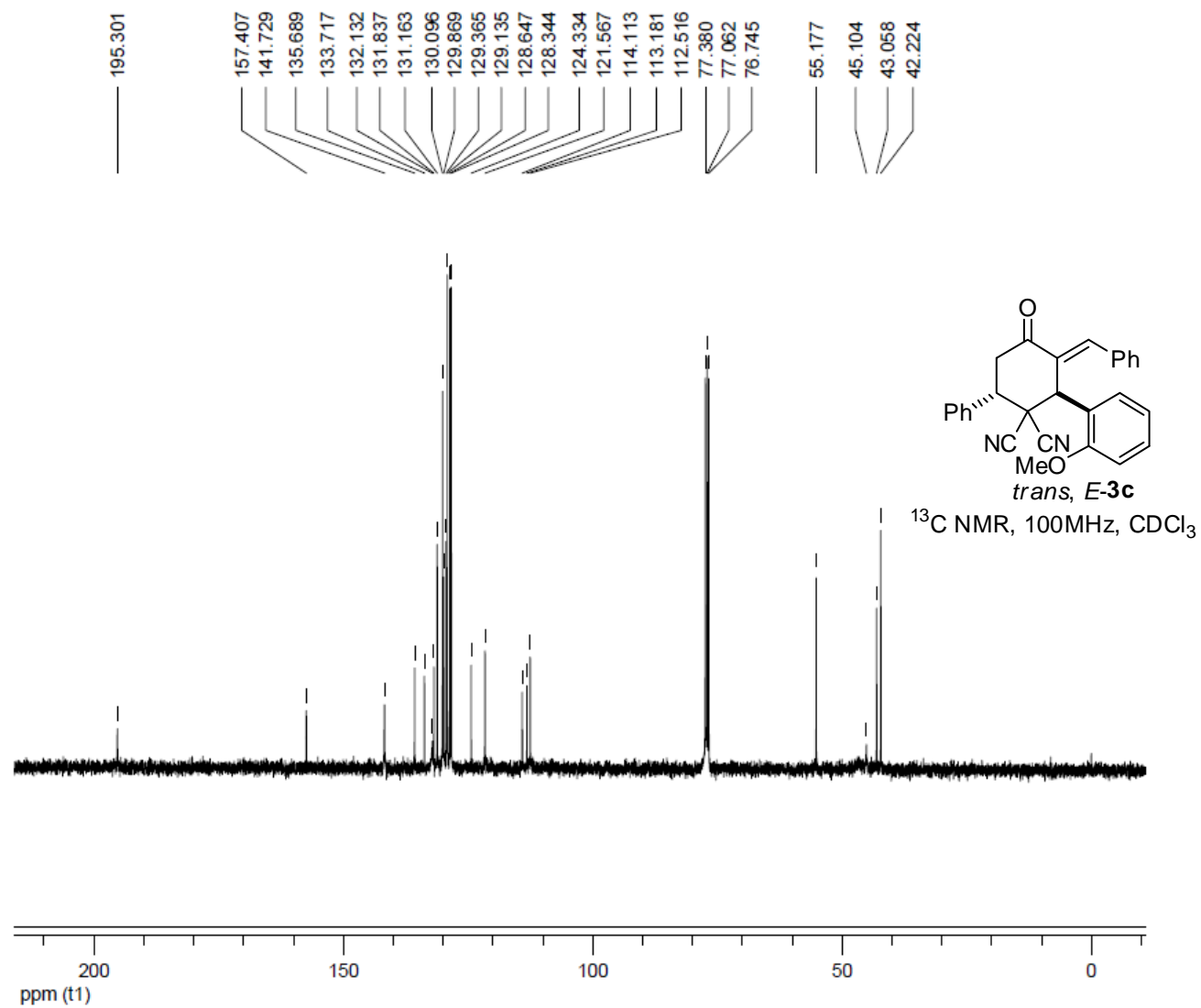
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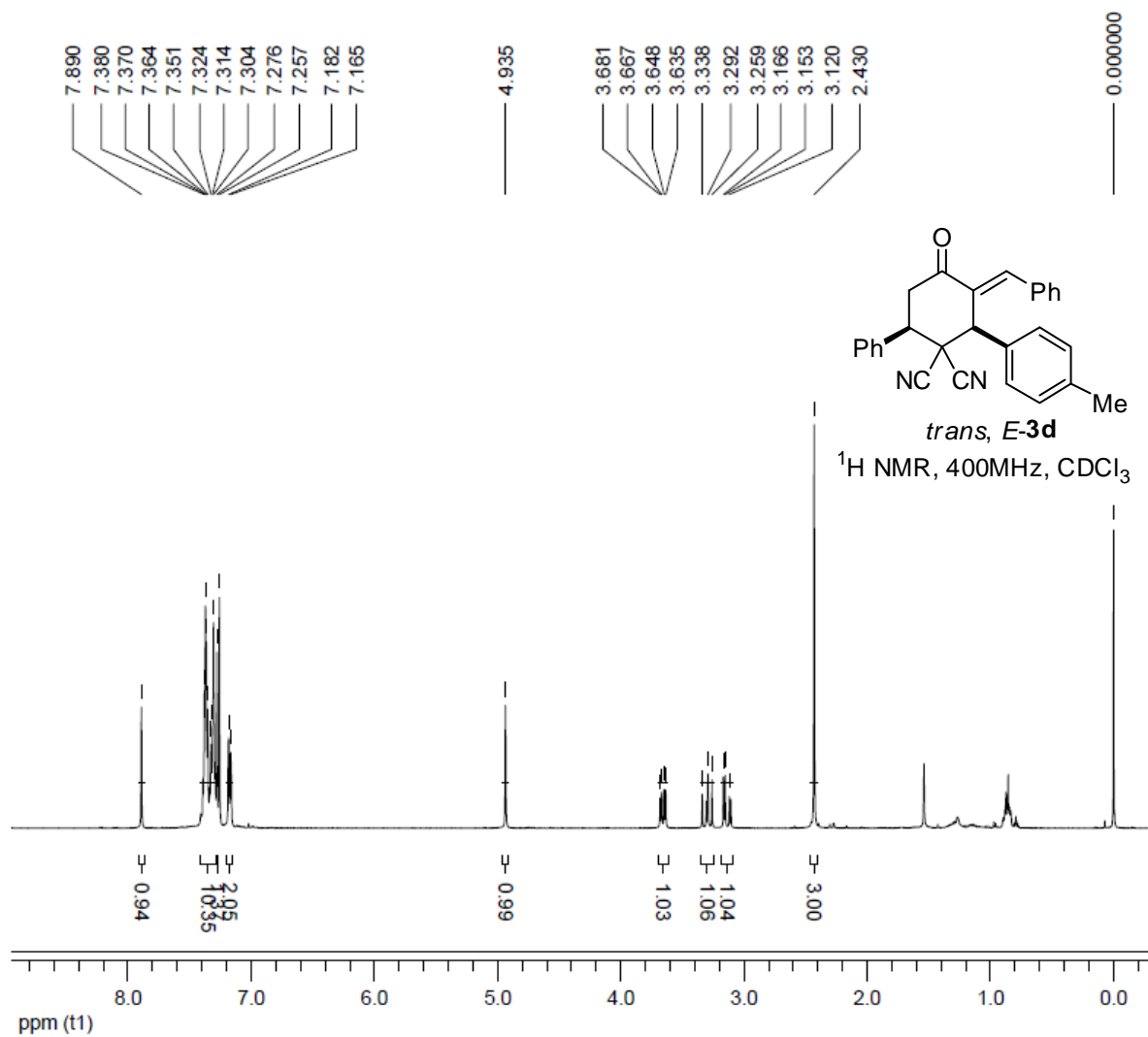
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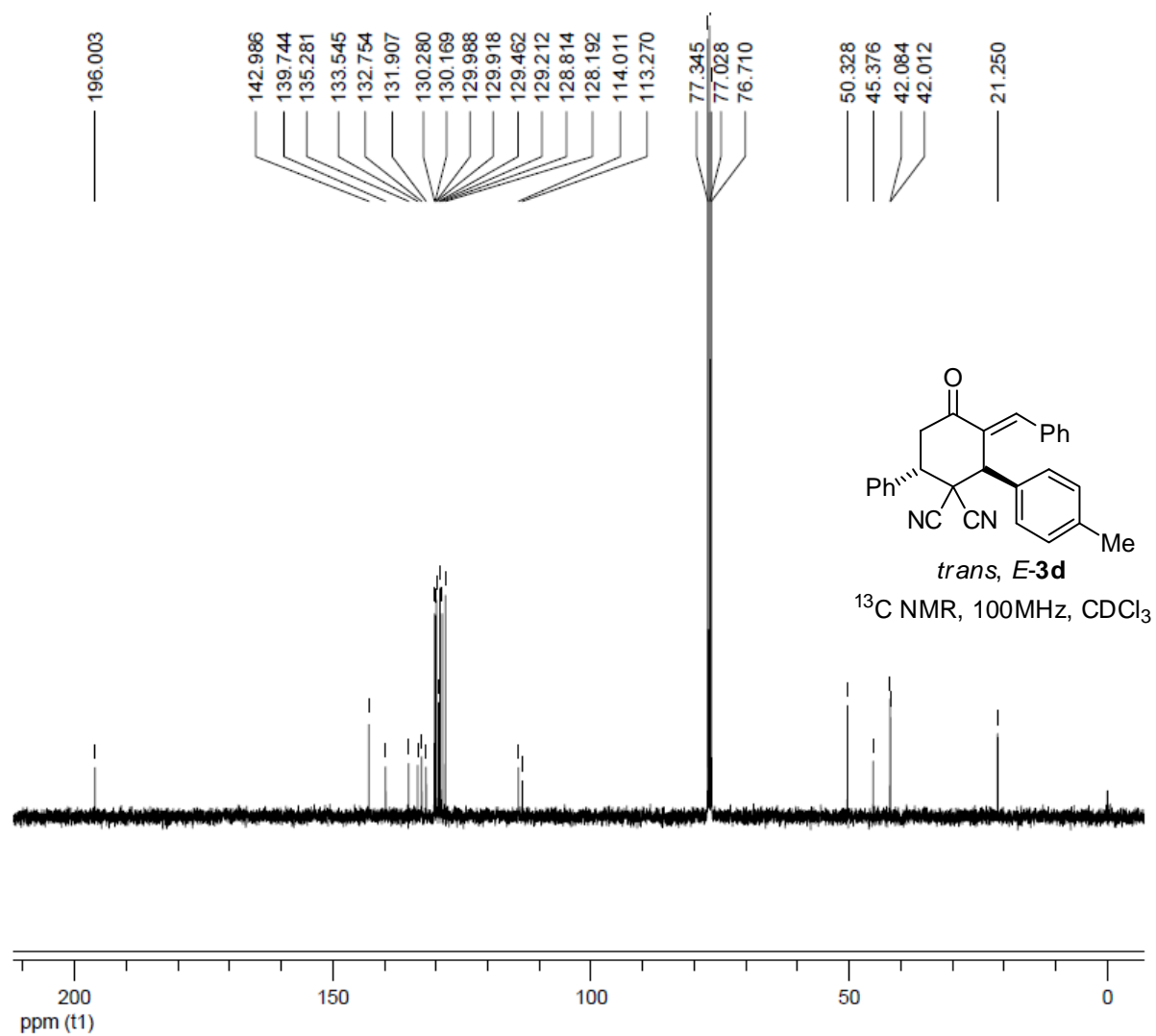
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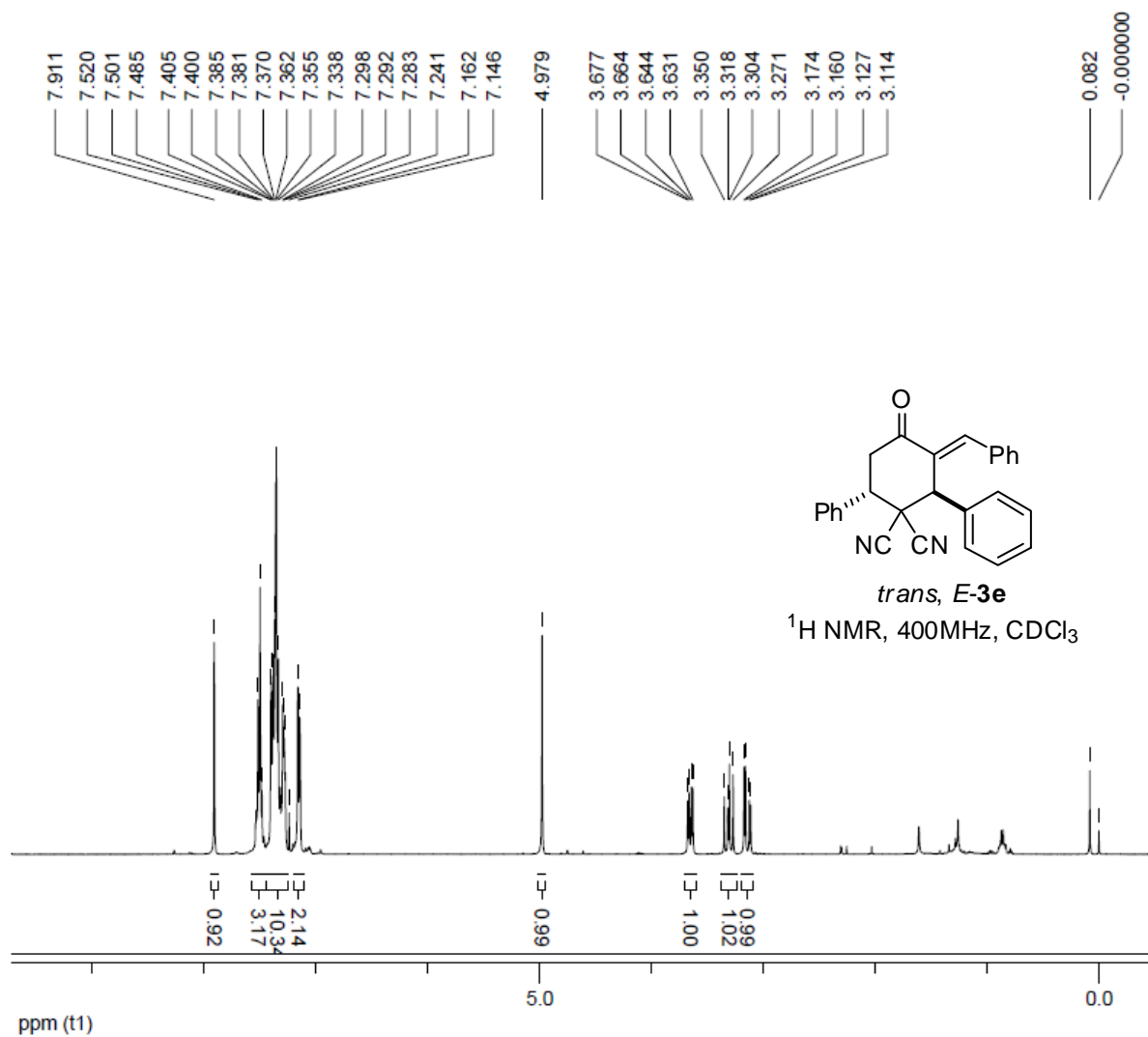
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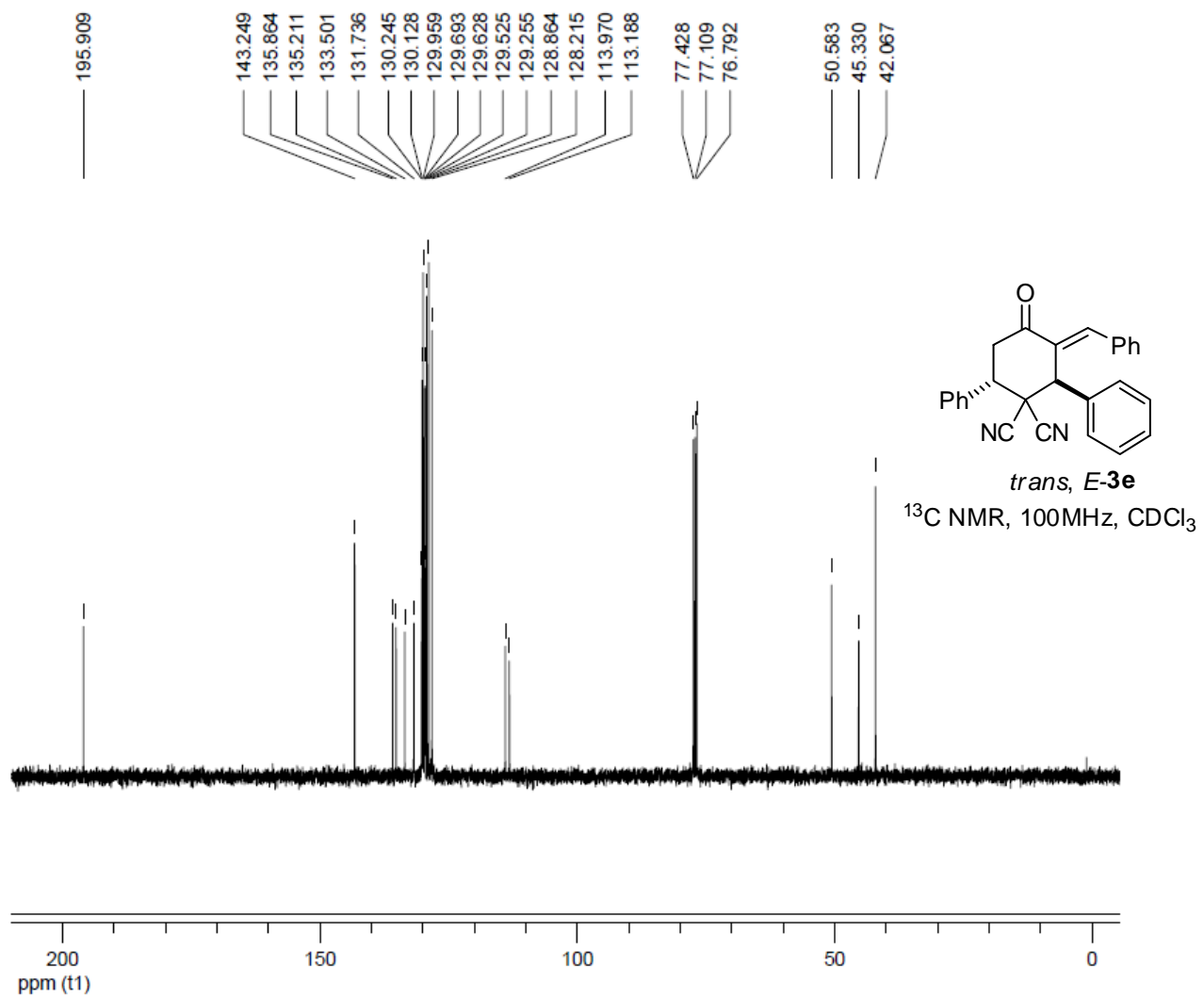
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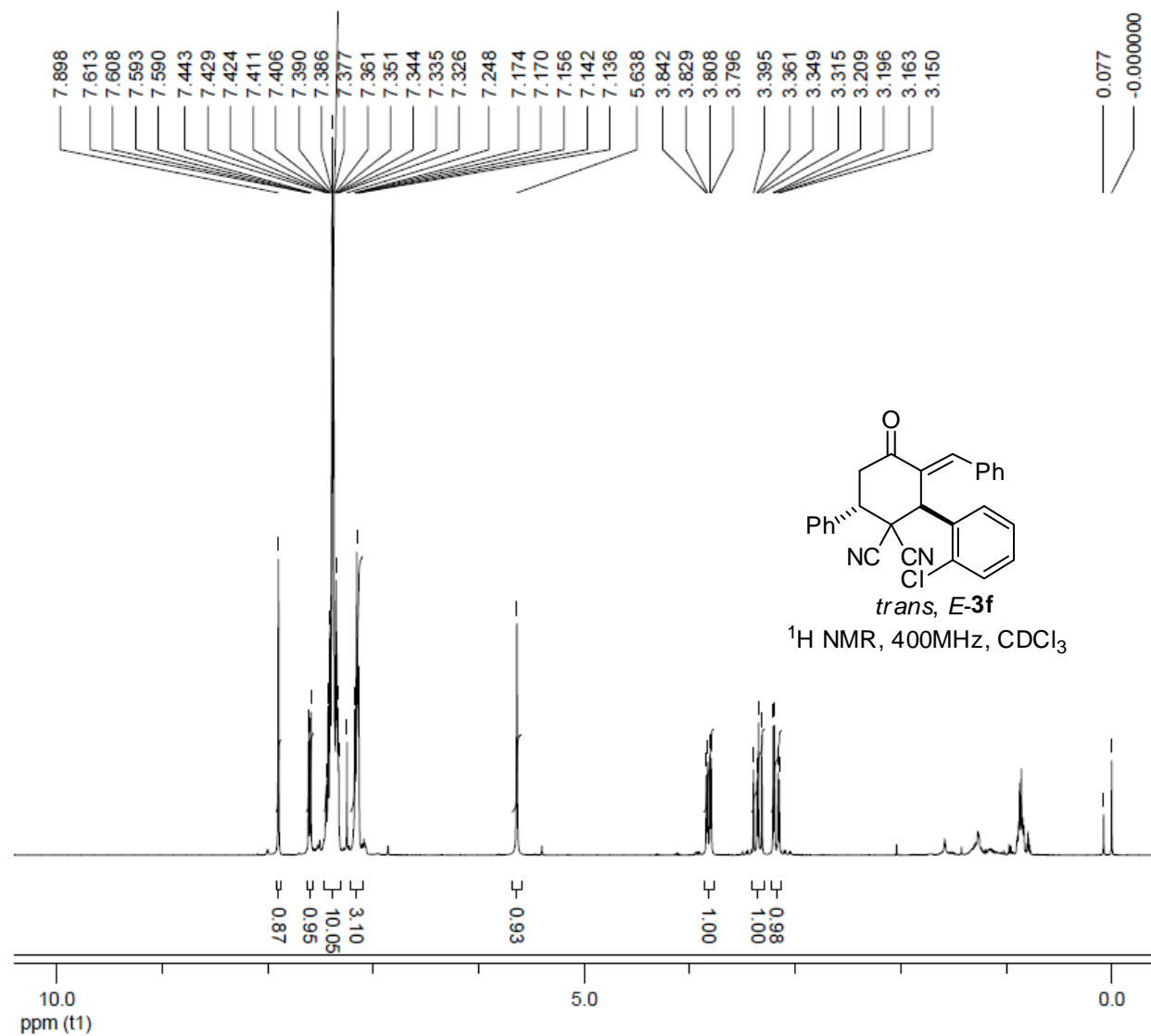
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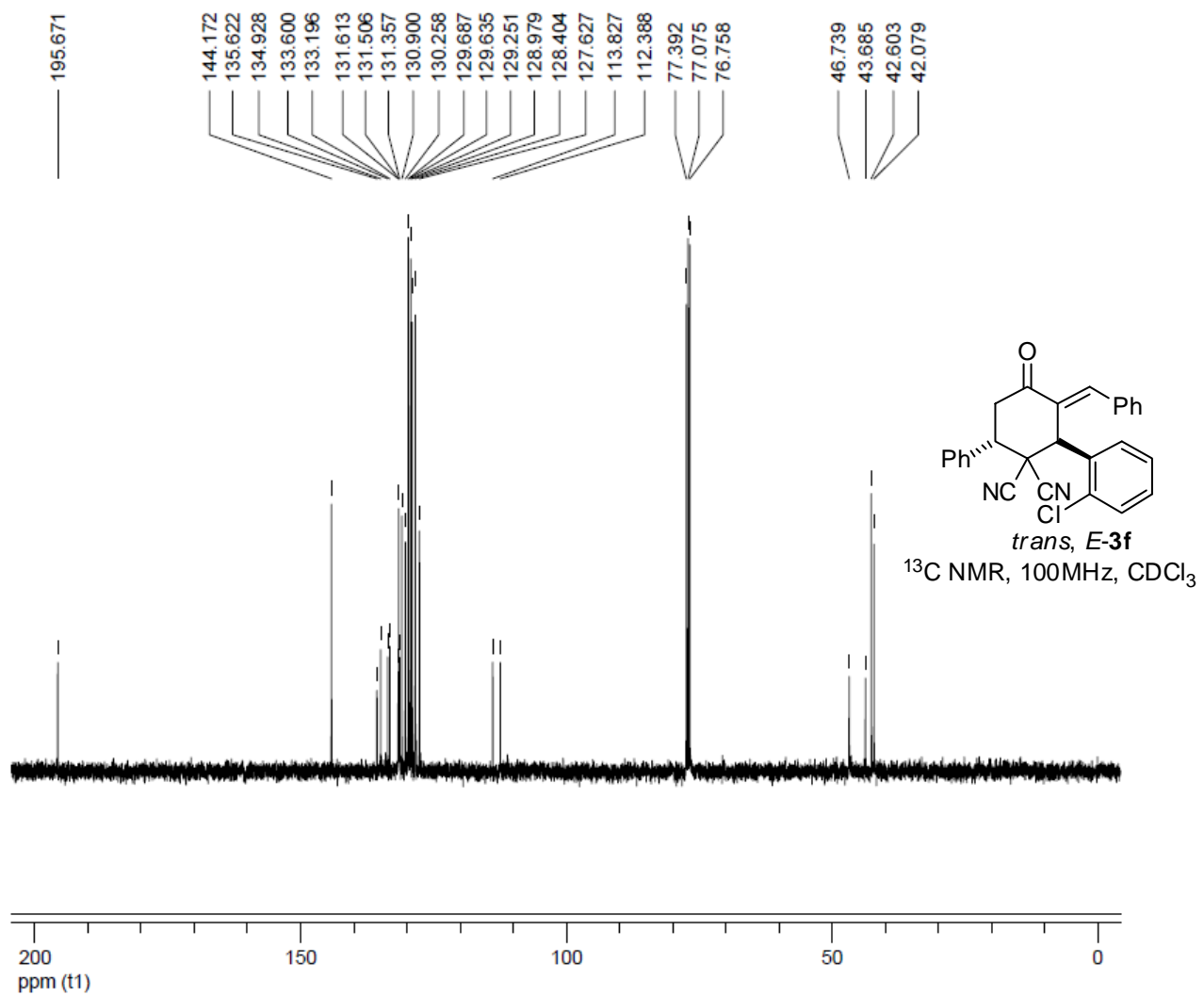
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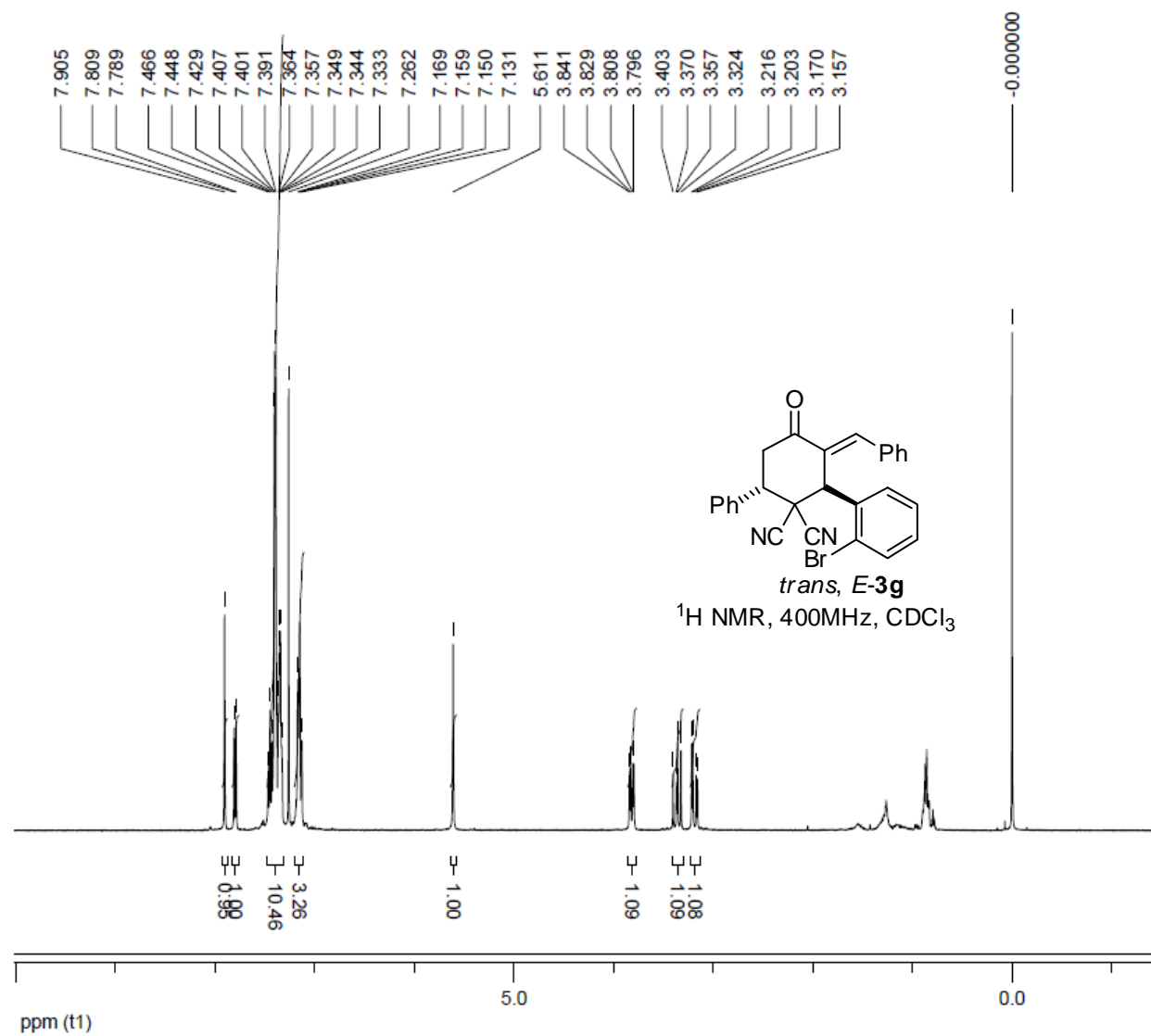
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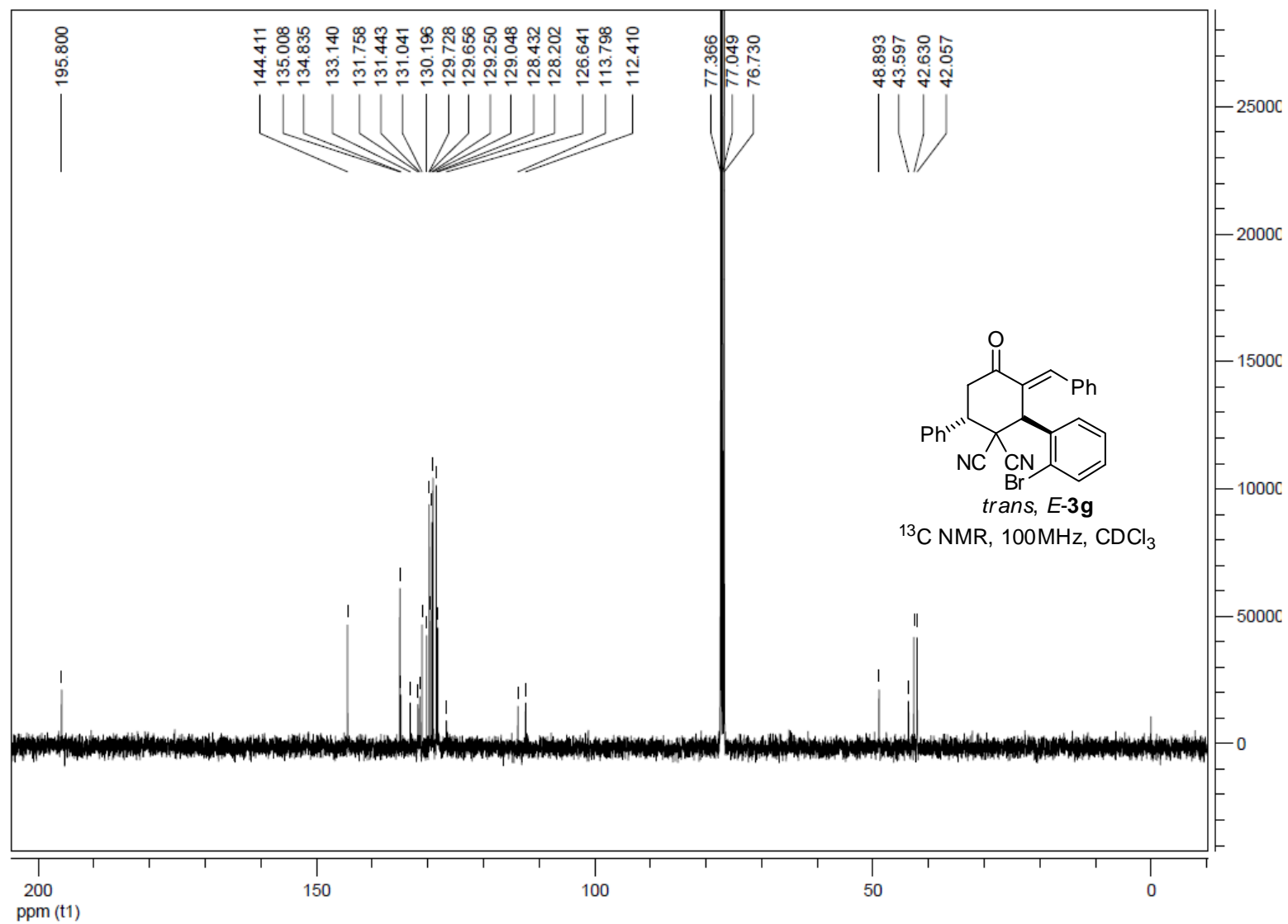
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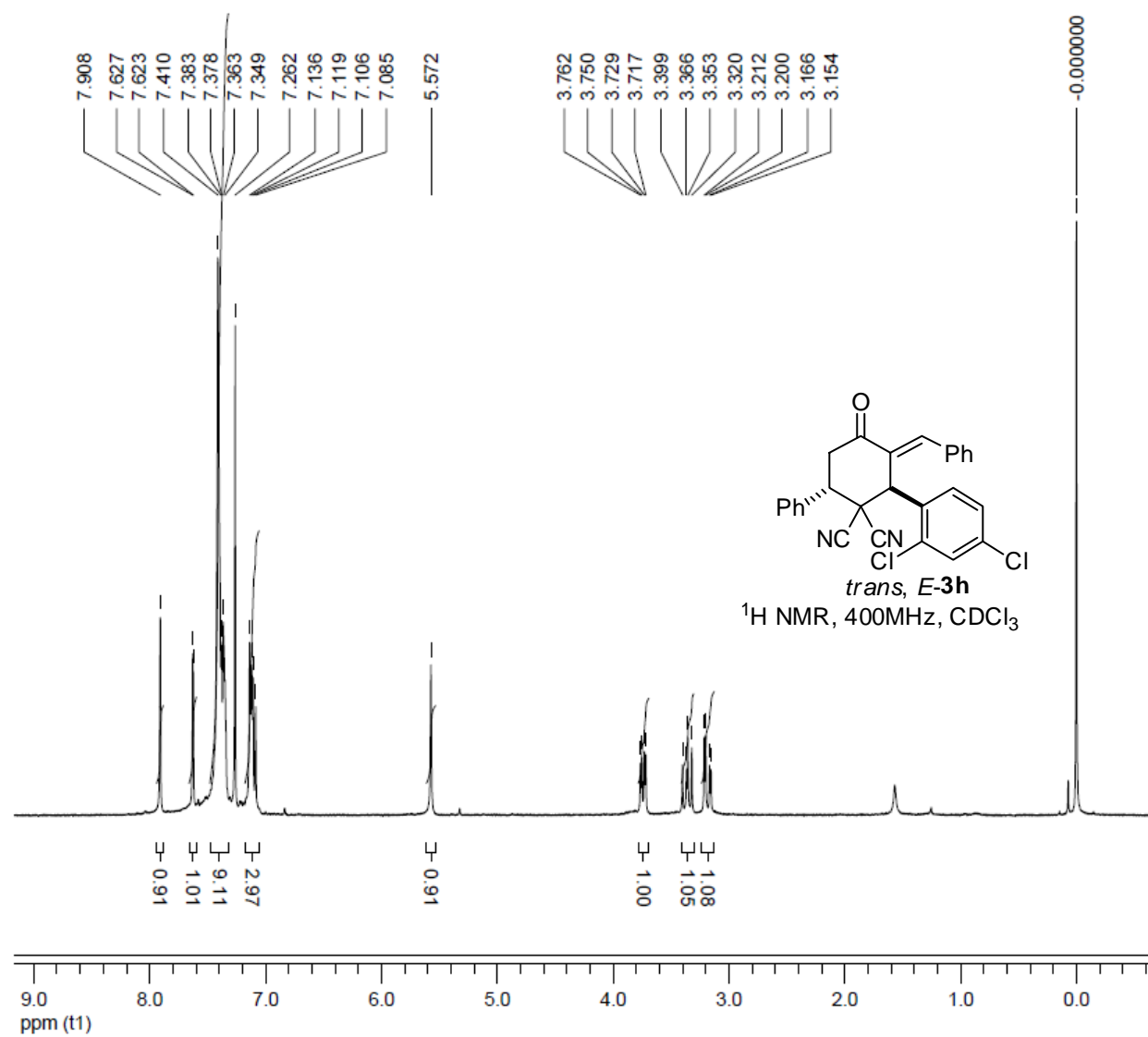
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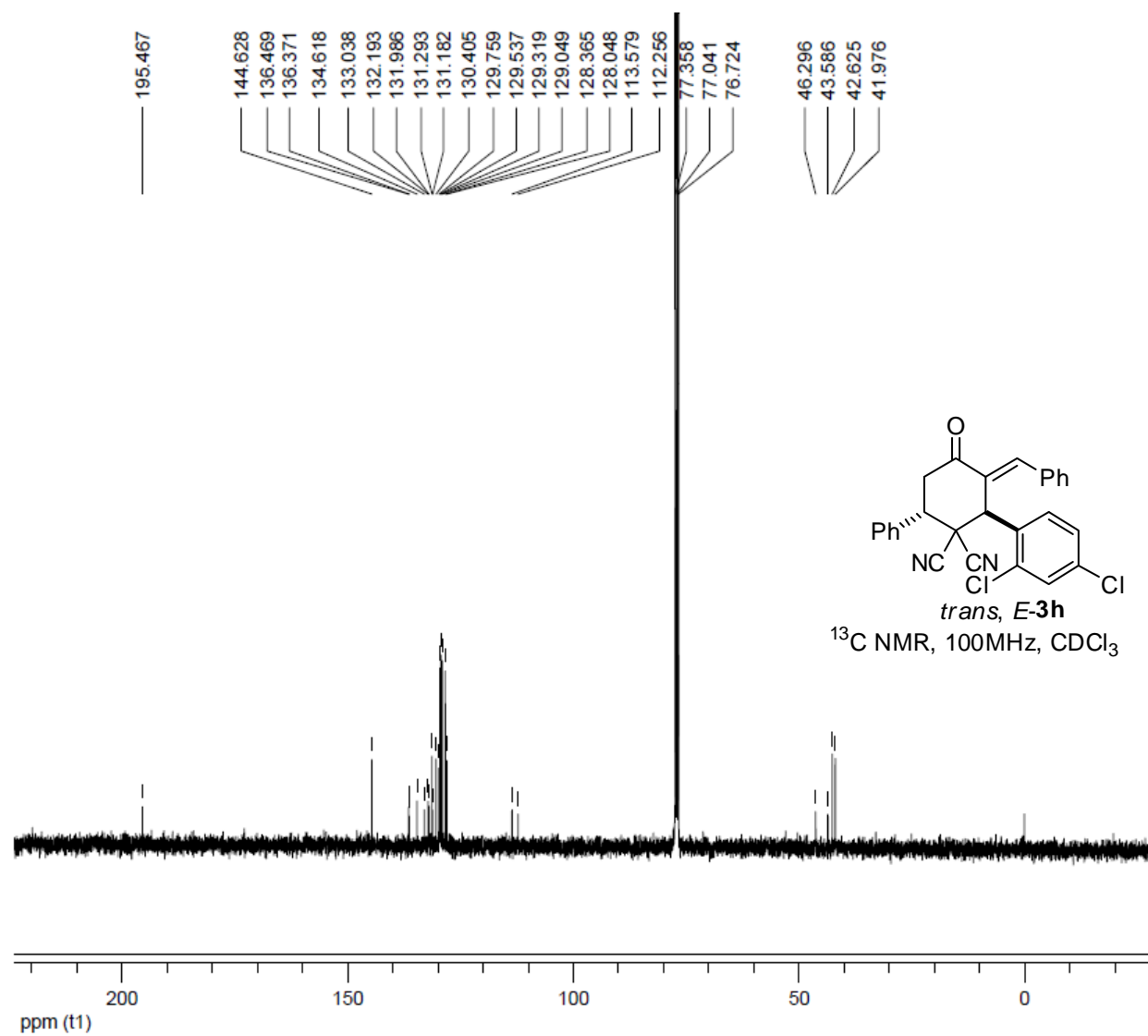
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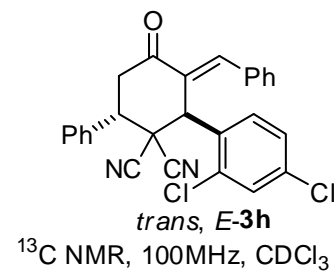


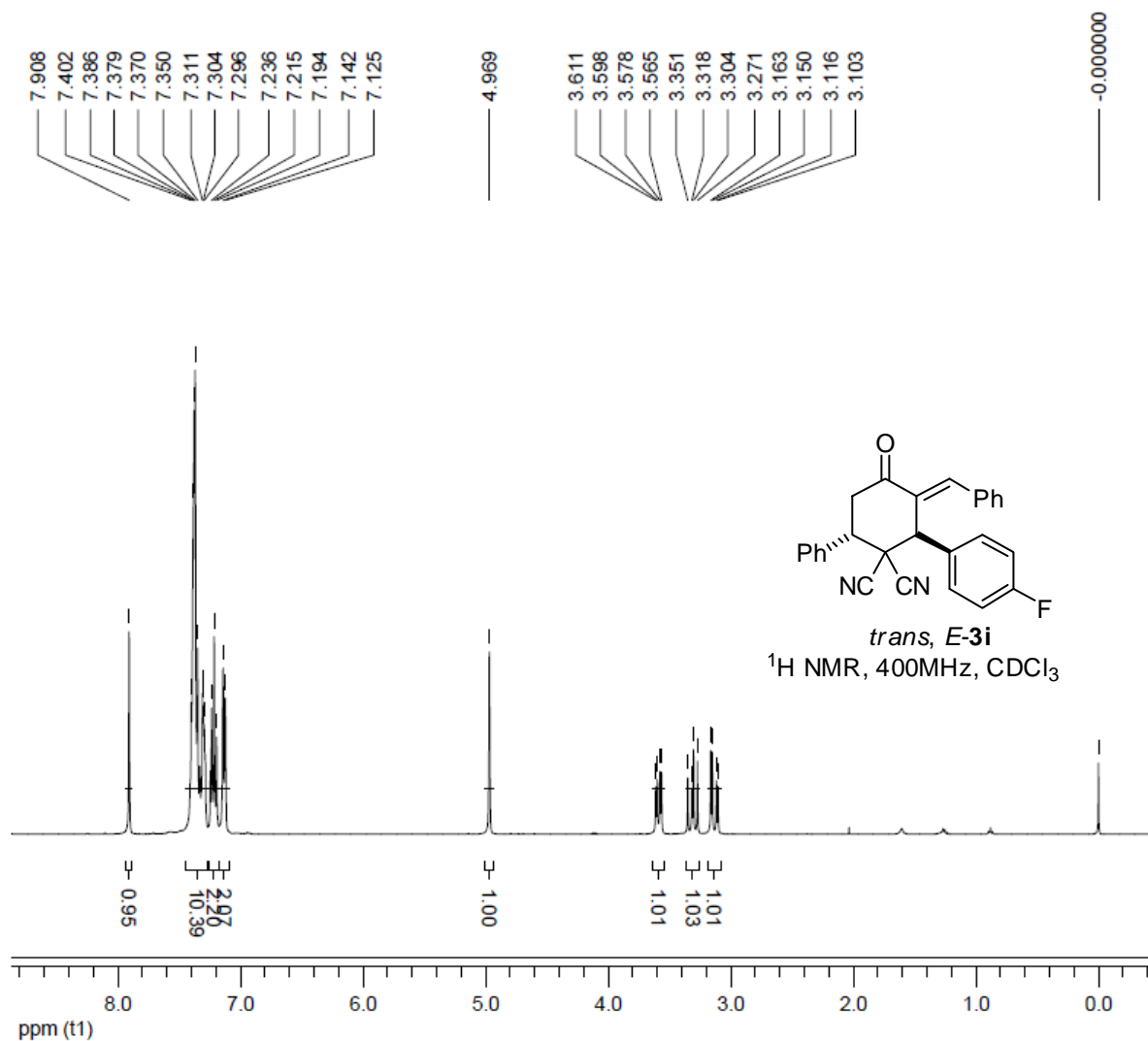


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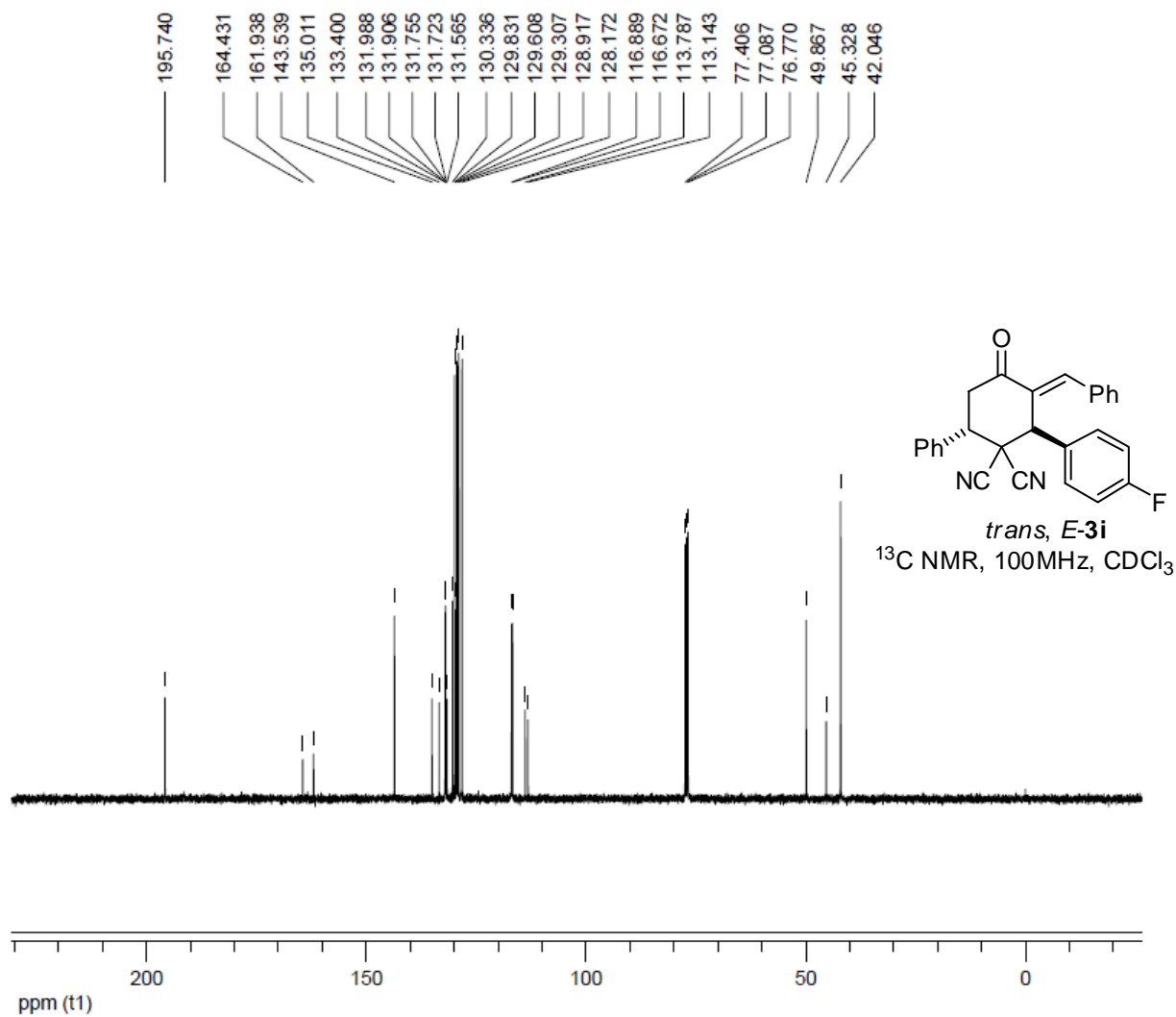
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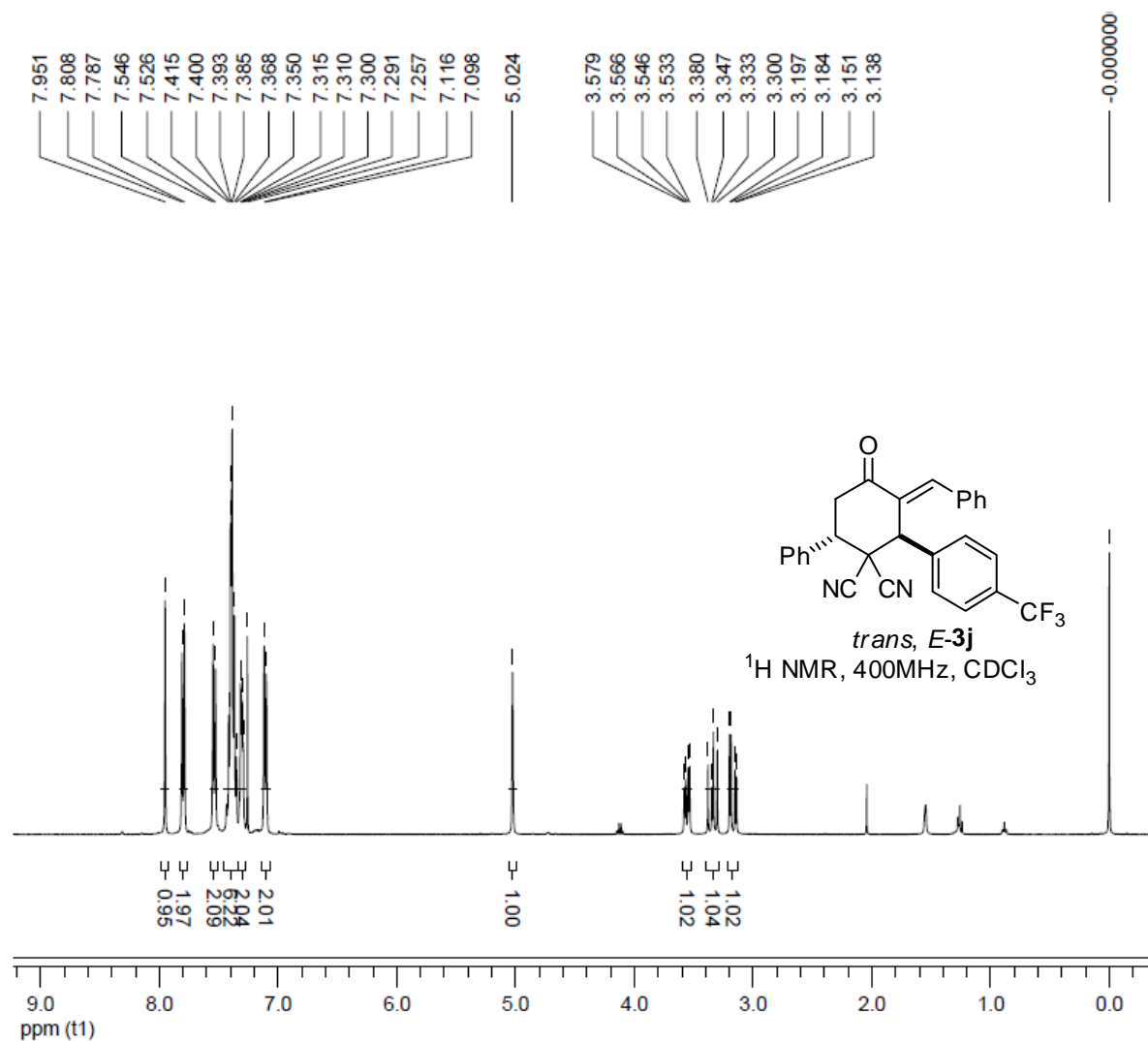
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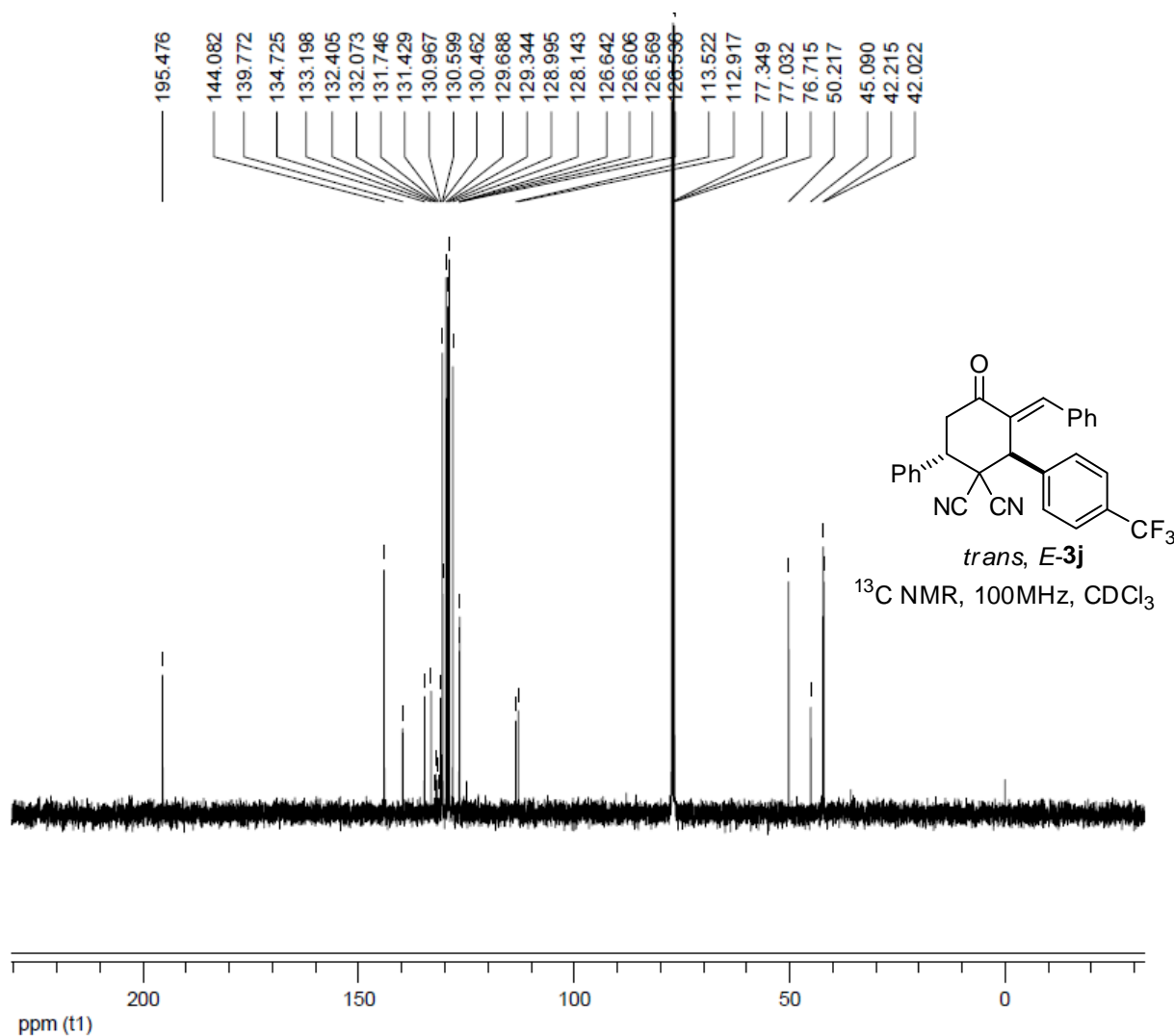
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Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

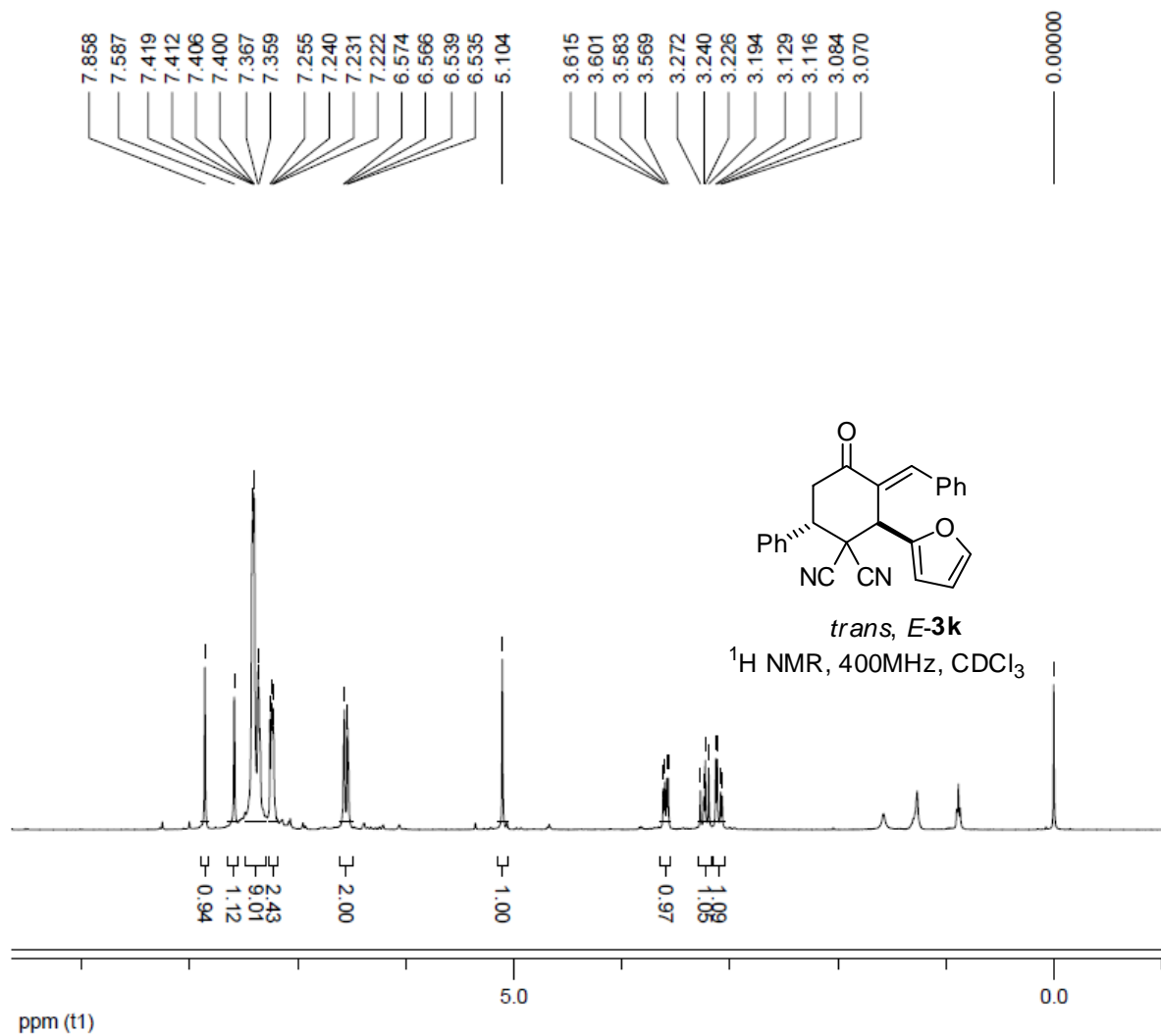
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

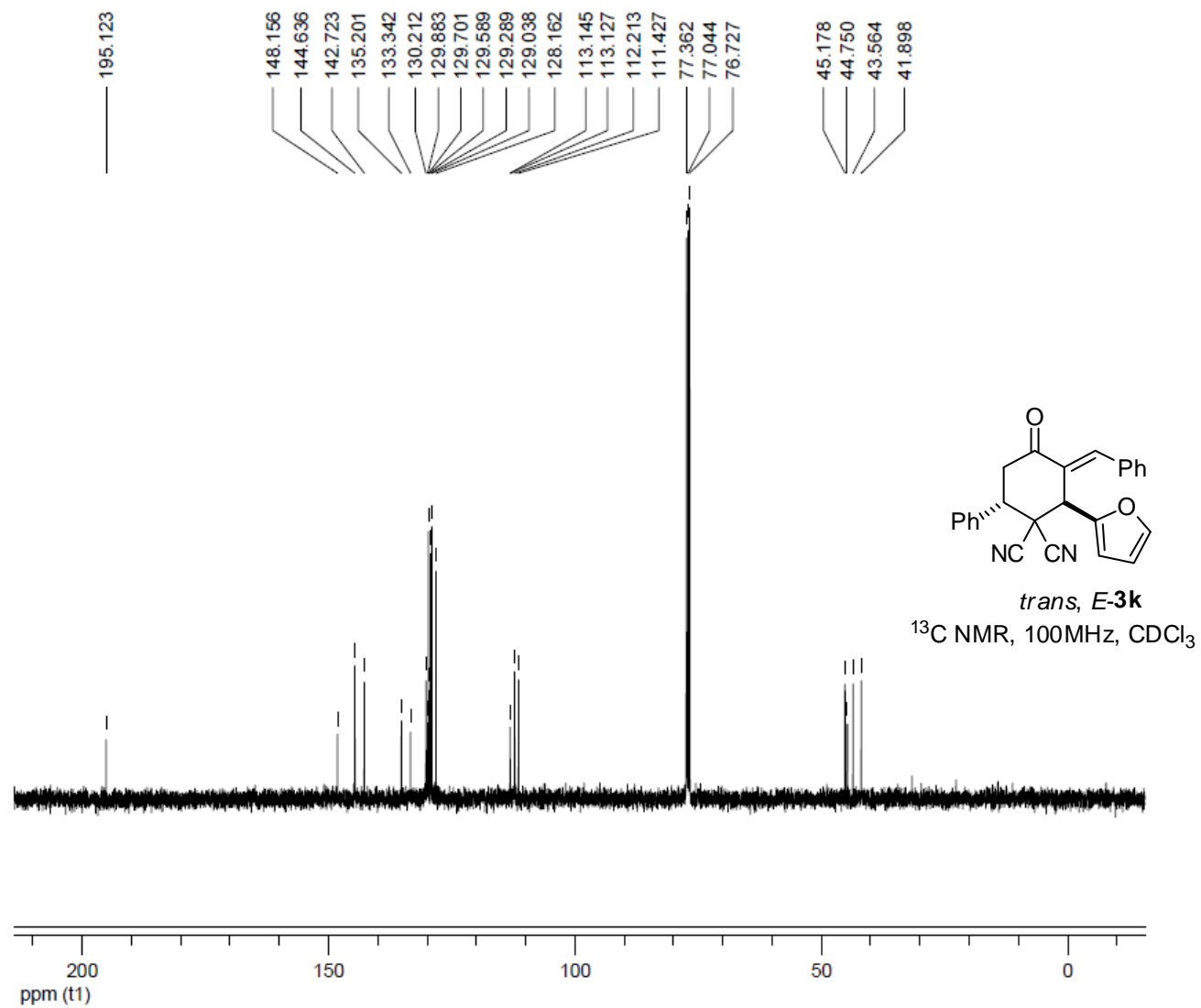
(f1) 3.9846

Spectral Width (ppm):

(f1) 20.553

Pulse Program:

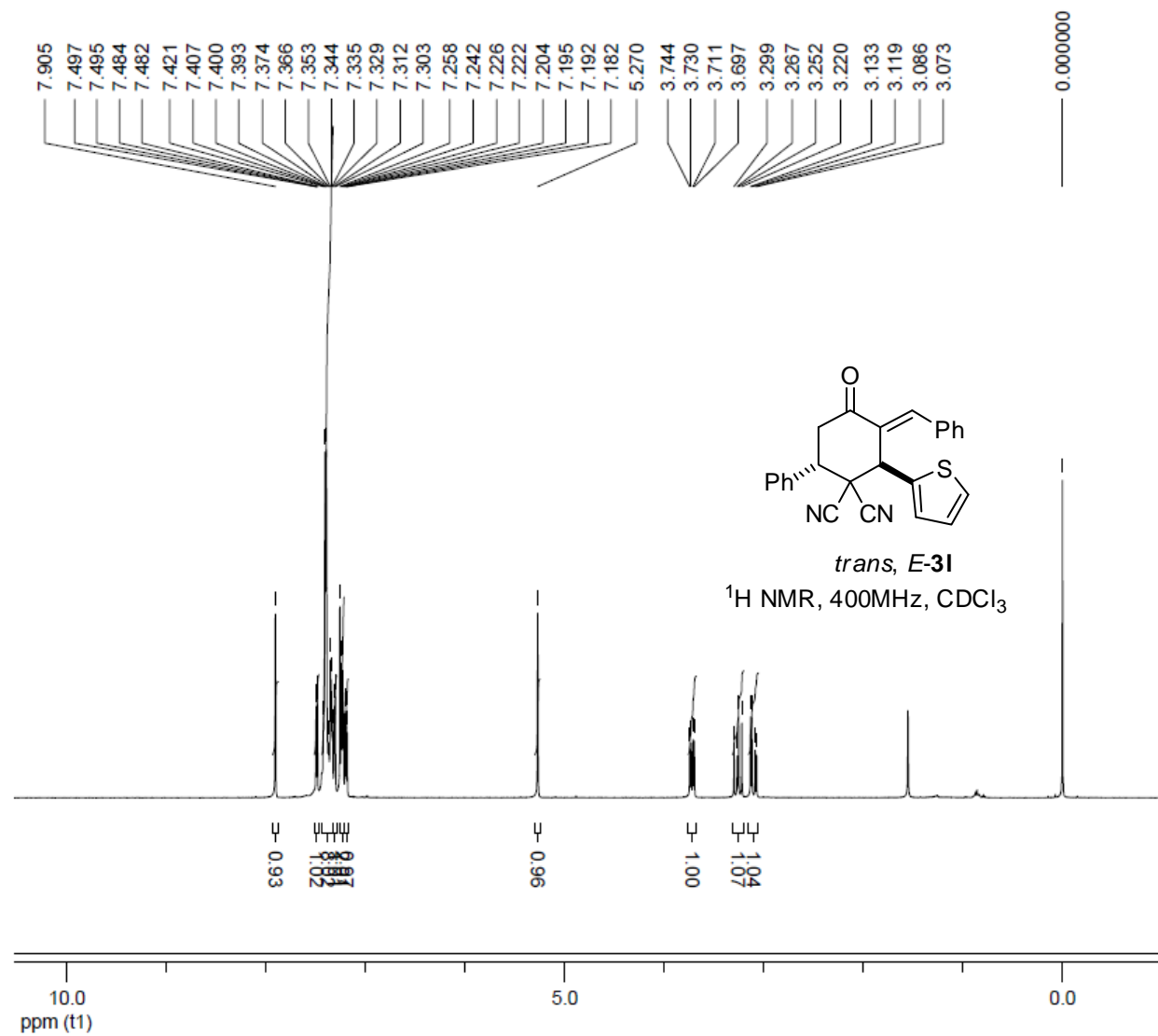
Unknown



Date:  
5 Jul 2011  
Document's Title:  
nc

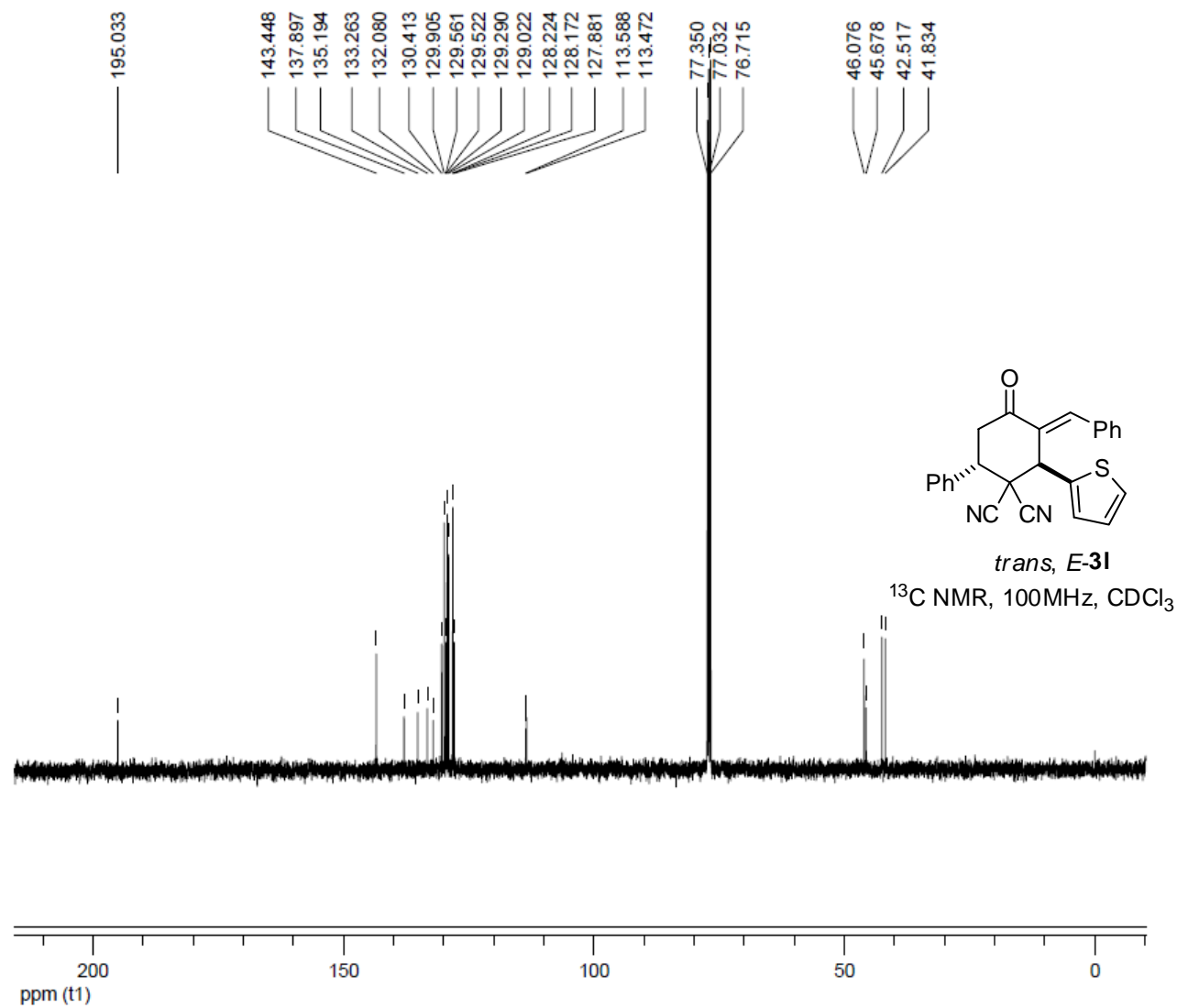
Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown



Date:  
5 Jul 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown

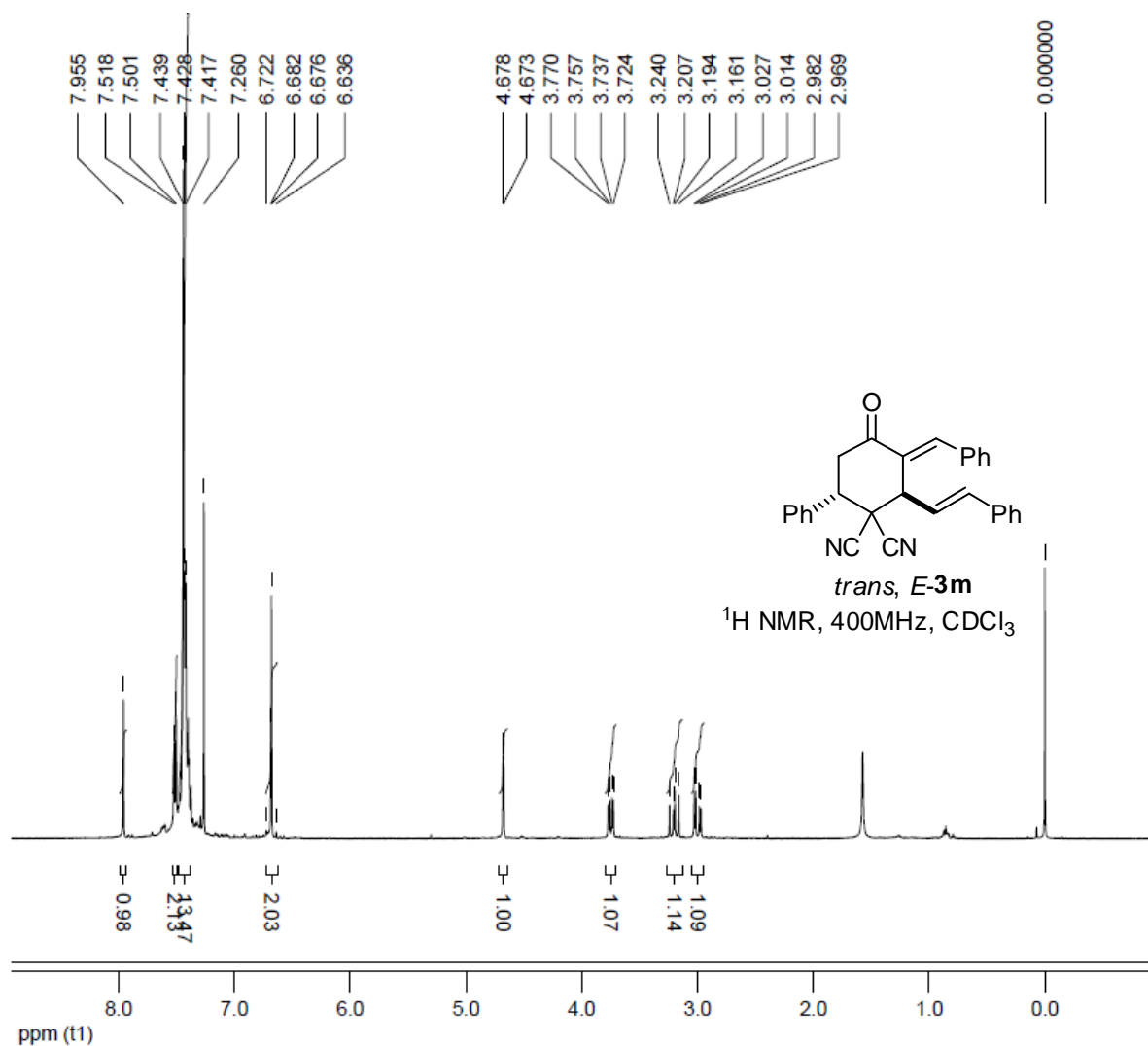




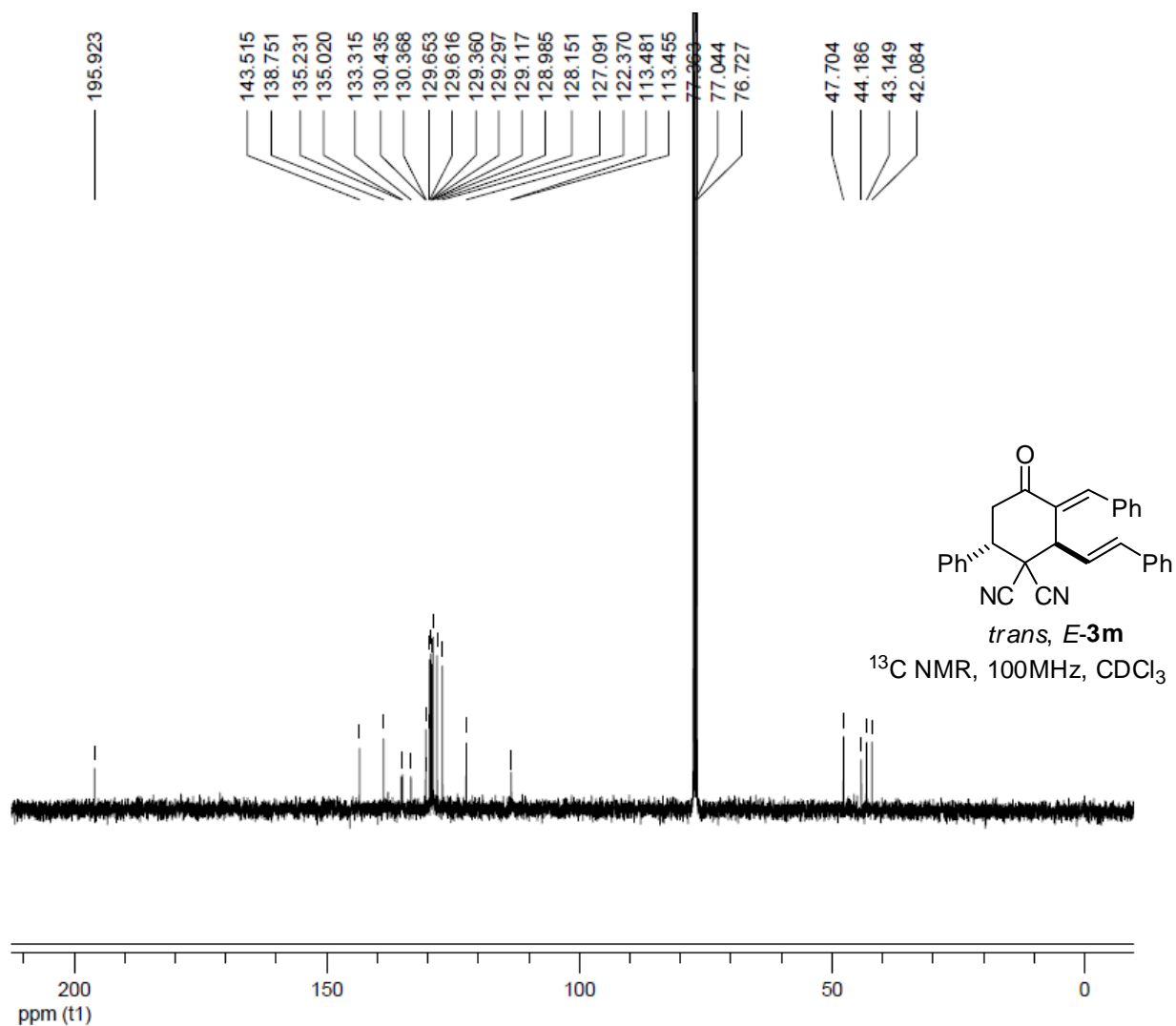
Date:  
5 Jul 2011  
Document's Title:  
nc

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown



Date:  
5 Jul 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown



Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

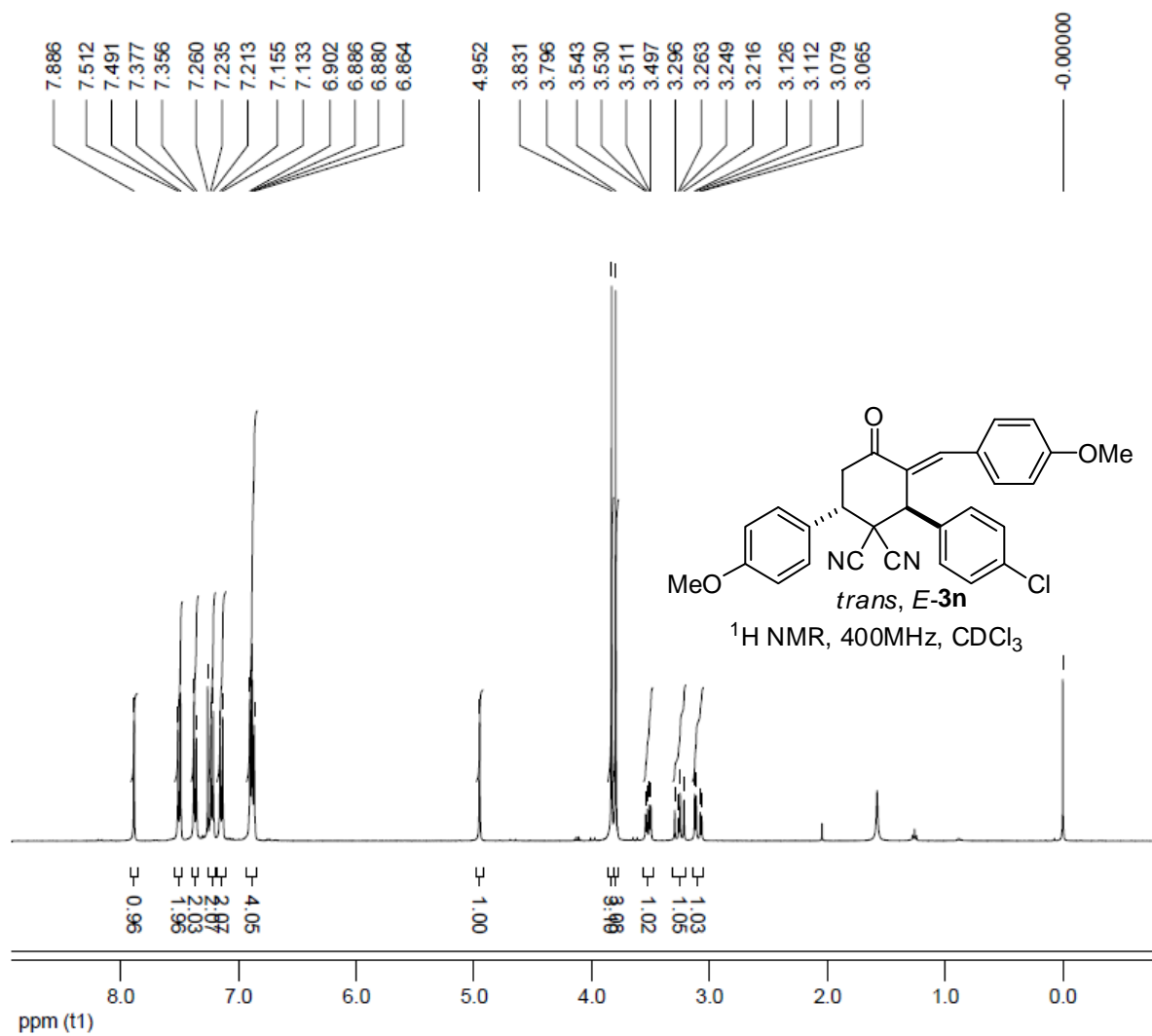
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

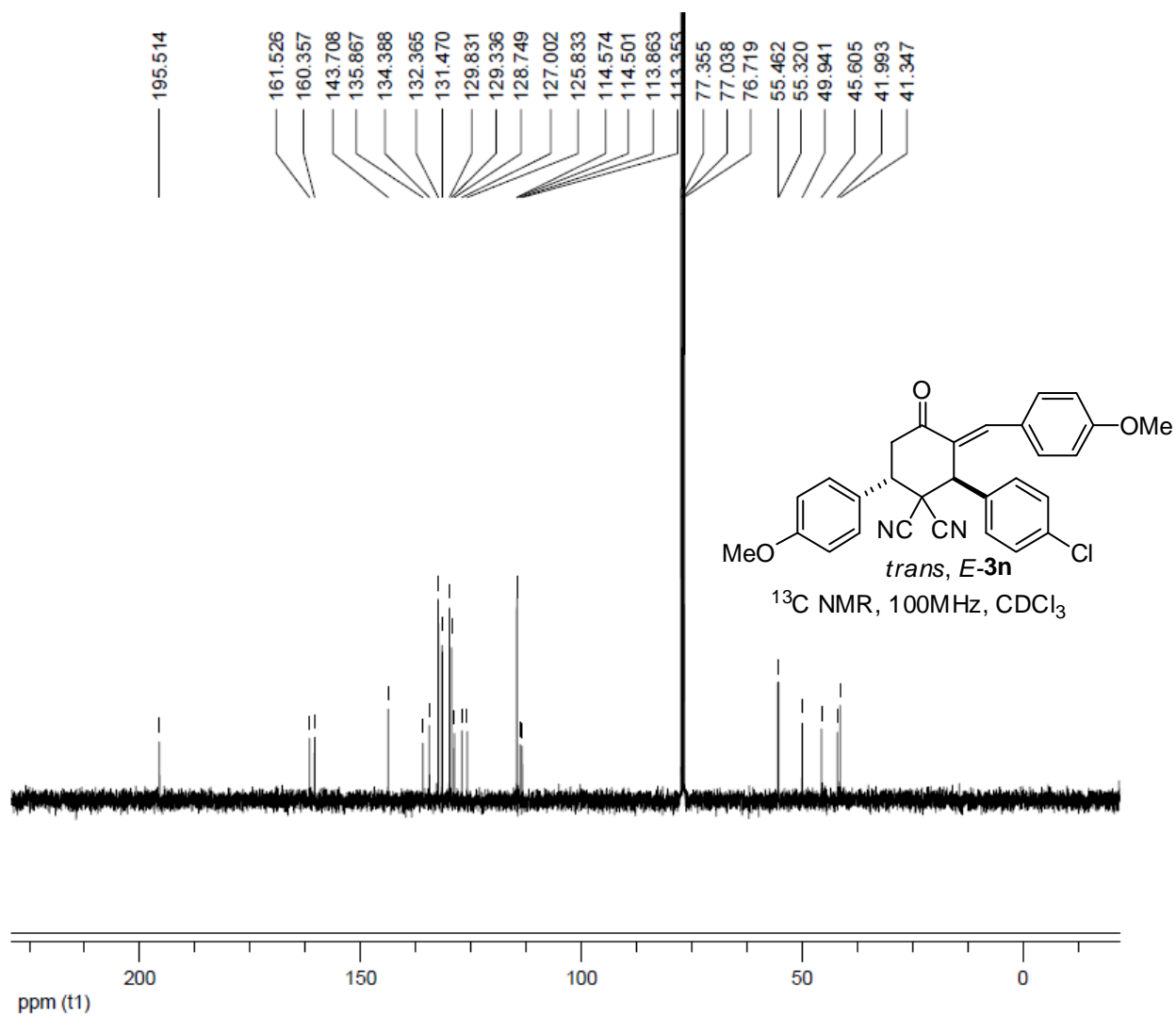
(f1) 3.9846

Spectral Width (ppm):

(f1) 20.553

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

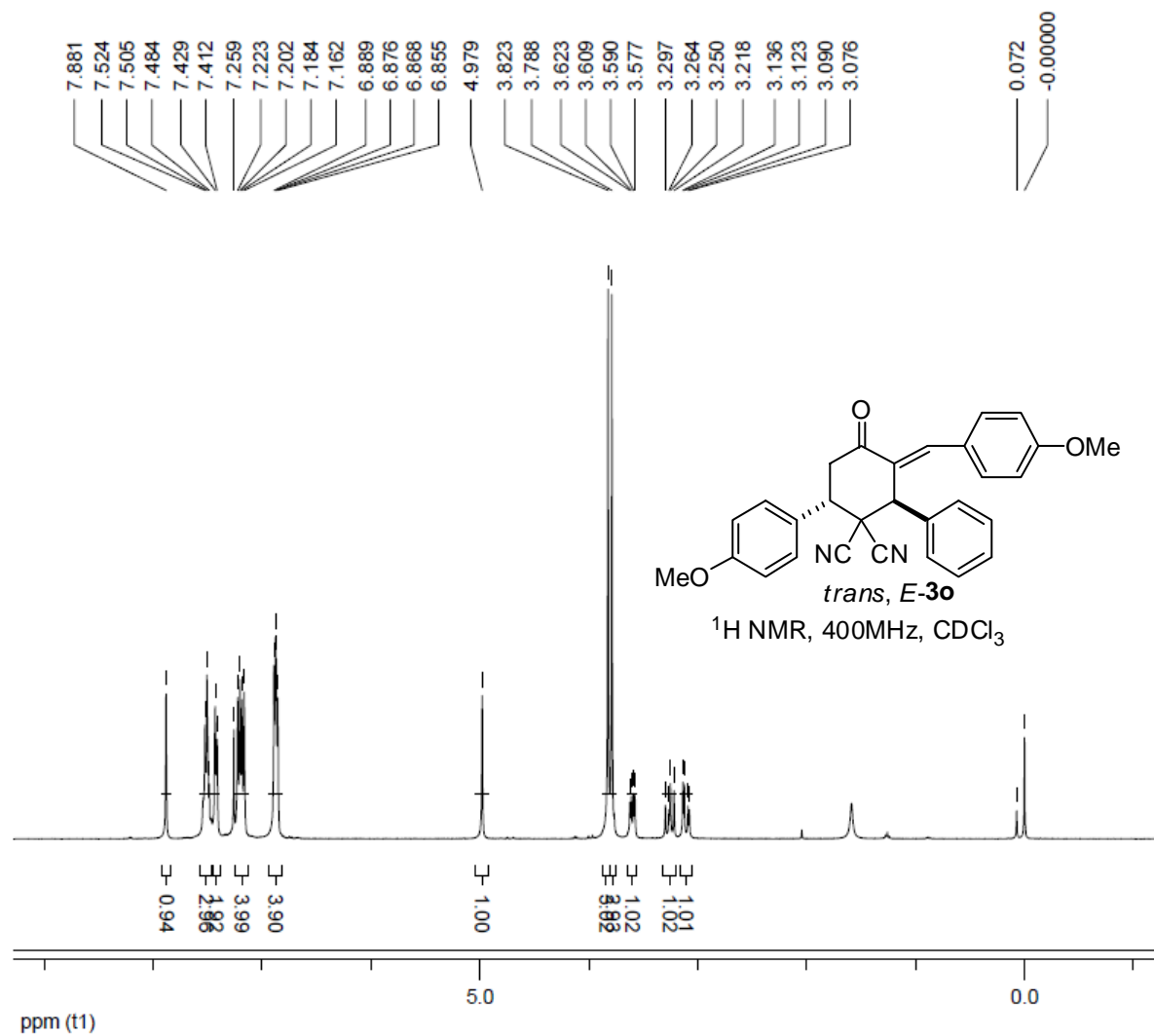
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

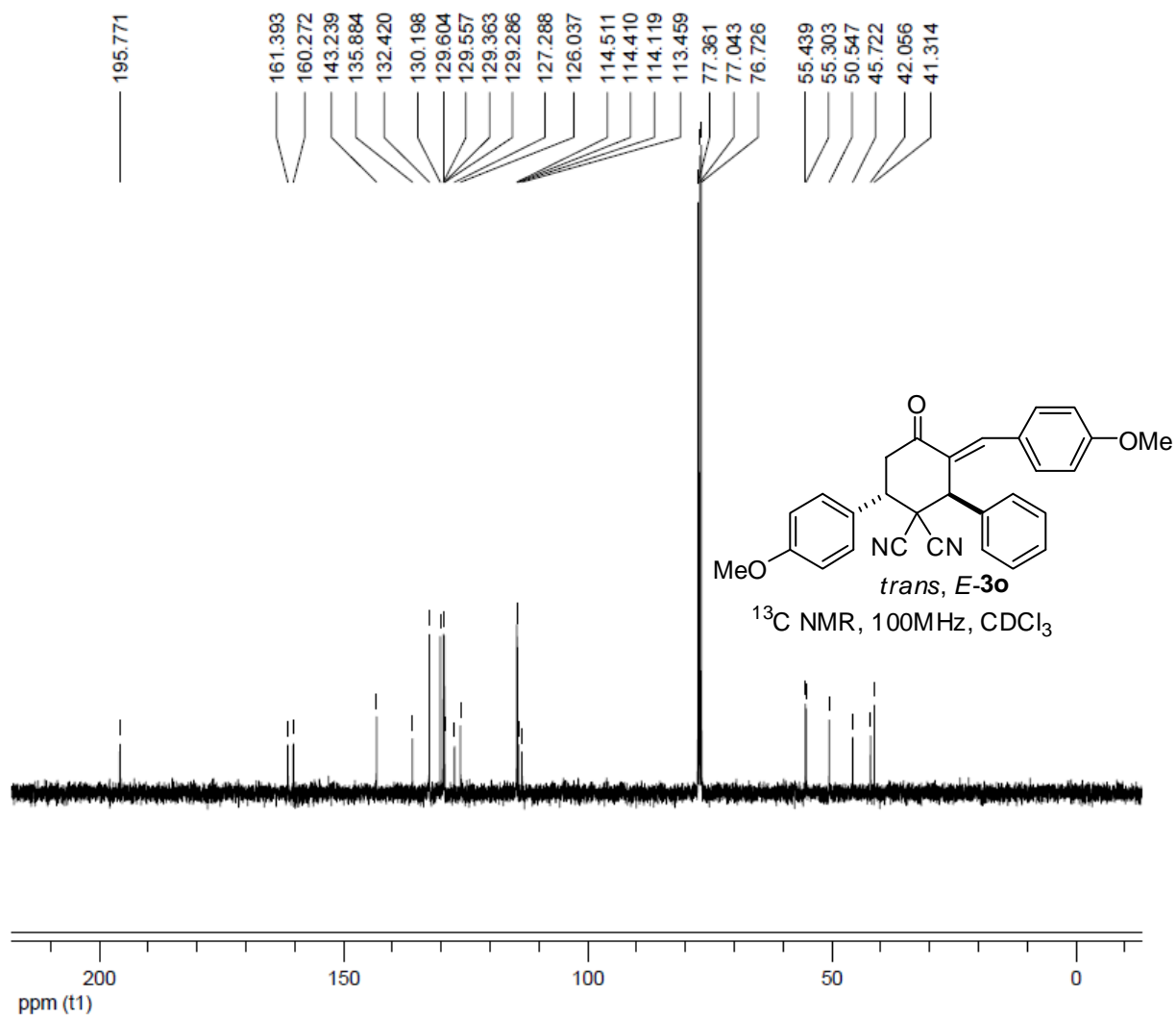
(f1) 3.9846

Spectral Width (ppm):

(f1) 20.553

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

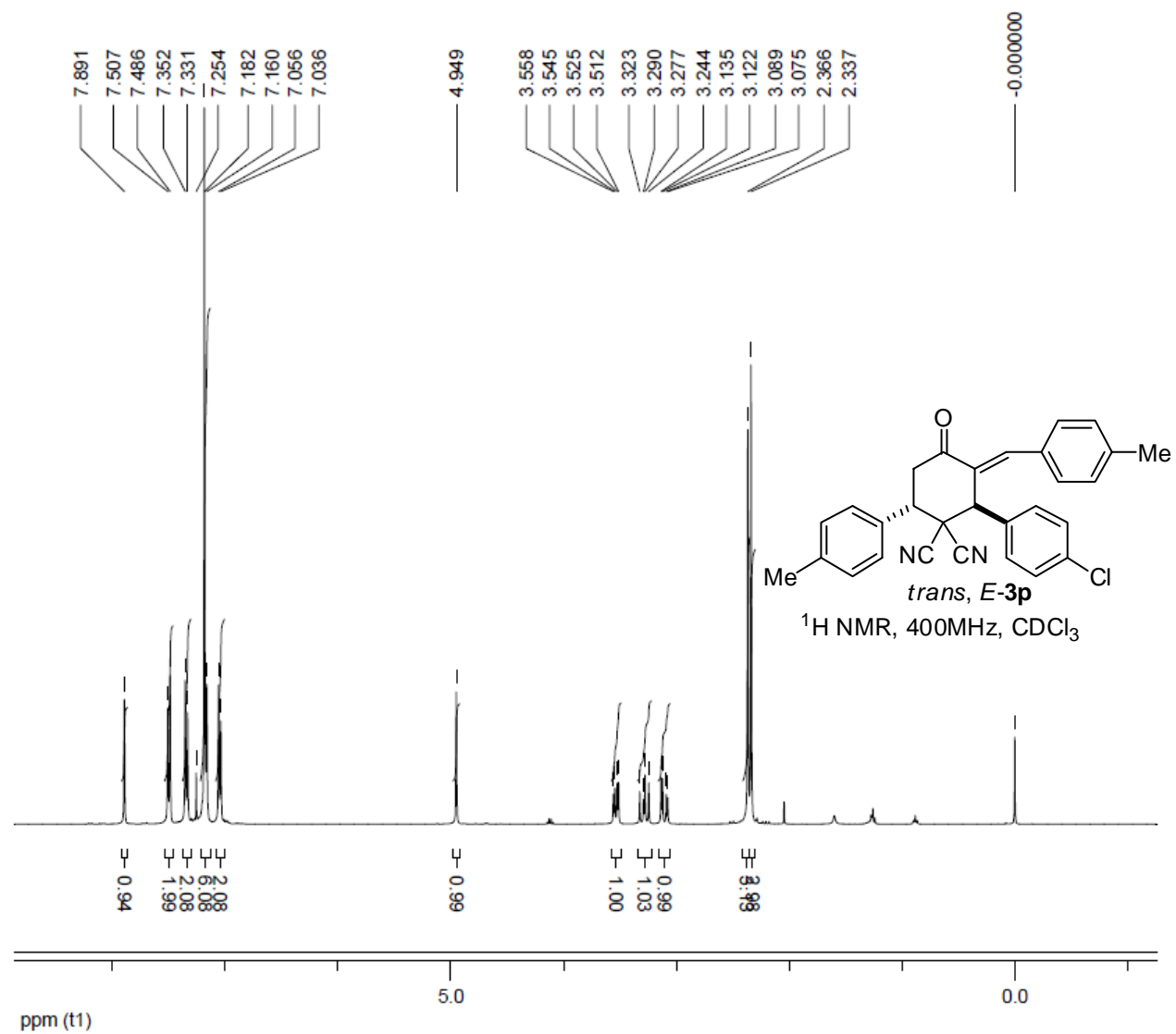
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

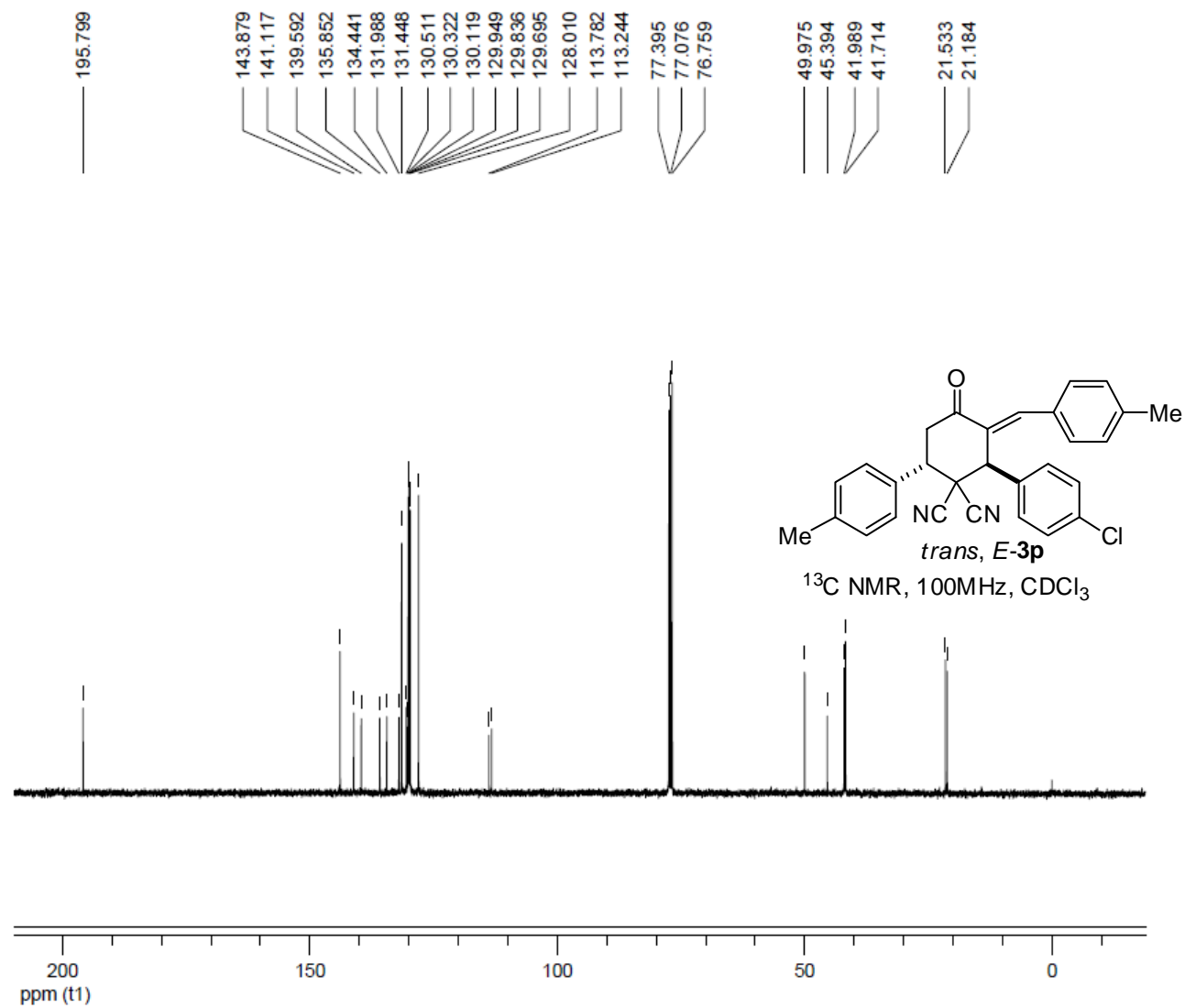
Pulse Program:

Unknown



Date:  
5 Jul 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown

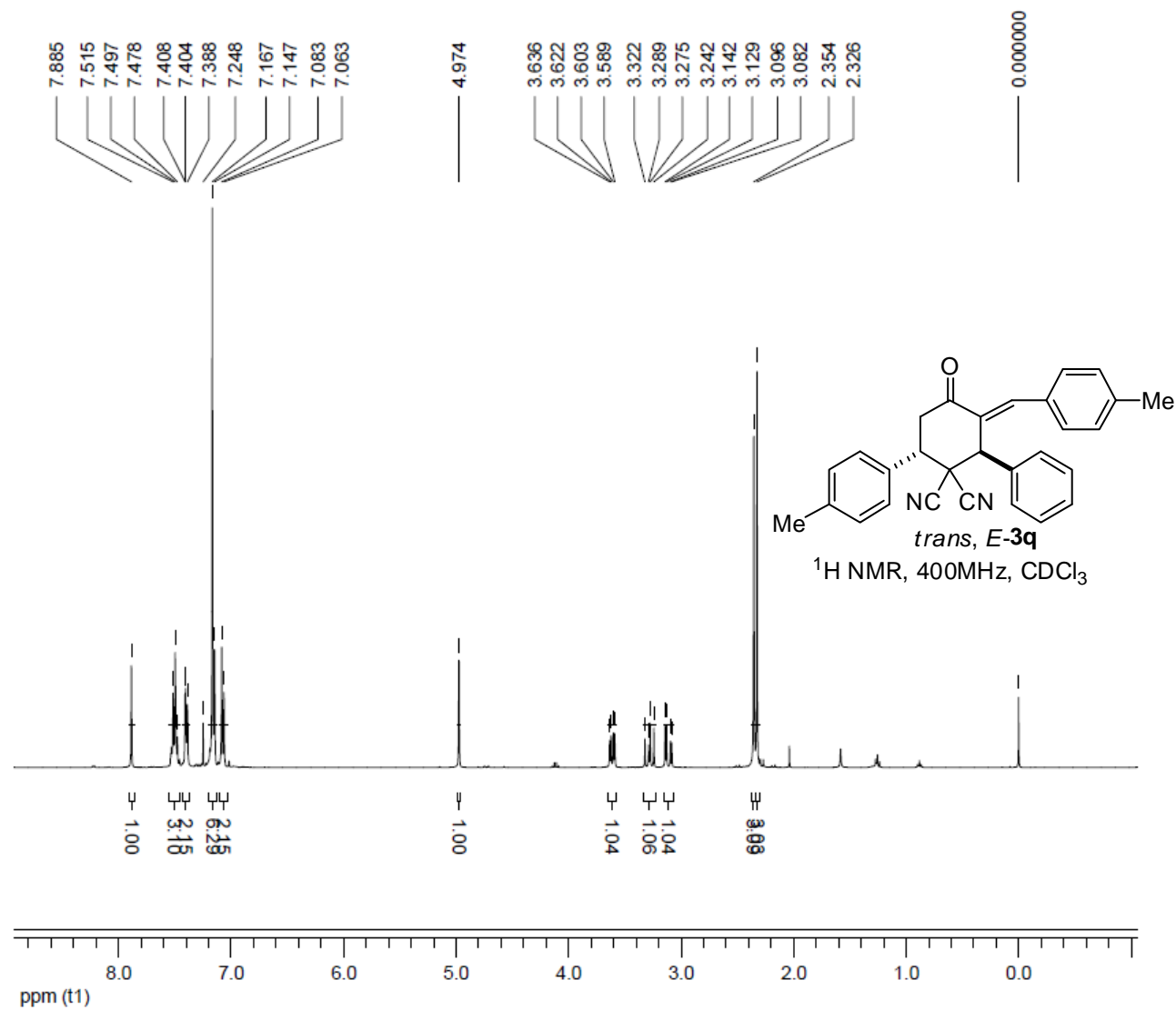




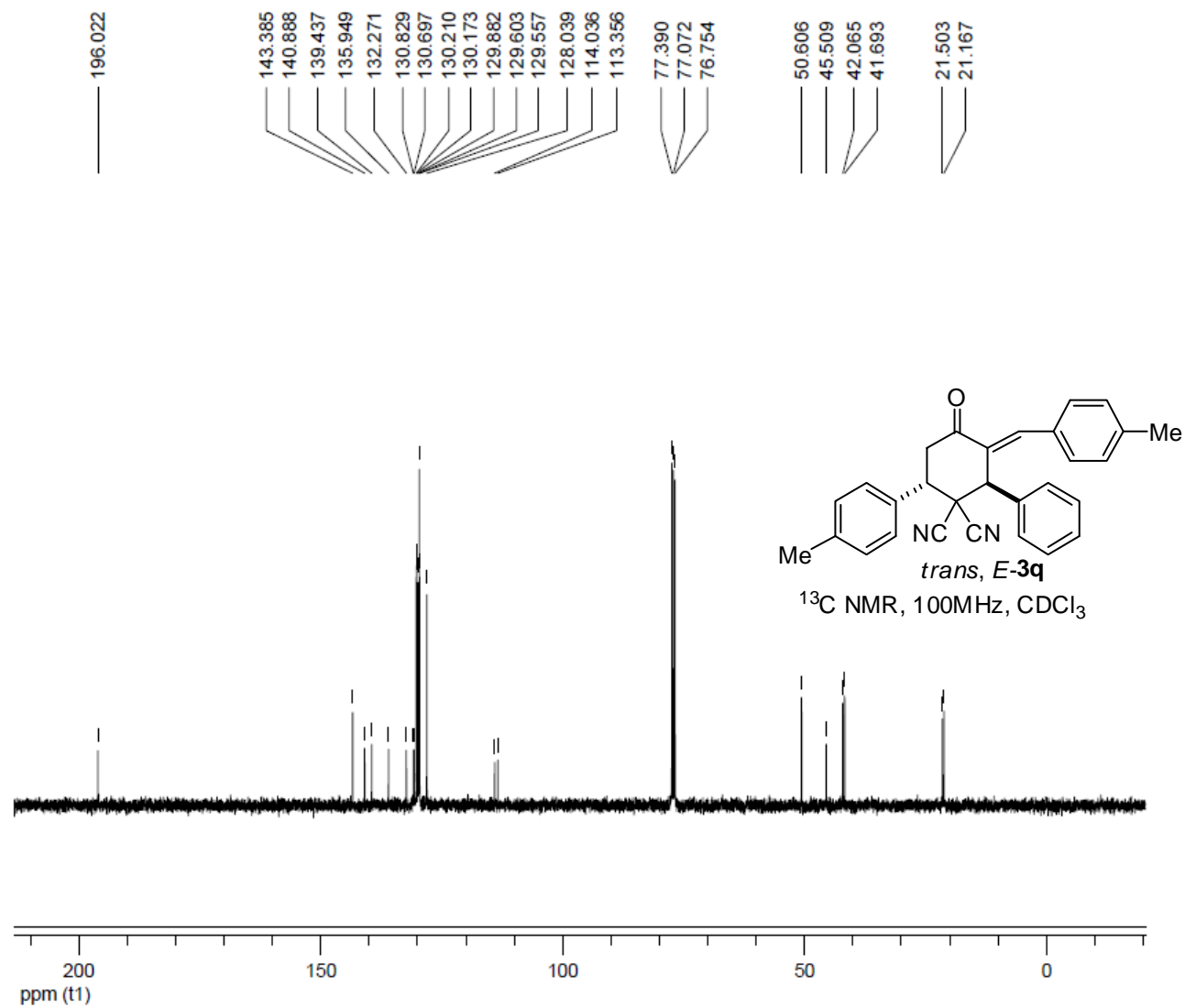
Date:  
5 Jul 2011  
Document's Title:  
1r

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown



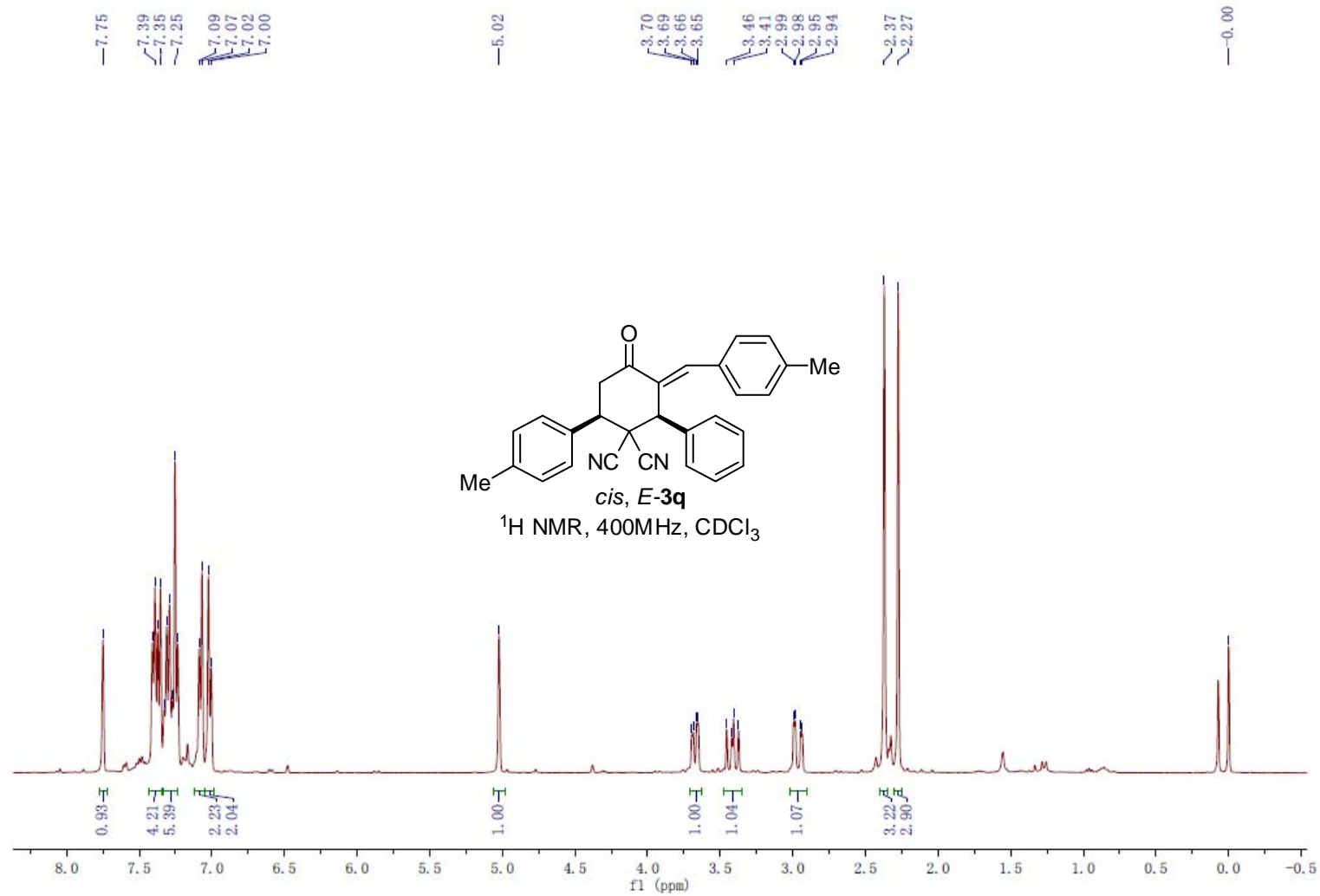
Date:  
5 Jul 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown

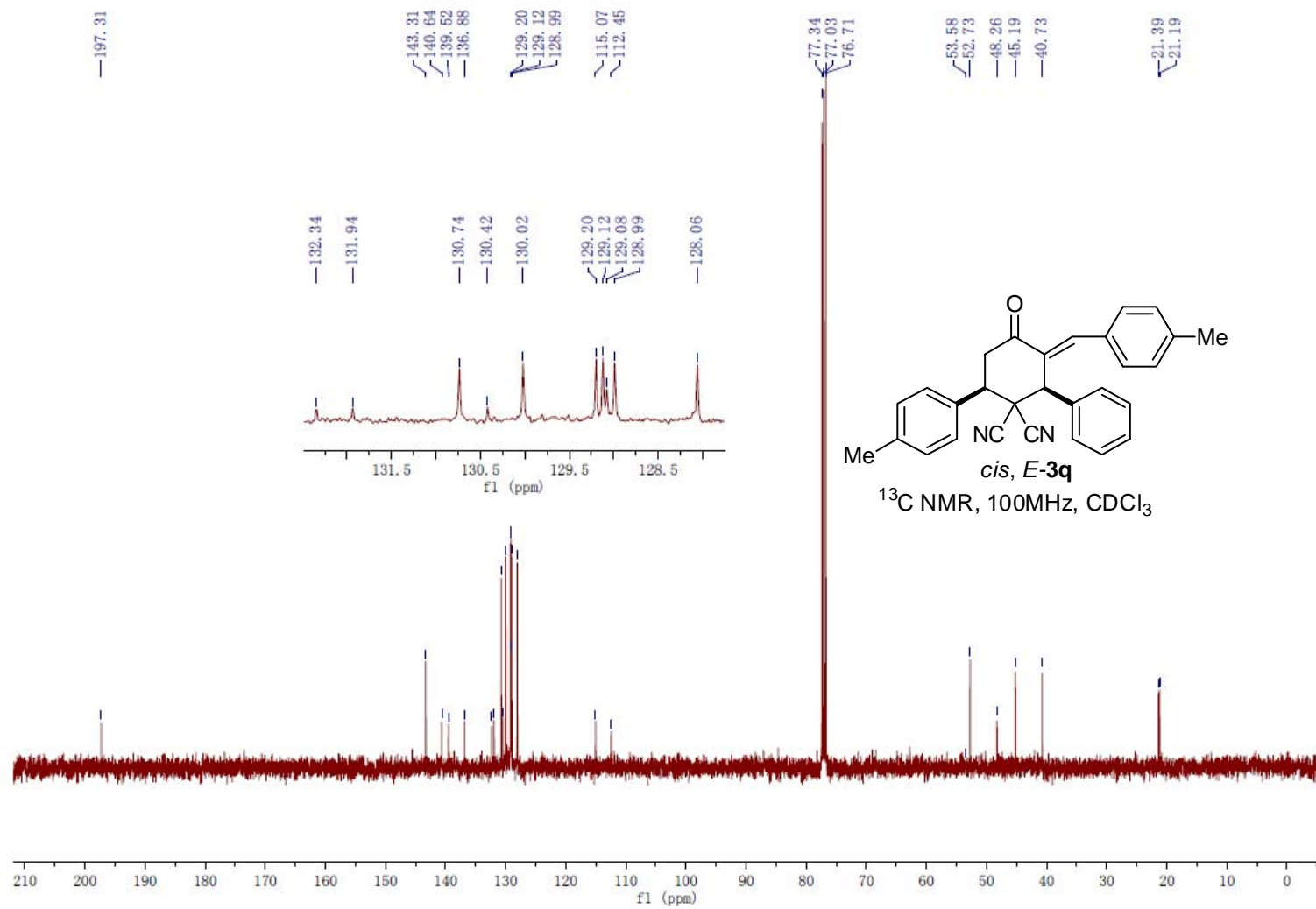


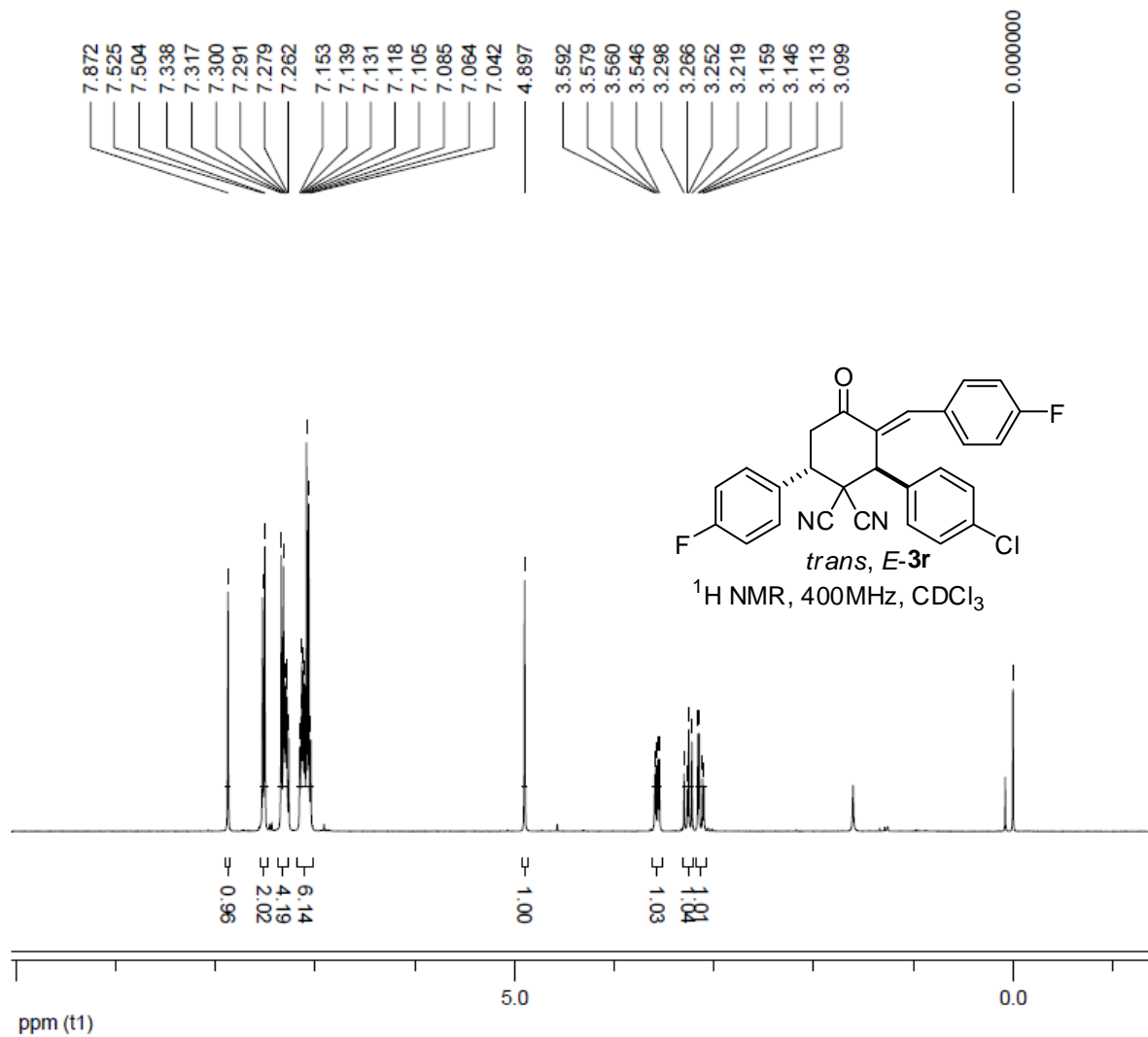
Date:  
5 Jul 2011  
Document's Title:  
1r

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 1.1010  
Spectral Width (ppm):  
(f1) 295.806  
Pulse Program:  
Unknown







Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

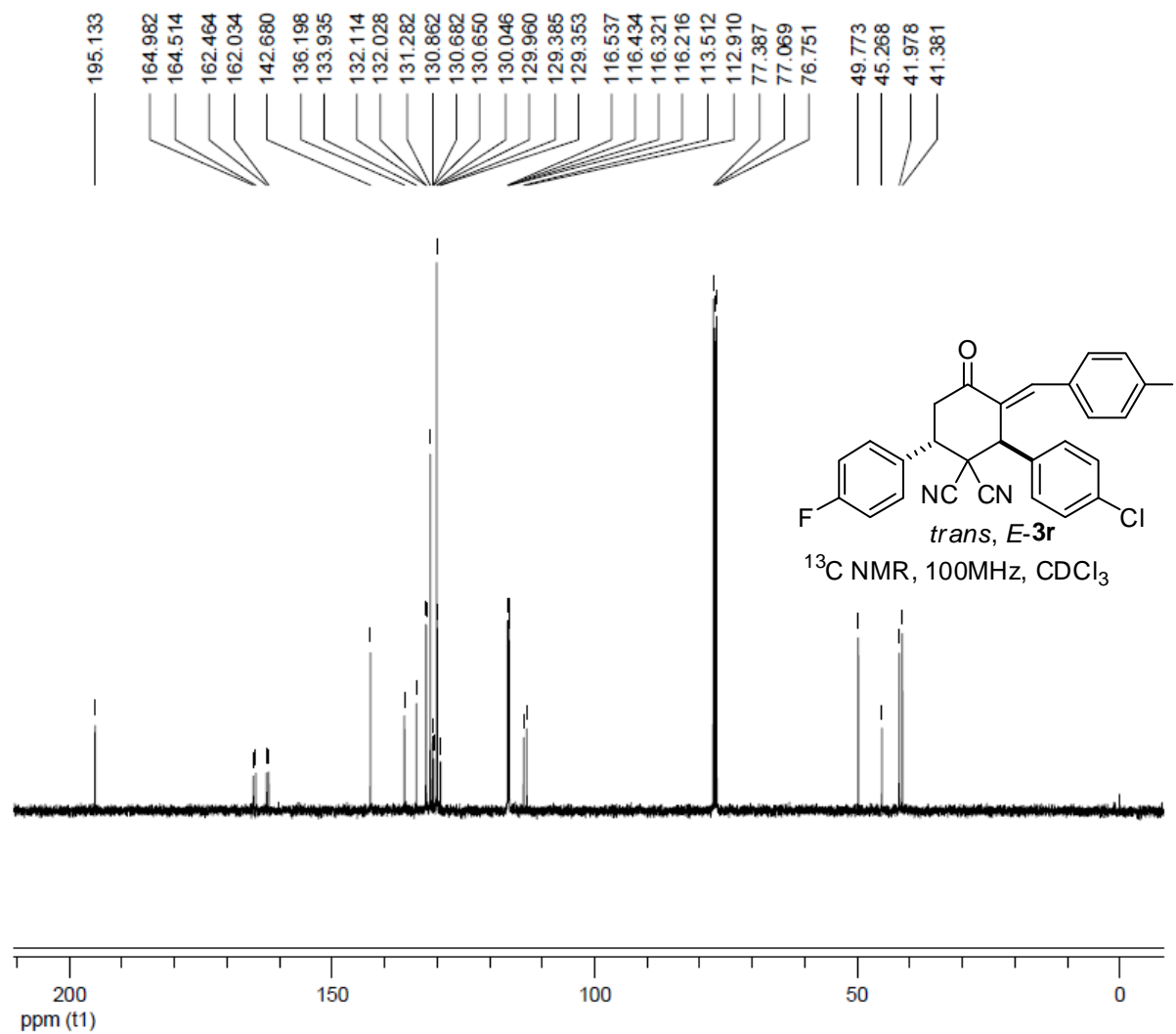
(f1) 3.9846

Spectral Width (ppm):

(f1) 20.553

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

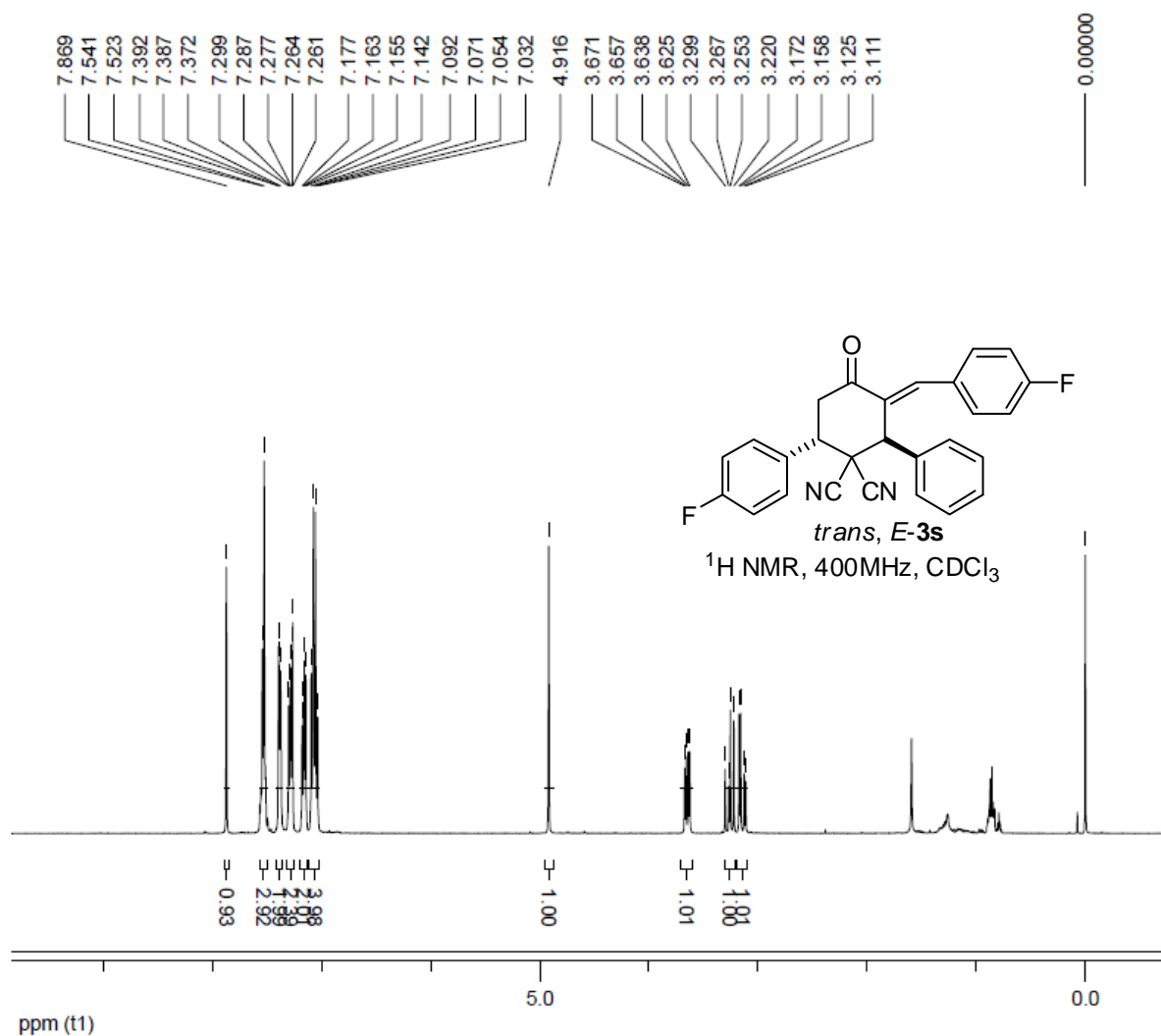
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

Pulse Program:

Unknown



Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

(f1) 3.9846

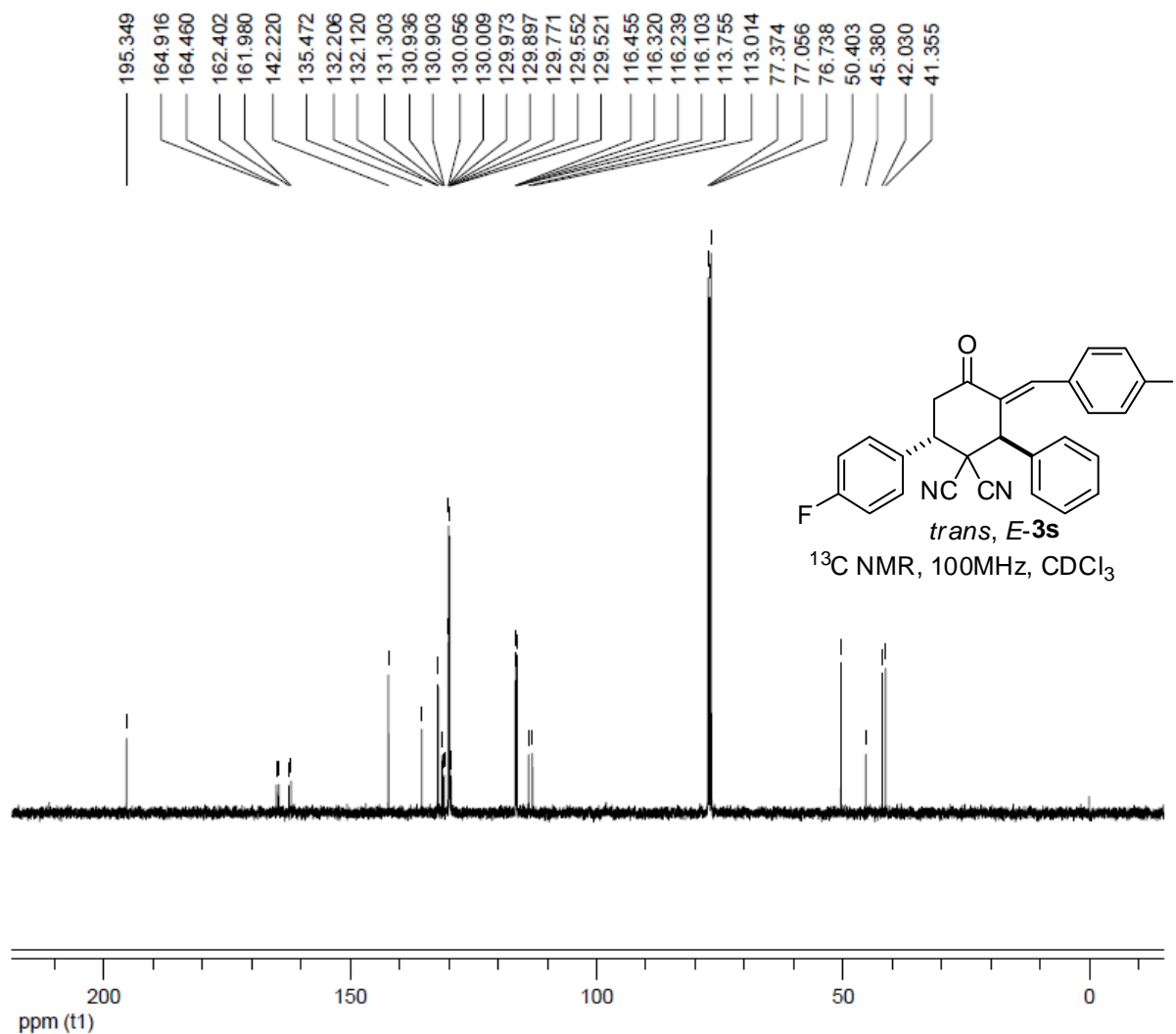
Spectral Width (ppm):

(f1) 20.553

Pulse Program:

Unknown





Date:

5 Jul 2011

Document's Title:

nc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.613

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

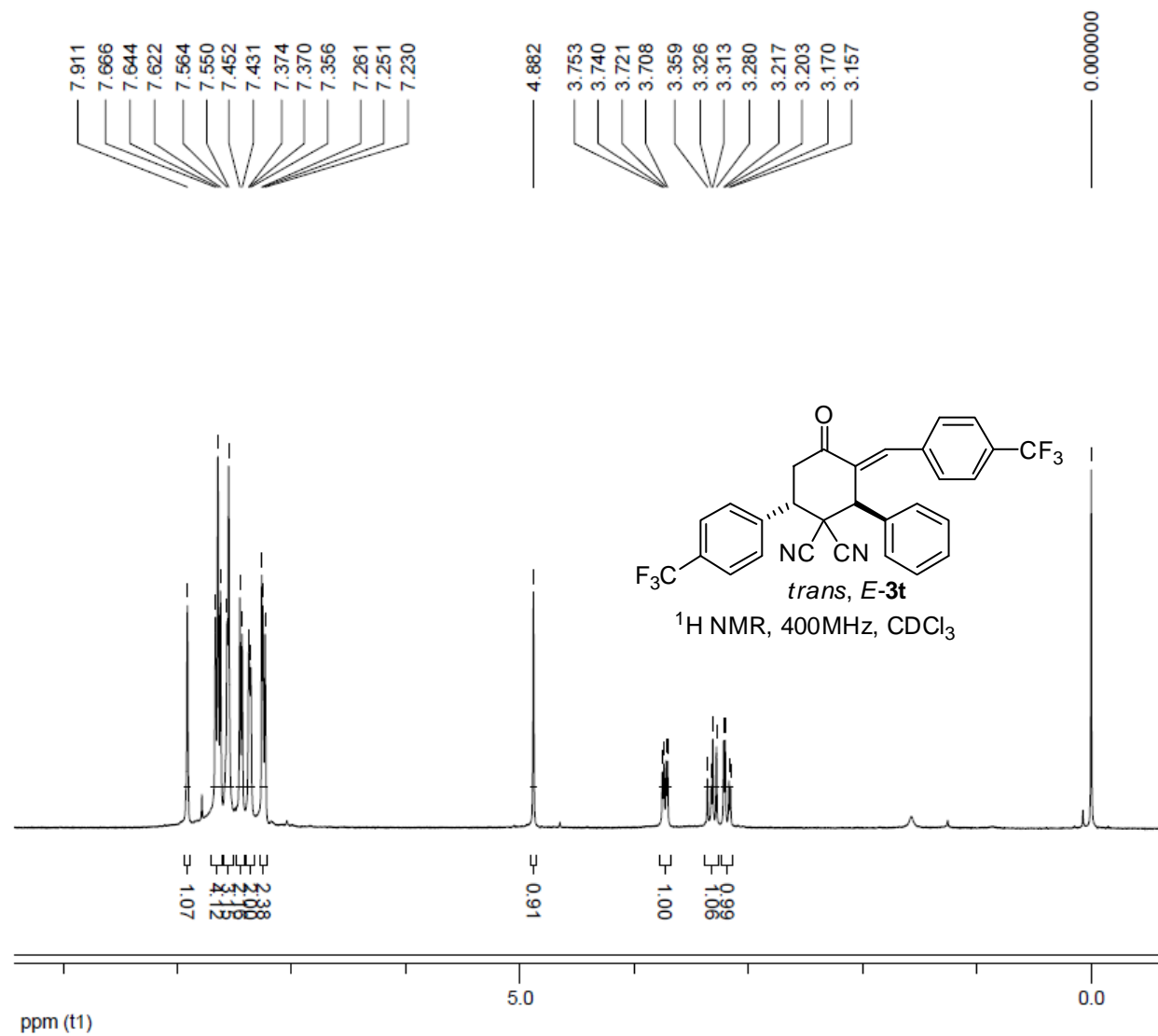
(f1) 0.9175

Spectral Width (ppm):

(f1) 354.968

Pulse Program:

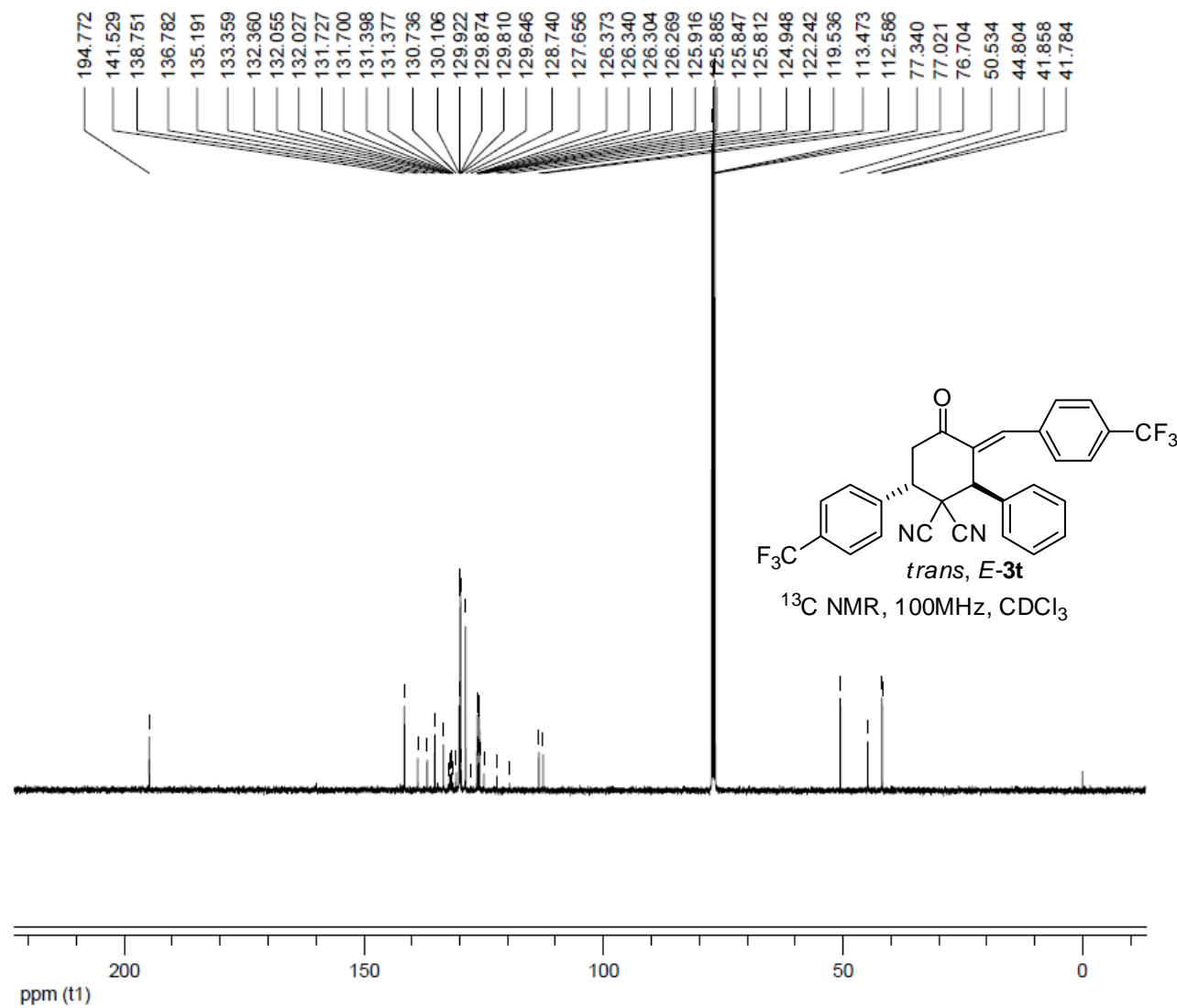
Unknown



Date:  
5 Jul 2011  
Document's Title:  
n

Spectrum Title:  
PROTON

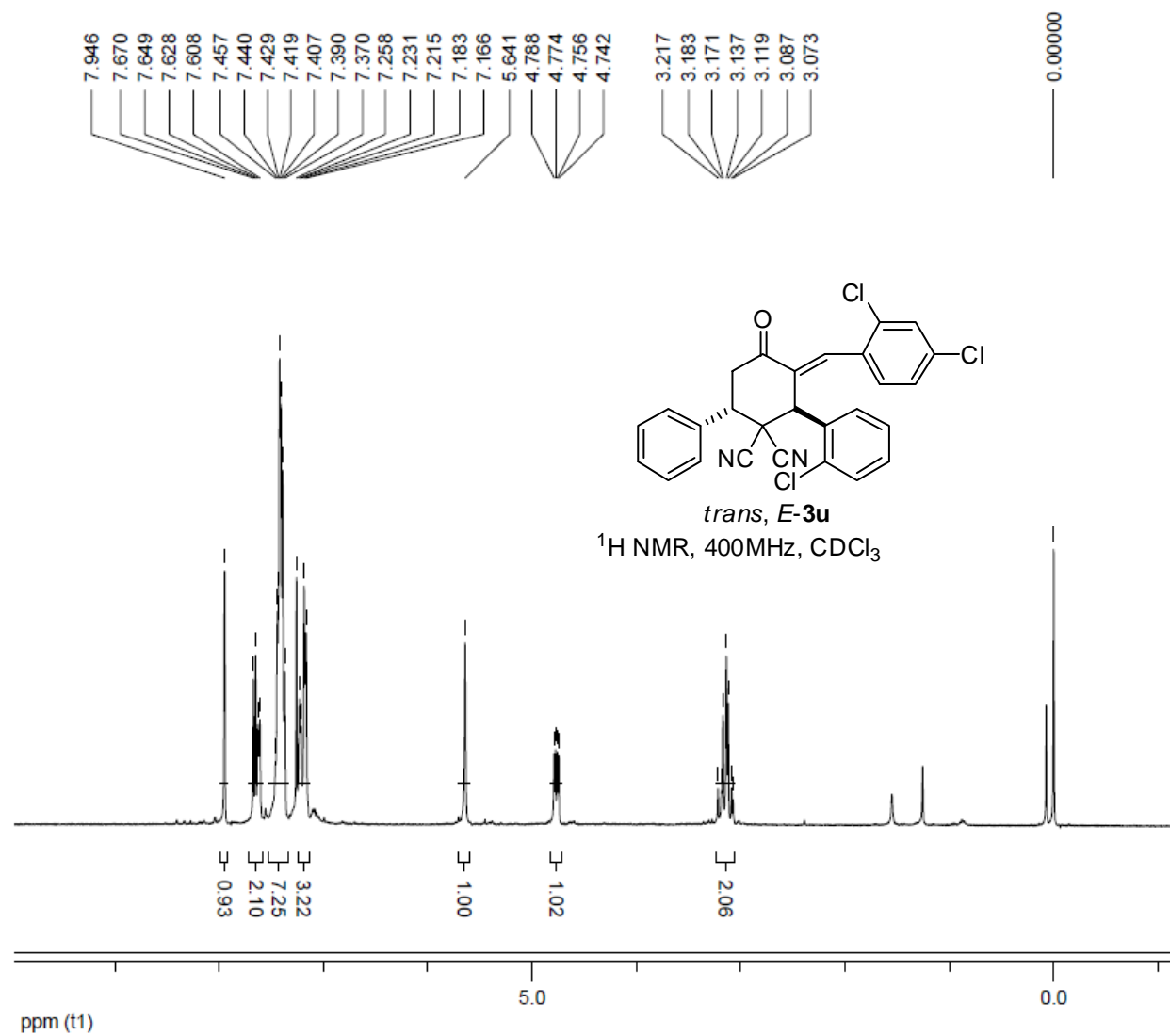
Frequency (MHz):  
(f1) 400.230  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.547  
Pulse Program:  
Unknown



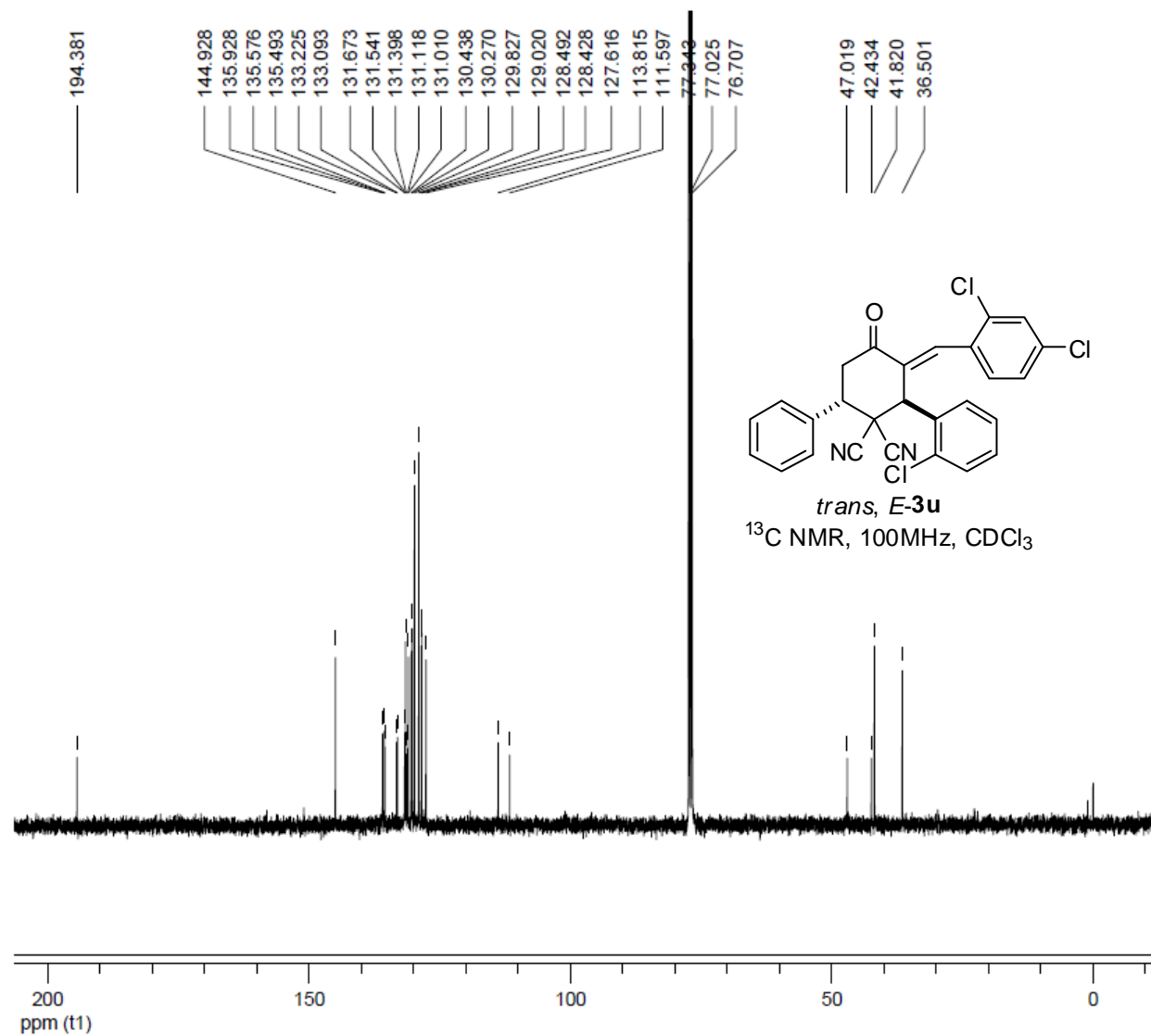
Date:  
5 Jul 2011  
Document's Title:  
nc

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown



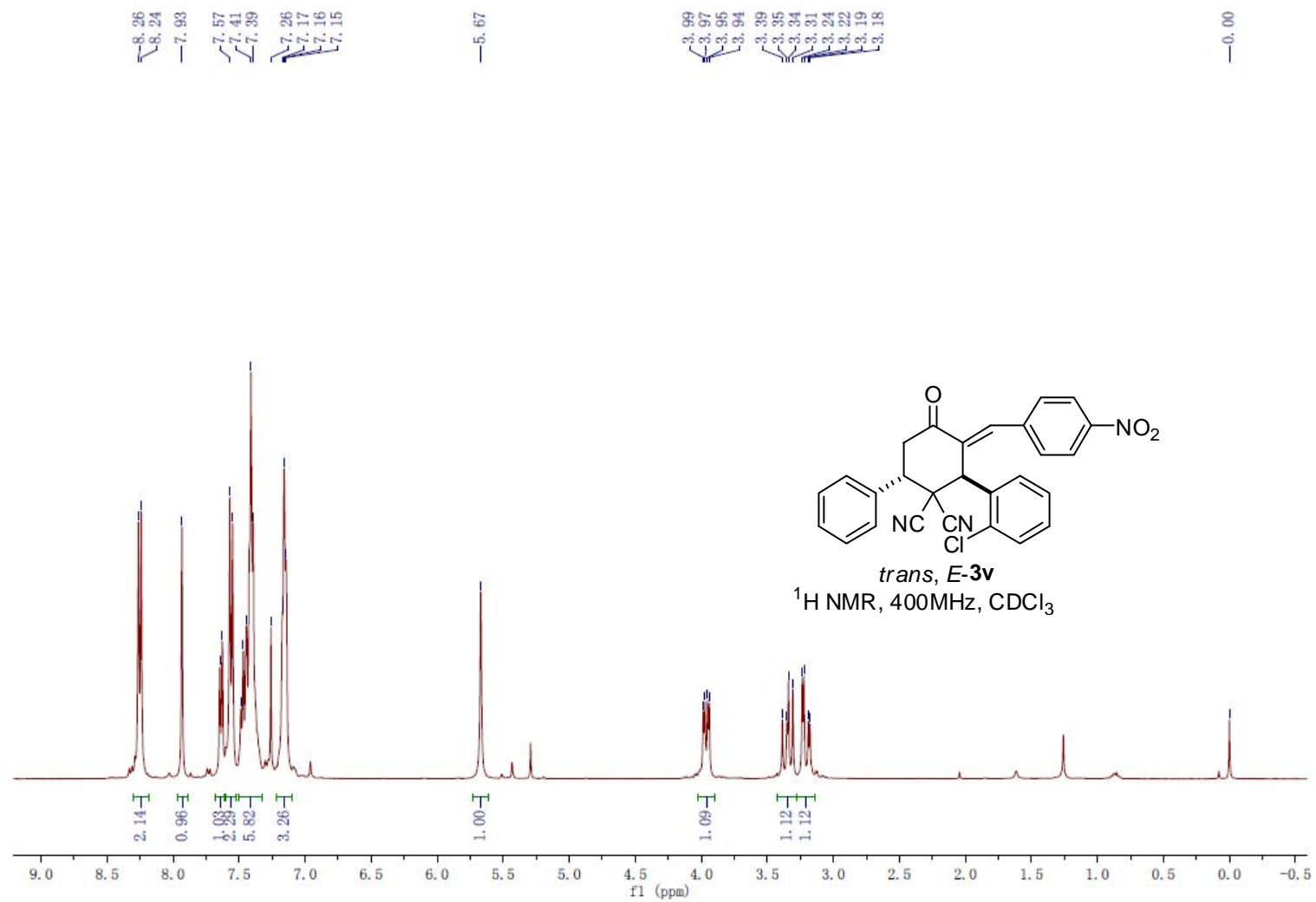
Date:  
5 Jul 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.230  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.547  
Pulse Program:  
Unknown

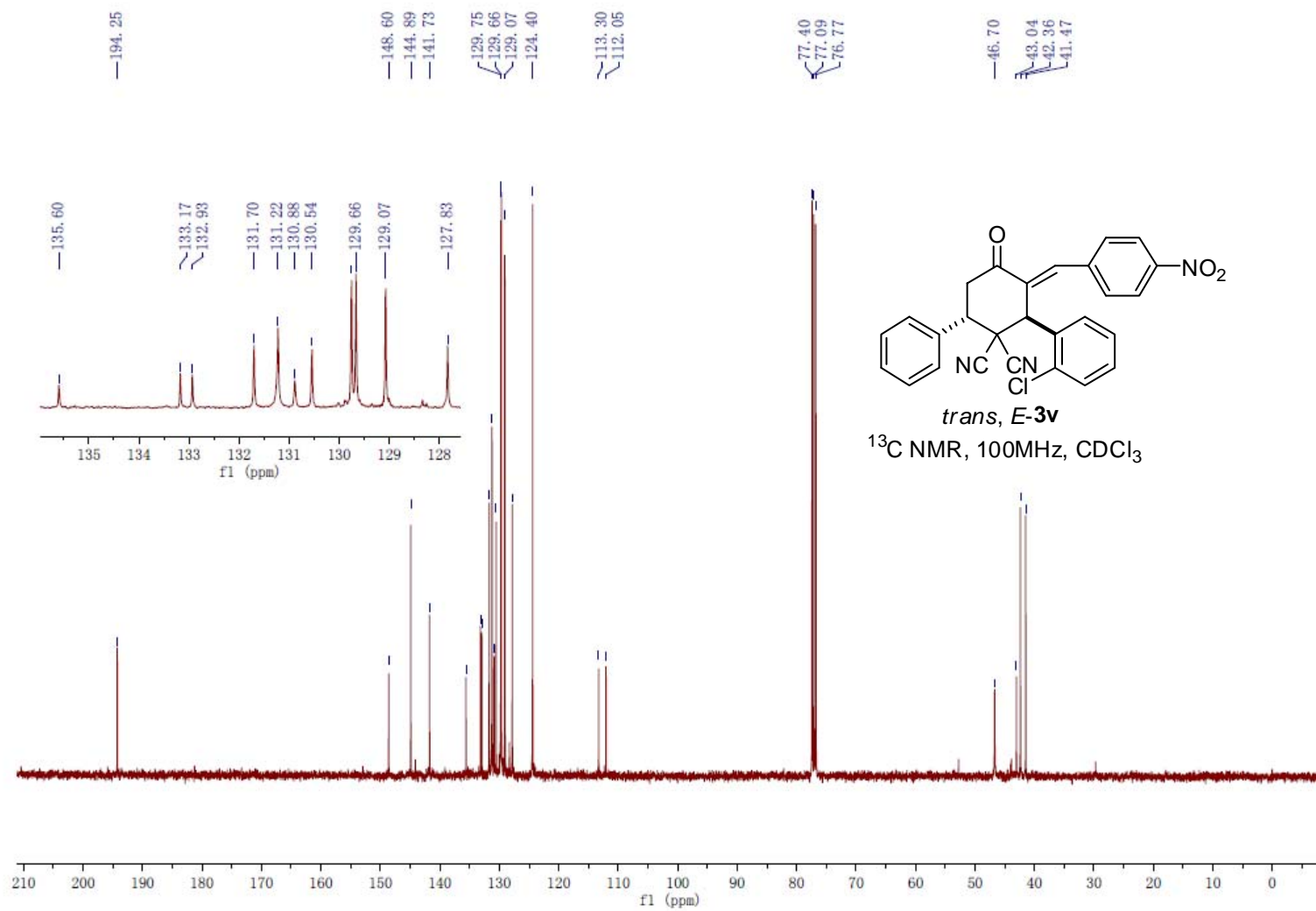


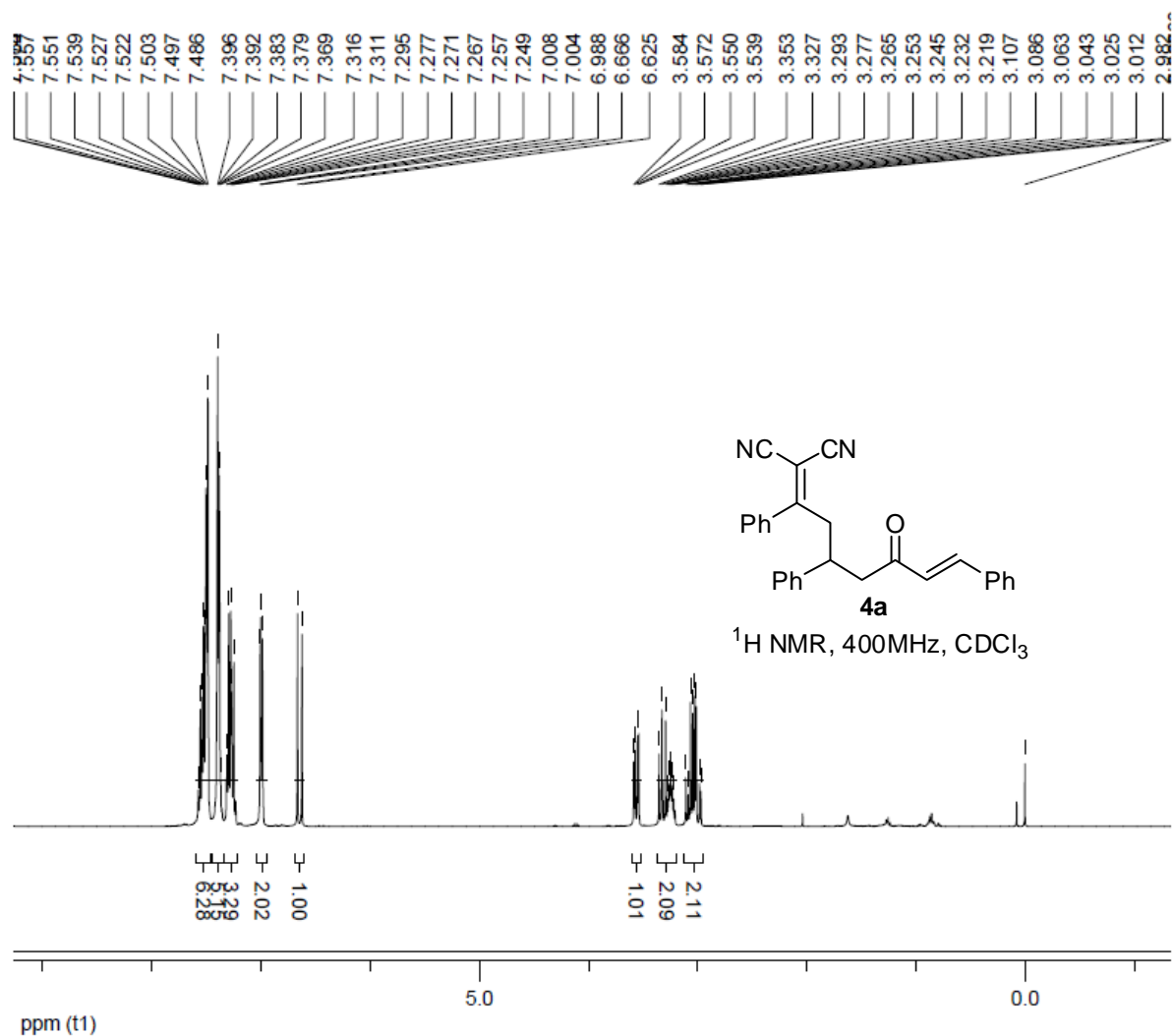
Date:  
5 Jul 2011  
Document's Title:  
nc

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.638  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 1.1010  
Spectral Width (ppm):  
(f1) 295.733  
Pulse Program:  
Unknown







Date:

5 Jul 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.130

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

(f1) 3.9846

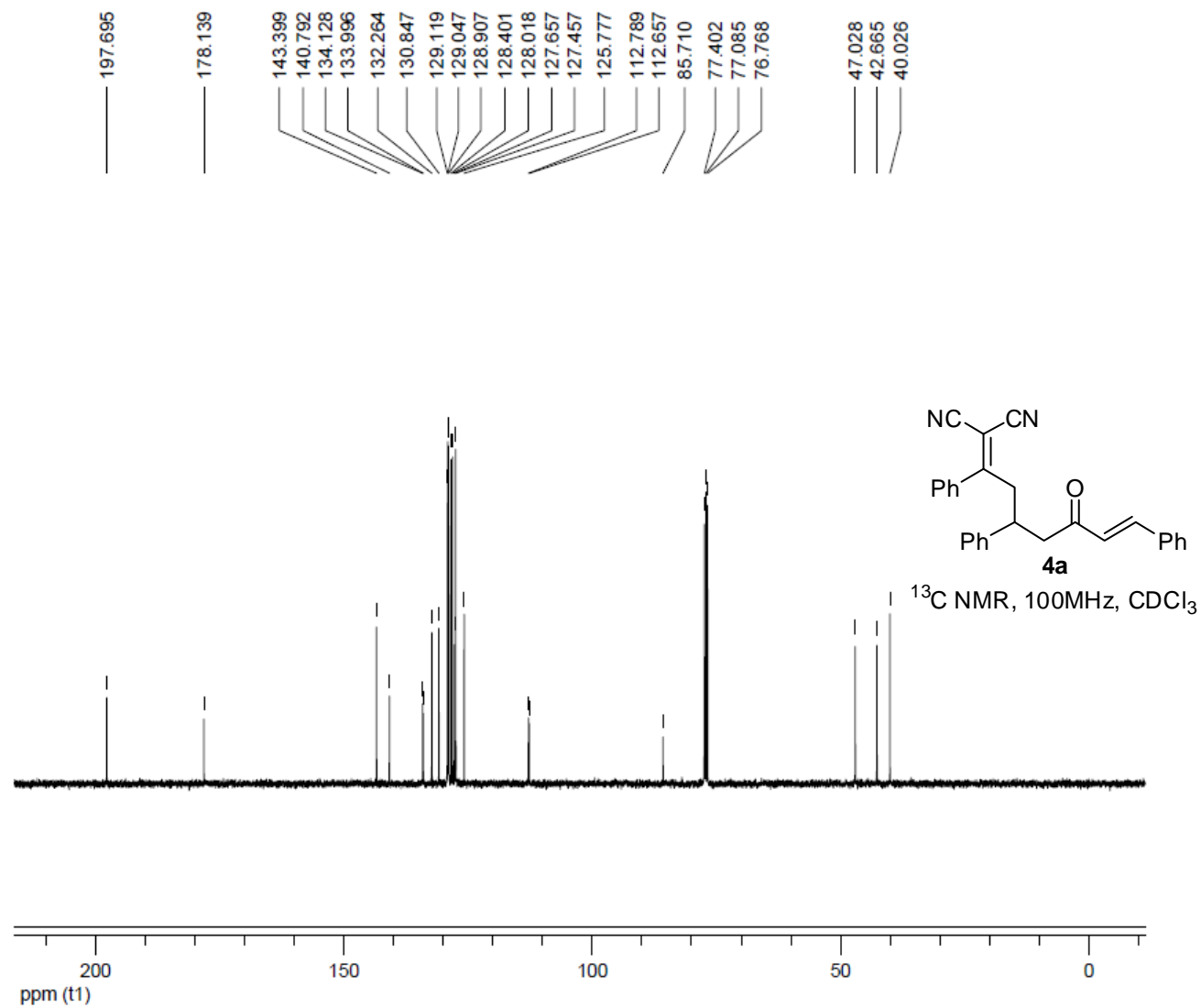
Spectral Width (ppm):

(f1) 20.553

Pulse Program:

Unknown

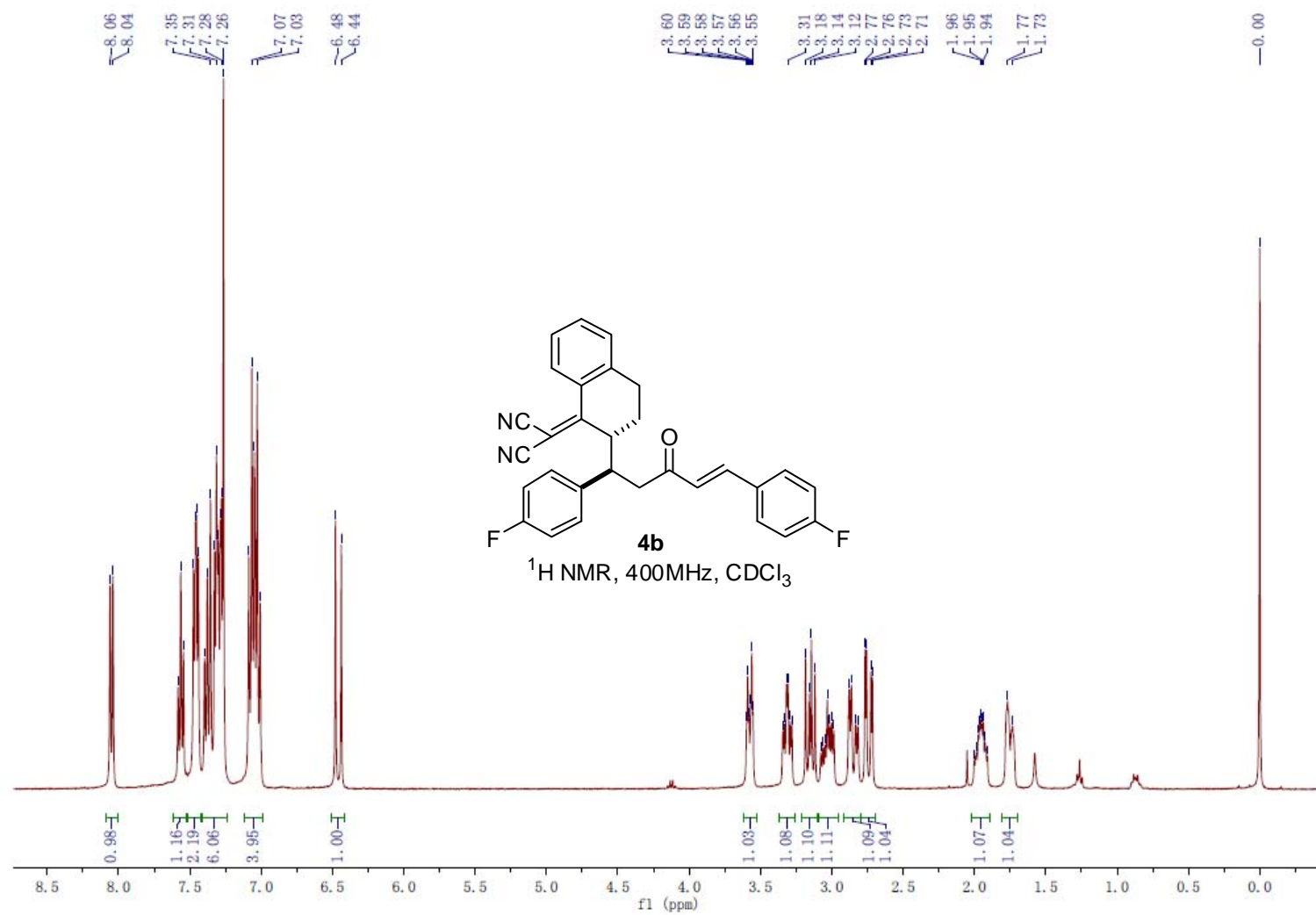


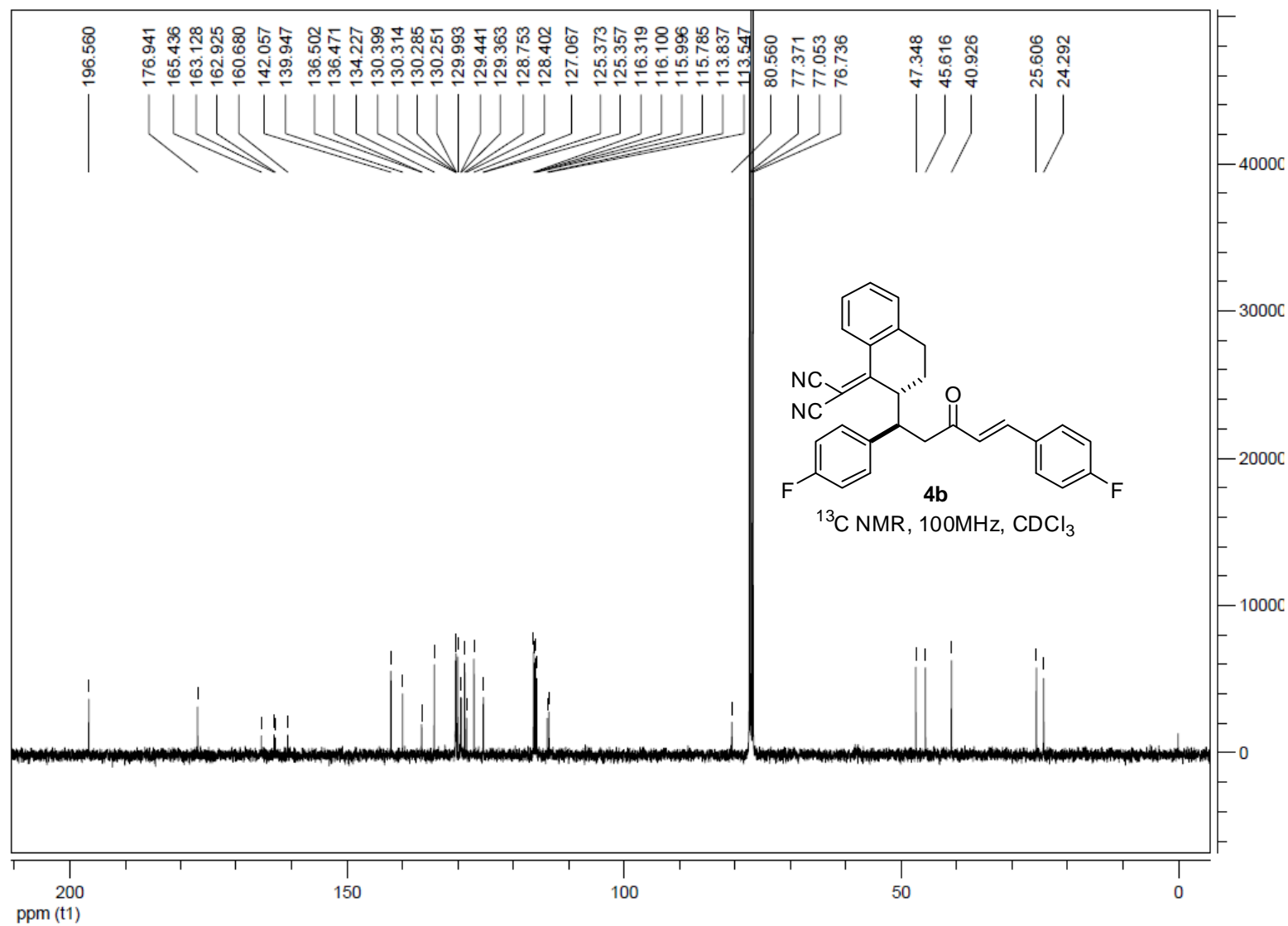


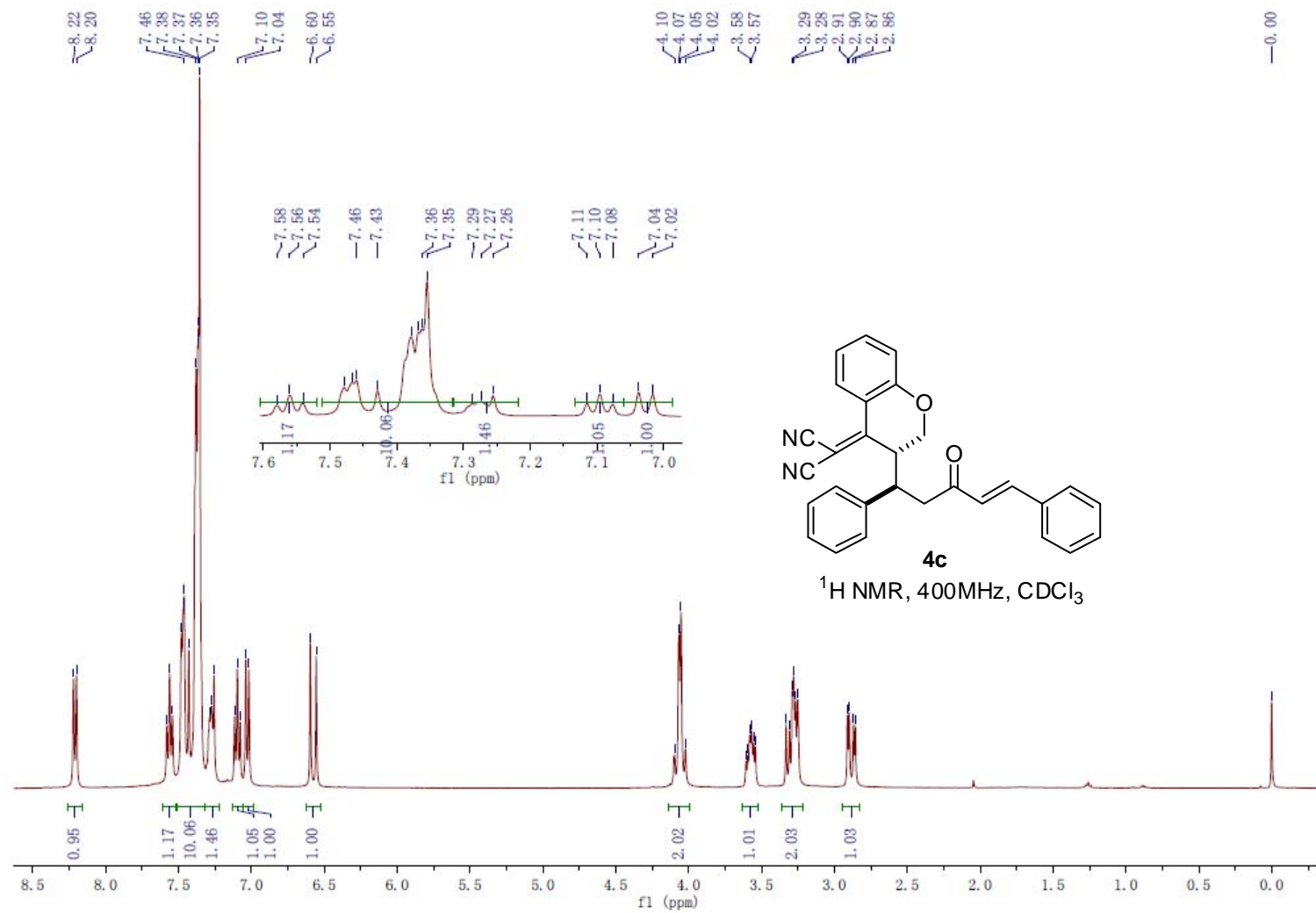
Date:  
5 Jul 2011  
Document's Title:  
nc

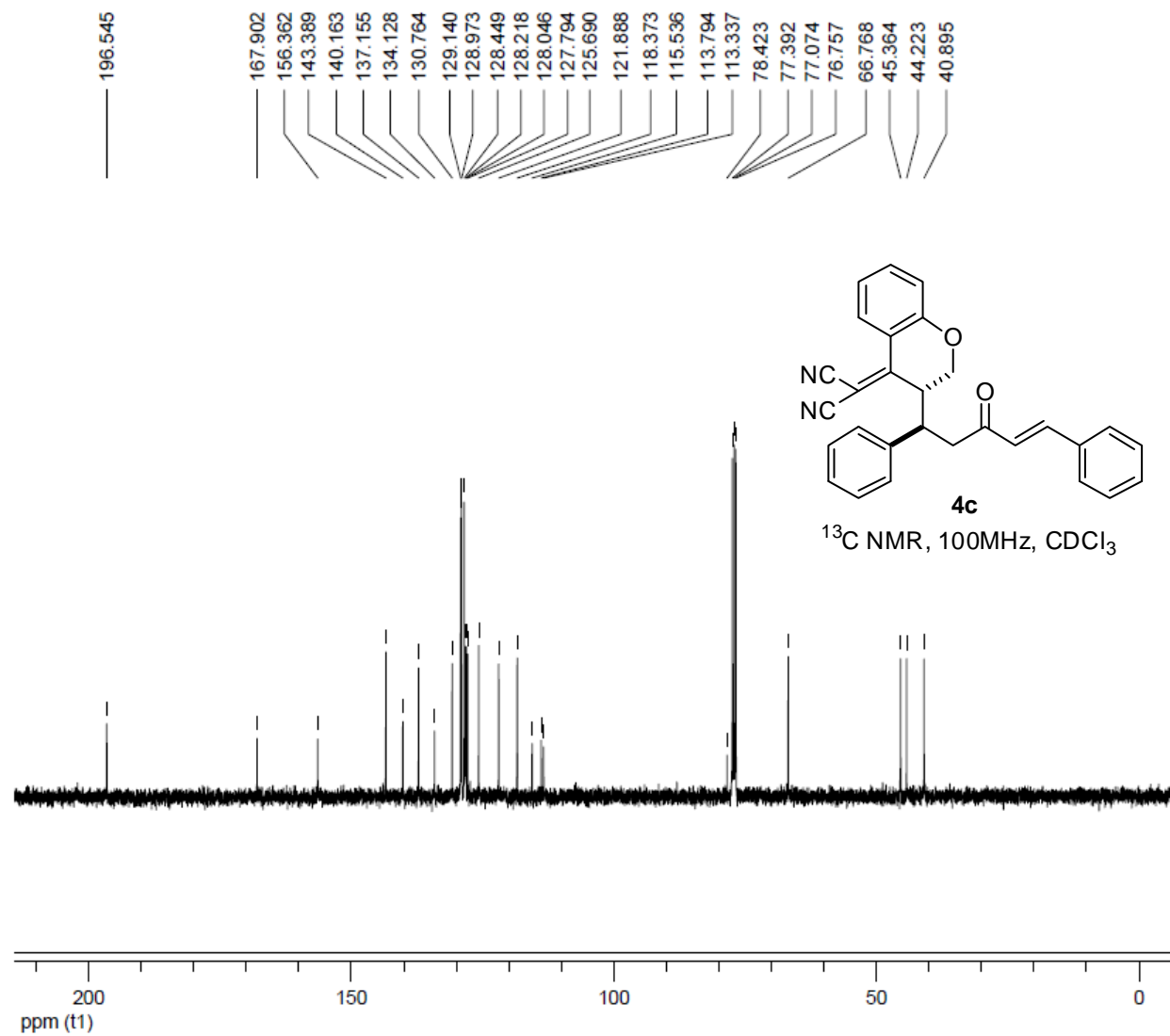
Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown





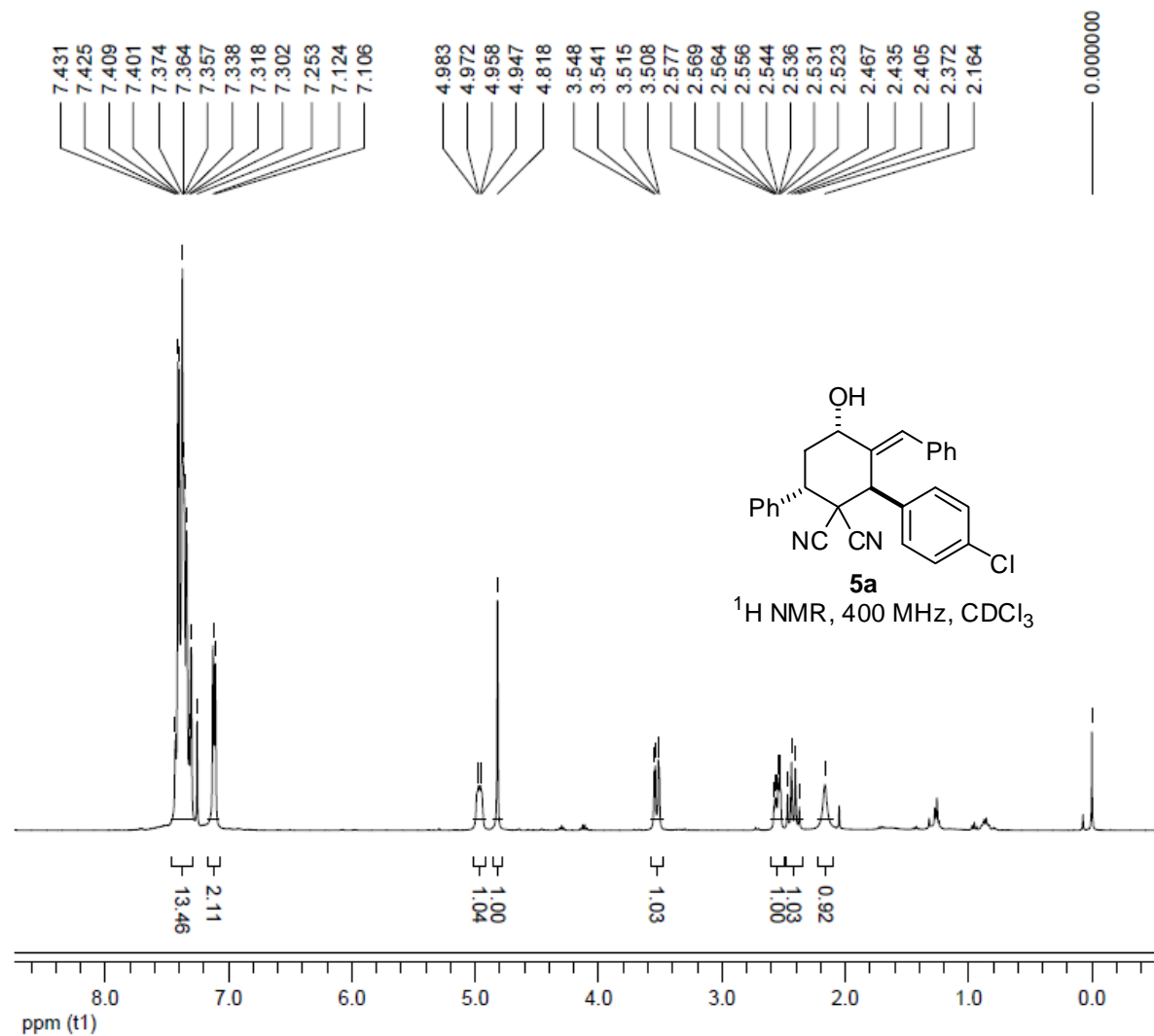




Date:  
5 Jul 2011  
Document's Title:  
nc

Spectrum Title:  
C13CPD

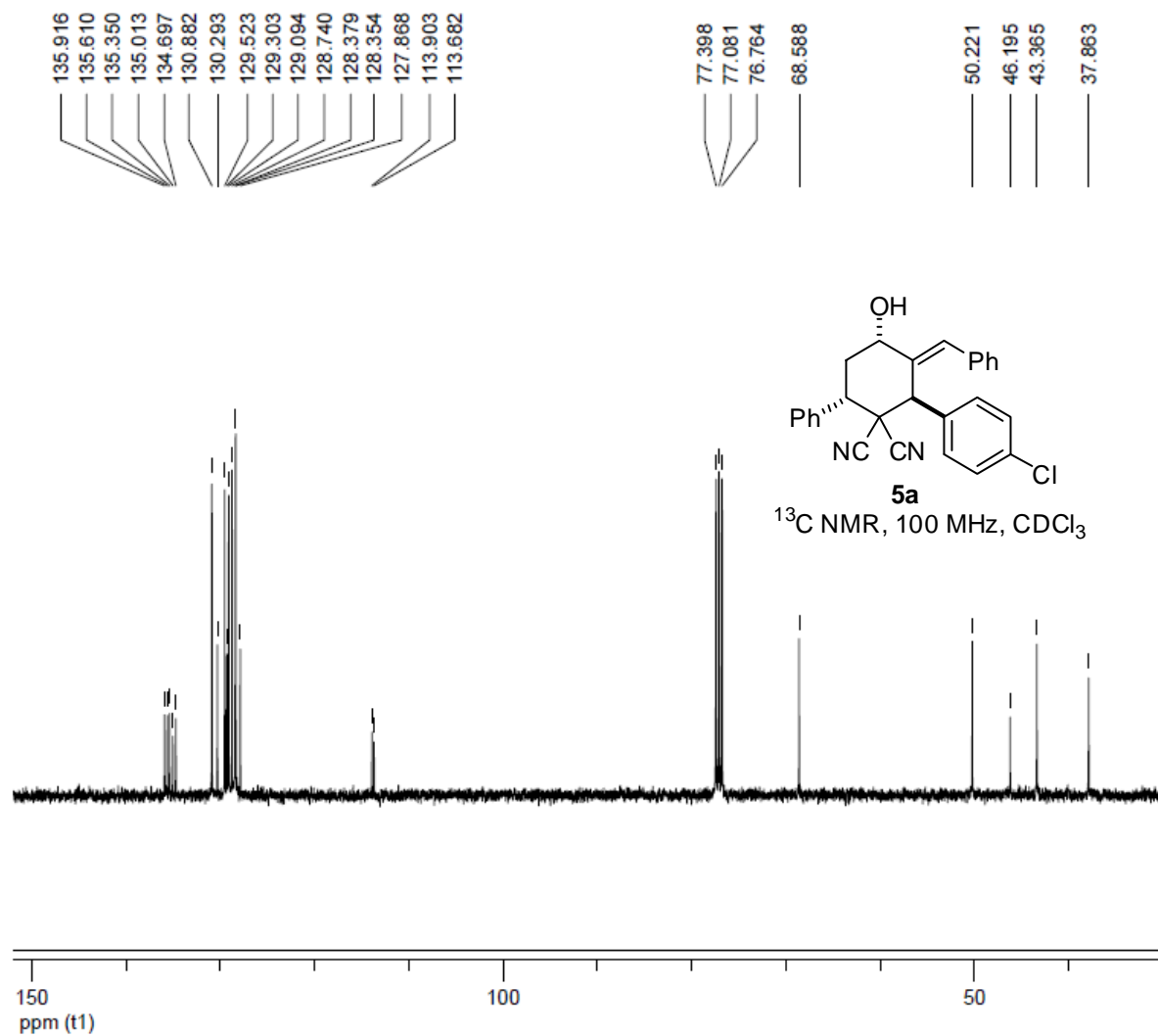
Frequency (MHz):  
(f1) 100.638  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 1.1010  
Spectral Width (ppm):  
(f1) 295.733  
Pulse Program:  
Unknown



Date:  
13 Sep 2011  
Document's Title:  
n.mrc

Spectrum Title:  
PROTON

Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown



Date:

13 Sep 2011

Document's Title:

n.mrc

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.638

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

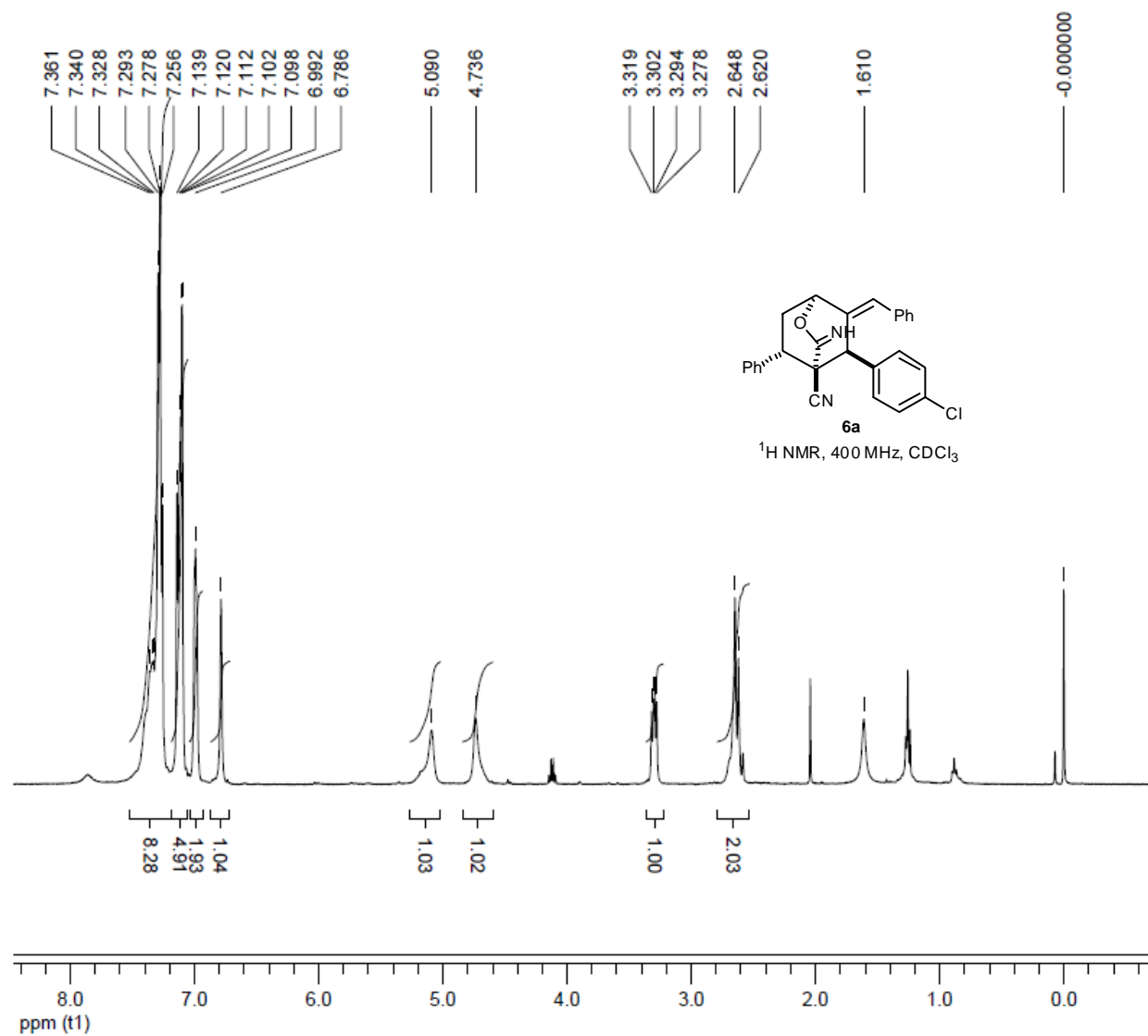
(f1) 1.1010

Spectral Width (ppm):

(f1) 295.733

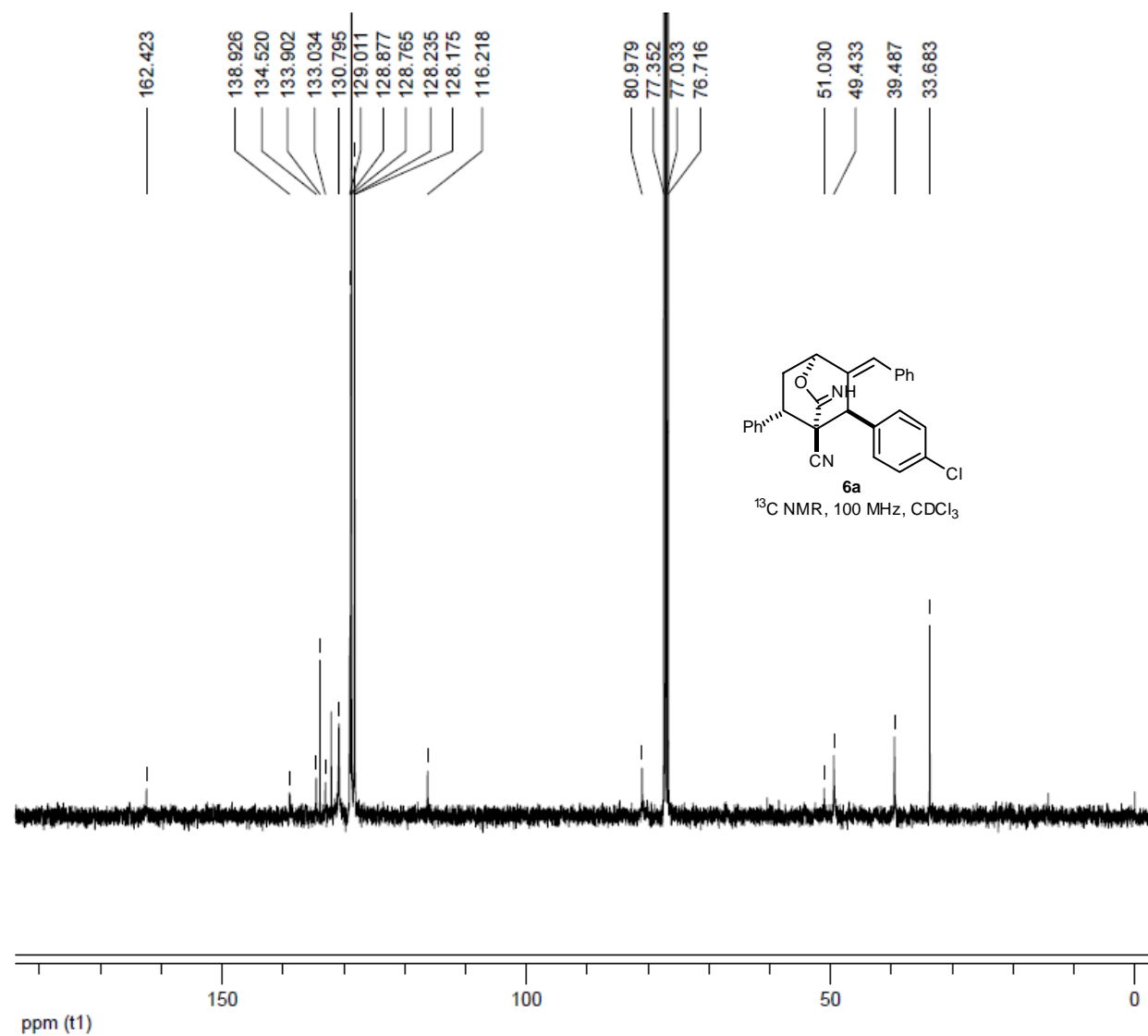
Pulse Program:

Unknown



Date:  
13 Sep 2011  
Document's Title:  
n  
Spectrum Title:  
PROTON  
Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown

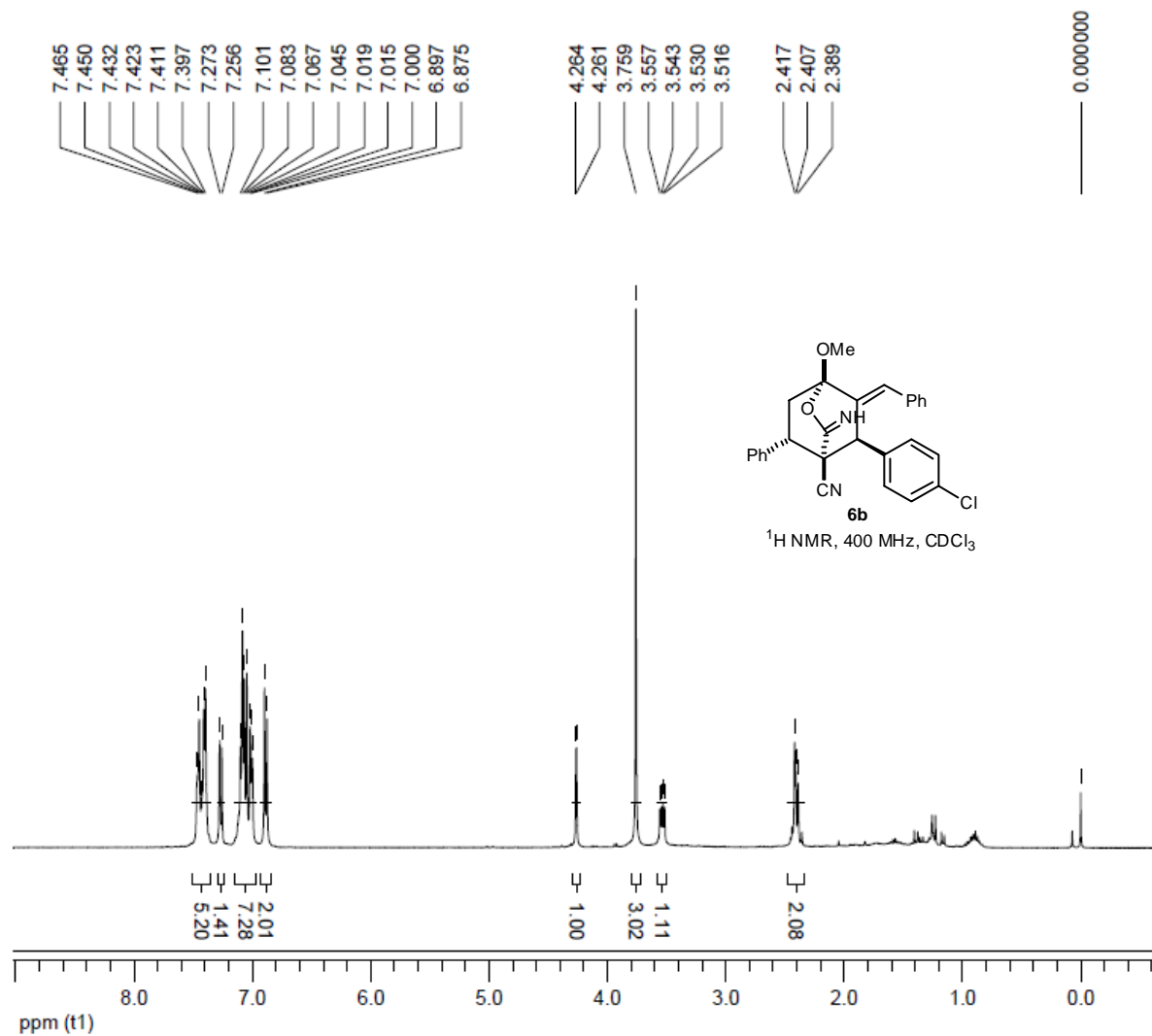




Date:  
13 Sep 2011  
Document's Title:  
n

Spectrum Title:  
C13CPD

Frequency (MHz):  
(f1) 100.613  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 0.9175  
Spectral Width (ppm):  
(f1) 354.968  
Pulse Program:  
Unknown



Date:

13 Sep 2011

Document's Title:

n

Spectrum Title:

PROTON

Frequency (MHz):

(f1) 400.230

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

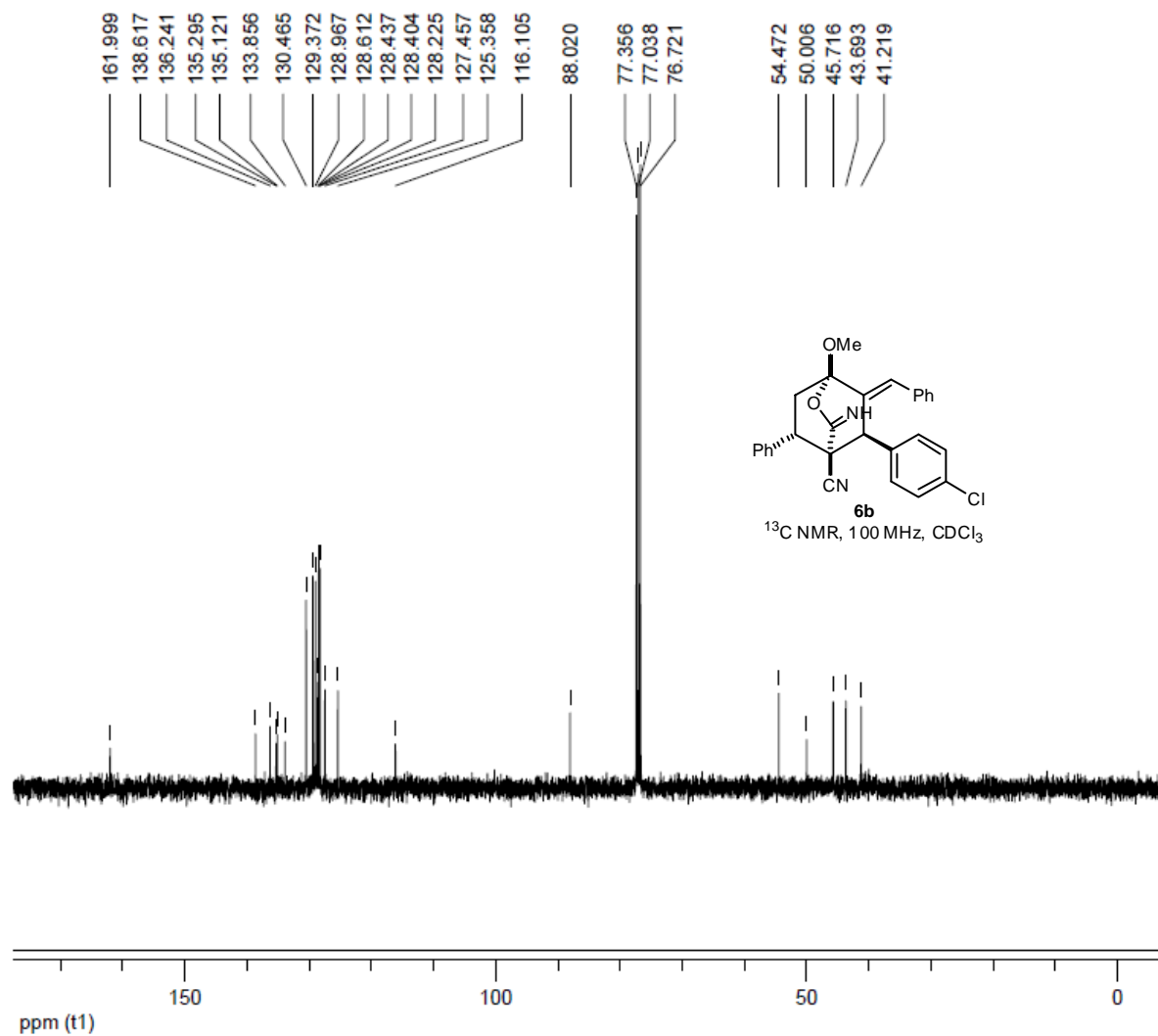
(f1) 3.9846

Spectral Width (ppm):

(f1) 20.547

Pulse Program:

Unknown



Date:

13 Sep 2011

Document's Title:

n

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.638

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

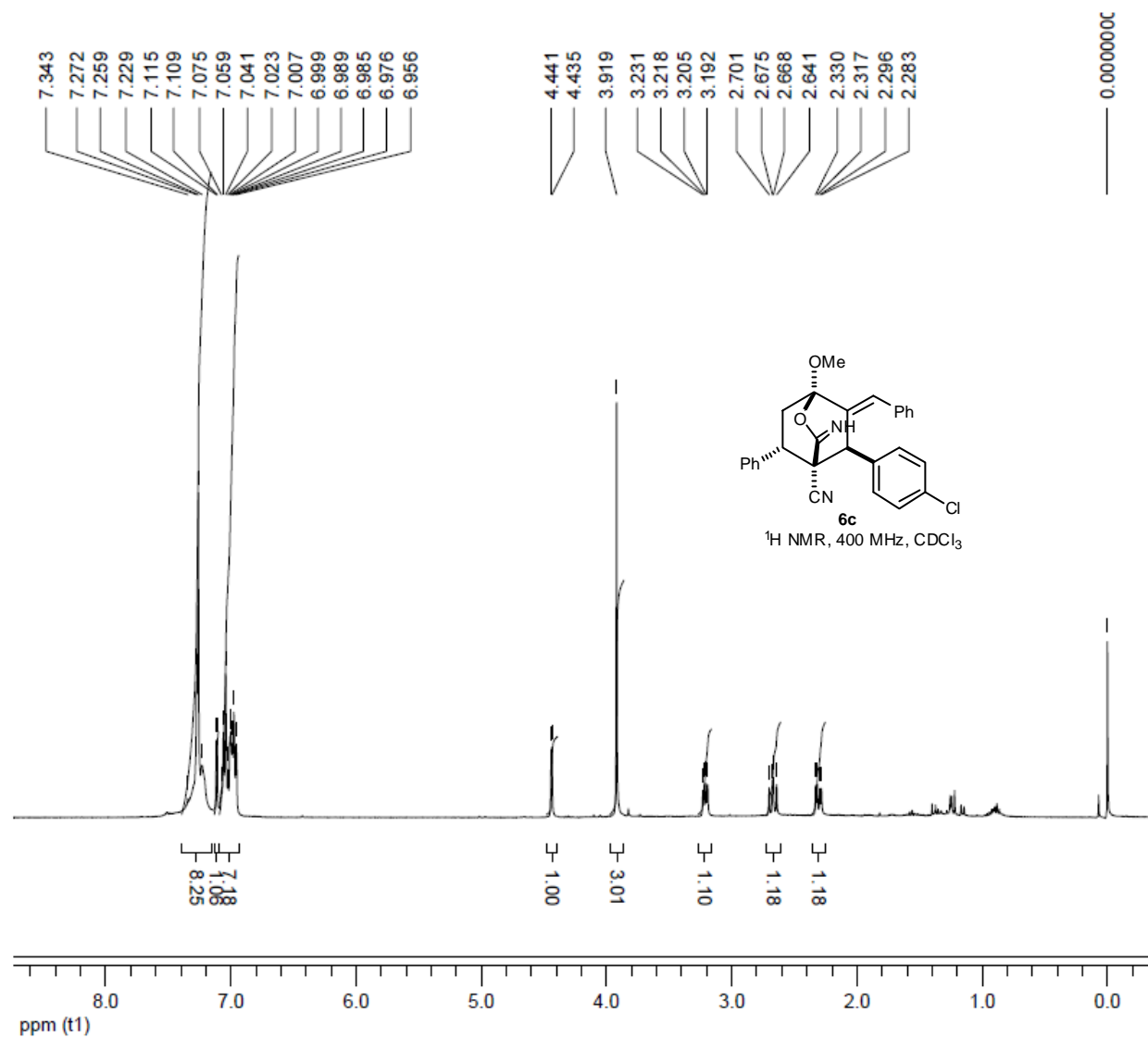
(f1) 1.1010

Spectral Width (ppm):

(f1) 295.733

Pulse Program:

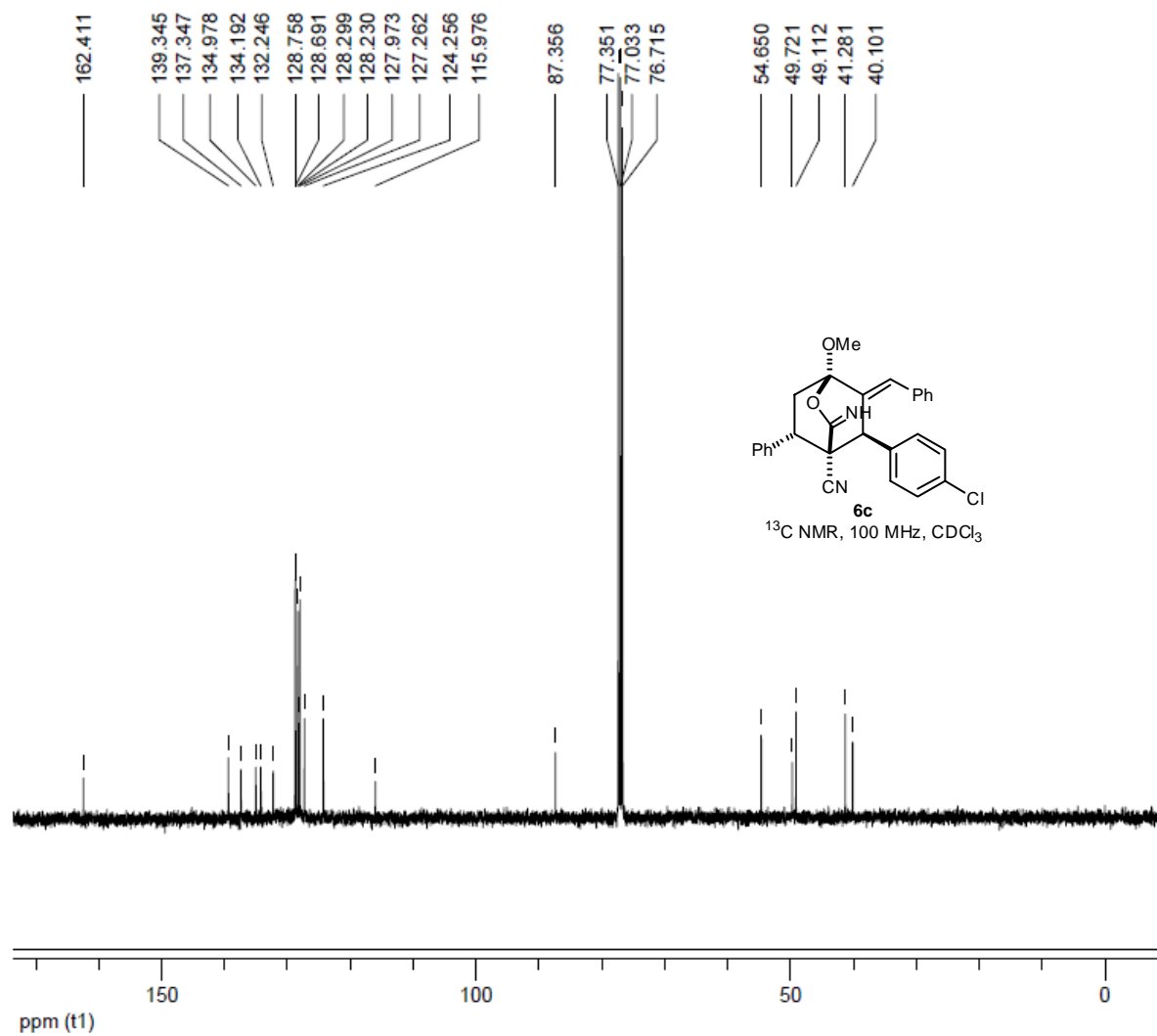
Unknown



Date:  
13 Sep 2011  
Document's Title:  
n

Spectrum Title:  
PROTON

Frequency (MHz):  
(f1) 400.130  
Original Points Count:  
(f1) 32768  
Actual Points Count:  
(f1) 32768  
Acquisition Time (sec):  
(f1) 3.9846  
Spectral Width (ppm):  
(f1) 20.553  
Pulse Program:  
Unknown



Date:

13 Sep 2011

Document's Title:

n

Spectrum Title:

C13CPD

Frequency (MHz):

(f1) 100.638

Original Points Count:

(f1) 32768

Actual Points Count:

(f1) 32768

Acquisition Time (sec):

(f1) 1.1010

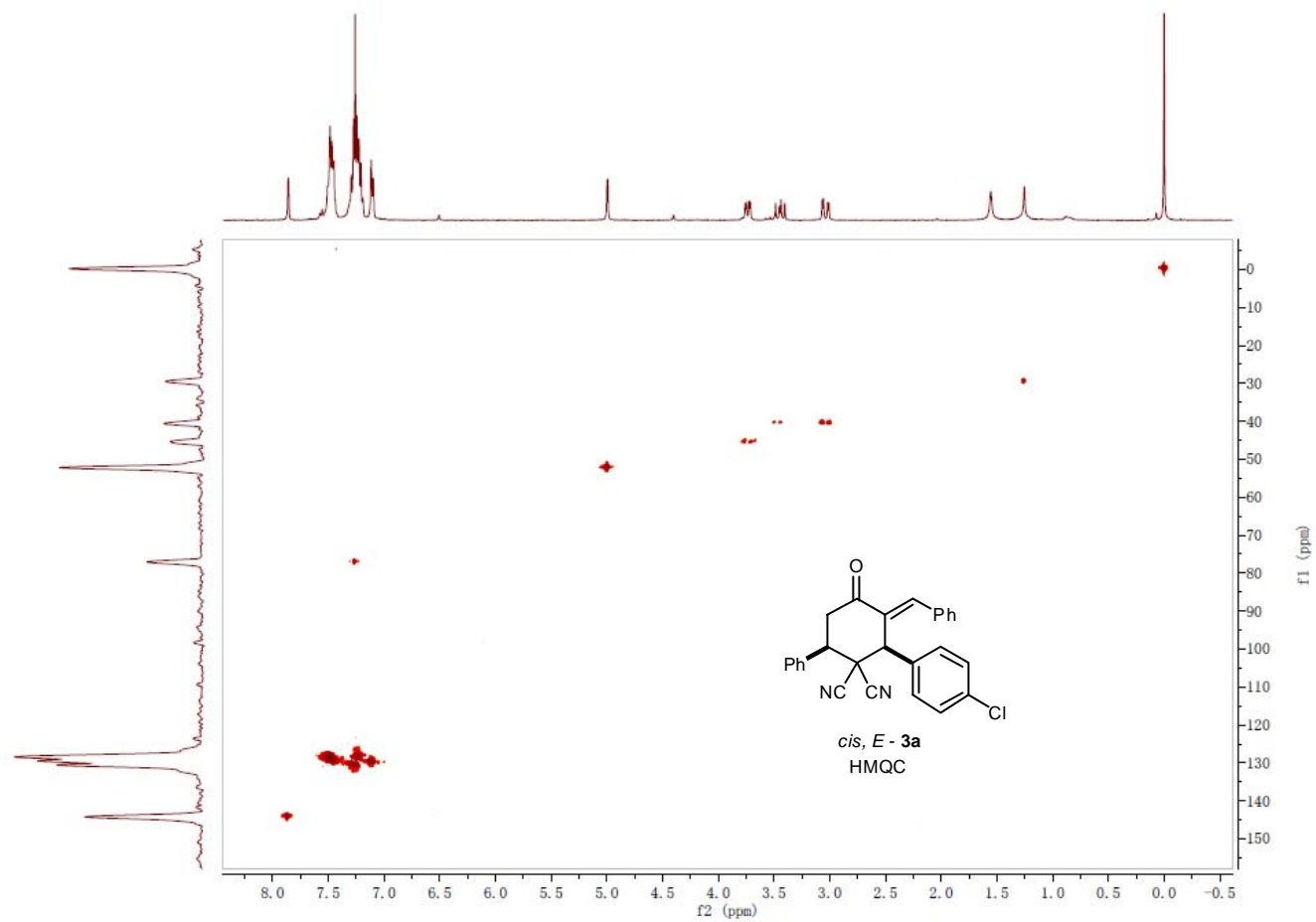
Spectral Width (ppm):

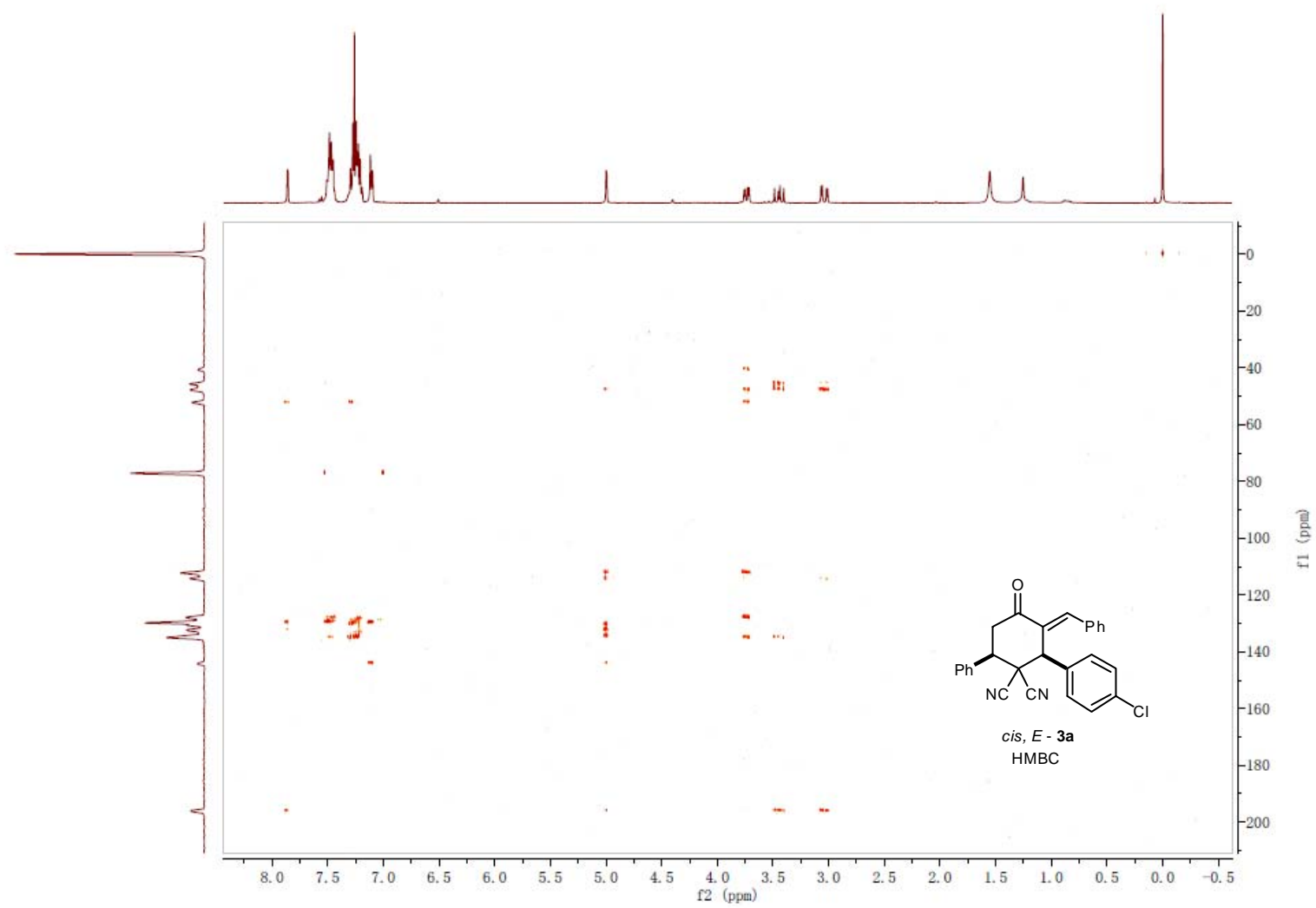
(f1) 295.733

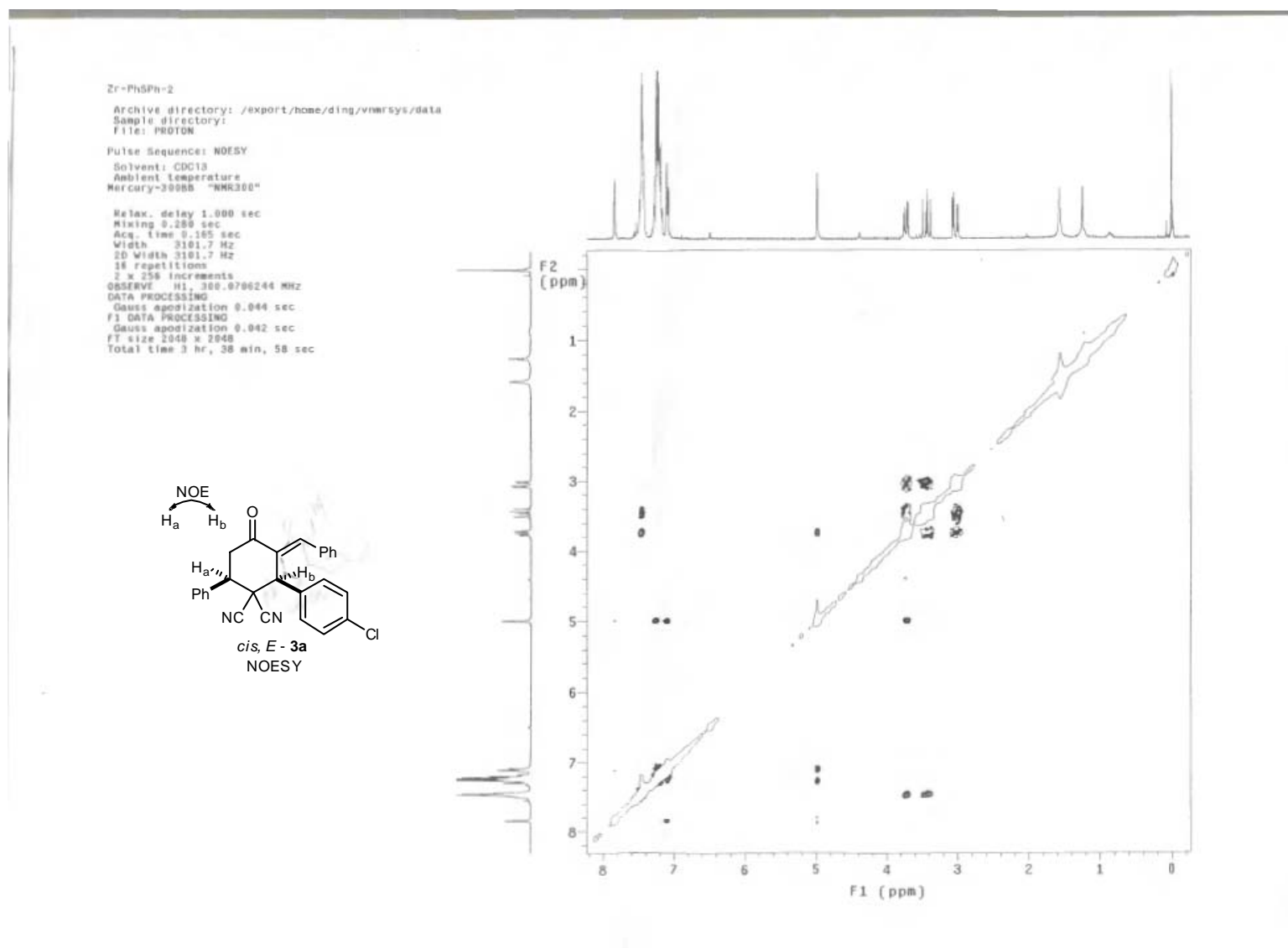
Pulse Program:

Unknown

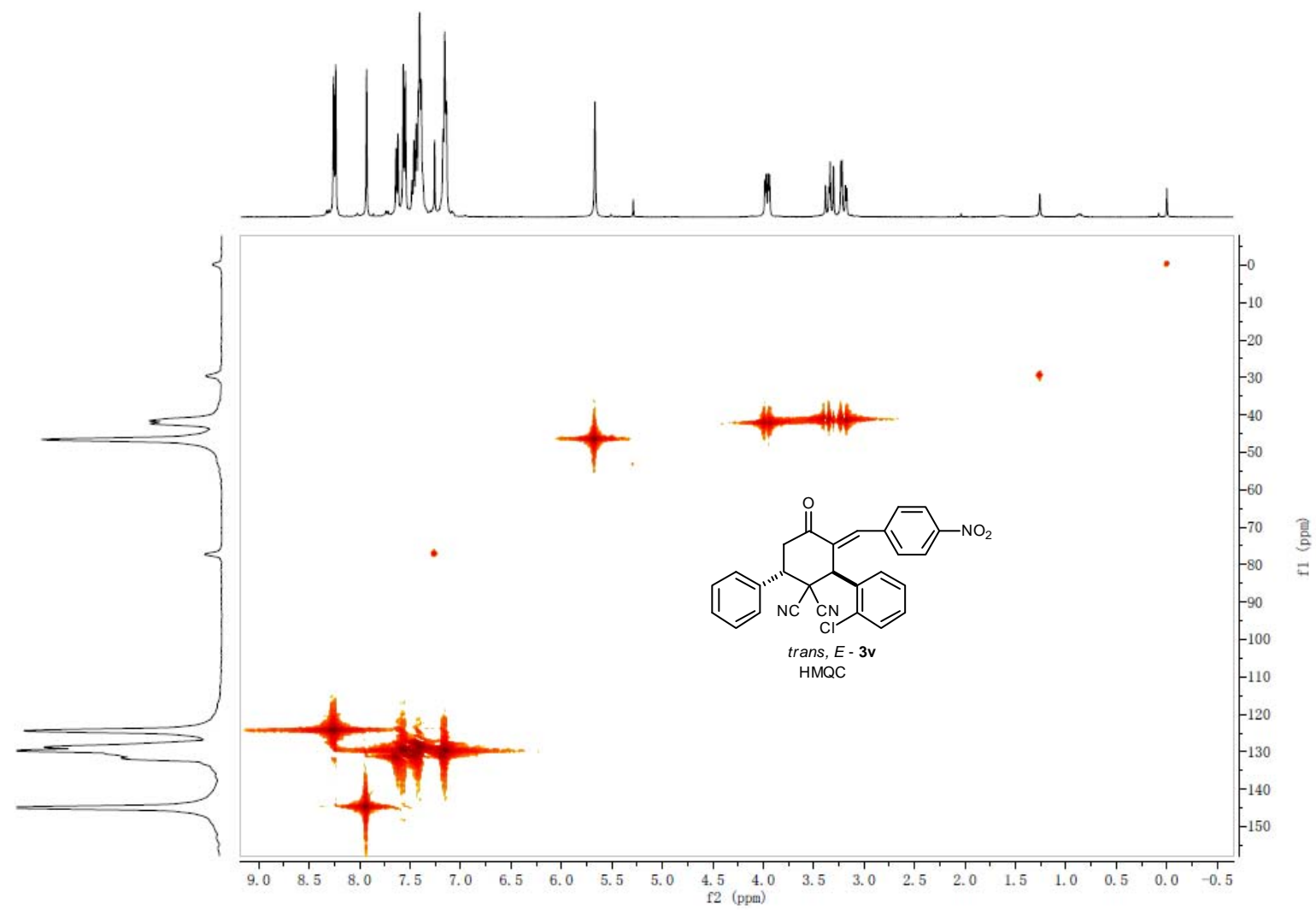
## IV. HMQC, HMBC and NOSEY Spectra

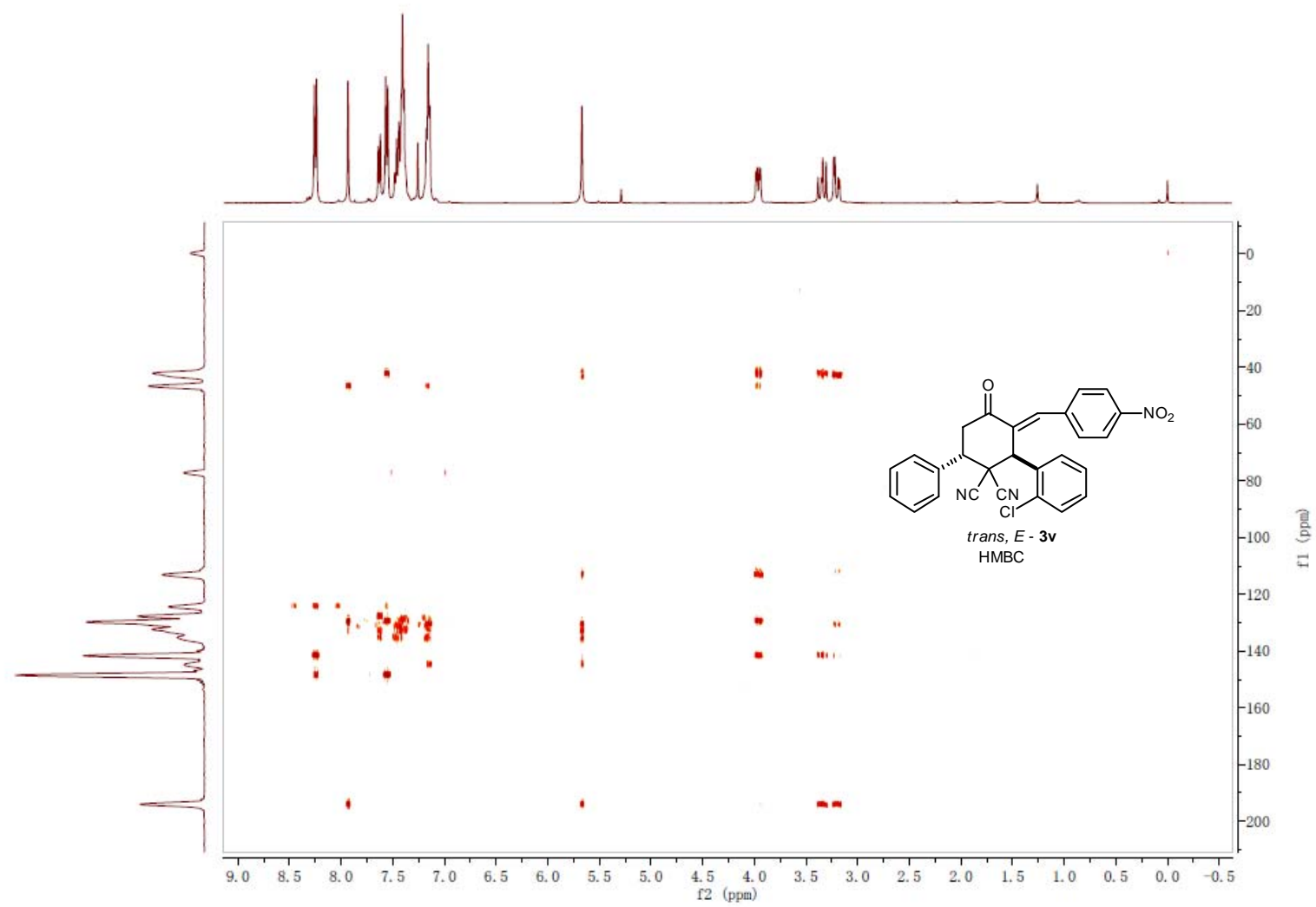










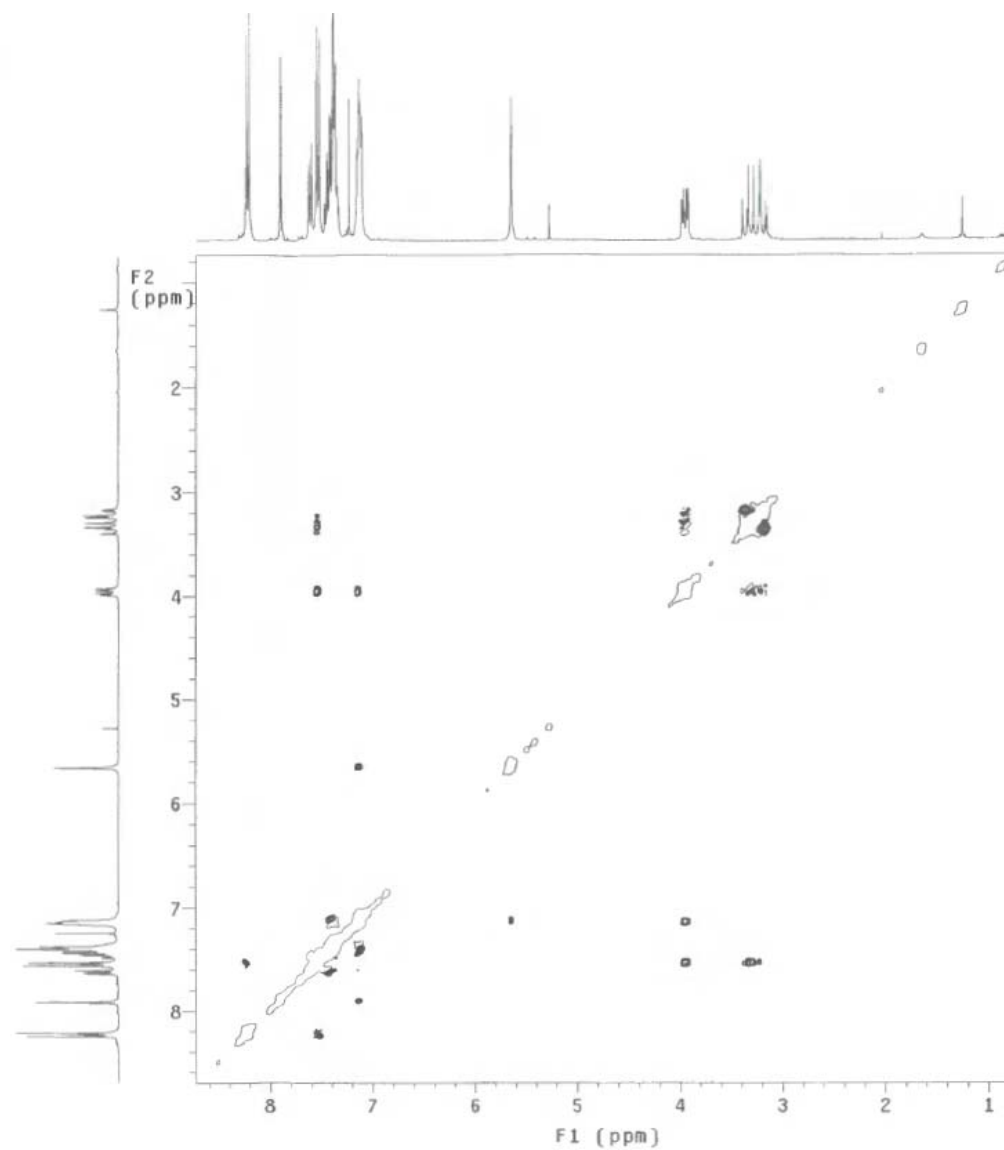
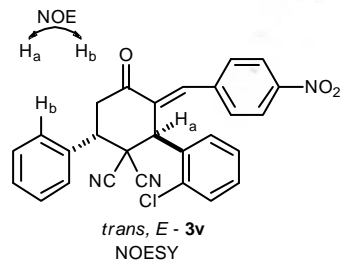


Zr-PhPh02S-0C1

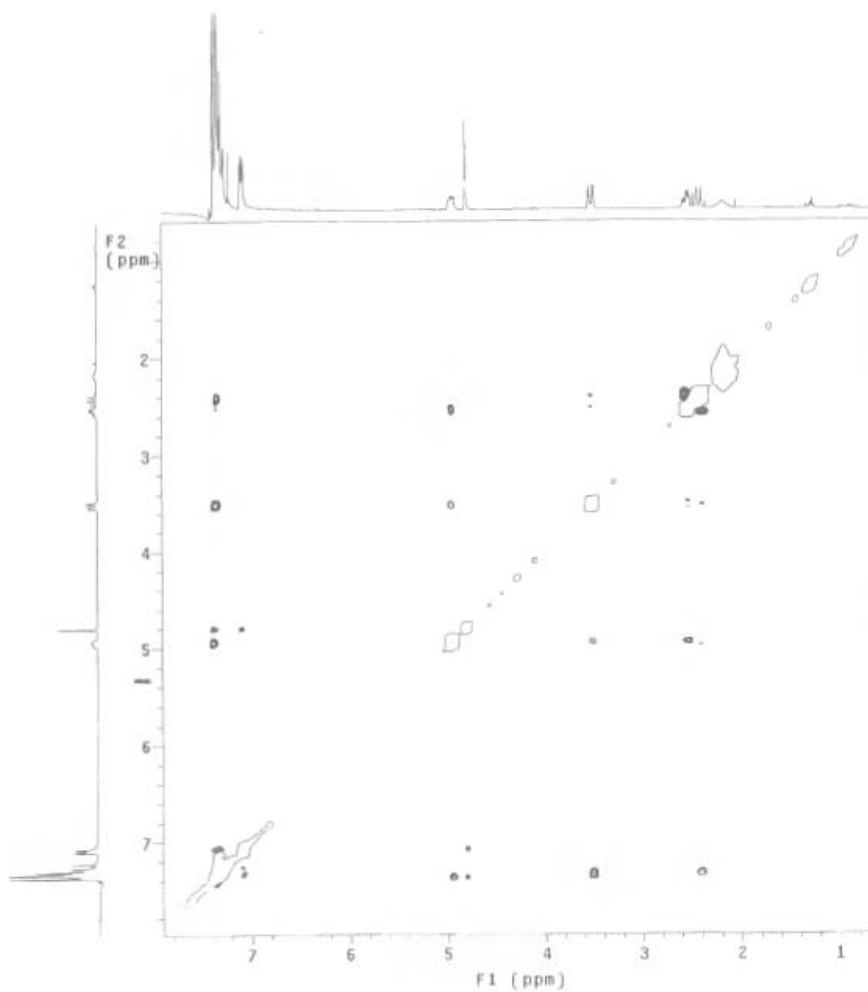
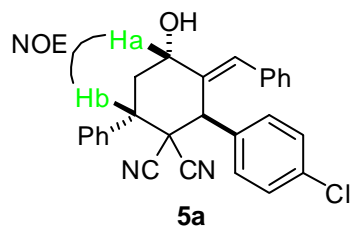
Archive directory: /export/home/ding/vnmrsys/data  
Sample directory:  
File: PROTON

Pulse Sequence: NOESY  
Solvent: CDCl3  
Ambient temperature  
Mercury-300BB "NMR300"

Relax. delay 1.000 sec  
Mixing 0.250 sec  
Acq. Time 0.155 sec  
Width 3301.4 Hz  
2D Width 3301.4 Hz  
15 repetitions  
2 x 256 increments  
OBSERVE H1, 300.0706281 MHz  
DATA PROCESSING  
Gauss apodization 0.057 sec  
F1 DATA PROCESSING  
Gauss apodization 0.040 sec  
FT size 2048 x 2048  
Total time 3 hr, 33 min, 5 sec



zr-reduc-1  
Archive directory: /export/home/ding/vnmrsys/data  
Sample directory:  
File: PROTON  
Pulse Sequence: NOESY  
Solvent: CDCl3  
Ambient temperature  
Mercury-300RS "NMR300"  
Relax. delay 1.000 sec  
Mixing 0.280 sec  
Acq. time 0.171 sec  
Width 2305.5 Hz  
2D Width 2305.5 Hz  
8 repetitions  
2 x 256 increments  
OBSERVE H1, 300.0706313 MHz  
DATA PROCESSING  
Gauss apodization 0.045 sec  
F1 DATA PROCESSING  
Gauss apodization 0.029 sec  
FT size 2048 x 2048  
Total time 1 hr, 50 min, 29 sec



zr-spd-1  
Archive directory: /export/home/ding/vnmrsys/data  
Sample directory:  
File: PROTON  
Pulse Sequence: NQESY  
Solvent: CDCl3  
Ambient temperature  
Mercury-300SB "NMR300"  
Relax. delay 1.000 sec  
Mixing 8.278 sec  
Acq. time 0.170 sec  
Width 3016.6 Hz  
2D Width 3016.6 Hz  
18 repetitions  
2 x 256 increments  
OBSERVE H1, 300.0706244 MHz  
DATA PROCESSING  
Gauss apodization 0.038 sec  
F1 DATA PROCESSING  
Gauss apodization 0.033 sec  
FT size 2048 x 2048  
Total time 3 hr, 38 min, 24 sec

