

## **Expeditious Synthesis of 1-Aminoindane Derivatives by [1,4]-Hydride Shift Mediated C(sp<sup>3</sup>)-H Bond Functionalization**

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Gakushuin University,  
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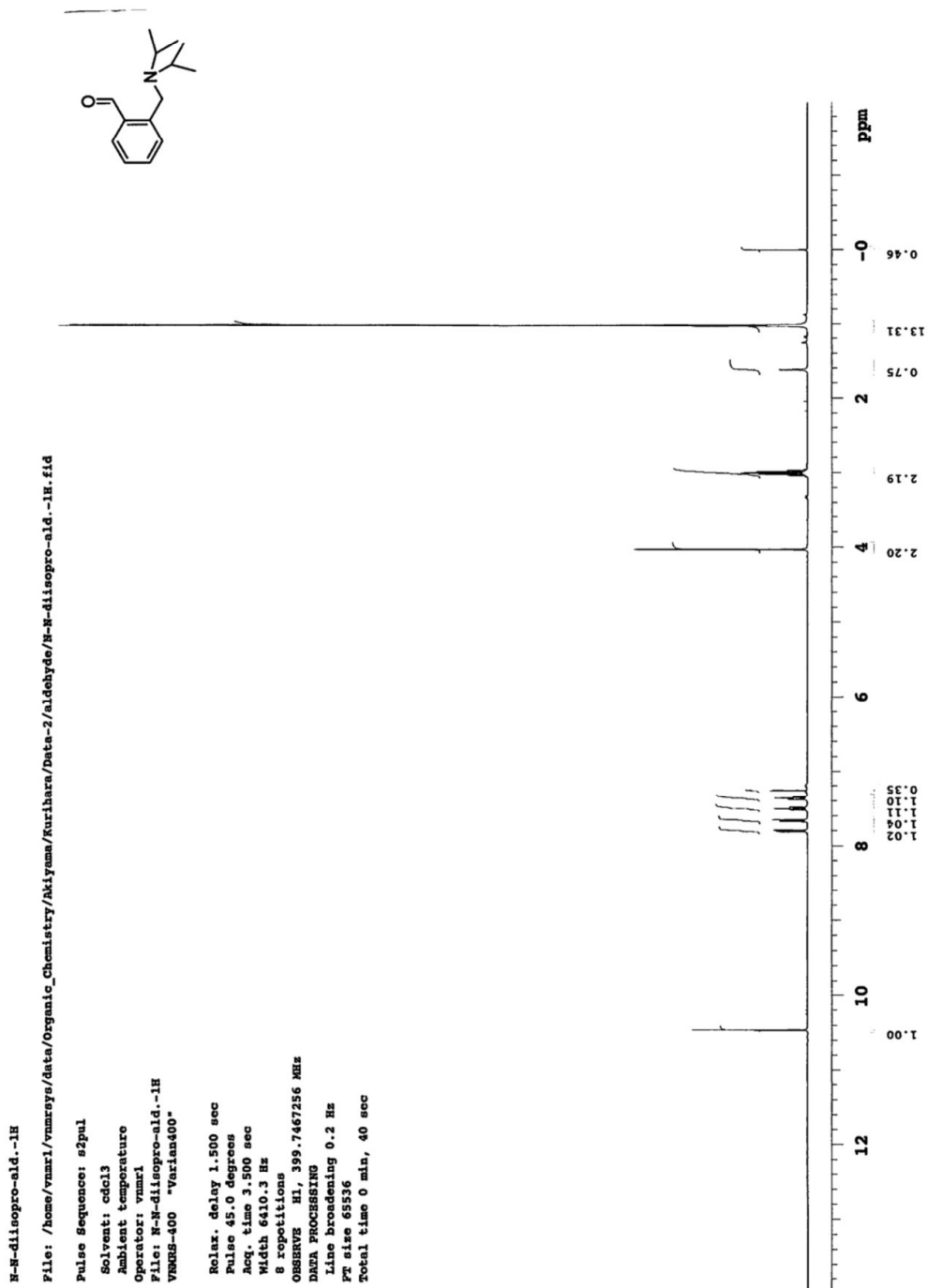
*takahiko.akiyama@gakushuin.ac.jp*

### ***Supporting Information***

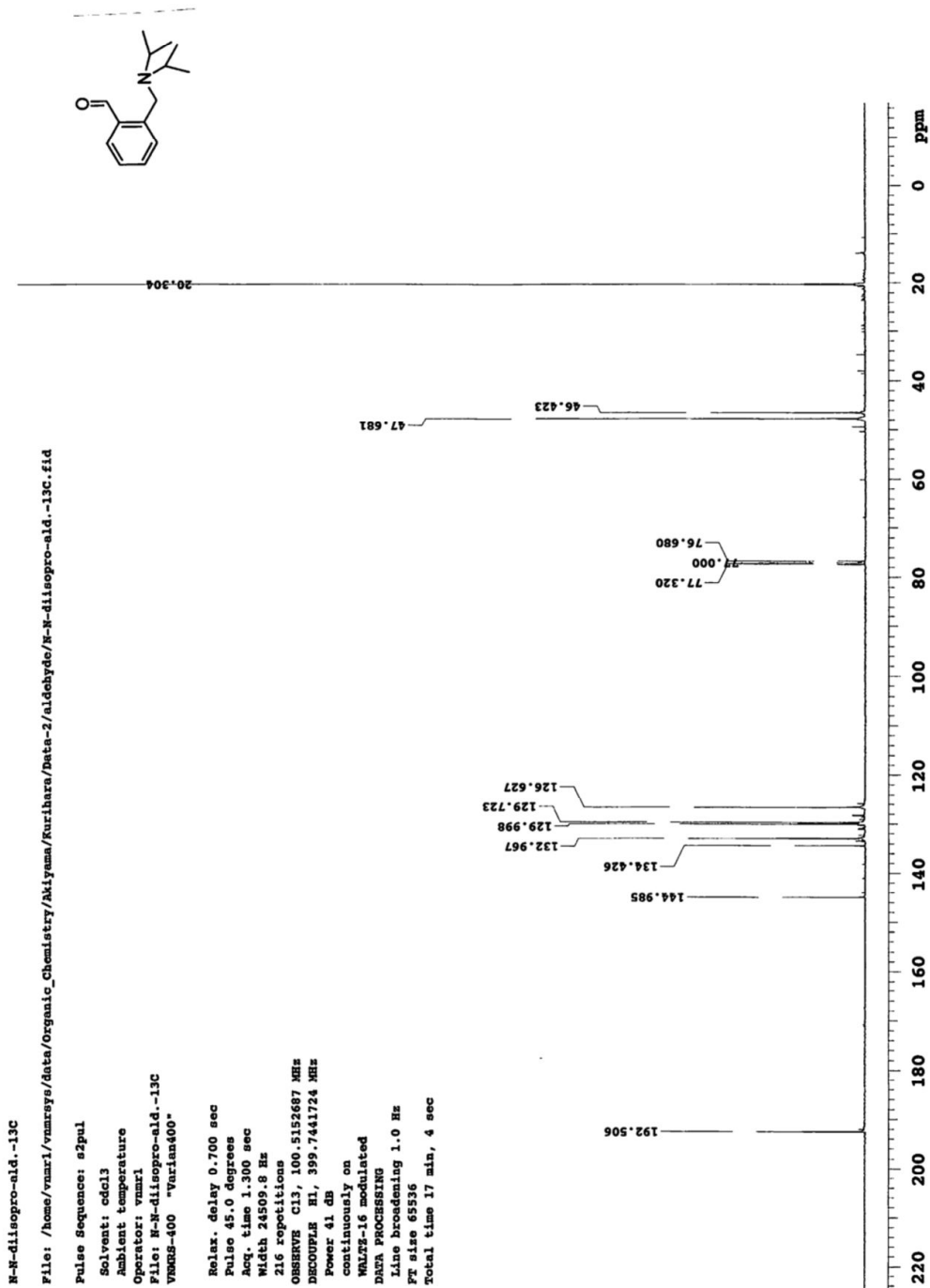
Scanned images of <sup>1</sup>H-, <sup>13</sup>C-NMR of new compounds

S1

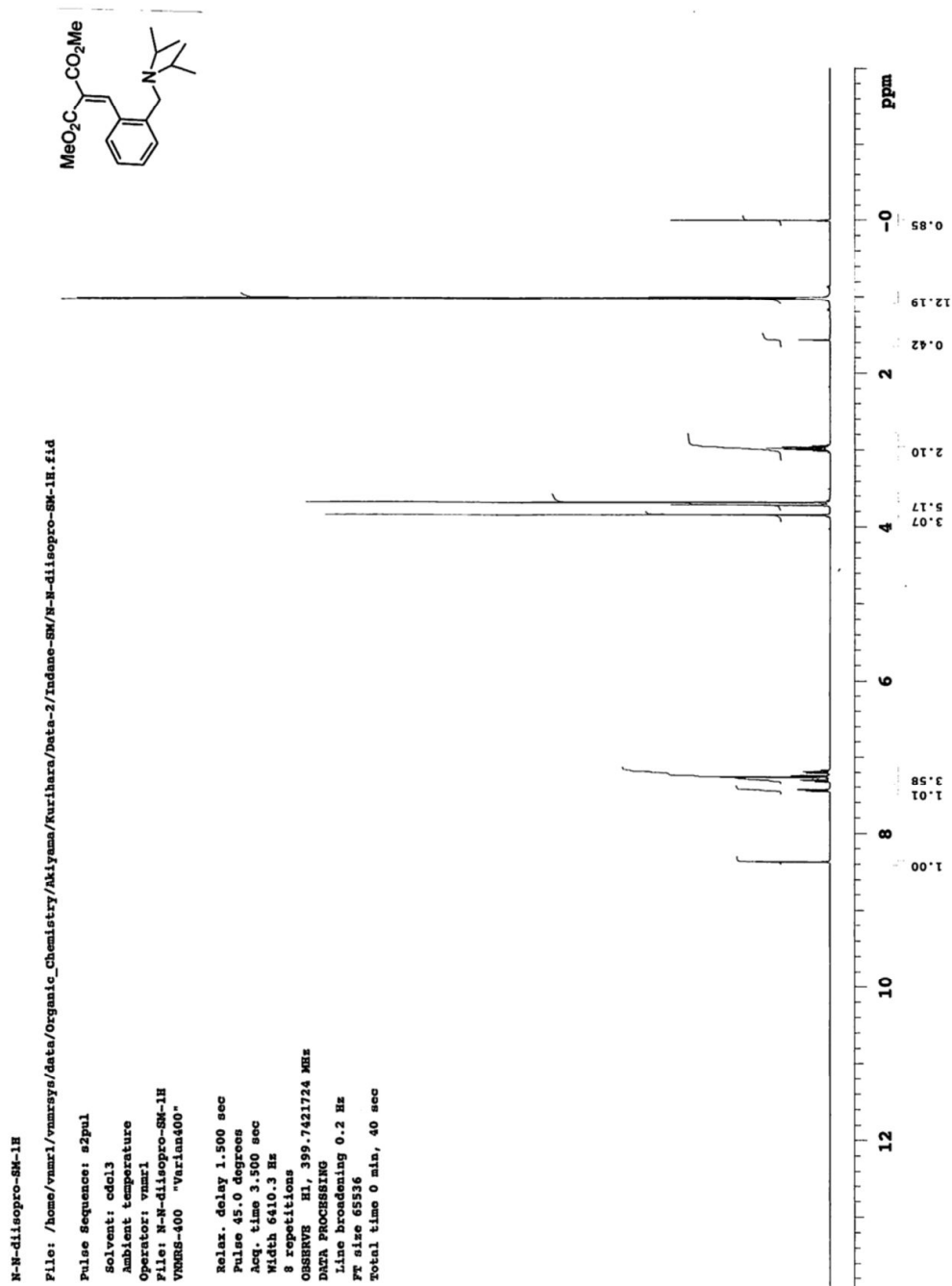
<sup>1</sup>H NMR spectrum of s3.



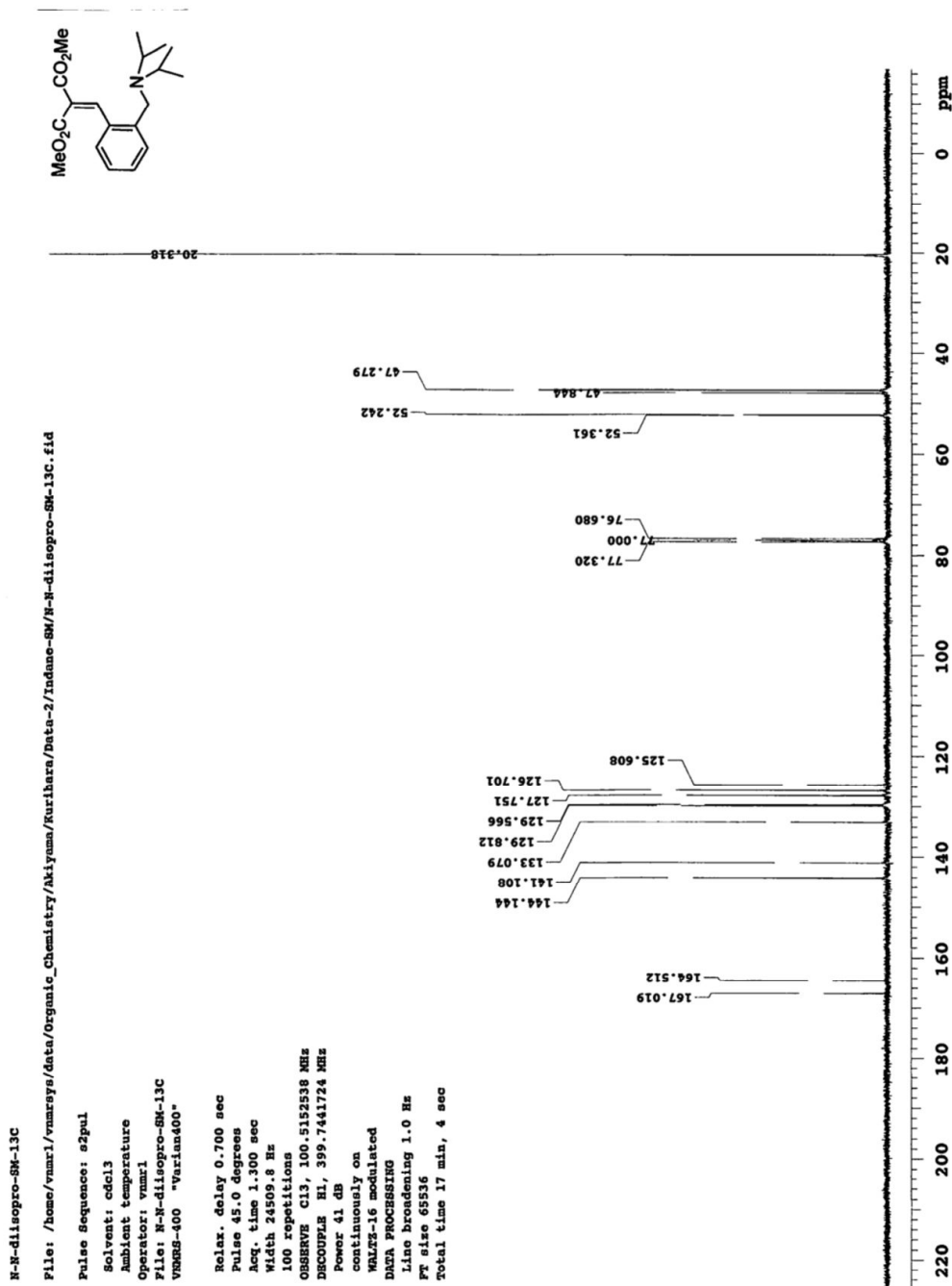
<sup>13</sup>C NMR spectrum of **s3**.



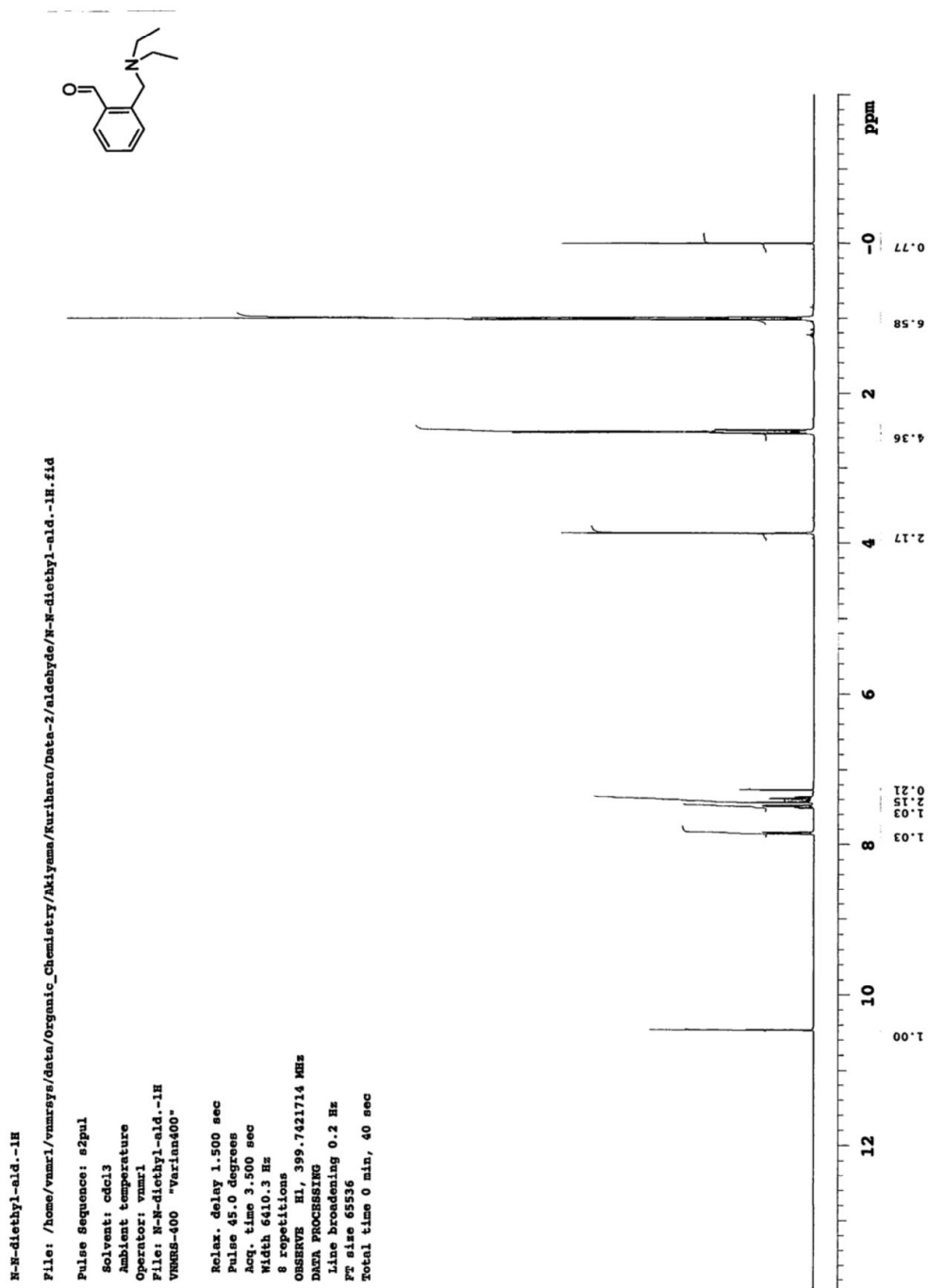
<sup>1</sup>H NMR spectrum of **3a**.



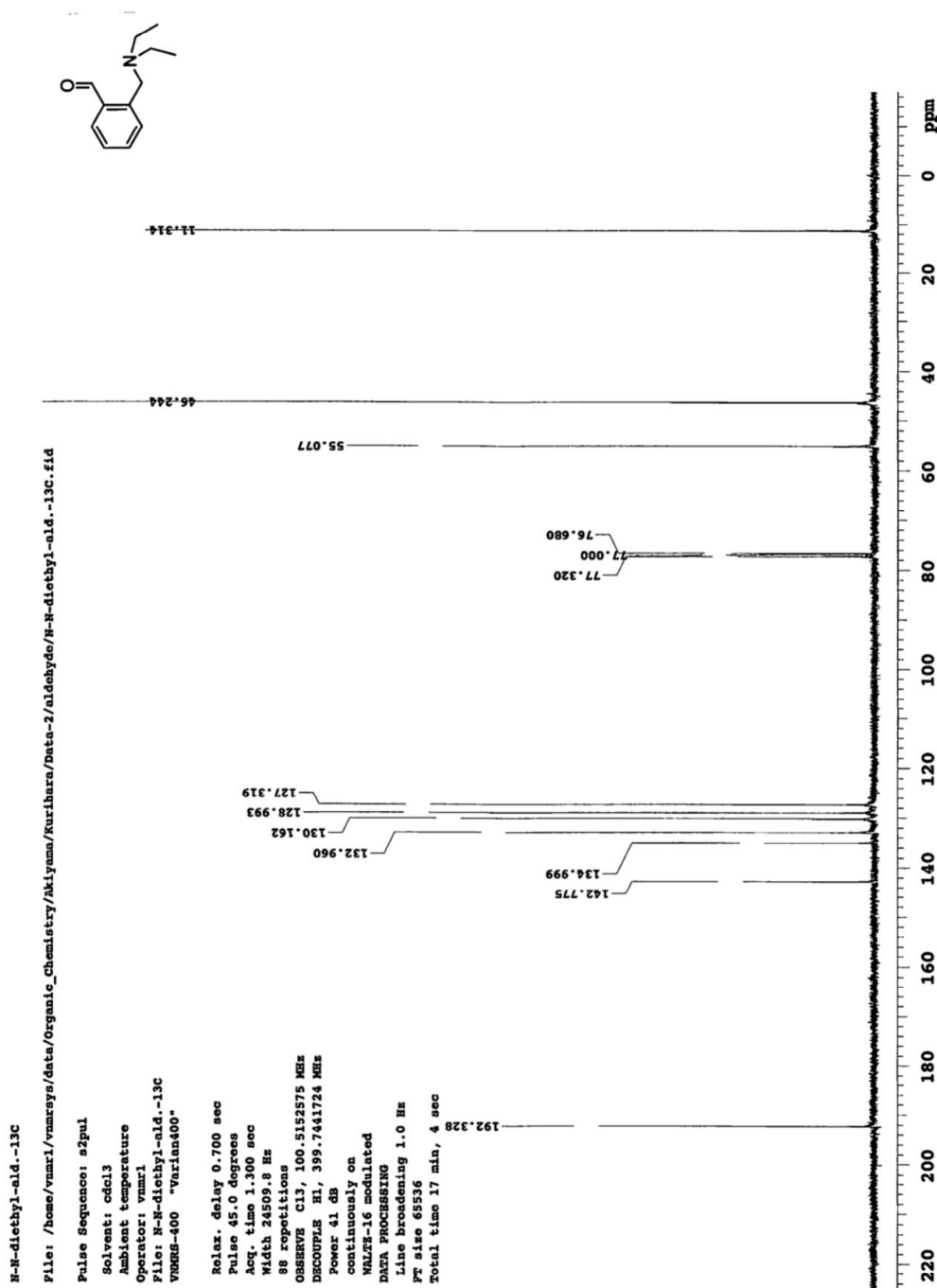
<sup>13</sup>C NMR spectrum of 3a.



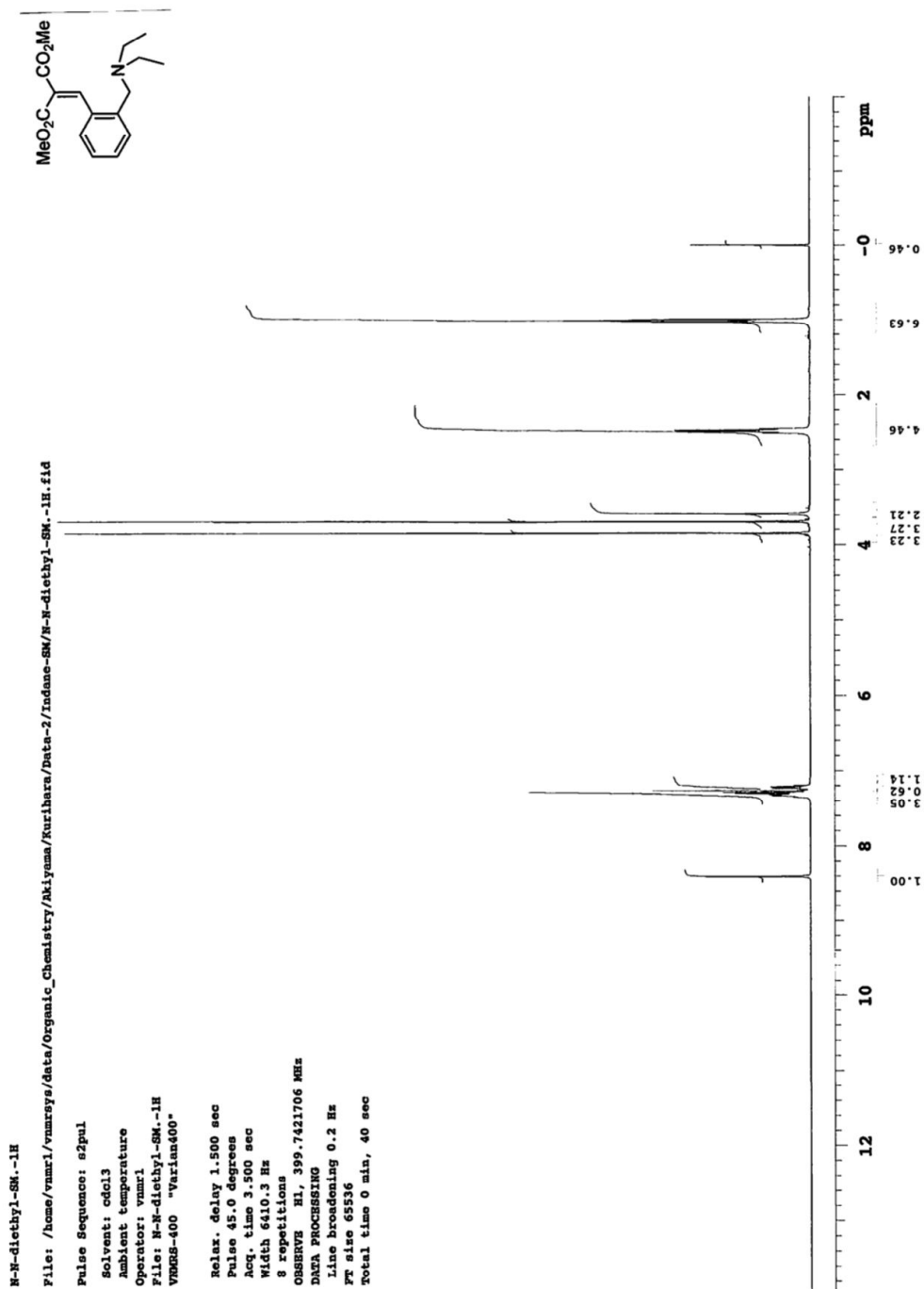
<sup>1</sup>H NMR spectrum of **5**.



<sup>13</sup>C NMR spectrum of **5**.

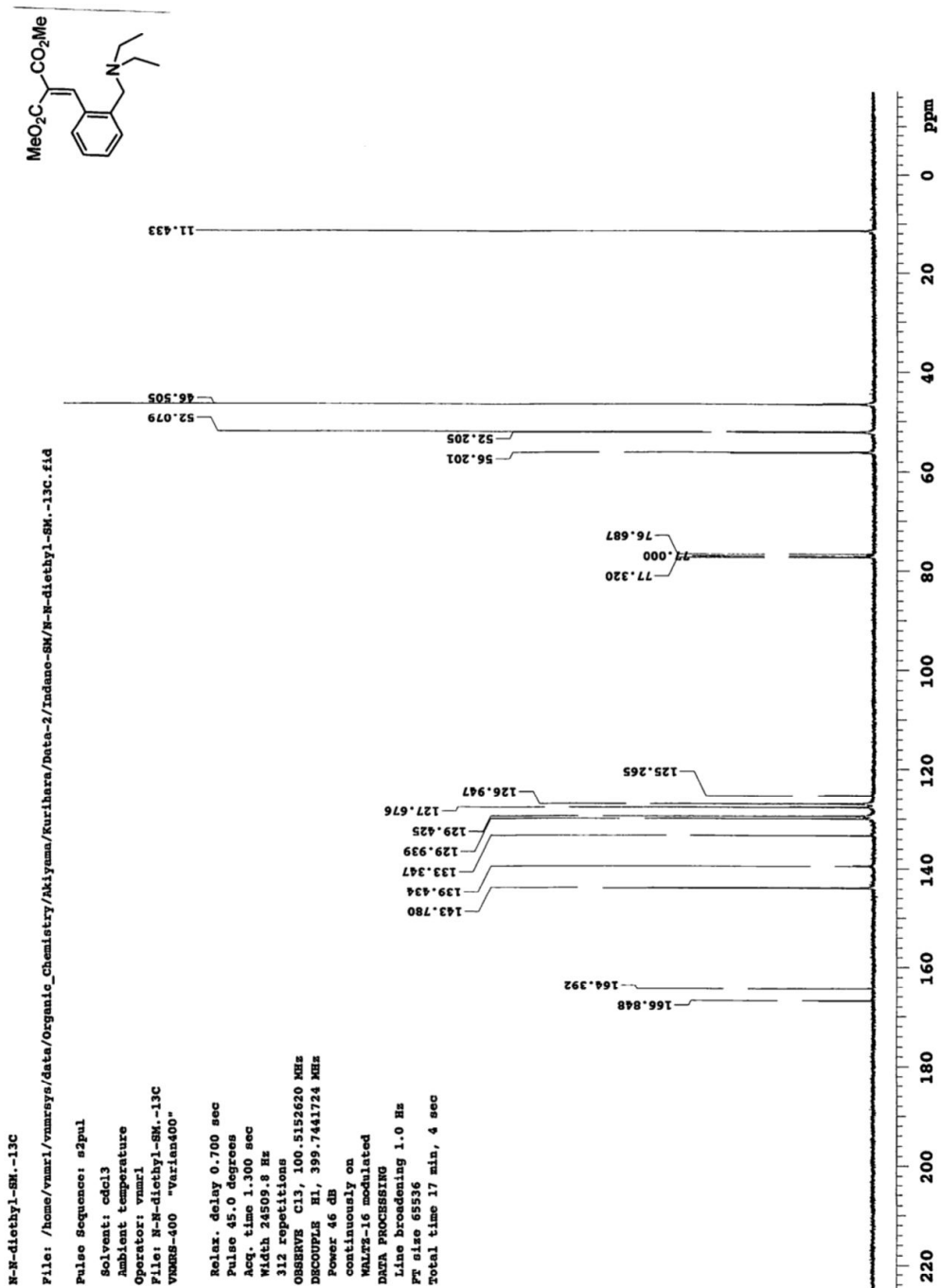


$^1\text{H}$  NMR spectrum of **3b**.

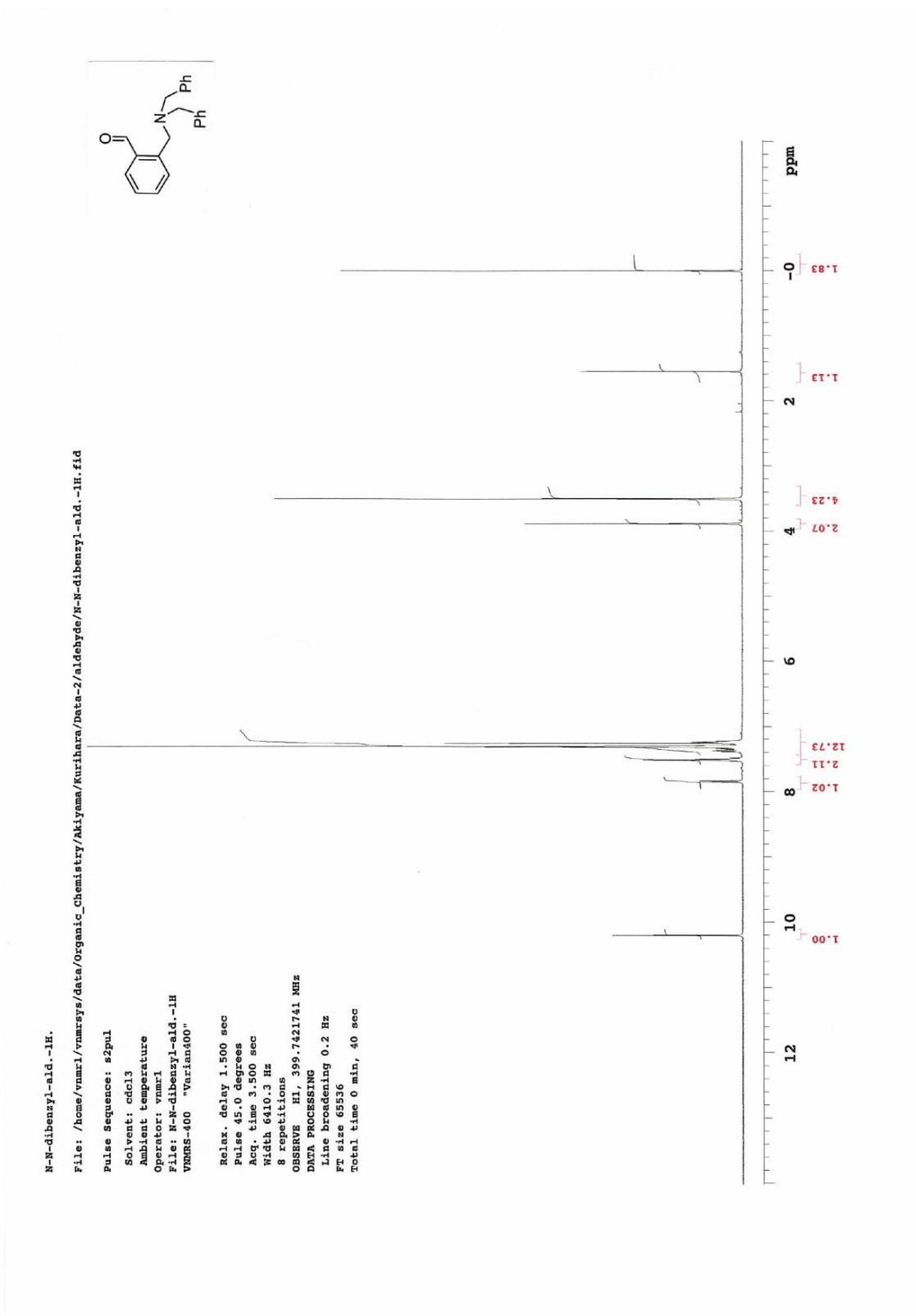




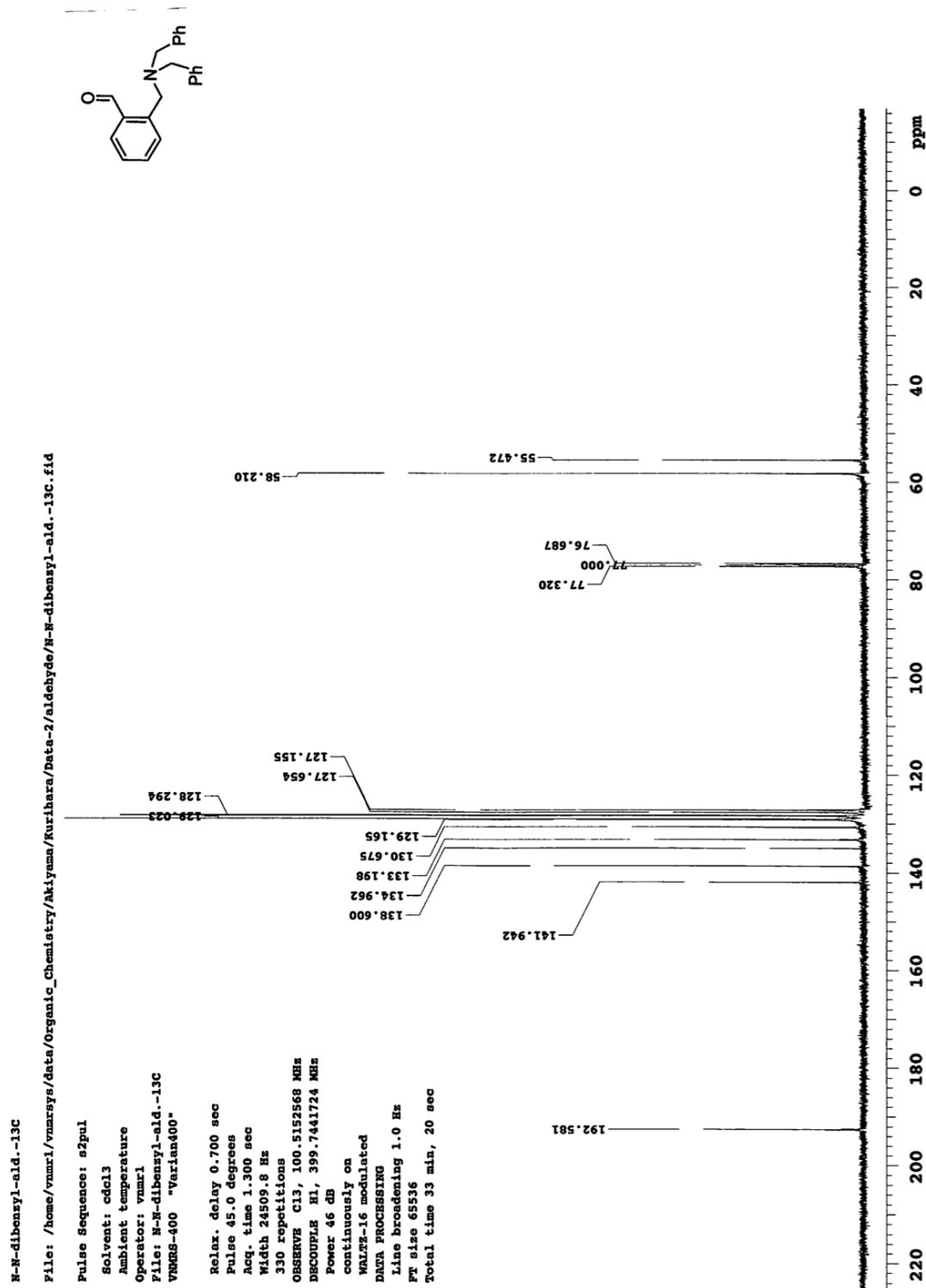
$^{13}\text{C}$  NMR spectrum of **3b**.



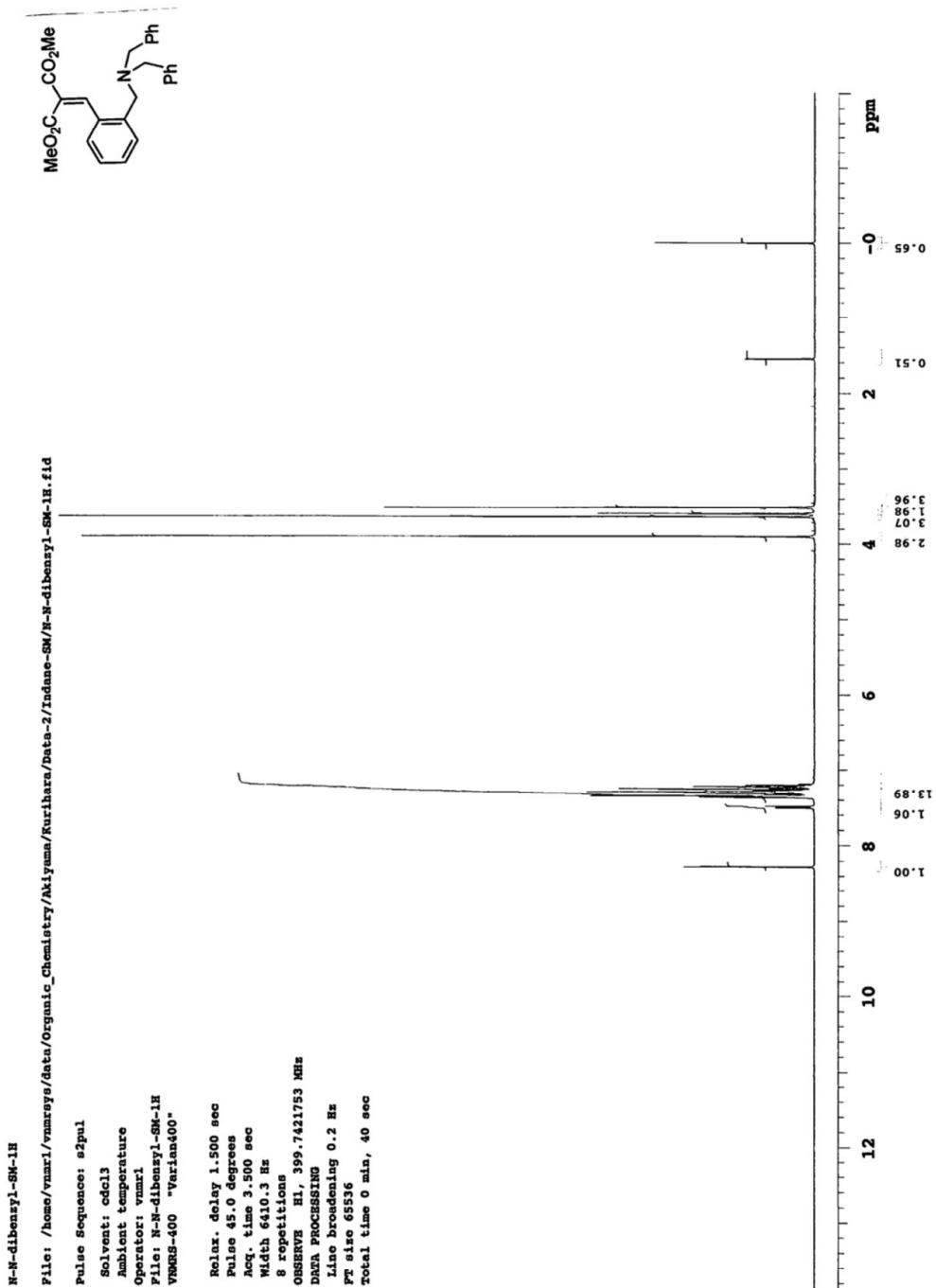
<sup>1</sup>H NMR spectrum of **s4**.



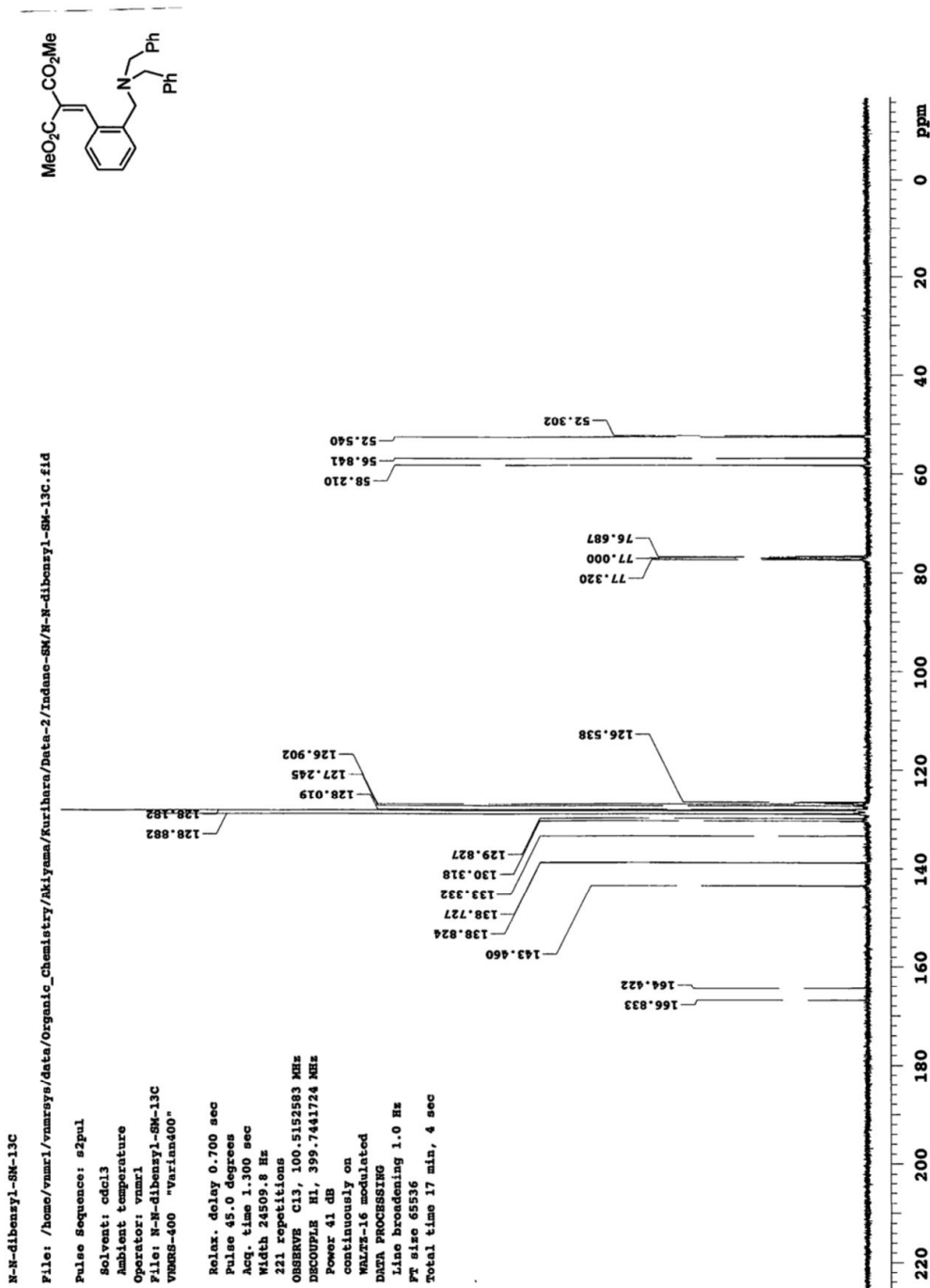
<sup>13</sup>C NMR spectrum of **s4**.



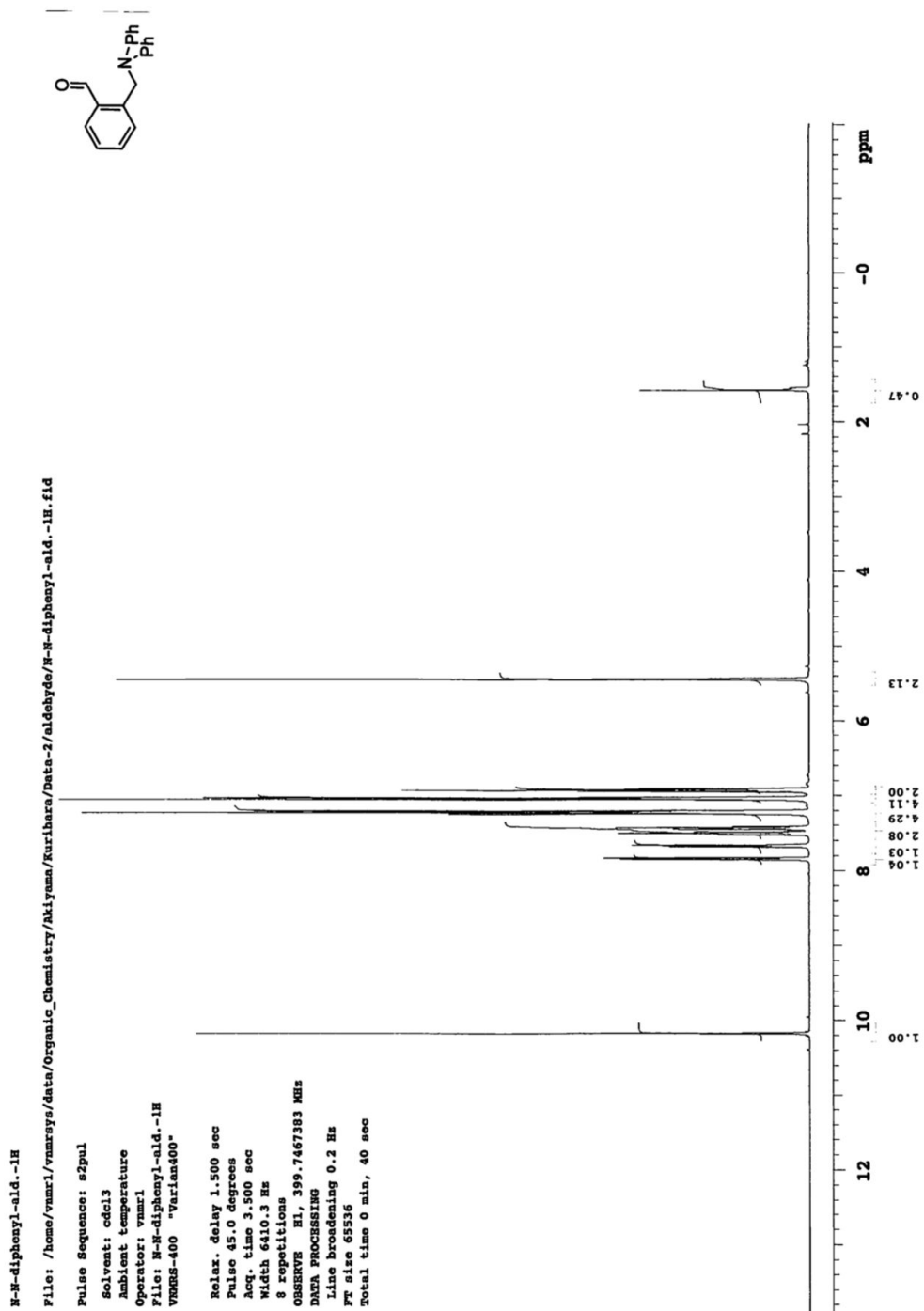
$^1\text{H}$  NMR spectrum of **3c**.



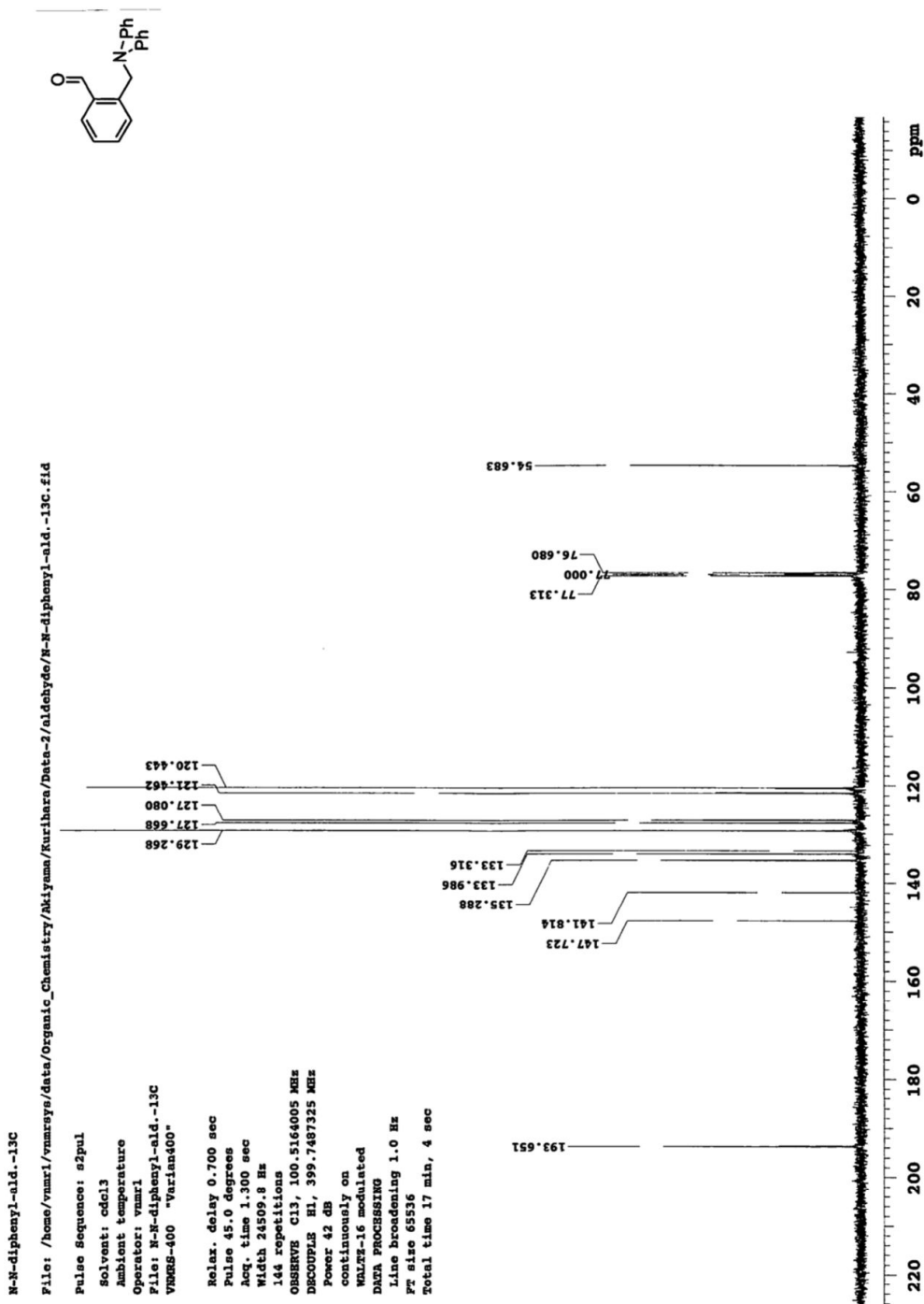
<sup>13</sup>C NMR spectrum of **3c**.



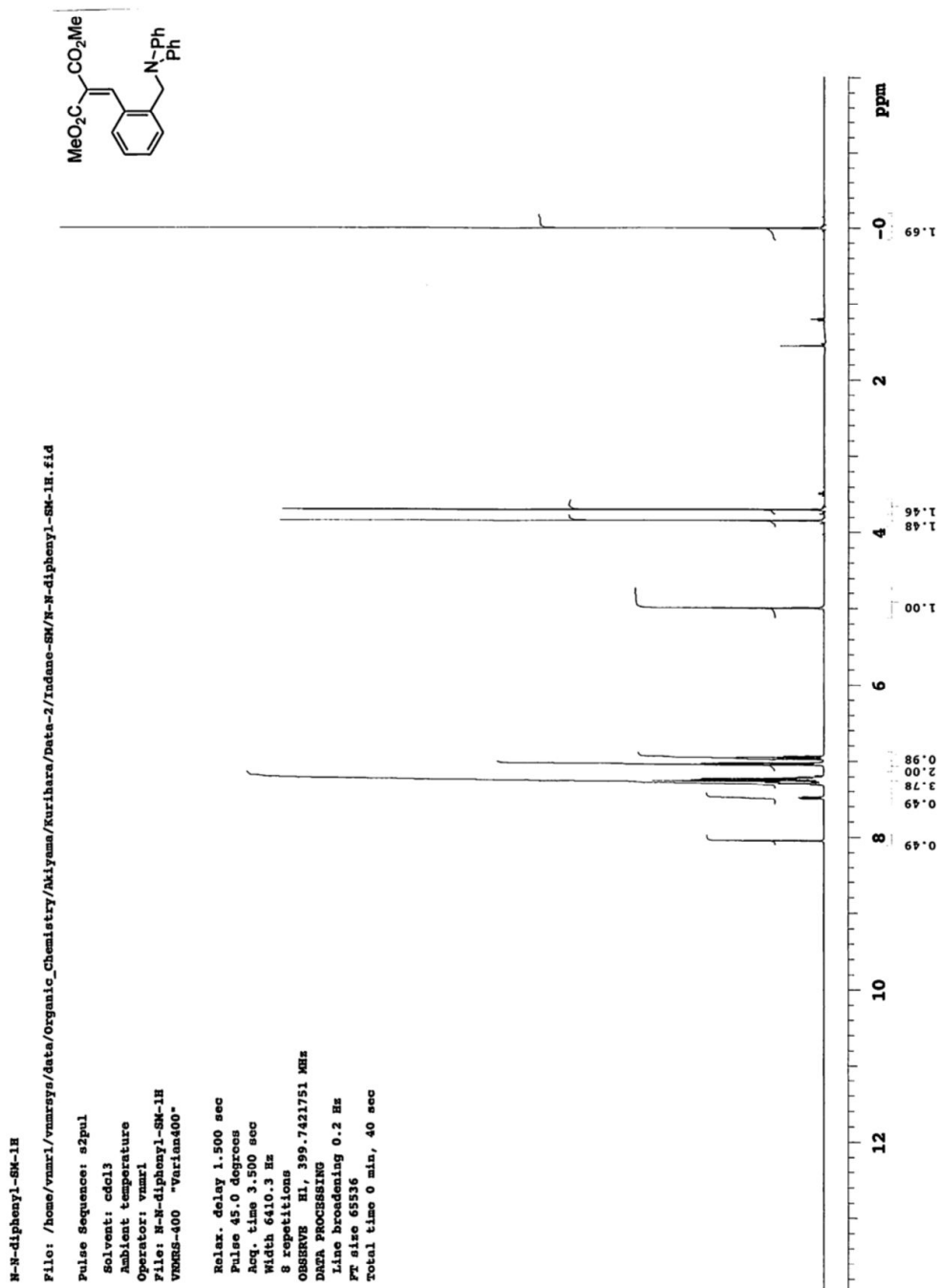
<sup>1</sup>H NMR spectrum of s5.



<sup>13</sup>C NMR spectrum of **s5**.

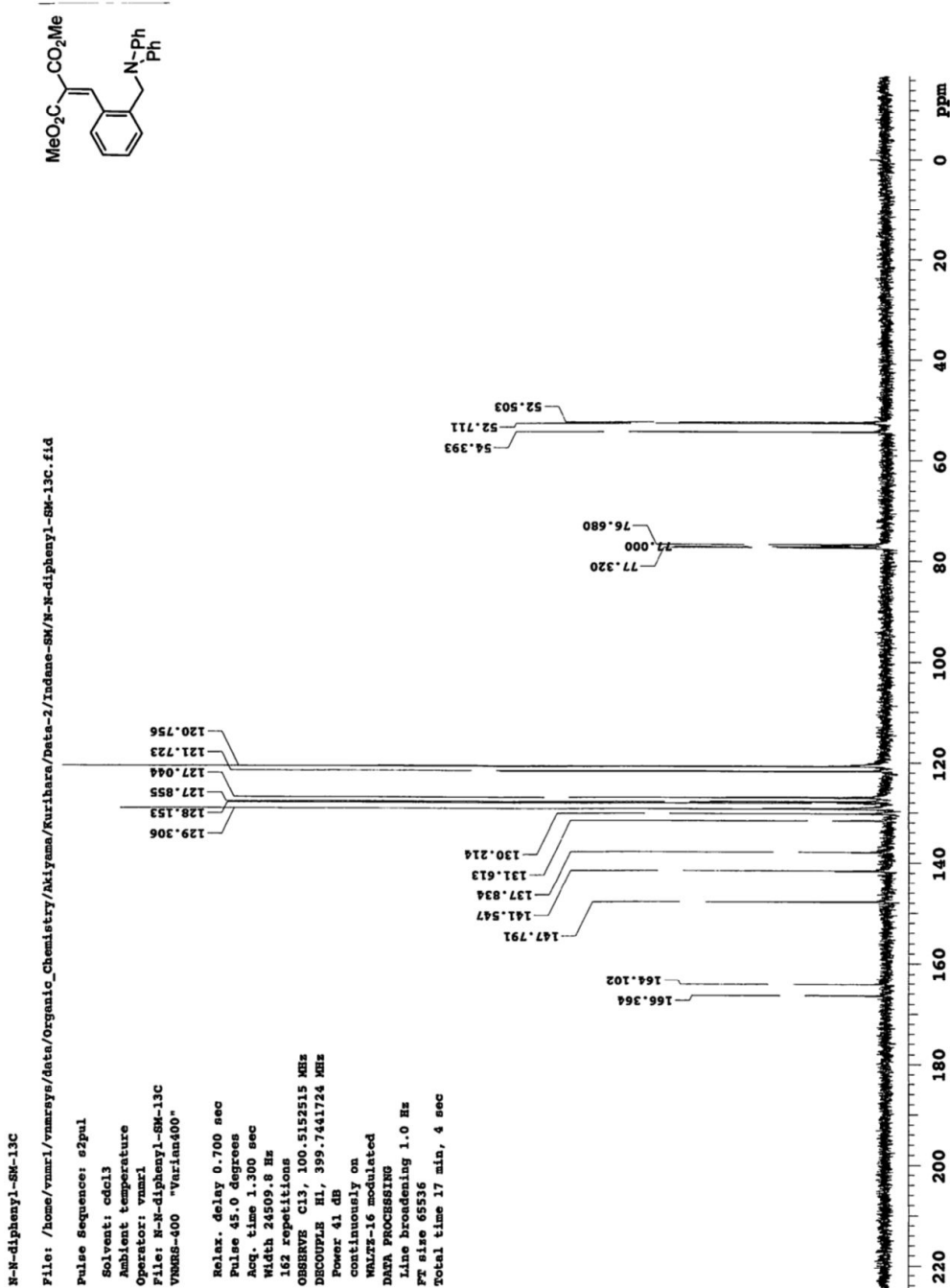


$^1\text{H}$  NMR spectrum of **3d**.

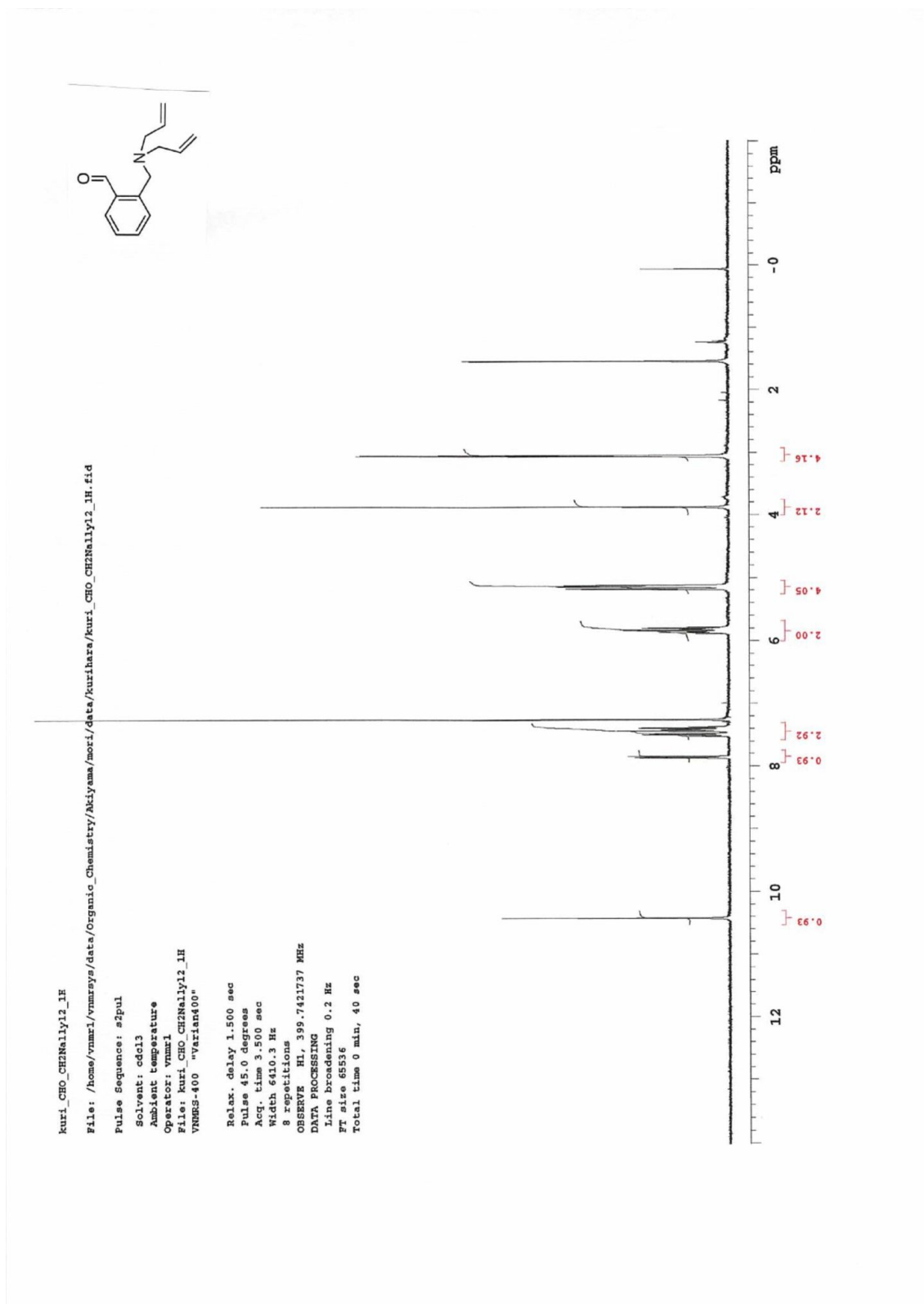




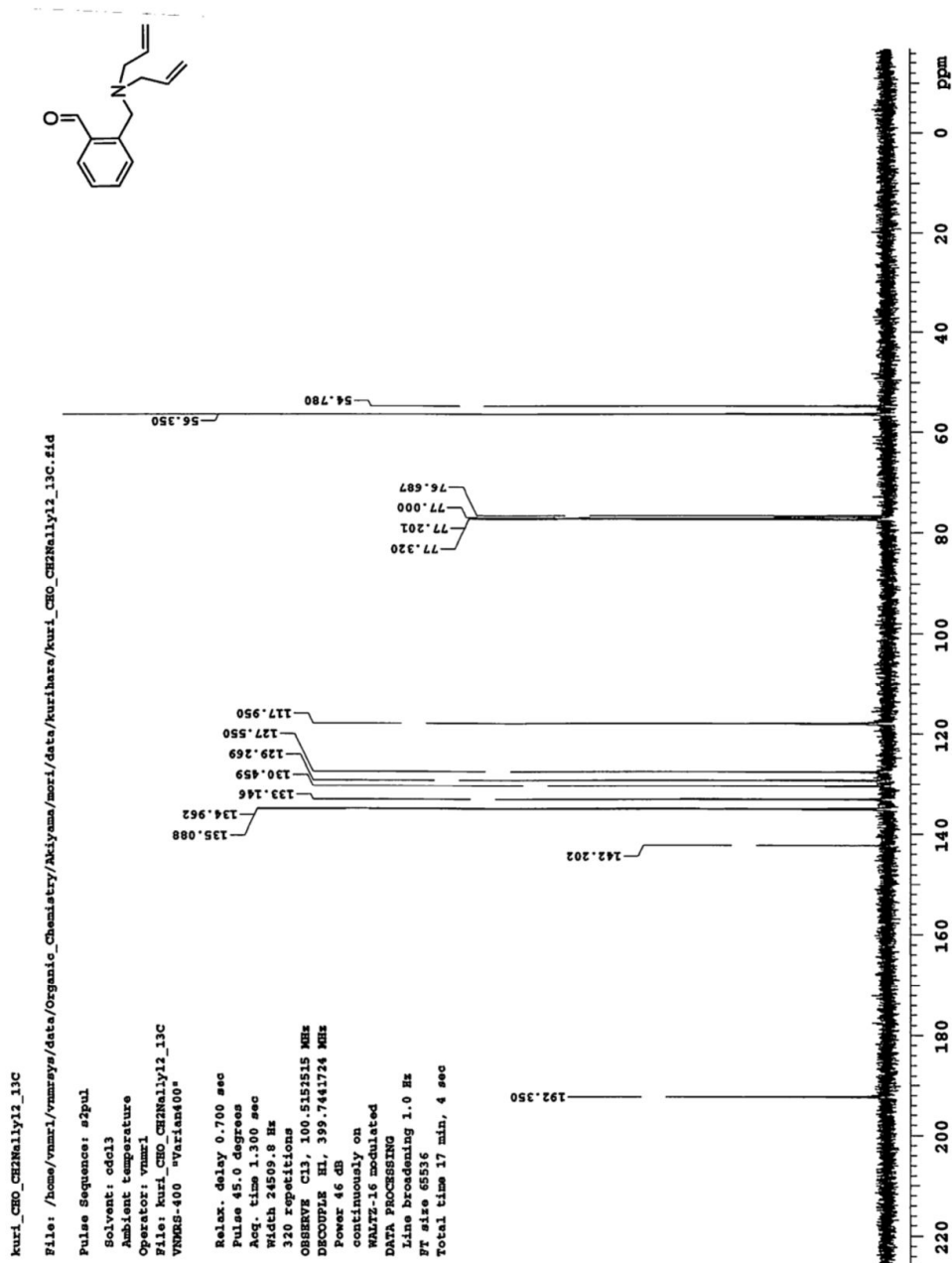
<sup>13</sup>C NMR spectrum of **3d**.



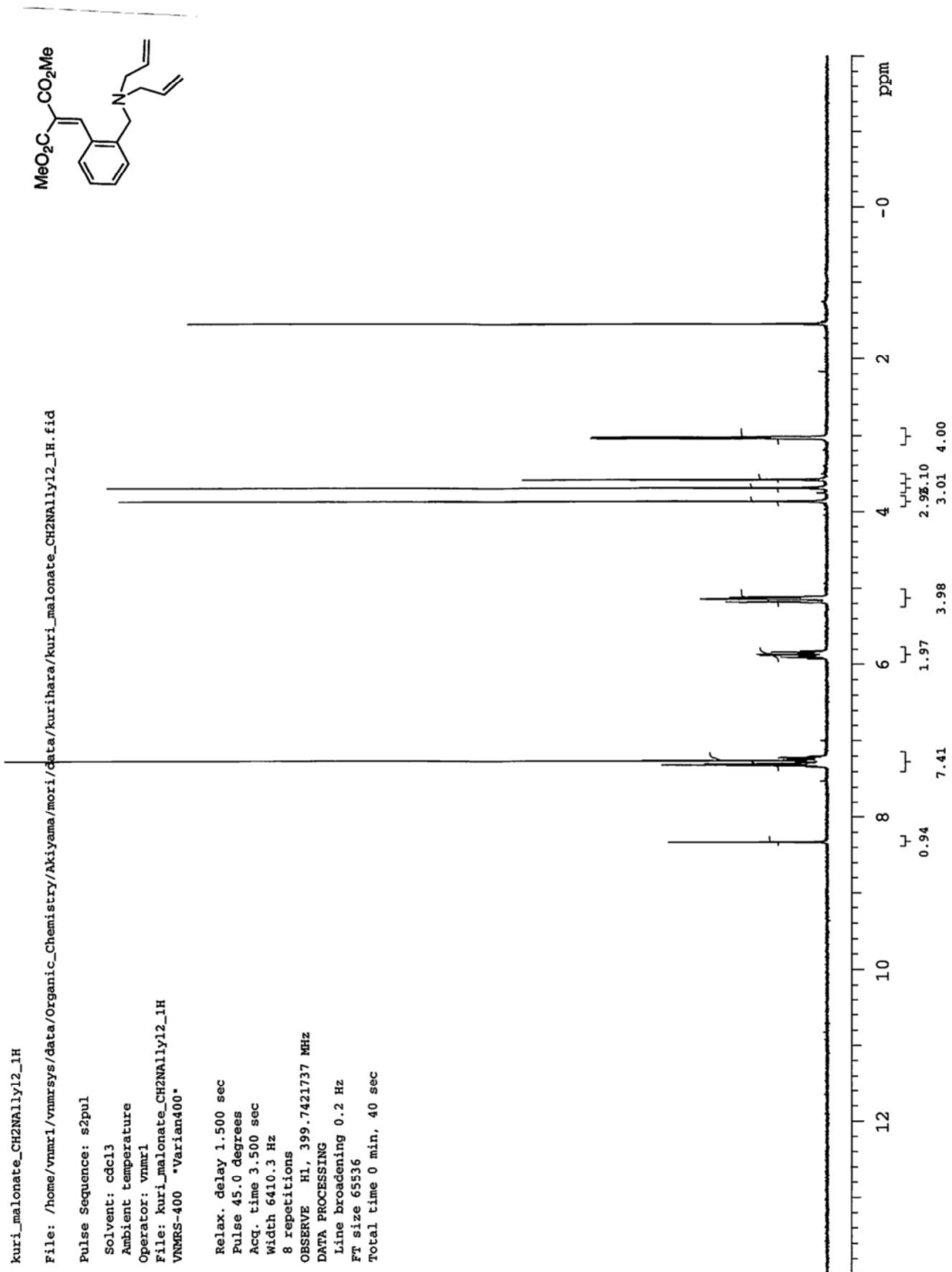
<sup>1</sup>H NMR spectrum of **s6**.



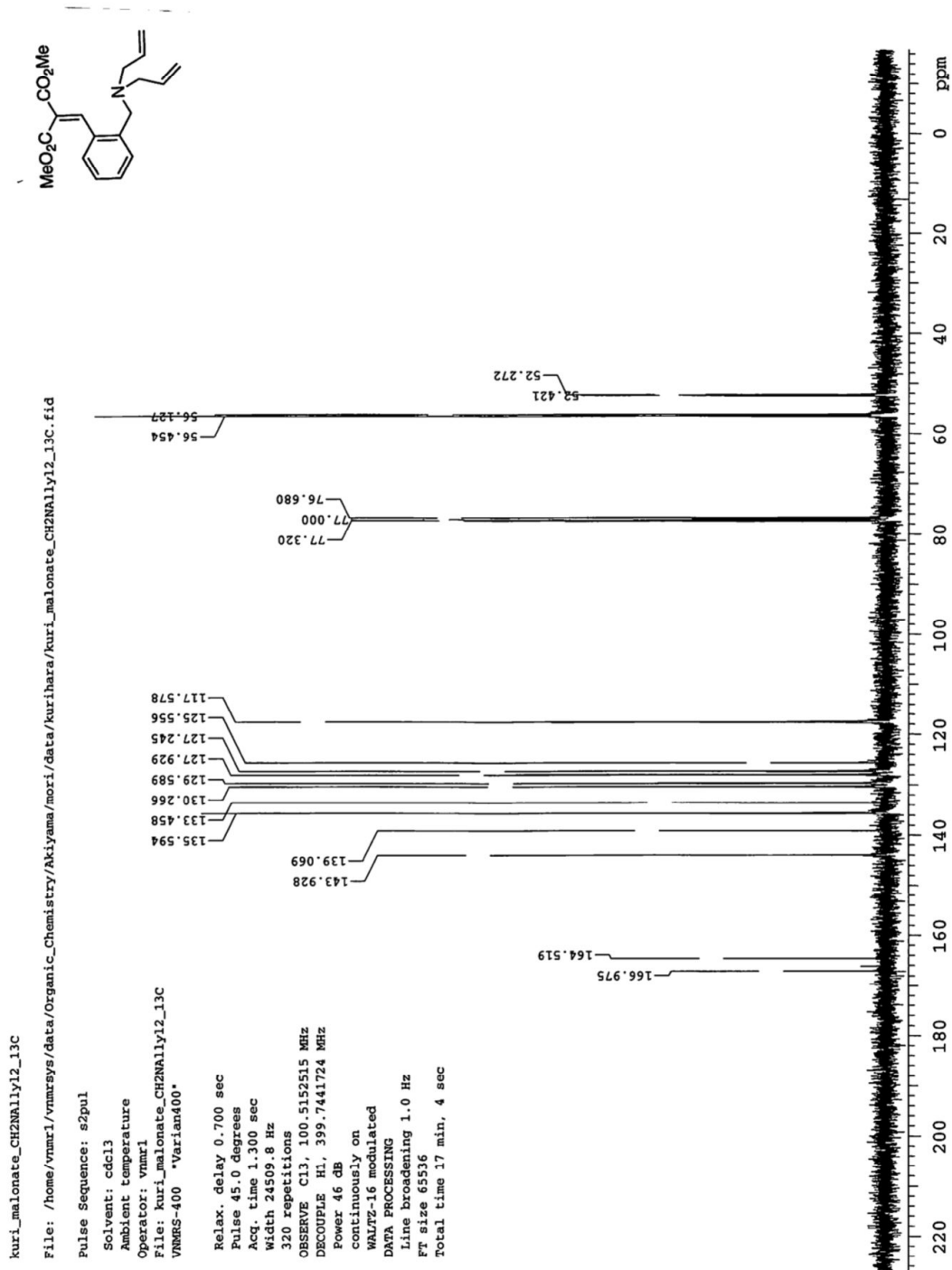
<sup>13</sup>C NMR spectrum of **s6**.



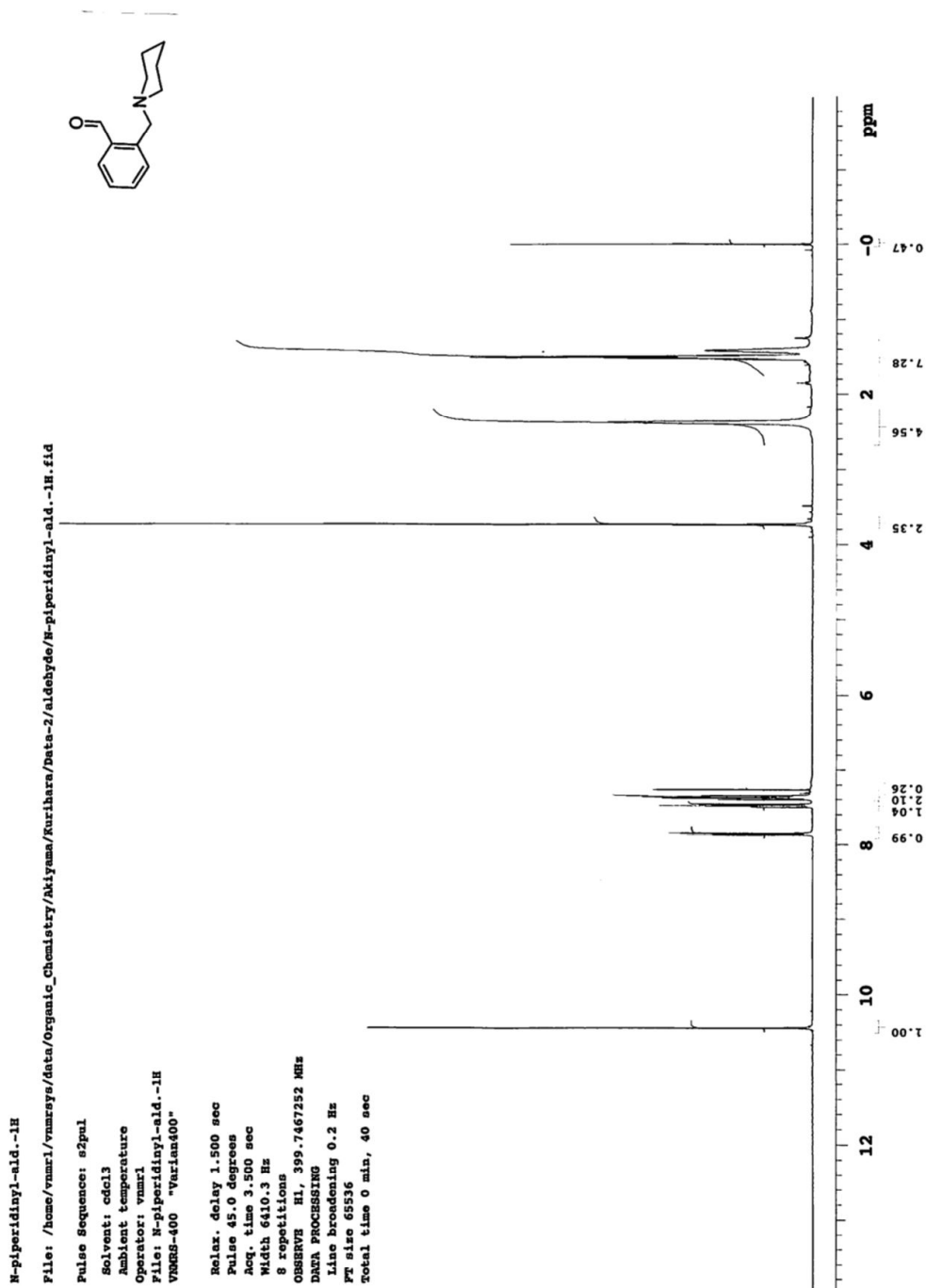
<sup>1</sup>H NMR spectrum of **3e**.



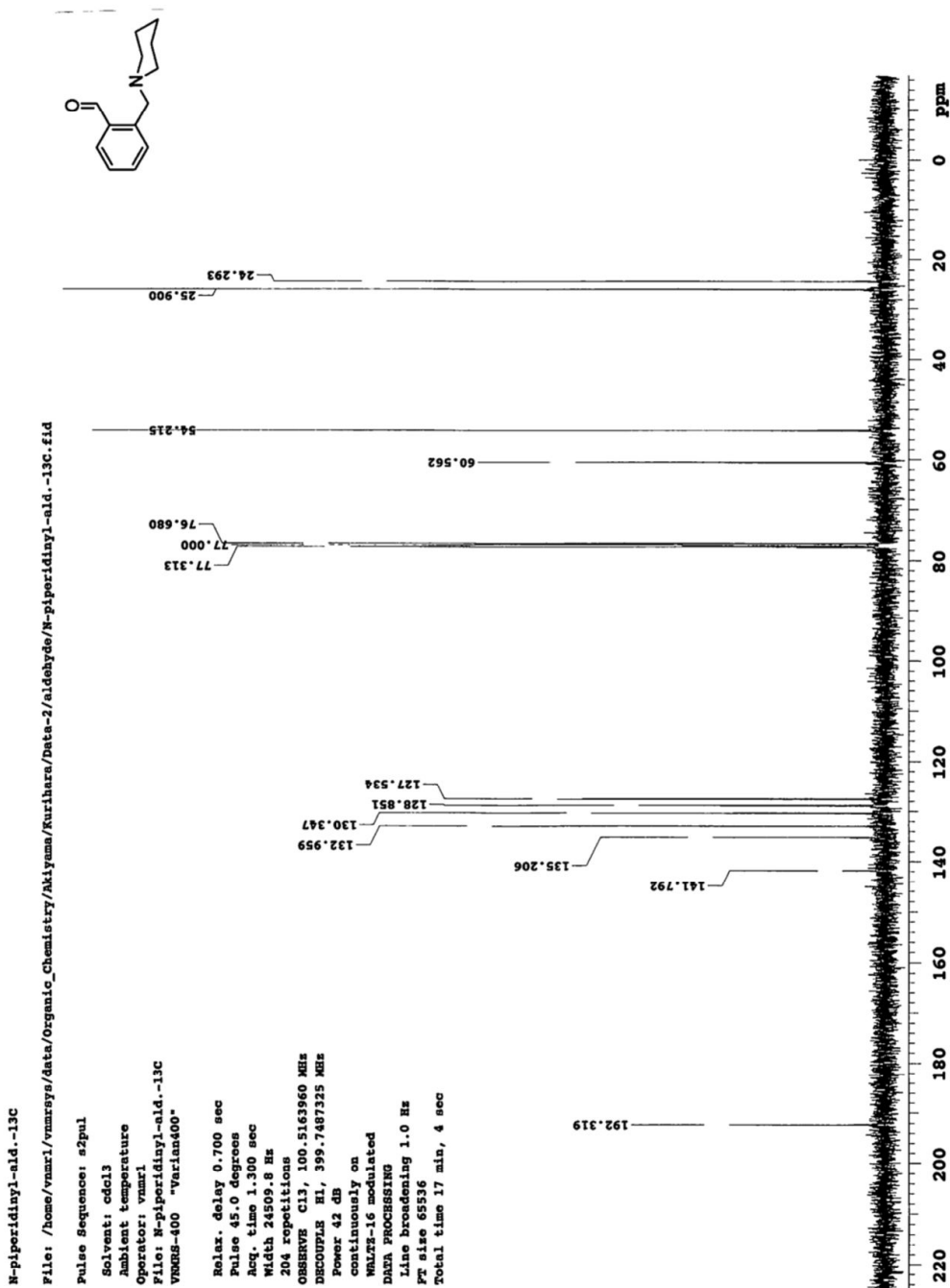
<sup>13</sup>C NMR spectrum of **3e**.



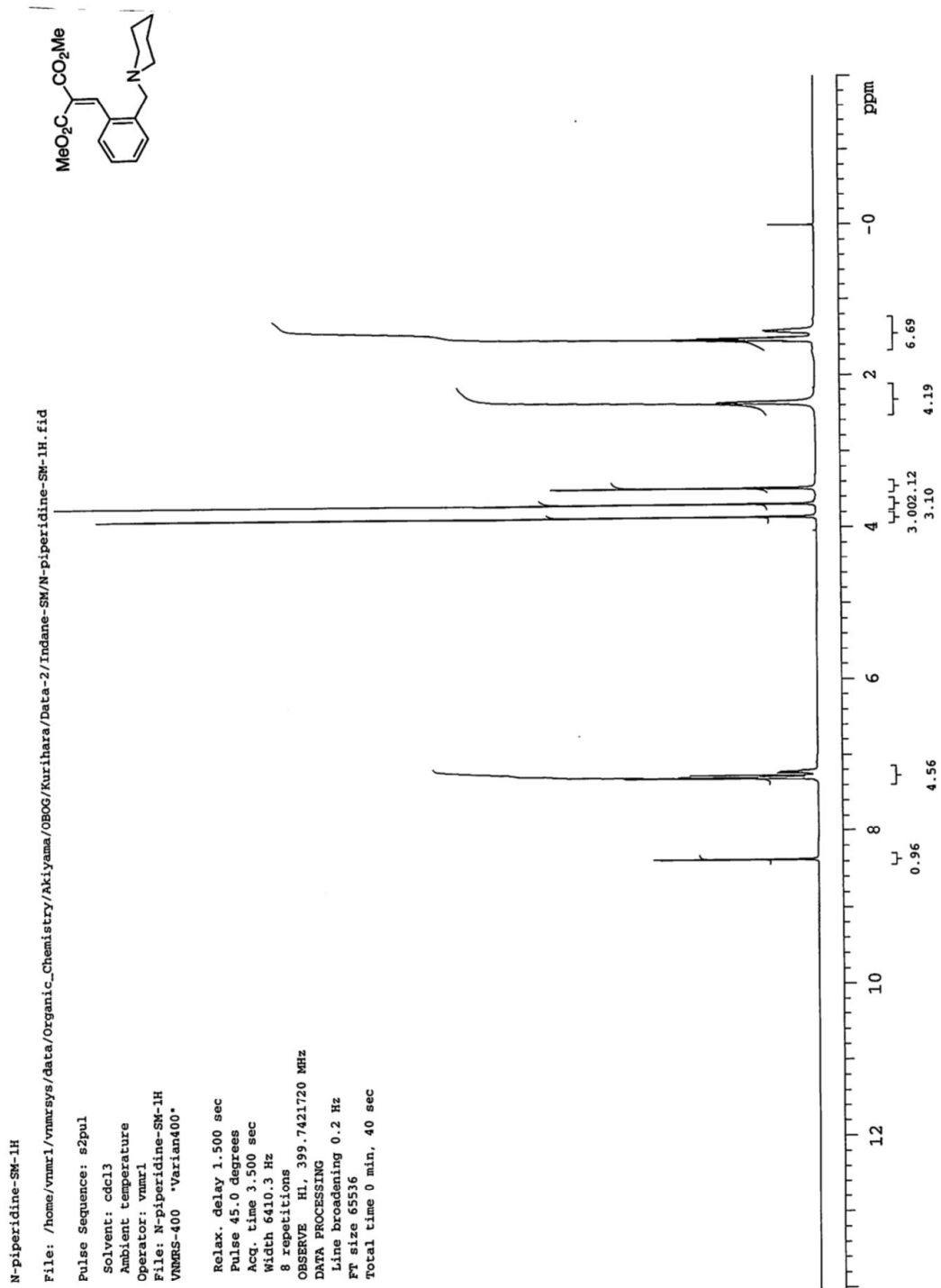
<sup>1</sup>H NMR spectrum of s7.



<sup>13</sup>C NMR spectrum of s7.

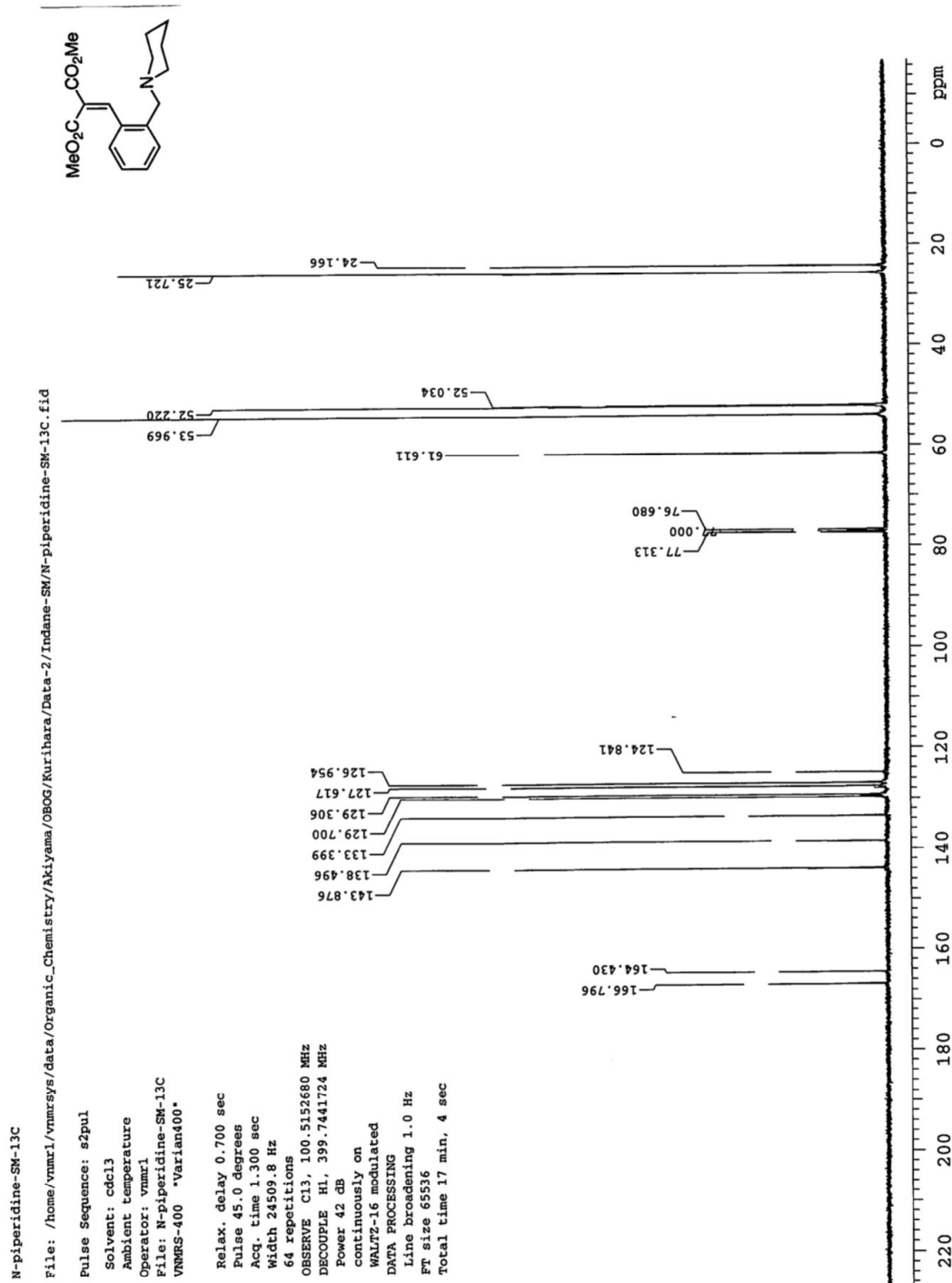


<sup>1</sup>H NMR spectrum of **3f**.

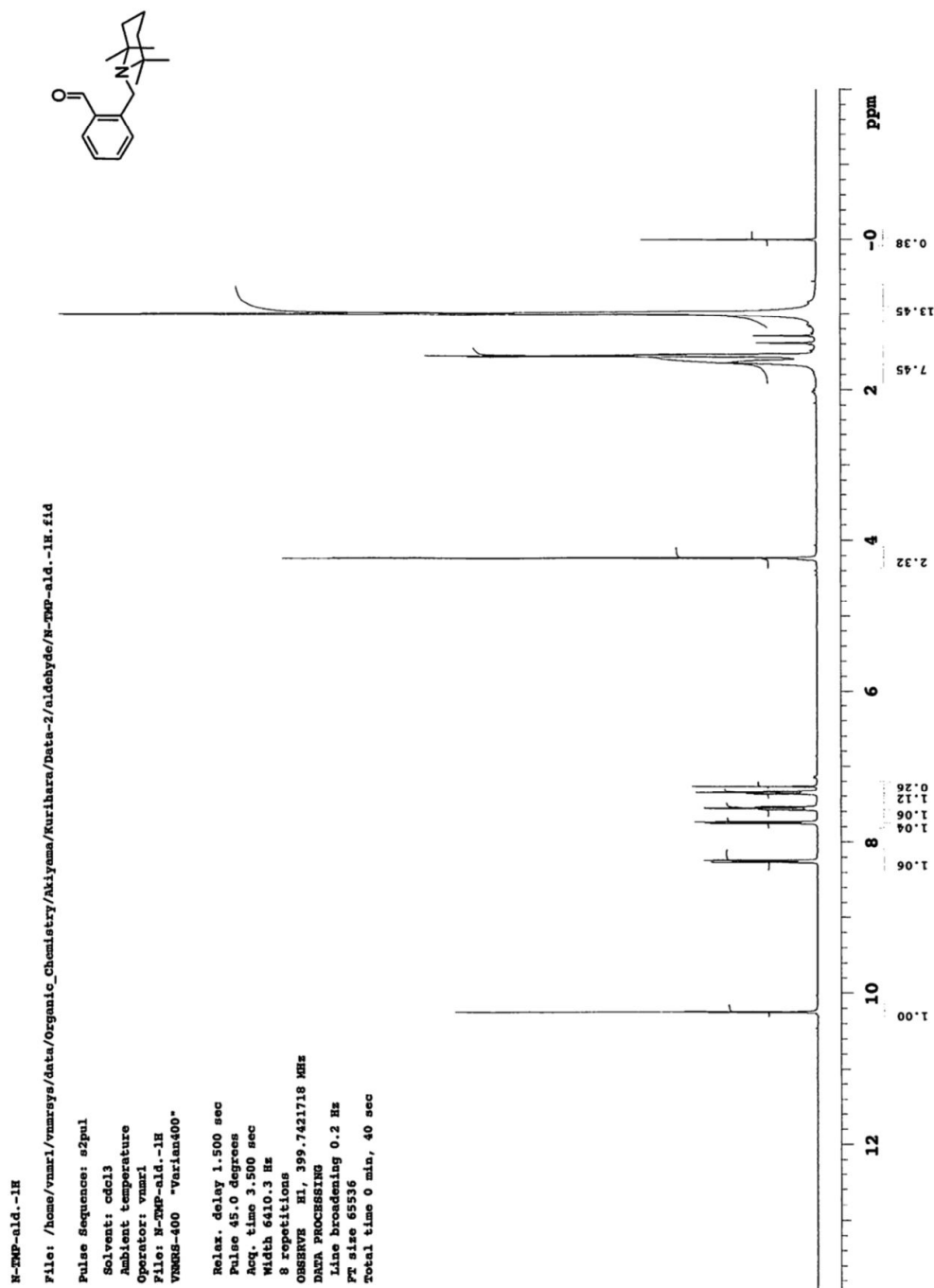




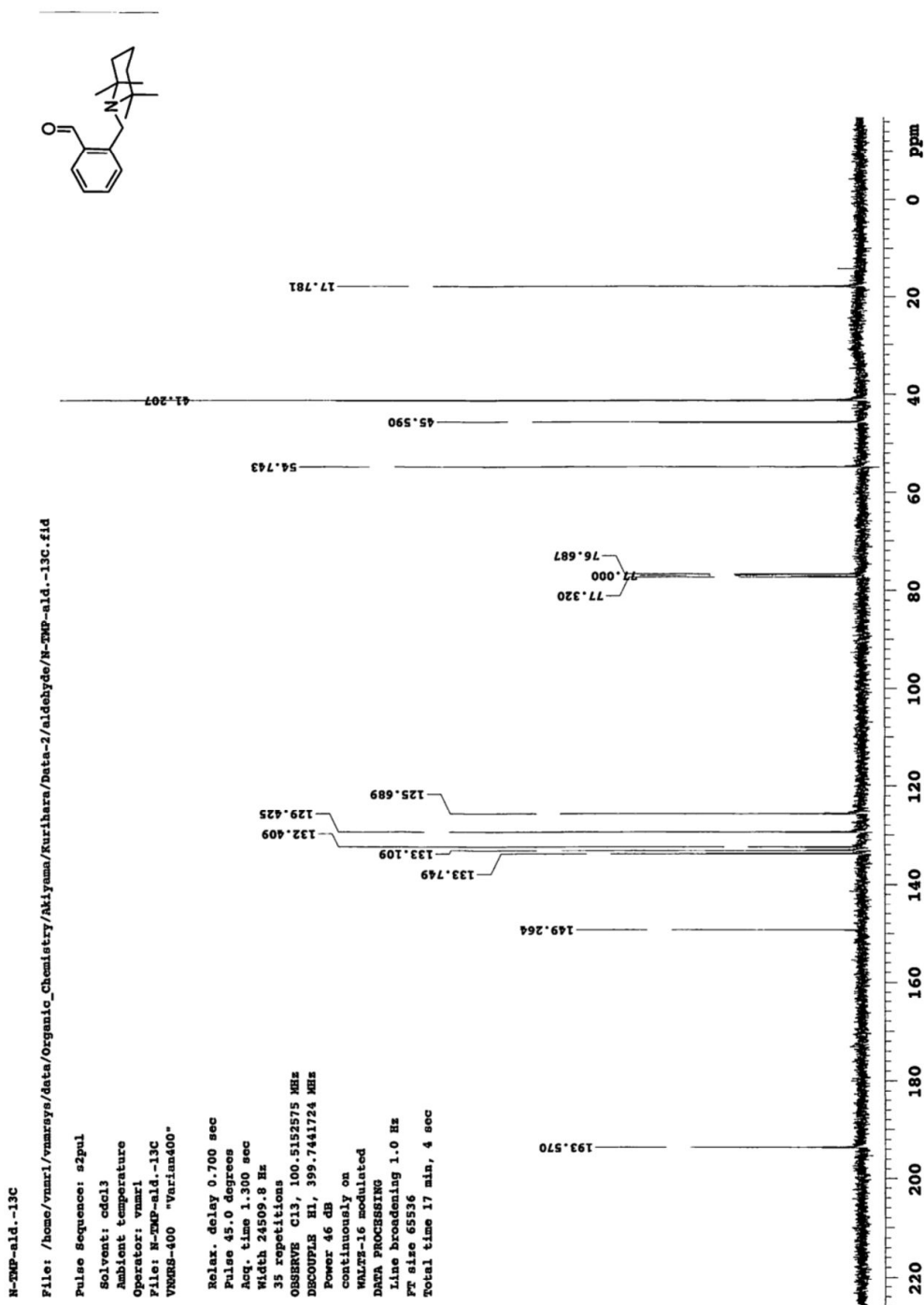
<sup>13</sup>C NMR spectrum of **3f**.



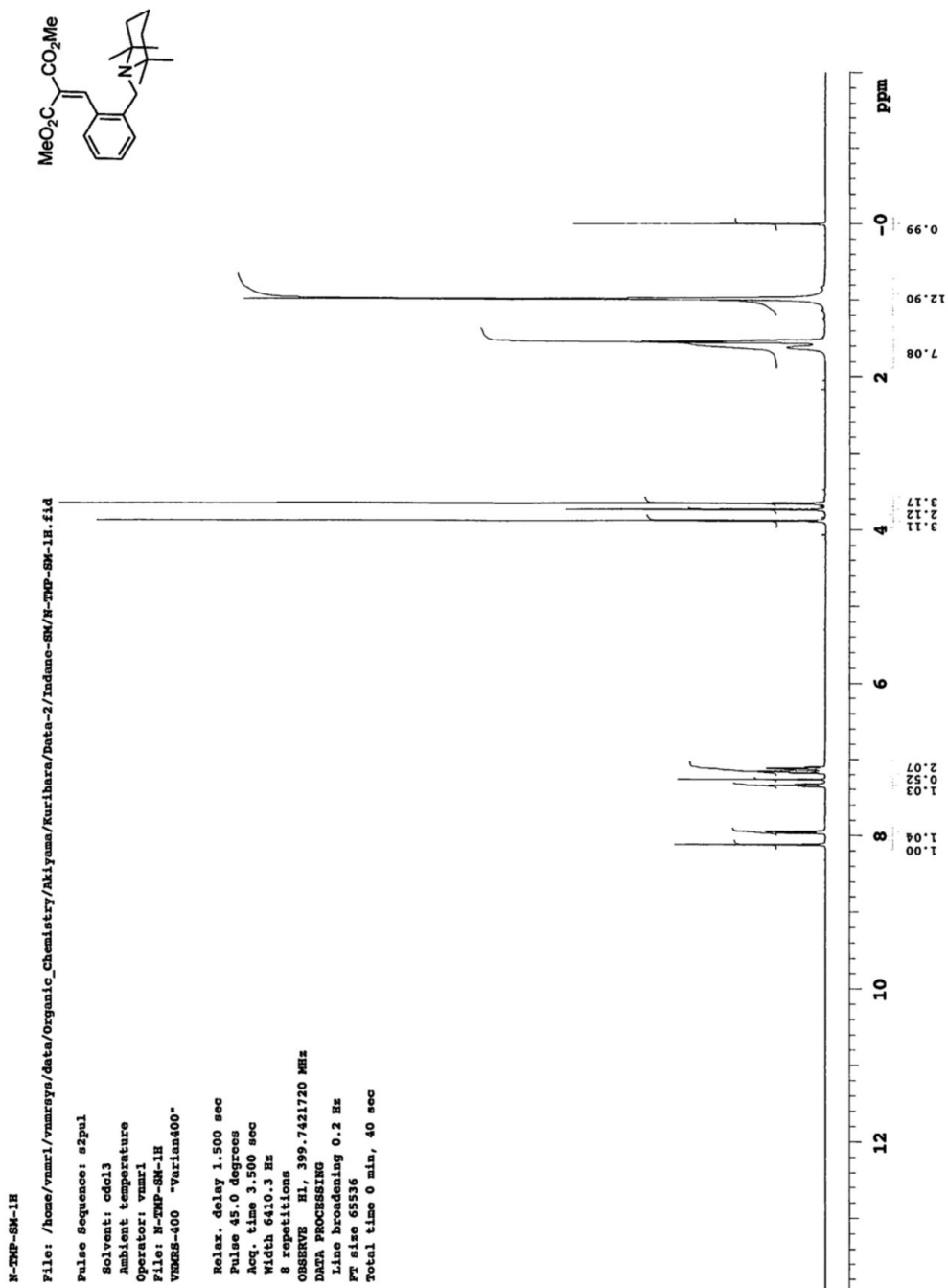
$^1\text{H}$  NMR spectrum of **s8**.



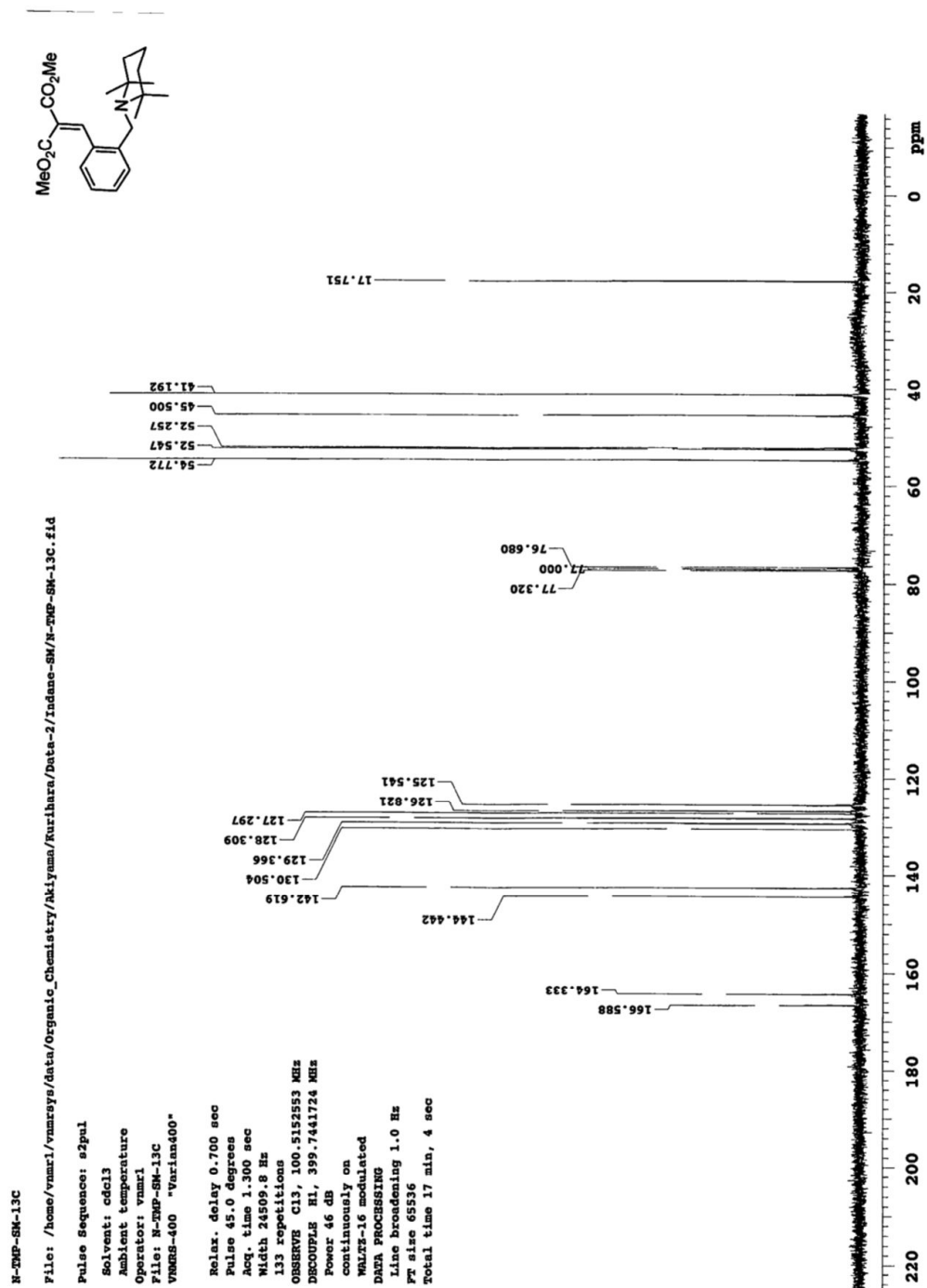
<sup>13</sup>C NMR spectrum of **s8**.



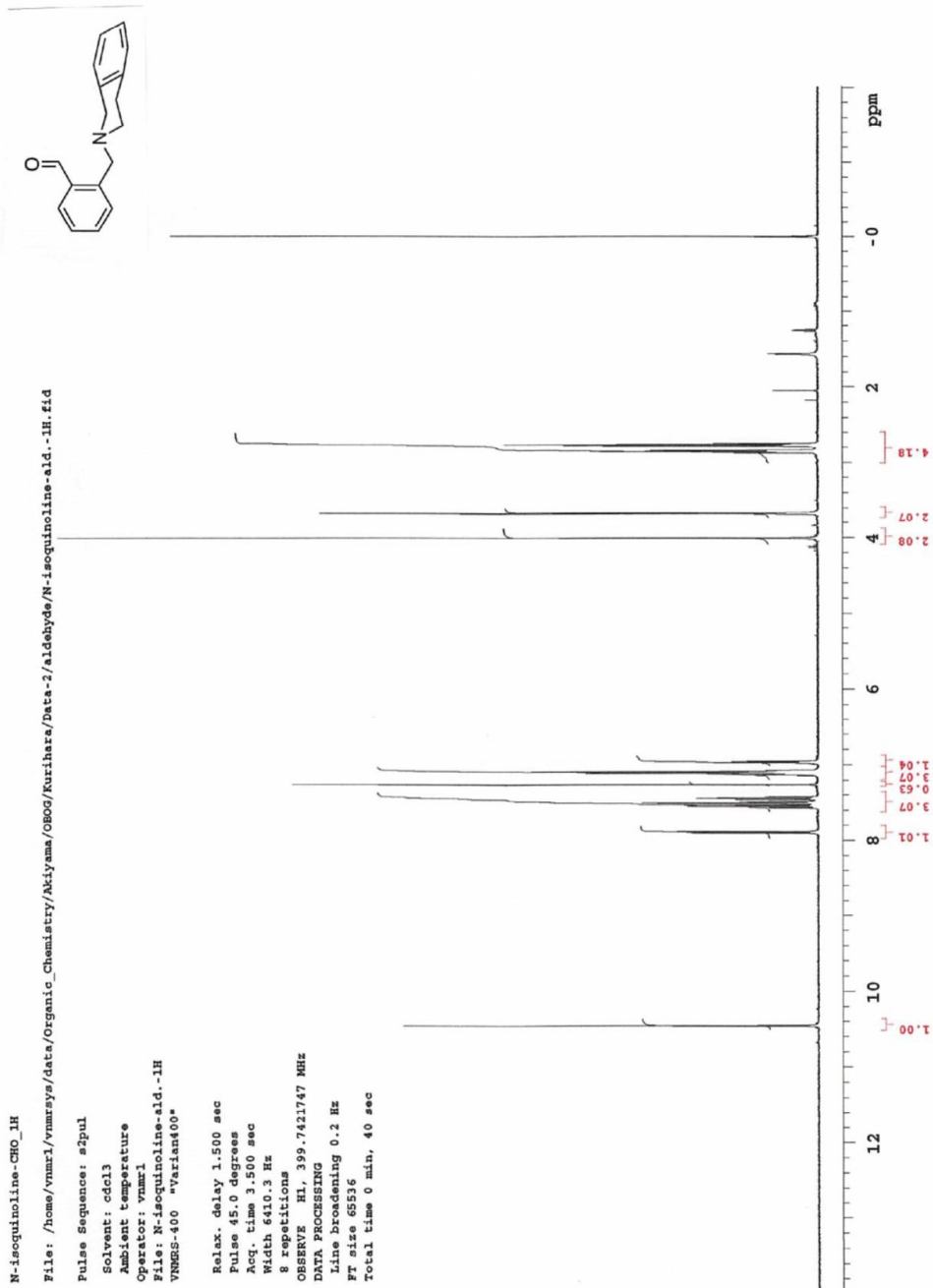
<sup>1</sup>H NMR spectrum of **3g**.



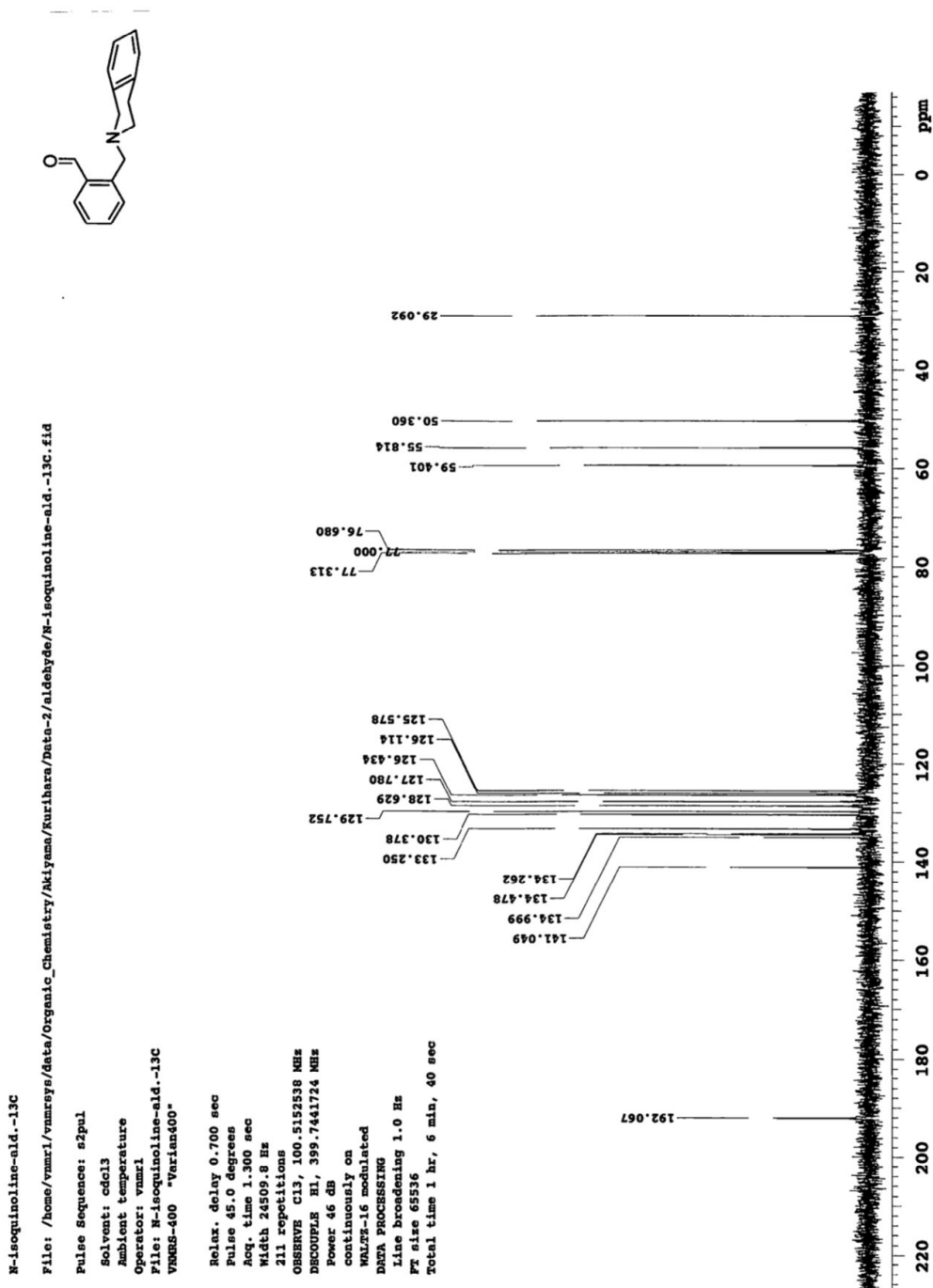
$^{13}\text{C}$  NMR spectrum of **3g**.



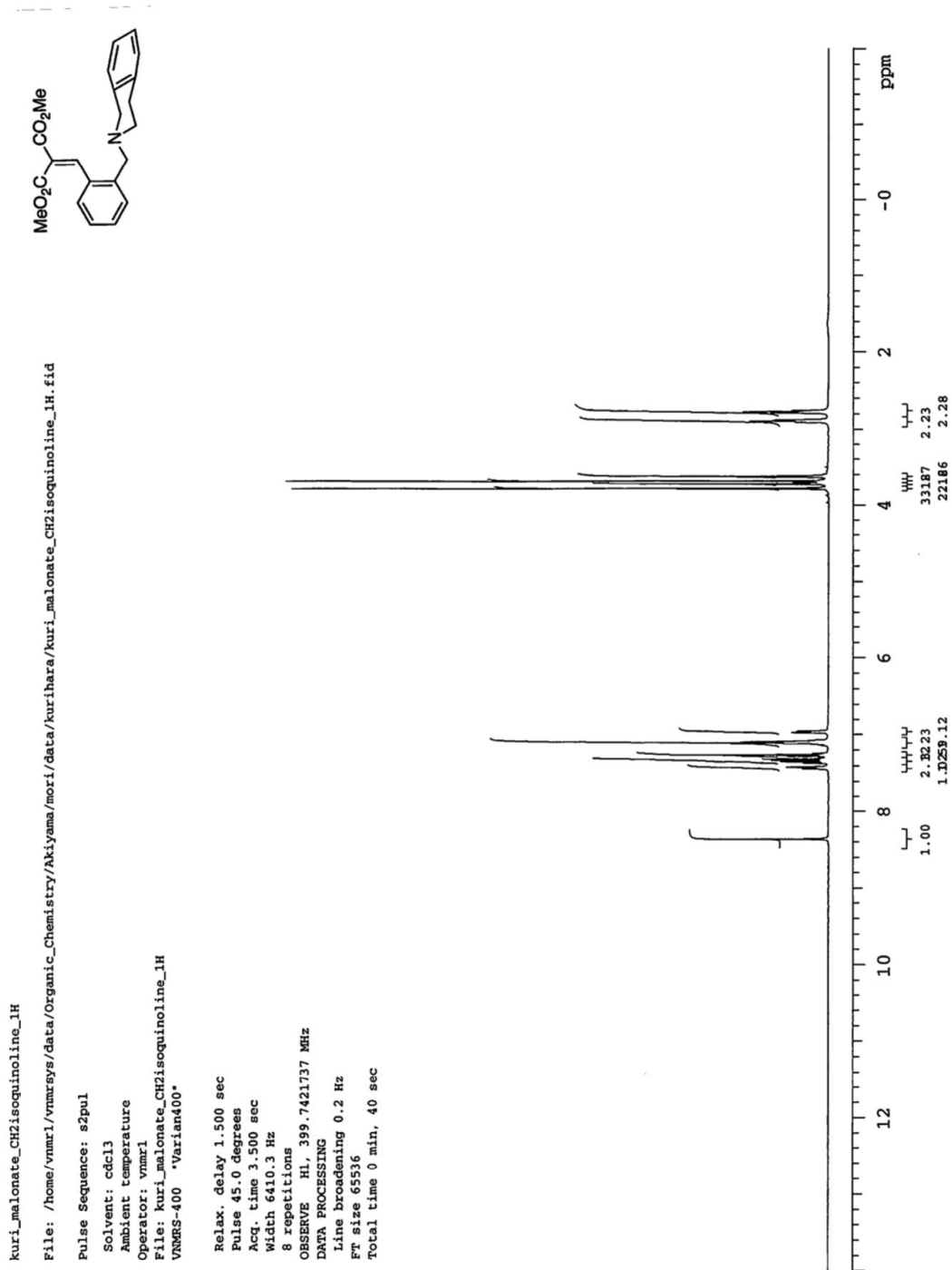
<sup>1</sup>H NMR spectrum of **s9**.



<sup>13</sup>C NMR spectrum of **s9**.

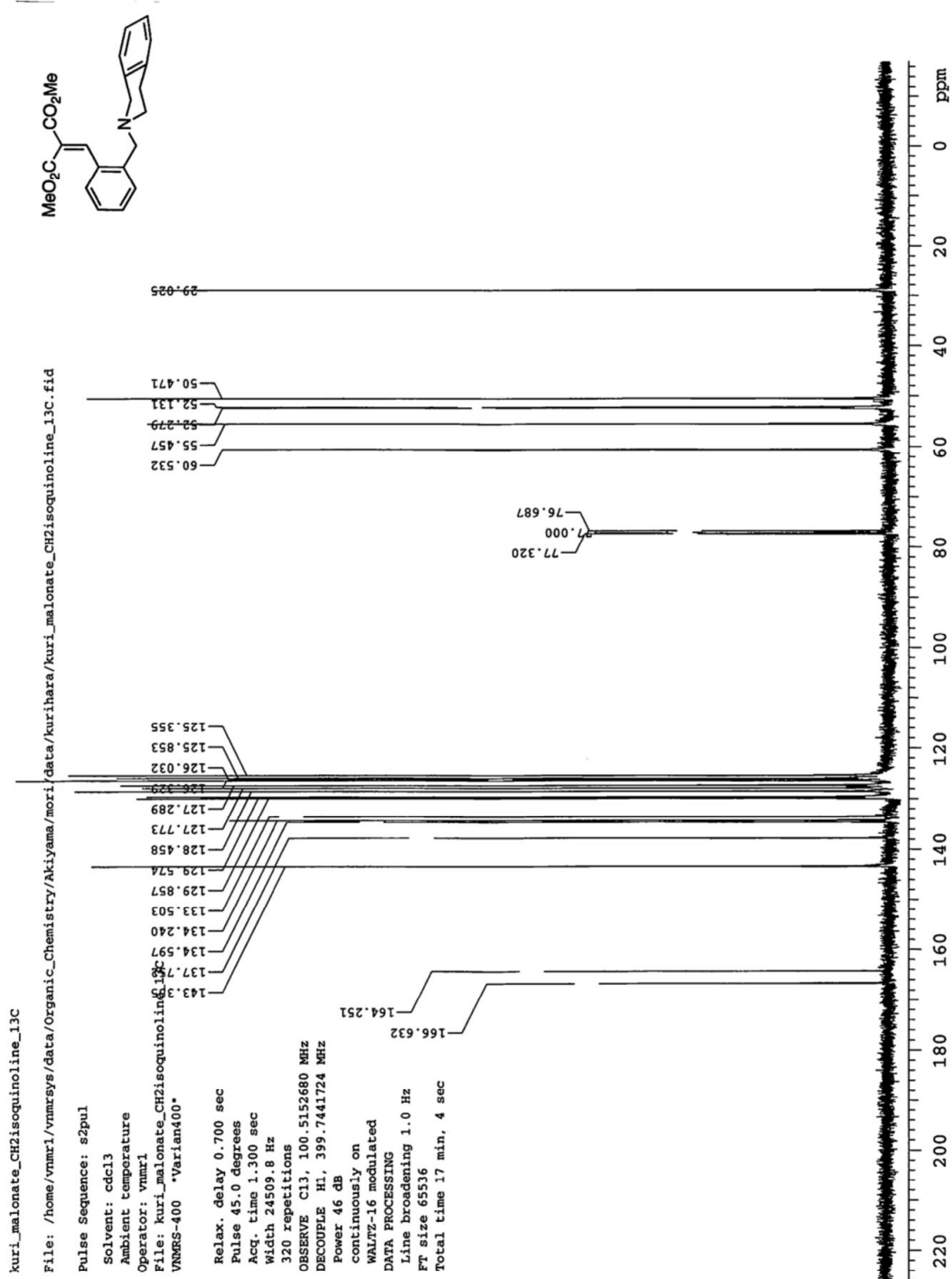


<sup>1</sup>H NMR spectrum of **3i**.

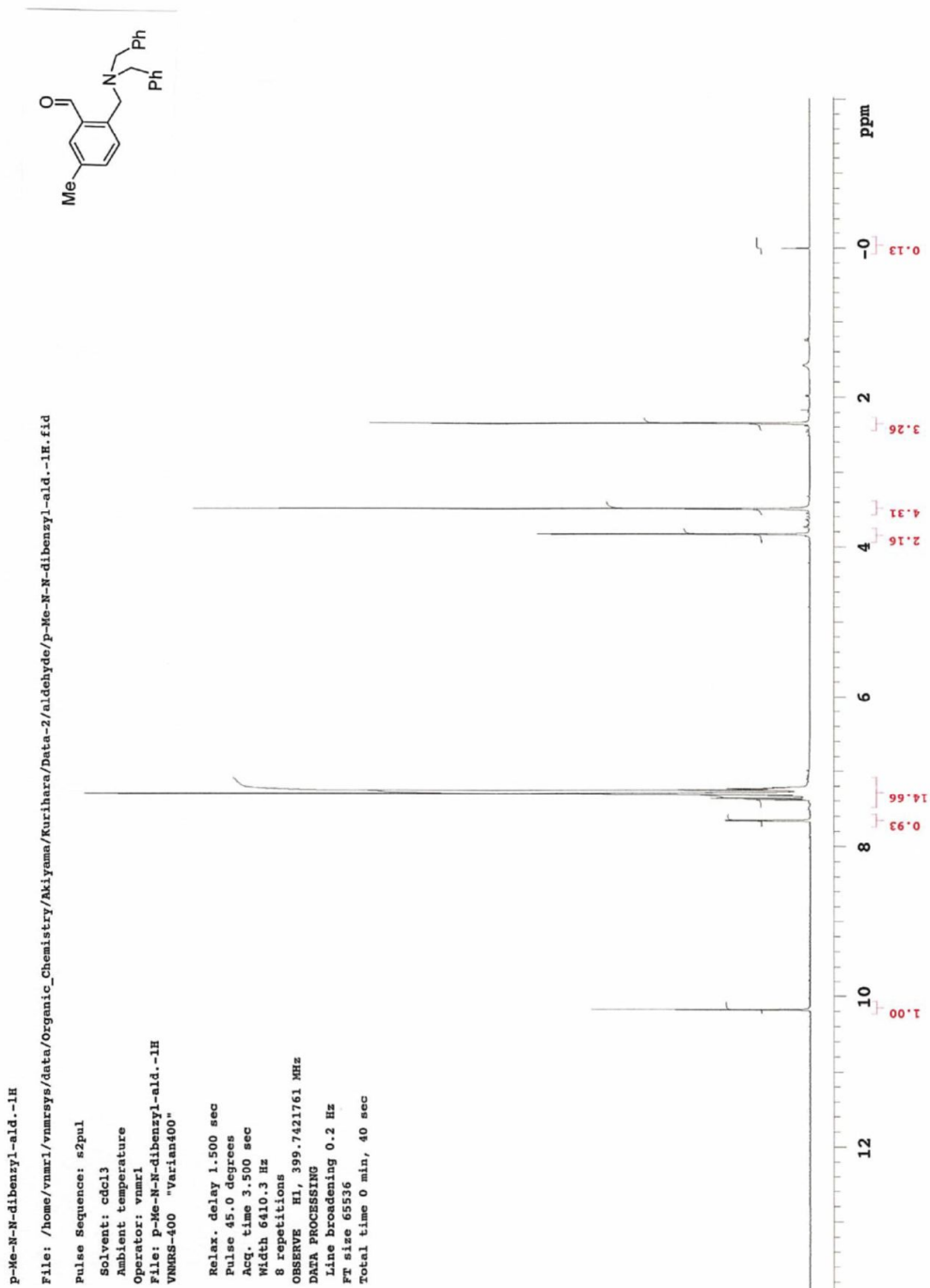




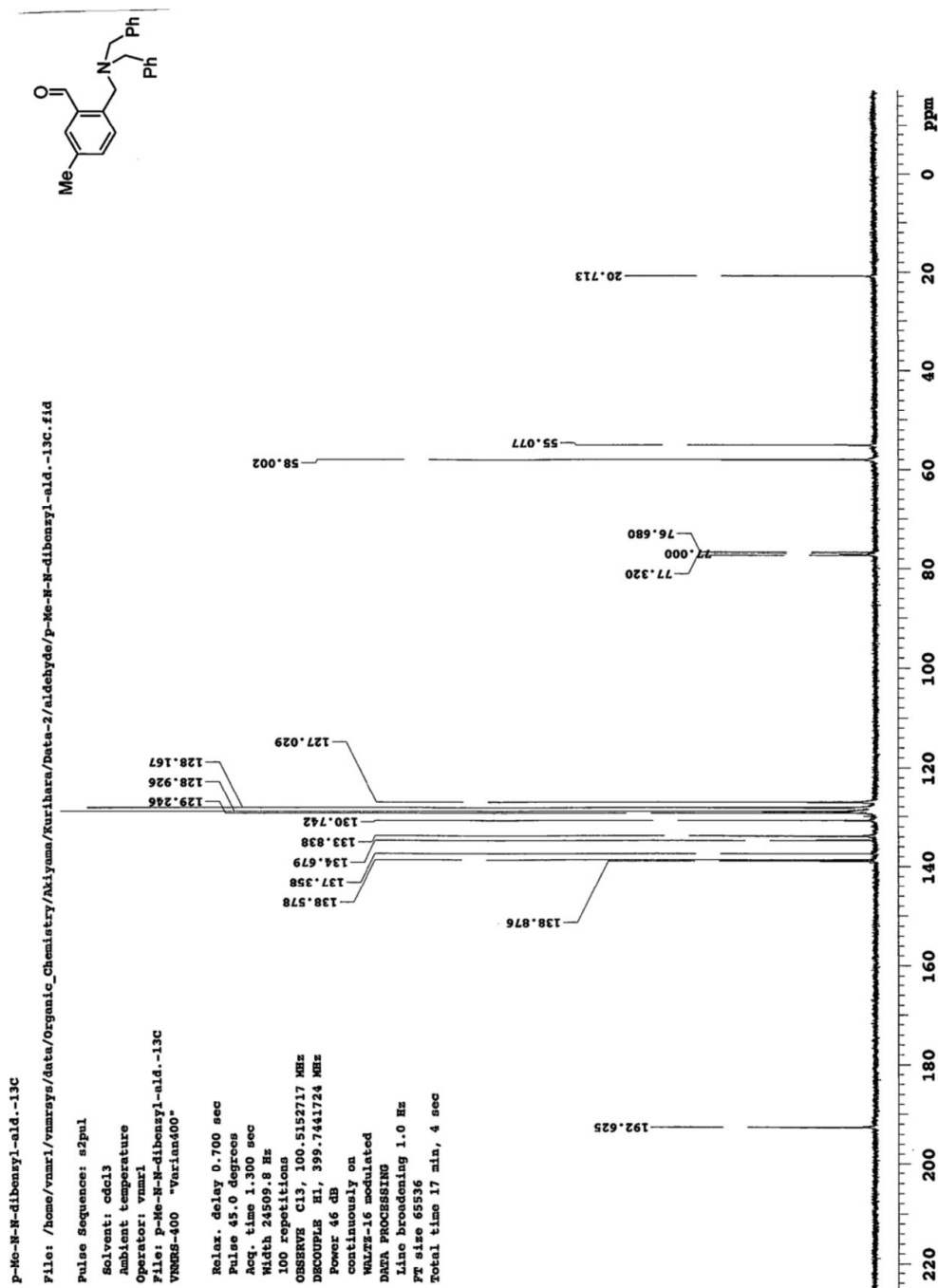
<sup>13</sup>C NMR spectrum of **3i**.



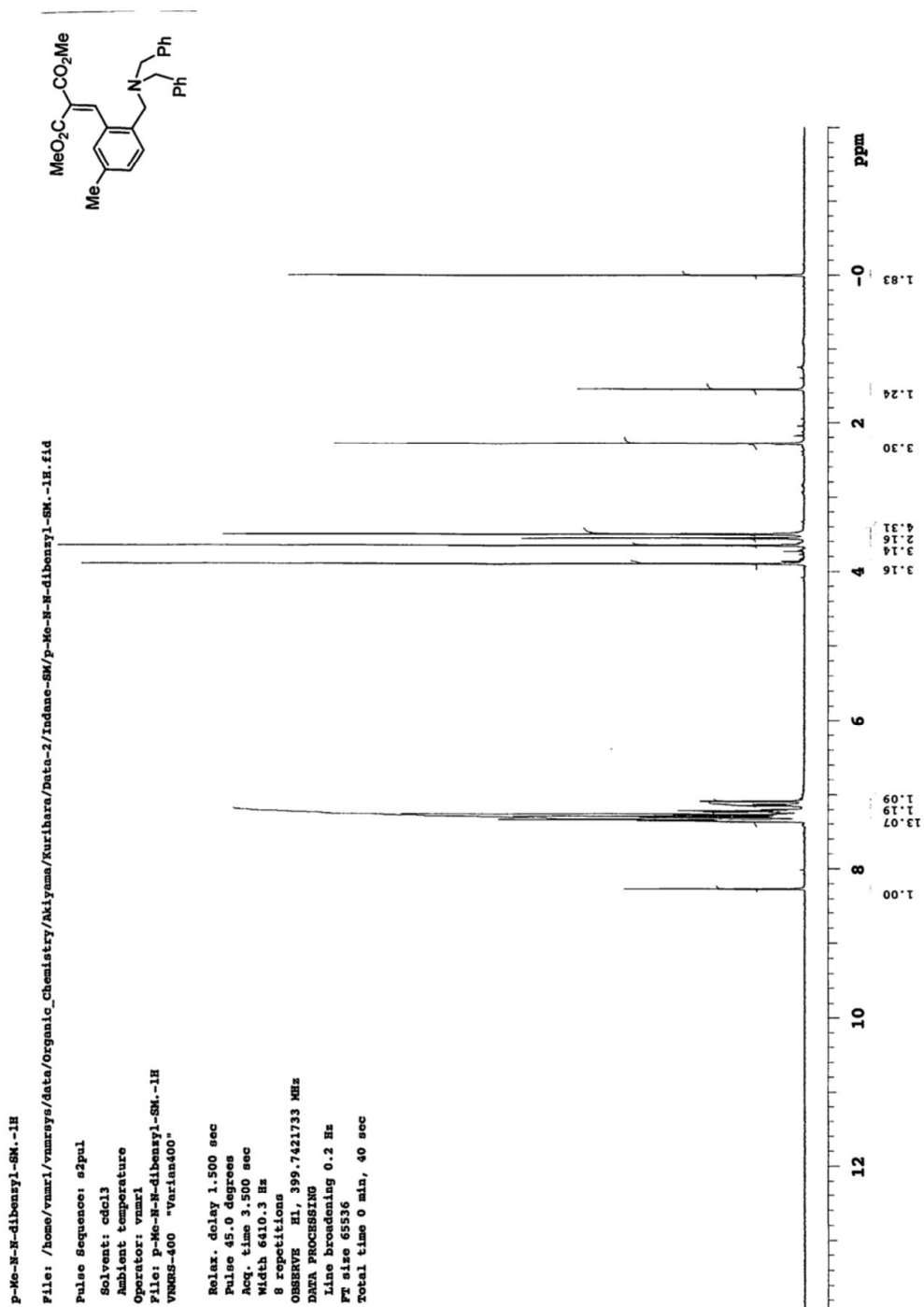
<sup>1</sup>H NMR spectrum of **s10**.



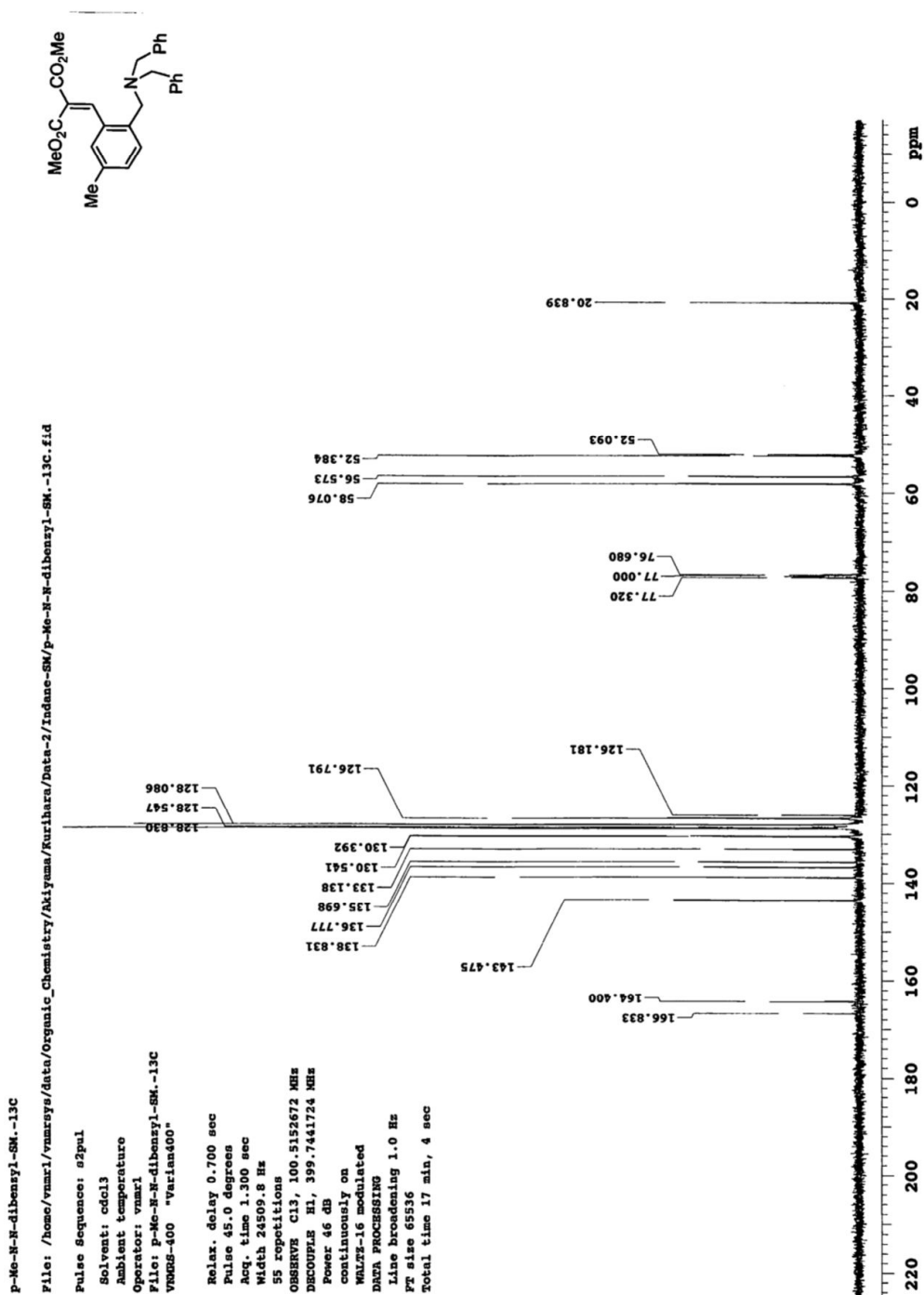
<sup>13</sup>C NMR spectrum of **s10**.



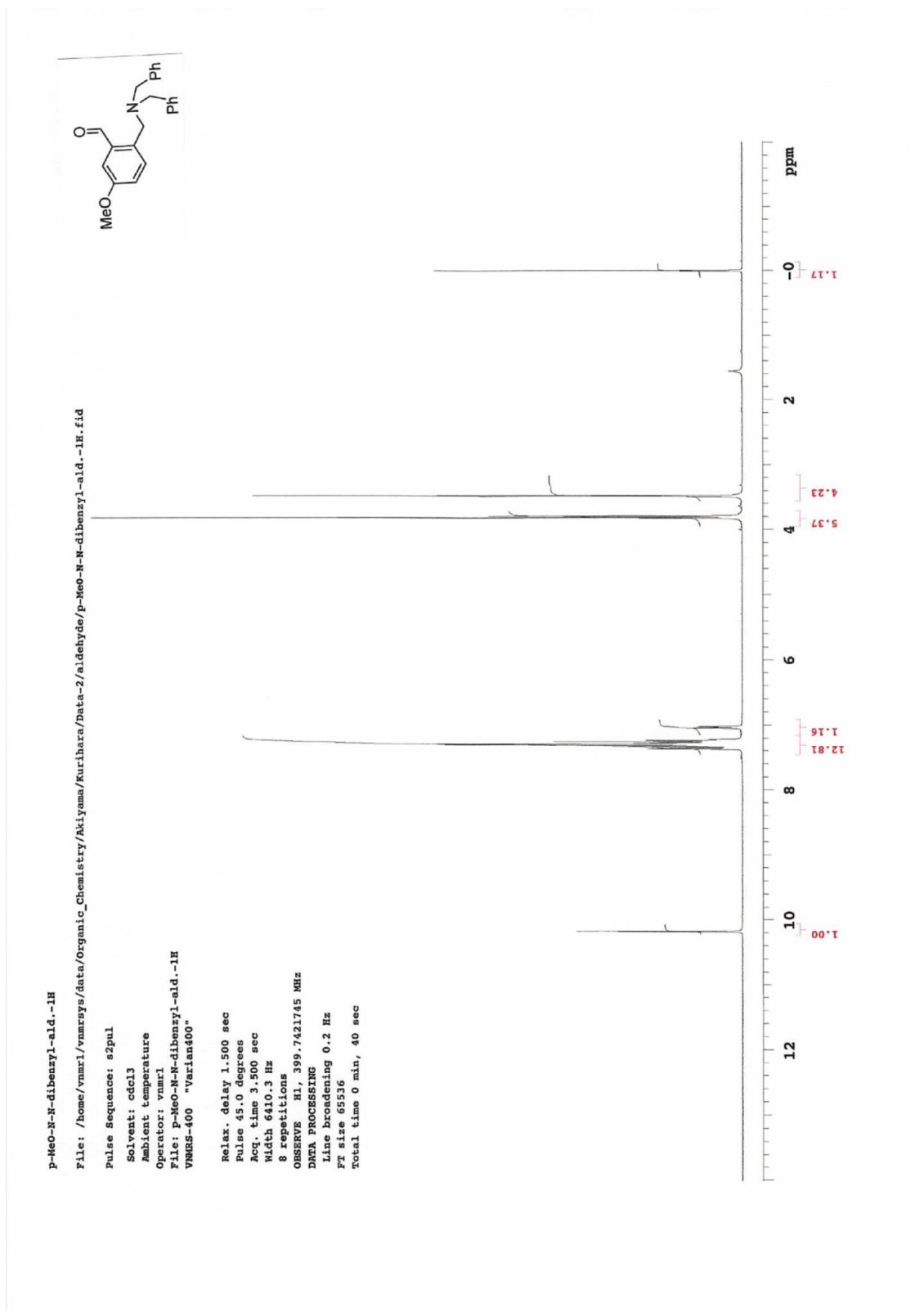
<sup>1</sup>H NMR spectrum of **3j**.



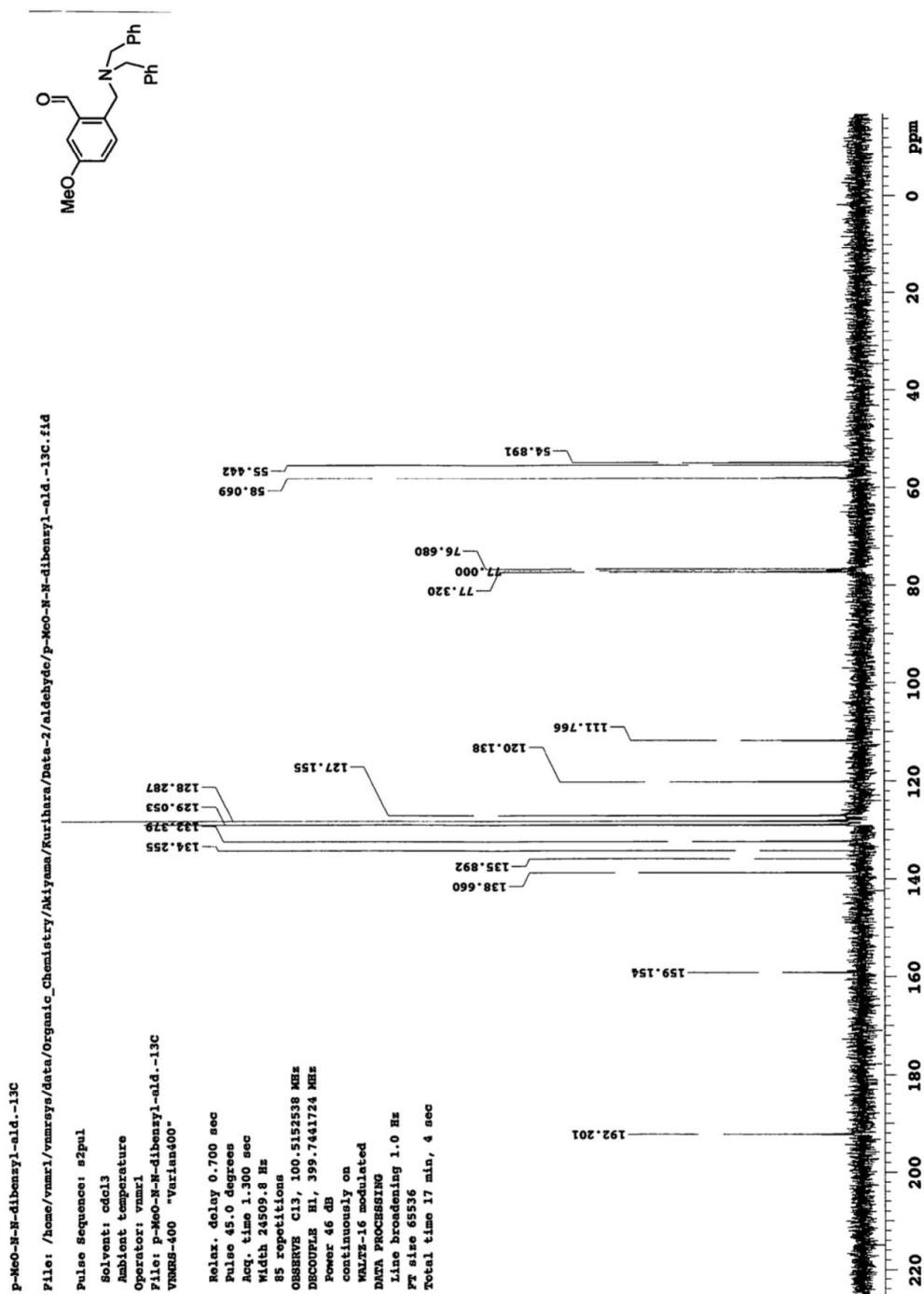
$^{13}\text{C}$  NMR spectrum of **3j**.



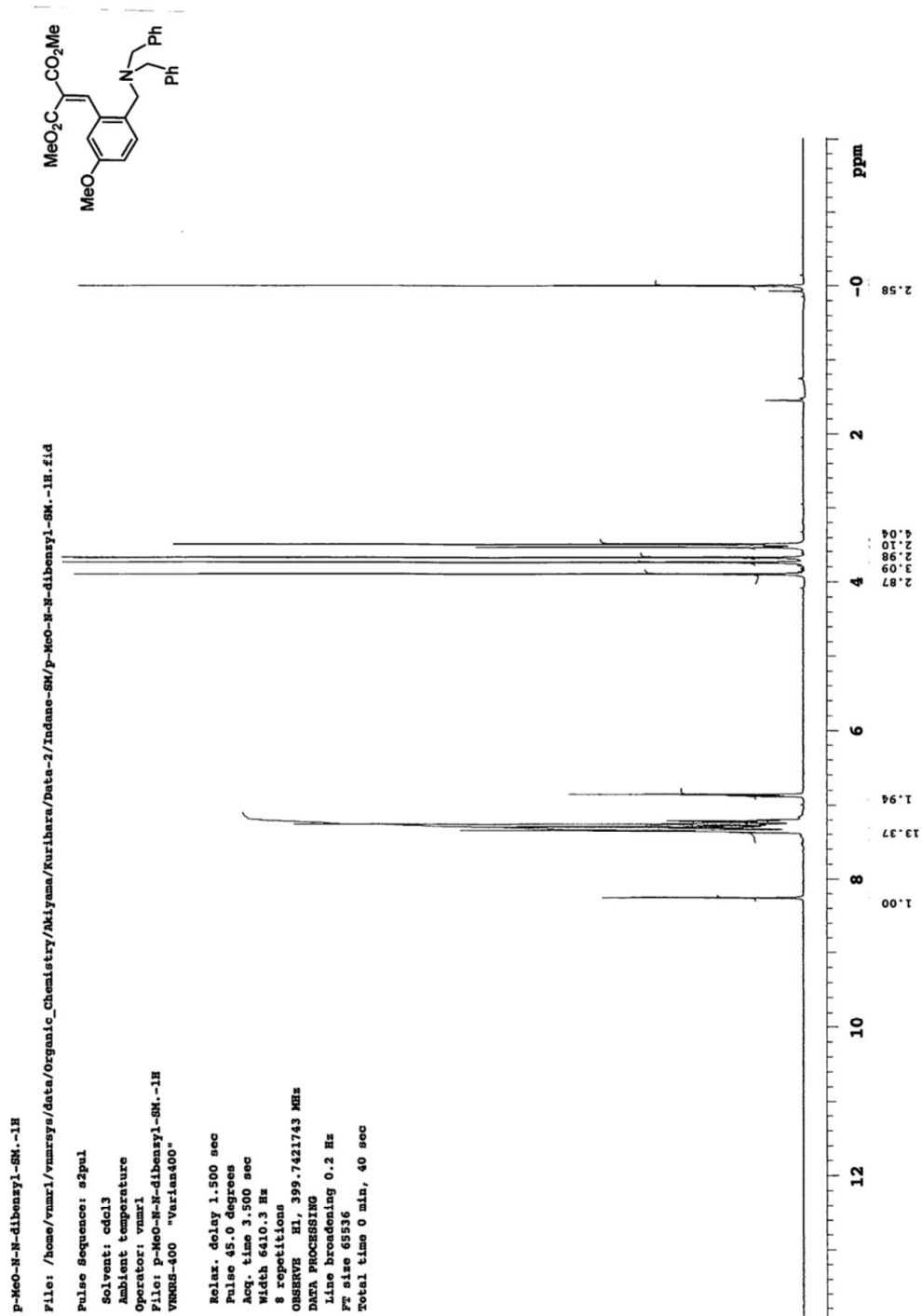
<sup>1</sup>H NMR spectrum of **s11**.



<sup>13</sup>C NMR spectrum of **s11**.

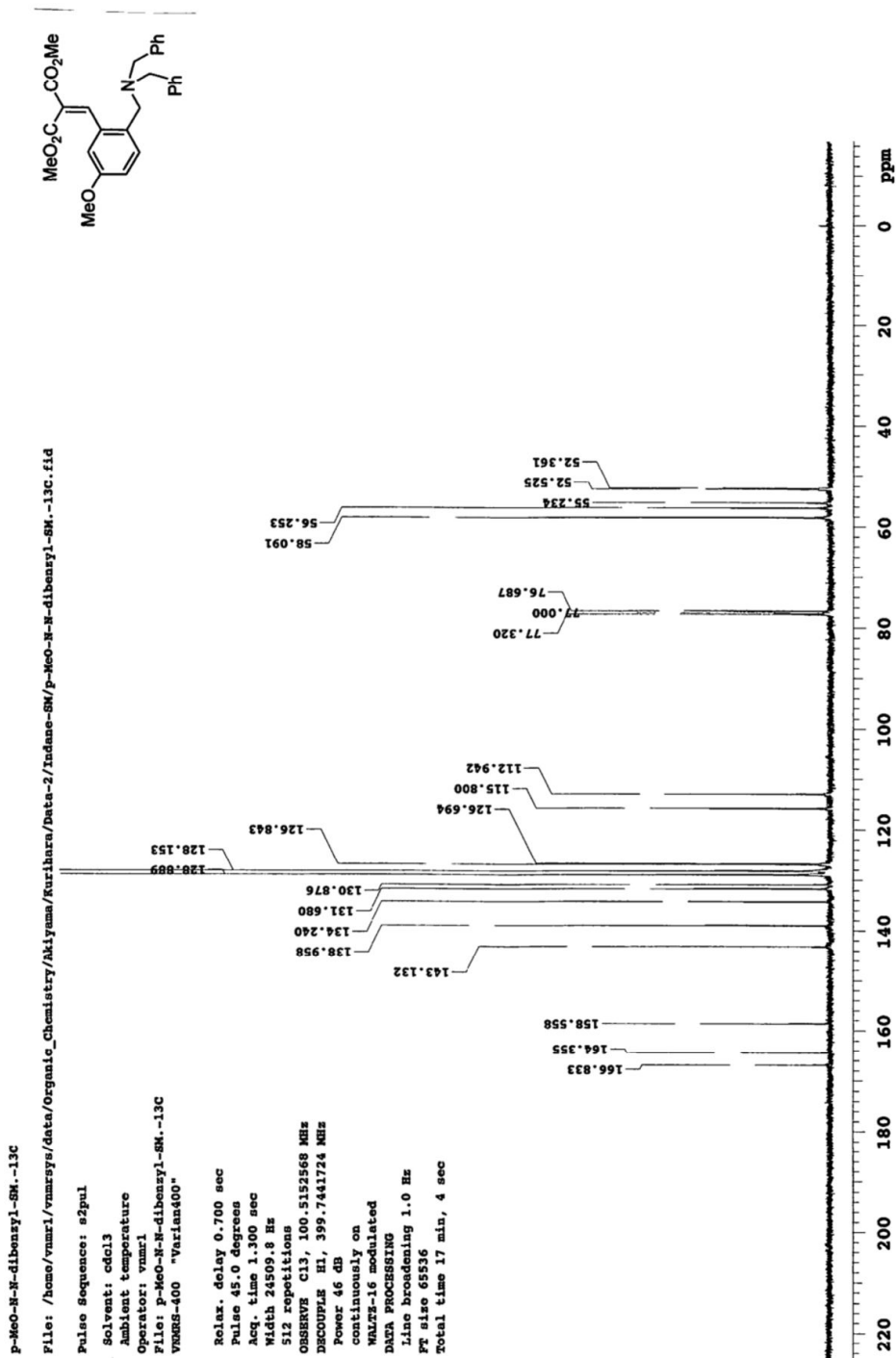


$^1\text{H}$  NMR spectrum of **3k**.

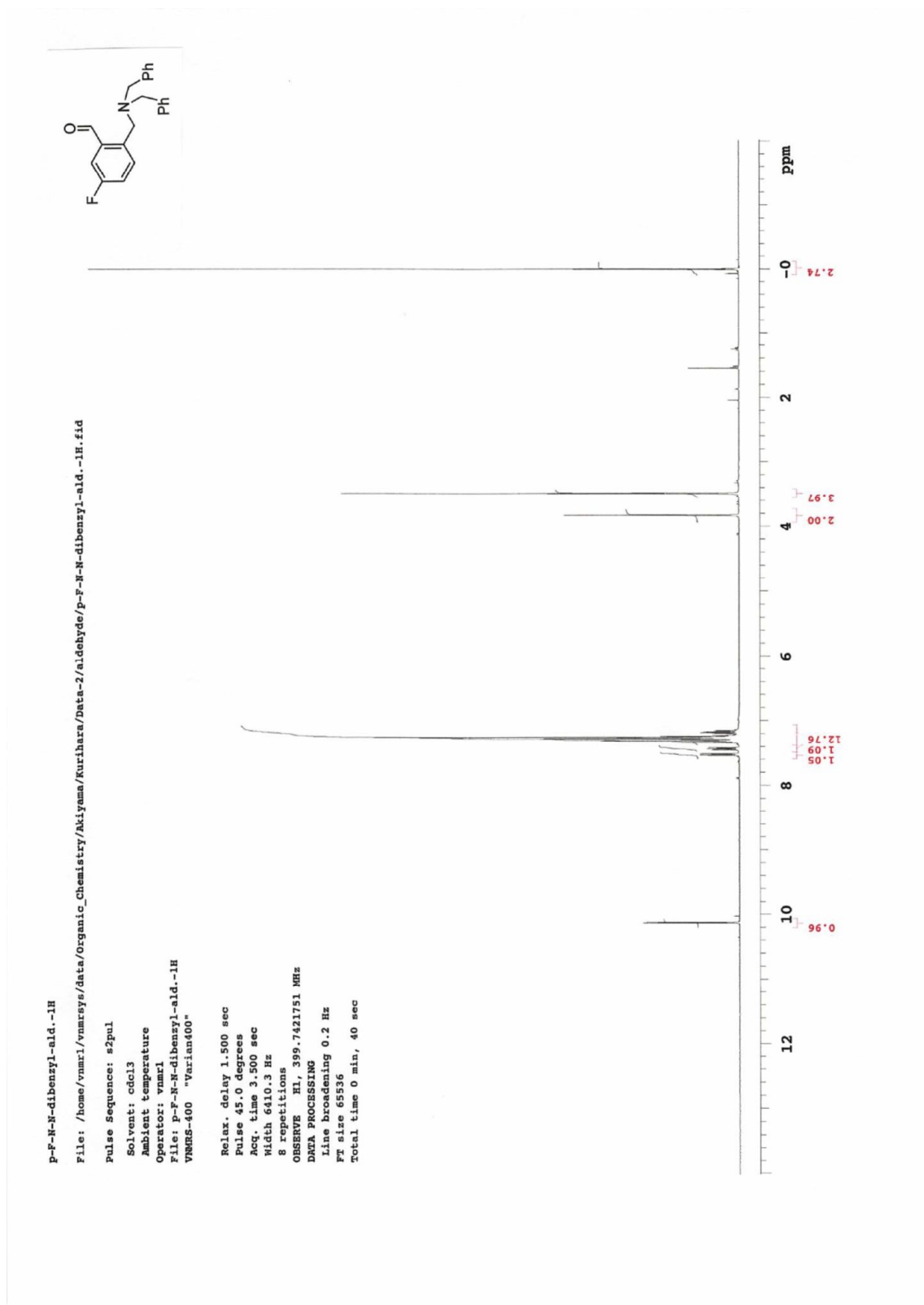




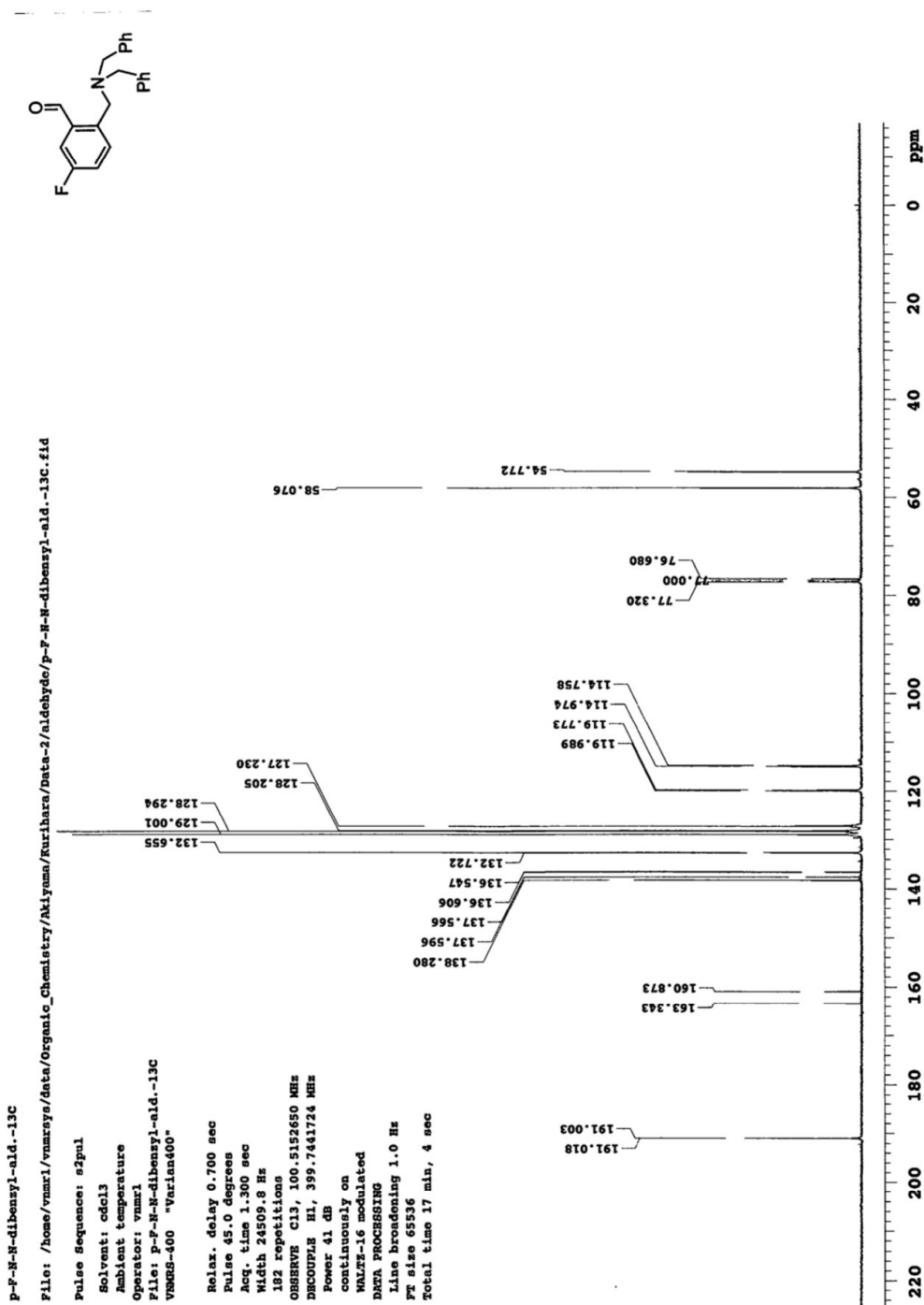
<sup>13</sup>C NMR spectrum of **3k**.



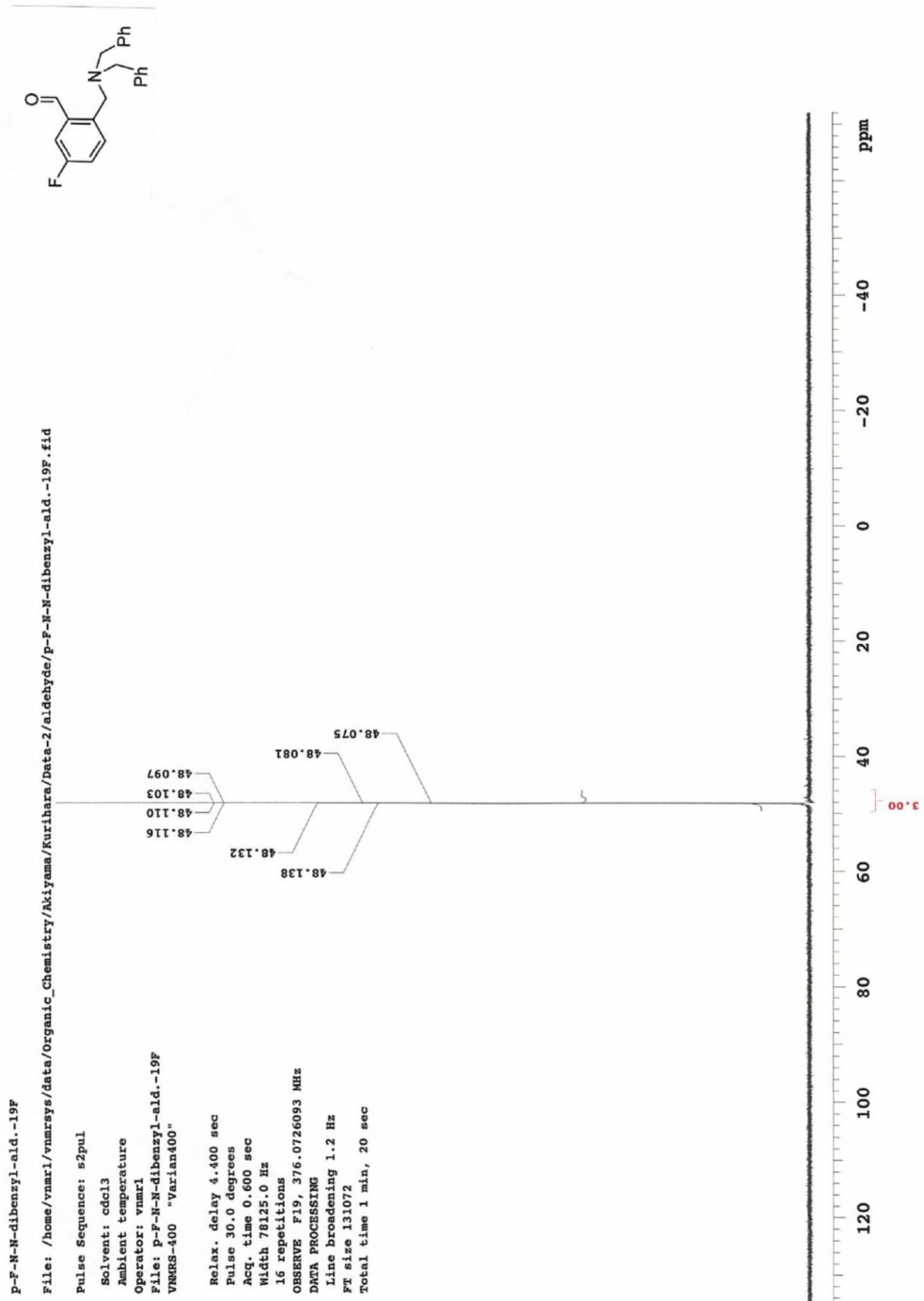
<sup>1</sup>H NMR spectrum of **s12**.



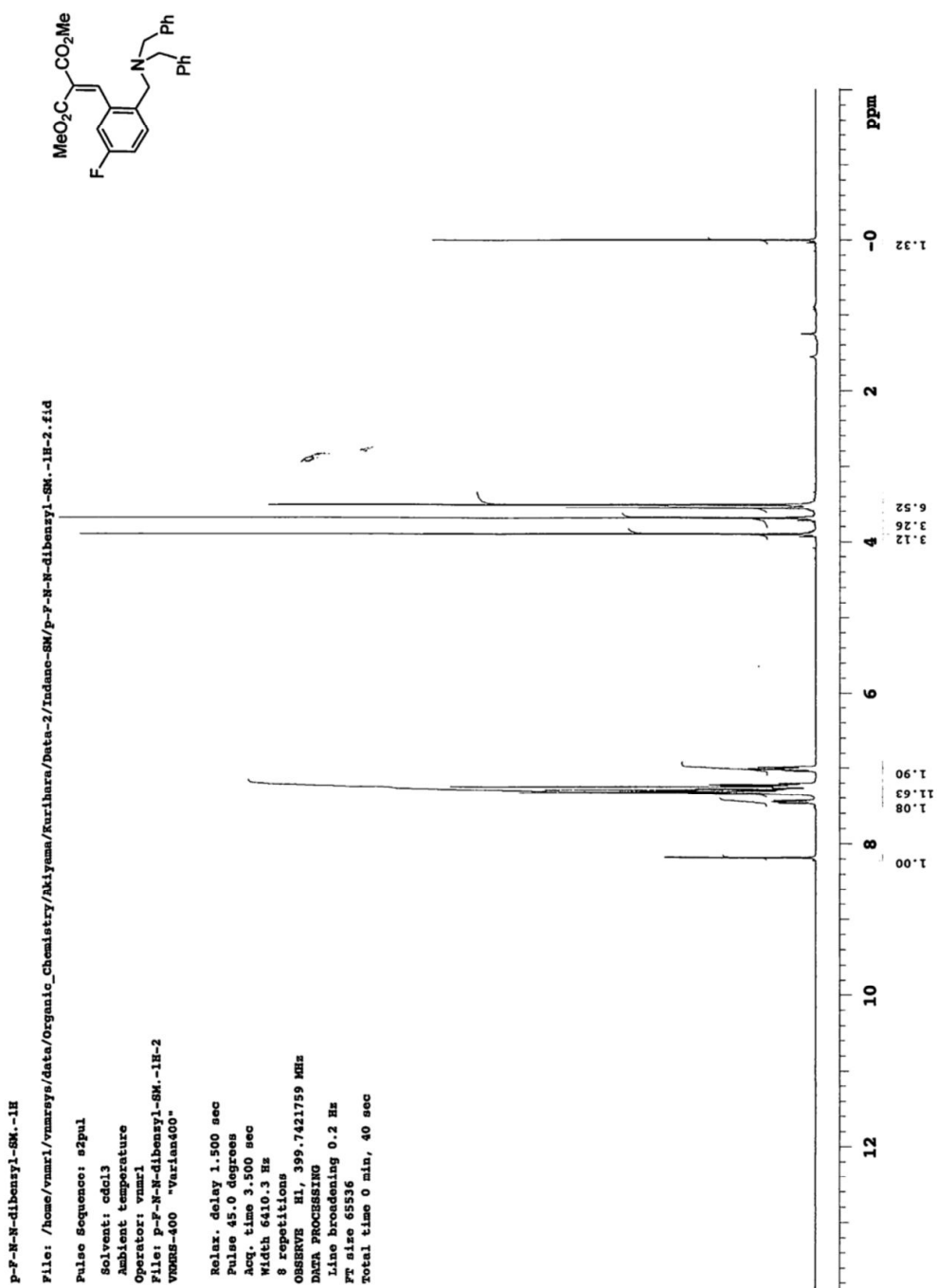
<sup>13</sup>C NMR spectrum of **s12**.



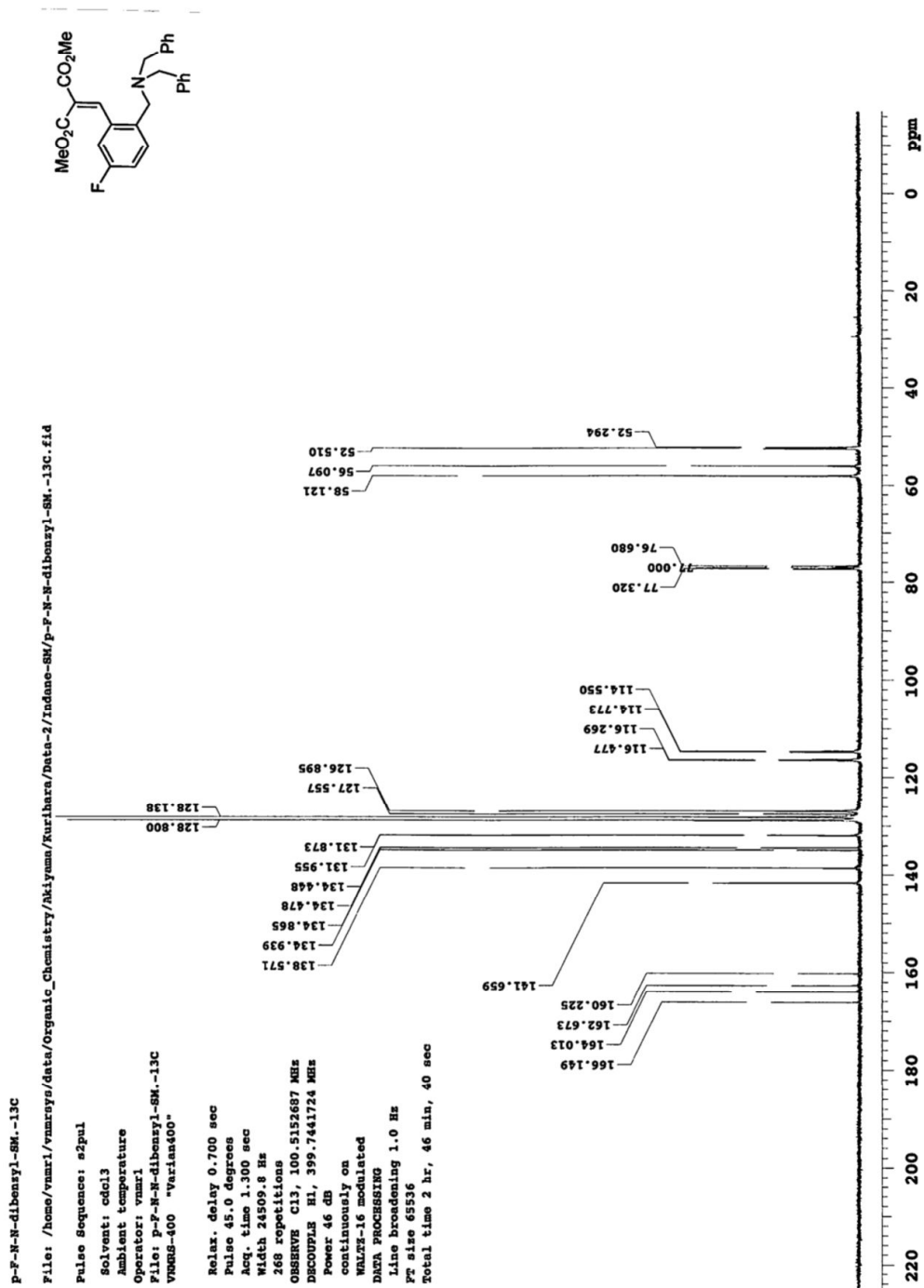
<sup>19</sup>F NMR spectrum of **s13**.



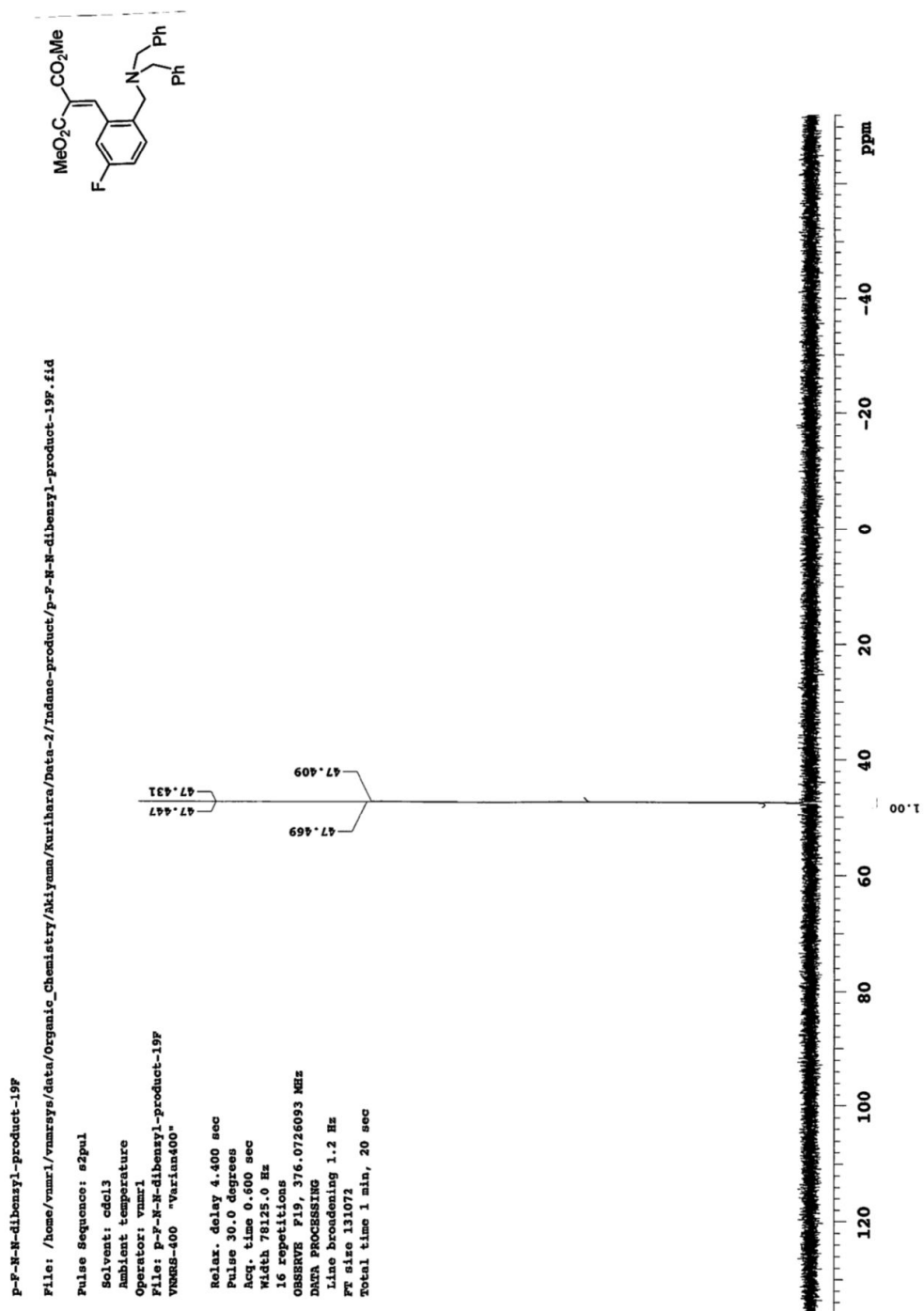
<sup>1</sup>H NMR spectrum of **31**.



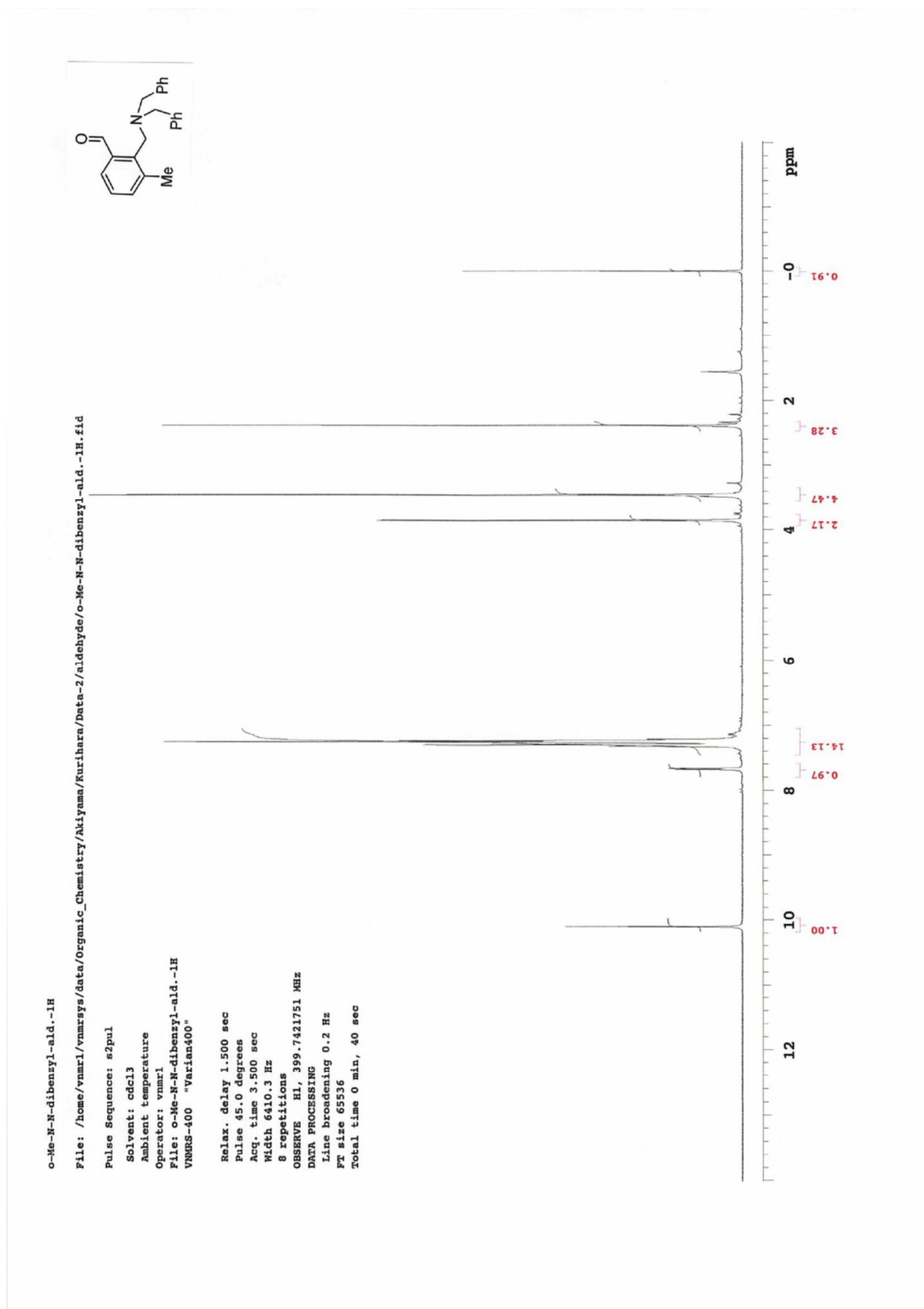
<sup>13</sup>C NMR spectrum of 31.



<sup>19</sup>F NMR spectrum of **31**.

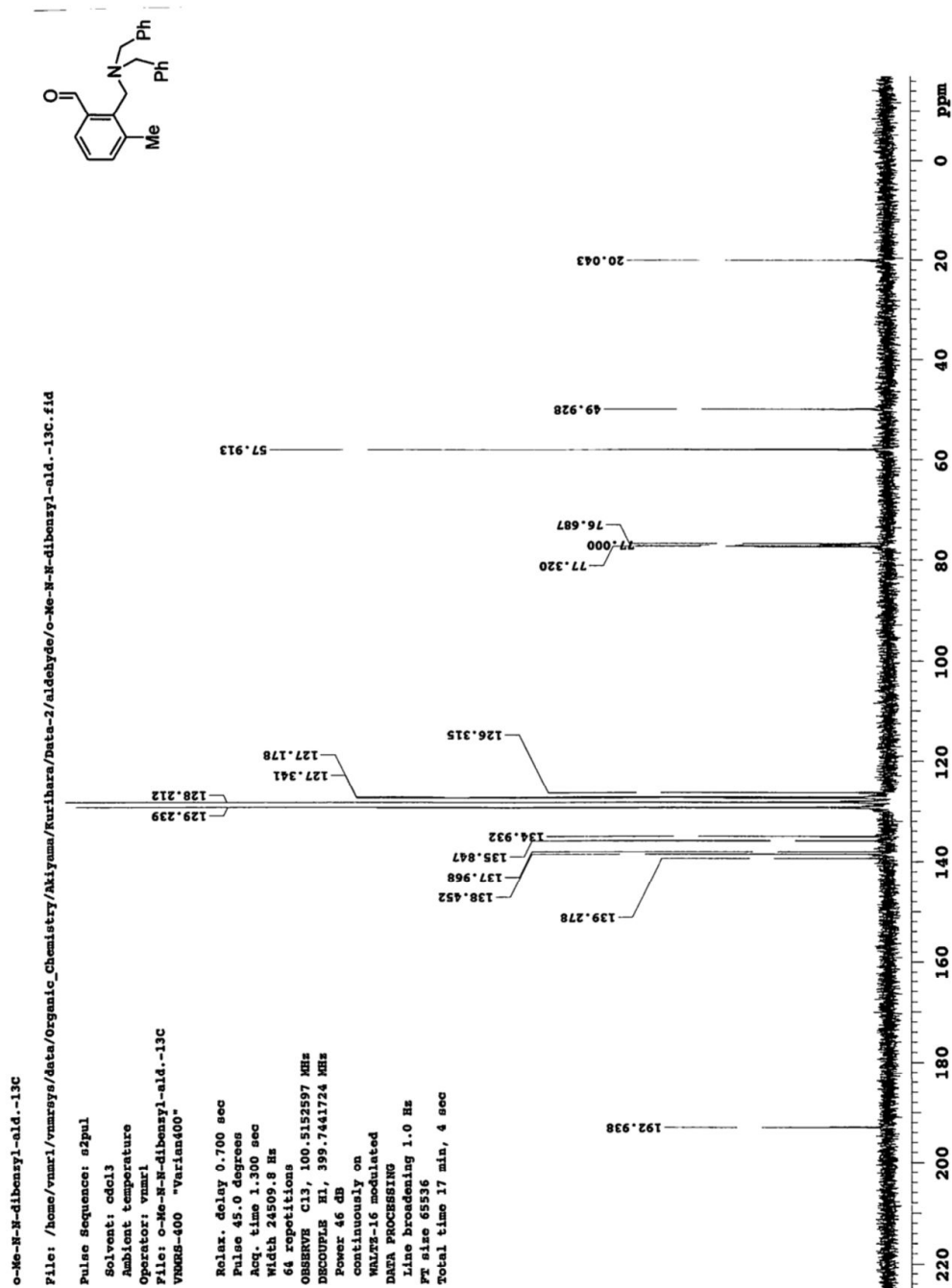


<sup>1</sup>H NMR spectrum of **s13**

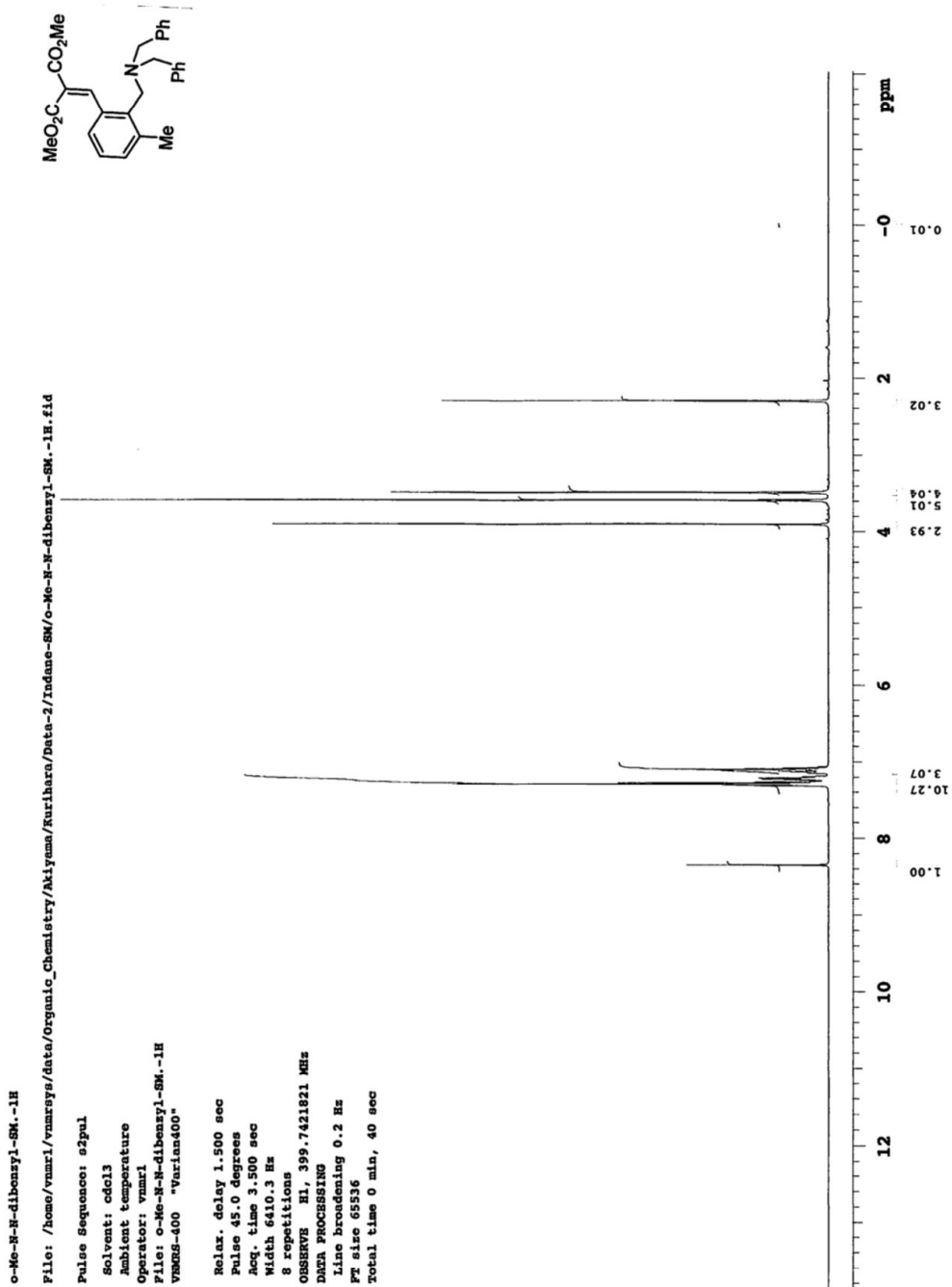




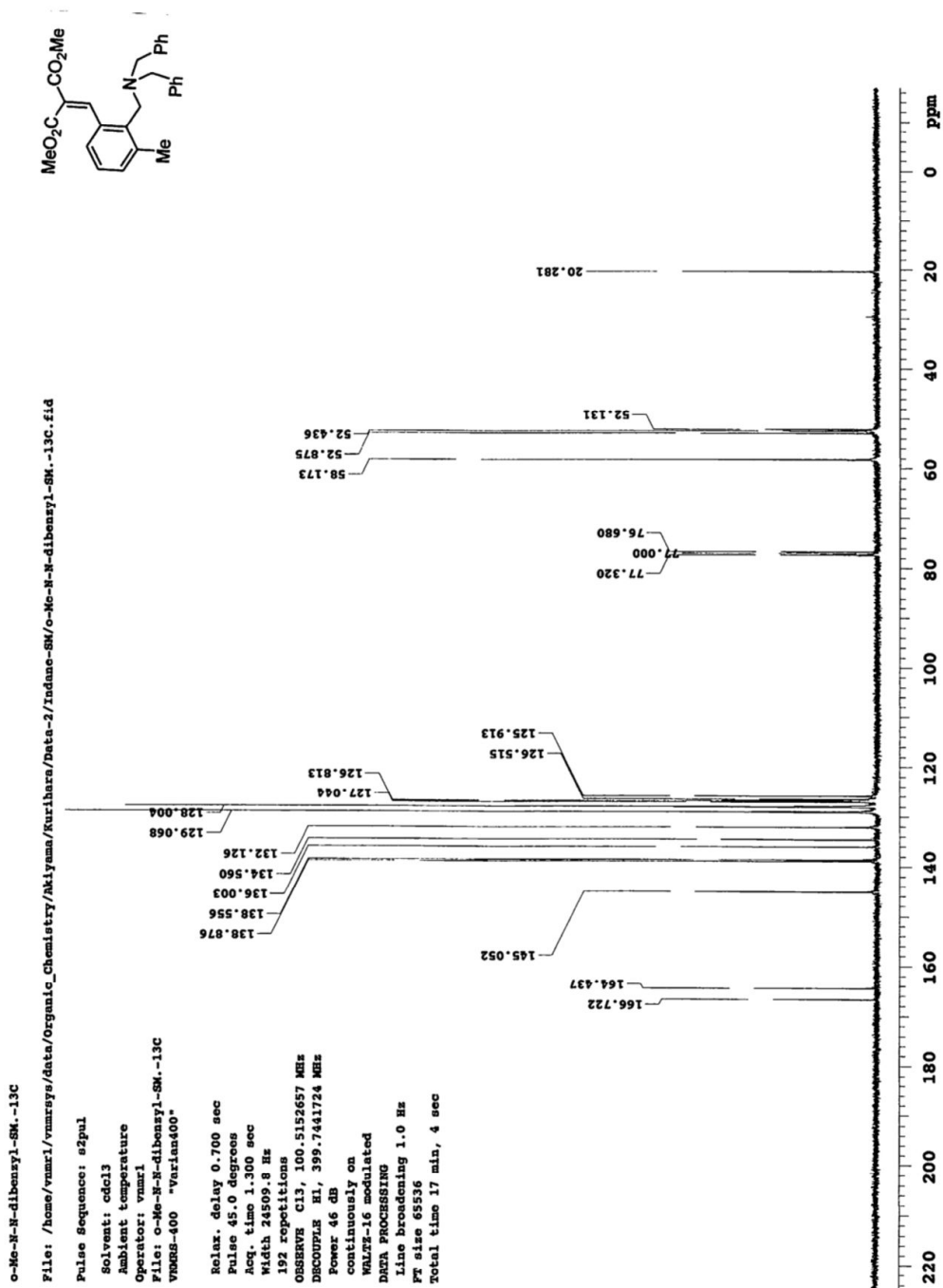
<sup>13</sup>C NMR spectrum of **s13**.



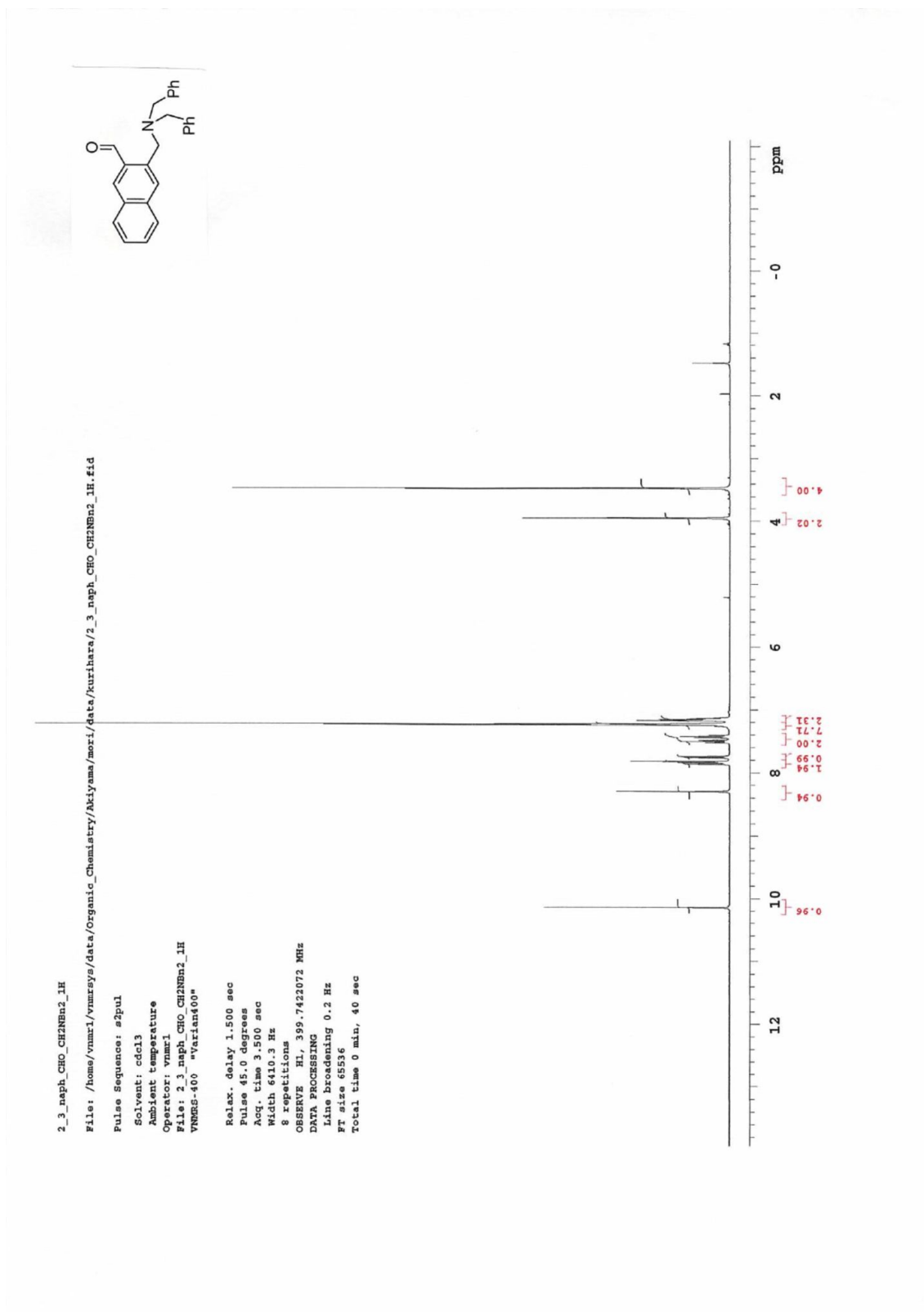
<sup>1</sup>H NMR spectrum of **3m**.



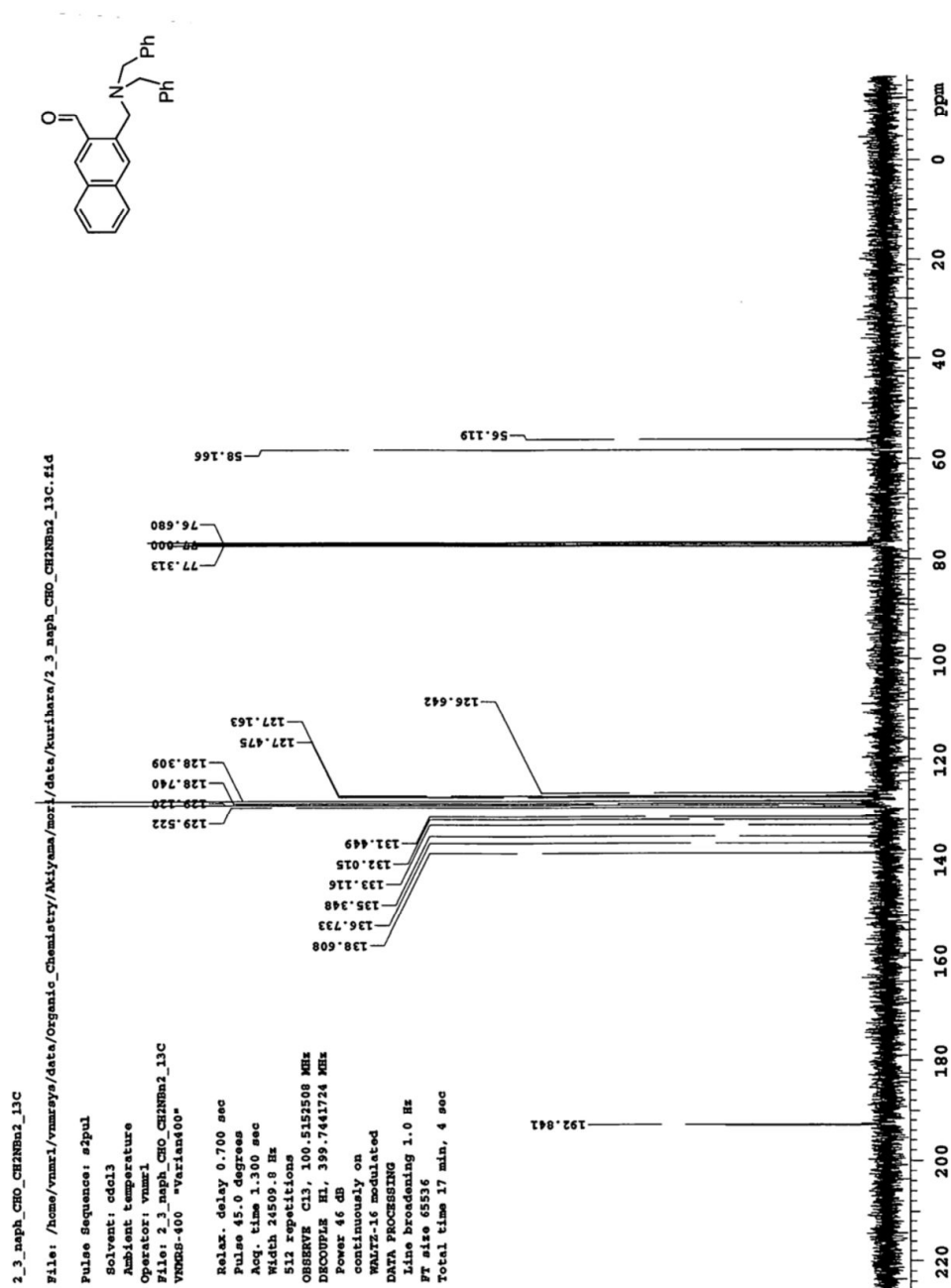
<sup>13</sup>C NMR spectrum of **3m**.



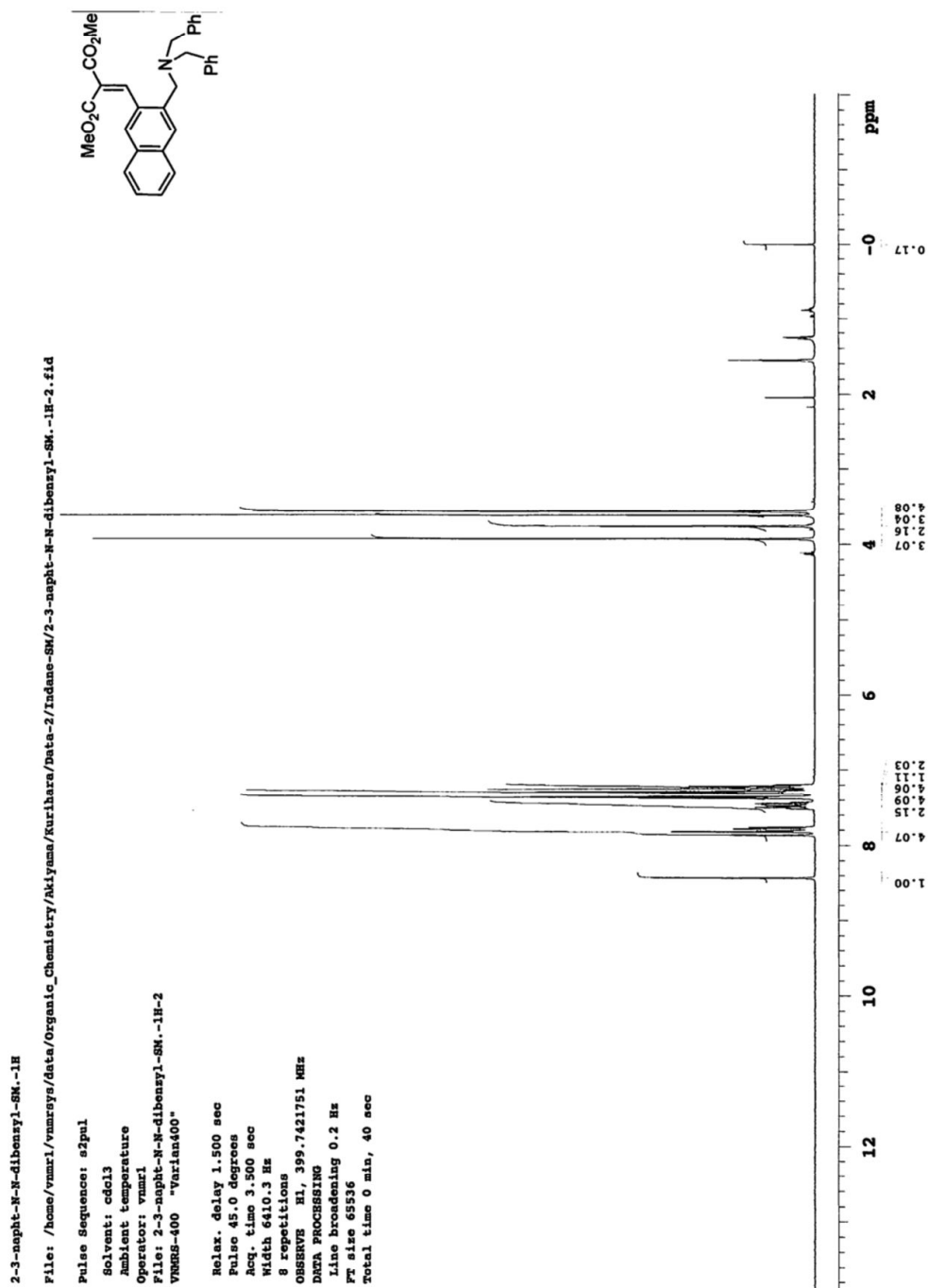
<sup>1</sup>H NMR spectrum of **s14**.



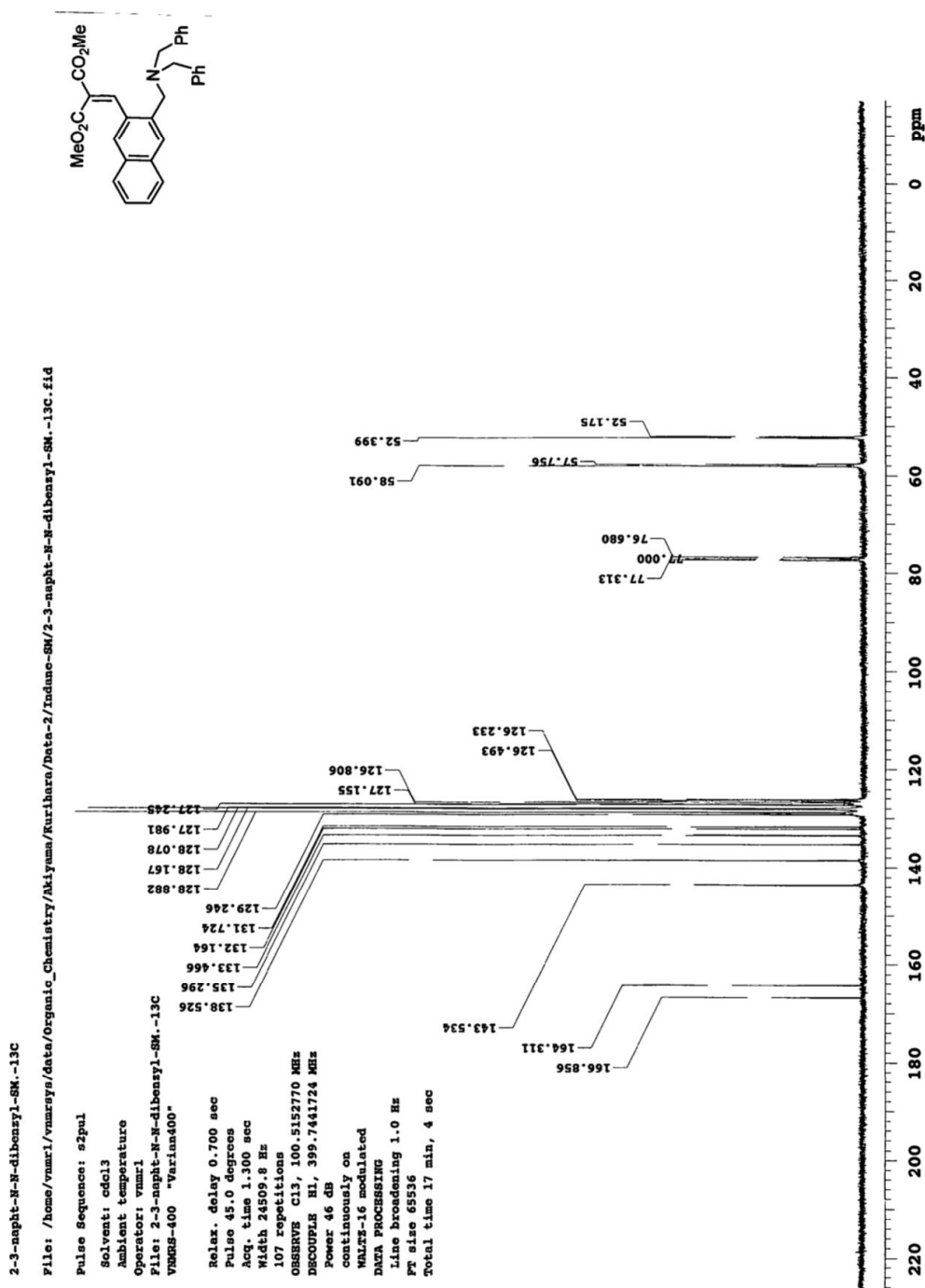
<sup>13</sup>C NMR spectrum of **s14**.



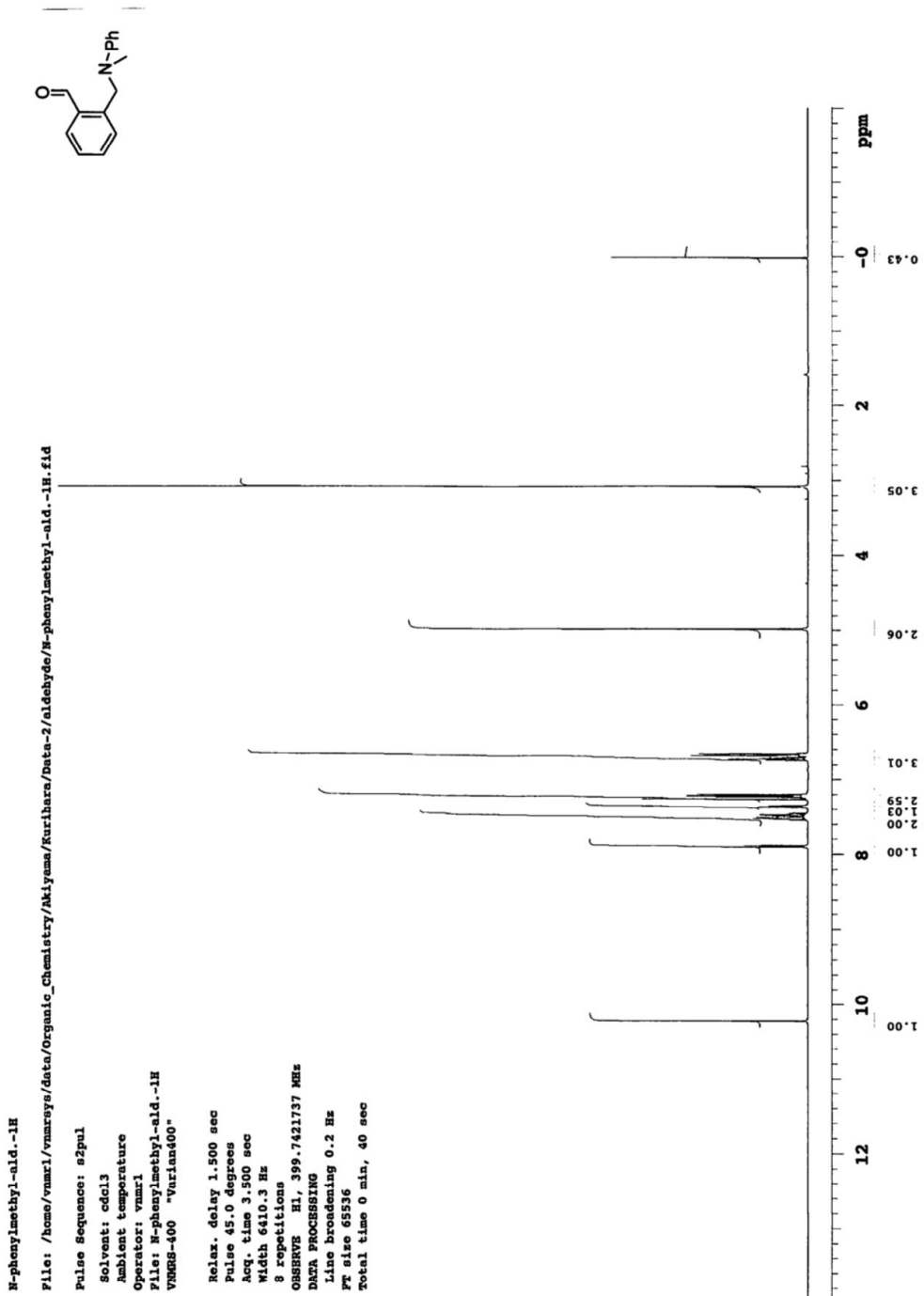
<sup>1</sup>H NMR spectrum of **3n**.



<sup>13</sup>C NMR spectrum of **3n**.

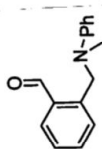


<sup>1</sup>H NMR spectrum of **s15**.





<sup>13</sup>C NMR spectrum of **s15**.



N-phenylmethyl-ald.-13C

File: /home/vnmr1/vnmrsys/data/Organic\_Chemistry/Kurihara/Data-2/aldehyde/N-phenylmethyl-ald.-13C.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: vnmr1

File: N-phenylmethyl-ald.-13C

VMRS-400 "Varian400"

Relax. delay 0.700 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24509.8 Hz

232 repetitions

OBSERVE C13, 100.5152538 MHz

DECOUPLE H1, 399.7441724 MHz

Power 41 dB

continuously on

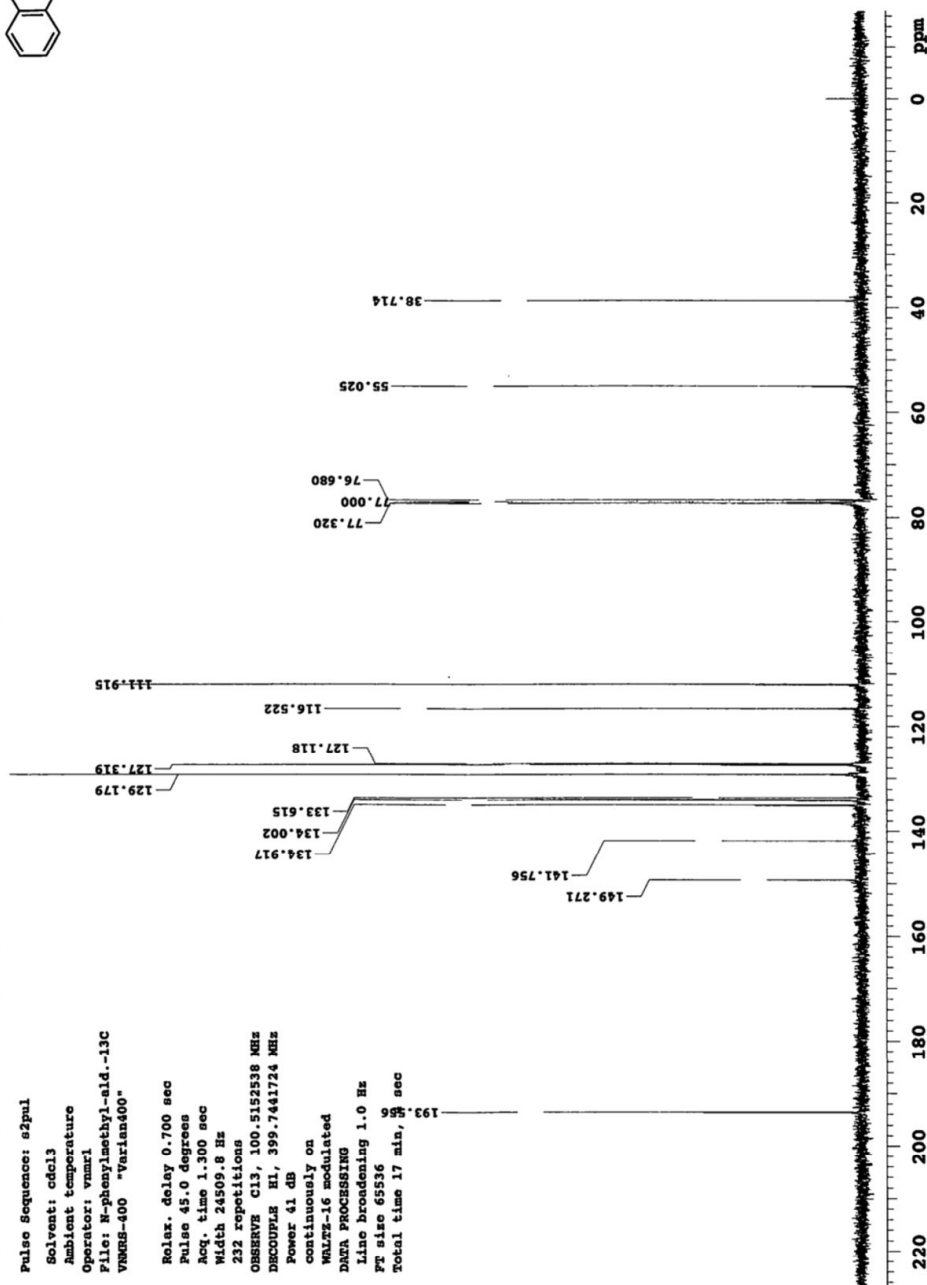
WALTZ-16 modulated

DMCA PROCESSING

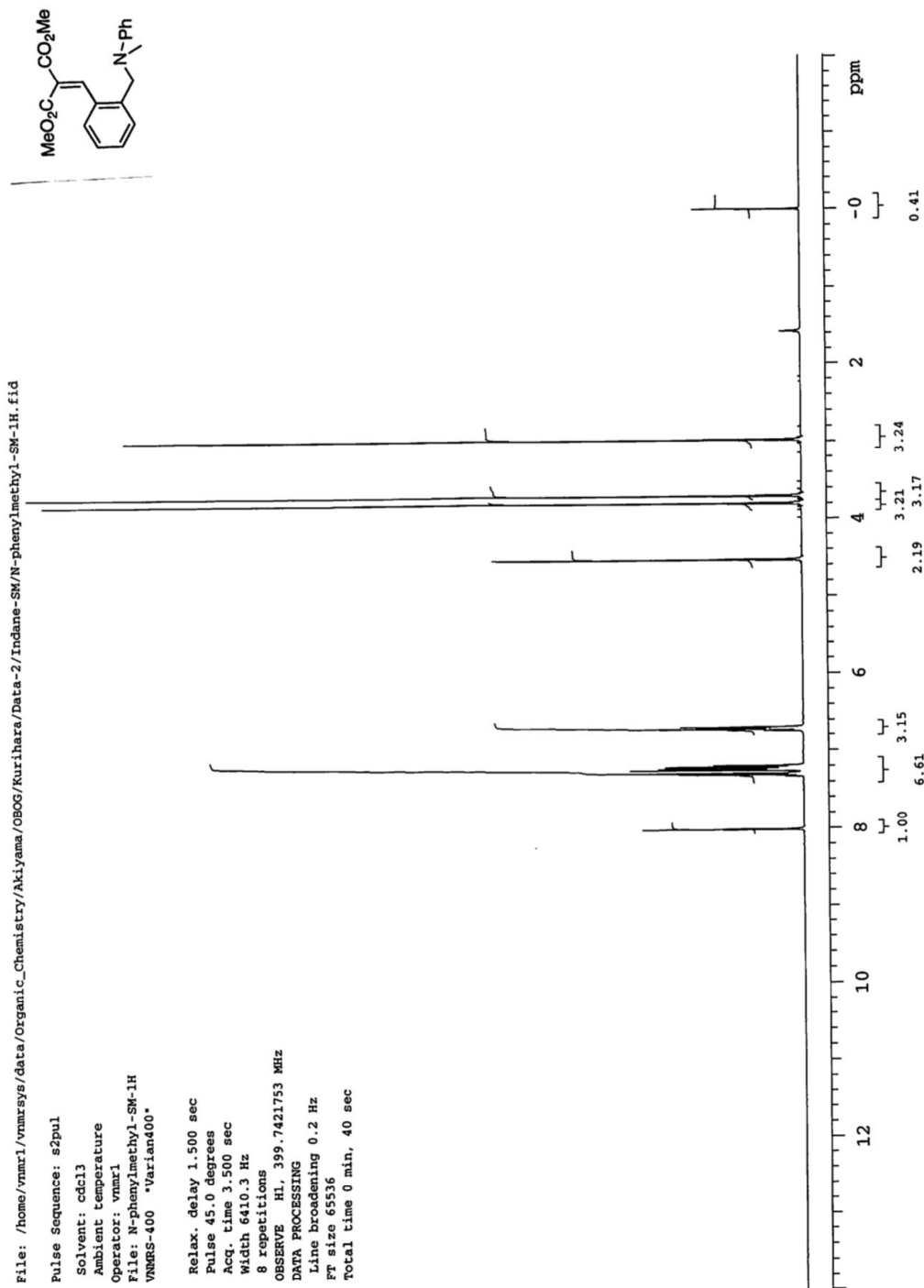
Line Broadening 1.0 Hz

FT size 65836

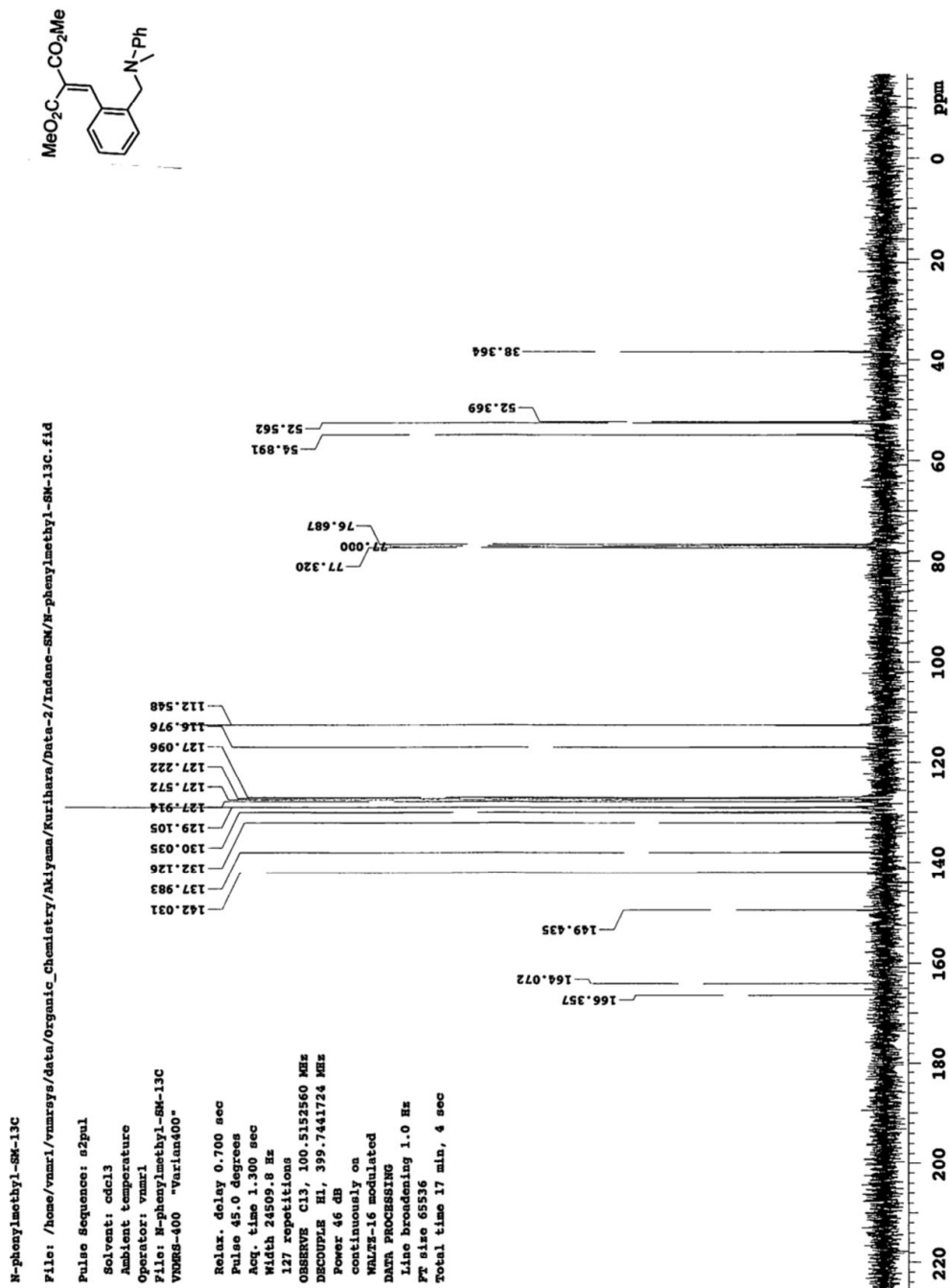
Total time 17 min, 36 sec



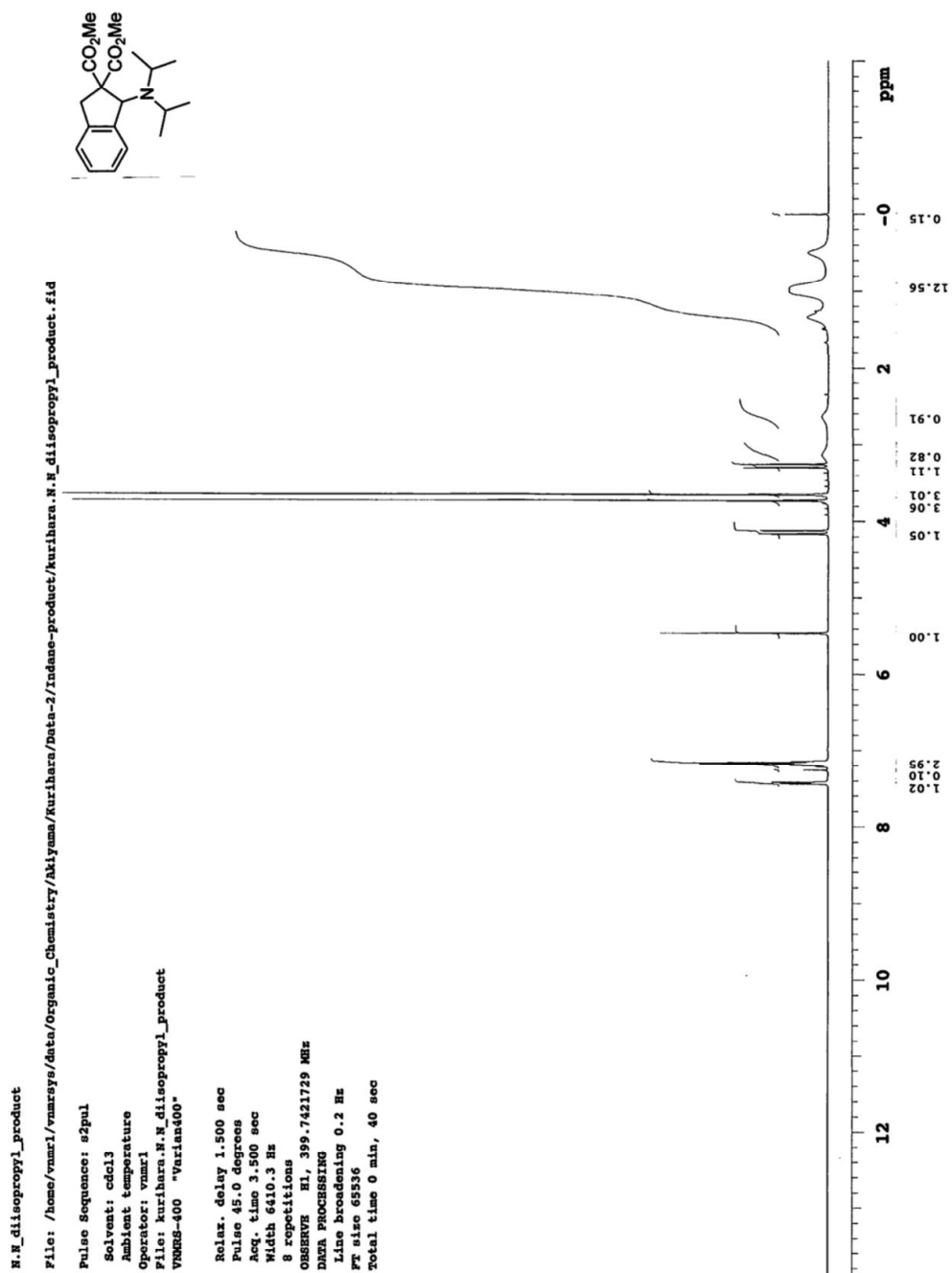
<sup>1</sup>H NMR spectrum of **3o**.



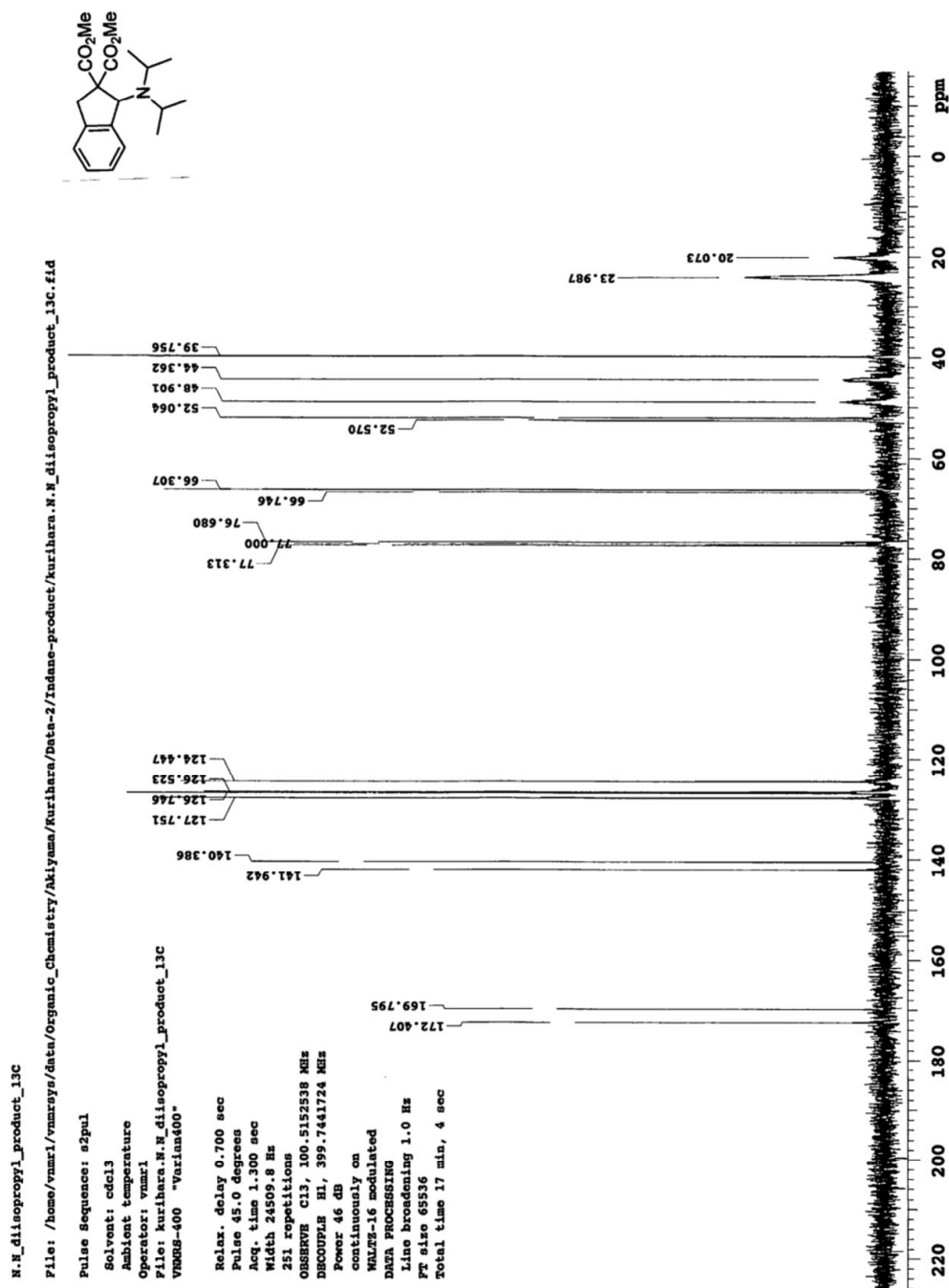
<sup>13</sup>C NMR spectrum of **30**.



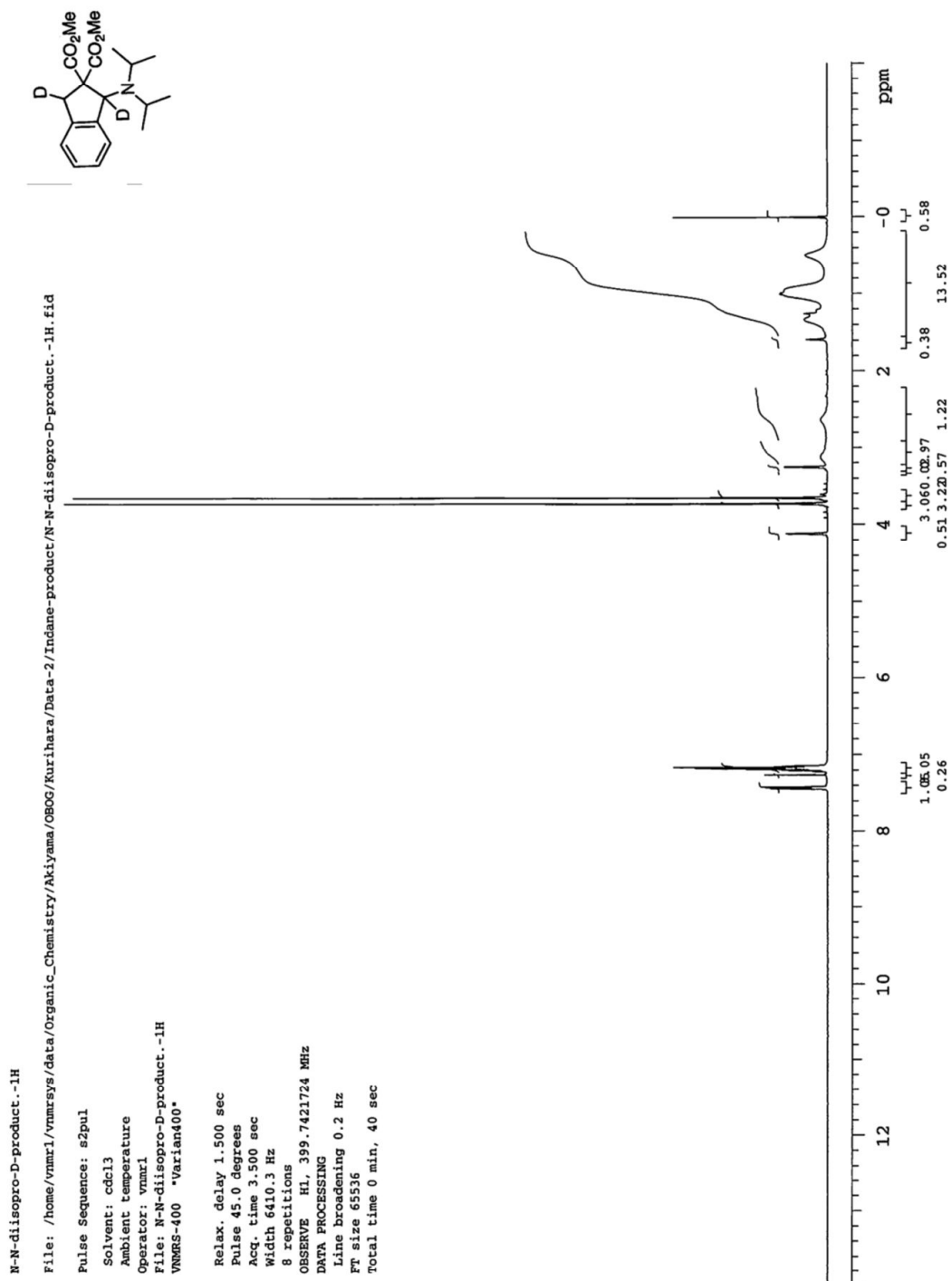
<sup>1</sup>H NMR spectrum of **4a**.



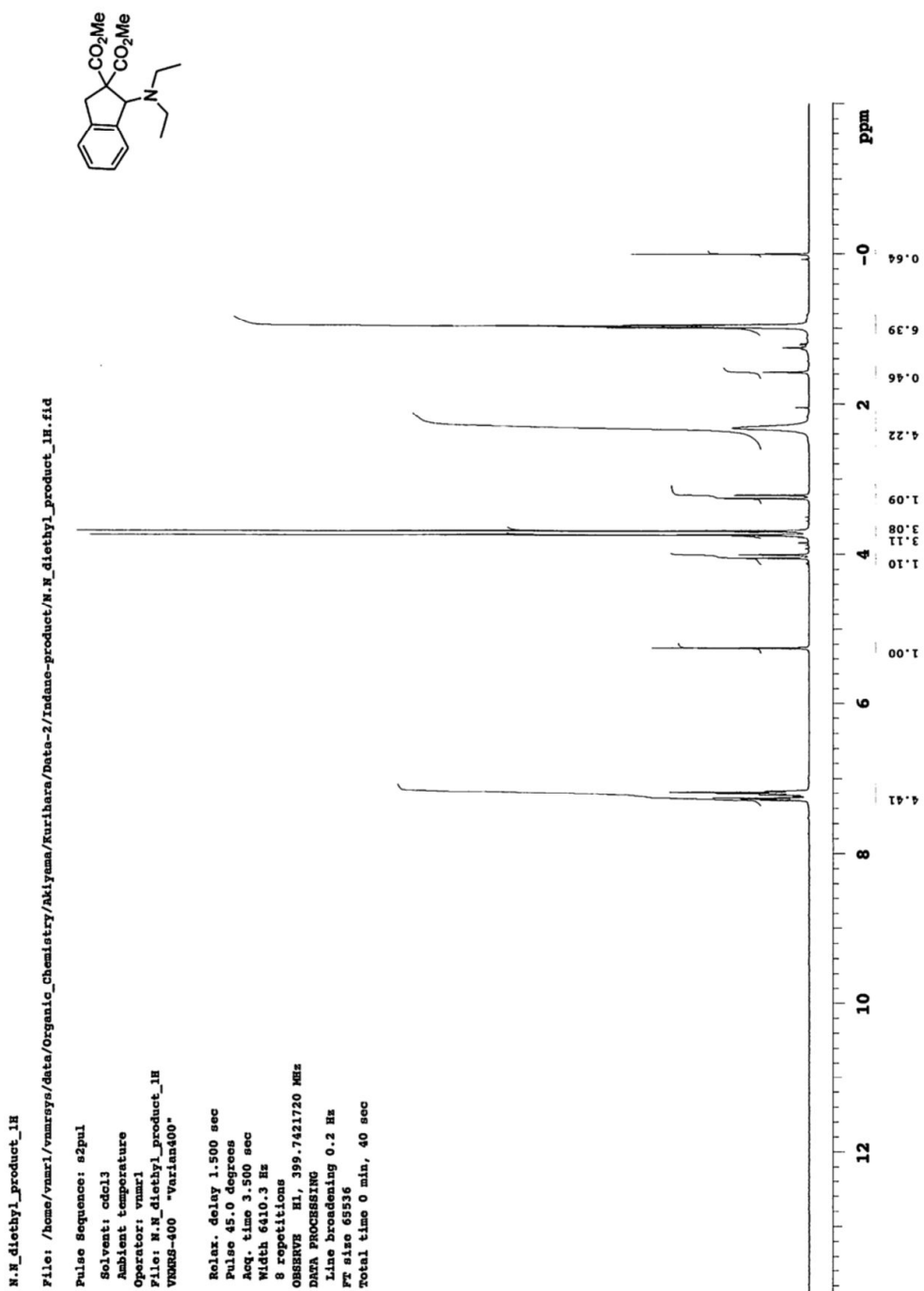
<sup>13</sup>C NMR spectrum of 4a.



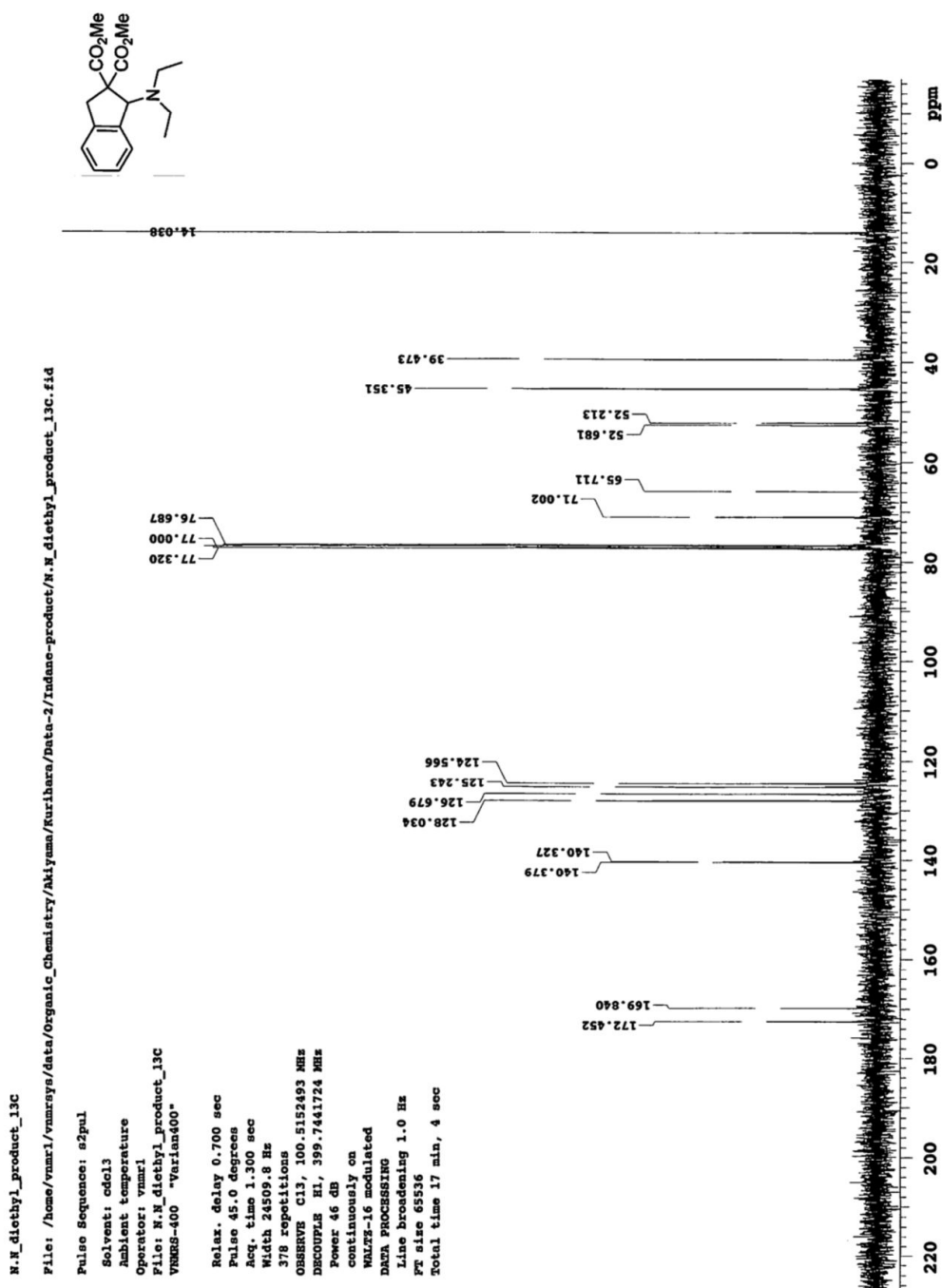
<sup>1</sup>H NMR spectrum of *d*-4a.



<sup>1</sup>H NMR spectrum of **4b**.

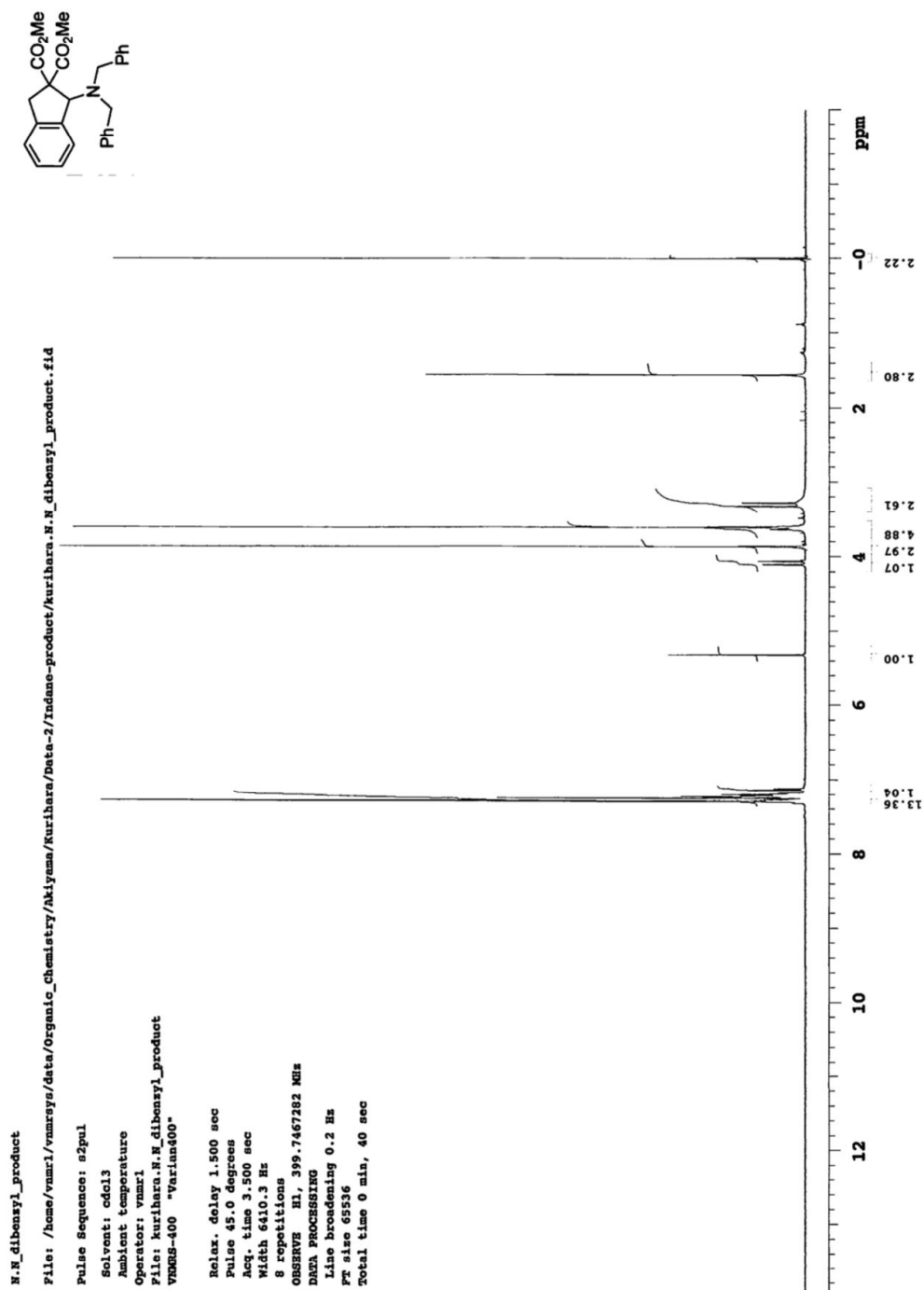


$^{13}\text{C}$  NMR spectrum of **4b**.

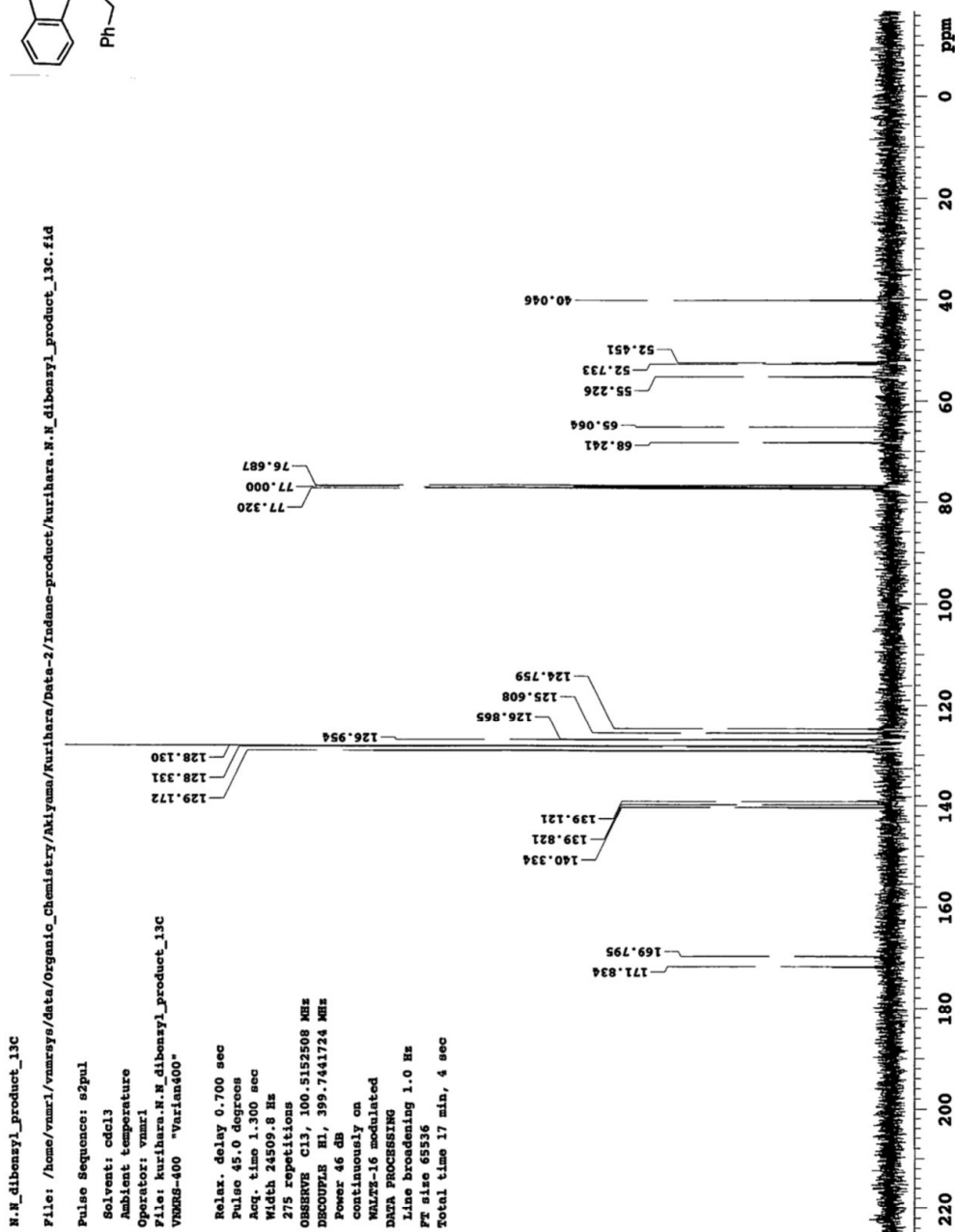
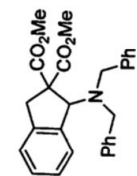




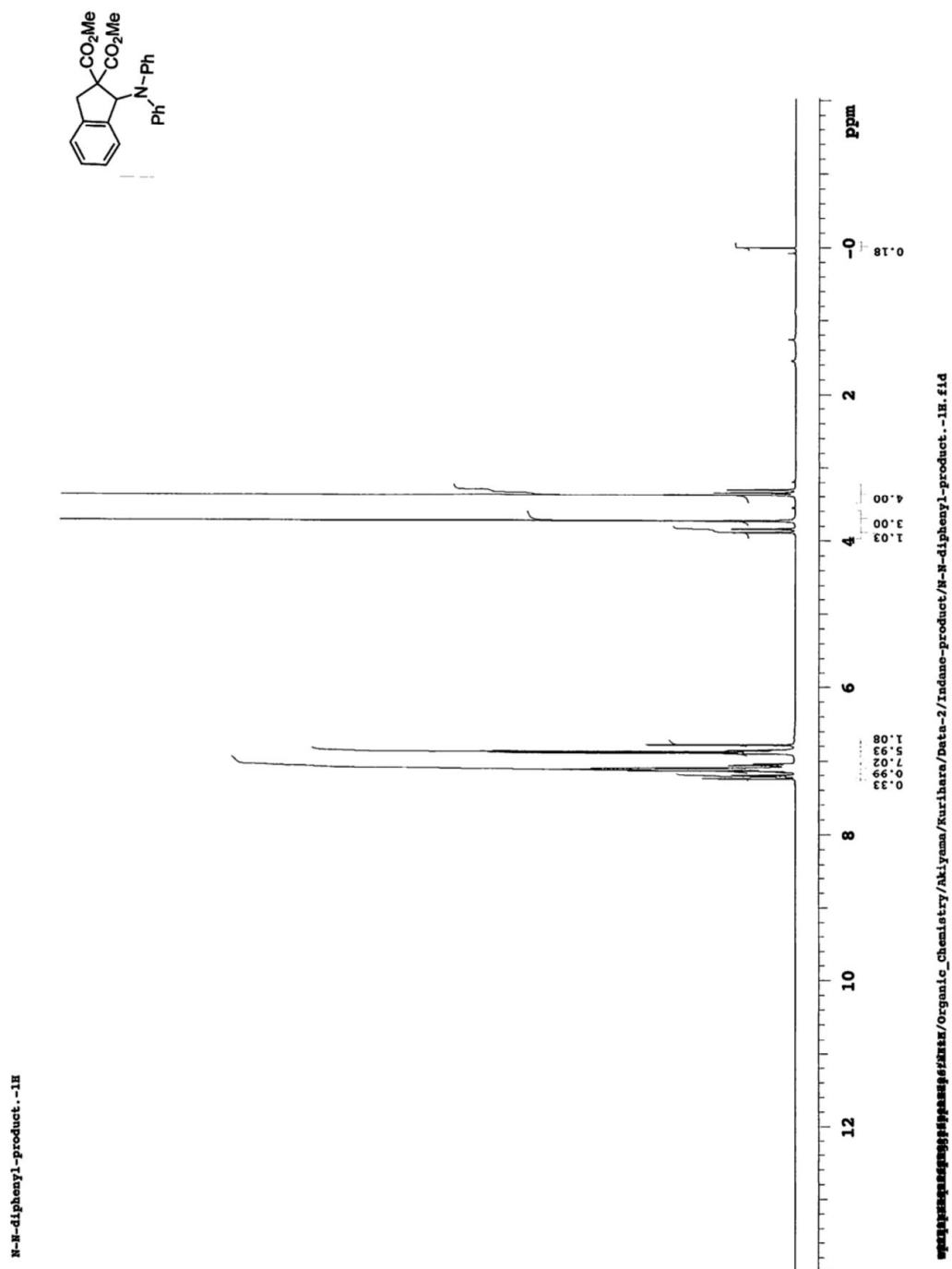
<sup>1</sup>H NMR spectrum of **4c**.



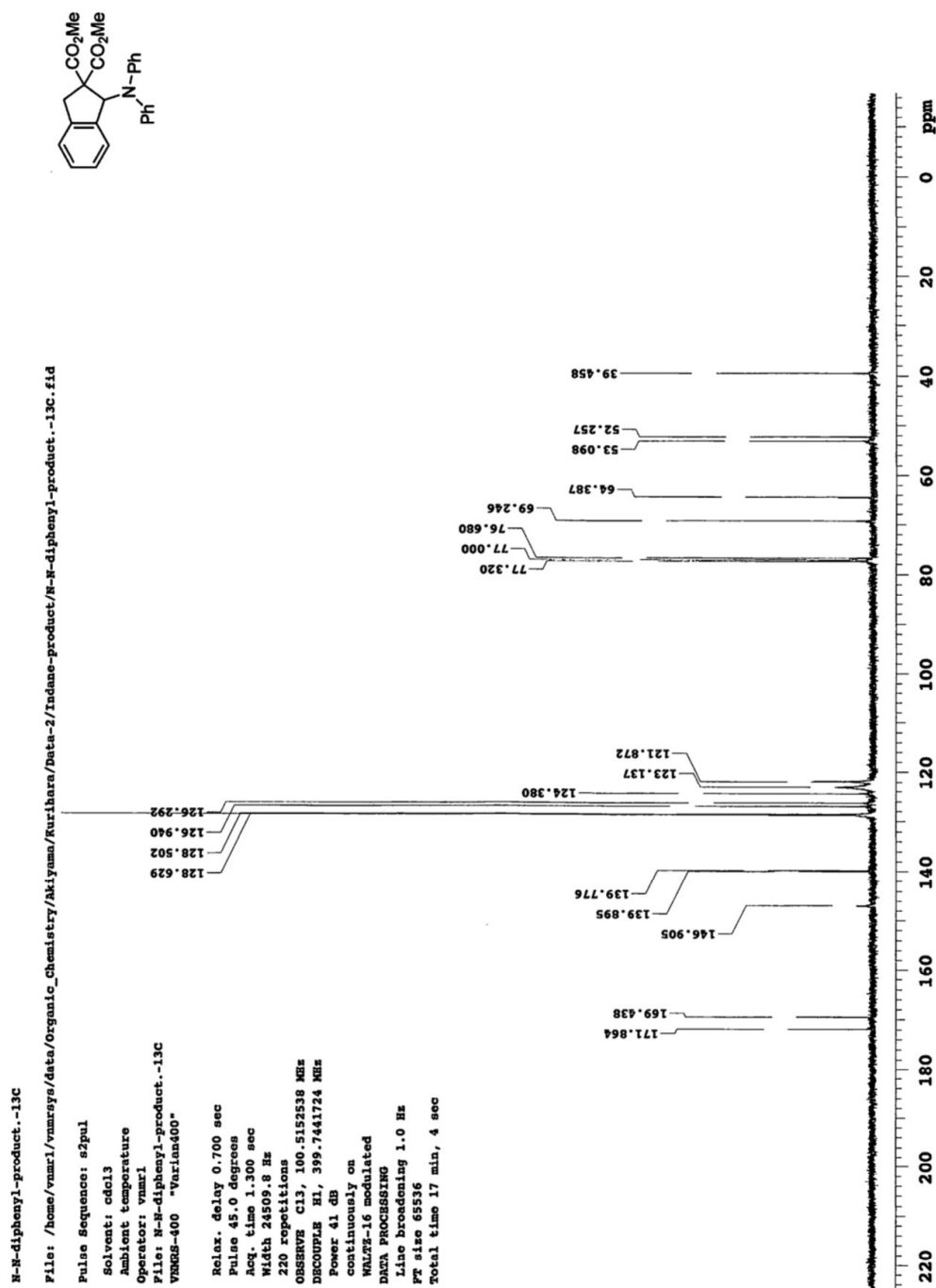
<sup>13</sup>C NMR spectrum of **4c**.



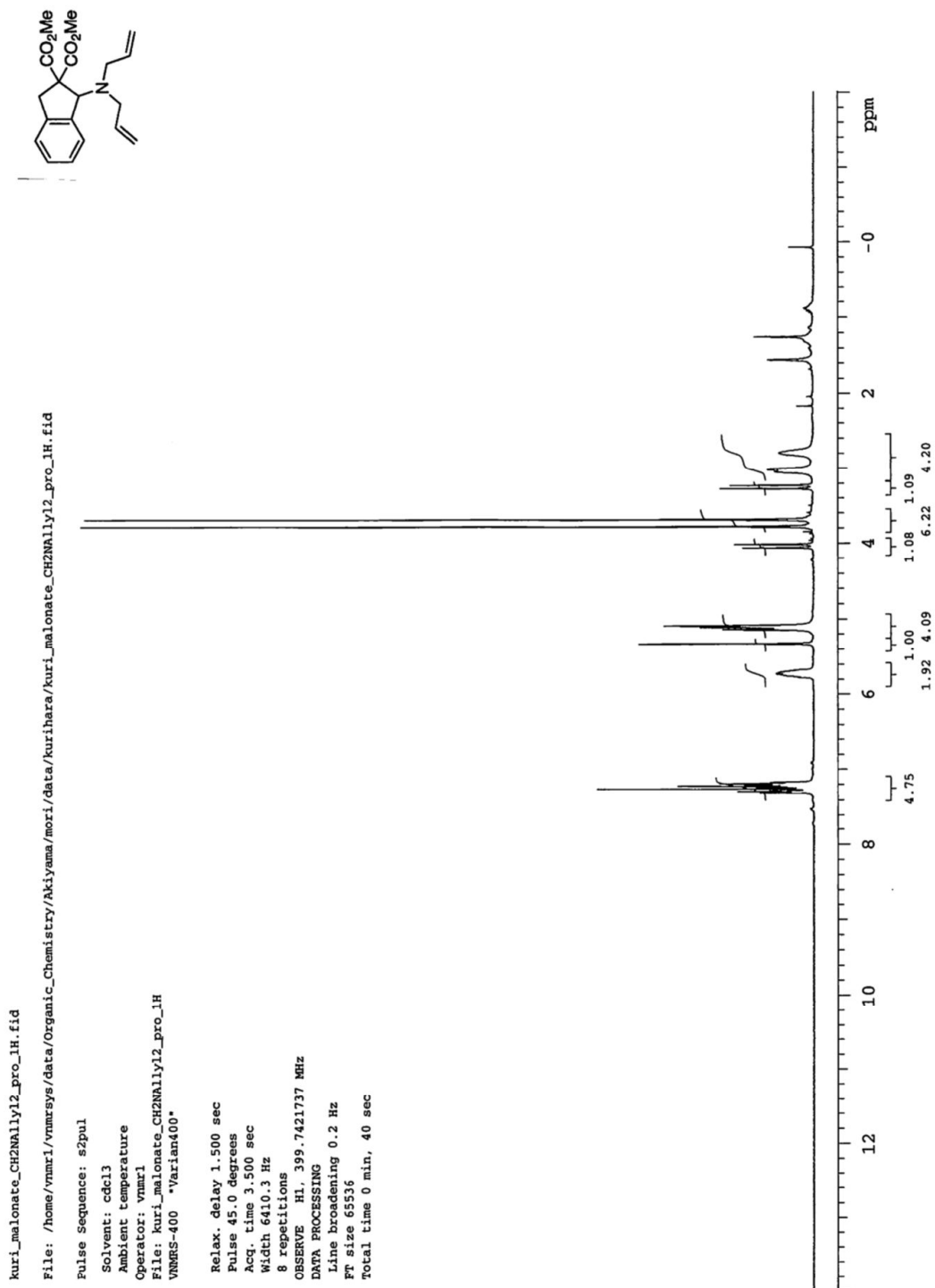
<sup>1</sup>H NMR spectrum of **4d**.



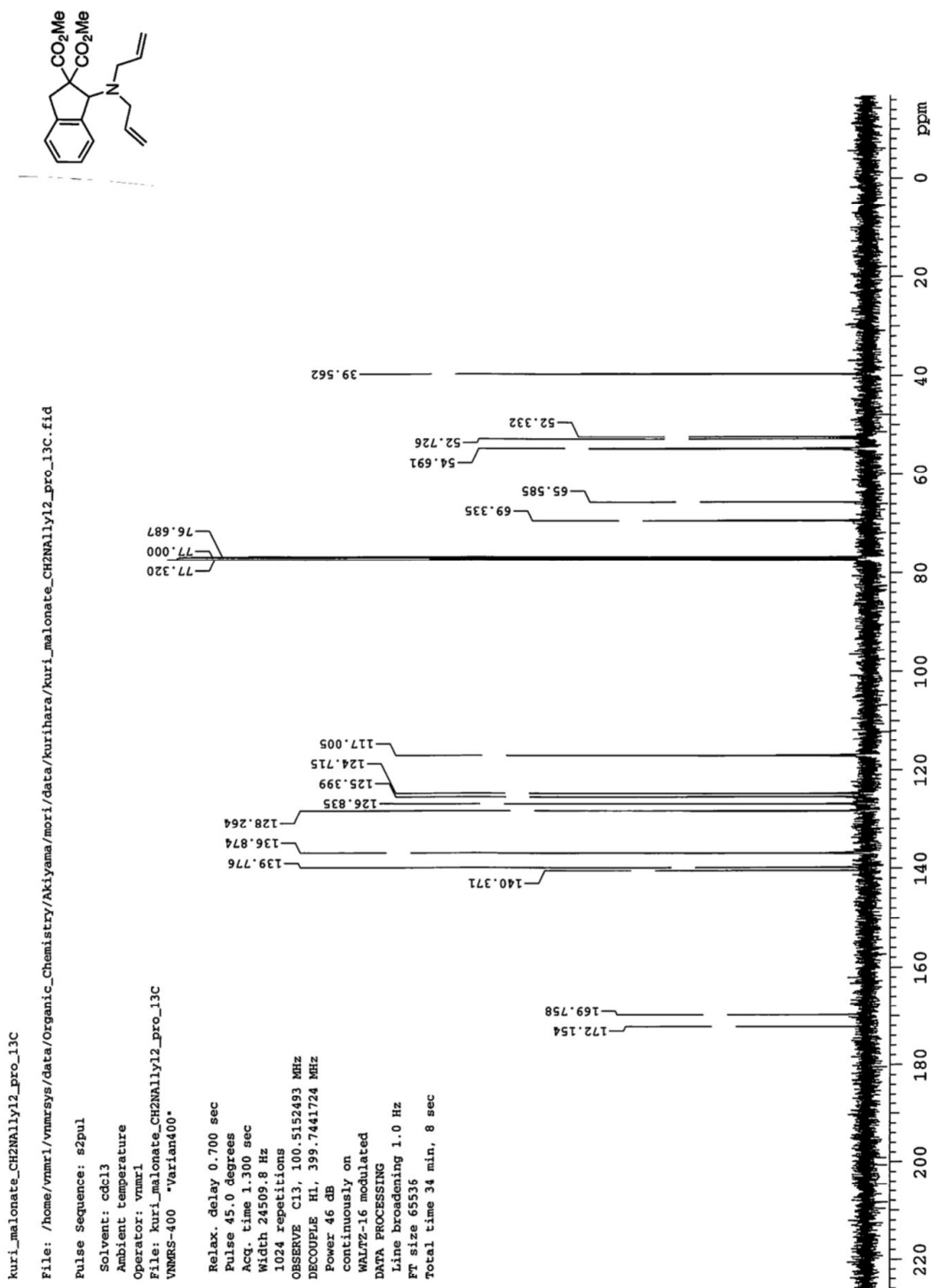
<sup>13</sup>C NMR spectrum of **4d**.



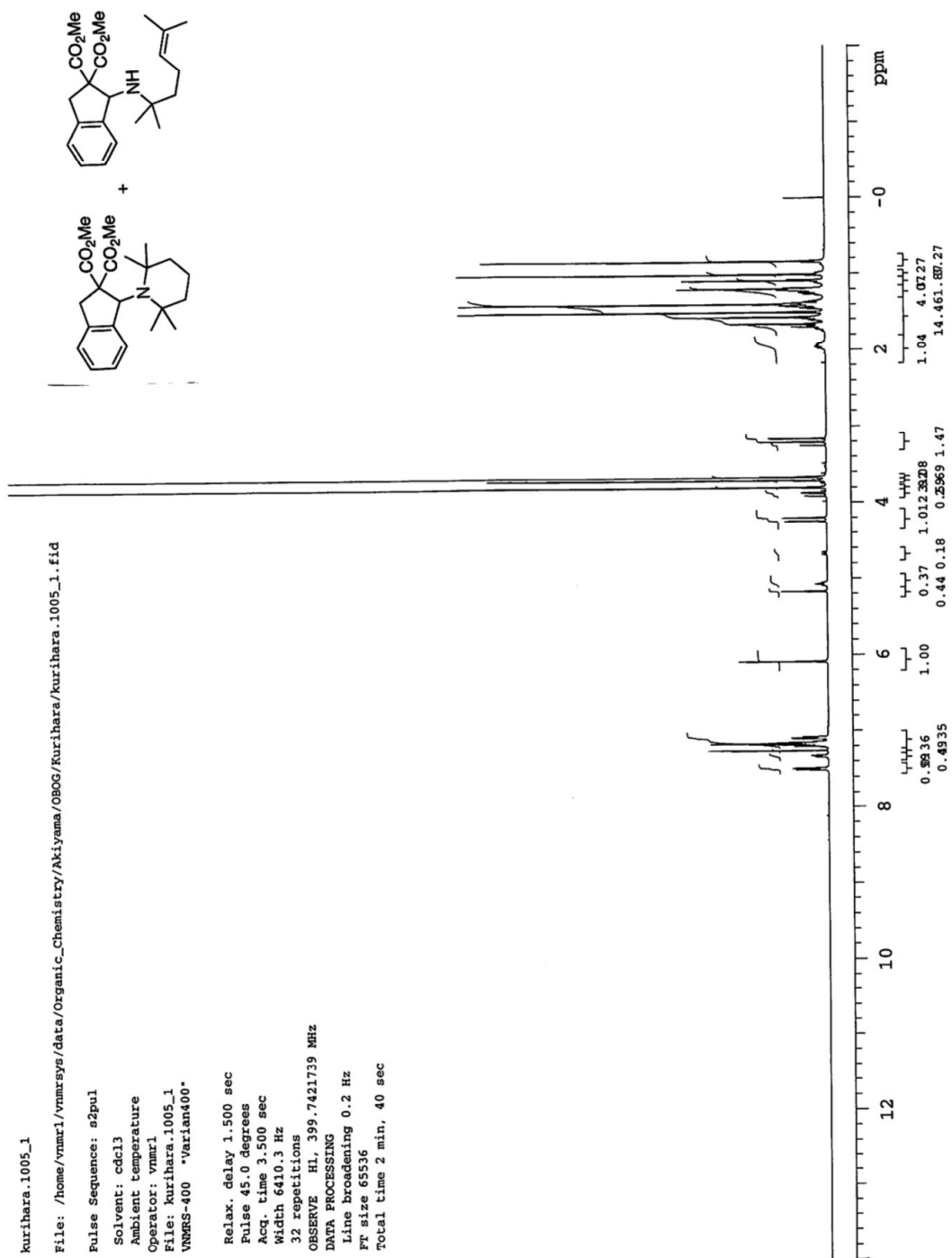
<sup>1</sup>H NMR spectrum of **4e**.



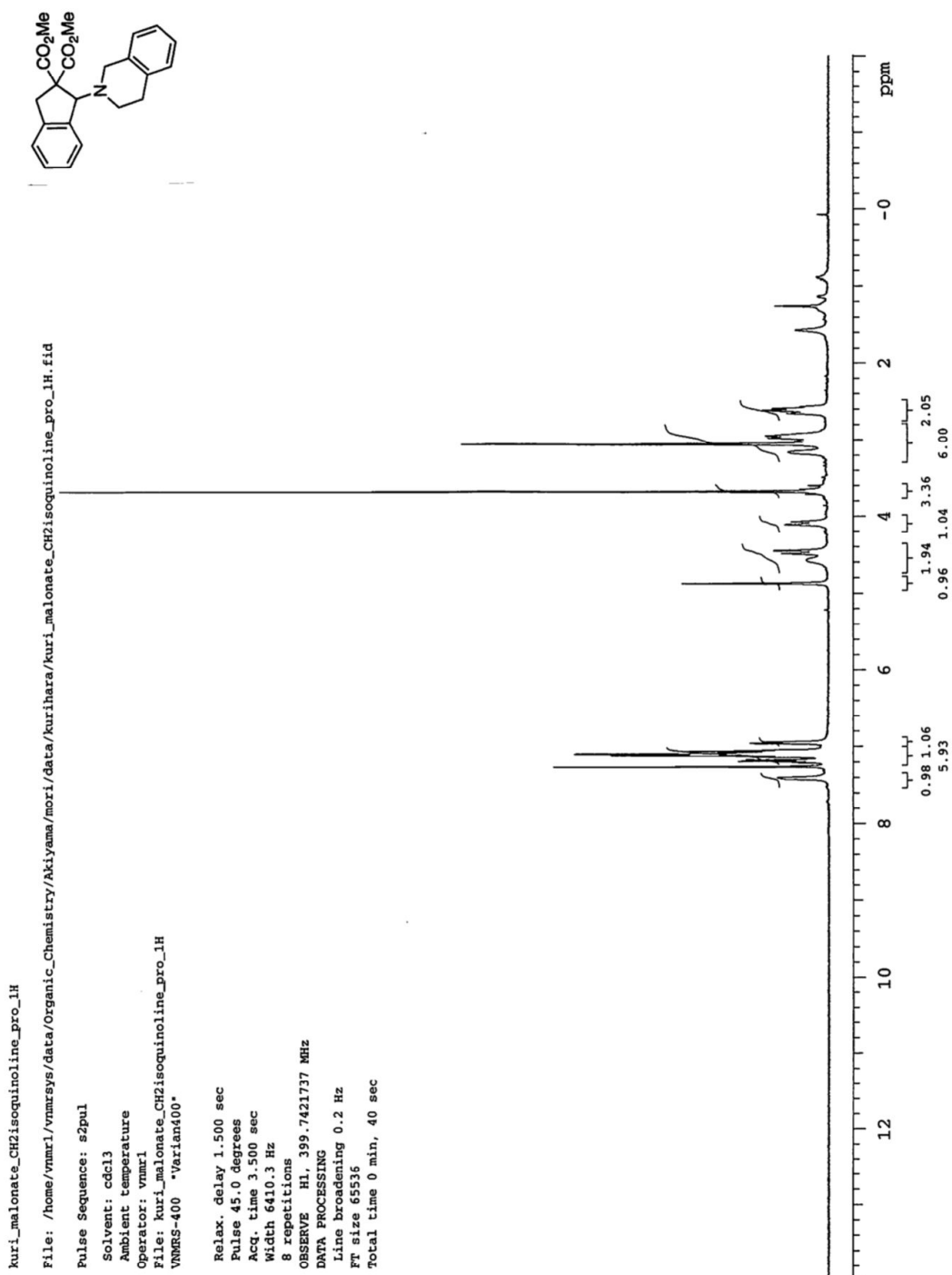
<sup>13</sup>C NMR spectrum of **4e**.



<sup>1</sup>H NMR spectrum of **4g+4h**.

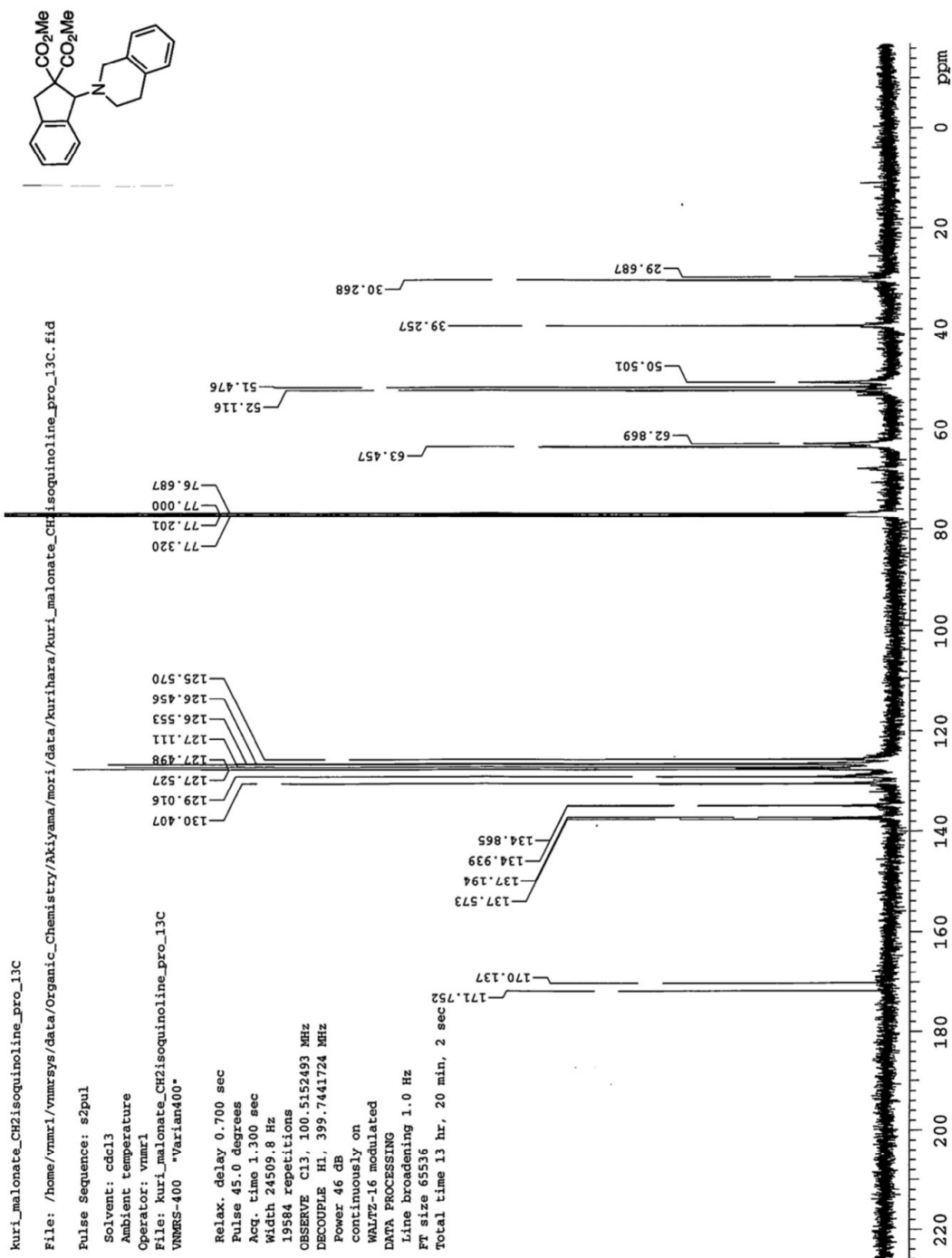


<sup>1</sup>H NMR spectrum of **4i**.

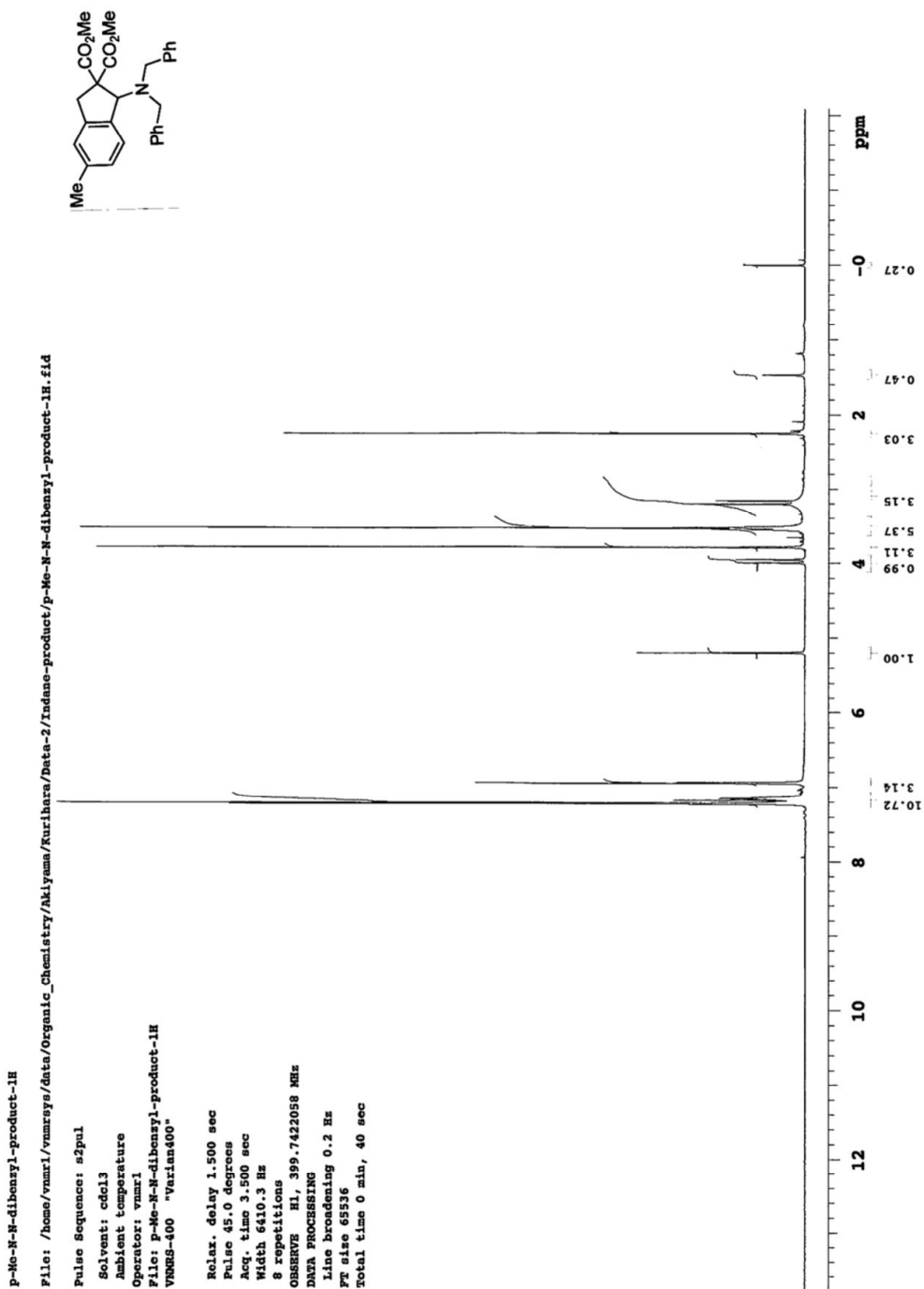




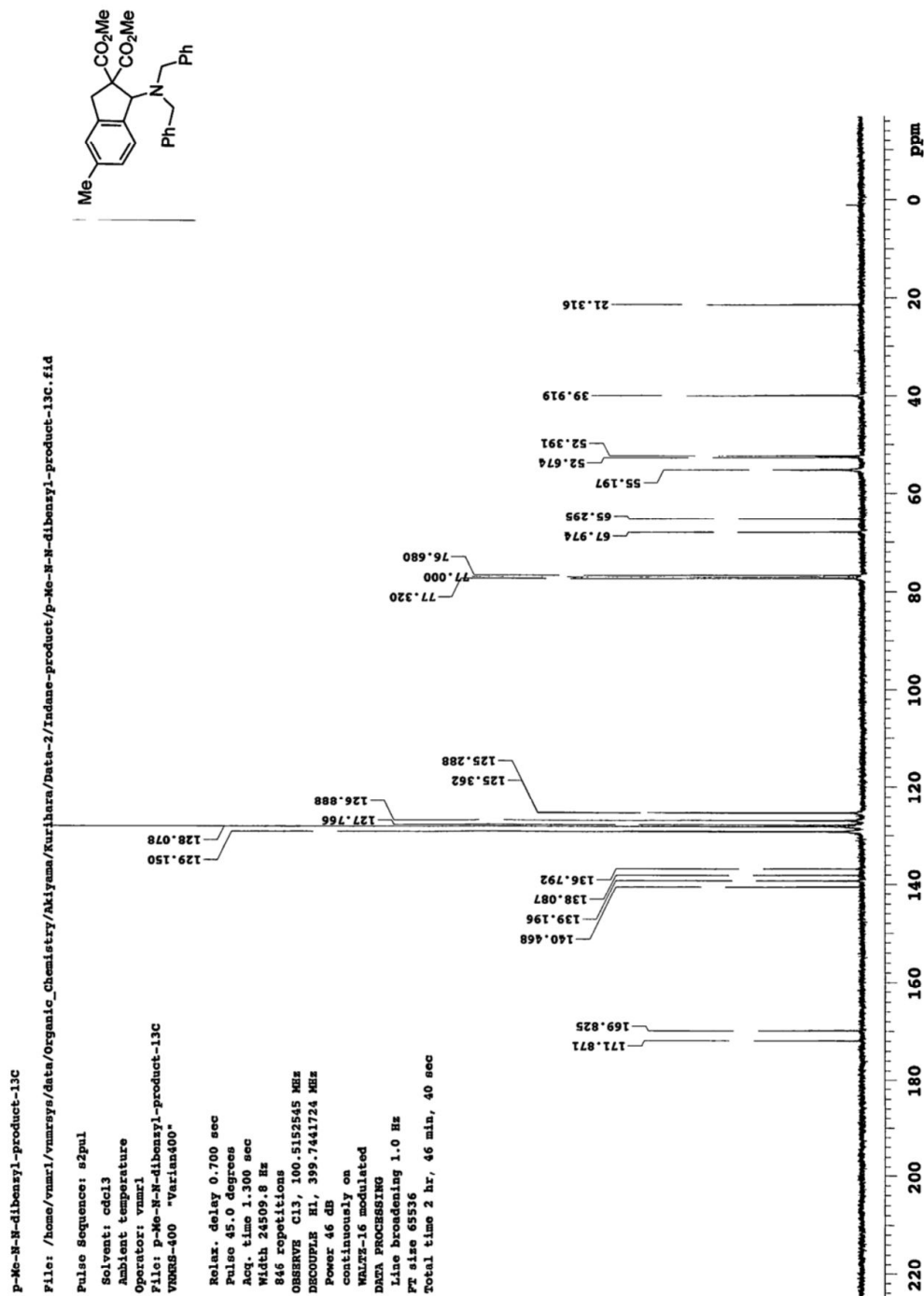
<sup>13</sup>C NMR spectrum of **4i**.



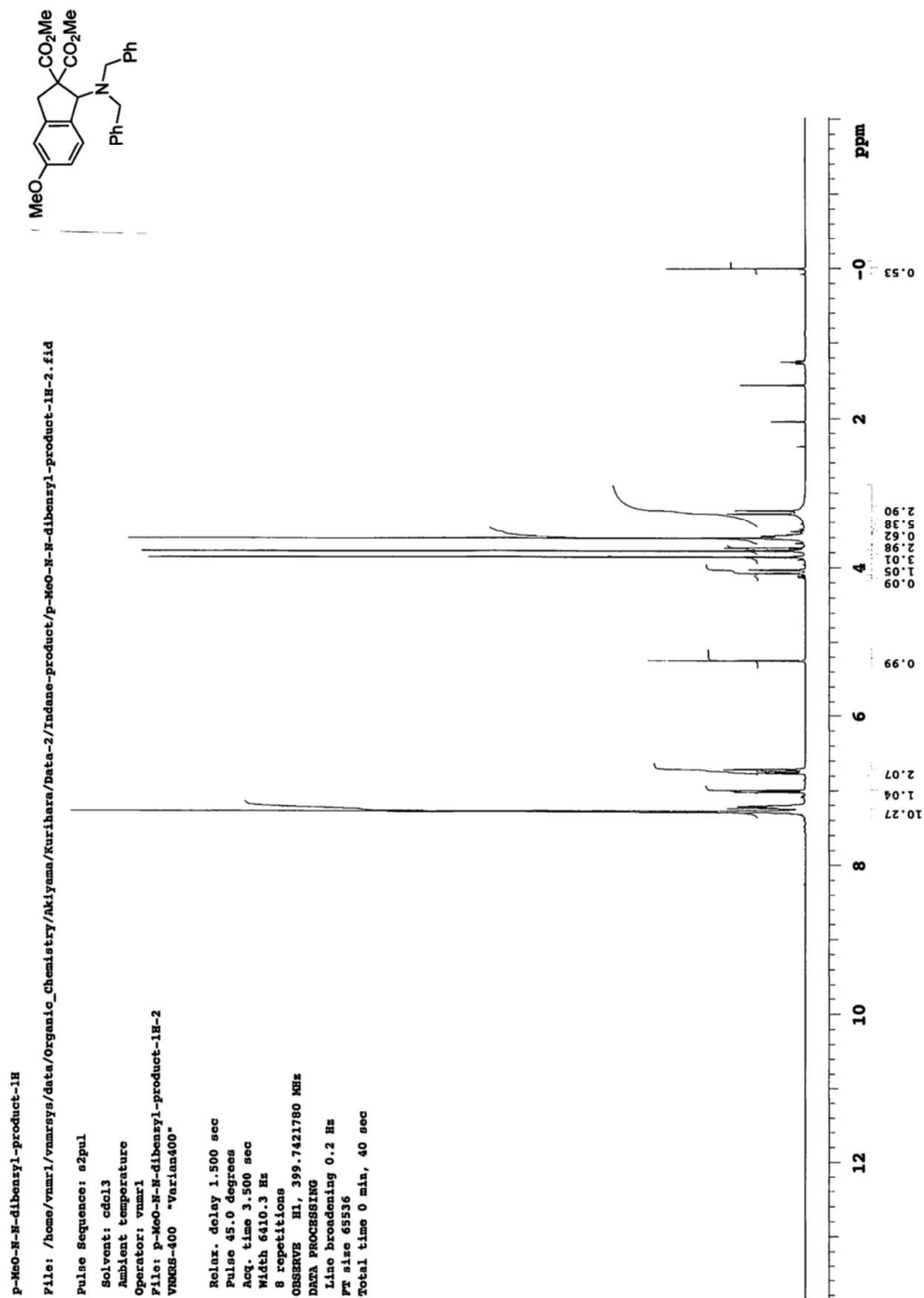
<sup>1</sup>H NMR spectrum of **4j**.



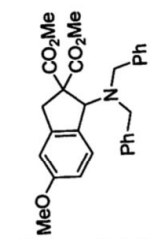
<sup>13</sup>C NMR spectrum of 4j.



<sup>1</sup>H NMR spectrum of **4k**.



$^{13}\text{C}$  NMR spectrum of **4k**.



p-MeO-N,N-dibenzyl-product-13c  
 File: /home/vmar1/vmar1s/data/Organic\_chemistry/Akiyama/Kurihara/Data-2/Todane-product/p-MeO-N,N-dibenzyl-product-13c.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: vmar1

File: p-MeO-N,N-dibenzyl-product-13c

VNMR-600 -Varian600-

Relax. delay 0.700 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24509.8 Hz

259 repetitions

OBSERVE C13, 100.5152553 MHz

DECOUPLE H1, 399.7441724 MHz

Power 46 dB

continually on

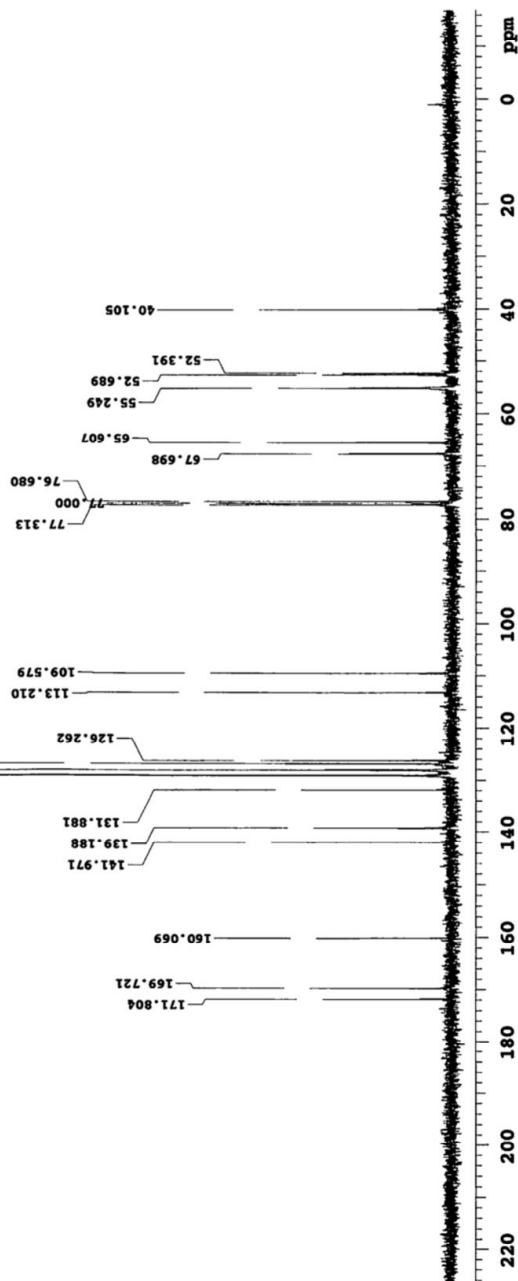
WALTZ-16 modulated

DATA PROCESSING

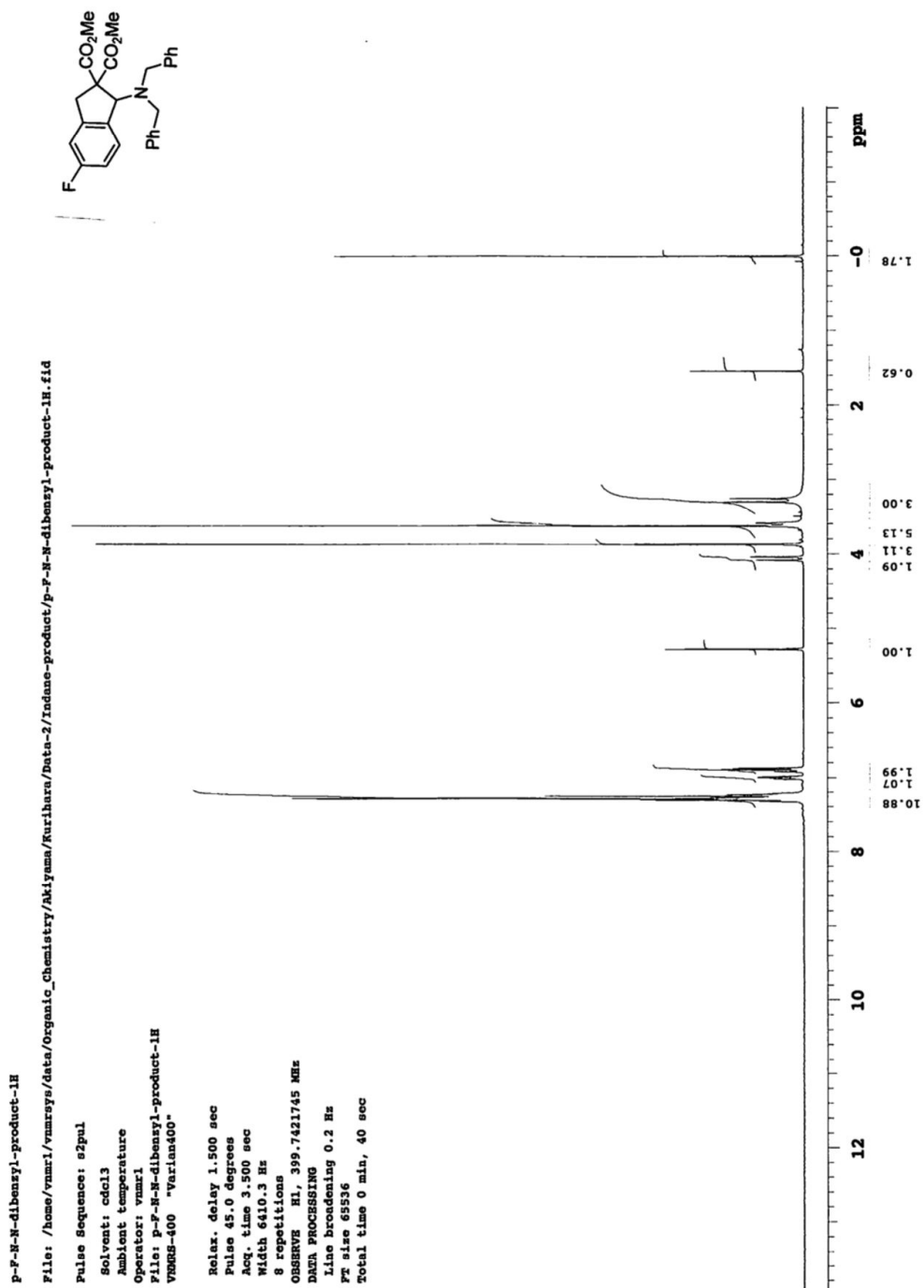
Line broadening 1.0 Hz

FT size 65536

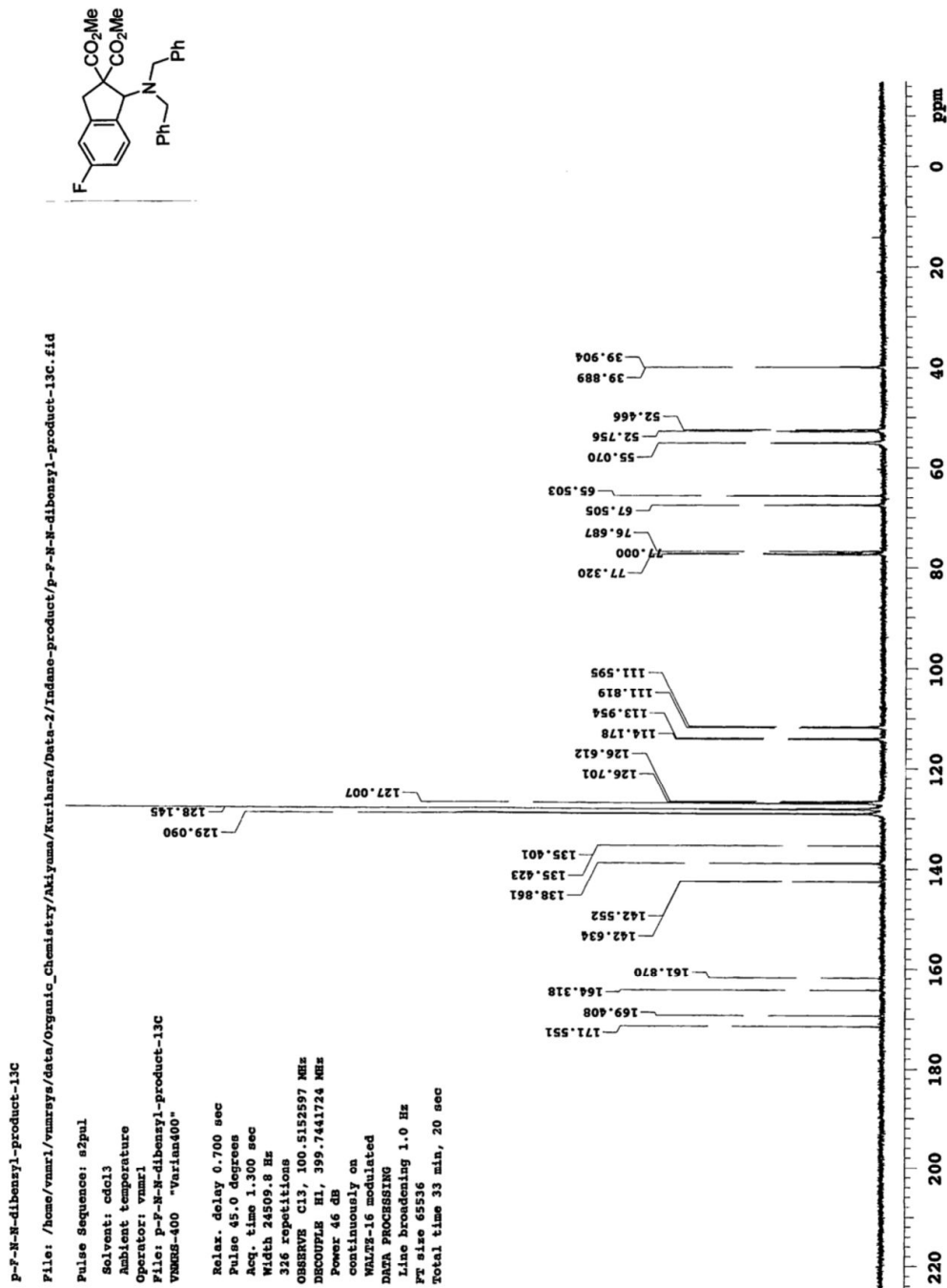
Total time 17 min, 4 sec



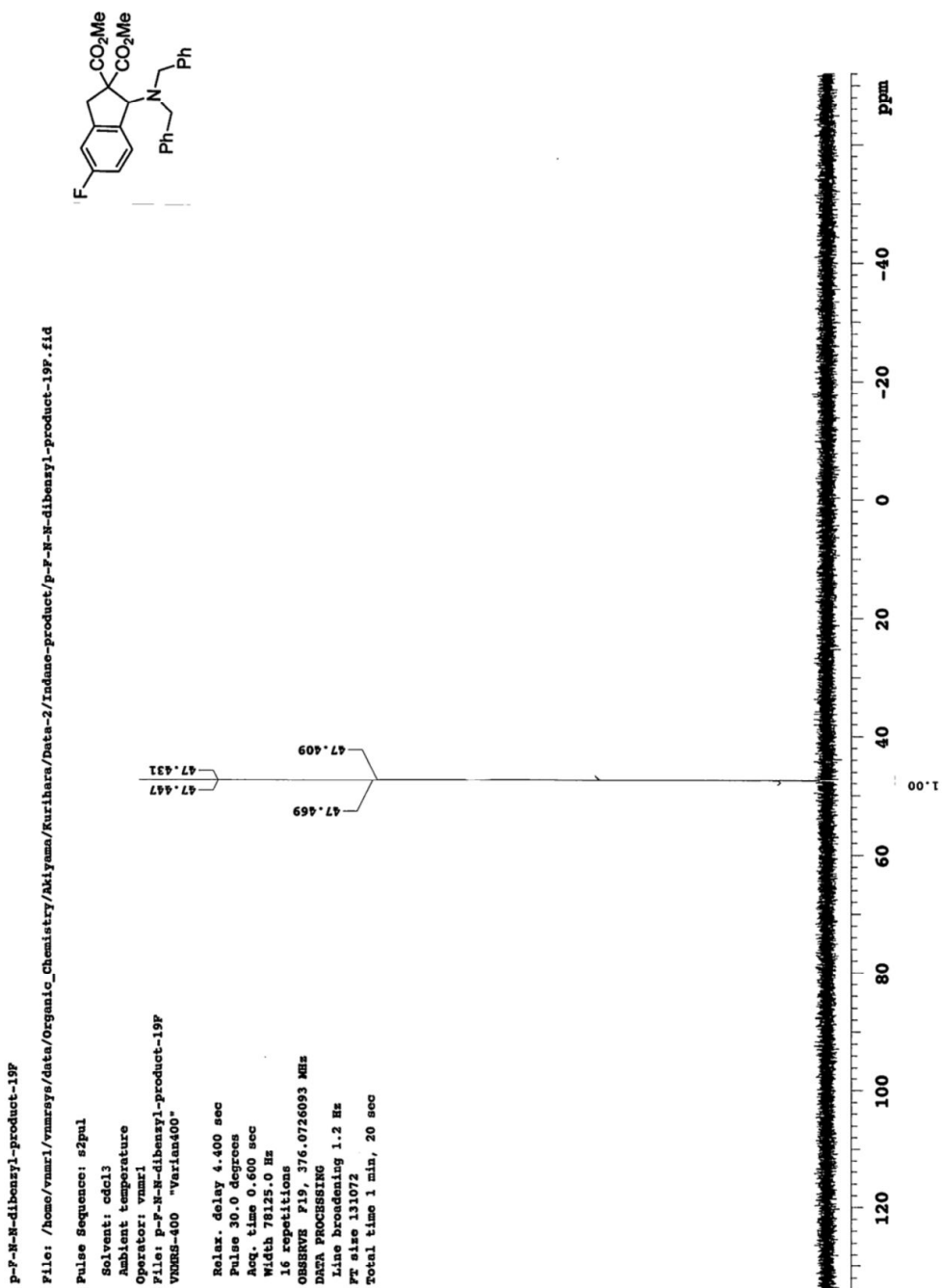
<sup>1</sup>H NMR spectrum of **4l**.



<sup>13</sup>C NMR spectrum of **4l**.

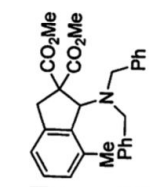


<sup>19</sup>F NMR spectrum of **4l**.





<sup>1</sup>H NMR spectrum of **4m**.



o-Me-N-N-dibenzyl-product-1H  
File: /home/vmar1/vmarsys/data/Organic\_chemistry/Akiyama/Kurihara/Data-2/Indunc-product/o-Me-N-N-dibenzyl-product-1H.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: vmar1

File: o-Me-N-N-dibenzyl-product-1H  
VNMRS-400 "Varian400"

Relax. delay 1.500 sec

Pulse 45.0 degrees

Acq. time 3.500 sec

Width 6410.3 Hz

8 repetitions

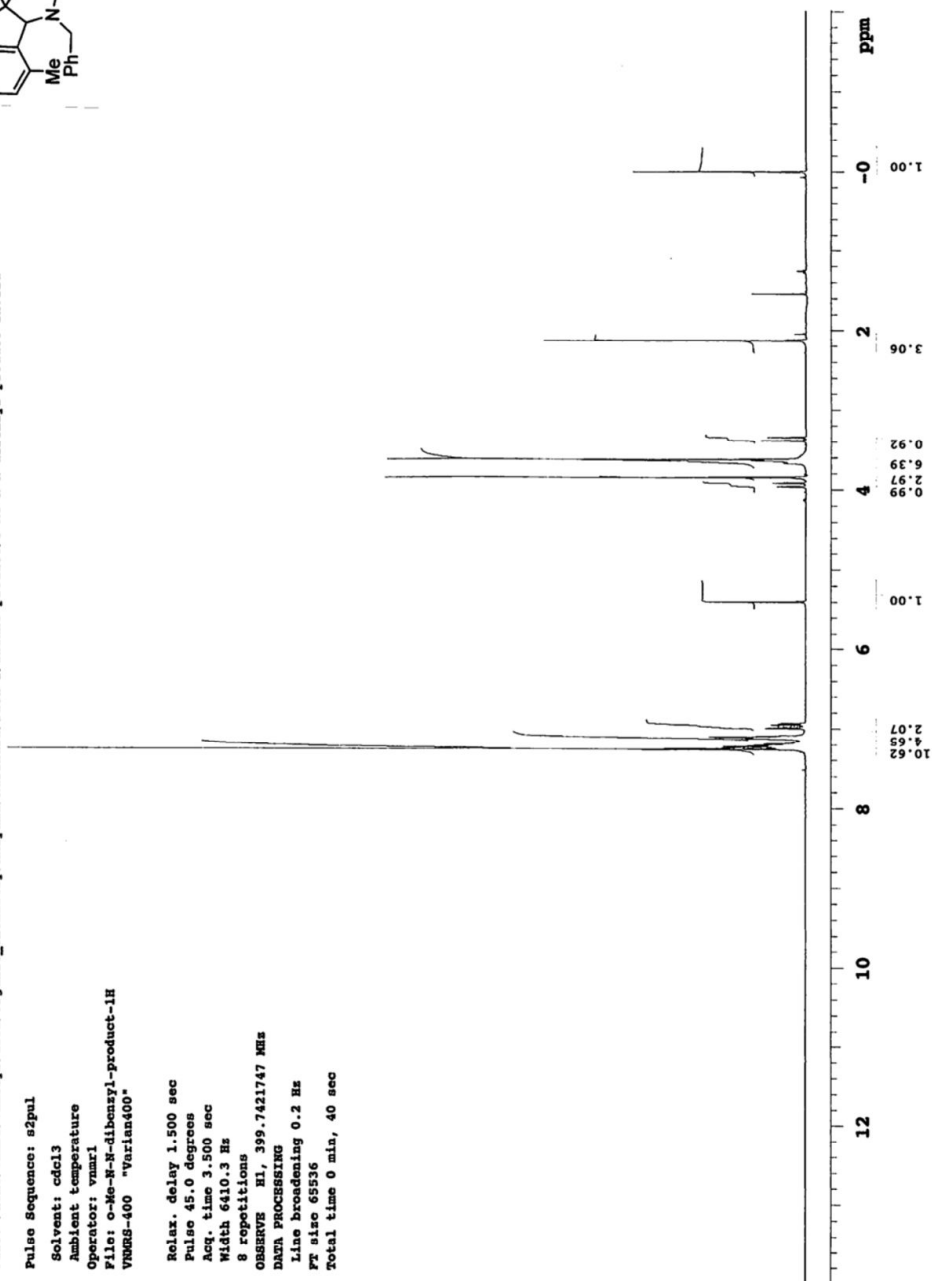
OBSERVE F1, 399.7421747 MHz

DATA PROCESSING

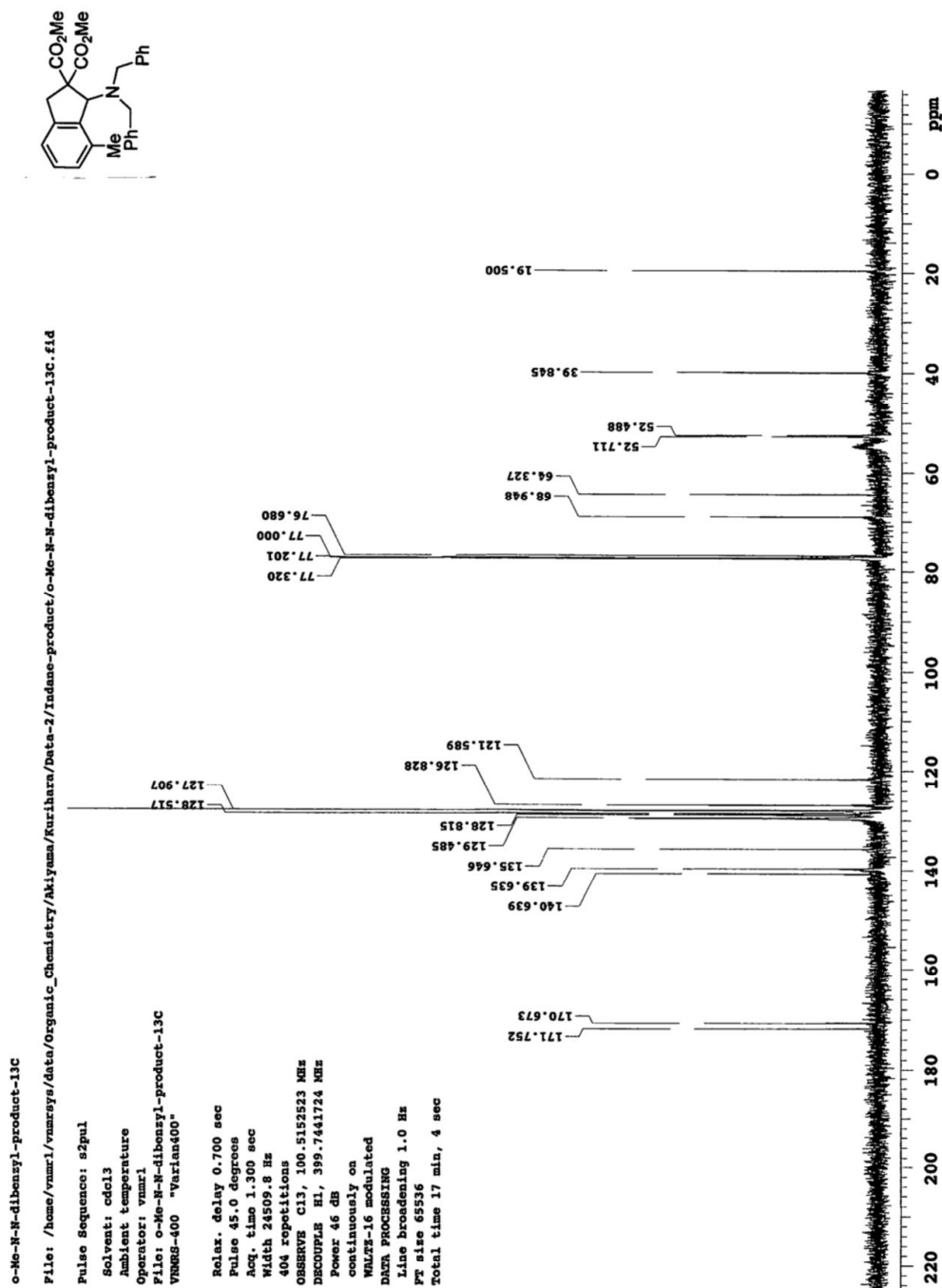
Line broadening 0.2 Hz

FT size 65536

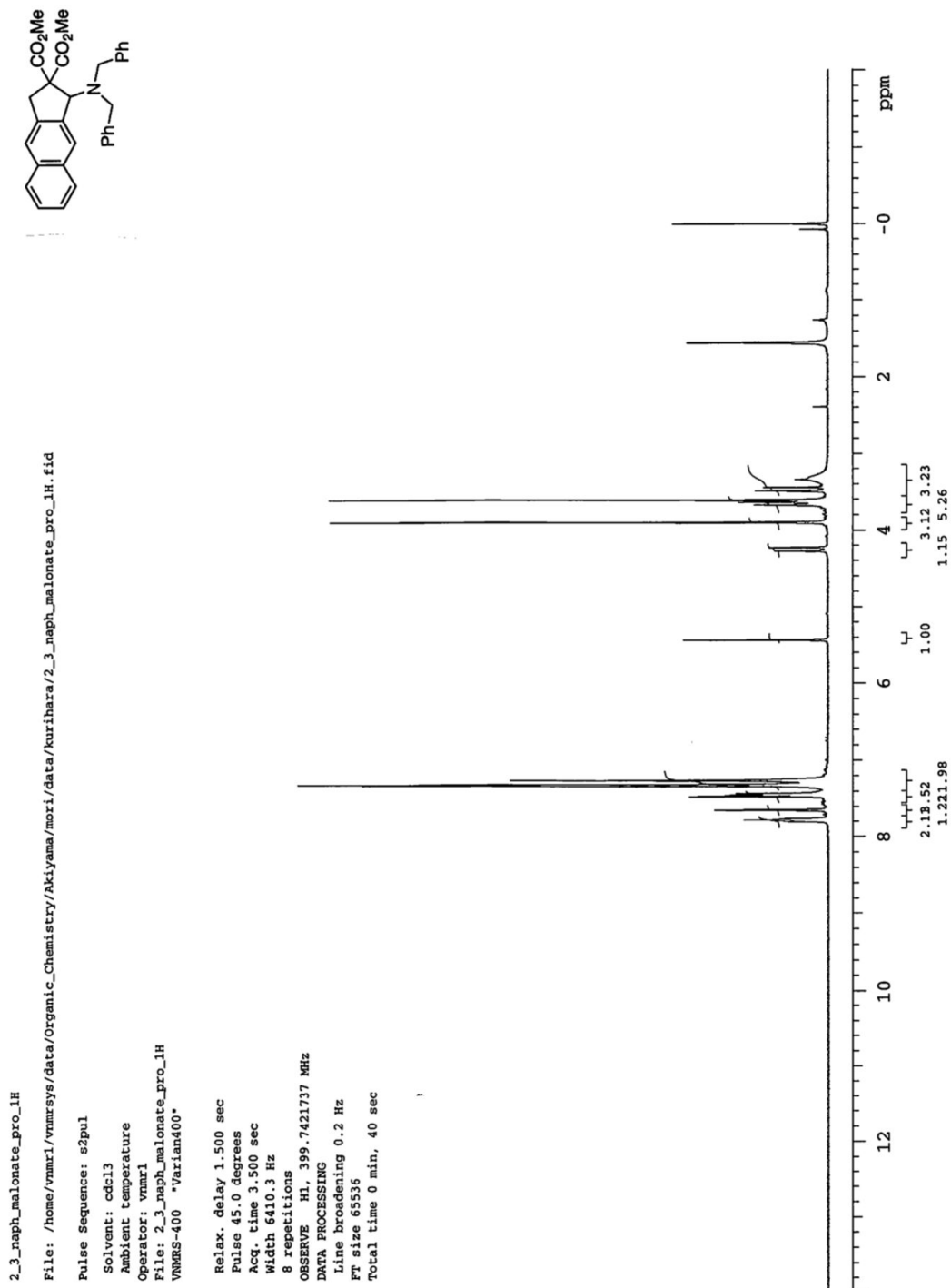
Total time 0 min, 40 sec



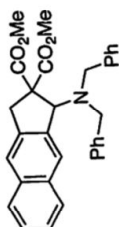
$^{13}\text{C}$  NMR spectrum of **4m**.



<sup>1</sup>H NMR spectrum of **4n**.



$^{13}\text{C}$  NMR spectrum of **4n**.



File: /home/vnmr1/vnmrSYS/data/Organic\_Chemistry/Akiyama/OB06/Kurihara/Data-2/Indane-product/2-3-naph-2-N-diphenyl-product-13c.fid

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Operator: vnmr1

File: 2-3-naph-2-N-diphenyl-product-13c

VNMR-400 \*varian400\*

Relax. delay 0.700 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 24509.8 Hz

150 repetitions

OBSERVE C13, 100.5152590 MHz

DECOUPLE H1, 399.7441724 MHz

Power 46 dB

continuously on

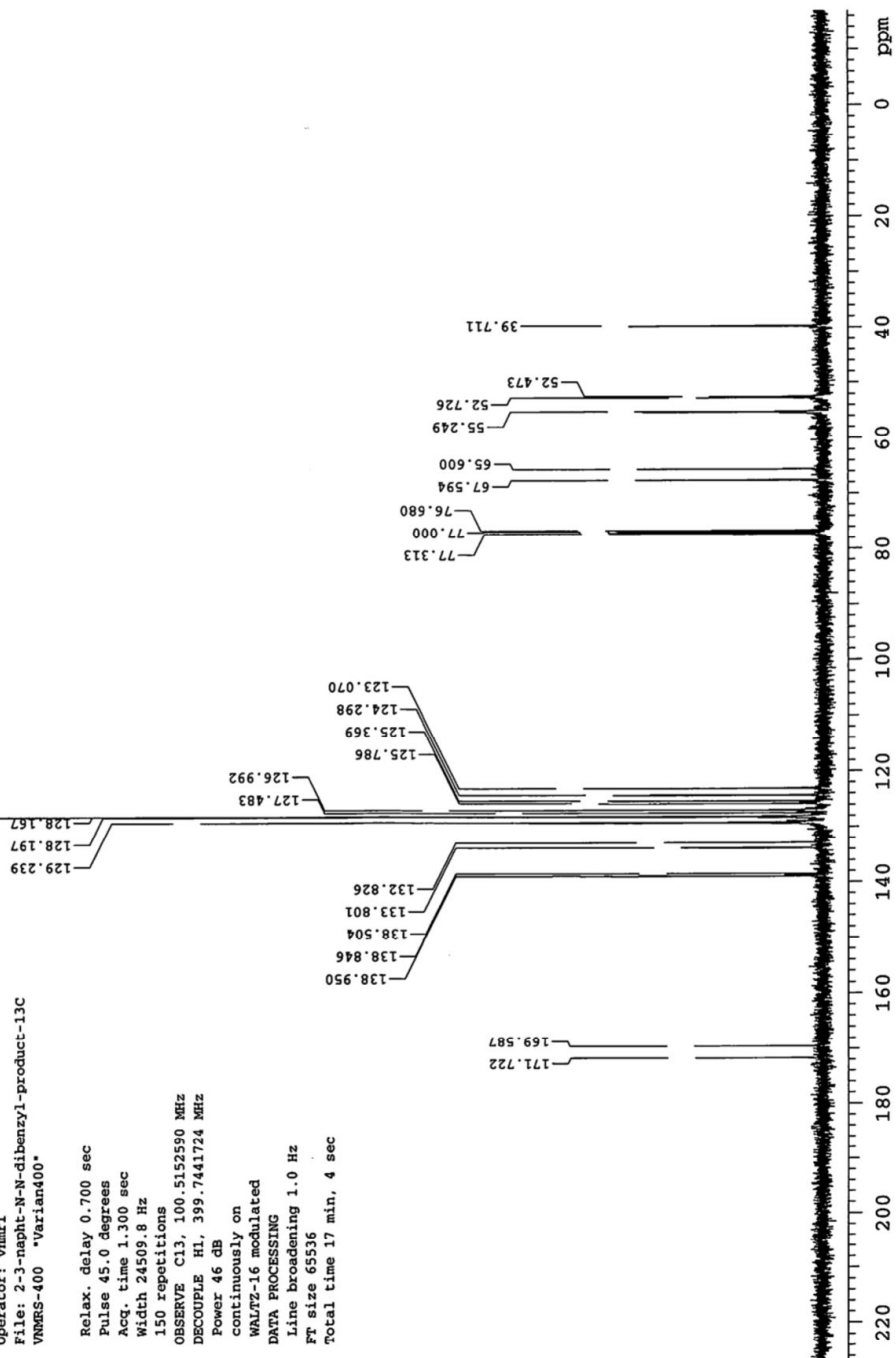
WALTZ-16 modulated

DATA PROCESSING

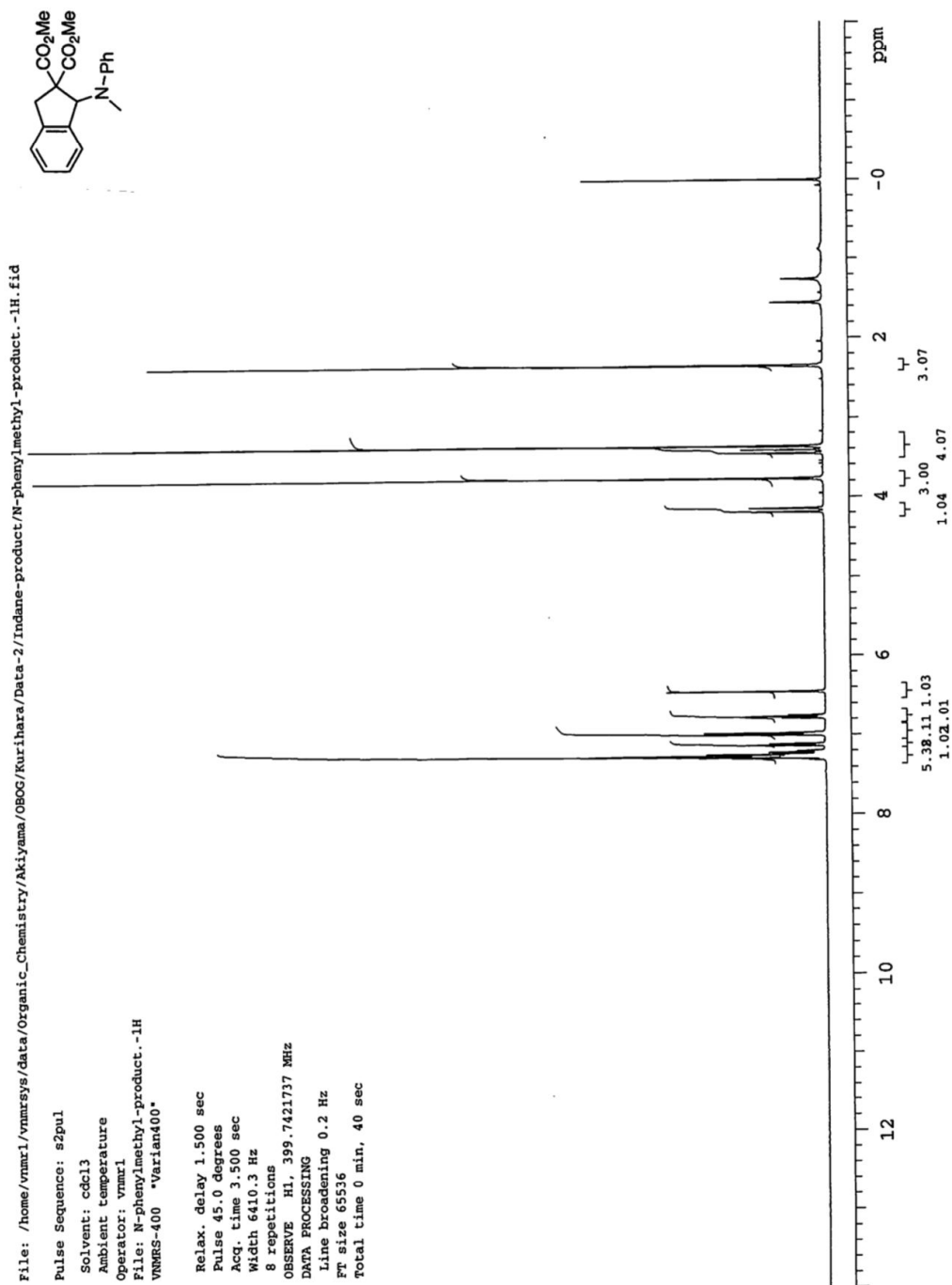
Line broadening 1.0 Hz

FT size 65536

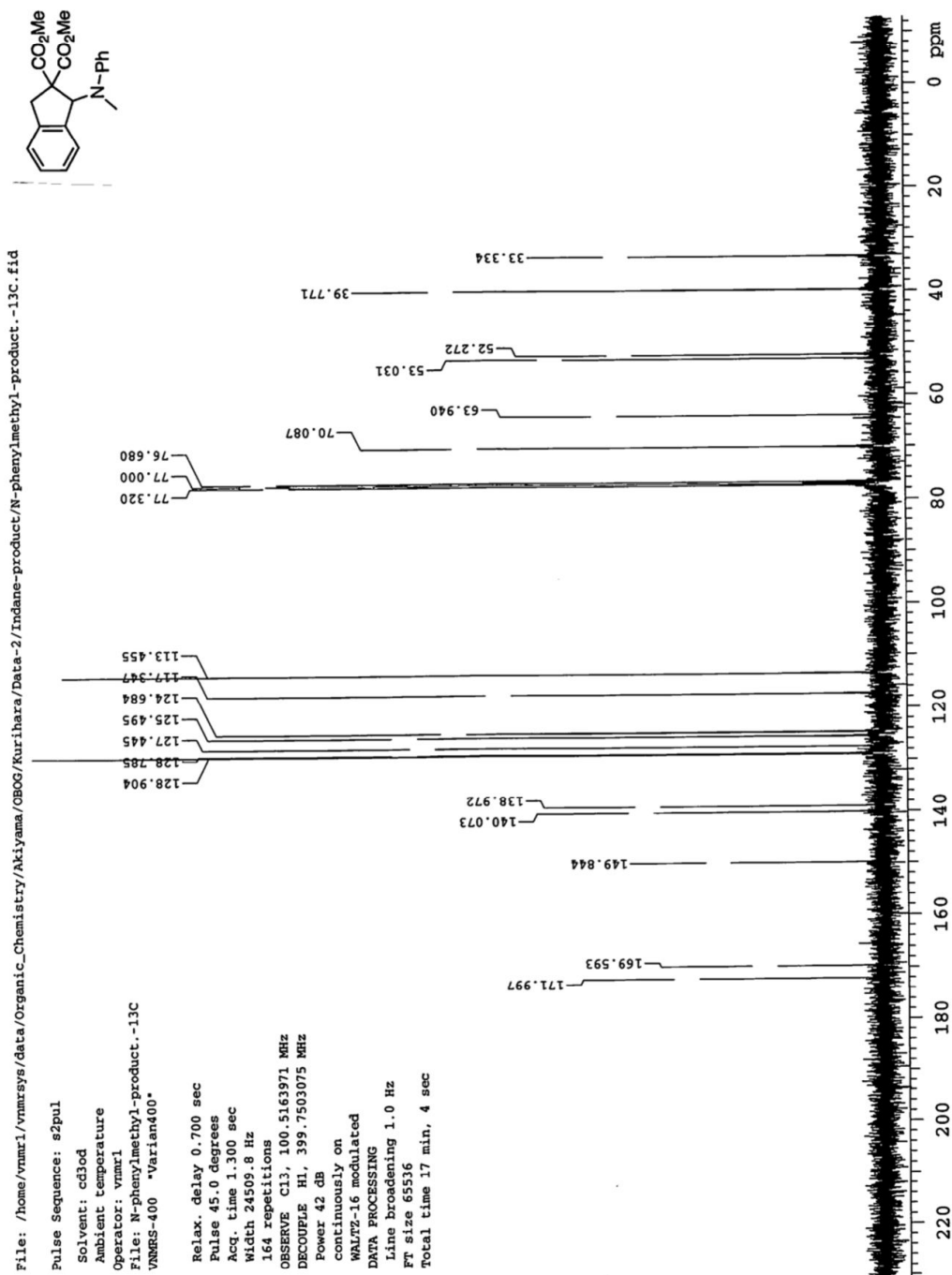
Total time 17 min, 4 sec



<sup>1</sup>H NMR spectrum of **4o**.



<sup>13</sup>C NMR spectrum of **40**.



<sup>1</sup>H NMR spectrum of 7.

