

Supporting Information

**Isolation and Characterization of Atropisomers of
Seven-Membered-Ring Benzolactams**

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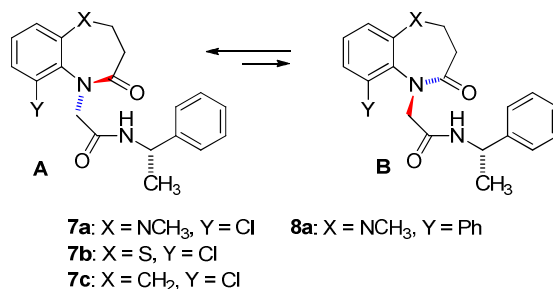
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1. General Remarks

NMR Spectra were recorded on a spectrometer at 400 MHz or 600 MHz for ¹H NMR, and 100 MHz or 150 MHz for ¹³C NMR. Chemical shifts are given in parts per million (ppm) downfield from tetramethylsilane as an internal standard and coupling constants (*J*) are reported in hertz (Hz). Splitting patterns are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), quintet (quin) and multiplet (m). The high resolution mass spectra (HRMS) were obtained with an ionization mode of ESI. Melting points were taken on a melting point apparatus and are uncorrected. Optical rotations were determined with a digital polarimeter. Analytical thin layer chromatography was performed on pre-coated, glass-backed silica gel plates. Column chromatography was performed using silica gel (45–60 μm). Extracted solutions were dried over anhydrous MgSO₄ or Na₂SO₄. Solvents were evaporated under reduced pressure.

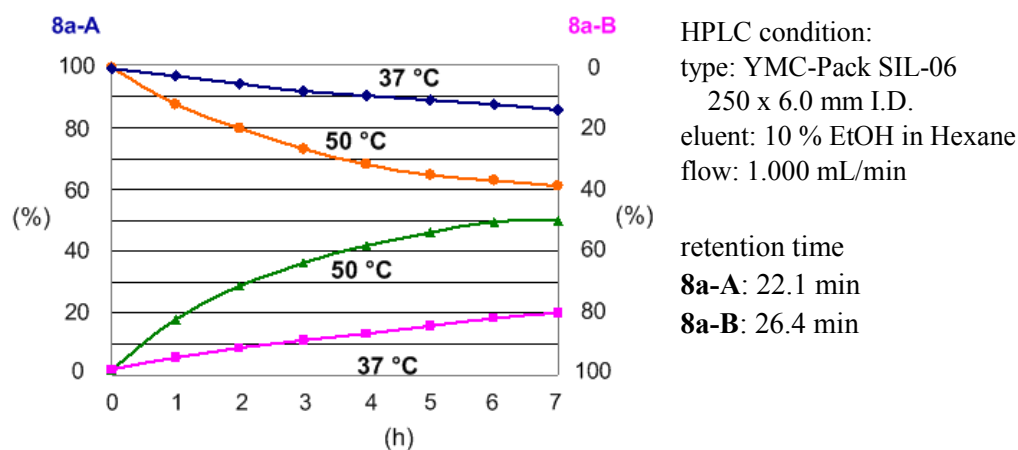
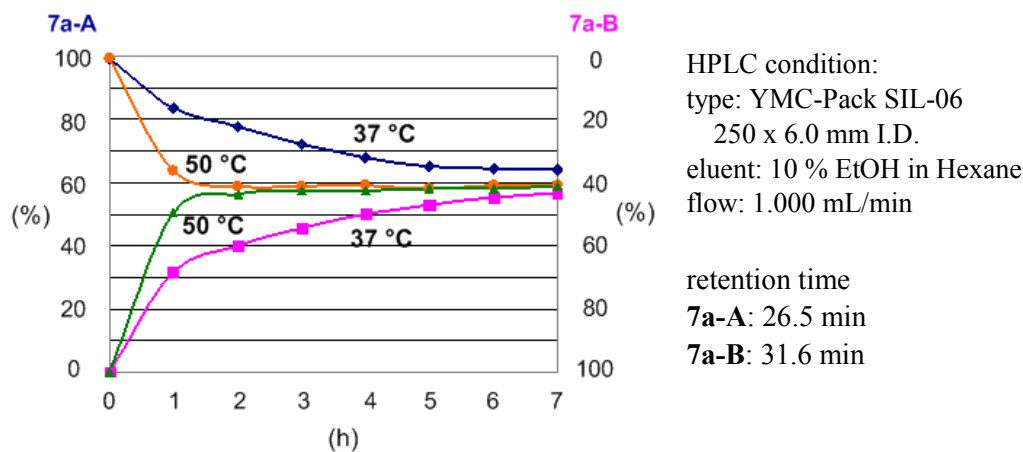
2. Stereochemical (Thermodynamic) Stability of Diastereomers

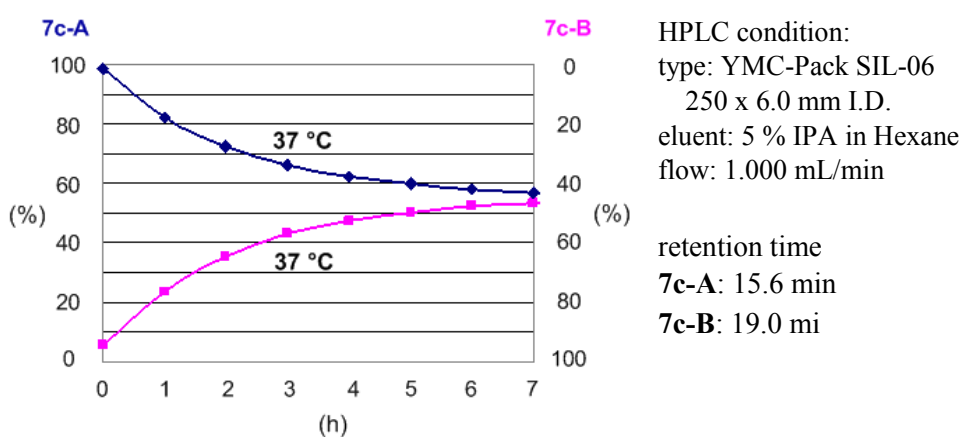
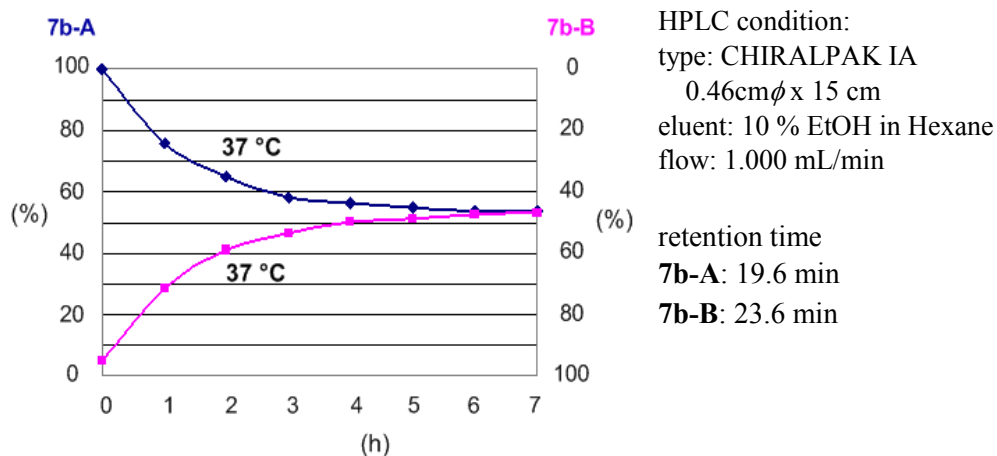
The ΔG^\ddagger values were determined according to the protocol reported for the literature: see ref. 17) in the main text.



Compd (axial chirality ^a)	ΔG^\ddagger kJ/mol	condition for isomerization ^b	equilibrium ratio (A:B)
7a-A (aR)	102.5	37 °C, 10 h ^c	1:0.7
B (aS)	99.4	37 °C, 8 h	
8a-A (aS)	106.9	50 °C, 14 h ^d	1:0.9
B (aR)	105.8	50 °C, 12 h ^e	
7b-A (aR)	100.8	37 °C, 8 h	1:0.9
B (aS)	99.2	37 °C, 7 h	
7c-A (aR)	101.9	37 °C, 9 h	1:0.8
B (aS)	99.8	37 °C, 8 h	

^a See, ref.14) in the main text. ^b To the equilibrium state in toluene. ^c At 50 °C, 2 h.
^d At 37 °C after 7 h, isomerized to 71 % de. ^e At 37 °C after 7 h, isomerized to 60 % de.

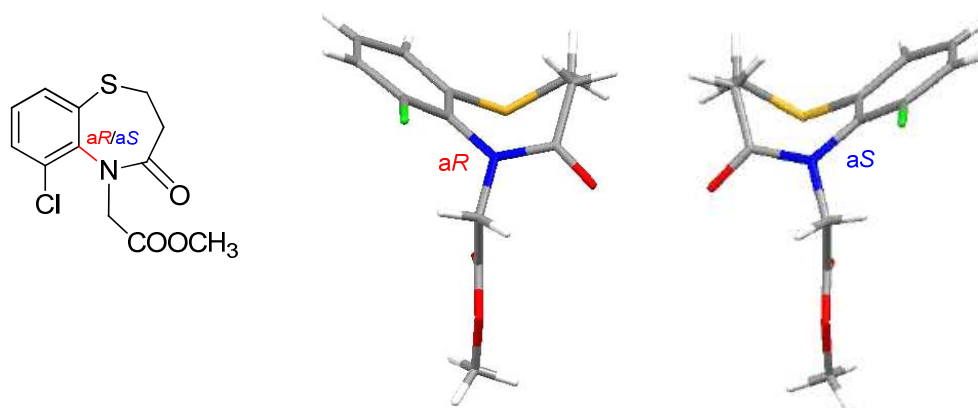




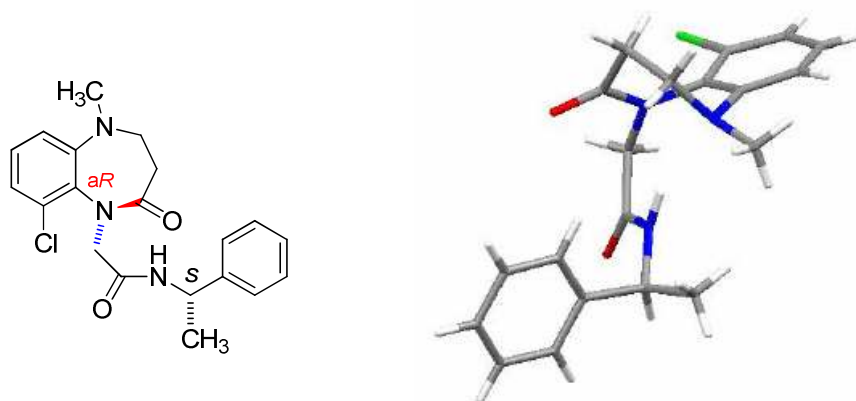
3. X-ray crystal structures of **5b**, **7a-A** (*aR,S*), **7a-B** (*aS,S*), **7b-A** (*aR,S*)

5b (racemate): (*aR*)-form (left) and (*aS*)-form (right) present in a unit cell.

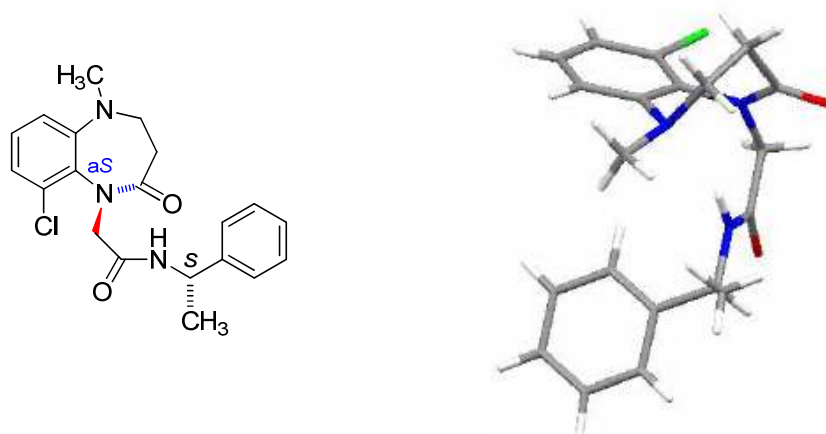
(note: Structure for **5b** is presented as Figure 4 in the manuscript)



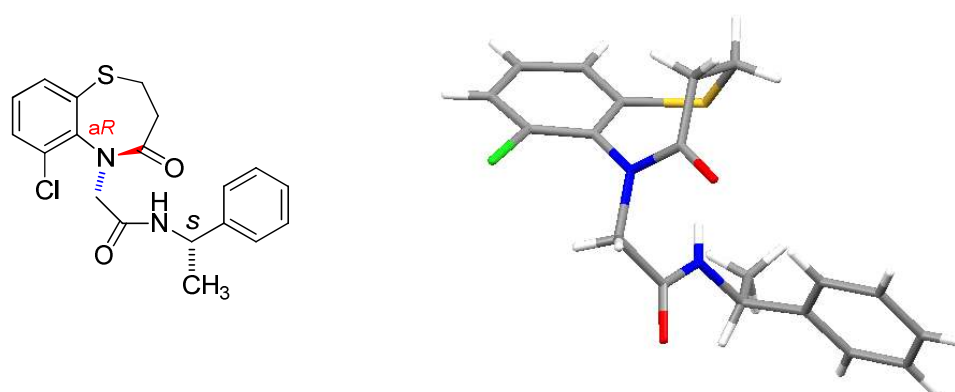
7a-A (aR,S): [note: Structure for **7a-A** is presented as Figure 5 (left) and in the manuscript and Table of Contents]



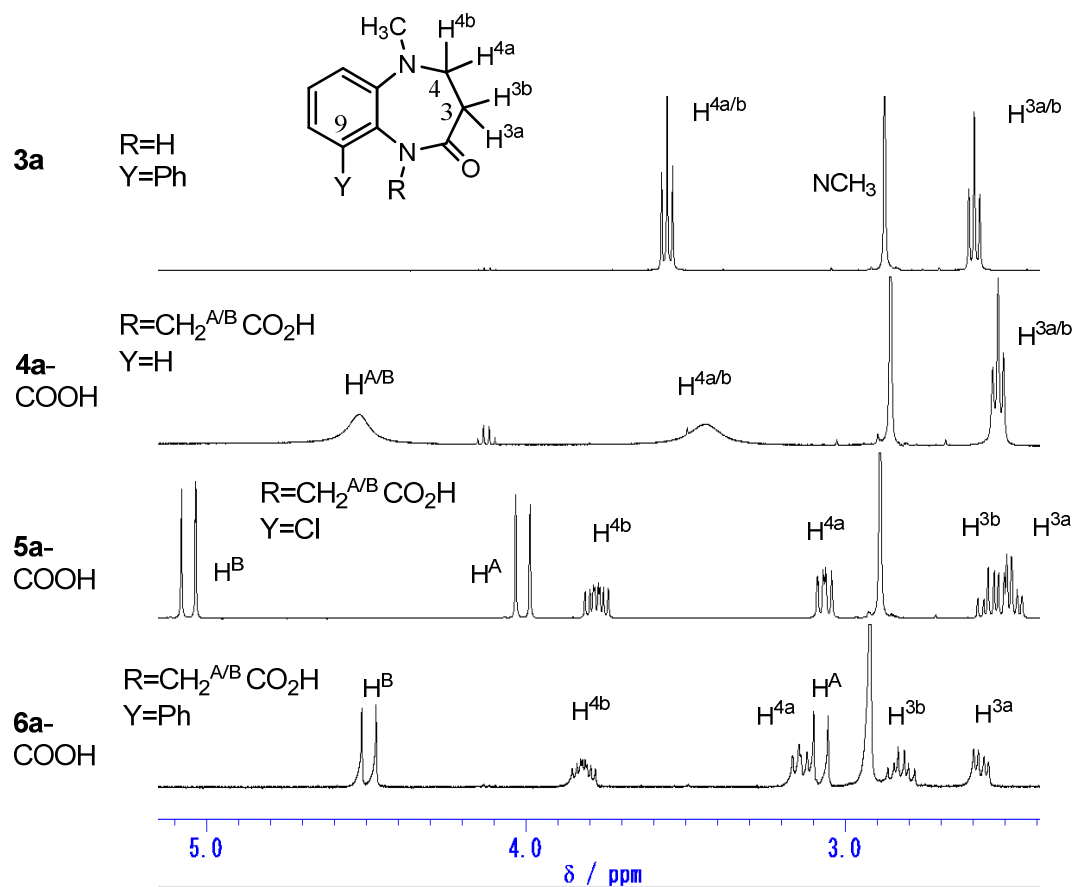
7a-B (aS,S): [note: Structure for **7a-B** is presented as Figure 5 (right) in the manuscript and Table of Contents]



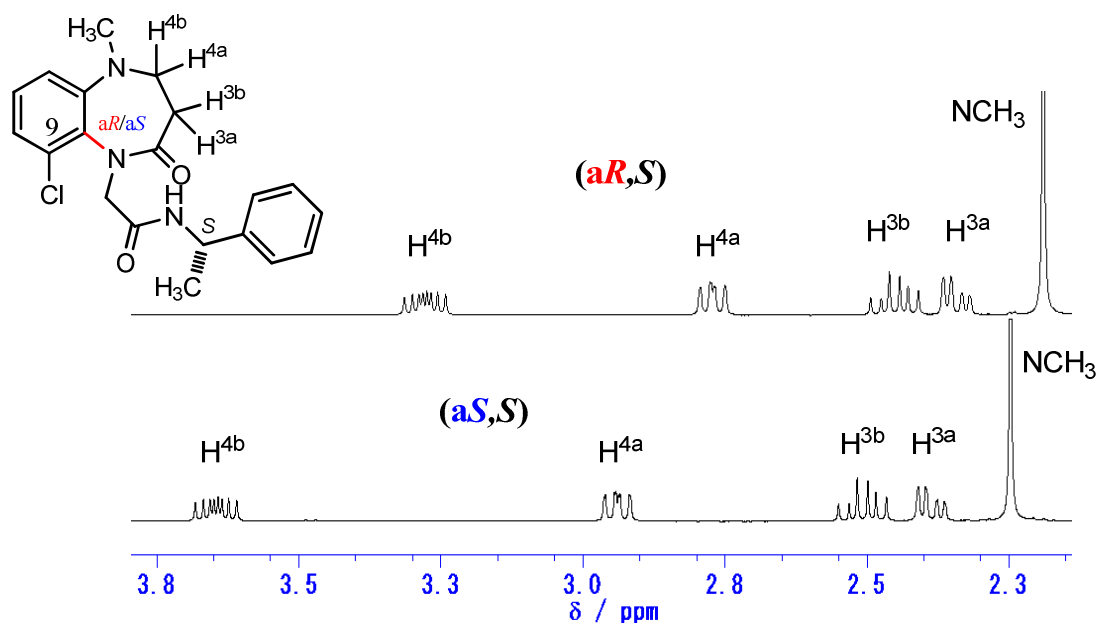
7b-A (aR,S): [note: Structure for **7b-A** is presented as Figure 7 in the manuscript]



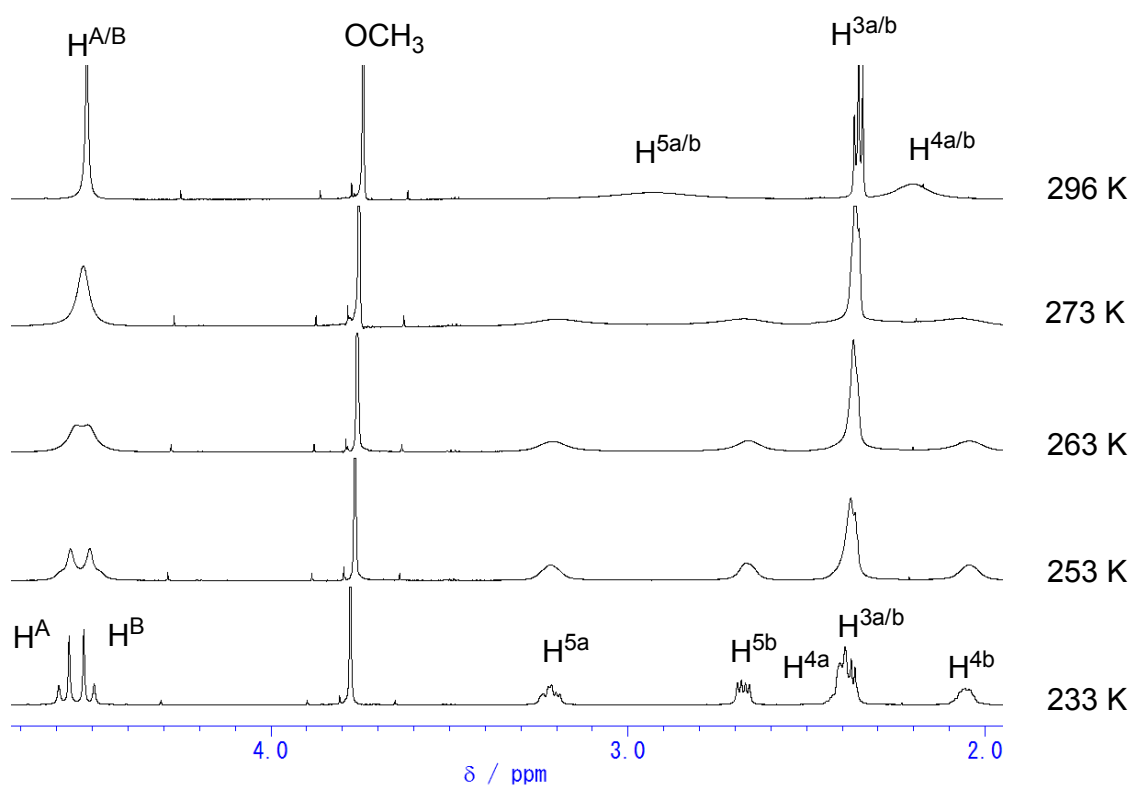
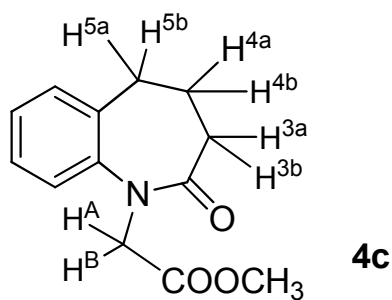
4. ^1H NMR spectra (magnified) of 3a, 4a-COOH, 5a-COOH, and 6a-COOH (400 MHz, CDCl_3)
(note: This chart is presented as Figure 3 in the manuscript)



5. ^1H NMR spectra (magnified) of 7a-A (aR,S) (upper) and 7a-B (aS,S) (lower) (400 MHz, CDCl_3)
(note: This chart is presented as Figure 6 in the manuscript)



6. Temperature dependence of the ^1H NMR signals of **4c** (600 MHz, CDCl_3)

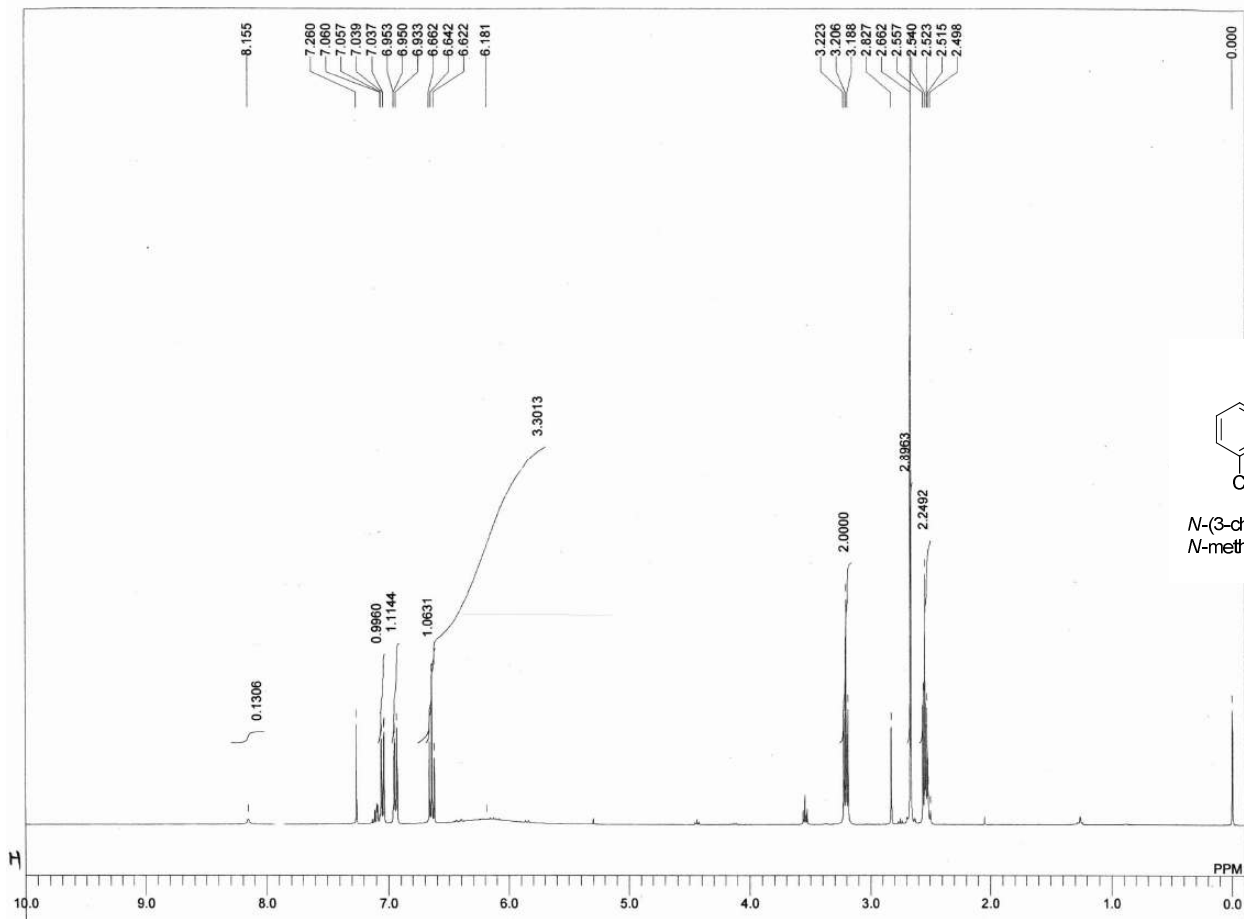


$$\Delta G^\ddagger = 56.3 \text{ kJ/mol}^*$$

$$T_c = 273 \text{ K}$$

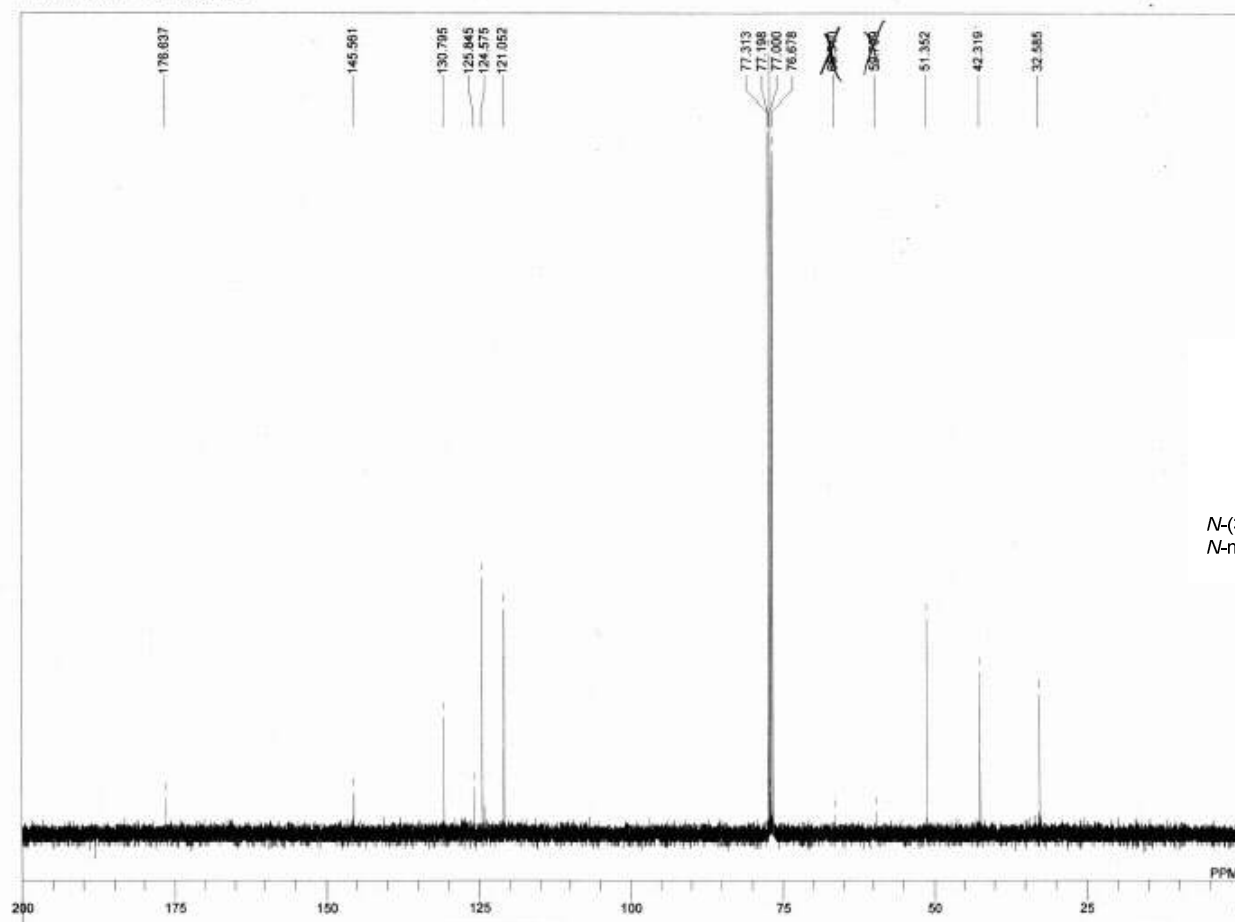
* determined by the method reported by Boiadjev et al.,
lit. Boiadjev, S. E.; Lightner, D. A. *Tetrahedron* **2002**, 58, 7411–7421.

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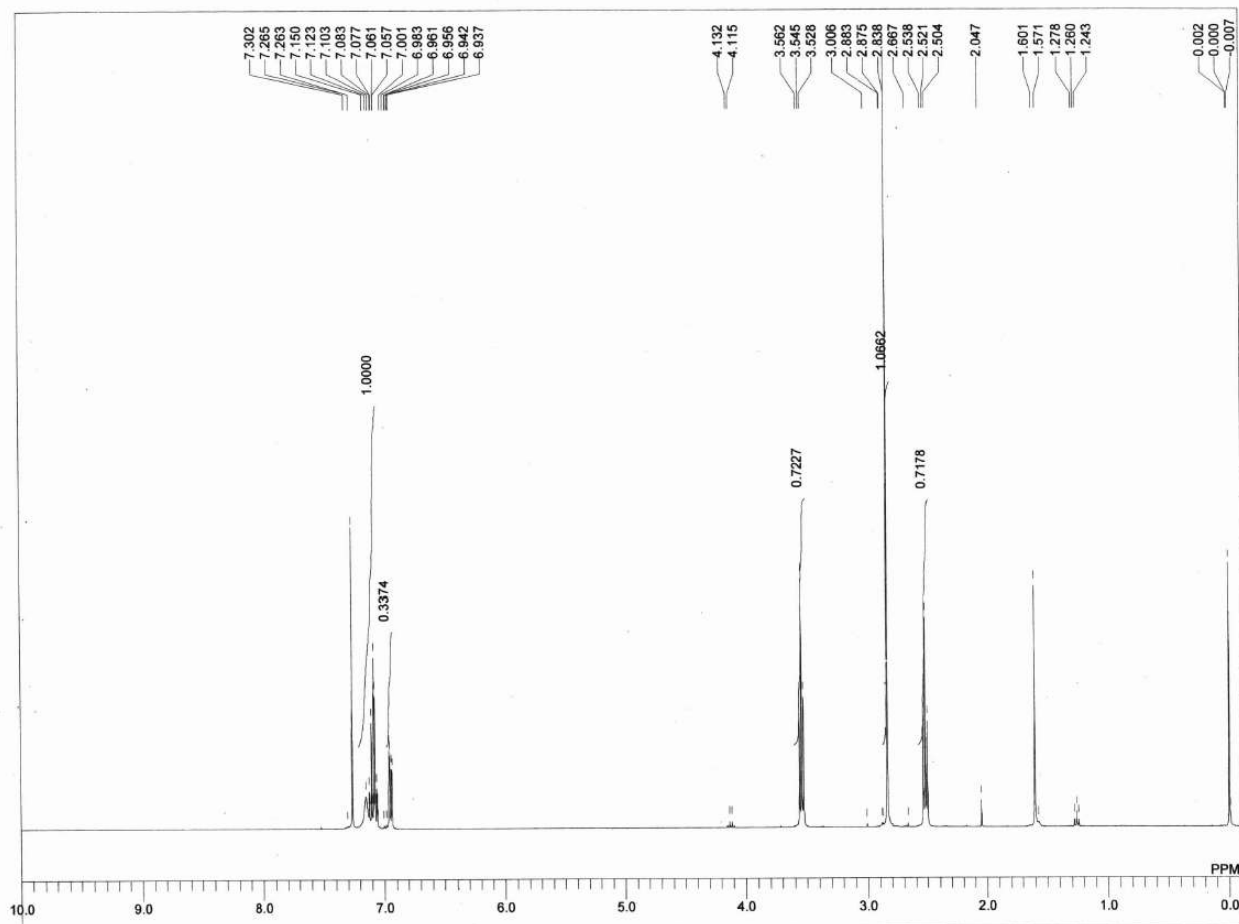
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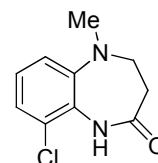


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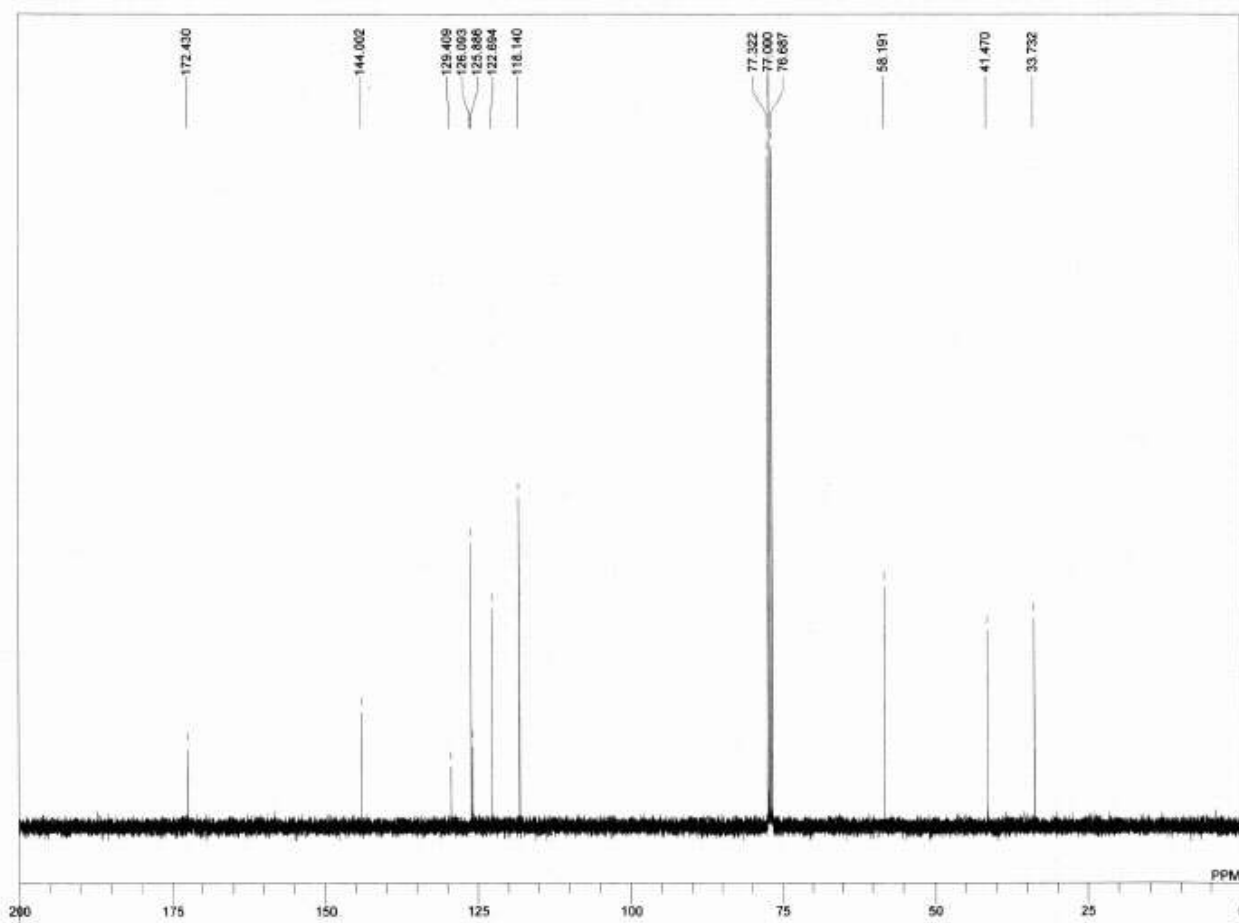


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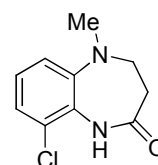


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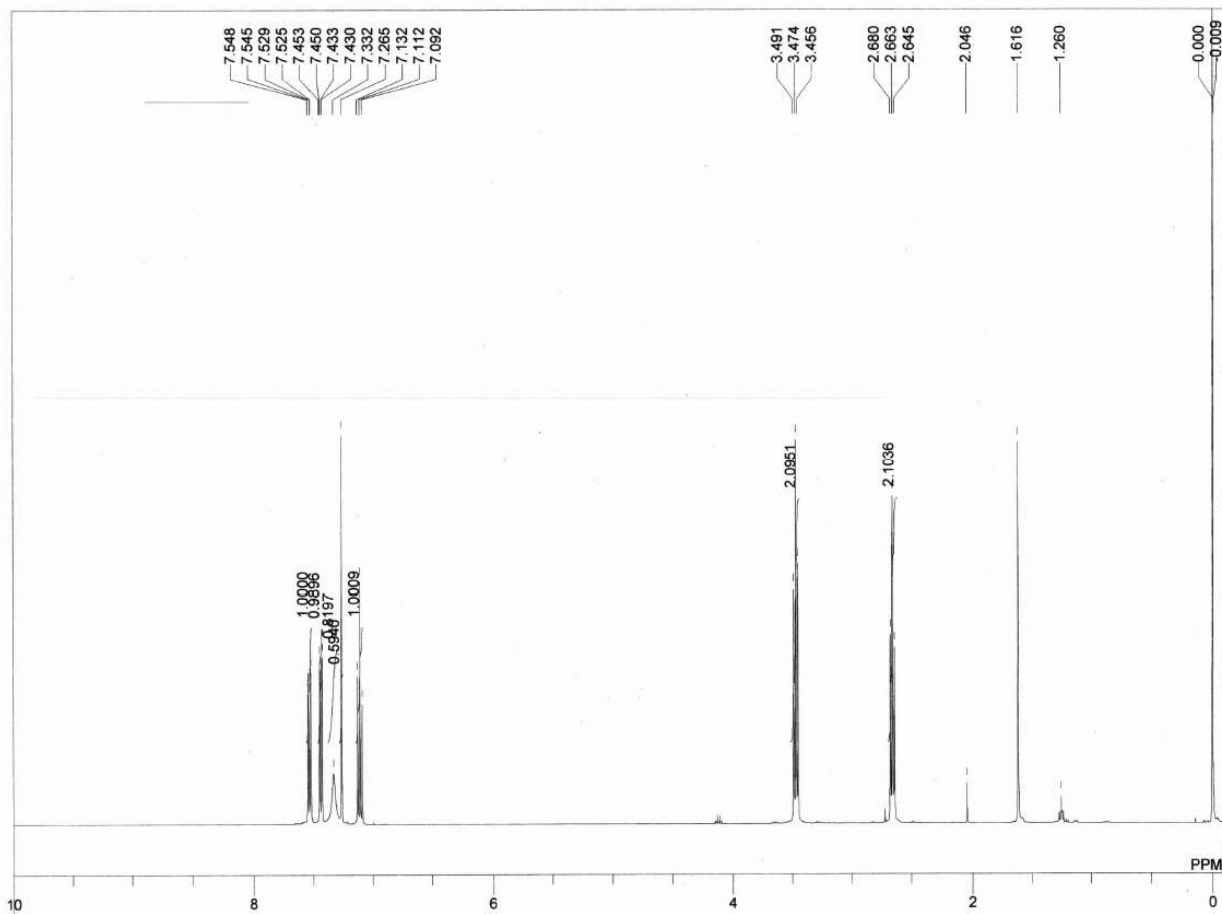


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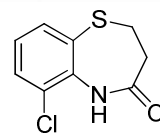


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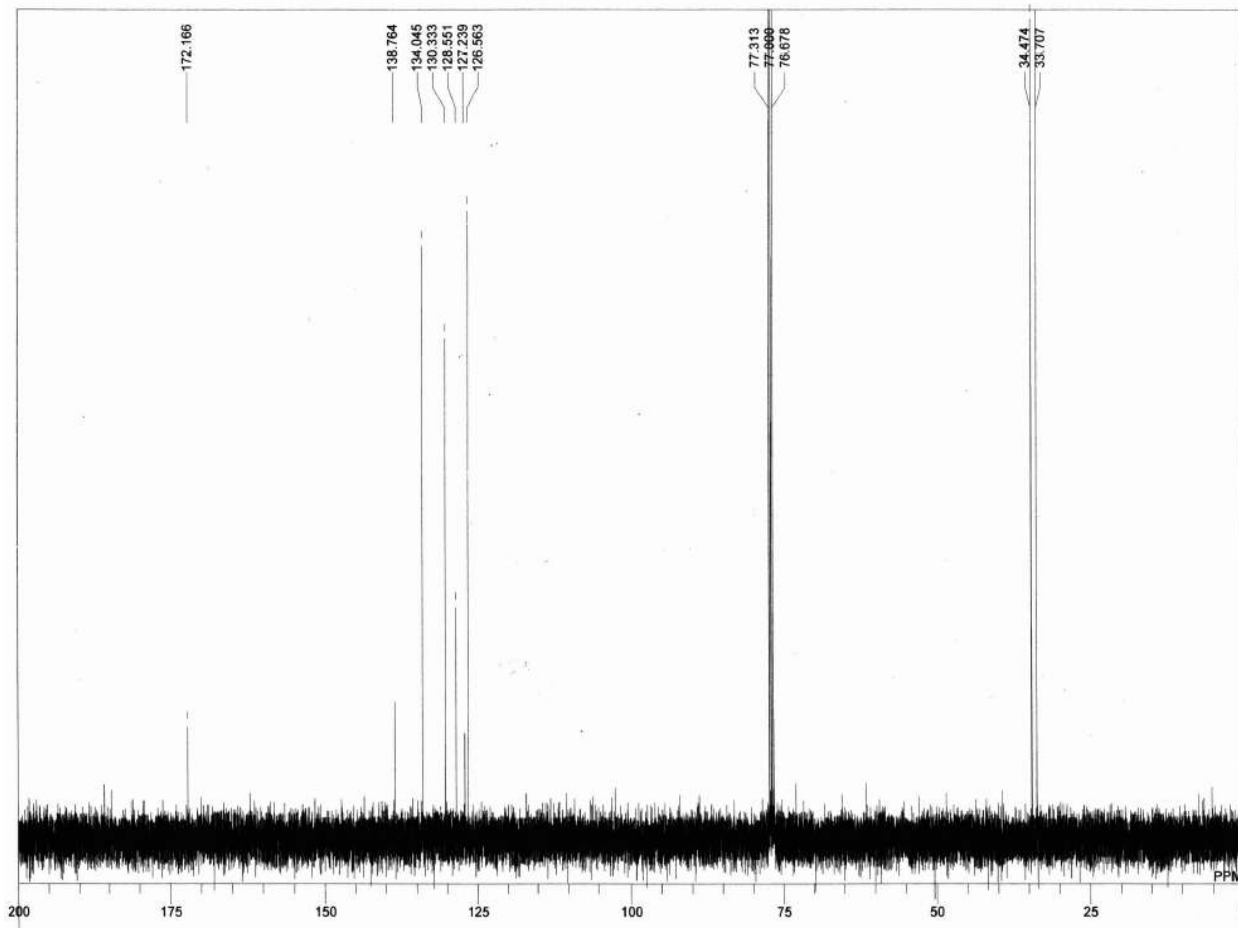


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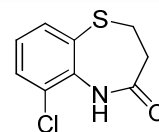


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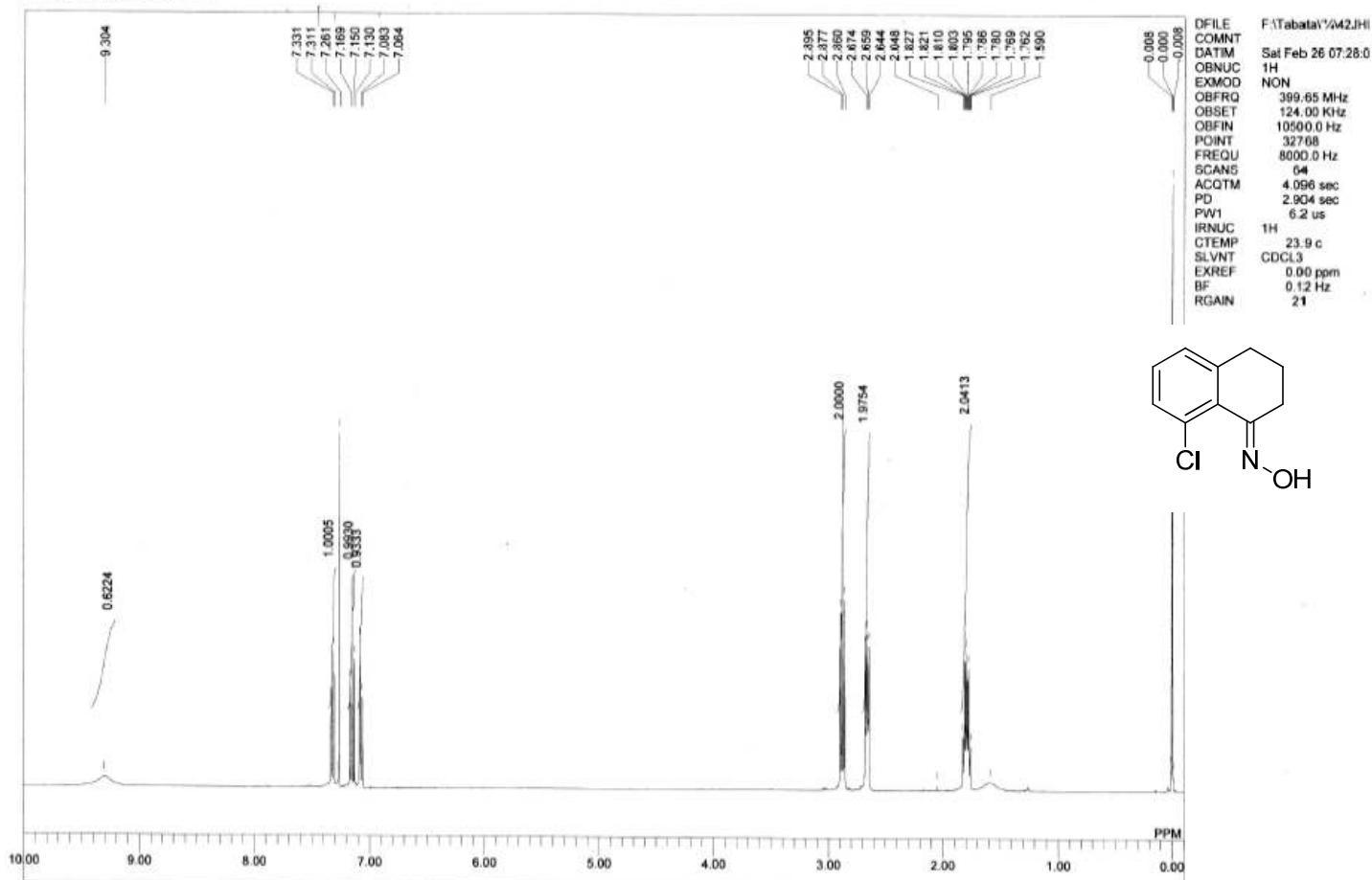


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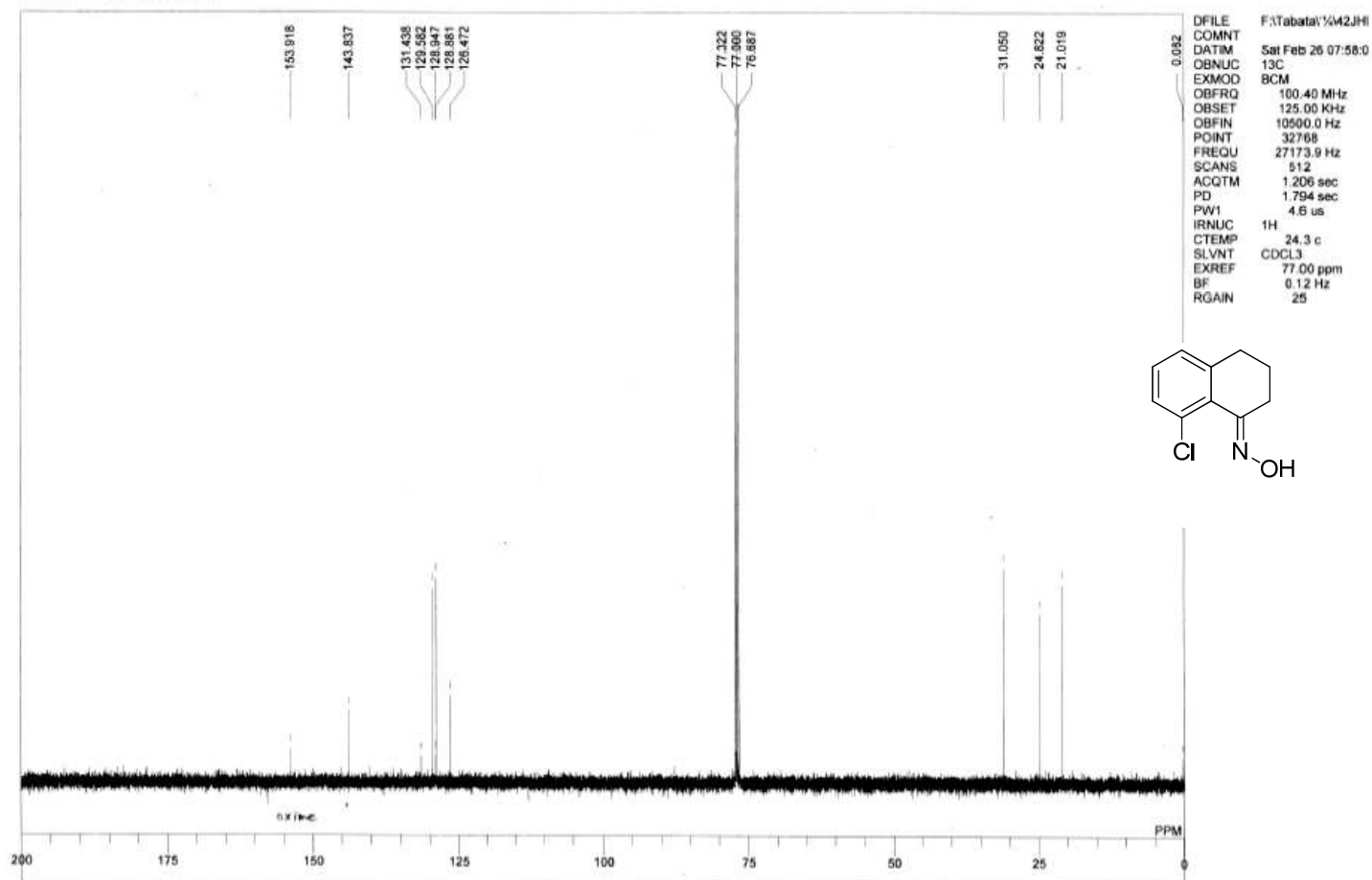


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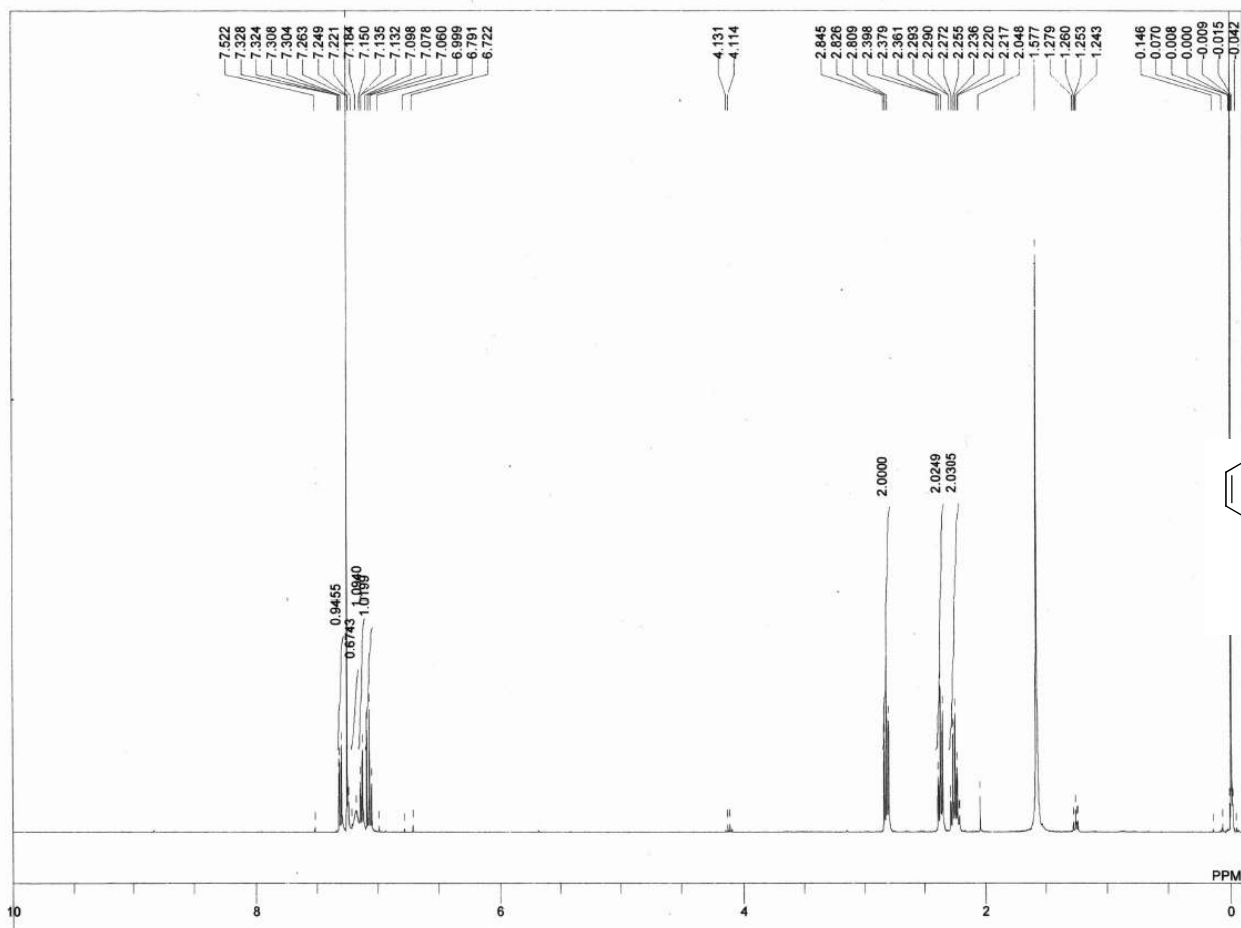
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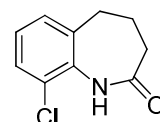
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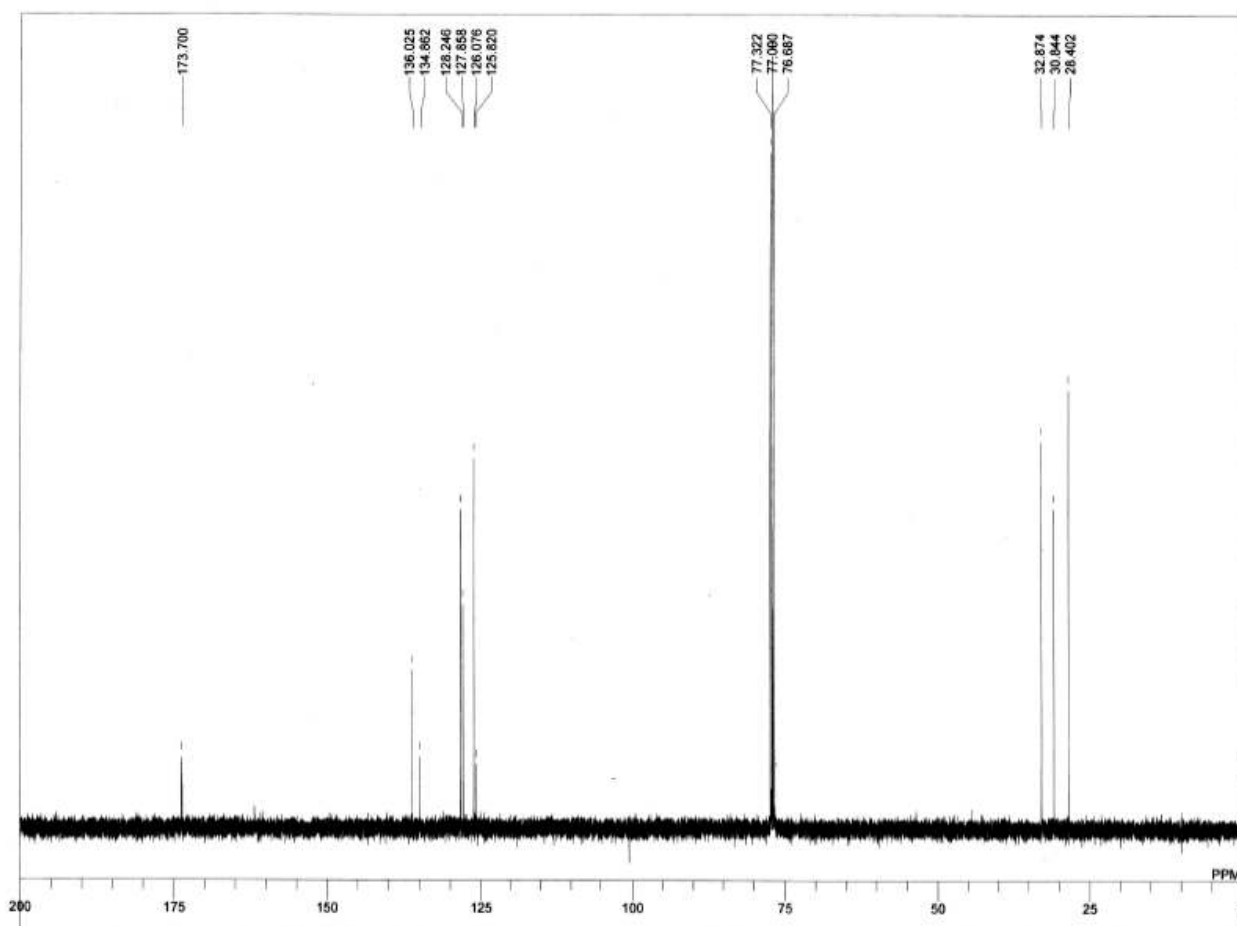


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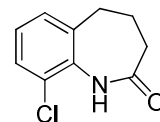


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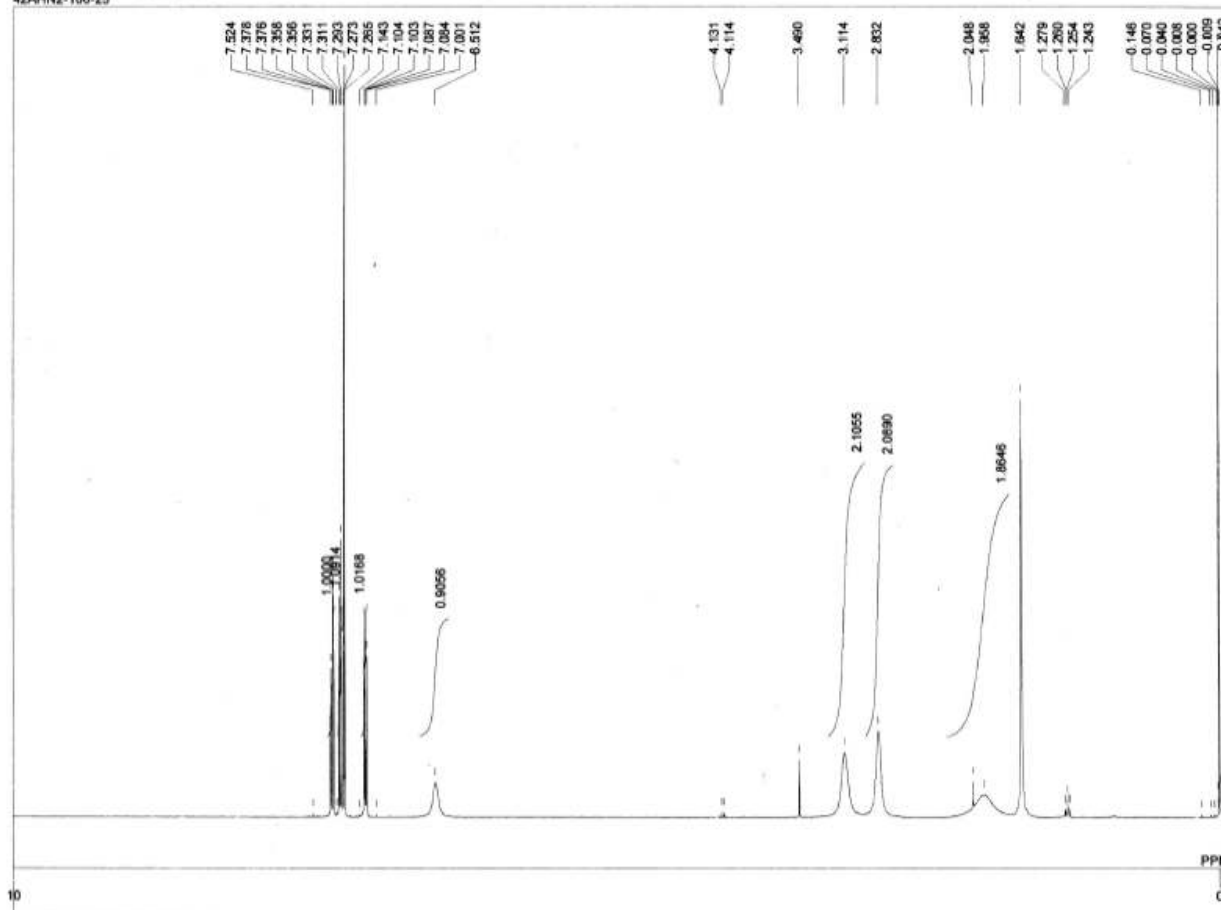


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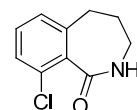


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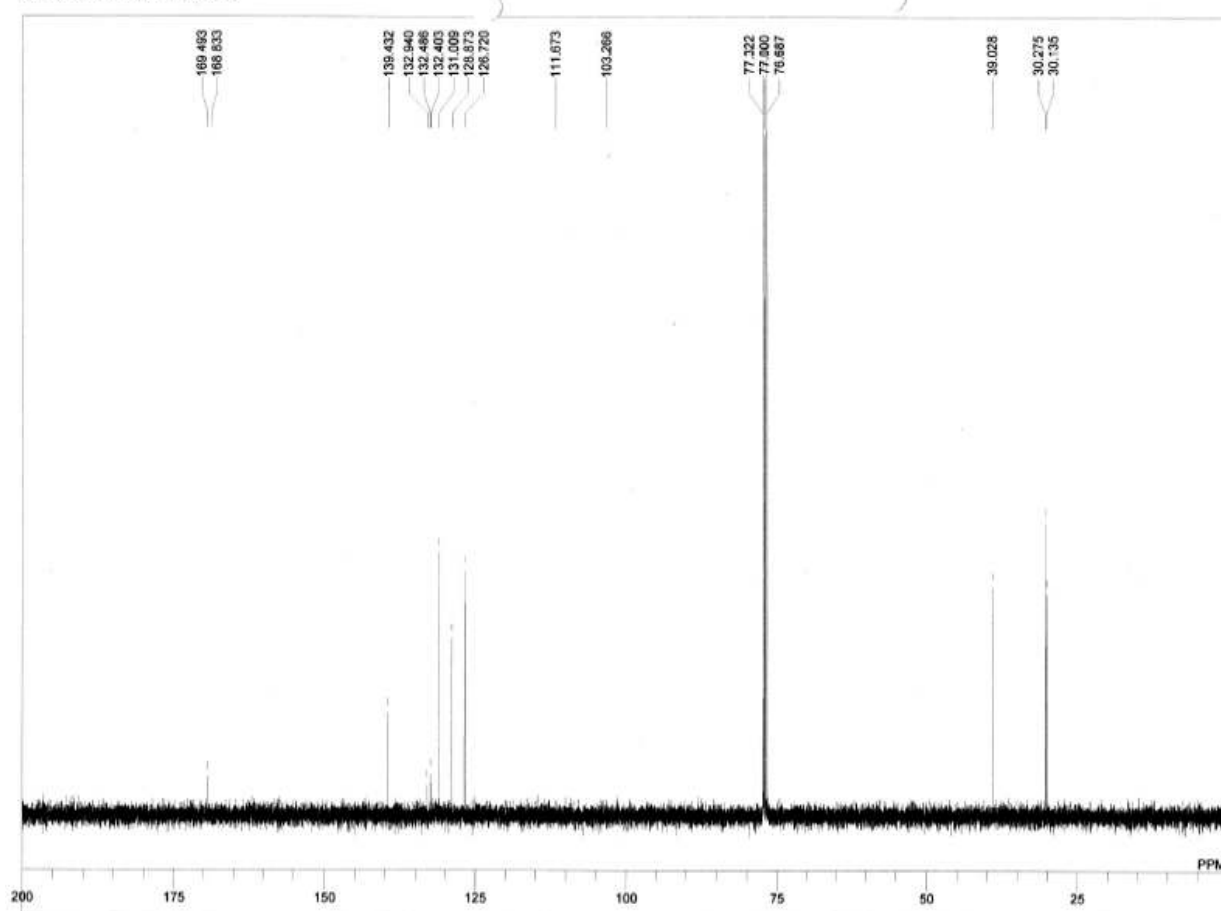


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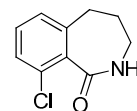


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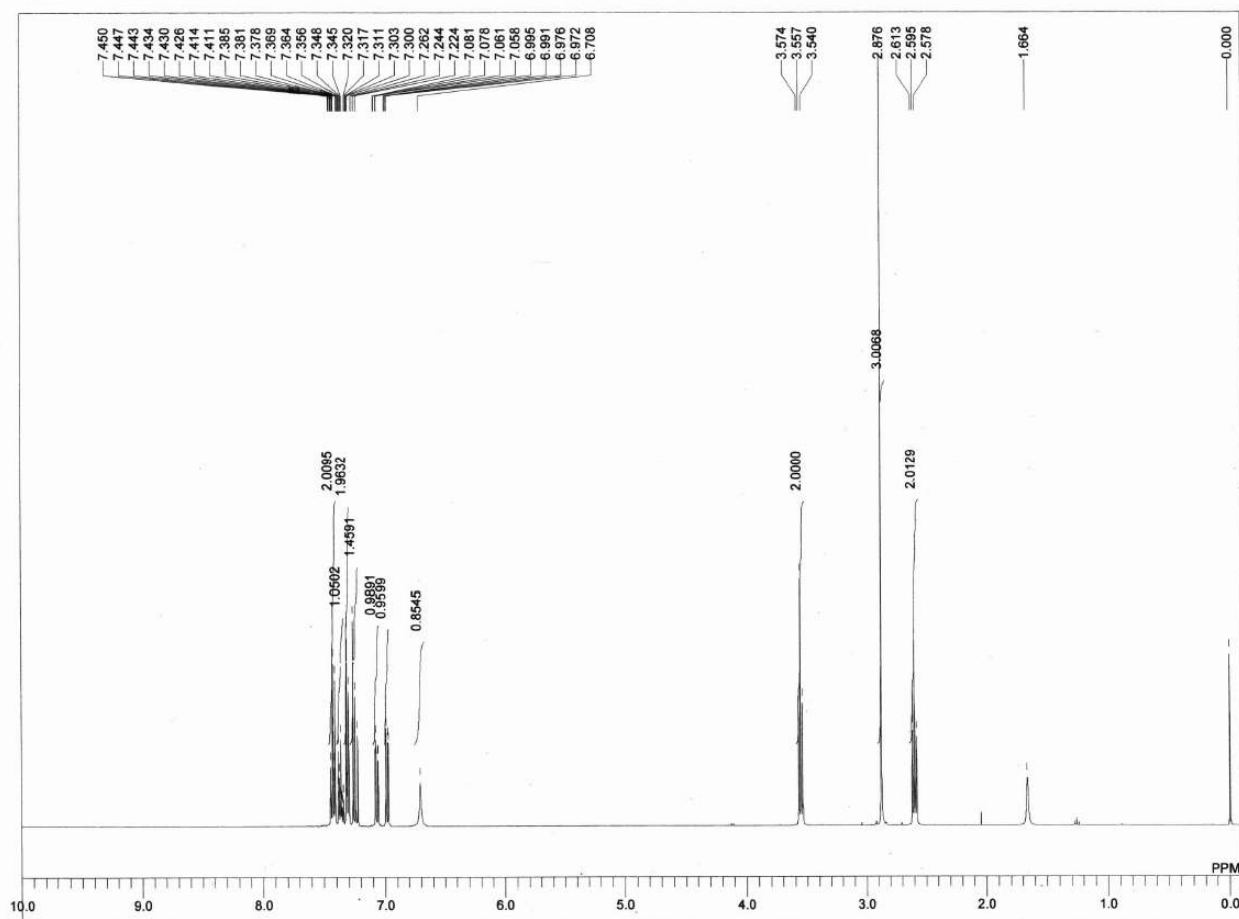


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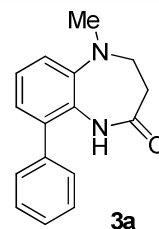


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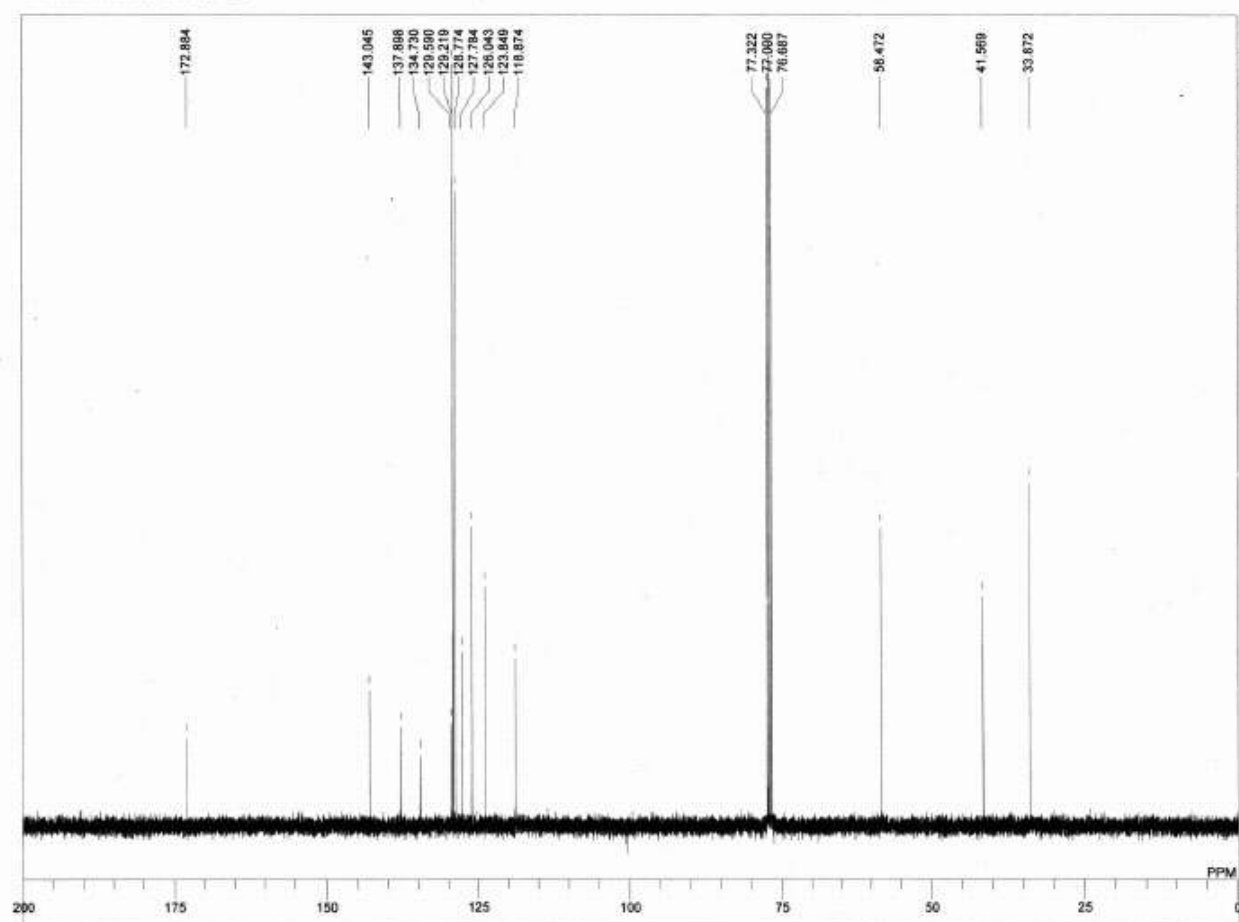
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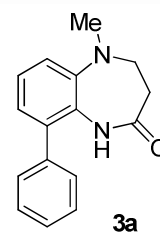
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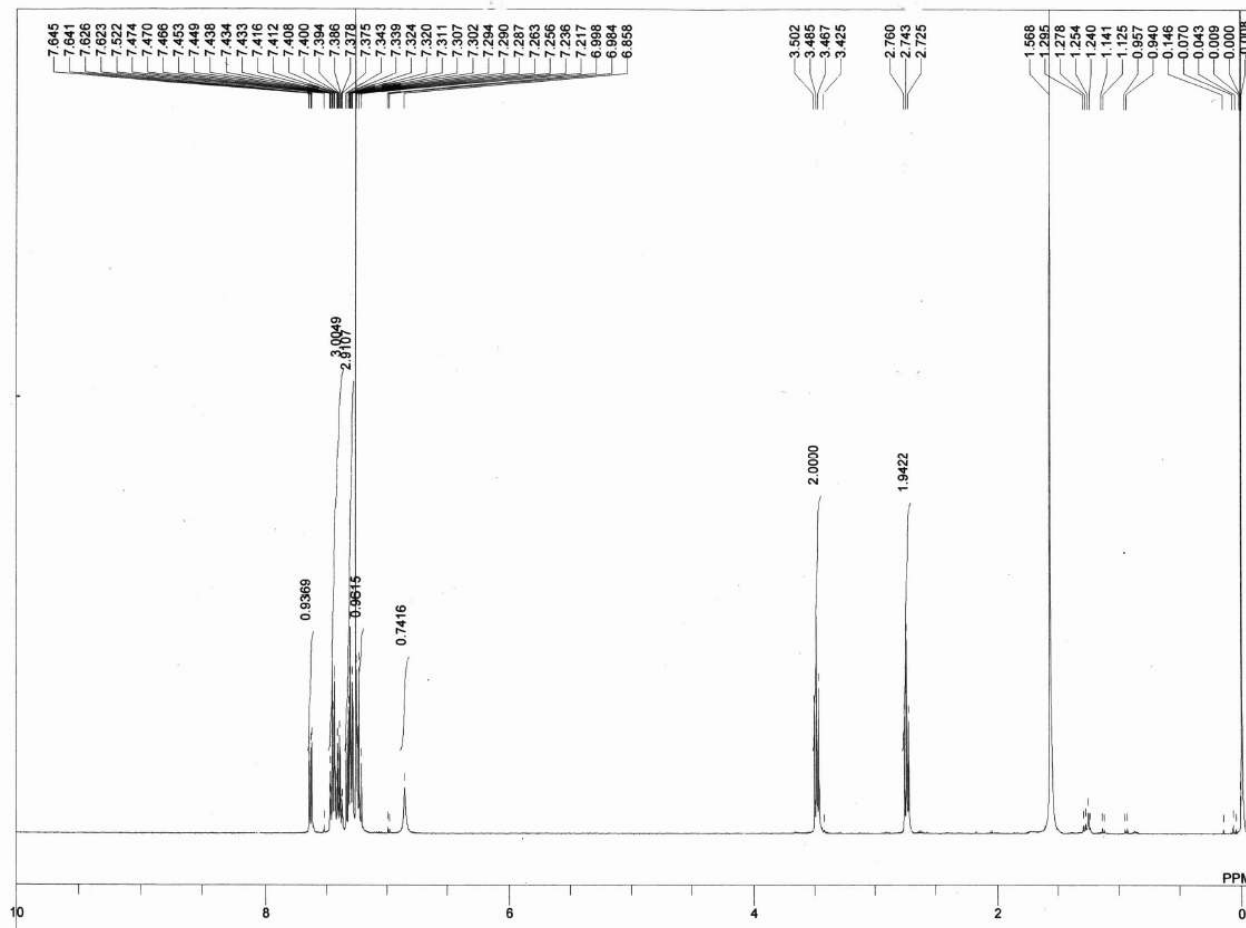
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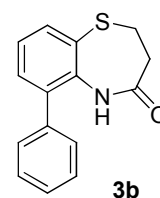
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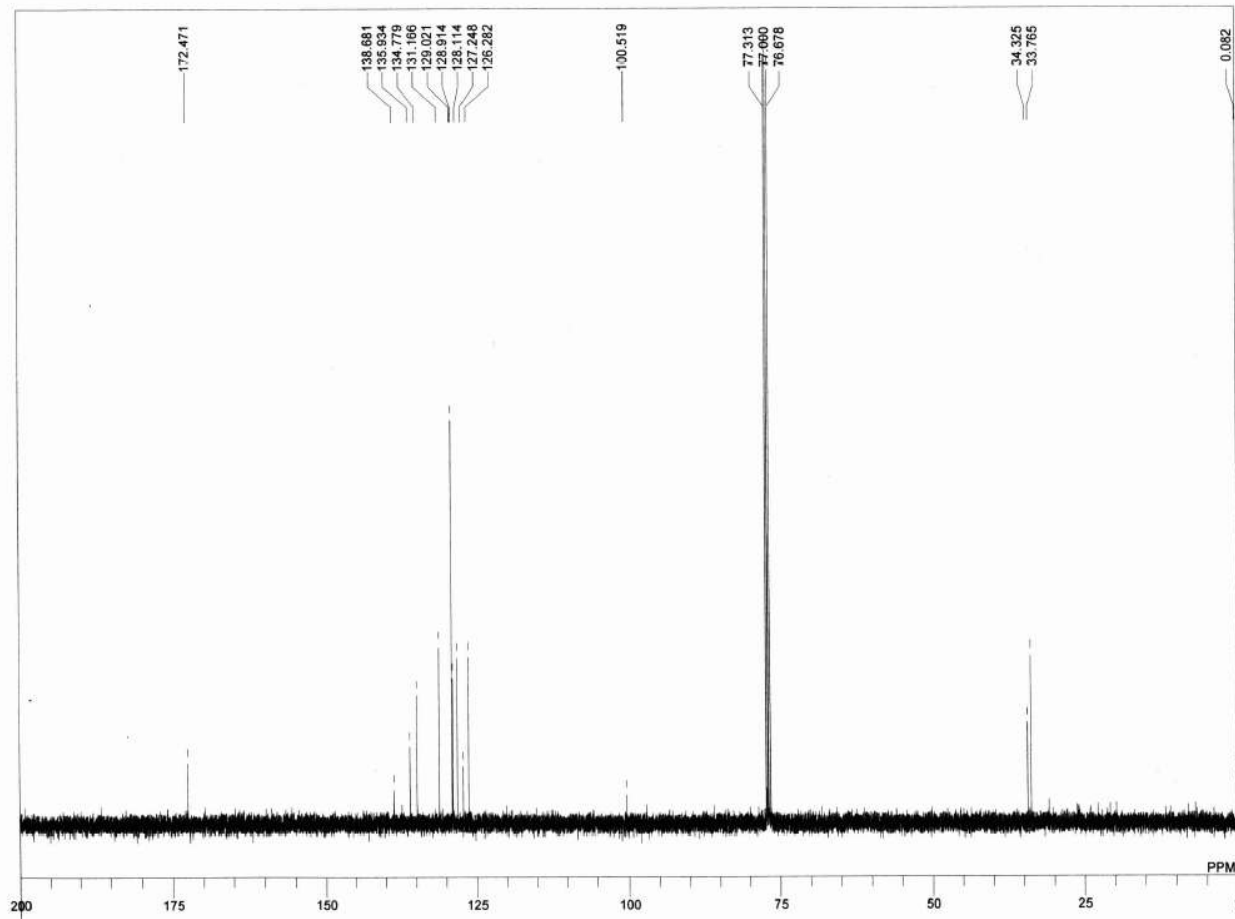
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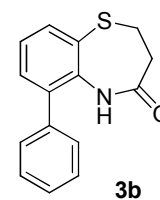
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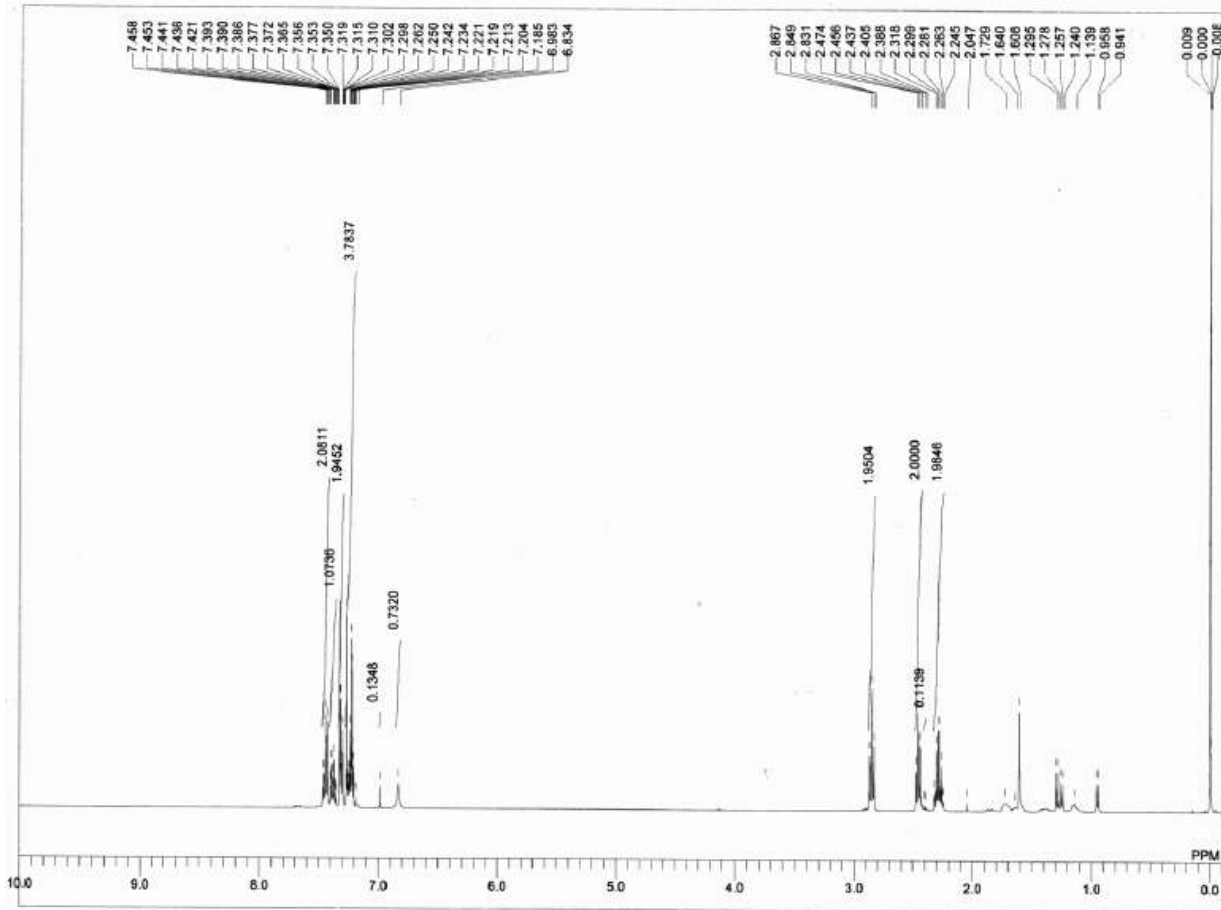
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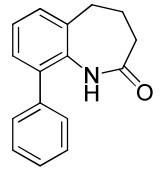
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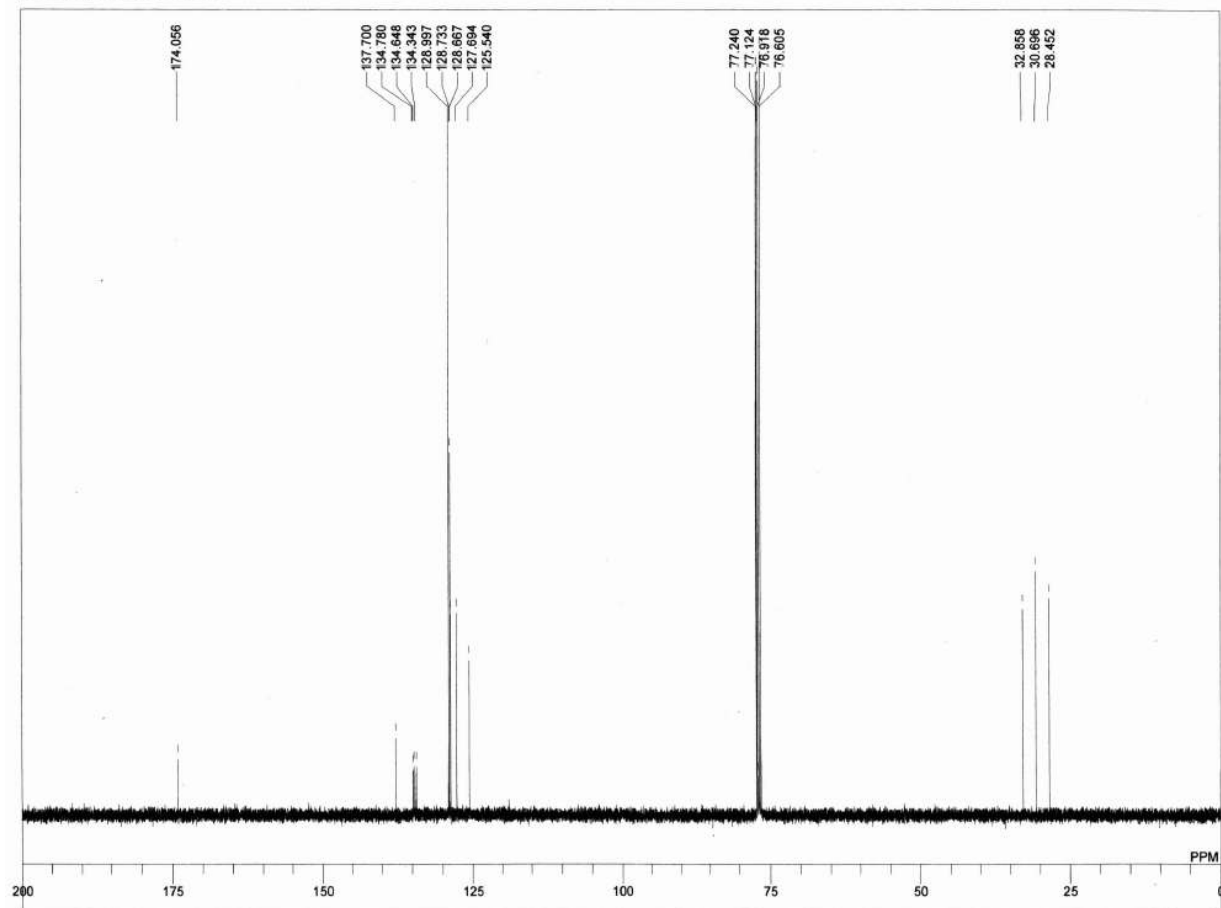


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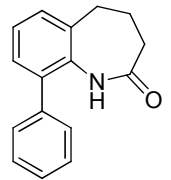


3c

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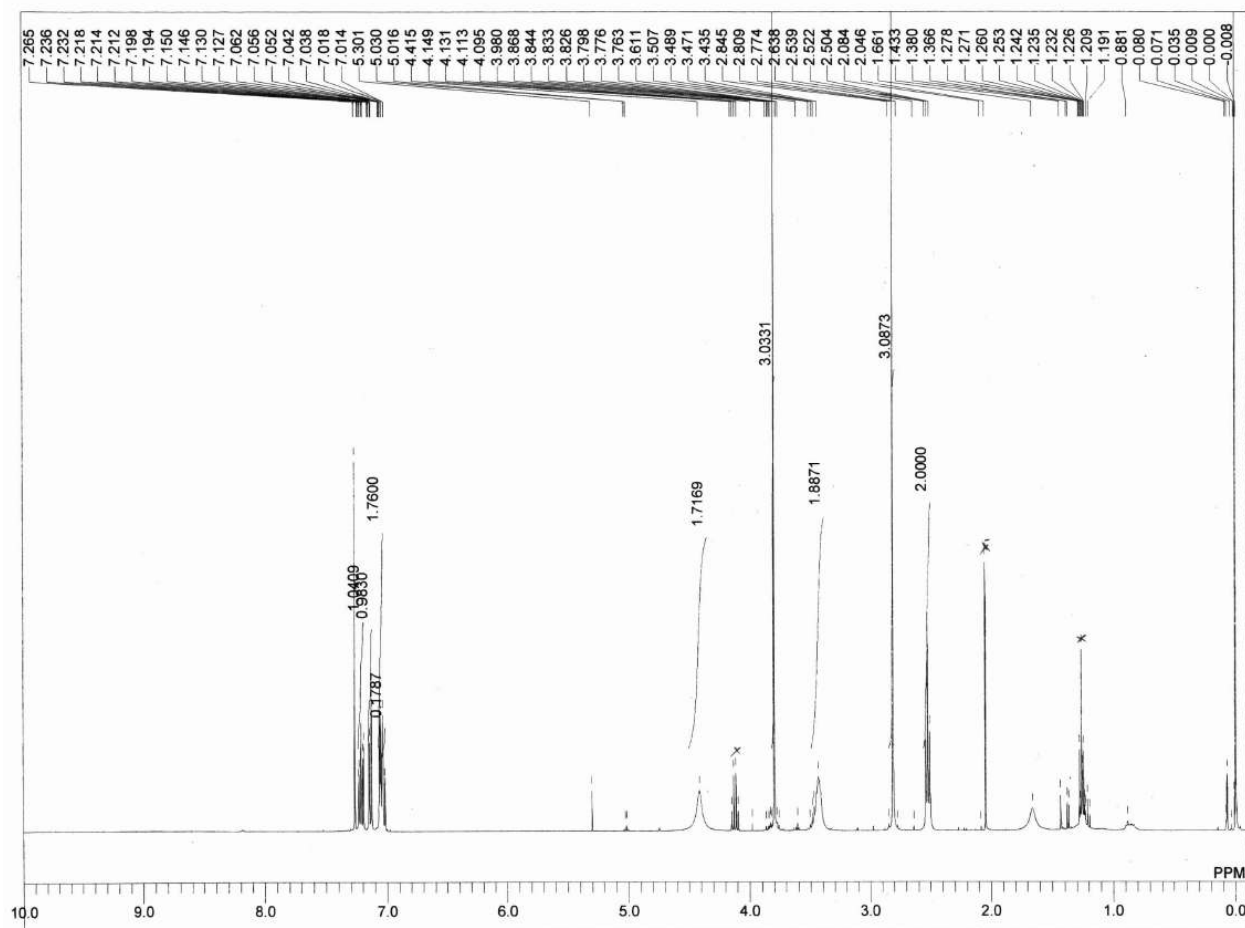


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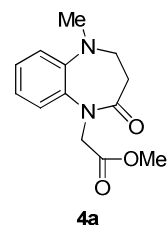


3c

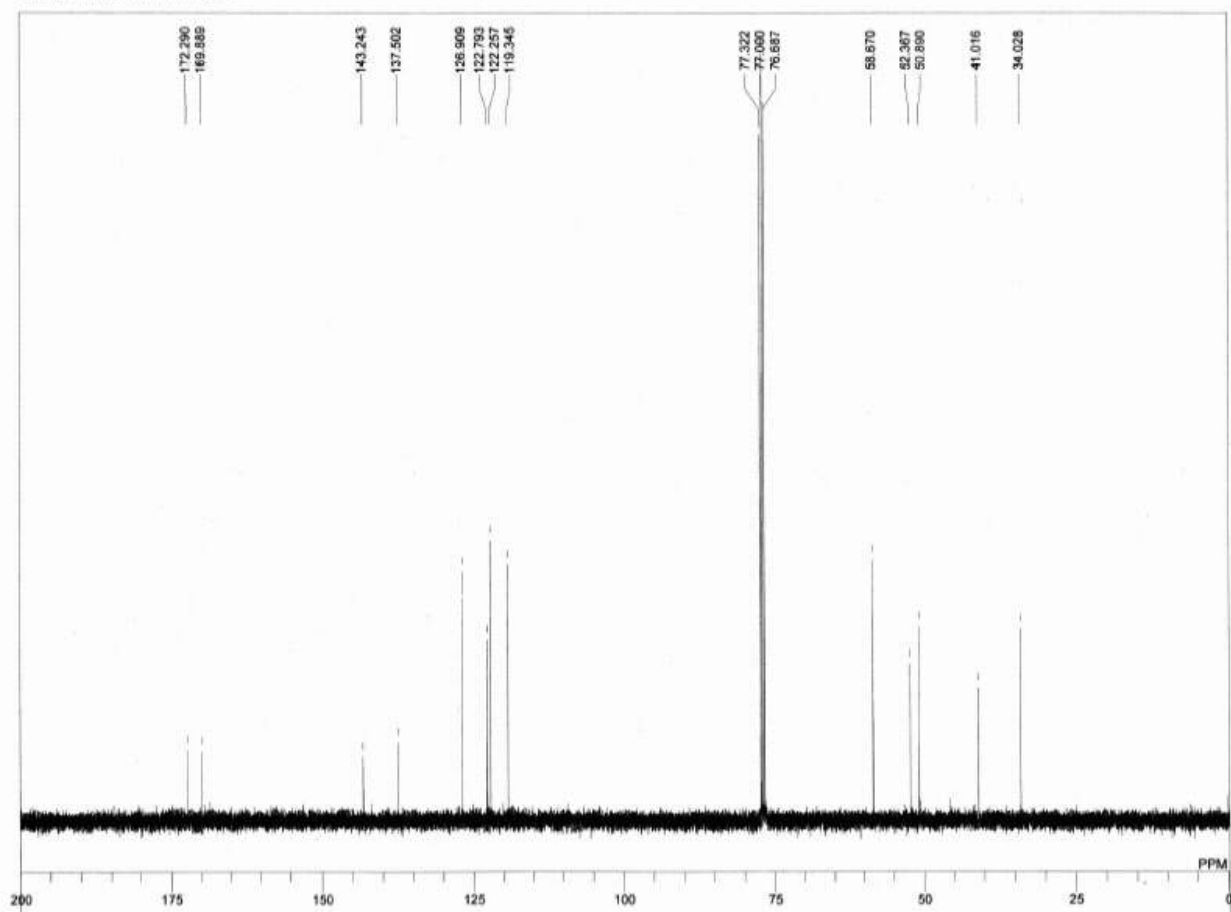
G:\Wada\42PNW1-54-26.als



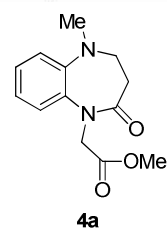
DFILE G:\Wada\42PN
COMNT Tue Jun 10 18:
DATIM 1H
OBNUC NON
EXMOD 399.65 MHz
OBFRQ 124.00 KHz
OBSET 10500.0 Hz
OBFIN 32768
POINT 8000.0 Hz
FREQU 16
SCANS 4.096 sec
ACQTM 2.904 sec
PD 6.2 us
PW1 1H
IRNUC 24.3 c
CTEMP CDCL3
SLVNT 0.00 ppm
EXREF 0.12 Hz
BF F

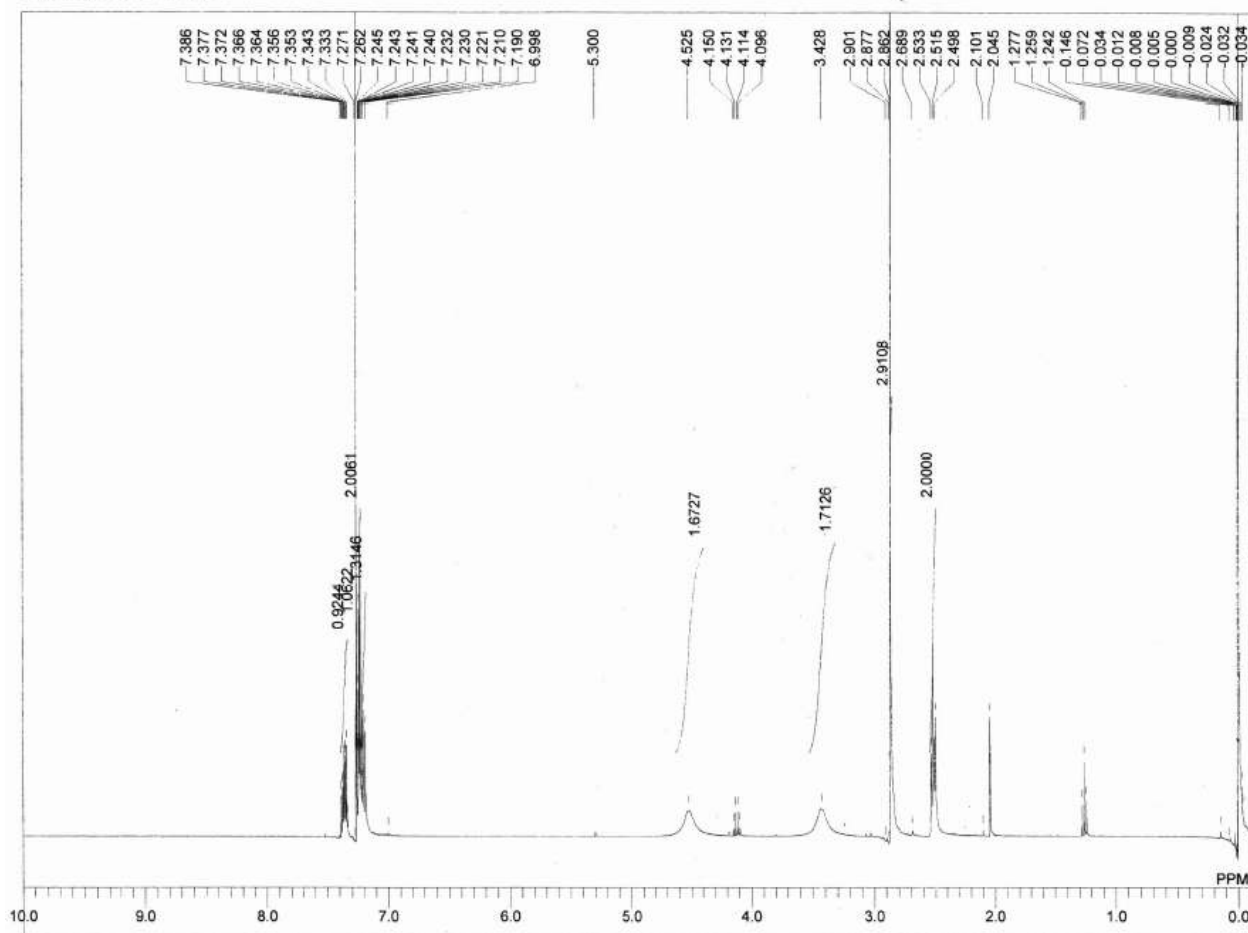


F:\Wada\42PNW3-18-30-carbon.als

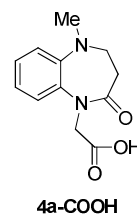


DFILE F:\Wada\42PNW3-
COMNT Fri Nov 06 05:30:31
DATIM 13C
OBNUC BCM
EXMOD 100.40 MHz
OBFRQ 125.00 KHz
OBSET 10500.0 Hz
OBFIN 32768
POINT 27173.9 Hz
FREQU 512
SCANS 1.206 sec
ACQTM 1.794 sec
PD 4.6 us
PW1 1H
IRNUC 23.8 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF 0.12 Hz
BF 25
RGAIN

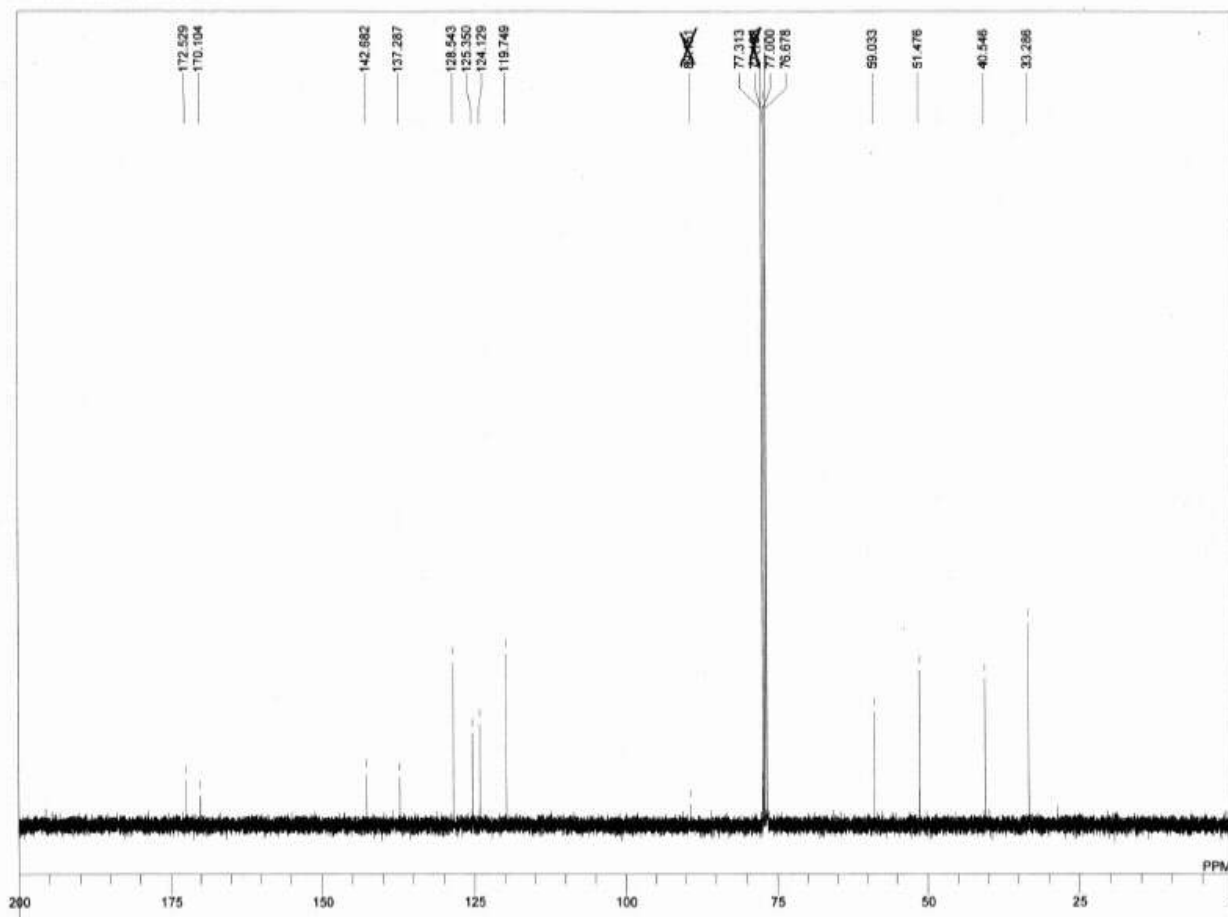




DFILE	G:\Wada42P
COMNT	
DATIM	Tue Jun 17 05
OBNUC	1H
EXMOD	NON
OBFRQ	399.65 MHz
OBSET	124.00 KHz
OBFIN	10500.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANG	16
ACQTM	4.096 sec
PD	2.904 sec
PW1	6.2 us
IRNUC	1H
CTEMP	26.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	20



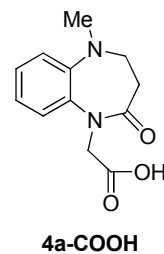
F:\Wada\42PNW1-60-25-carbon.xls



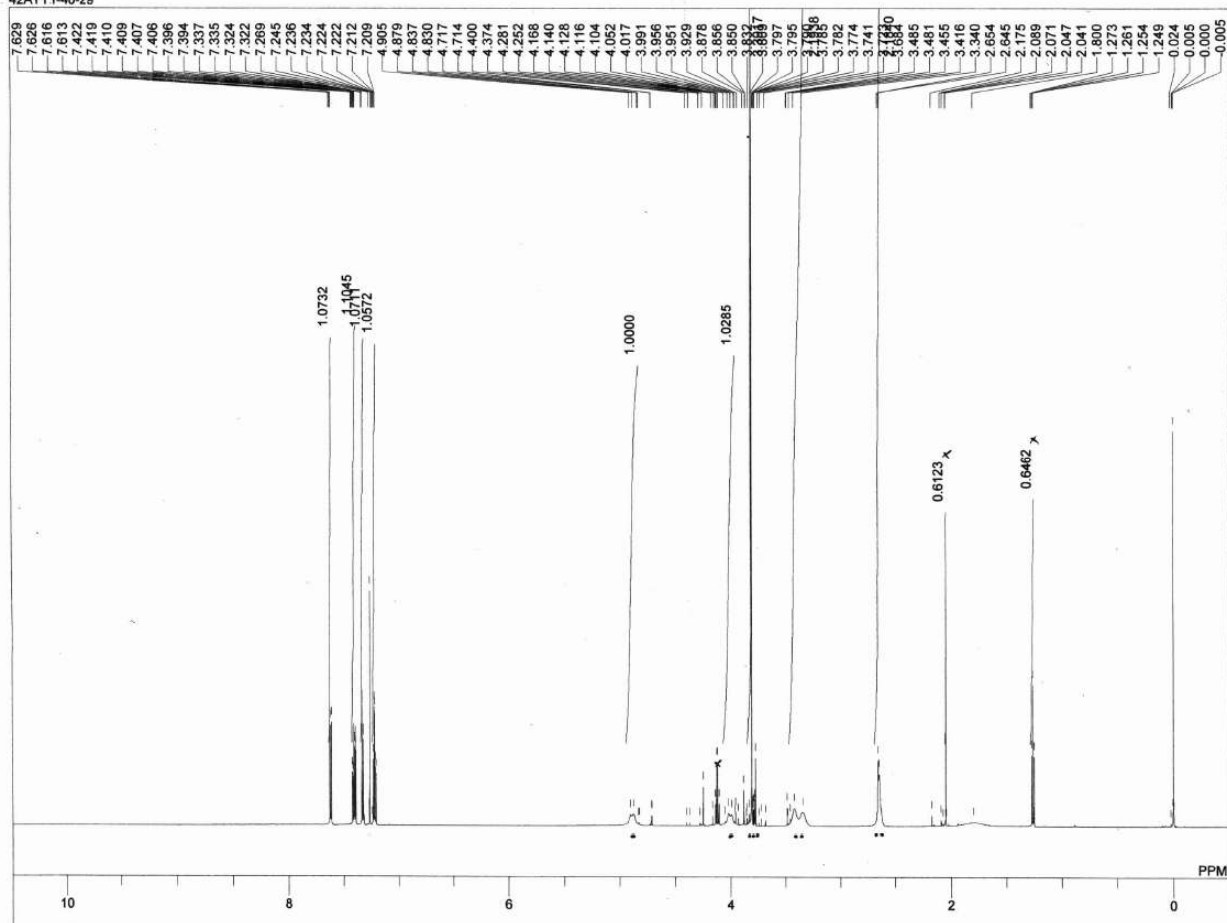
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DFILE      F:\Wada42PNW1-
COMNT
DATIM      Sat Oct 31 13:21:5
OBNUC      13C
EXMOD      BCM
OBFRQ      100.40 MHz
OBSET      125.00 KHz
OBFIN      10500.0 Hz
POINT
FREQU      27173.9 Hz
SCANS      512
AQOTM      1.266 sec
PD          1.794 sec
PW1         4.6 us
IRNUC      1H
CTEMP      22.6 c
SLVNT      CDCL3
EXREF      77.00 ppm
BF          0.12 Hz
RGAIN      24

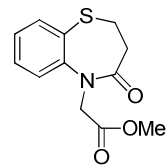
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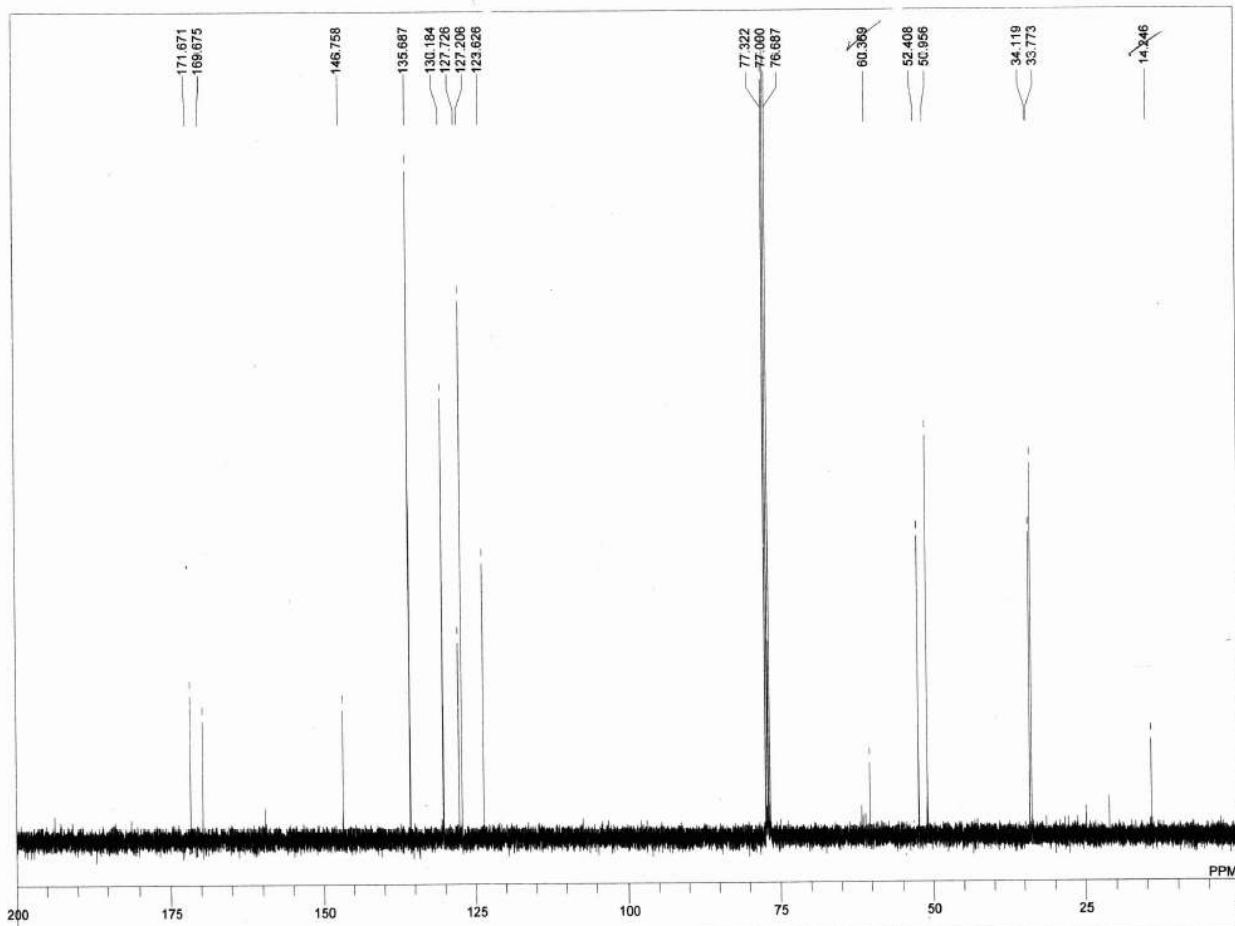
H:\Takada\Sw-42AYT1-40-29.als
42AYT1-40-29



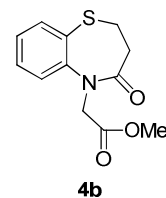
DFILE H:\Takada\Sw-42
COMNT 42AYT1-40-29
DATIM 22-NOV-2007 11:1
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 600.00 MHz
OBSET 175.00 KHz
OBFIN 305.5 Hz
POINT 32768
FREQU 9009.0 Hz
SCANS 64
ACQTM 3.637 sec
PD 4.000 sec
PW1 6.2 us
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19



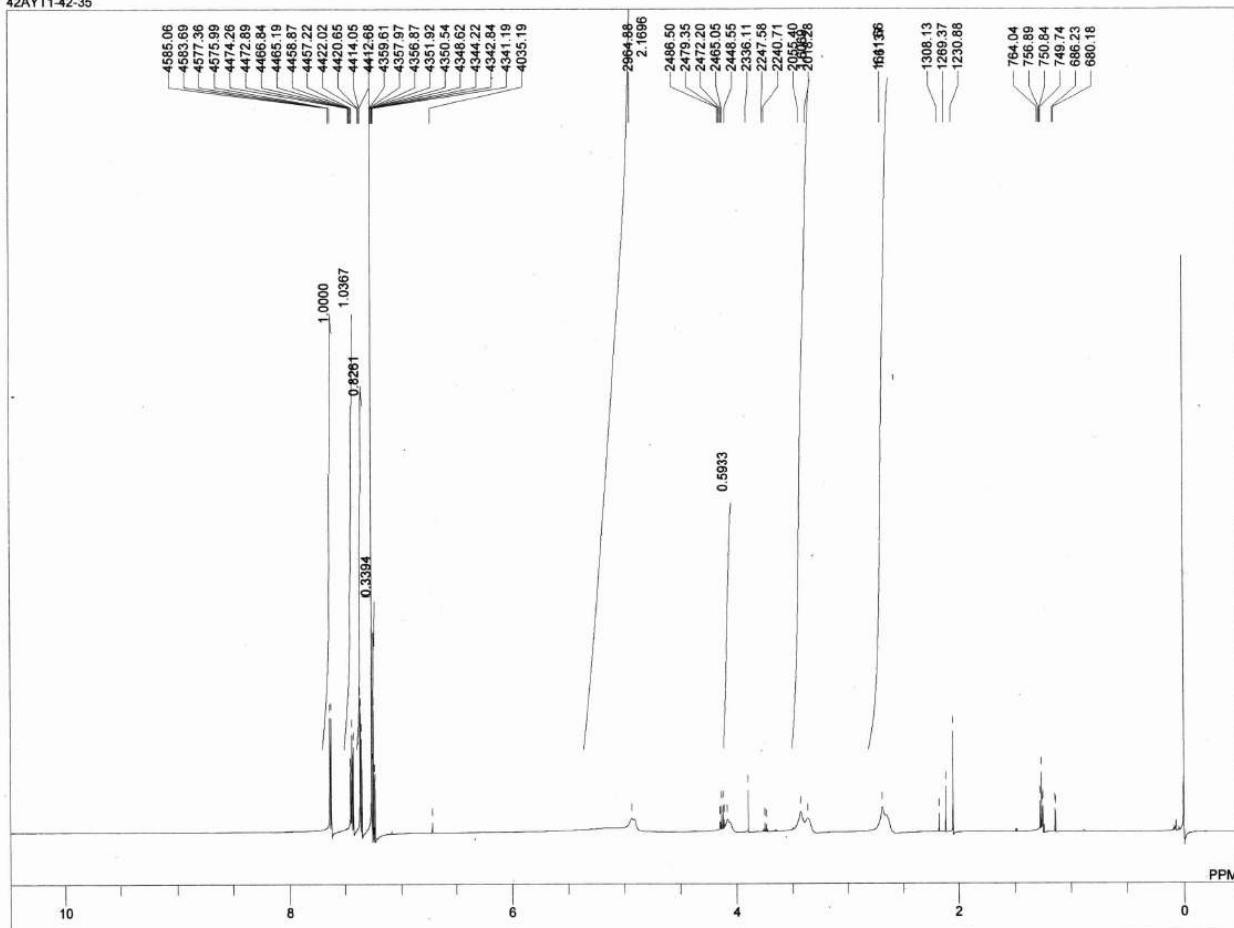
F:\Takada\42Y-YT1-182-35.als



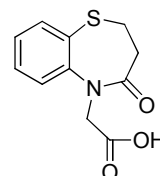
DFILE F:\Takada\42Y-YT
COMNT Tue Feb 08 06:23:1
DATIM 13C
OBNUC BCM
EXMOD 100.40 MHz
OBFRQ 125.00 KHz
OBSET 10500.0 Hz
OBFIN 32768
POINT 27173.9 Hz
FREQU 512
SCANS 1.206 sec
ACQTM 1.794 sec
PD 4.6 us
PW1 1H
IRNUC 25.2 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF 0.12 Hz
BF 24
RGAIN



H:\Takada\Sw-142AYT1-42-35.als
42AYT1-42-35

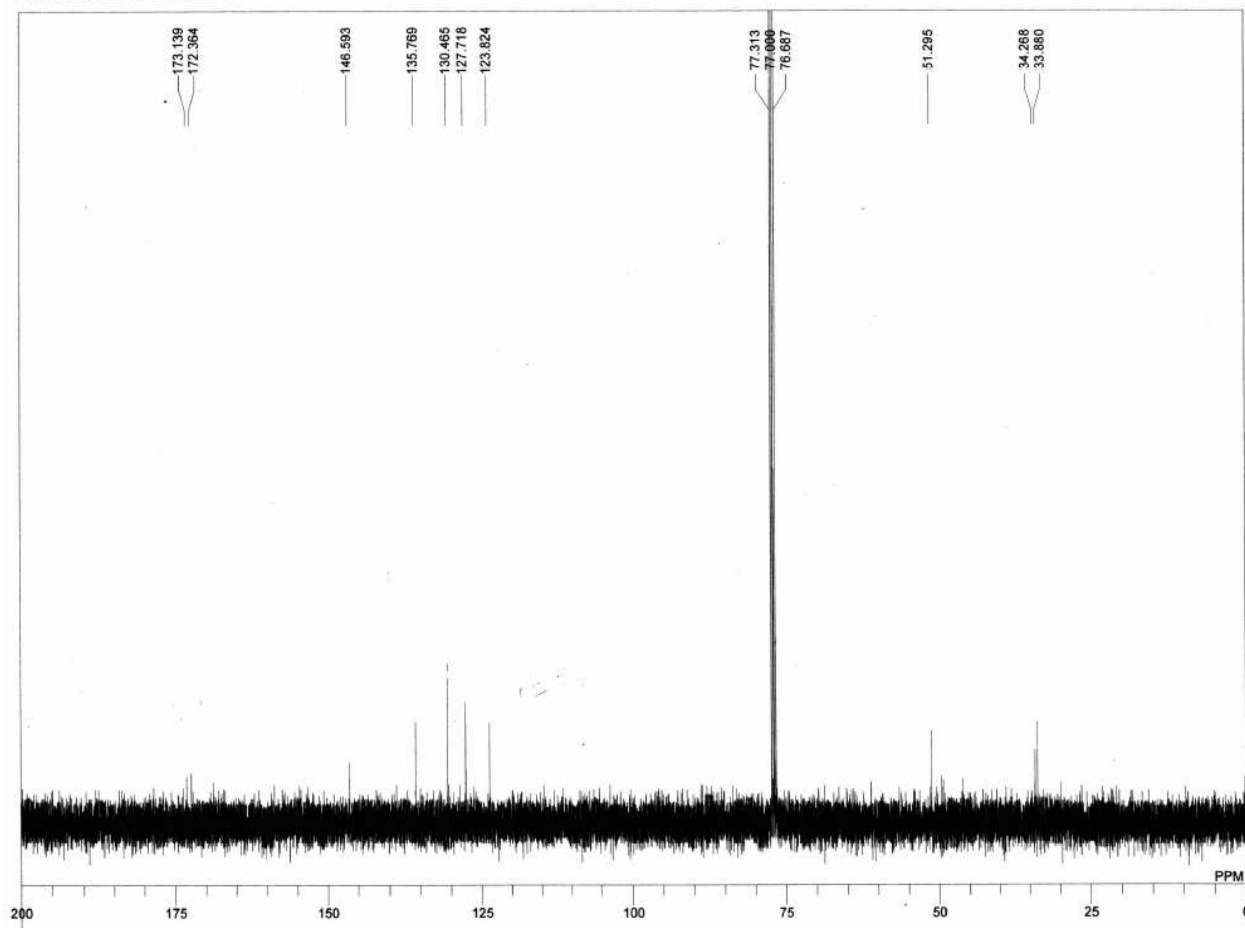


DFILE H:\Takada\Sw-14
COMNT 42AYT1-42-35
DATIM 26-NOV-2007 09:
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 600.00 MHz
OBSET 175.00 KHz
OBFIN 305.5 Hz
POINT 32768
FREQU 9009.0 Hz
SCANS 64
ACQTM 3.637 sec
PD 4.000 sec
PW1 6.2 us
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20

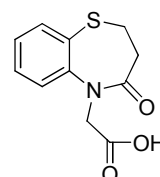


4b-COOH

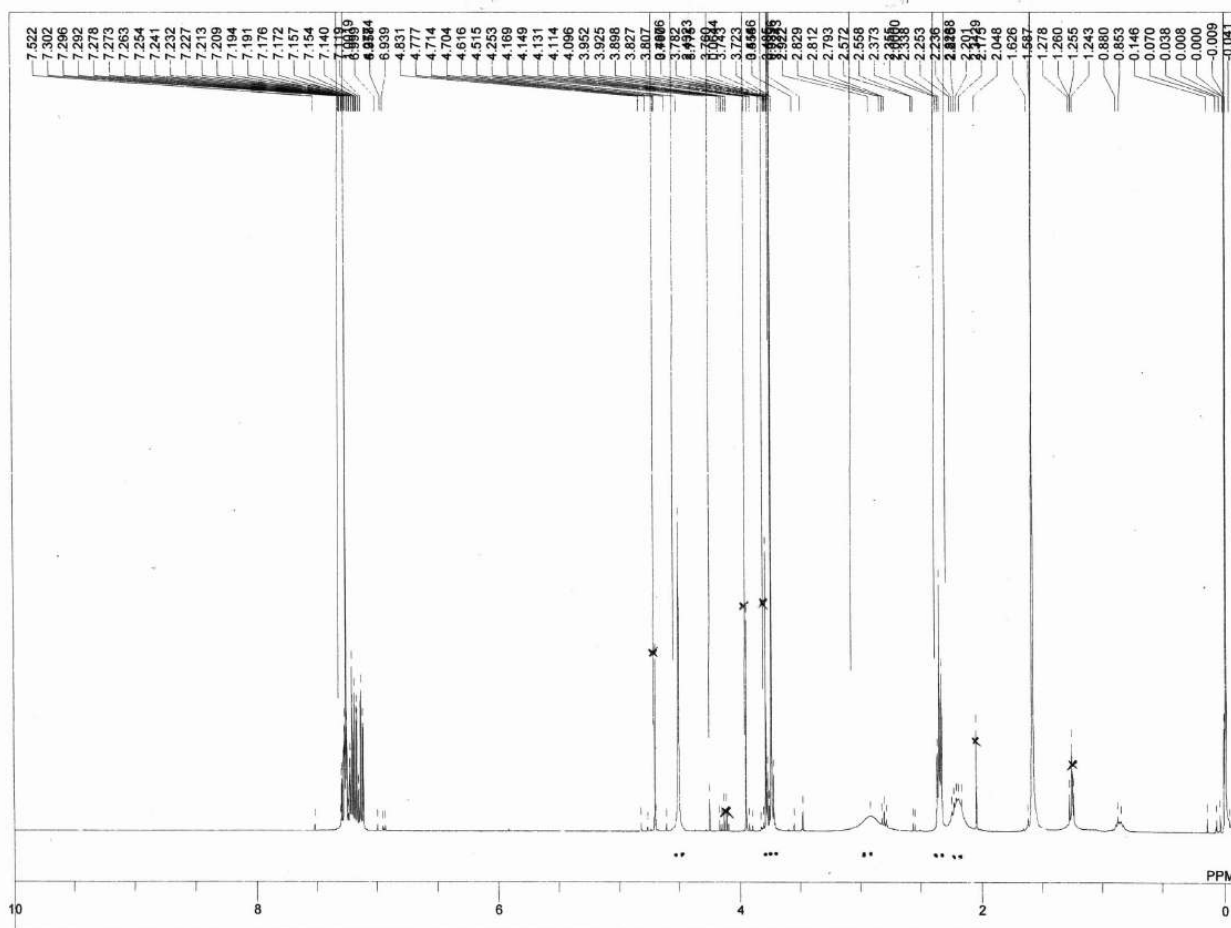
F:\Takada\carbon\42YYT1-52-20.als



DFILE F:\Takada\carbon\
COMNT Mon Nov 08 15:27:
DATIM 13C
OBNUC BCM
EXMOD 100.40 MHz
OBFRQ 125.00 KHz
OBSET 10500.0 Hz
OBFIN 32768
POINT 27173.9 Hz
FREQU 200
SCANS 1.206 sec
ACQTM 1.794 sec
PD 4.6 us
PW1 1H
IRNUC 23.9 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF 0.12 Hz
BF 25
RGAIN



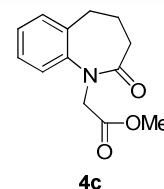
4b-COOH



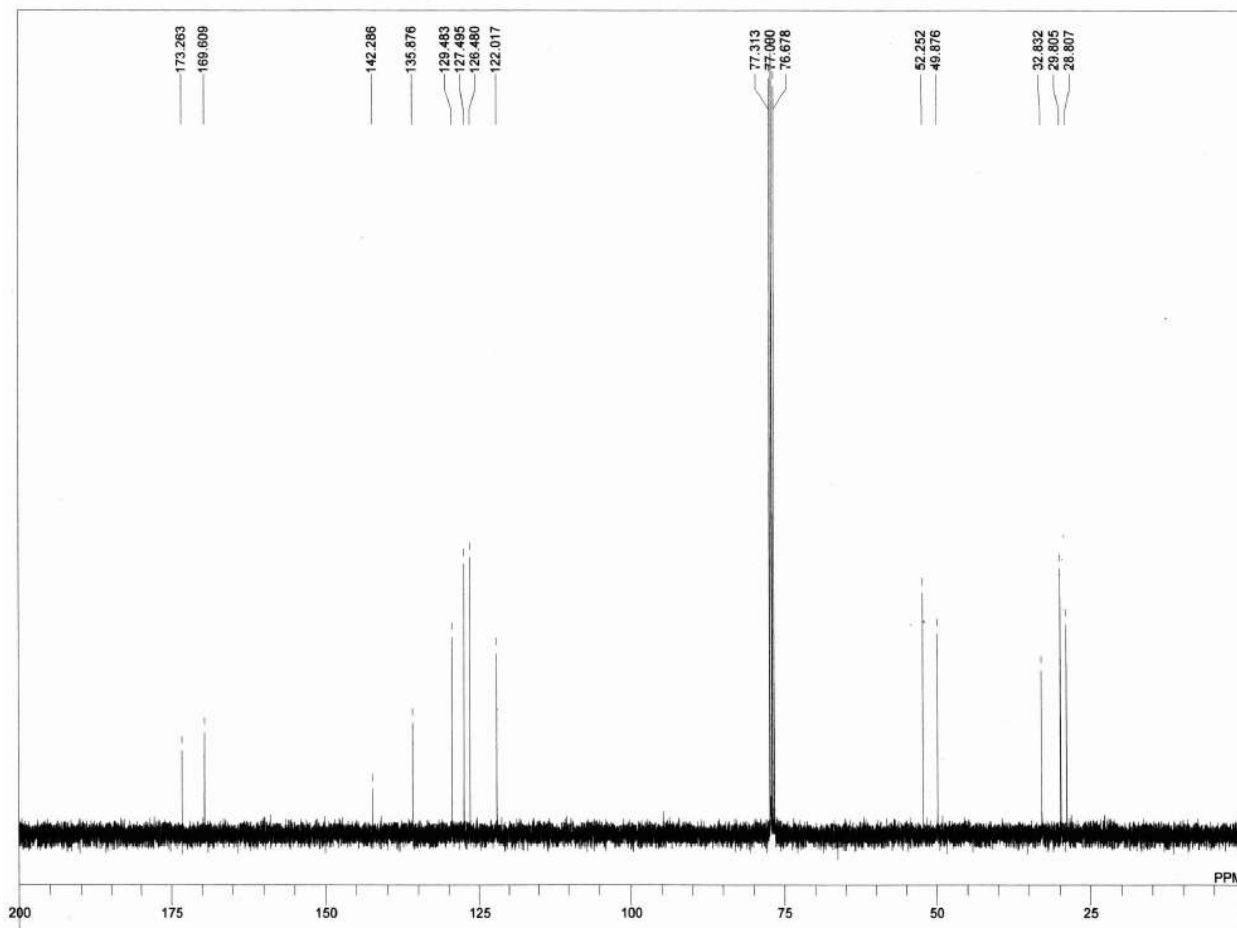
```

DFILE      F:\Takada\42Y-YT-
COMNT
DATIM      Tue Jul 28 13:00:3
OBNUC      1H
EXMOD      NON
OBFRQ      399.65 MHz
OBSET      124.00 KHz
OBFIN      10500.0 Hz
POINT      32768
FREQU      8000.0 Hz
SCANS      128
ACQTM      4.096 sec
PD          2.904 sec
PW1         6.2 us
IRNUC      1H
CTEMP      22.2 c
SLVNT      CDCl3
EXREF      0.00 ppm
BF          0.12 Hz
RGAIN      21

```



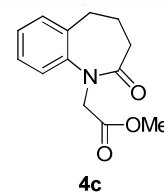
F:\Tabata\Hta9\42JHTA9-106-35C.als



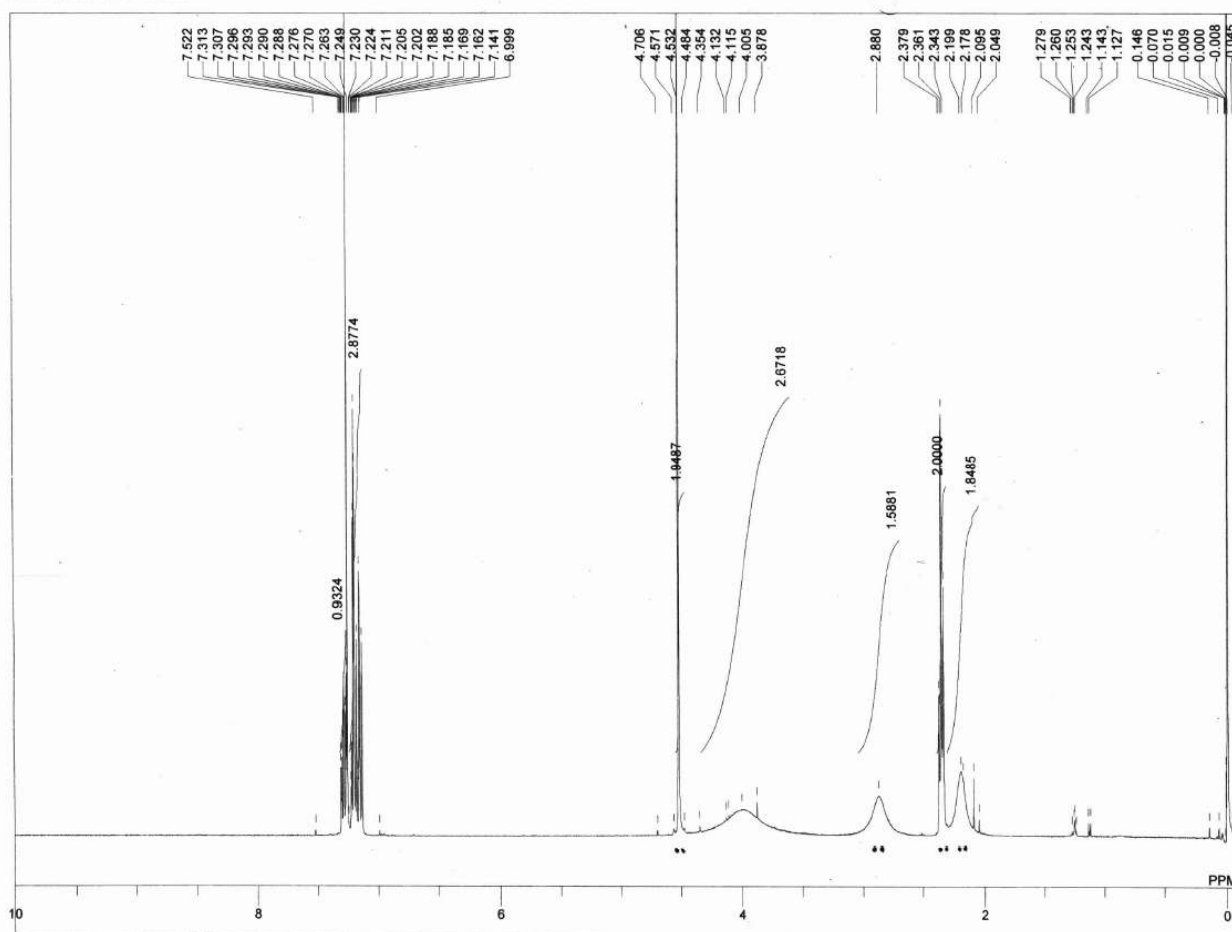
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DFILE      F:\Tabata\Hta9W42.
COMNT
DATIM      Thu Mar 10 11:22:
OBNUC      13C
EXMOD      BCM
OBFREQ     100.40 MHz
OBSET      125.00 KHz
OBFIN      10500.0 Hz
POINT      32768
FREQU      27173.9 Hz
SCANS      512
ACQTM      1.206 sec
PD         1.794 sec
PW1        4.6 us
IRNUC      1H
CTEMP      24.2 c
SLVNT      CDCL3
EXREF      77.00 ppm
BF         0.12 Hz
RGAIN      24

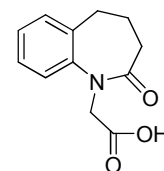
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F:\Takada\42Y-YT1-67-20.als

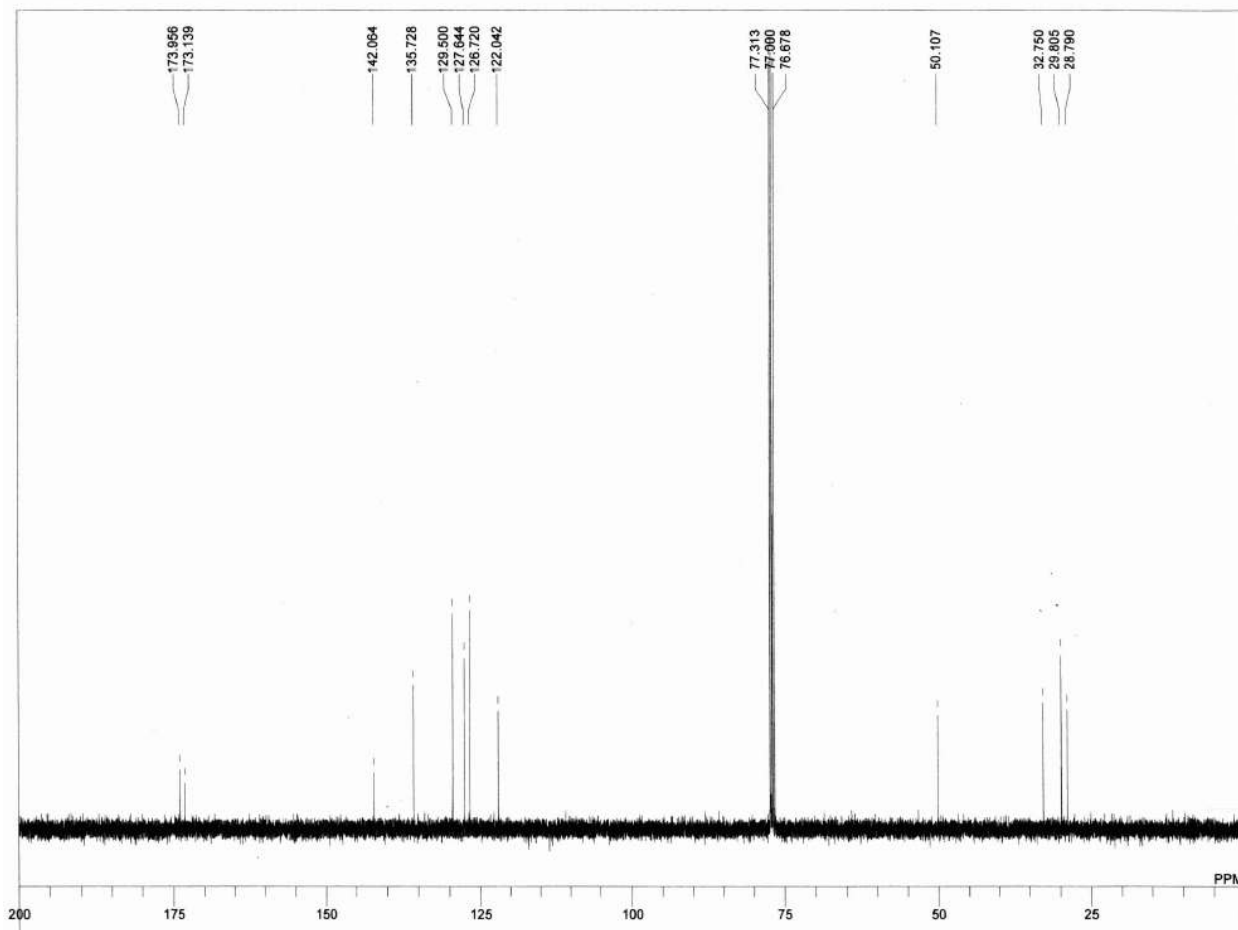


D:\Takada\42Y-YT1-67-20.als
 Thu Jul 30 14:31:5
 1H
 NON
 399.65 MHz
 124.00 KHz
 10500.0 Hz
 32768
 8000.0 Hz
 32
 4.096 sec
 2.904 sec
 6.2 us
 1H
 22.6 c
 CDCL3
 0.00 ppm
 0.12 Hz
 20

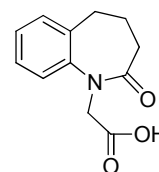


4c-COOH

F:\Takada\carbon\42Y-YT1-67-20.als

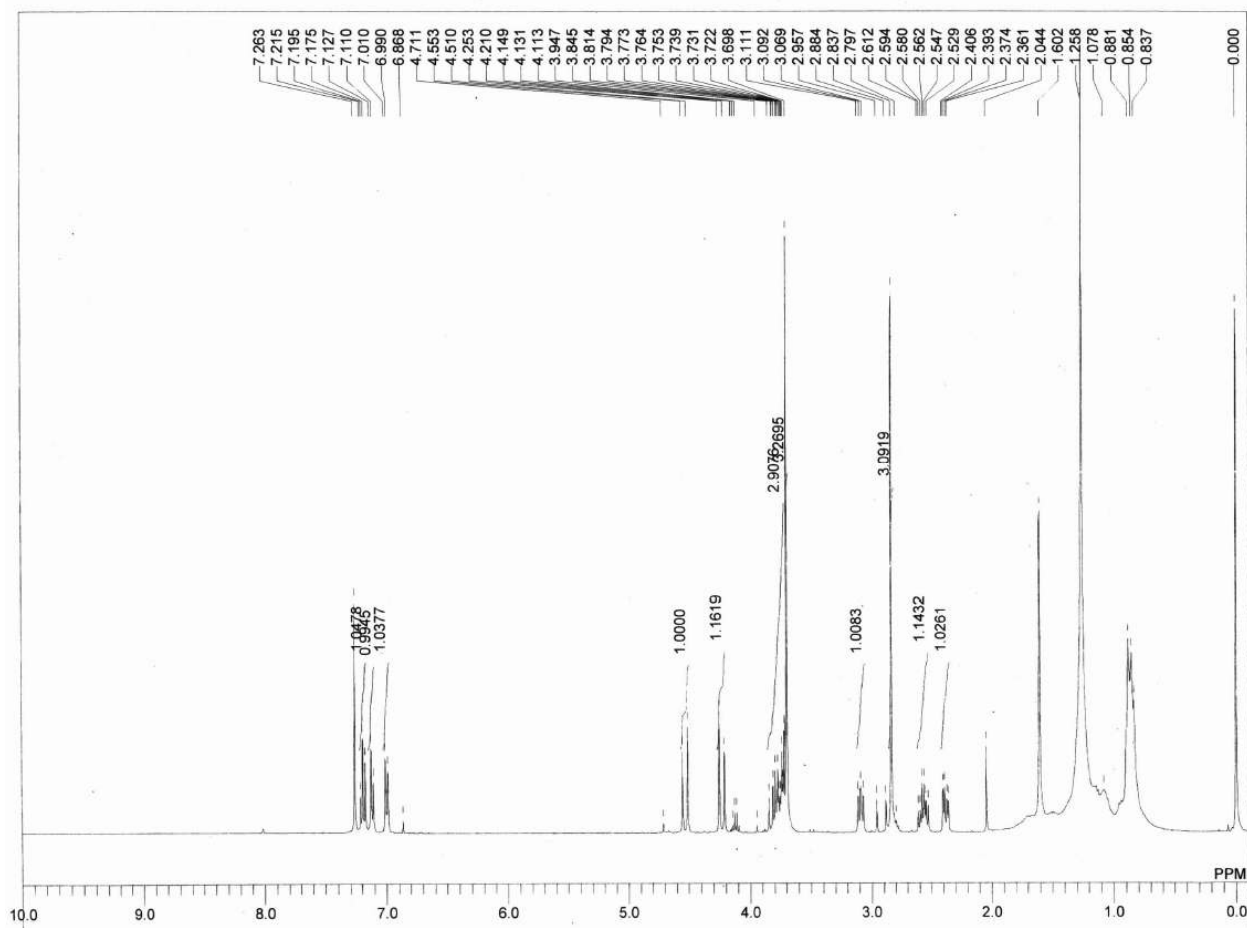


D:\Takada\carbon\42Y-YT1-67-20.als
 Sat Feb 19 14:05:2
 13C
 BCM
 100.40 MHz
 125.00 KHz
 10500.0 Hz
 32768
 27173.9 Hz
 512
 1.206 sec
 1.794 sec
 4.6 us
 1H
 25.5 c
 CDCL3
 77.00 ppm
 0.12 Hz
 24

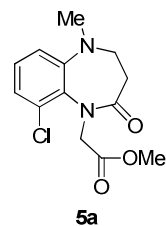


4c-COOH

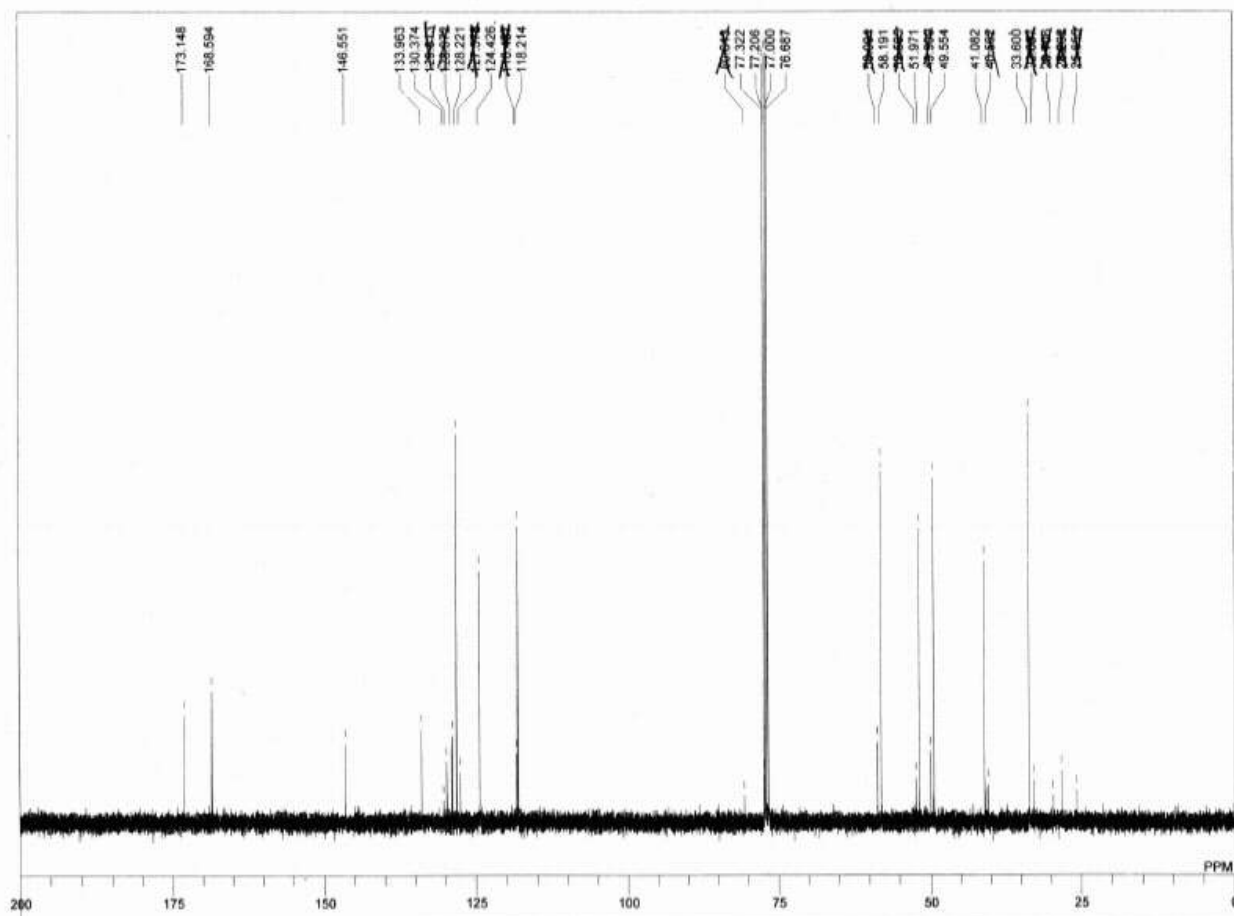
G:\Wada\42PNW1-138-25.als



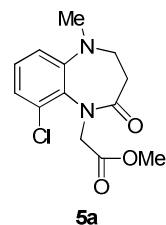
DFILE G:\Wada\42PN
COMNT Fri Aug 01 17:2
DATIM 1H
OBNUC NON
EXMOD
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 26.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 16



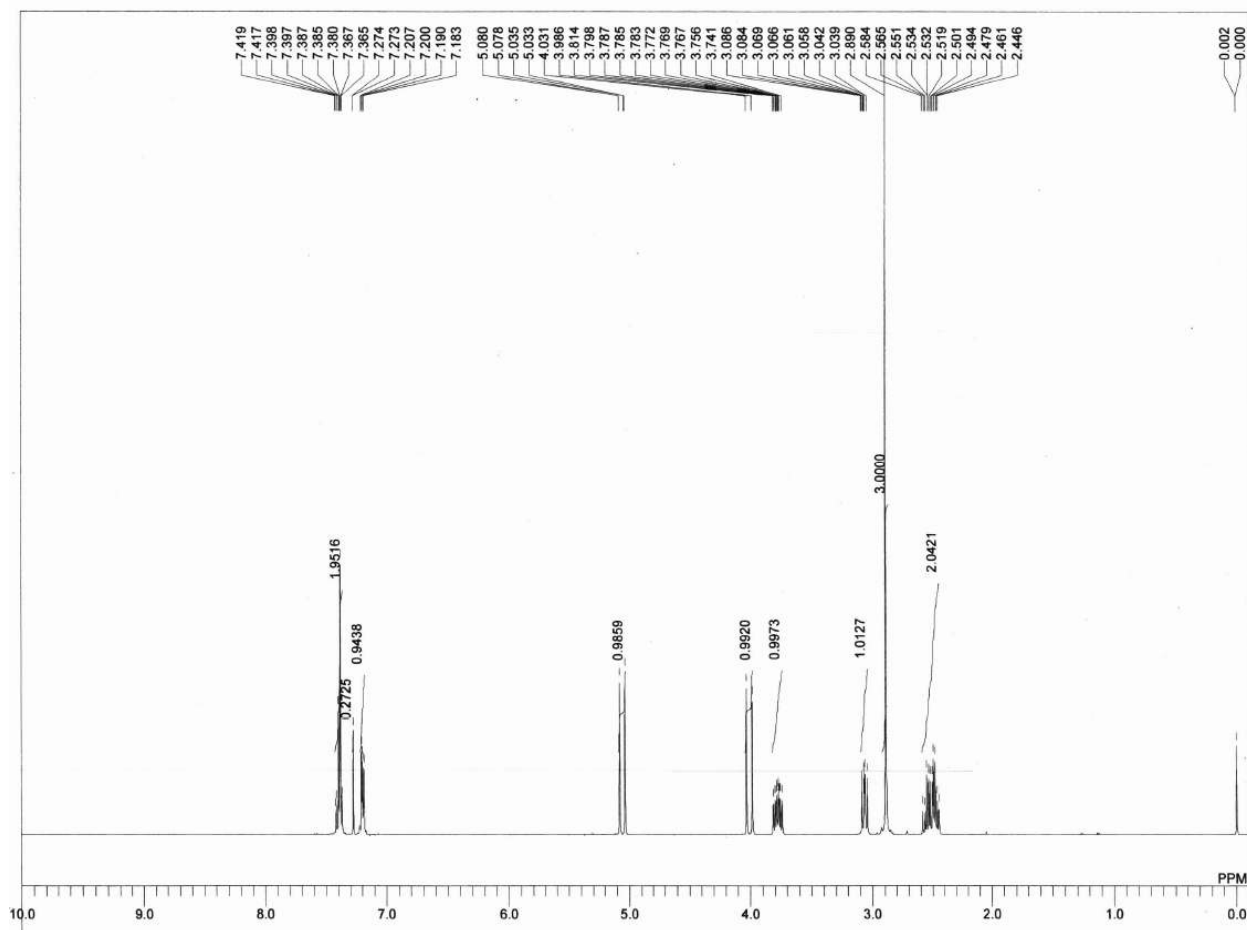
F:\Wada\42PNW-138-25-carbon.als



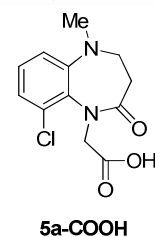
DFILE F:\Wada\42PNW-2
COMNT Thu Nov 12 14:21:
DATIM 13C
OBNUC BCM
EXMOD
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 512
ACQTM 1.206 sec
PD 1.794 sec
PW1 4.5 us
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24



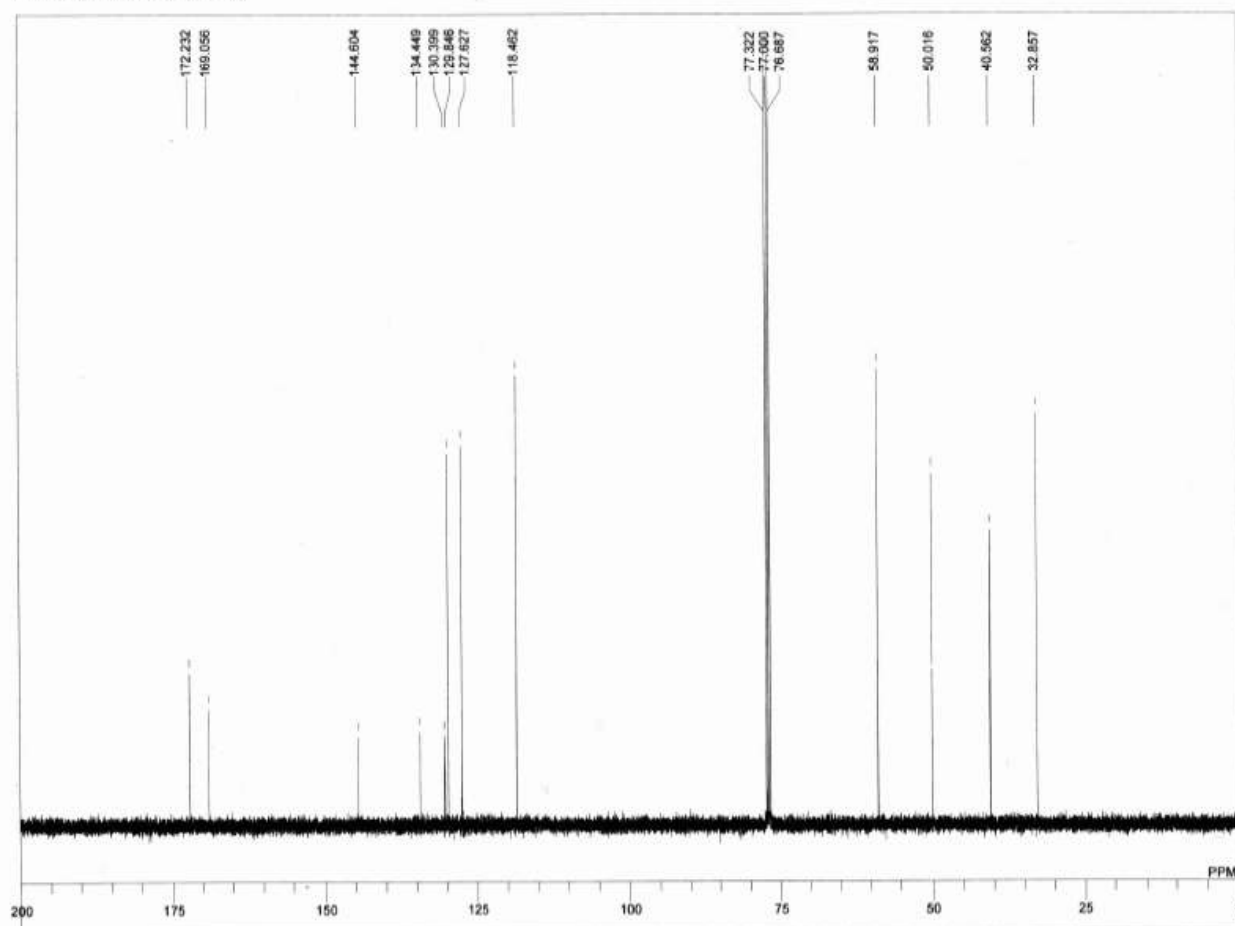
F:\Wada\42PNW-2-122-49.als



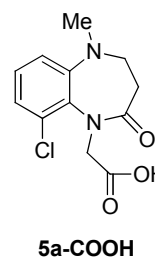
DFILE F:\Wada\42PNW-2
 COMNT Thu Nov 12 15:08:
 DATIM 1H
 OBNUC NON
 EXMOD 399.65 MHz
 OBFRQ 124.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 8000.0 Hz
 FREQU 16
 SCANS 4.096 sec
 ACQTM 2.904 sec
 PD 6.2 us
 PW1 1H
 IRNUC 22.7 c
 CTEMP CDCL3
 SLVNT 0.00 ppm
 EXREF 0.12 Hz
 BF 16
 RGAIN



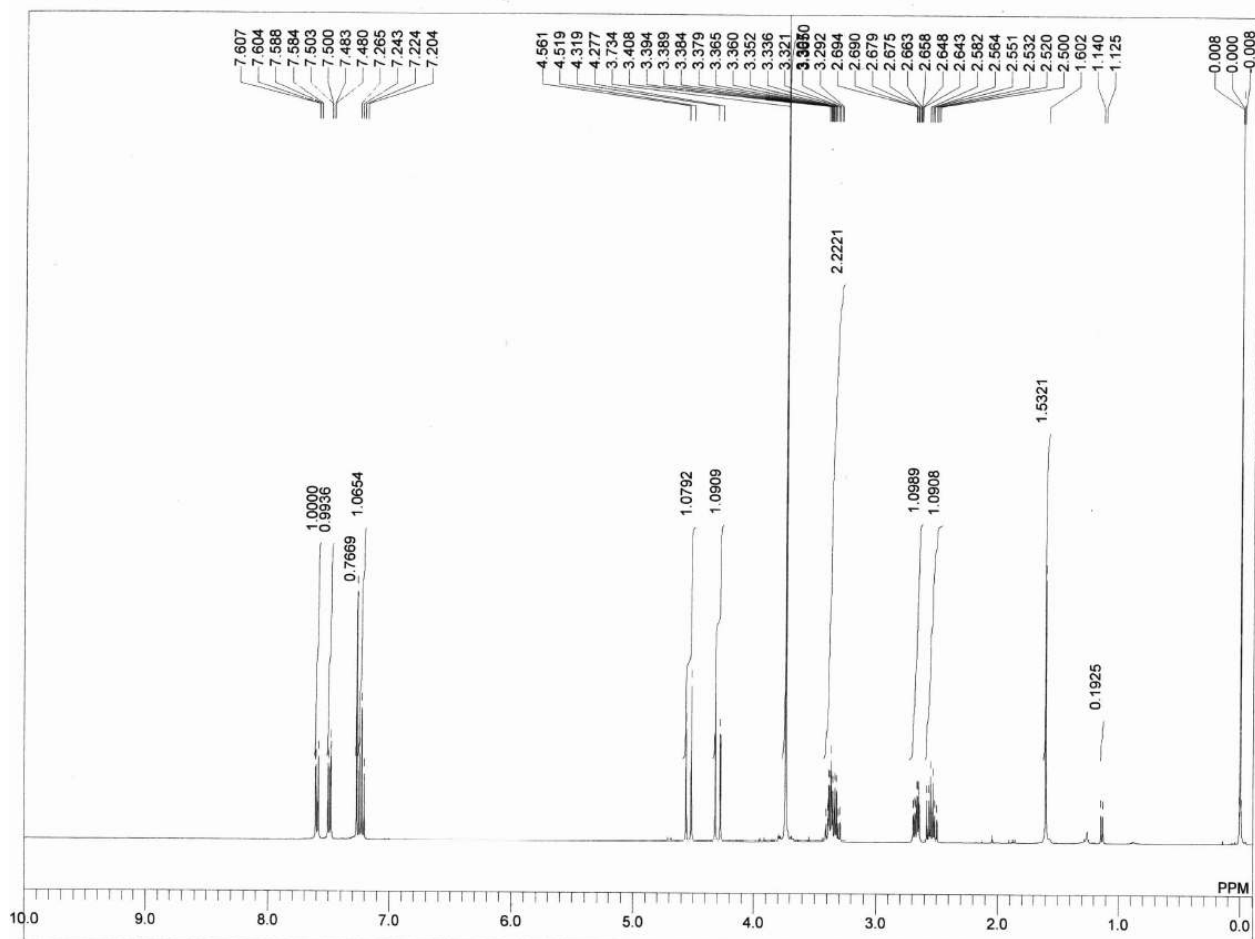
F:\Wada\42PNW-2-122-49-carbon.als



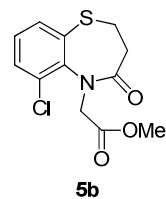
DFILE F:\Wada\42PNW-2
 COMNT Thu Nov 12 15:34:
 DATIM 13C
 OBNUC BCM
 EXMOD 100.40 MHz
 OBFRQ 125.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 27173.9 Hz
 FREQU 512
 SCANS 1.206 sec
 ACQTM 1.794 sec
 PD 4.6 us
 PW1 1H
 IRNUC 23.0 c
 CTEMP CDCL3
 SLVNT 77.00 ppm
 EXREF 0.12 Hz
 BF 24
 RGAIN



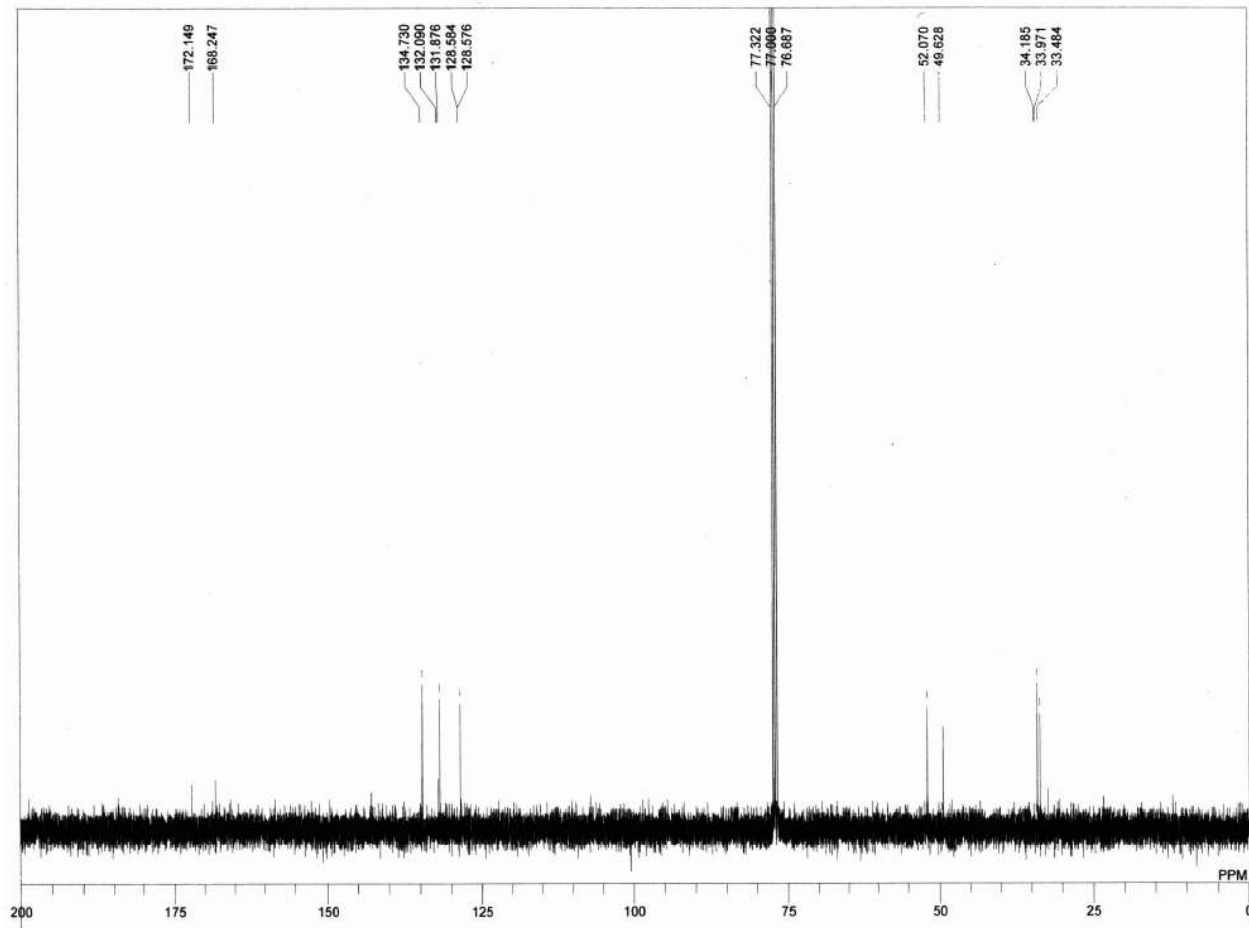
G:\Natsugari\42AHN2-65-25.als



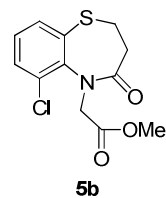
DFILE G:\Natsugari
COMNT Thu Dec 27 1
DATIM 1H
OBNUC NON
EXMOD
OBFRQ 399.65 MH
OBSET 124.00 KH
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 64
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20



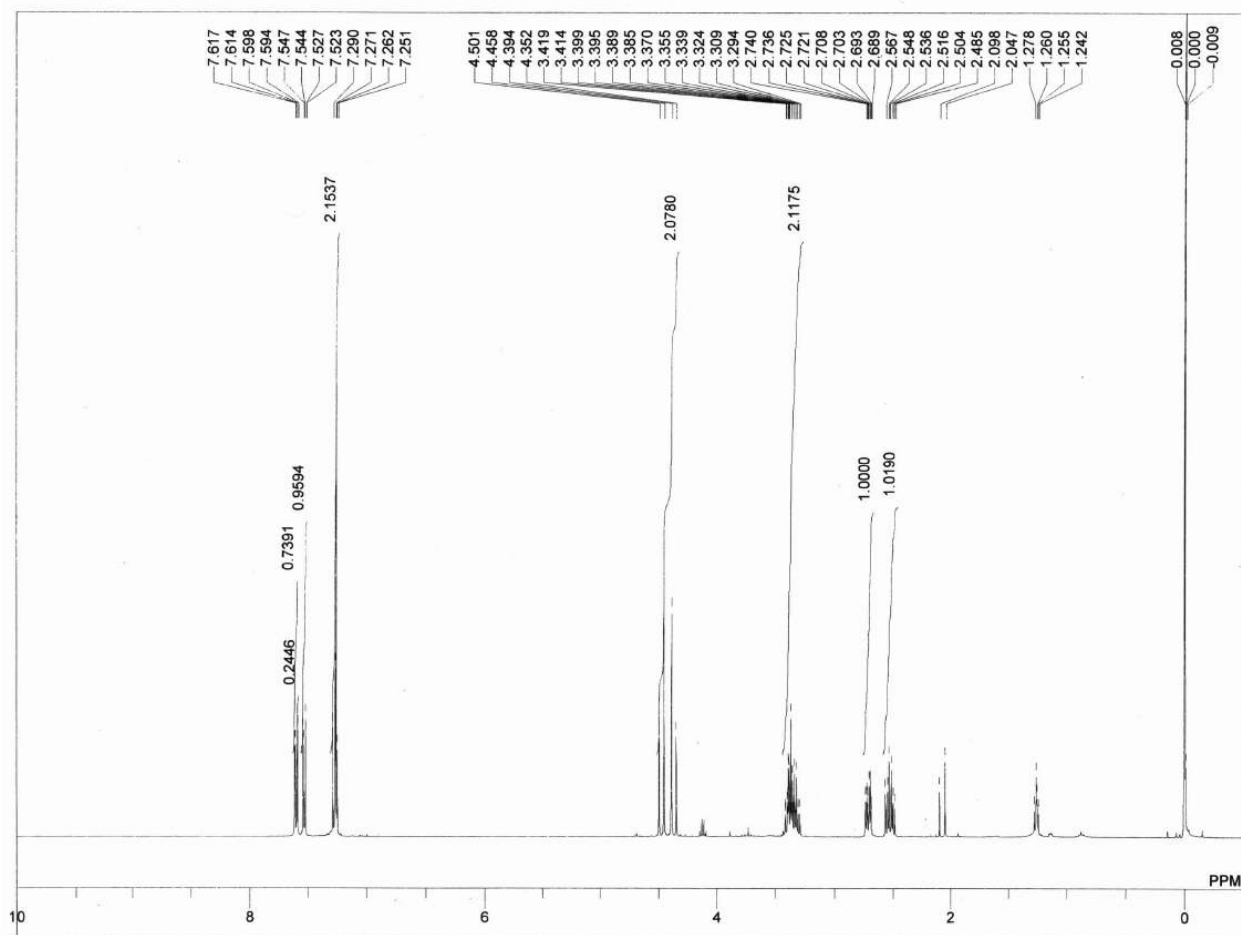
F:\Takada\carbon\42YYT1-174-32.als



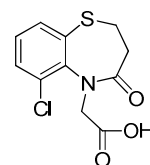
DFILE F:\Takada\carbon
COMNT Mon Nov 08 13:51
DATIM 13C
OBNUC BCM
EXMOD
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 200
ACQTM 1.206 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 25



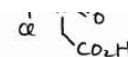
G:\Natsugari\42AHN2-68-20.als



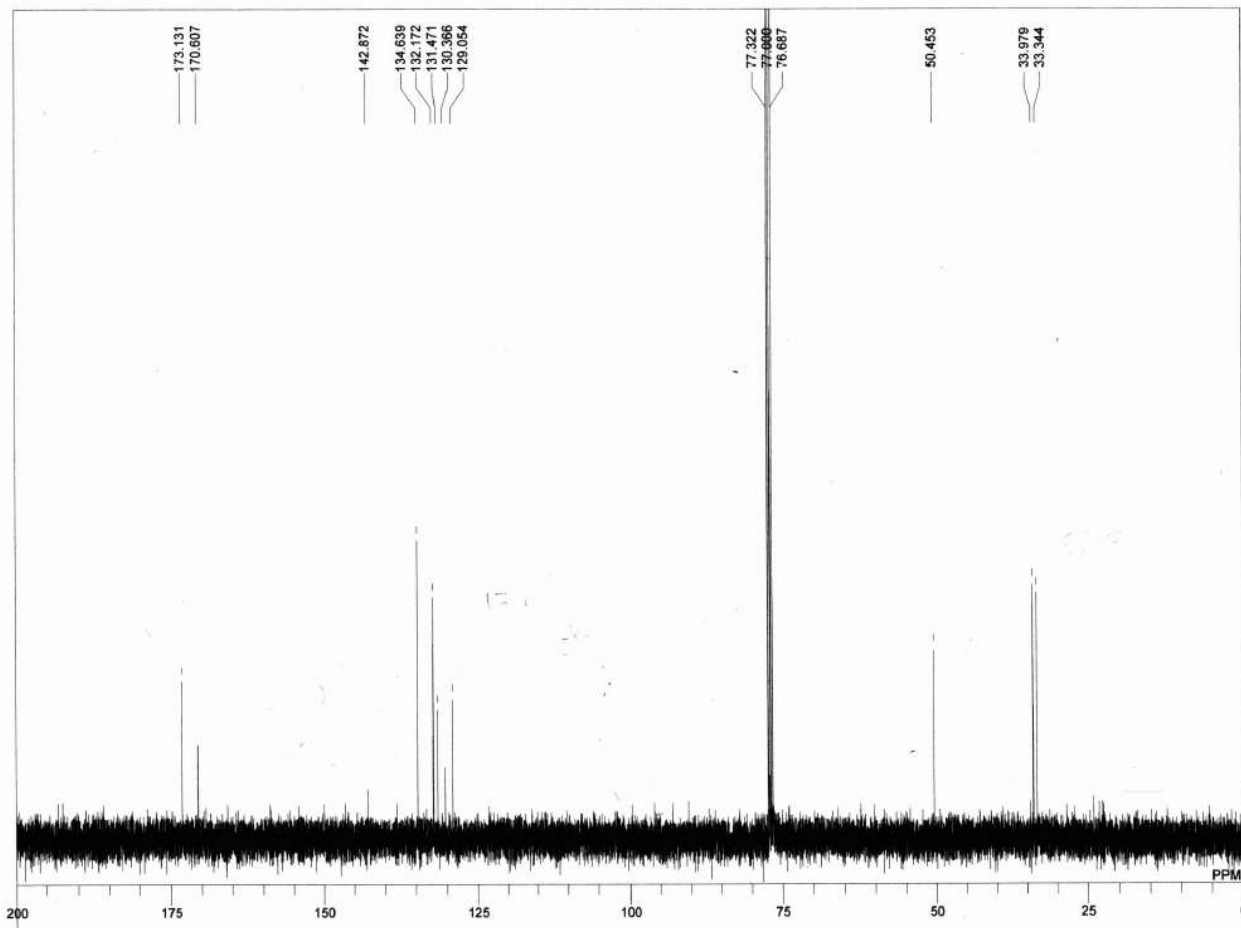
DFILE G:\Natsugari\4
COMINT
DATIM Sat Jan 12 13:
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 64
AQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 24.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 21



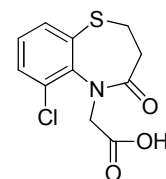
5b-COOH



P:\Takada\carbon\42YYT1-99-40.als

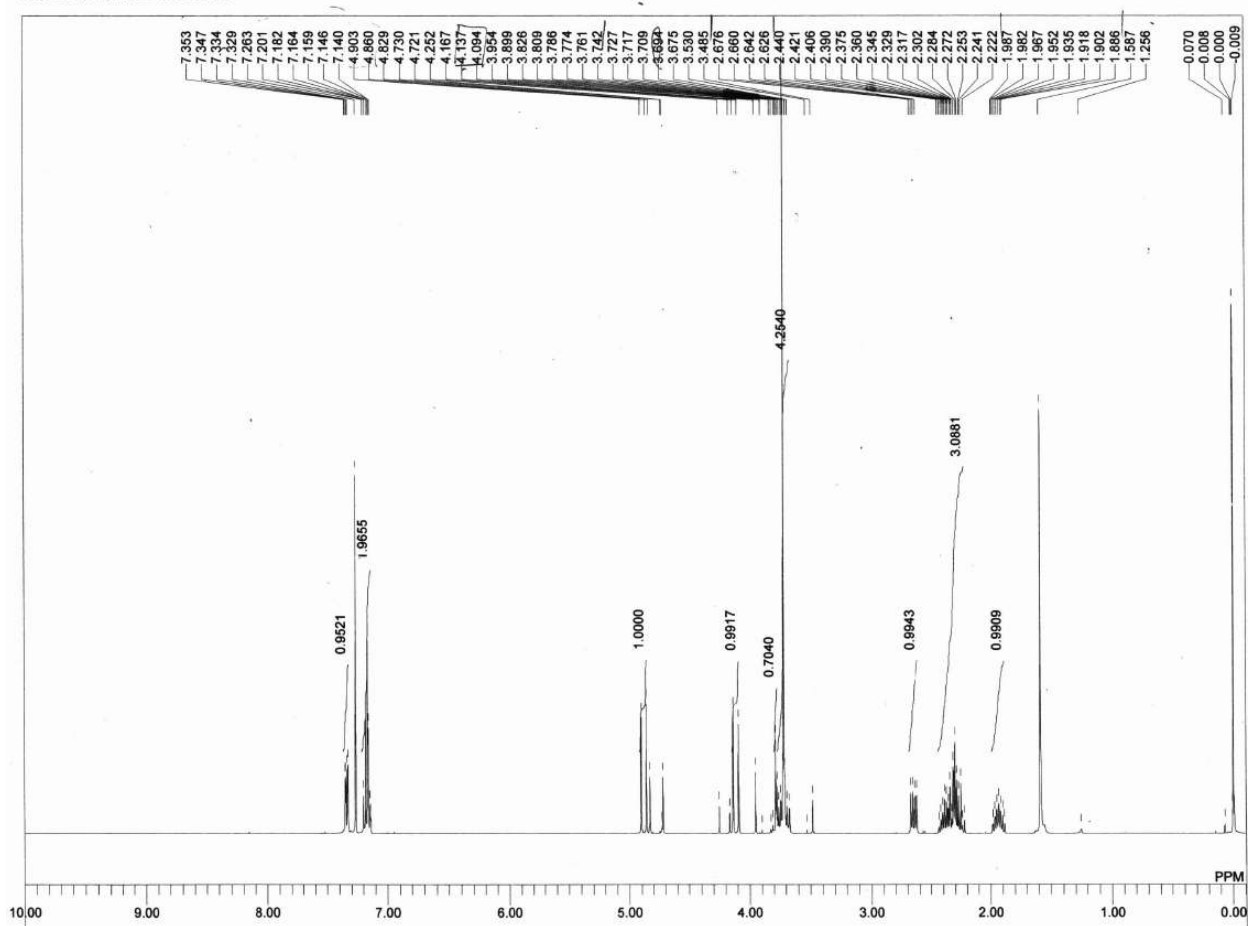


DFILE F:\Takada\carbon\4
COMINT
DATIM Tue Aug 10 09:52:
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 256
AQTM 1.206 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24

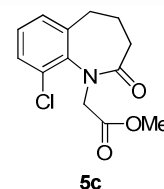


5b-COOH

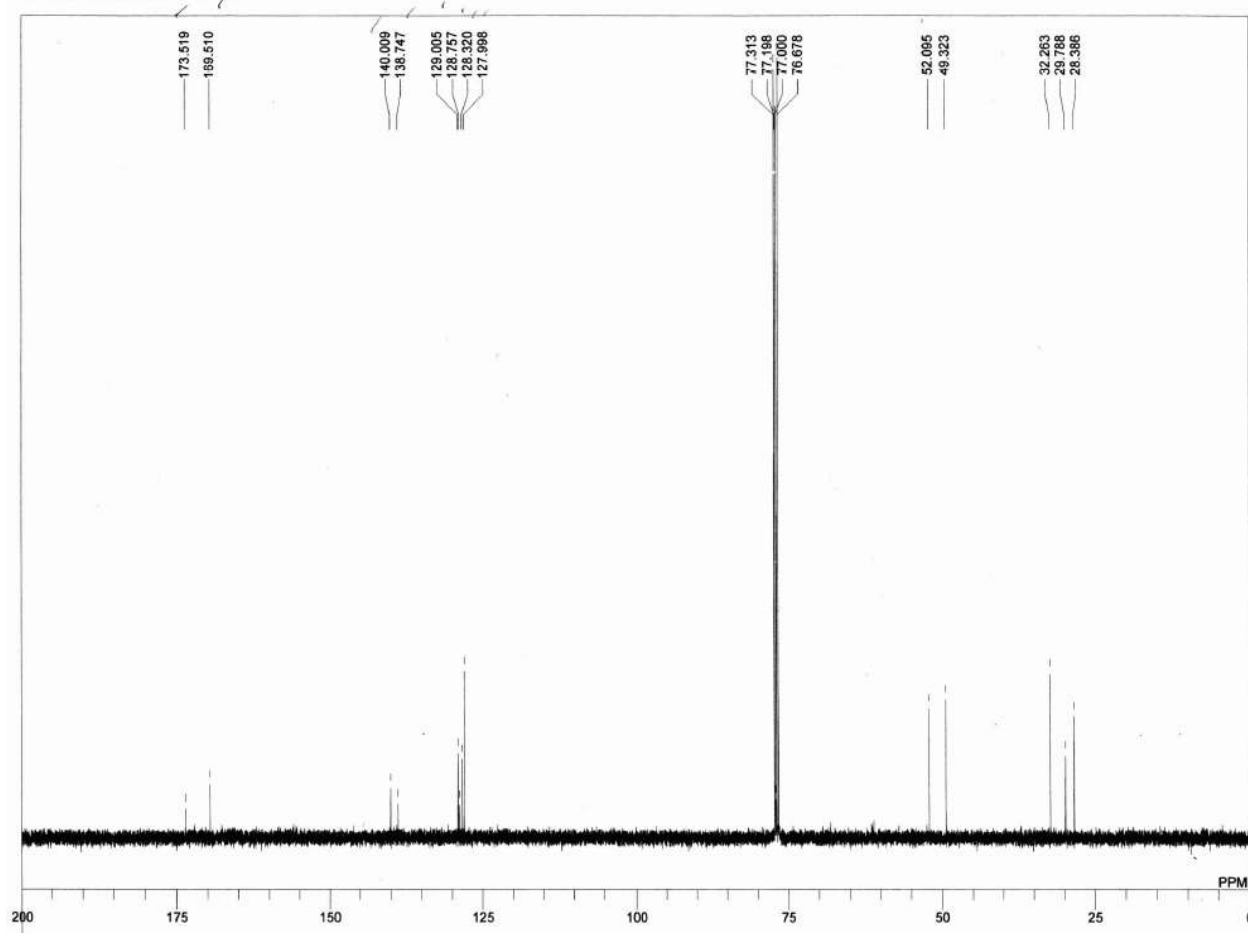
F:\Tabata\Hta942\JHTA9-60-37.als



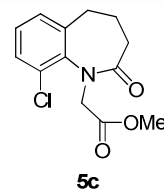
DFILE F:\Tabata\Hta942.J
 COMNT Sun Aug 29 12:51:
 DATIM 1H
 OBNUC NON
 EXMOD 399.65 MHz
 OBFRQ 124.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 8000.0 Hz
 FREQU 128
 SCANS 4.096 sec
 ACQTM 2.904 sec
 PD 6.2 us
 PW1 1H
 IRNUC 24.2 c
 CTEMP CDCL3
 SLVNT 0.00 ppm
 EXREF 0.12 Hz
 BF 20
 RGAIN



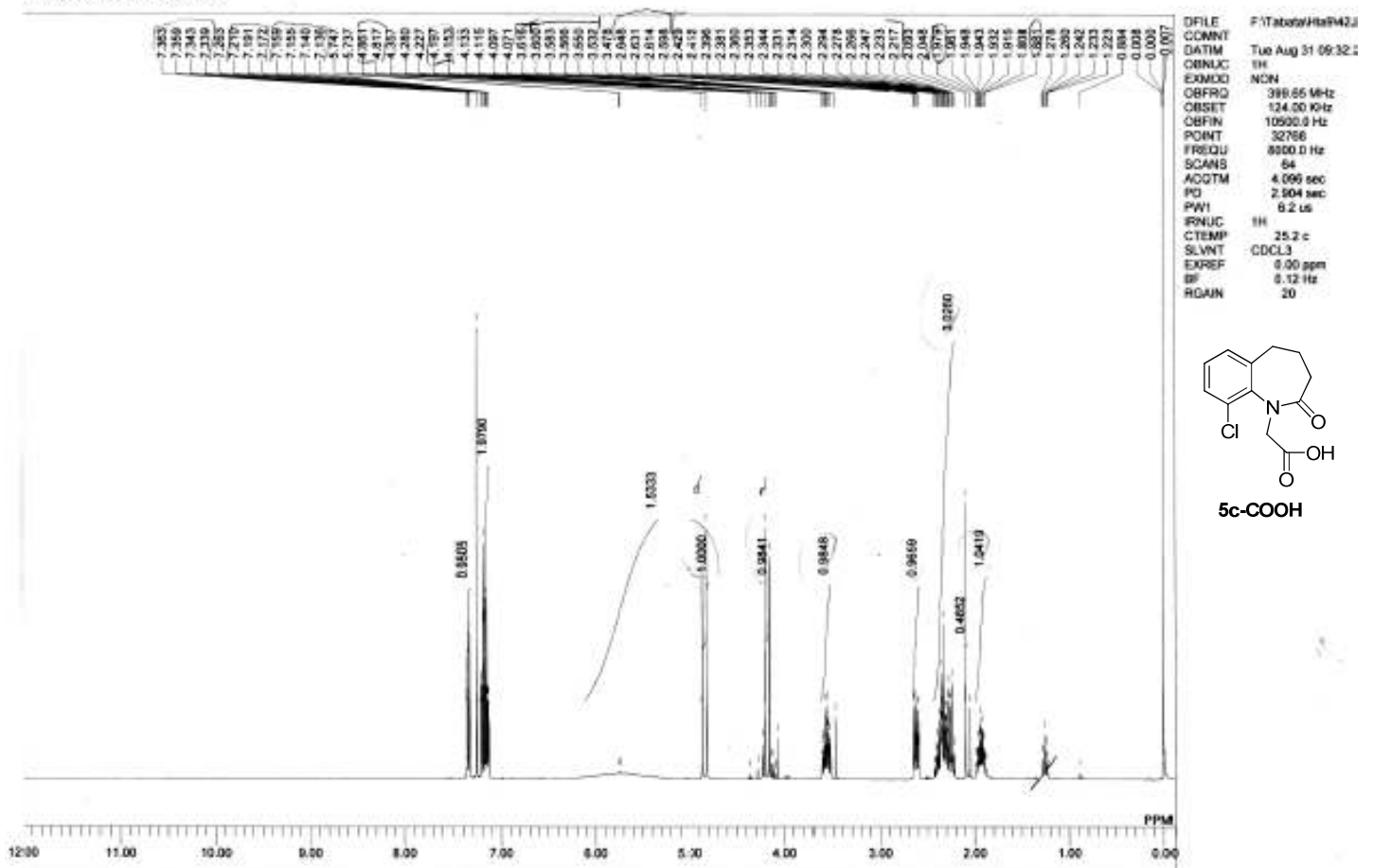
F:\Tabata\Hta942\JHTA9-60-37-C.als



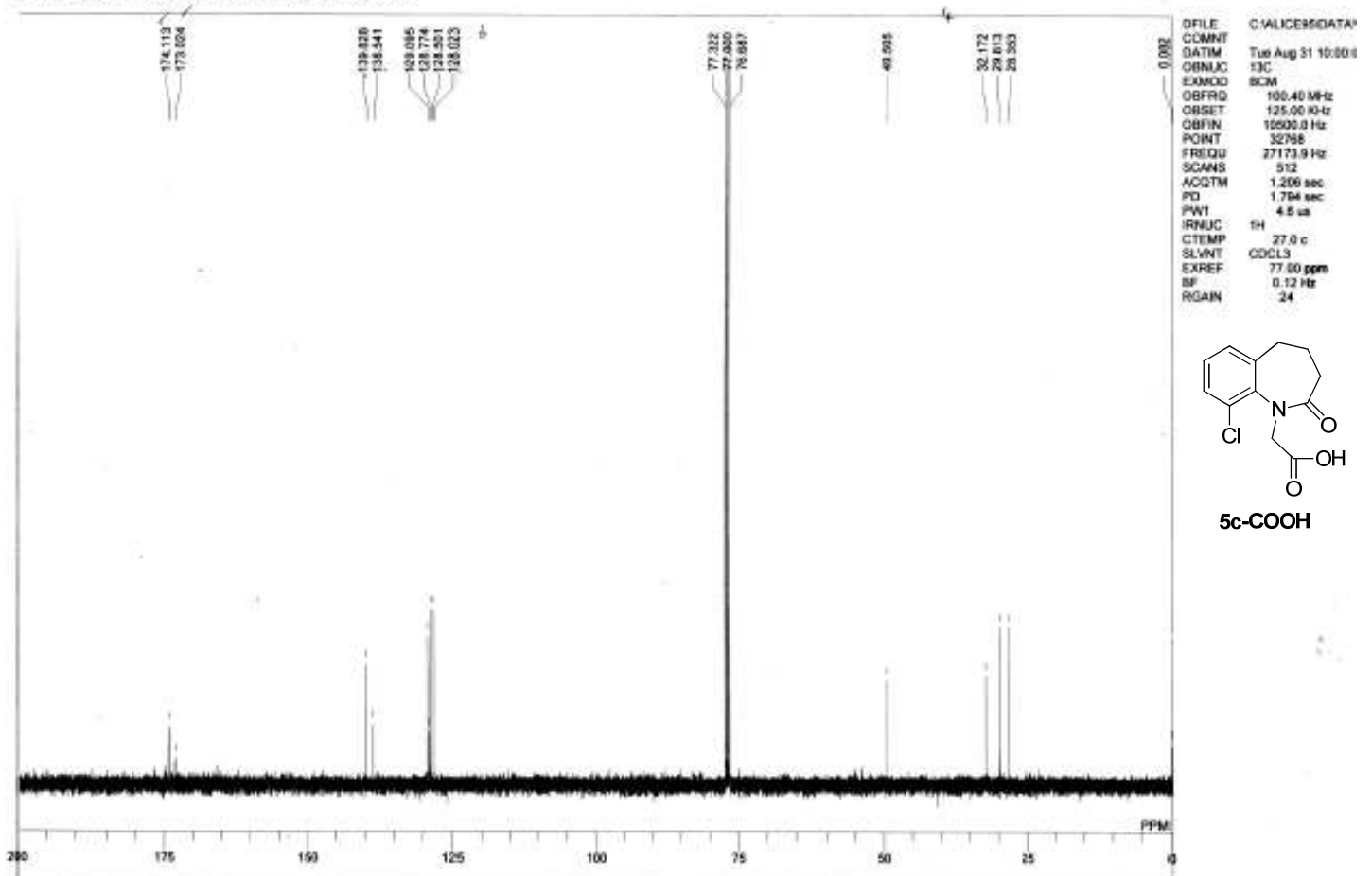
DFILE F:\Tabata\Hta942.J
 COMNT Sun Aug 29 13:47:
 DATIM 13C
 OBNUC BCM
 EXMOD 100.40 MHz
 OBFRQ 125.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 27173.9 Hz
 FREQU 1024
 SCANS 1.206 sec
 ACQTM 1.794 sec
 PD 4.6 us
 PW1 1H
 IRNUC 25.4 c
 CTEMP CDCL3
 SLVNT 77.00 ppm
 EXREF 0.12 Hz
 BF 25
 RGAIN



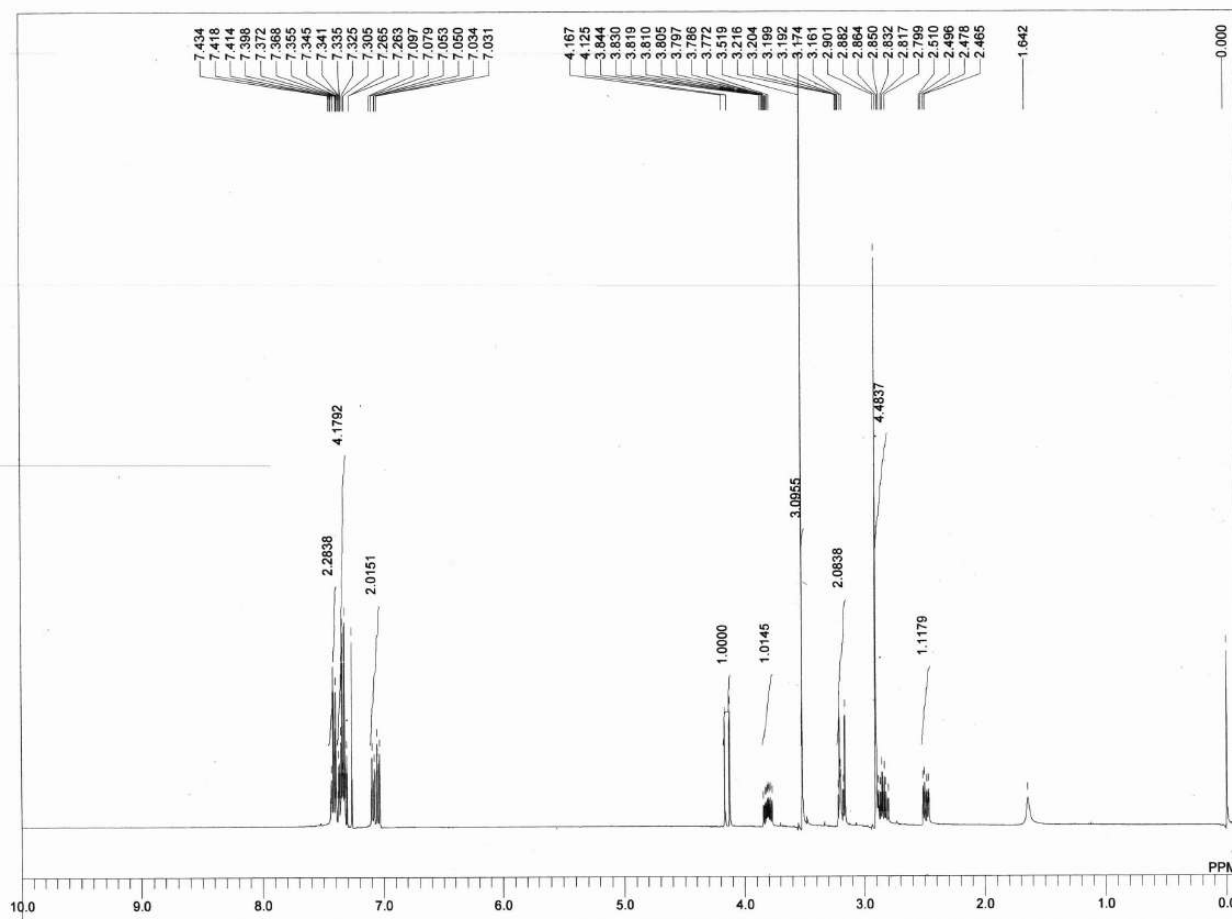
F:\Tabata\Hmr\H42\HTA9-80-49.ab



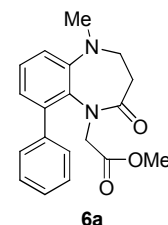
C:\ALICER5\DATA\Tabata\2006.10\H42\HTA9-80-49-C.ab



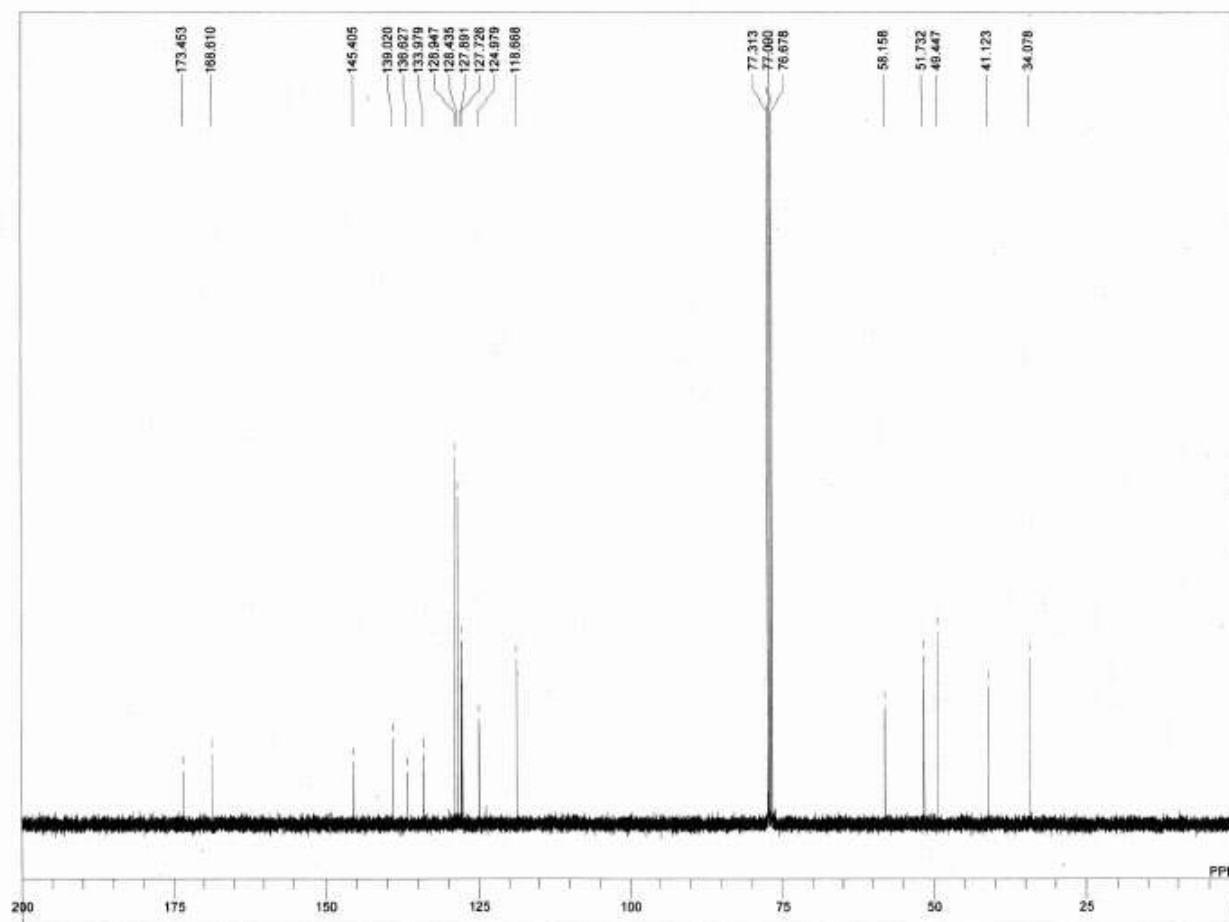
F:\Wada\42PNW-2-117-25.als



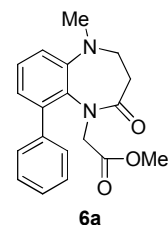
DFILE F:\Wada\42PNW-2
 COMNT Wed Nov 11 20:06
 DATIM 1H
 OBNUC NON
 EXMOD 399.65 MHz
 QBFRQ 124.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 8000.0 Hz
 FREQU 16
 SCANS 4.096 sec
 ACQTM 2.904 sec
 PD 6.2 us
 PW1 1H
 IRNUC 21.8 c
 CTEMP CDCL3
 SLVNT 0.00 ppm
 EXREF BF 0.12 Hz
 RGAIN 16

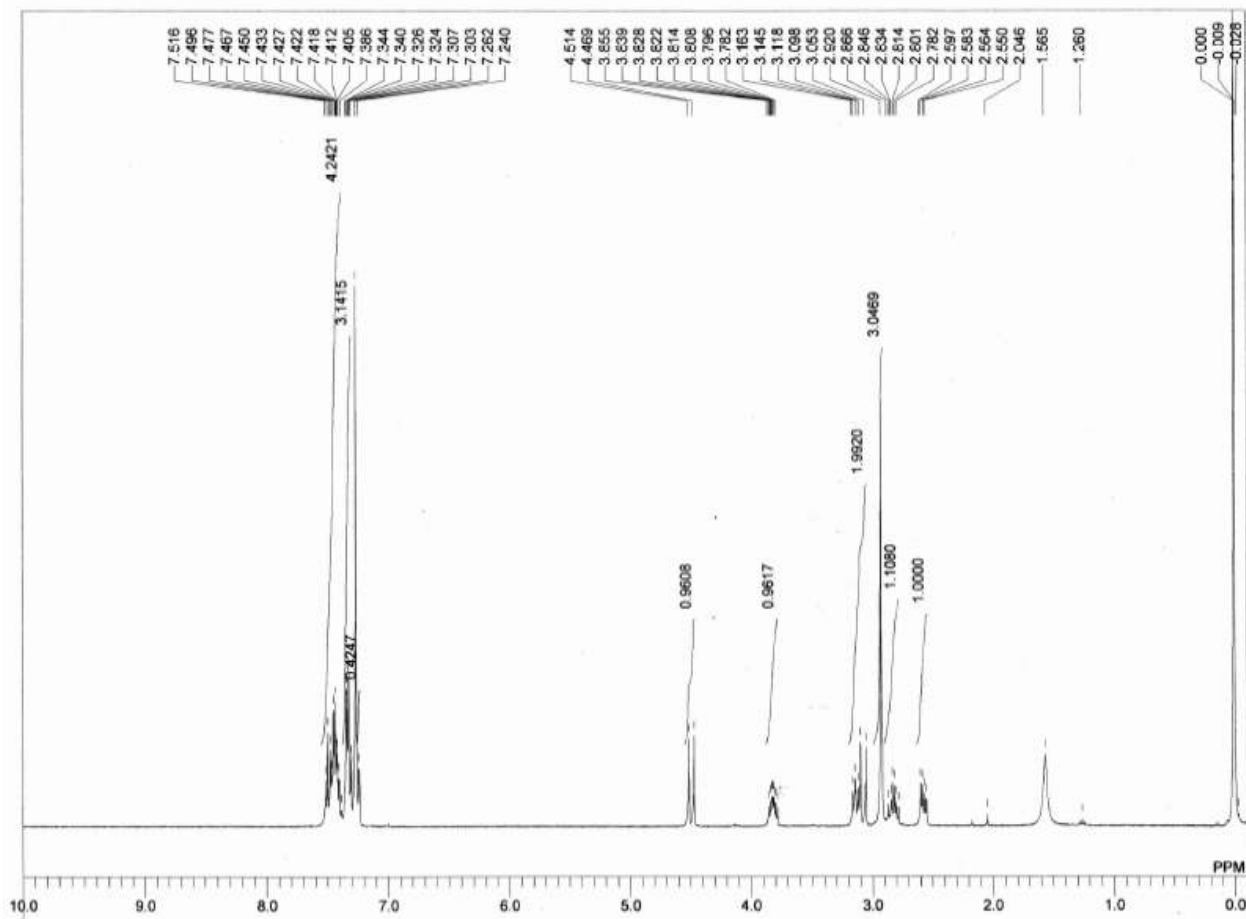


F:\Wada\42PNW-2-117-25-carbon.als

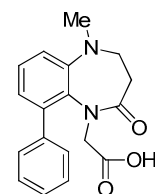


DFILE F:\Wada\42PNW-2
 COMNT Wed Nov 11 20:32
 DATIM 13C
 OBNUC BCM
 EXMOD 100.40 MHz
 QBFRQ 125.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 27173.9 Hz
 FREQU 512
 SCANS 1.206 sec
 ACQTM 1.794 sec
 PD 4.6 us
 PW1 1H
 IRNUC 22.6 c
 CTEMP CDCL3
 SLVNT 77.00 ppm
 EXREF BF 0.12 Hz
 RGAIN 24



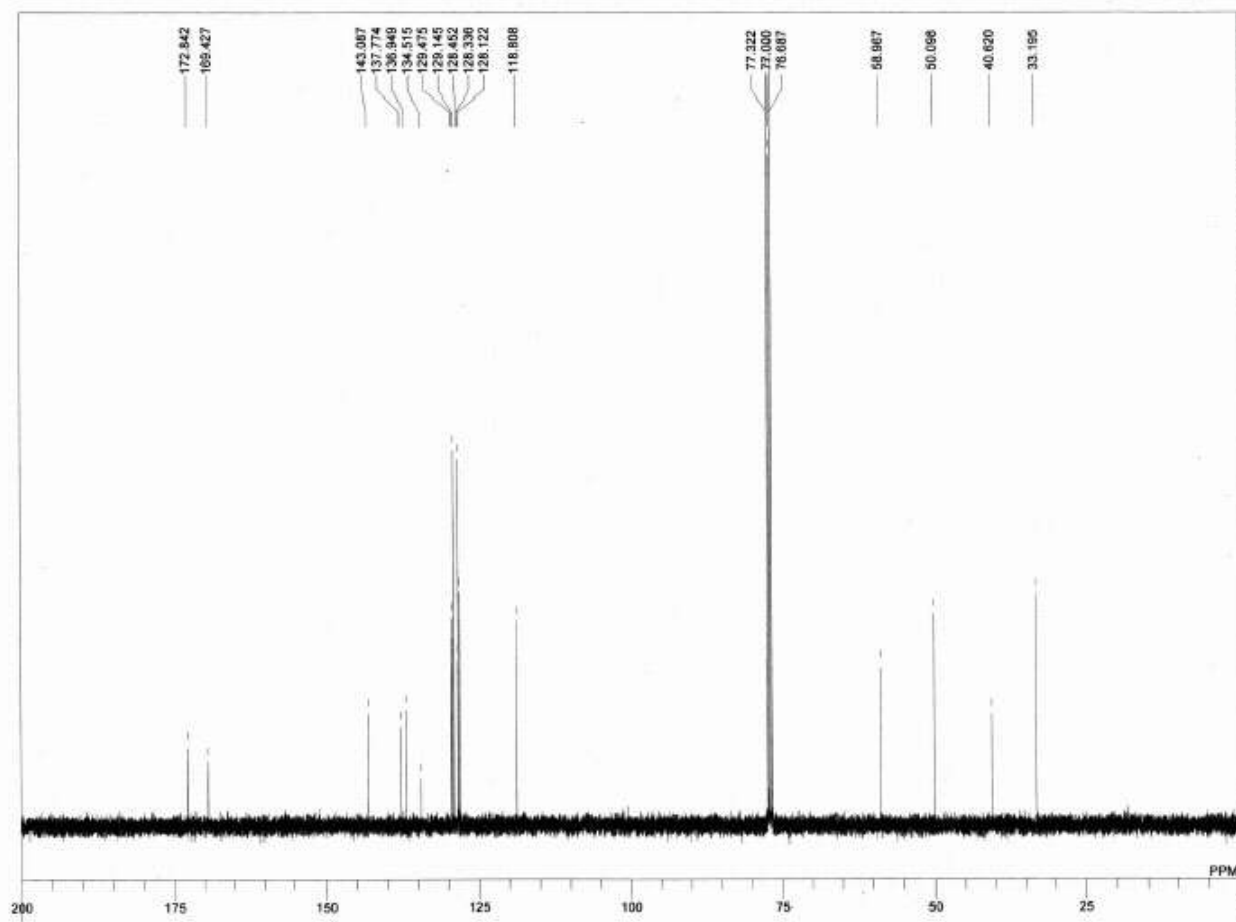


DFILE G:\Wada\42PNW-2
COMNT
DATIM Fri Apr 24 19:21
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 16
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 21

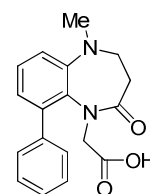


6a-COOH

F:\Wada\42PNW-2-189-39-carbon.als

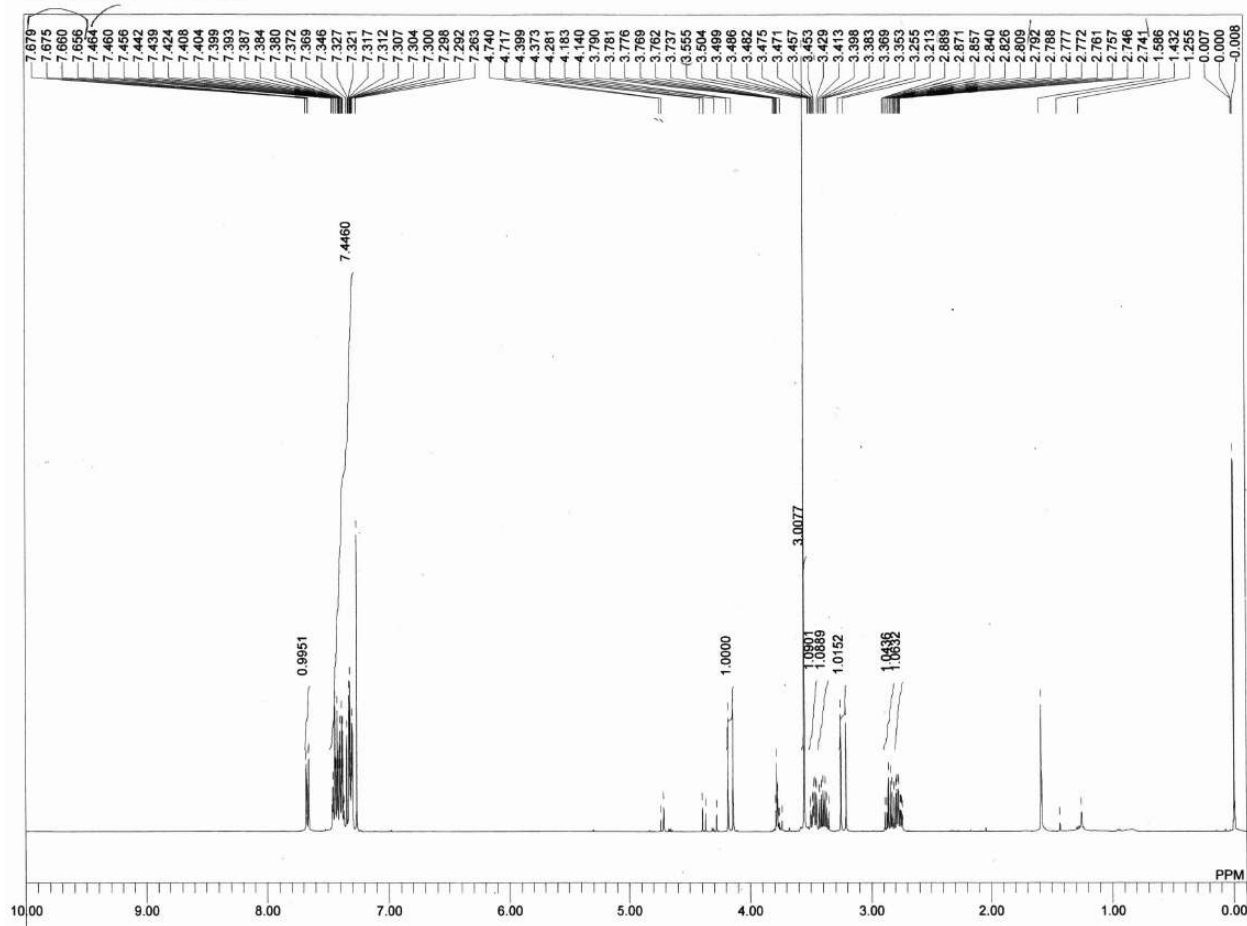


DFILE F:\Wada\42PNW-2
COMNT
DATIM Wed Nov 11 21:07
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 512
ACQTM 1.206 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24

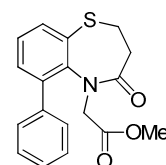


6a-COOH

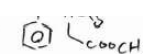
F:\Tabata\Hta9\42JHTA9-105-35H.als



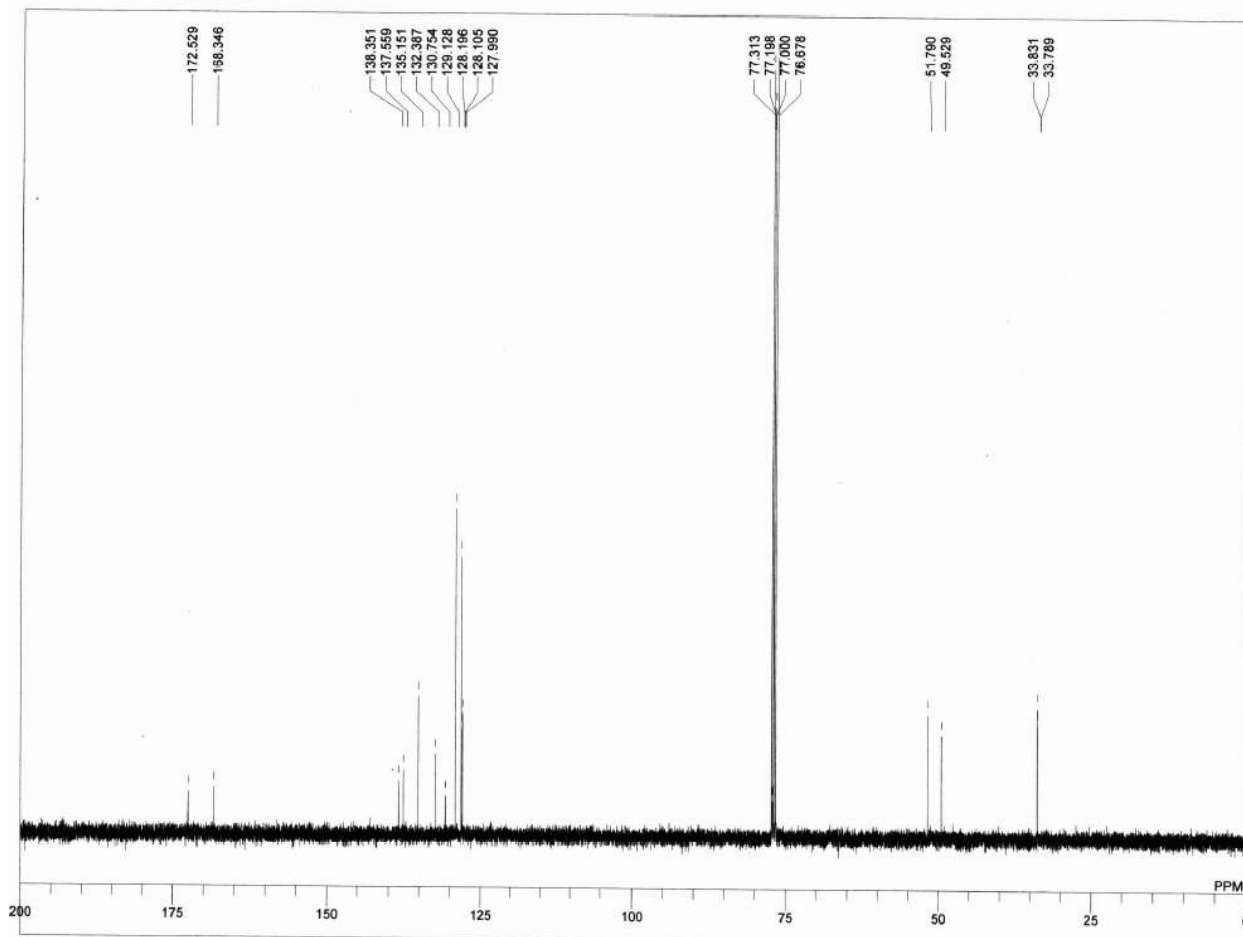
DFILE F:\Tabata\Hta9\42J
COMNT
DATIM Tue Mar 08 15:51:1
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 64
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19



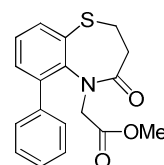
6b



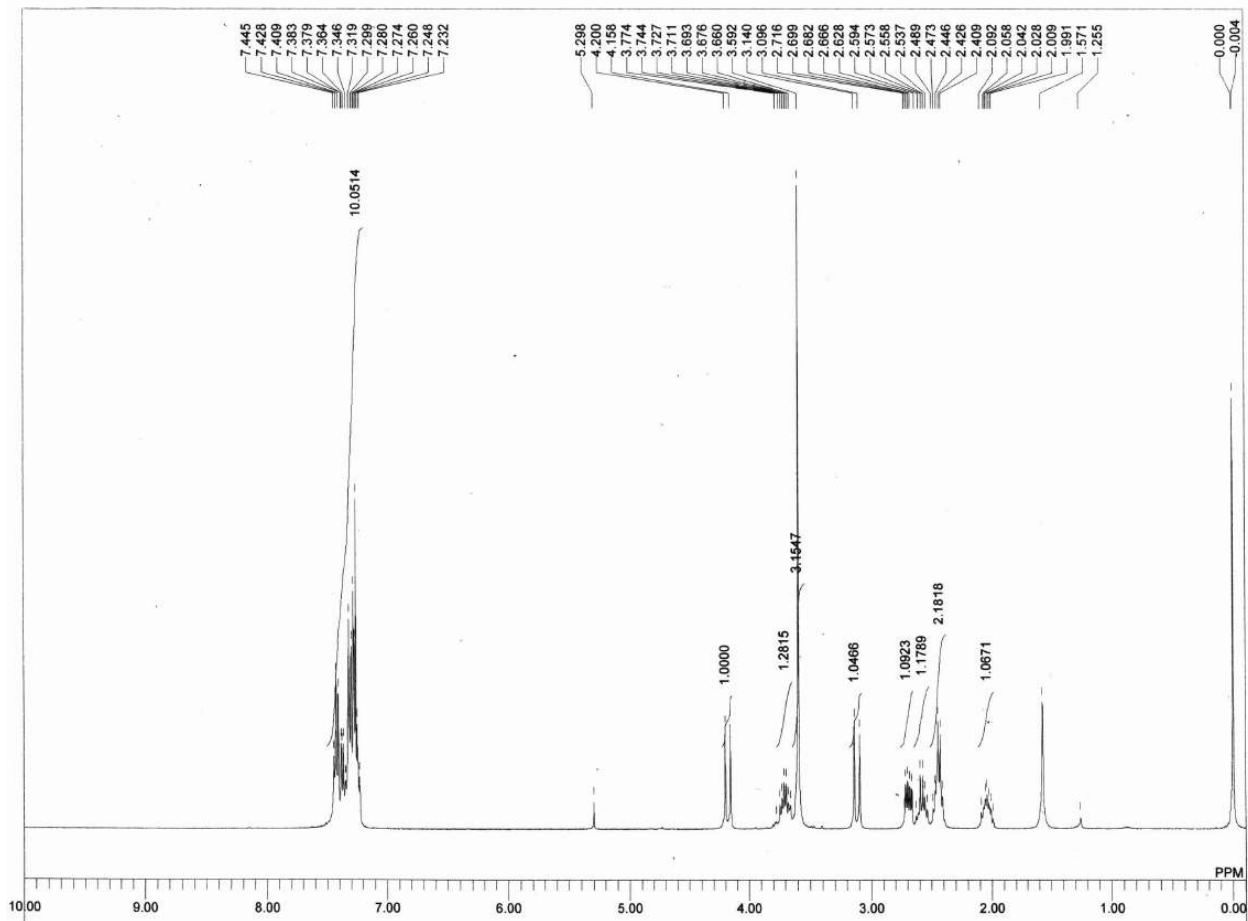
F:\Tabata\Hta9\42JHTA9-105-35C.als



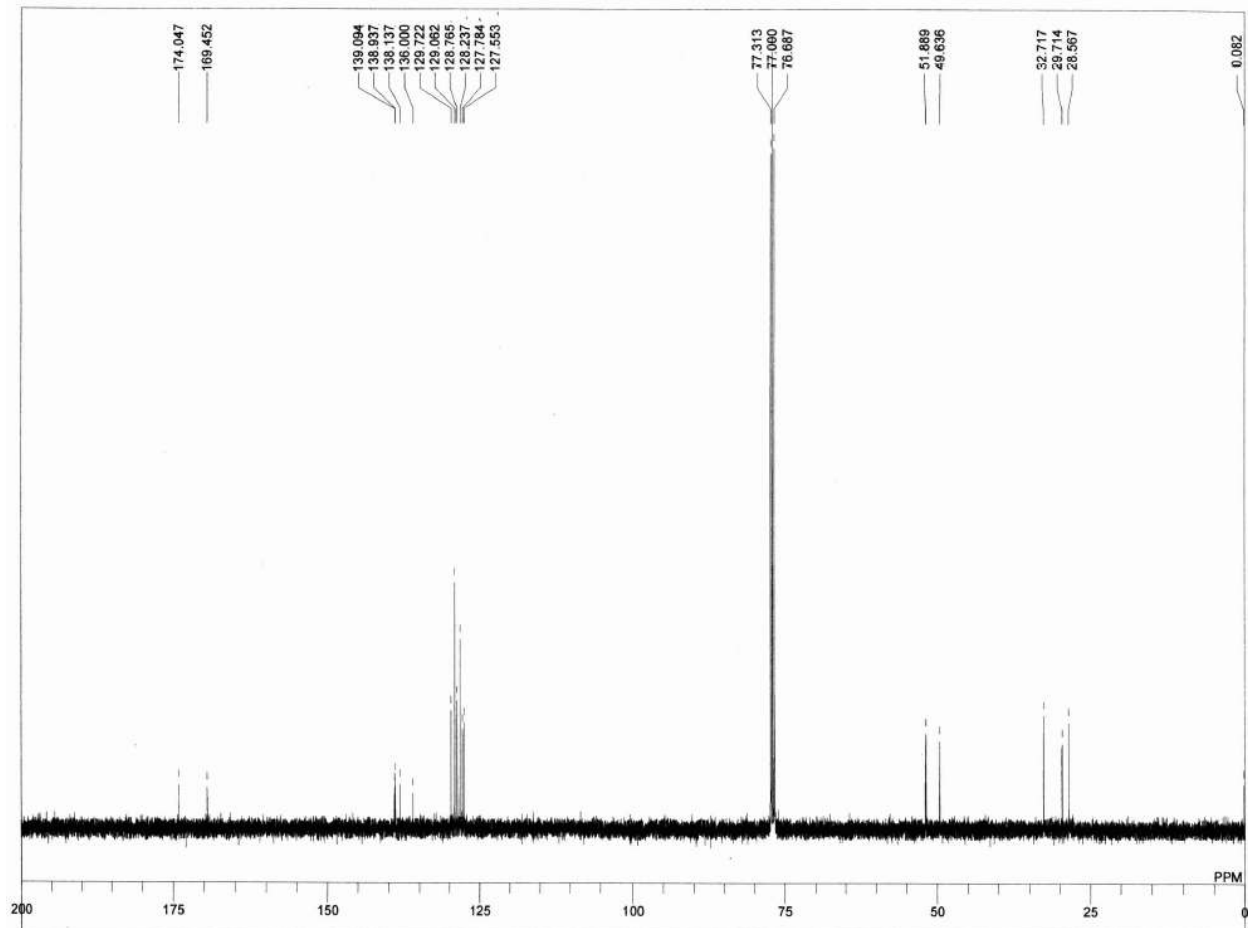
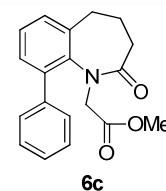
DFILE F:\Tabata\Hta9\42J
COMNT
DATIM Tue Mar 08 16:24:
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 512
ACQTM 1.208 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 24.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24



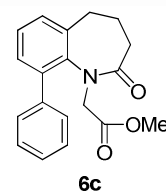
6b



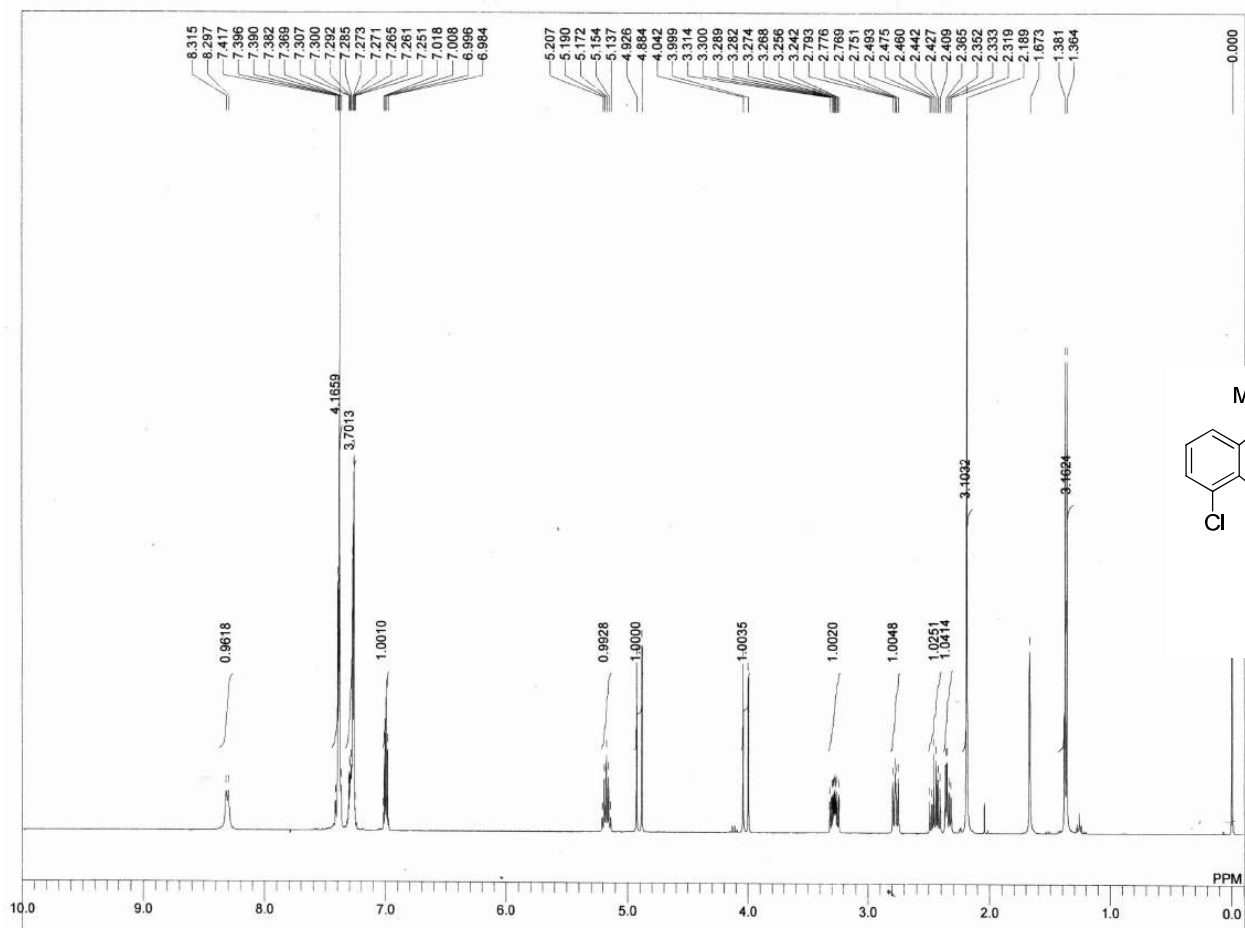
DFILE F:\Tabata\Hta9\42J
 COMNT Mon Feb 07 16:10:
 DATIM 1H
 OBNUC 1H
 EXMOD NON
 OBFRQ 399.65 MHz
 OBSET 124.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 4.096 sec
 PD 2.904 sec
 PW1 6.2 us
 IRNUC 1H
 CTEMP 25.7 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 20



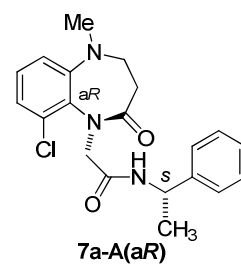
DFILE F:\Tabata\Hta9\42J
 COMNT Mon Feb 07 16:59:
 DATIM 13C
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27173.9 Hz
 SCANS 1024
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 4.6 us
 IRNUC 1H
 CTEMP 26.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24



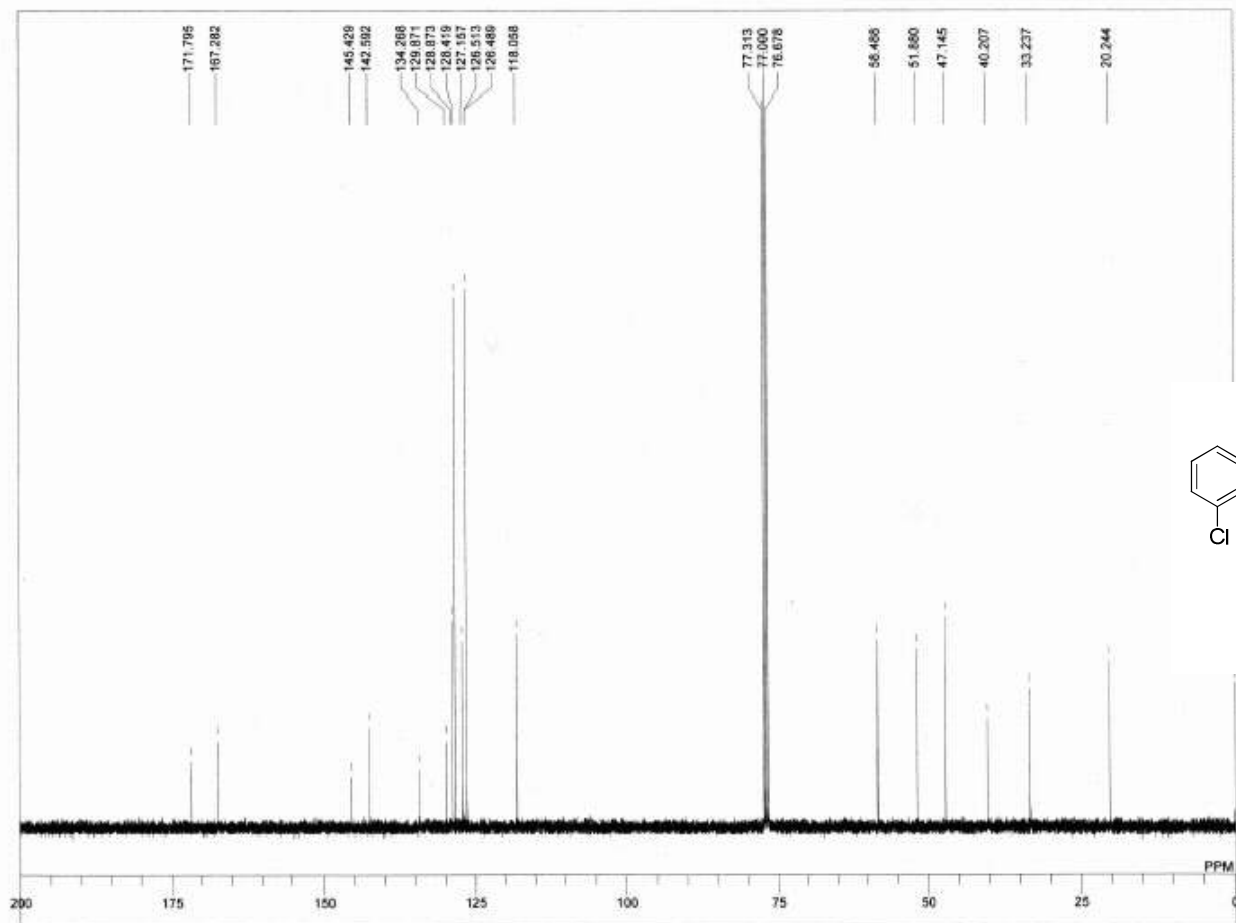
F:\Wada\42PNW2-69-35.als



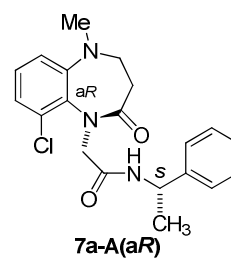
DFILE F:\Wada\42PNW2-
 COMNT Mon Dec 28 22:09:
 DATIM 1H
 OBNUC 1H
 EXMOD NON
 OBFRQ 399.65 MHz
 OBSET 124.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 4.096 sec
 PD 2.904 sec
 PW1 6.2 us
 IRNUC 1H
 CTEMP 23.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 18



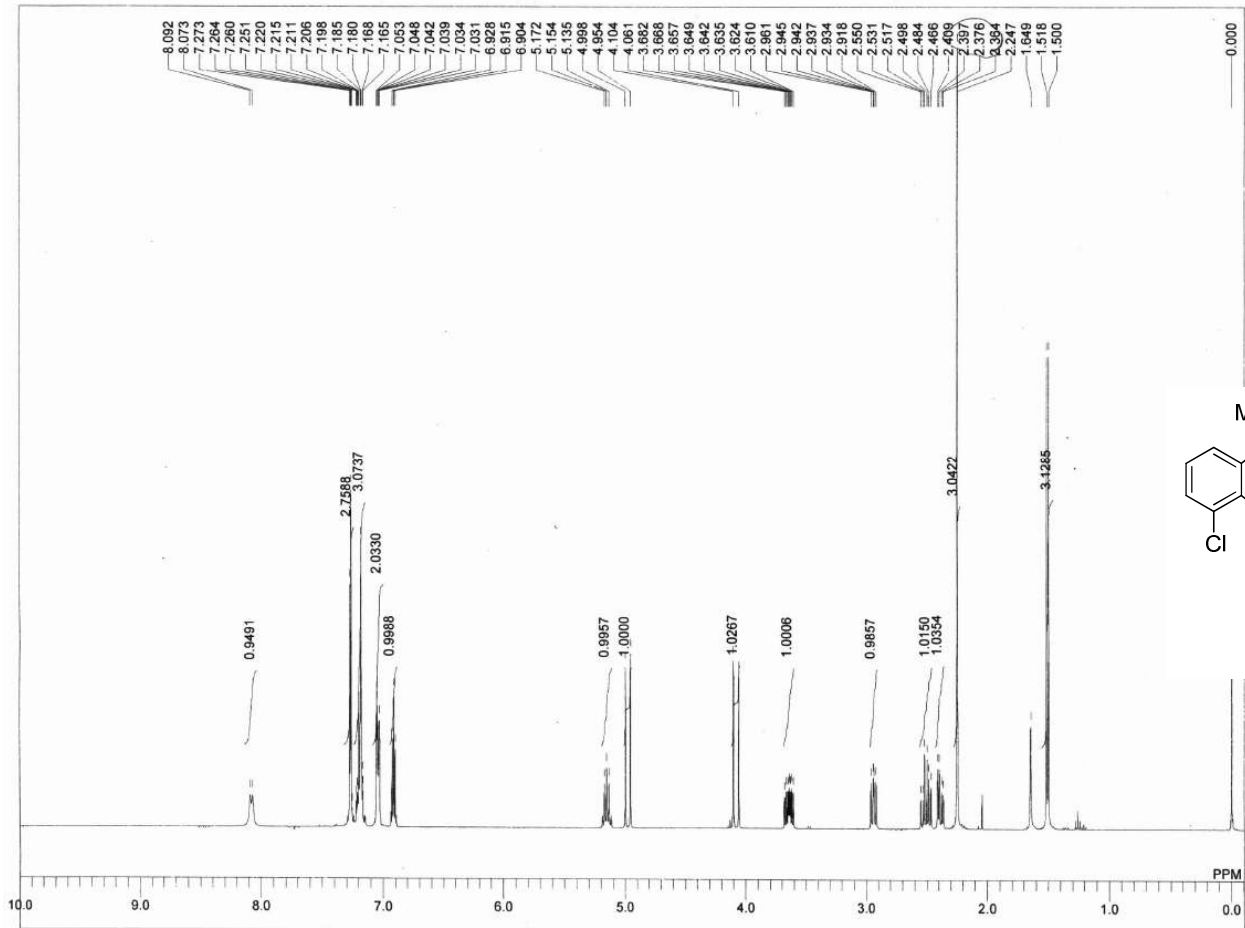
F:\Wada\42PNW2-69-35-carbon.als



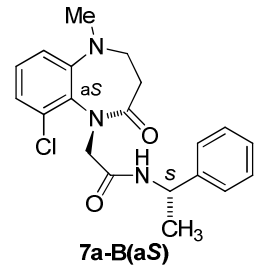
DFILE F:\Wada\42PNW2-
 COMNT Mon Dec 28 22:58:
 DATIM 13C
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27173.9 Hz
 SCANS 1024
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 4.6 us
 IRNUC 1H
 CTEMP 24.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24



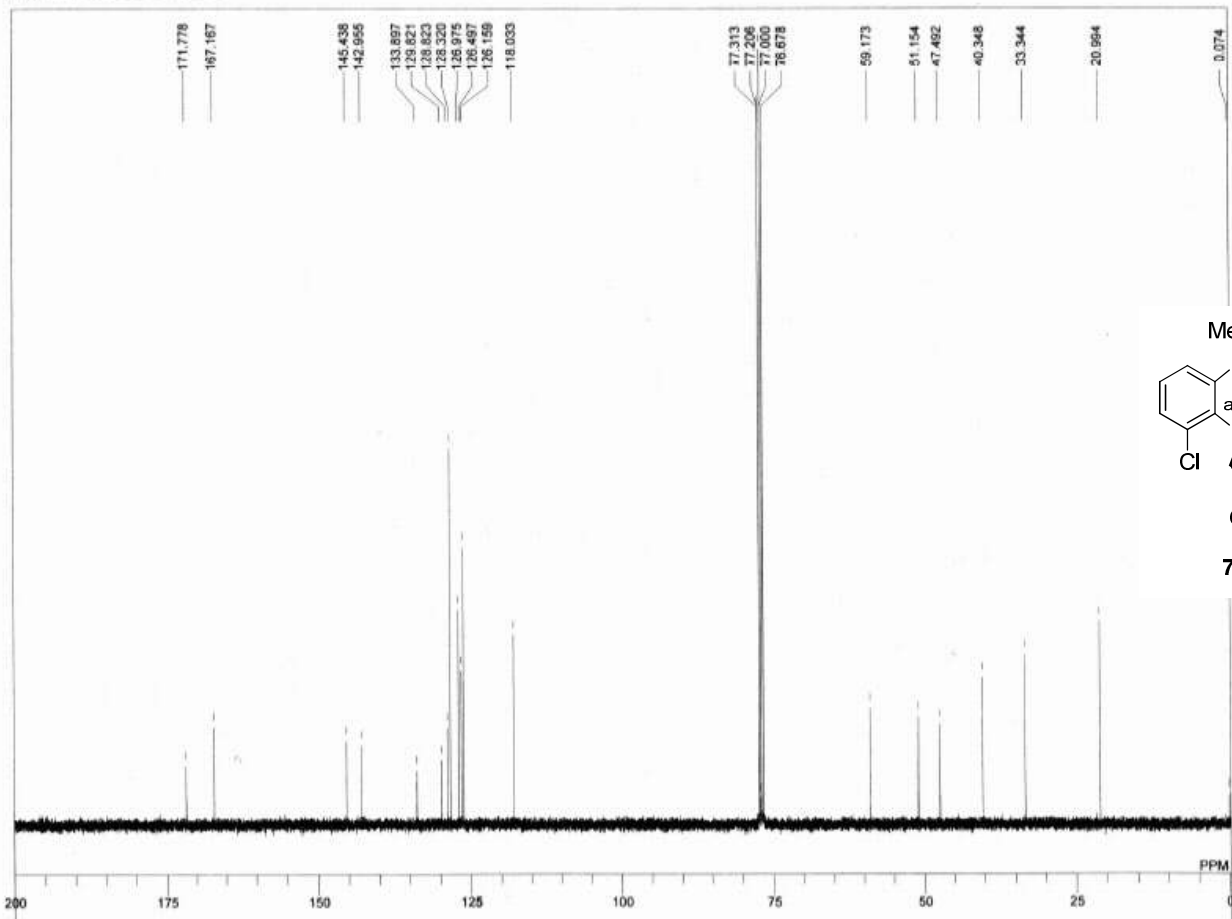
F:\Wada\42PNW2-69-51.als



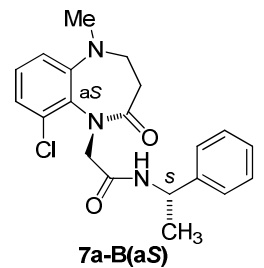
DFILE F:\Wada\42PNW2
 COMNT Mon Dec 28 23:05
 DATIM 1H
 OBNUC 399.65 MHz
 EXMOD 124.00 KHz
 OBFRQ 10500.0 Hz
 OBSET 32768
 OBFIN 8000.0 Hz
 POINT 16
 FREQU 4.096 sec
 SCANS 2.904 sec
 ACQTM 6.2 us
 PD 1H
 PW1 23.9 c
 IRNUC CDCL3
 CTMP 0.00 ppm
 SLVNT 0.12 Hz
 EXREF 18
 BF
 RGAIN



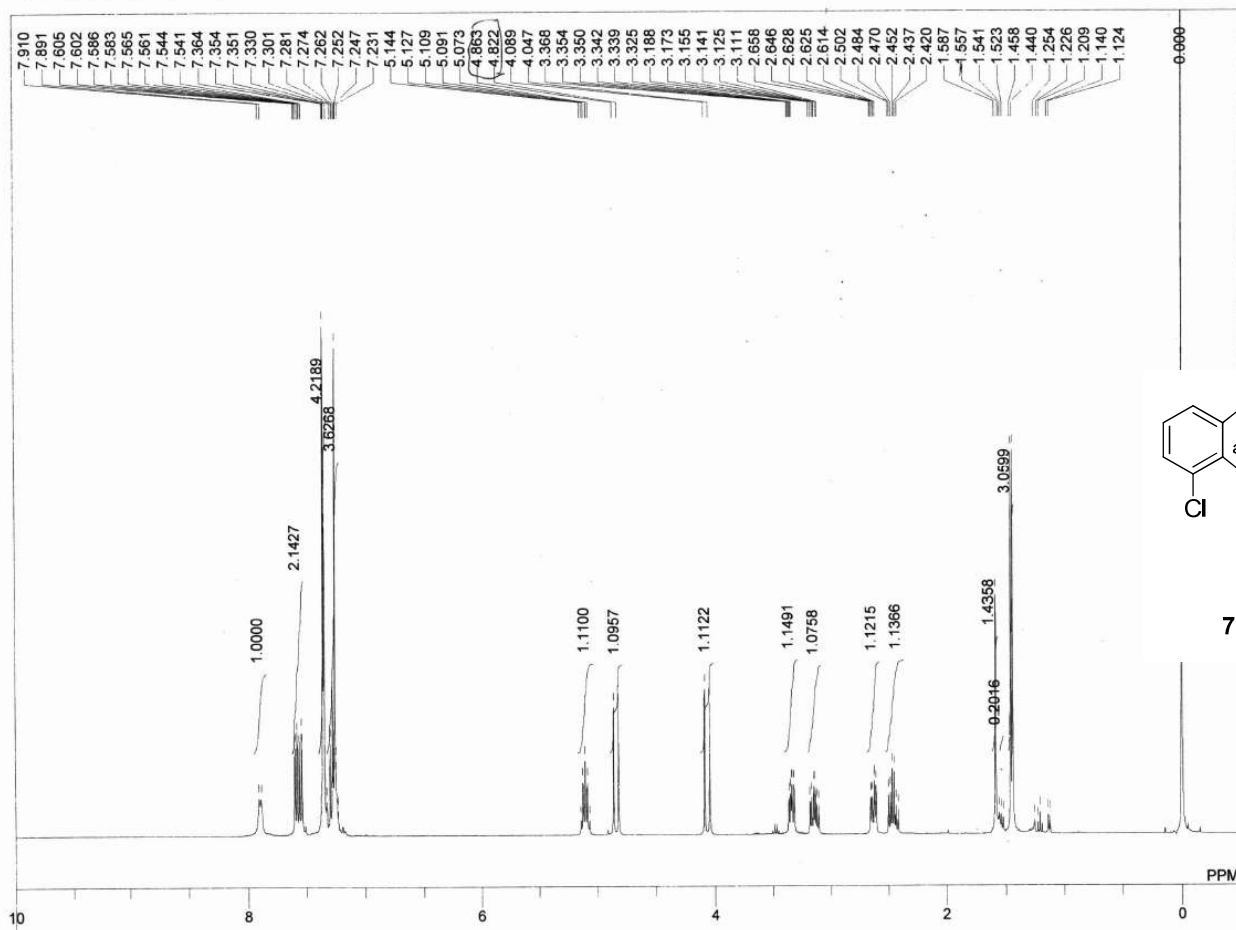
F:\Wada\42PNW2-69-51-carbon.als



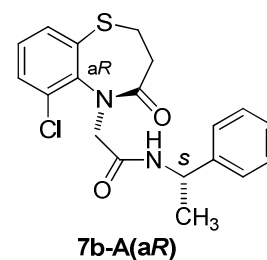
DFILE F:\Wada\42PNW2
 COMNT Mon Dec 28 23:55
 DATIM 13C
 OBNUC 100.40 MHz
 EXMOD 125.00 KHz
 OBFRQ 10500.0 Hz
 OBSET 32768
 OBFIN 27173.9 Hz
 POINT 1024
 FREQU 1.206 sec
 SCANS 1.794 sec
 ACQTM 4.6 us
 PD 1H
 PW1 24.6 c
 IRNUC CDCL3
 CTMP 77.00 ppm
 SLVNT 0.12 Hz
 EXREF 5a
 BF
 RGAIN



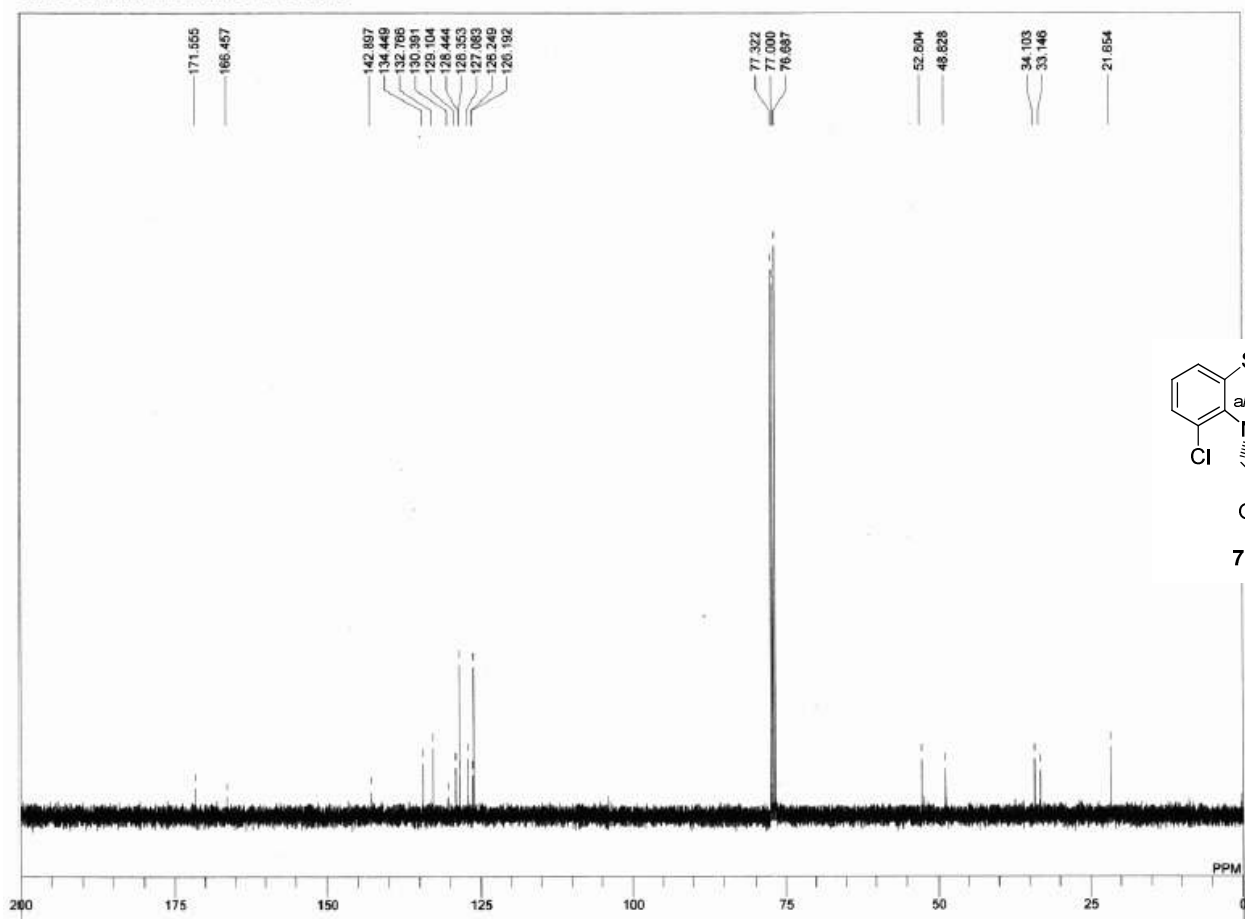
G:\Natsugari\42AHN2-69-30C.als



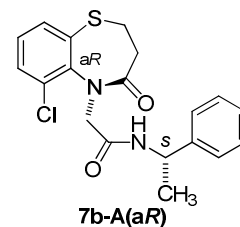
DFILE G:\Natsugari\4
COMNT Sat Jan 12 15:
DATIM 1H
OBNUC NON
EXMOD
OBFRQ 399.65 MH
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 64
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 24.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 20



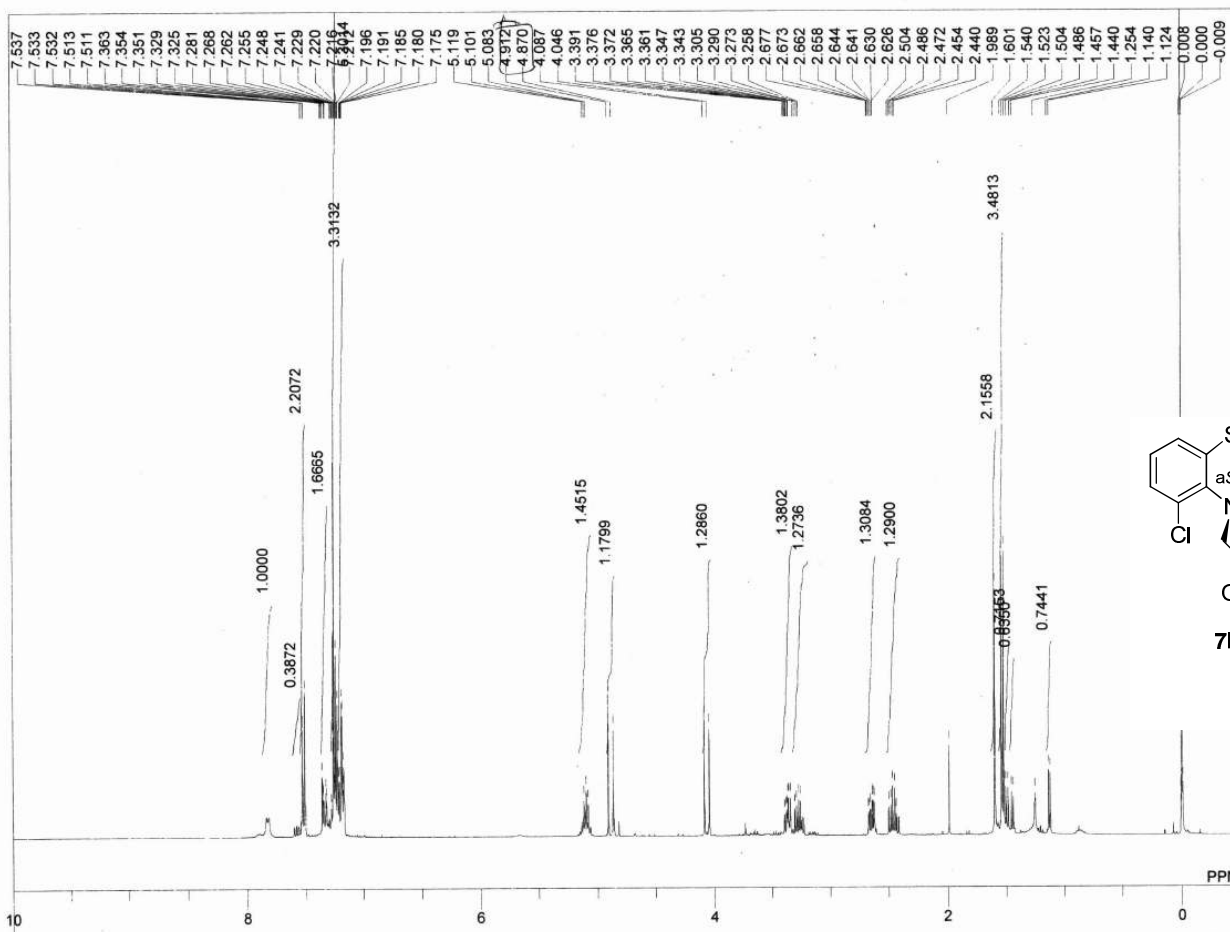
C:\ALICE95\DATA\Takada\carbon\42YYT1-167-31c.als



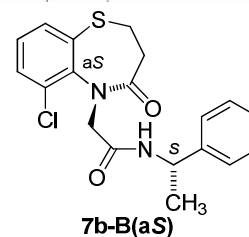
DFILE C:\ALICE95\DATA\
COMNT Mon Aug 23 12:03:
DATIM 13C
OBNUC BCM
EXMOD
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 256
ACQTM 1.206 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 27.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24



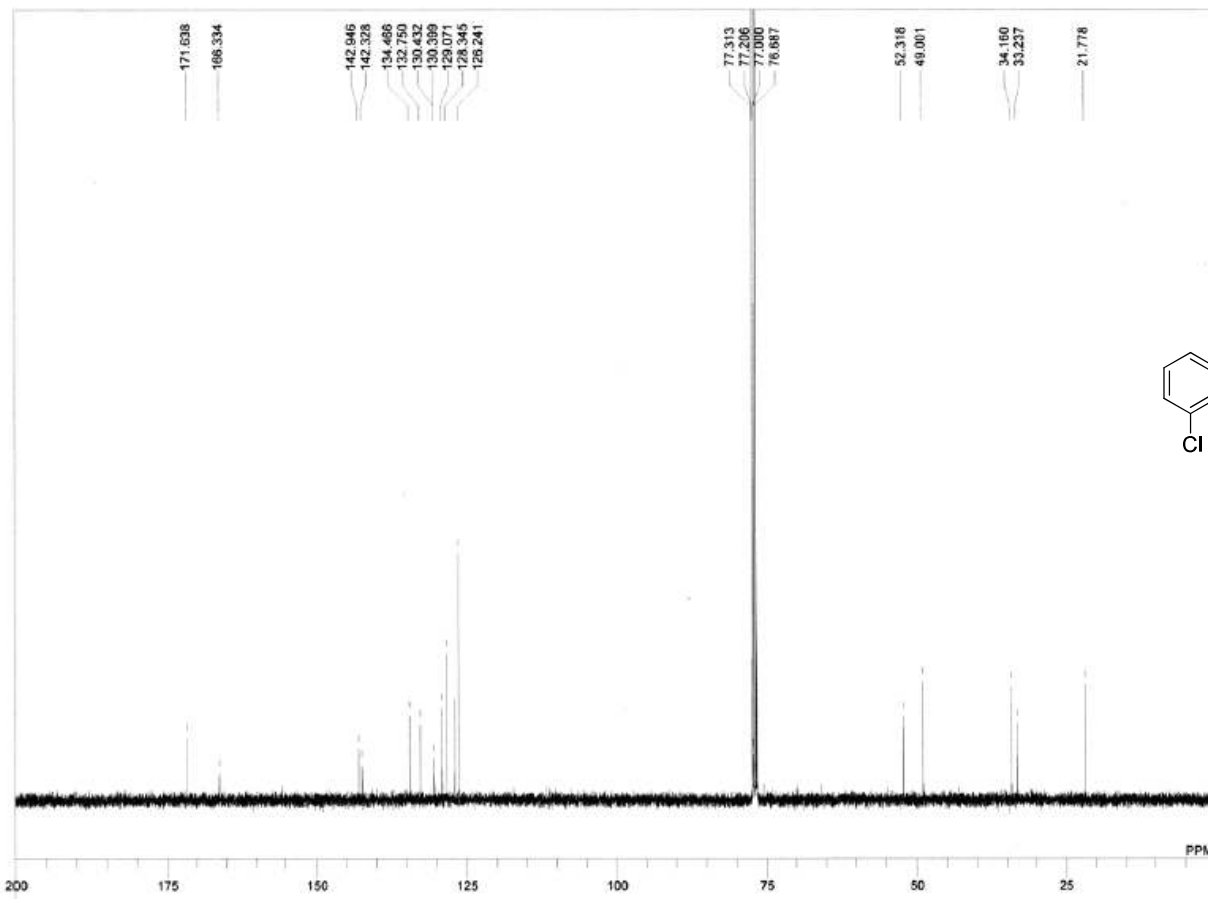
G:\Watsugari\42AHN2-69-33L.als



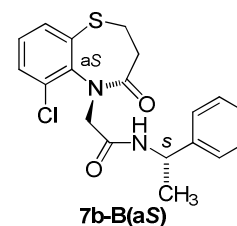
DFILE G:\Watsugari\42AHN2-69-33L.als
 COMNT Sat Jan 12 15:
 DATIM 1H
 OBNUC 399.65 MHz
 EXMOD 124.00 KHz
 OBFRQ 10500.0 Hz
 OBSET 32768
 OBFIN 8000.0 Hz
 POINT 64
 FREQU 4.096 sec
 SCANS 2.904 sec
 ACQTM 6.2 us
 PD 1H
 PW1 24.2 c
 IRNUC CDCL3
 CTEMP 0.00 ppm
 SLVNT 0.20 Hz
 EXREF 20
 BF
 RGAIN



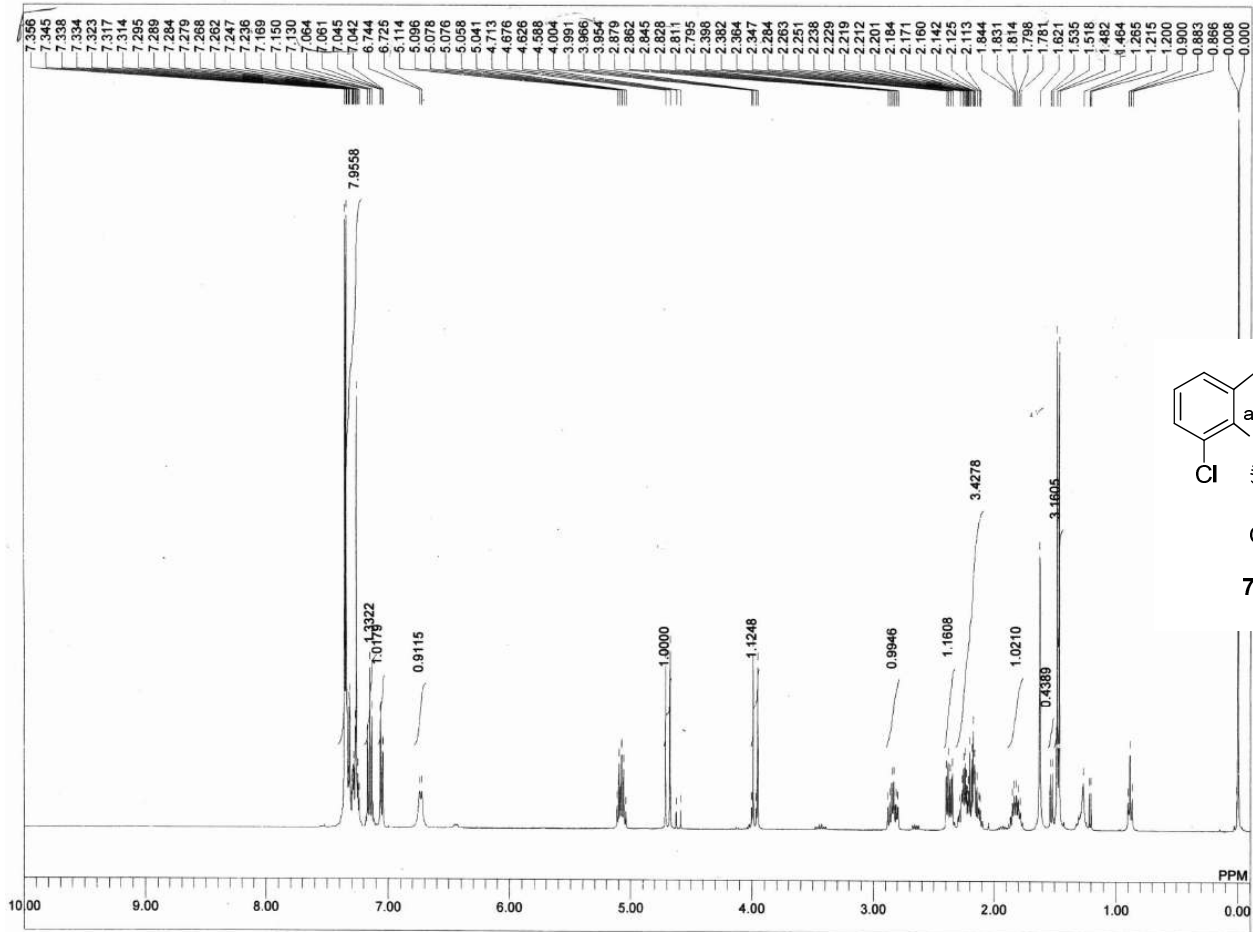
W10.20.10.243\40042\TABATA\42JHN-12.als



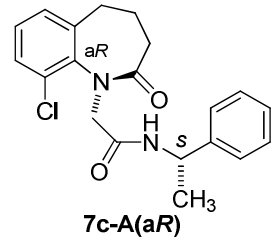
DFILE W10.20.10.243\400-
 COMNT Mon Mar 28 13:05:
 DATIM 13C
 OBNUC 100.40 MHz
 EXMOD 125.00 KHz
 OBFRQ 10500.0 Hz
 OBSET 32768
 OBFIN 27173.9 Hz
 POINT 2048
 FREQU 1.206 sec
 SCANS 1.794 sec
 ACQTM 4.5 us
 PD 1H
 PW1 23.2 c
 IRNUC CDCL3
 CTEMP 77.00 ppm
 SLVNT 0.12 Hz
 EXREF 24
 BF
 RGAIN



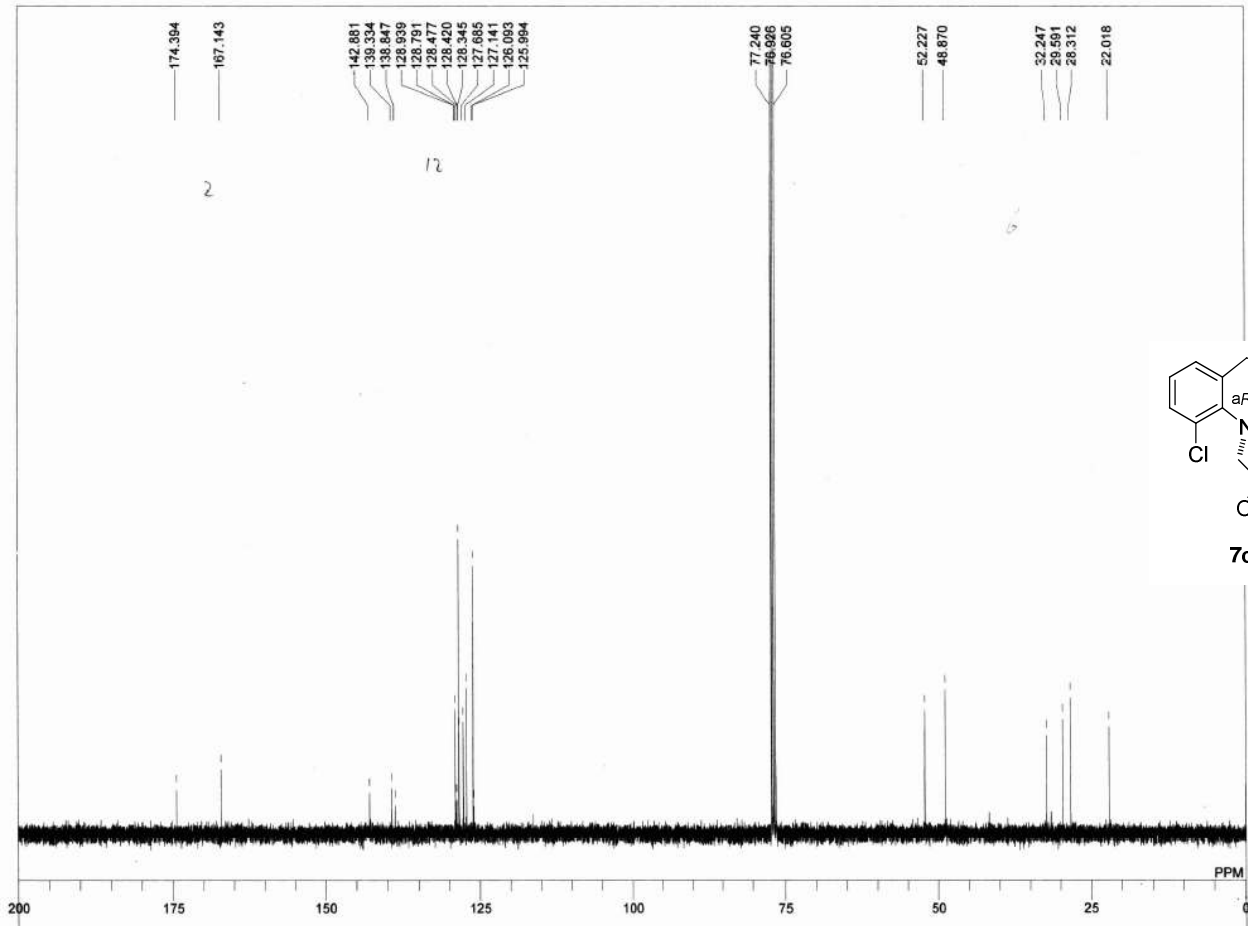
F:\Tabata\Hta9\42JHTA9-61-36-a.als



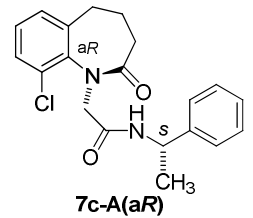
DFILE F:\Tabata\Hta9\42
COMNT Fri Sep 03 07:04:1
1H 1H
NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 64
ACQTM 4.096 sec
PD 2.904 sec
PW1 6.2 us
IRNUC 1H
CTEMP 25.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19



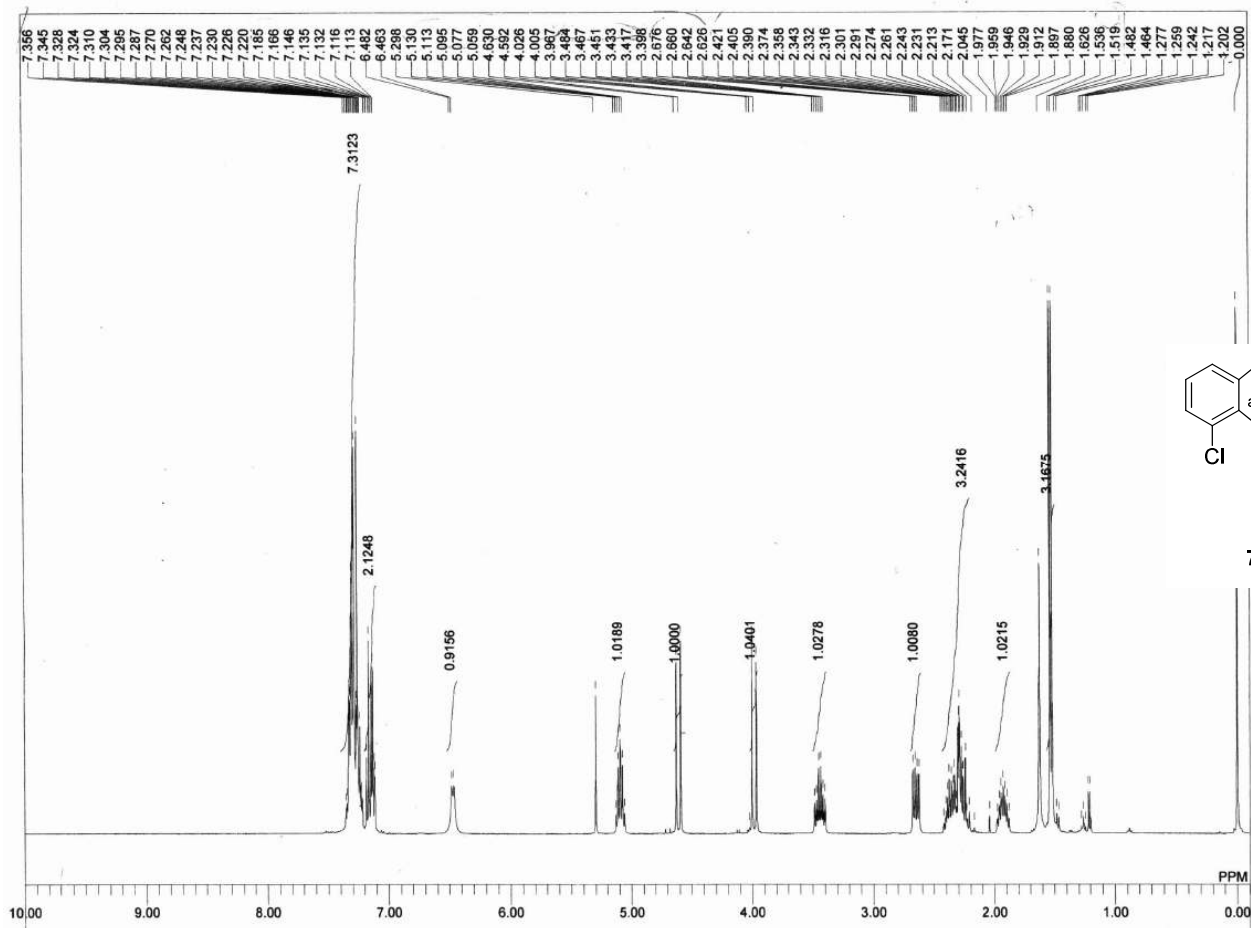
F:\Tabata\Hta9\42JHTA9-61-36-aC.als



DFILE F:\Tabata\Hta9\42
COMNT Fri Sep 03 07:31:4
13C 13C
BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 512
ACQTM 1.206 sec
PD 1.794 sec
PW1 4.6 us
IRNUC 1H
CTEMP 27.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 25

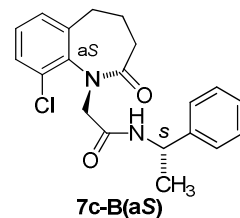


F:\Tabata\Hta9\42JHTA9-61-36-b.als

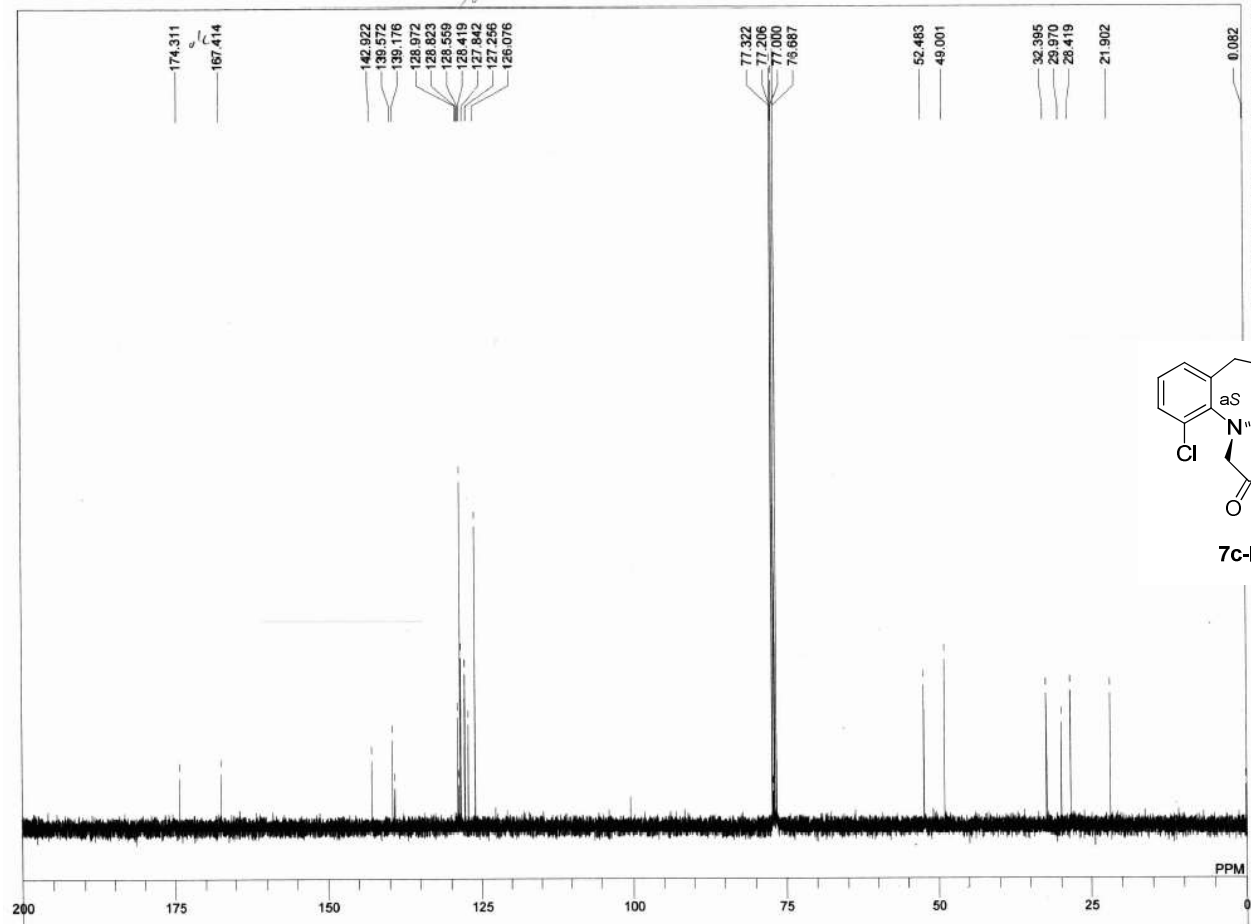


DFILE COMNT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

F:\Tabata\Hta9\42J
 Fri Sep 03 06:17:5
 1H
 NON
 399.65 MHz
 124.00 KHz
 10500.0 Hz
 32768
 8000.0 Hz
 64
 4.096 sec
 2.904 sec
 6.2 us
 1H
 24.8 c
 CDCL3
 0.00 ppm
 0.12 Hz
 19

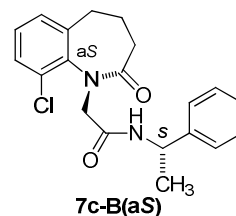


F:\Tabata\Hta9\42JHTA9-61-36-bC.als

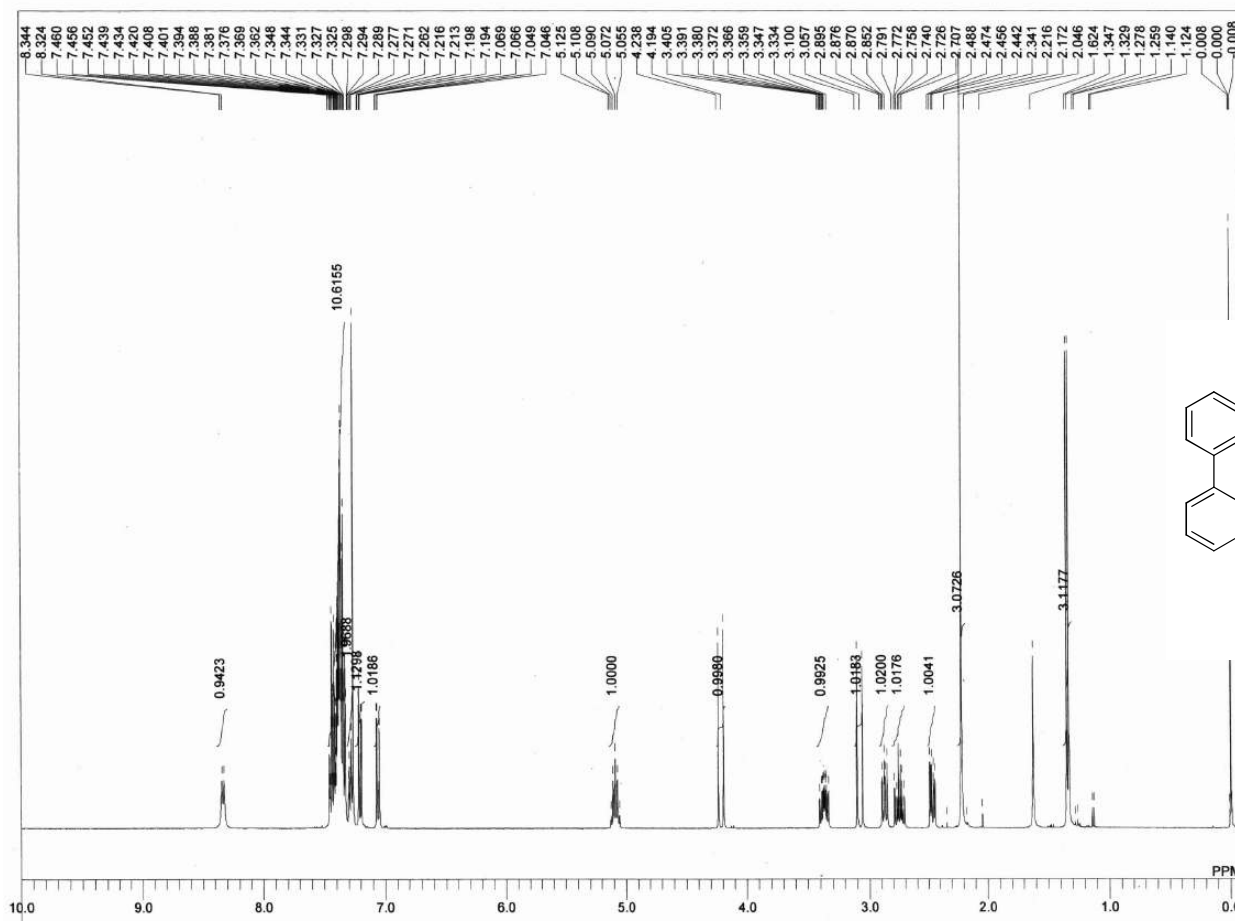


DFILE COMNT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

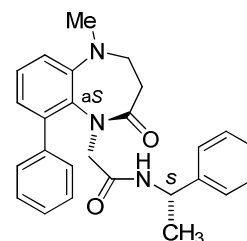
F:\Tabata\Hta9\42J
 Fri Sep 03 06:44:4
 13C
 BCM
 100.40 MHz
 125.00 KHz
 10500.0 Hz
 32768
 27173.9 Hz
 512
 1.206 sec
 1.794 sec
 4.6 us
 1H
 25.9 c
 CDCL3
 77.00 ppm
 0.12 Hz
 25



F:\Wada\42PNW3-3-37.als

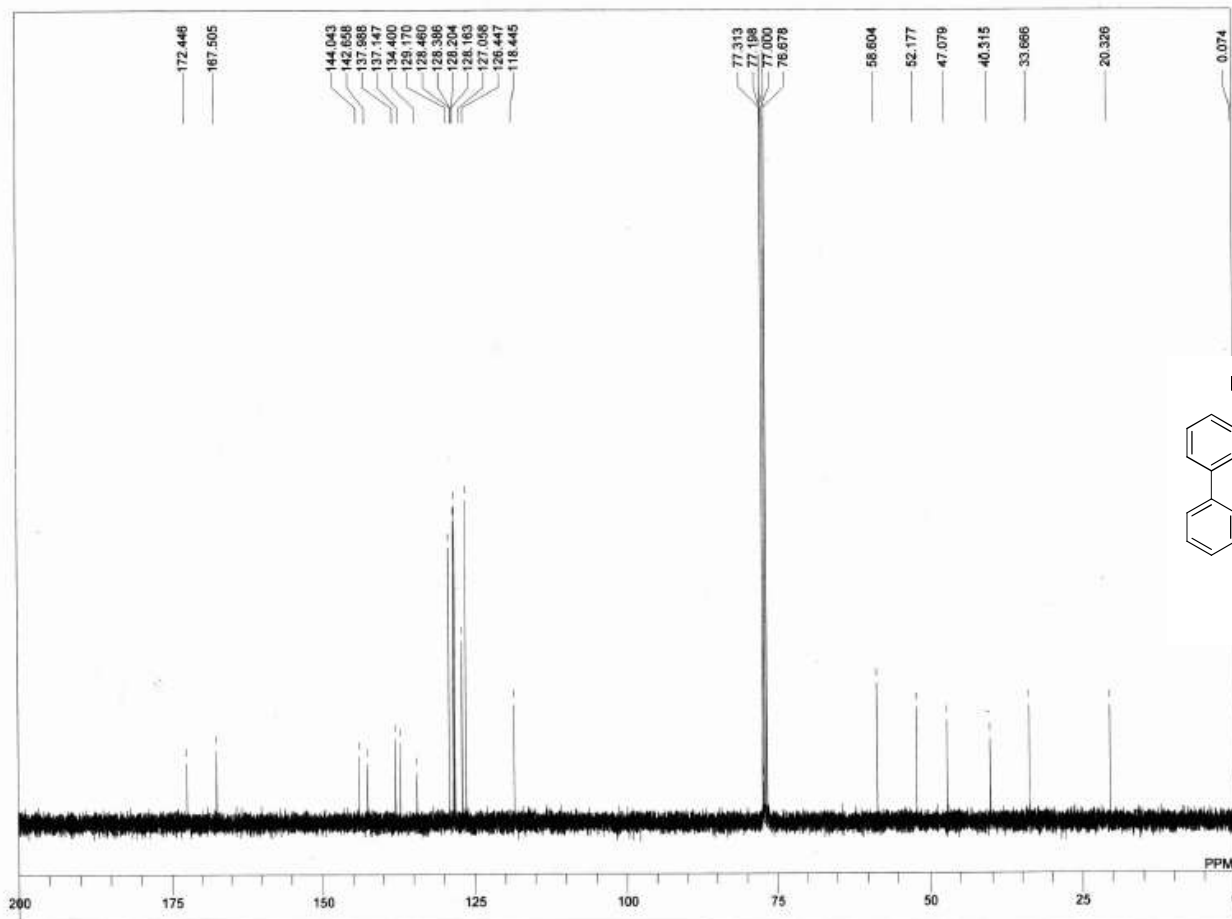


DFILE F:\Wada\42PNW3-
 COMNT Sat Nov 21 19:50:51
 DATIM 1H
 OBNUC NON
 EXMOD 399.65 MHz
 OBFRQ 124.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 8000.0 Hz
 FREQU 16
 SCANS 4.096 sec
 ACQTM 2.904 sec
 PD 6.2 us
 PW1 1H
 IRNUC 23.1 c
 CTMP CDCl3
 SLVNT 0.00 ppm
 EXREF BF 0.12 Hz
 RGAIN 19

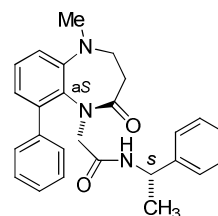


8a-A(aS)

F:\Wada\42PNW3-3-37-carbon.als

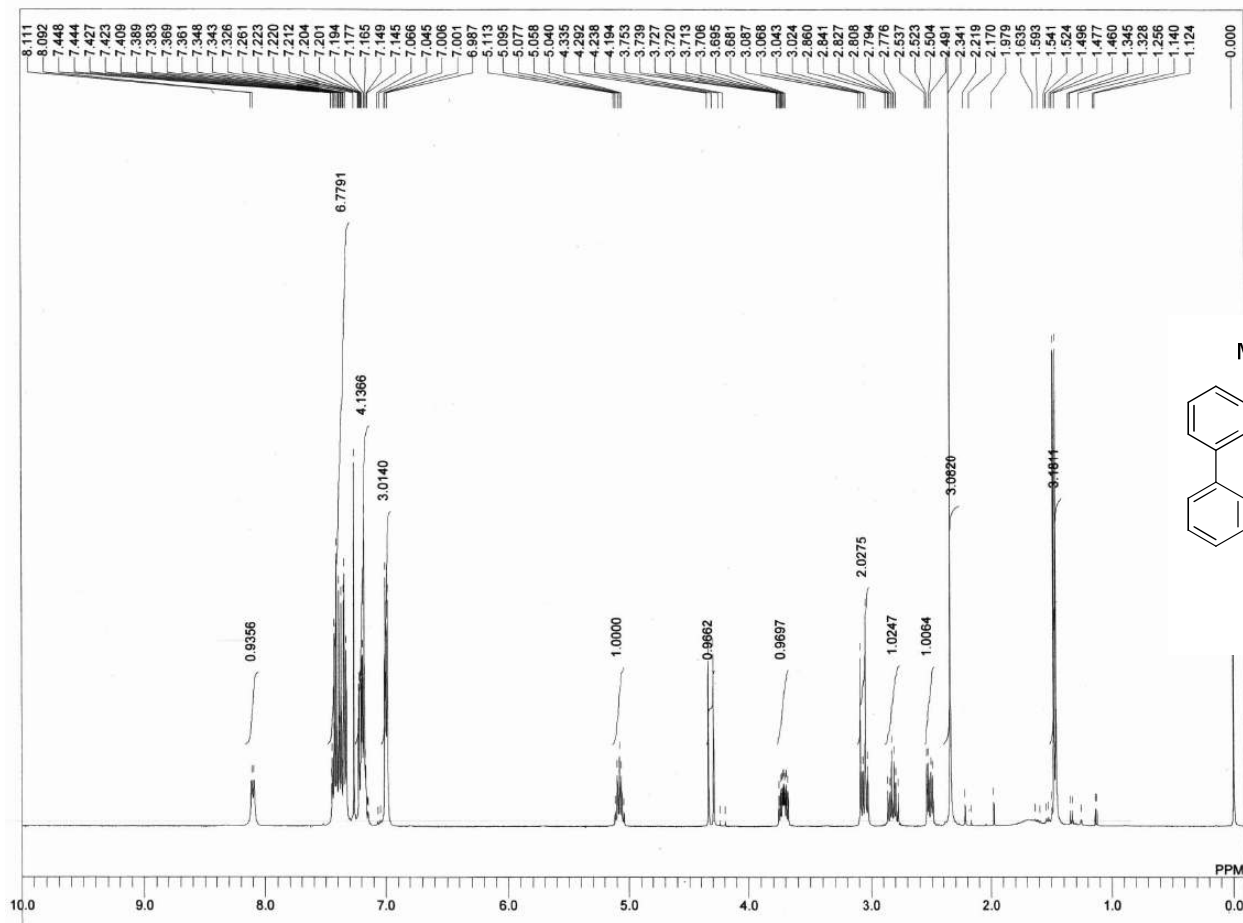


DFILE F:\Wada\42PNW3-
 COMNT Sat Nov 21 20:17:11
 DATIM 13C
 OBNUC BCM
 EXMOD 100.40 MHz
 OBFRQ 125.00 KHz
 OBSET 10500.0 Hz
 OBFIN 32768
 POINT 27173.9 Hz
 FREQU 512
 SCANS 1.206 sec
 ACQTM 1.794 sec
 PD 4.6 us
 PW1 1H
 IRNUC 25.2 c
 CTMP CDCl3
 SLVNT 77.00 ppm
 EXREF BF 0.12 Hz
 RGAIN 24

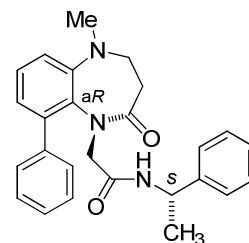


8a-A(aS)

F:\Wada\42PNW3-3-39.als

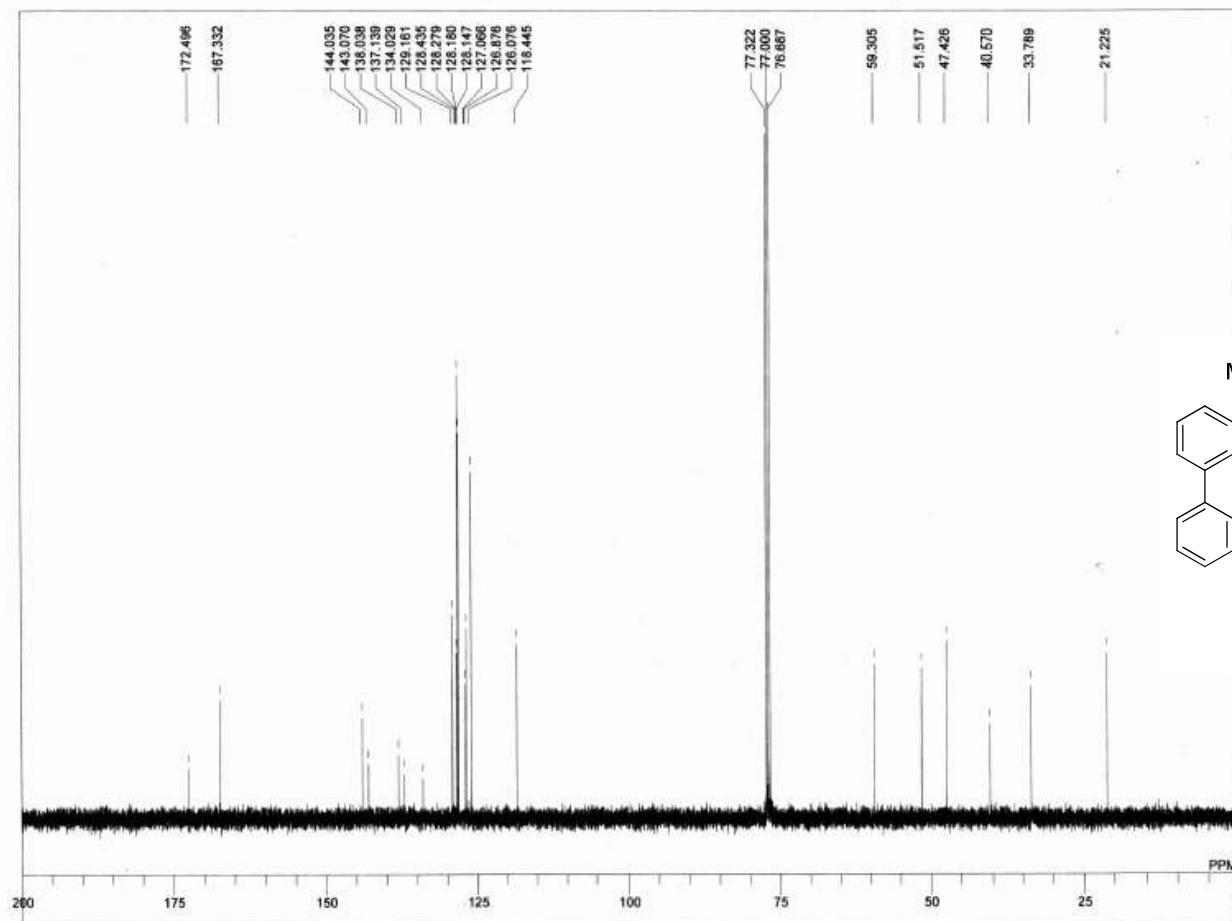


DFILE F:\Wada\42PNW3-
 COMNT Sat Nov 21 20:23:5
 1H
 NON
 OBFRQ 399.65 MHz
 OBSET 124.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 8000.0 Hz
 SCANS 16
 ACQTM 4.096 sec
 PD 2.904 sec
 PW1 6.2 us
 IRNUC 1H
 CTEMP 23.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 18

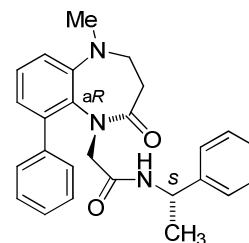


8a-B(aR)

F:\Wada\42PNW3-3-39-carbon.als



DFILE F:\Wada\42PNW3-
 COMNT Sat Nov 21 20:50:0
 13C
 BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.0 Hz
 POINT 32768
 FREQU 27173.9 Hz
 SCANS 512
 ACQTM 1.206 sec
 PD 1.794 sec
 PW1 4.6 us
 IRNUC 1H
 CTEMP 25.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 25



8a-B(aR)