

Electronic Supplementary Information

Highly Efficient and Enantioselective Biotransformations of β -Lactam Carbonitriles and Carboxamides and Their Synthetic Applications

Dong-Hui Leng,^a De-Xian Wang,^a Zhi-Tang Huang,^a and Mei-Xiang Wang^{*,a,b}

^a Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China, ^bThe Key Laboratory of Bioorganic Phosphorus Chemistry & Chemical Biology (Ministry of Education), Department of Chemistry, Tsinghua University, Beijing 100084, China

wangmx@mail.tsinghua.edu.cn

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1. General information

¹H and ¹³C NMR spectra were recorded on a 300 MHz or a 400 MHz NMR spectrometer. Chemical shifts are reported in ppm with tetramethylsilane or the residual solvent resonance as an internal standard. Melting points are uncorrected. Elemental analyses, mass spectrometry, and single crystal X-ray diffraction analyses were performed at the Analytical Laboratory of the Institute. Solvents were dried according to standard procedures prior to use. All other major chemicals were obtained from commercial sources and used without further

purification. The racemic nitriles **1a-g**, **5** were prepared following a literature methods¹, the racemic compound **8** was synthesized directly from catalytic hydrogenation of **5** in the presence of Pd/C catalyst.

2. Spectroscopic data of compounds **1**, **5** and **8**

(±)-1-Benzyl-4-oxoazetidine-2-carbonitrile (1a) : mp: 44.0-45.0°C. IR (KBr) ν 2247, 1764 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.28-7.43 (m, 5 H), 4.78 (d, $J=15.1$ Hz, 1H), 4.16 (d, $J=15.1$ Hz, 1H), 4.01 (dd, $J=3.5, 4.6$ Hz, 1H), 3.31-3.42 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 133.6, 129.2, 128.6, 128.5, 116.4, 46.0, 43.6, 38.0; MS (EI) m/z (%) 186 (18) $[\text{M}]^+$, 91 (100). Anal. Calcd. for $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}$: 186.0793 $[\text{M}]^+$; Found: 186.0795 $[\text{M}]^+$.

(±)-1-(4-Fluorobenzyl)-4-oxoazetidine-2-carbonitrile (1b) : oil. IR (KBr) ν 2242, 1768 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.05-7.12 (m, 2H), 7.26-7.30 (m, 2H), 4.70 (d, $J=15.2$ Hz, 1H), 4.18 (d, $J=15.2$ Hz, 1H), 4.02 (dd, $J=4.7, 3.2$ Hz, 1H), 3.31-3.43 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 162.7 (d, $J=246.2$ Hz, C-F), 130.4 (d, $J=8.3$ Hz, C-F), 129.6 (d, $J=3.3$ Hz, C-F), 116.4, 116.2 (d, $J=21.6$ Hz, C-F), 45.3, 43.7, 38.0. MS (EI) m/z (%) 204 (17) $[\text{M}]^+$, 109 (100). Anal. Calcd. for $\text{C}_{11}\text{H}_9\text{FN}_2\text{O}$: 204.0699 $[\text{M}]^+$; Found: 204.0702 $[\text{M}]^+$.

(±)-1-(4-Methylbenzyl)-4-oxoazetidine-2-carbonitrile (1c) : oil. IR (KBr) ν 2247, 1769 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.15-7.21 (m, 4H), 4.73 (d, $J=15.0$ Hz, 1H), 4.11 (d, $J=15.0$ Hz, 1H), 3.99 (t, $J=3.6$ Hz, 1H), 3.28-3.40 (m, 2H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 138.4, 130.6, 129.8, 128.6, 116.6, 45.7, 43.5, 37.9, 21.2; MS (EI) m/z (%) 200 (28) $[\text{M}]^+$, 105 (100). Anal. Calcd. for $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}$: 200.0950 $[\text{M}]^+$; Found: 200.0952 $[\text{M}]^+$.

(±)-1-(4-Bromobenzyl)-4-oxoazetidine-2-carbonitrile (1d) : oil. IR (KBr) ν 2242, 1768 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.52 (d, $J=8.6$ Hz, 2H), 7.18 (d, $J=8.3$ Hz, 2H), 4.69 (d, $J=15.2$ Hz, 1H), 4.15 (d, $J=15.2$ Hz, 1H), 4.03 (dd, $J=3.4, 4.6$ Hz, 1H), 3.32-3.44 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.9, 132.8, 132.3, 130.2, 122.6, 116.4, 45.4, 43.8, 38.2; MS (EI) m/z (%) 264 (19) $[\text{M}]^+$, 266 (16) $[\text{M}+2]^+$, 169 (100), 171 (68). Anal. Calcd. for $\text{C}_{11}\text{H}_9\text{BrN}_2\text{O}$: 263.9898 $[\text{M}]^+$, 265.9878 $[\text{M}+2]^+$; Found: 263.9901 $[\text{M}]^+$, 265.9882 $[\text{M}+2]^+$.

(±)-1-(3-Bromobenzyl)-4-oxoazetidine-2-carbonitrile (1e) : oil. IR (KBr) ν 2242, 1761 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.22-7.30 (m, 2H), 7.44-7.50 (m, 2H), 4.72 (d, $J=15.3$ Hz, 1H), 4.15 (d, $J=15.3$ Hz, 1H), 4.07 (dd, $J=3.1, 5.0$ Hz, 1H), 3.34-3.47 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 135.0, 131.7, 131.4, 130.8, 127.1, 123.2, 116.3, 45.3, 43.9, 38.3; MS (EI) m/z (%) 264 (21) $[\text{M}]^+$, 266 (18) $[\text{M}+2]^+$, 169(100), 171 (68). Anal. Calcd. for $\text{C}_{11}\text{H}_9\text{BrN}_2\text{O}$: 263.9898 $[\text{M}]^+$, 265.9878 $[\text{M}+2]^+$; Found: 263.9901 $[\text{M}]^+$, 265.9882 $[\text{M}+2]^+$.

(±)-1-(2-Bromobenzyl)-4-oxoazetidine-2-carbonitrile (1f) : mp: 83.0-84.0°C. IR (KBr) ν 2242, 1759 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.21-7.27 (m, 1H), 7.33-7.41 (m, 2H), 7.60-7.63 (m, 1H), 4.79 (d, $J=15.0$ Hz, 1H), 4.42 (d, $J=15.0$ Hz, 1H), 4.09 (dd, $J=2.9, 5.2$ Hz, 1H), 3.40 (dd, $J=5.1, 14.8$ Hz, 1H), 3.32 (dd, $J=2.8, 14.8$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 133.3, 133.1, 131.3, 130.4, 128.2, 124.0, 116.6, 46.2, 43.8, 38.7; MS (ESI) m/z (%) 265 $[\text{M}+\text{H}]^+$, 267 $[\text{M}+\text{H}+2]^+$; Anal. Calcd. for $\text{C}_{11}\text{H}_9\text{BrN}_2\text{O}$: C, 49.84; H, 3.42; N, 10.57. Found: C, 49.79; H, 3.49; N, 10.44.

(±)-1-(4-Methoxybenzyl)-4-oxoazetidine-2-carbonitrile (1g): mp: 43.0-44.0°C. IR (KBr) ν 2247, 1754 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 7.21 (d, $J=8.6$ Hz, 2H), 6.90 (d, $J=8.6$ Hz, 2H), 4.69 (d, $J=15.0$ Hz, 1H), 4.10 (d, $J=15.0$ Hz, 1H), 3.98 (dd, $J=3.5, 4.6$ Hz, 1H), 3.81 (s, 3H), 3.27-3.38 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.8, 159.7, 130.0, 125.6, 116.6, 114.5, 55.3, 45.4, 43.4, 37.8; MS (EI) m/z (%) 216 (43) $[\text{M}]^+$, 121 (100). Anal. Calcd. for $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2$: 216.0899 $[\text{M}]^+$; Found: 216.0901 $[\text{M}]^+$.

(±)-1-Allyl-4-oxoazetidine-2-carbonitrile (5) : oil. IR (KBr) ν 2247, 1768 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 5.72-5.86 (m, 1H), 5.32-5.38 (m, 2H), 4.20 (dd, $J=2.7, 5.3$ Hz, 1H), 4.10 (dd, $J=5.6, 15.5$ Hz, 1H), 3.77 (dd, $J=7.1, 15.5$ Hz, 1H), 3.42 (dd, $J=5.3, 14.8$ Hz, 1H), 3.32 (dd, $J=2.6, 14.8$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 163.9, 130.0, 120.6, 116.8, 44.5, 43.5, 38.2; MS (EI) m/z (%) 136 (51) $[\text{M}]^+$, 107 (58), 94 (53), 83 (32), 67 (100), 56 (87). Anal. Calcd. for $\text{C}_7\text{H}_8\text{N}_2\text{O}$: 136.0637 $[\text{M}]^+$; Found: 136.0639 $[\text{M}]^+$.

(±)-4-Oxo-1-propylazetidine-2-carbonitrile (8) : oil. IR (KBr) ν 2245, 1766 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 4.20 (dd, $J=2.7, 5.2$ Hz, 1H), 3.29-3.44 (m,

2H), 3.16-3.26 (m, 1H), 1.58-1.76 (m, 2H), 0.97 (t, $J=7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.3, 117.0, 43.9, 43.4, 38.7, 20.7, 11.4; MS (ESI) m/z (%) 139 $[\text{M}+\text{H}]^+$; Anal. Calcd. for $\text{C}_7\text{H}_{10}\text{N}_2\text{O}$: C, 60.85; H, 7.30; N, 20.28. Found: C, 60.55; H, 7.29; N, 19.93.

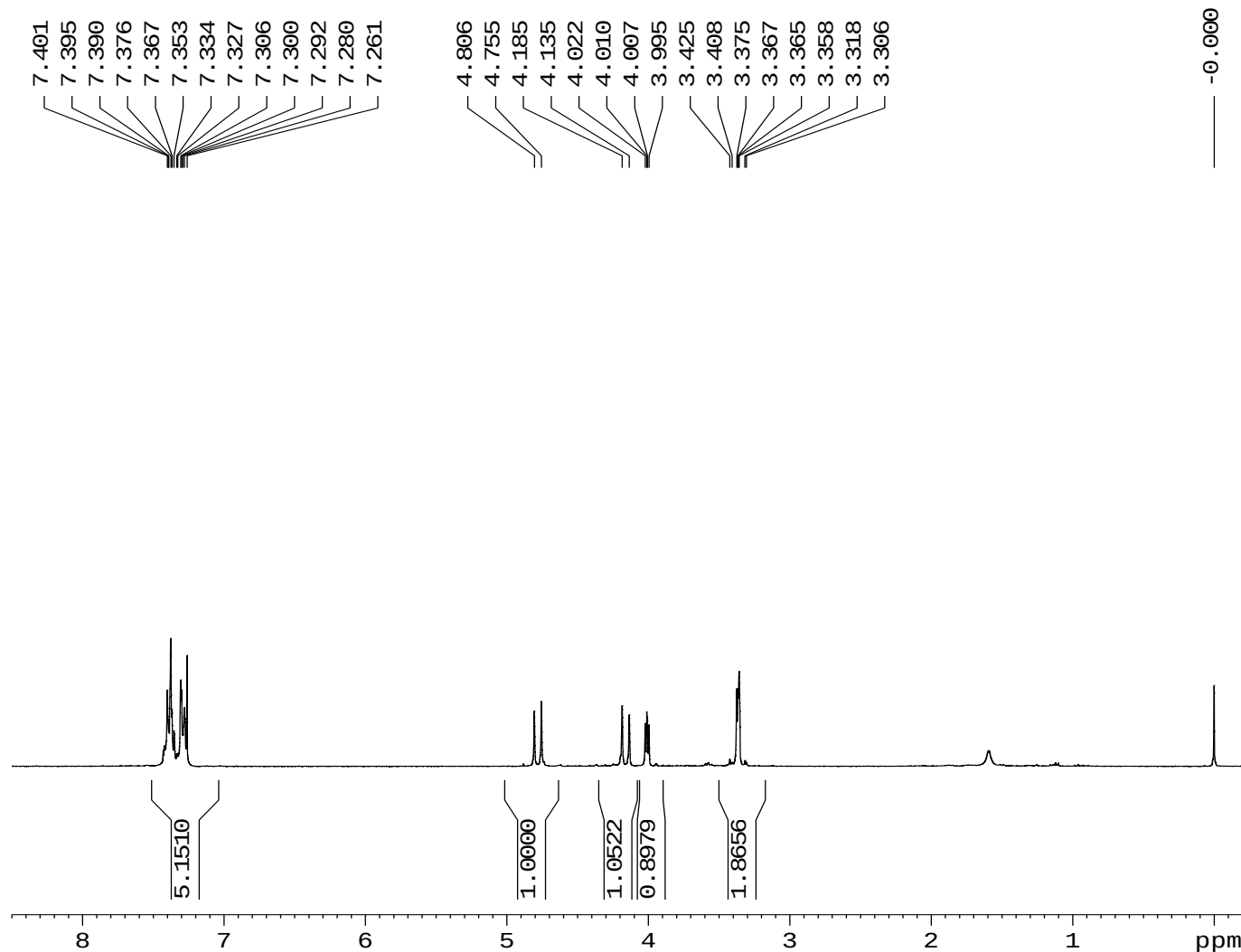
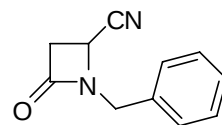
3. Chemical transformation of *R*-4a into *R*-2a and of *S*-6 into *S*-9

A 10 mL flask was charged with ester ***R*-4a** (101 mg, 0.46 mmol), 25-27% ammonia solution (1 mL) and acetone (0.46 mL). After complete dissolution, the resulting mixture was stirred overnight. The solvent was removed under reduced pressure, and the pure amide ***R*-2a** (94 mg, 100%) was collected after recrystallization with petroleum ether and ethyl acetate (1:1).

Catalytic hydrogenation of ***S*-6** (31 mg, 0.2 mol) in the presence of Pd/C (4 mg, 10%) in methanol (10 mL) using a hydrogen balloon at room temperature until the substrate disappeared. After filtration of the catalyst and removing of the solvent, pure ***S*-9** (31 mg, 100%) was left as white solid.

4. ^1H and ^{13}C NMR spectra of all compounds

1a-¹H NMR

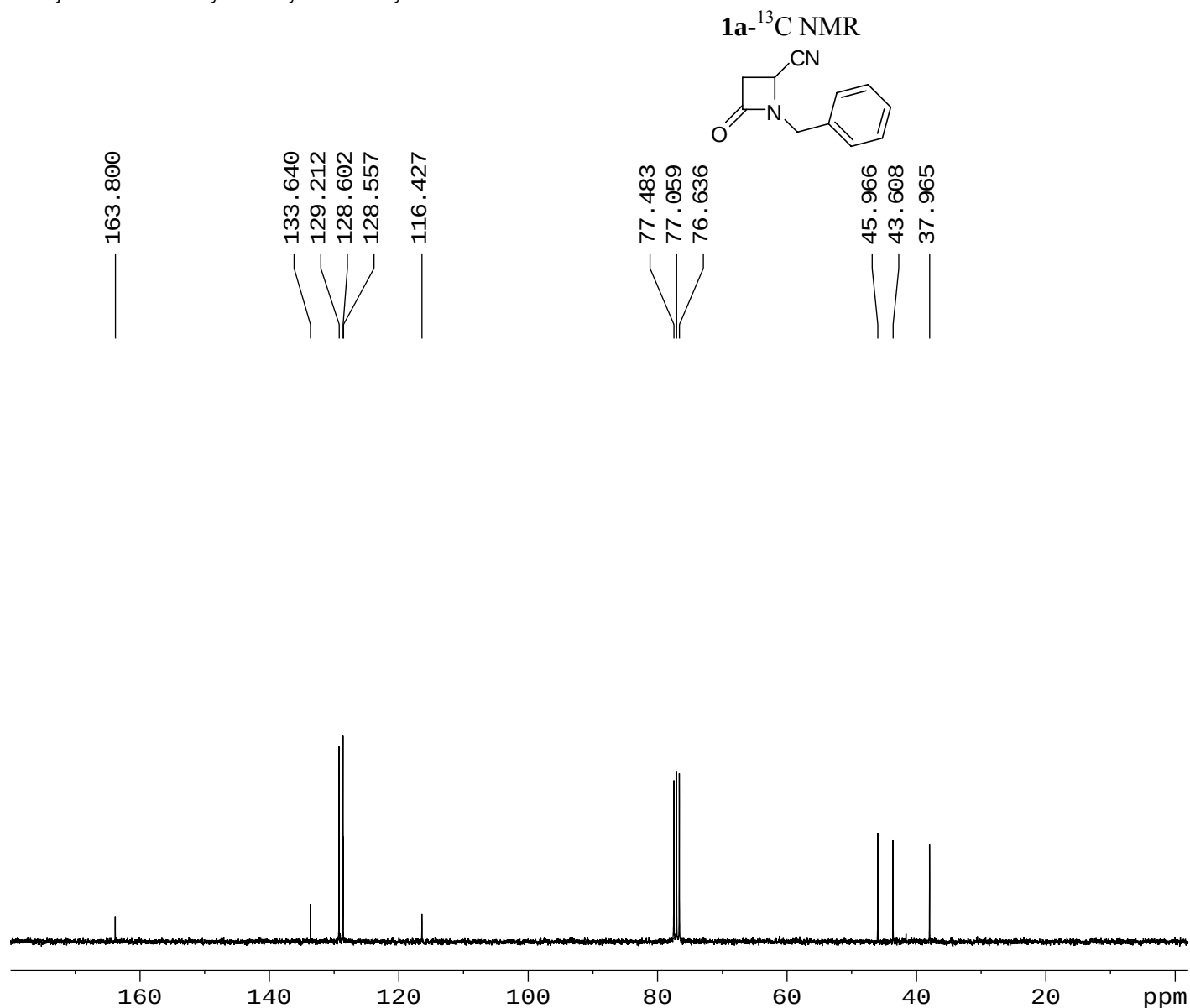


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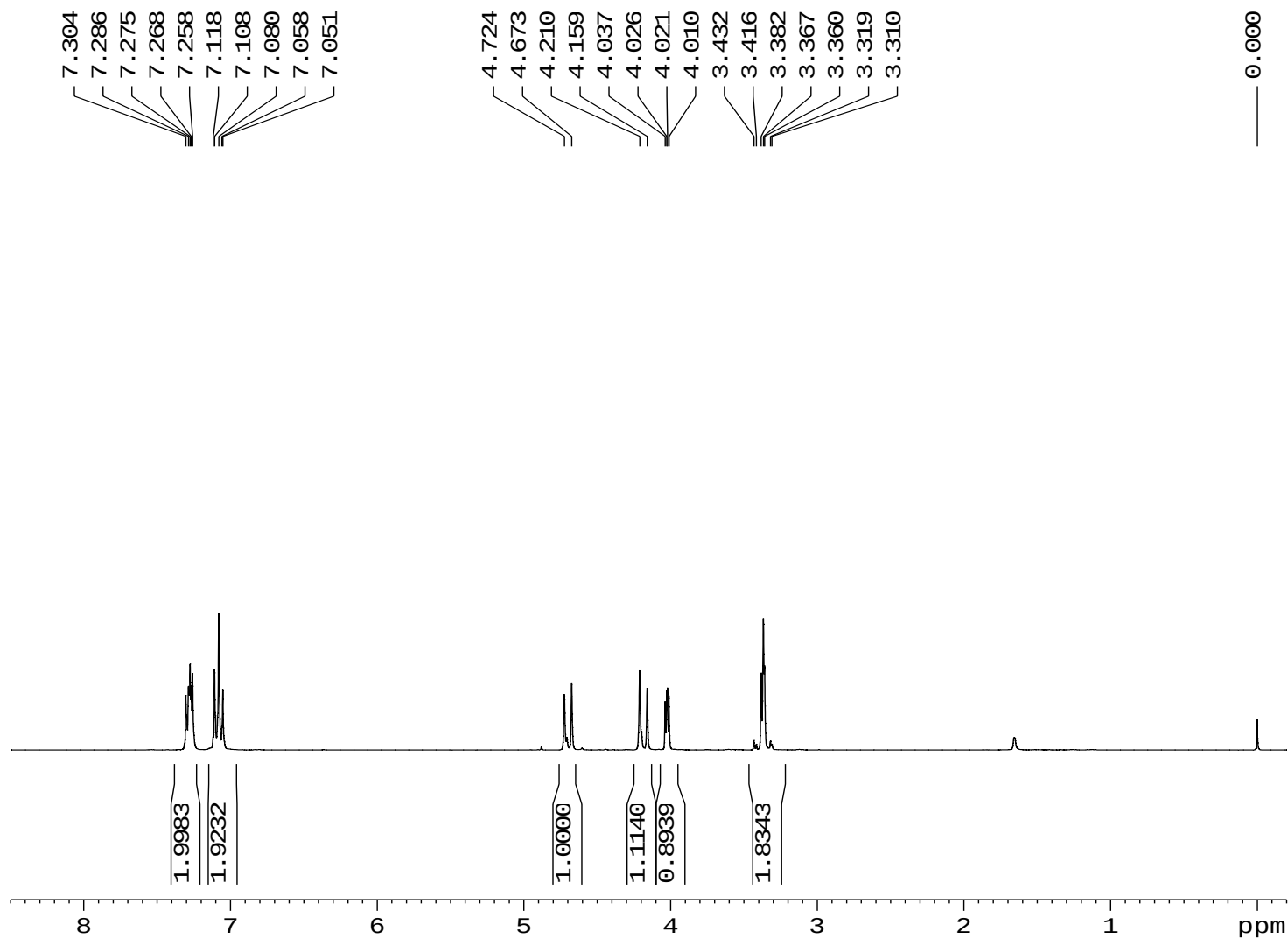
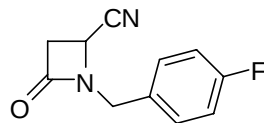
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1b-¹H NMR



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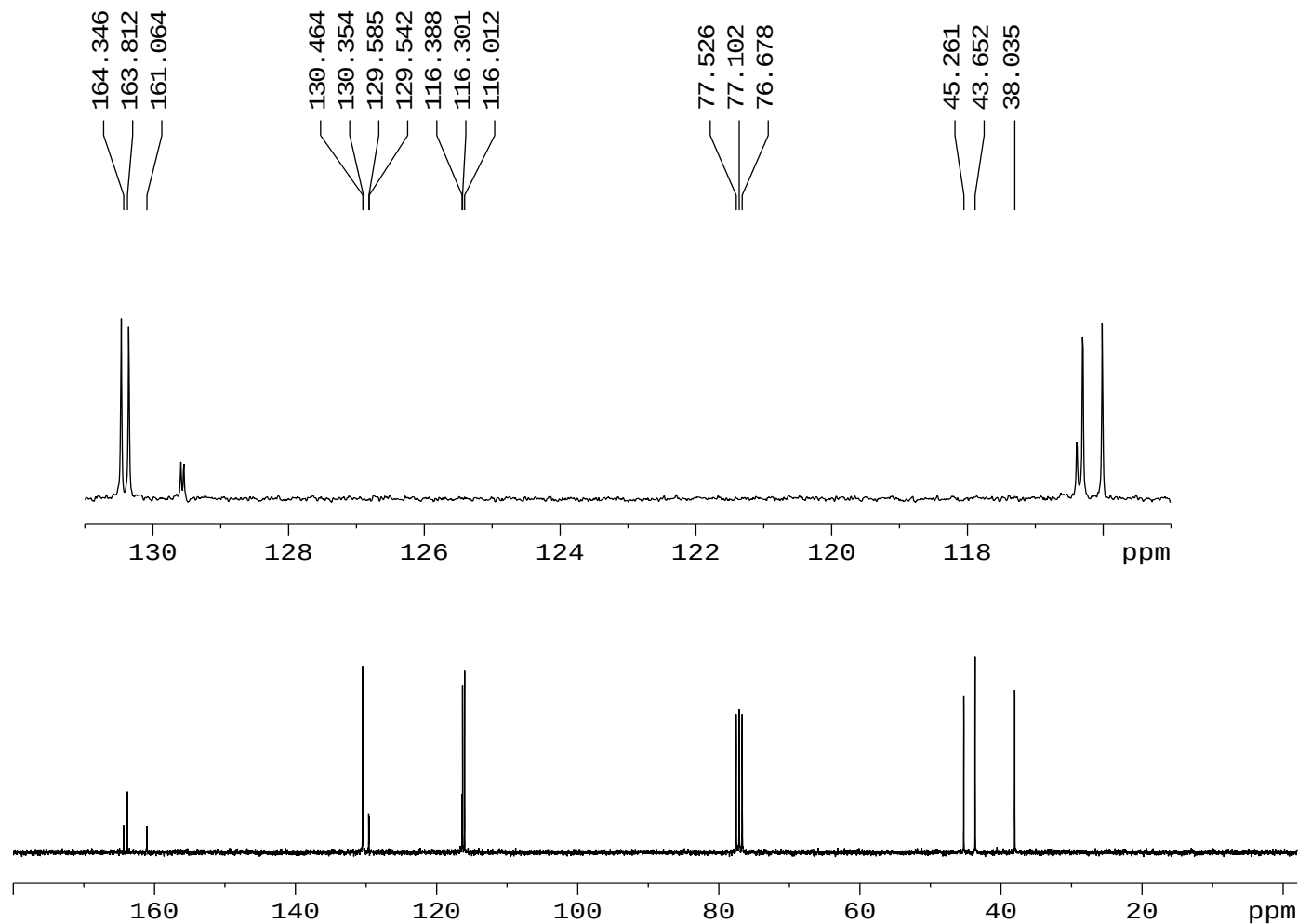
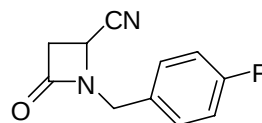
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1b-¹³C NMR



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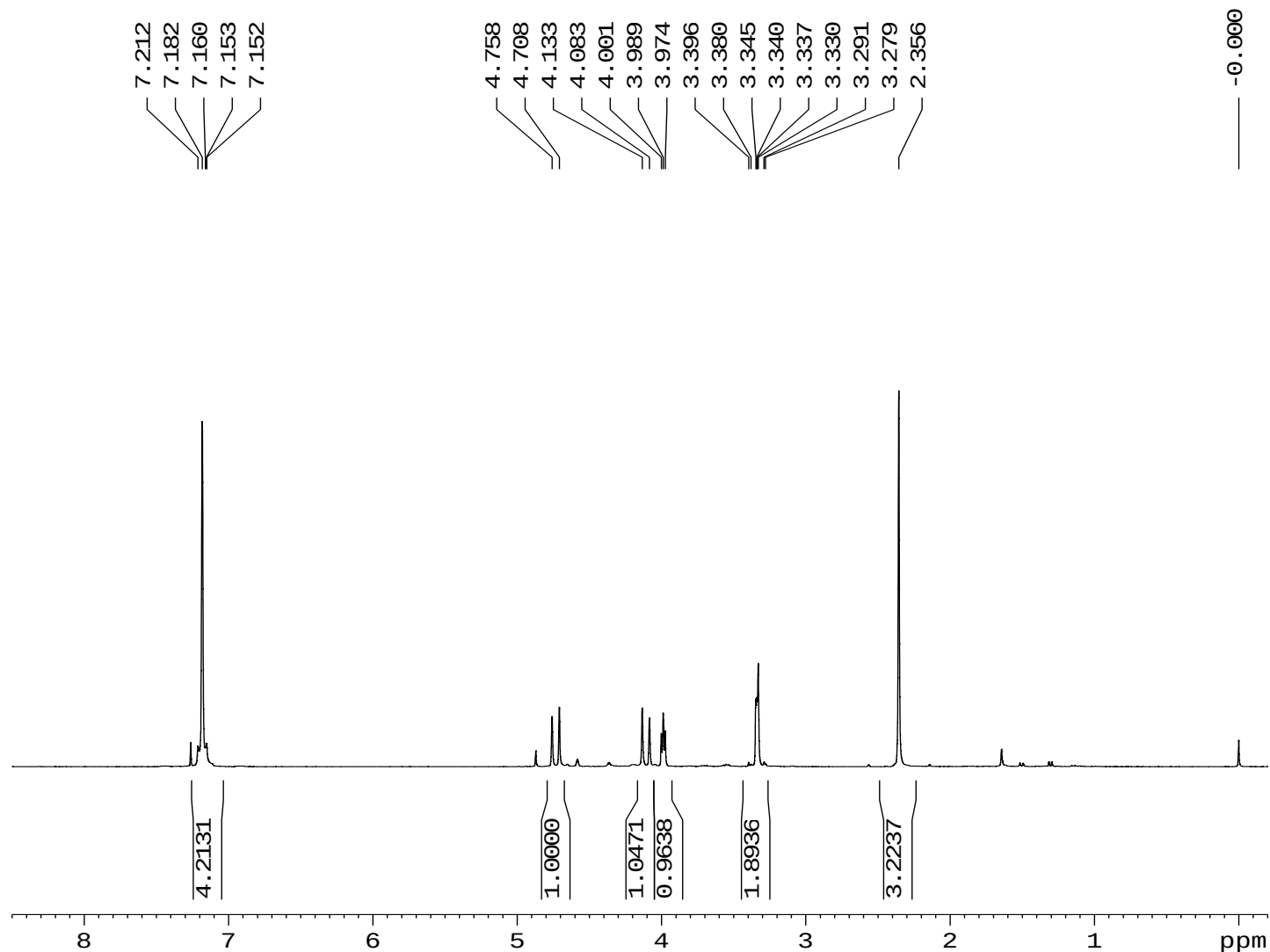
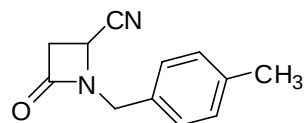
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1c-¹H NMR



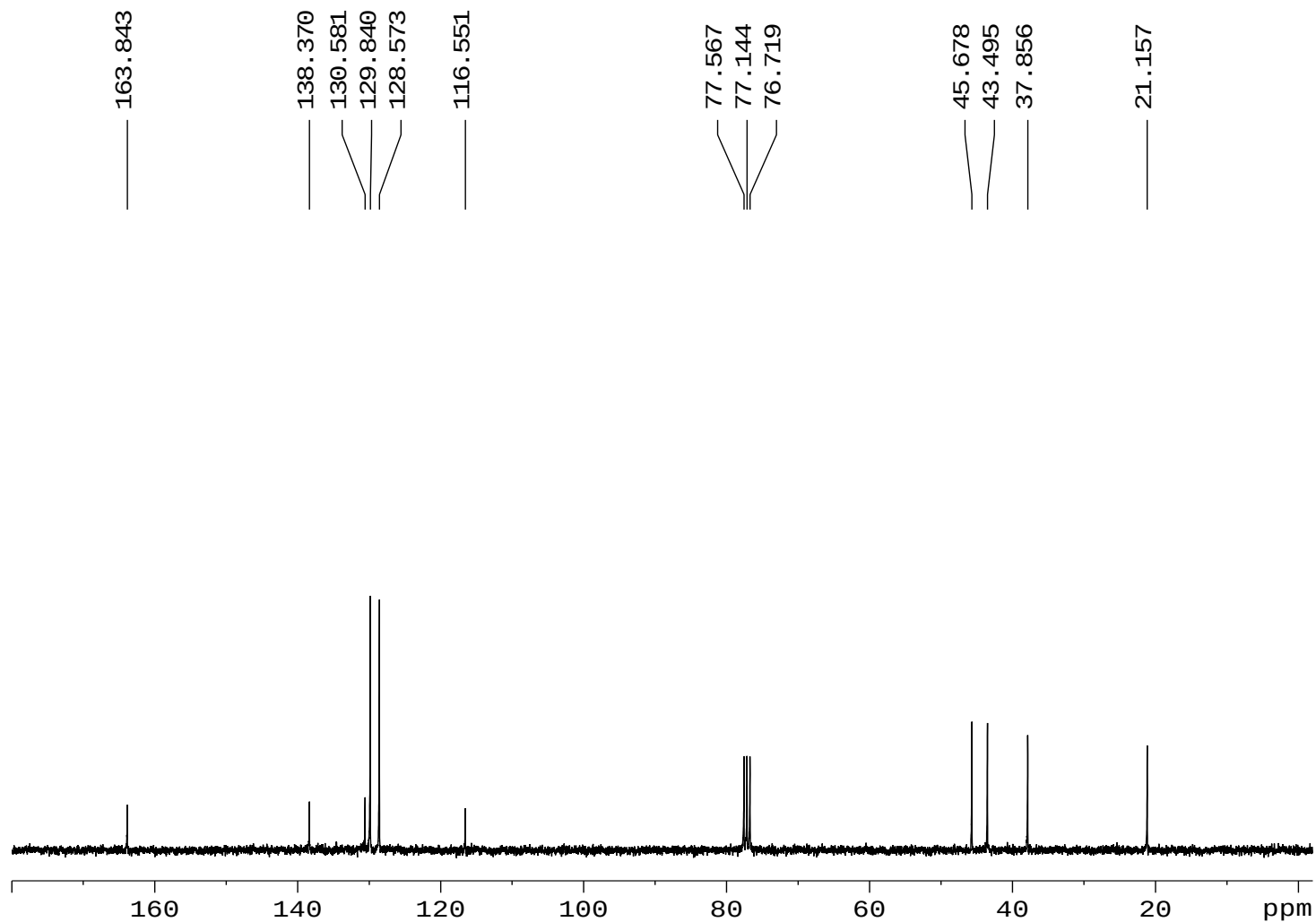
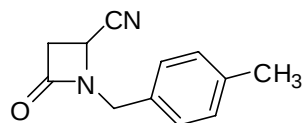
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1c-¹³C NMR



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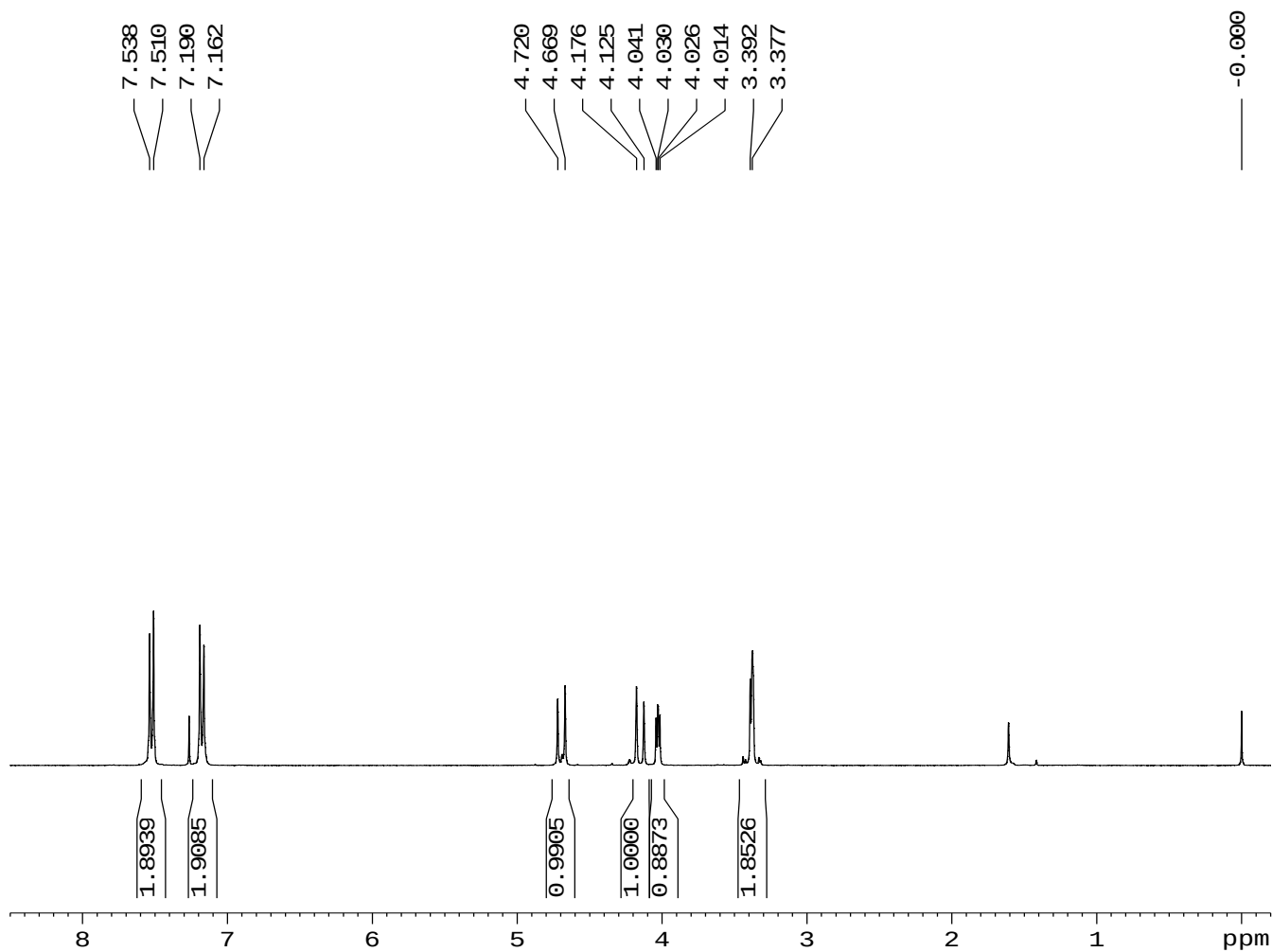
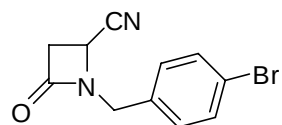
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1d-¹H NMR



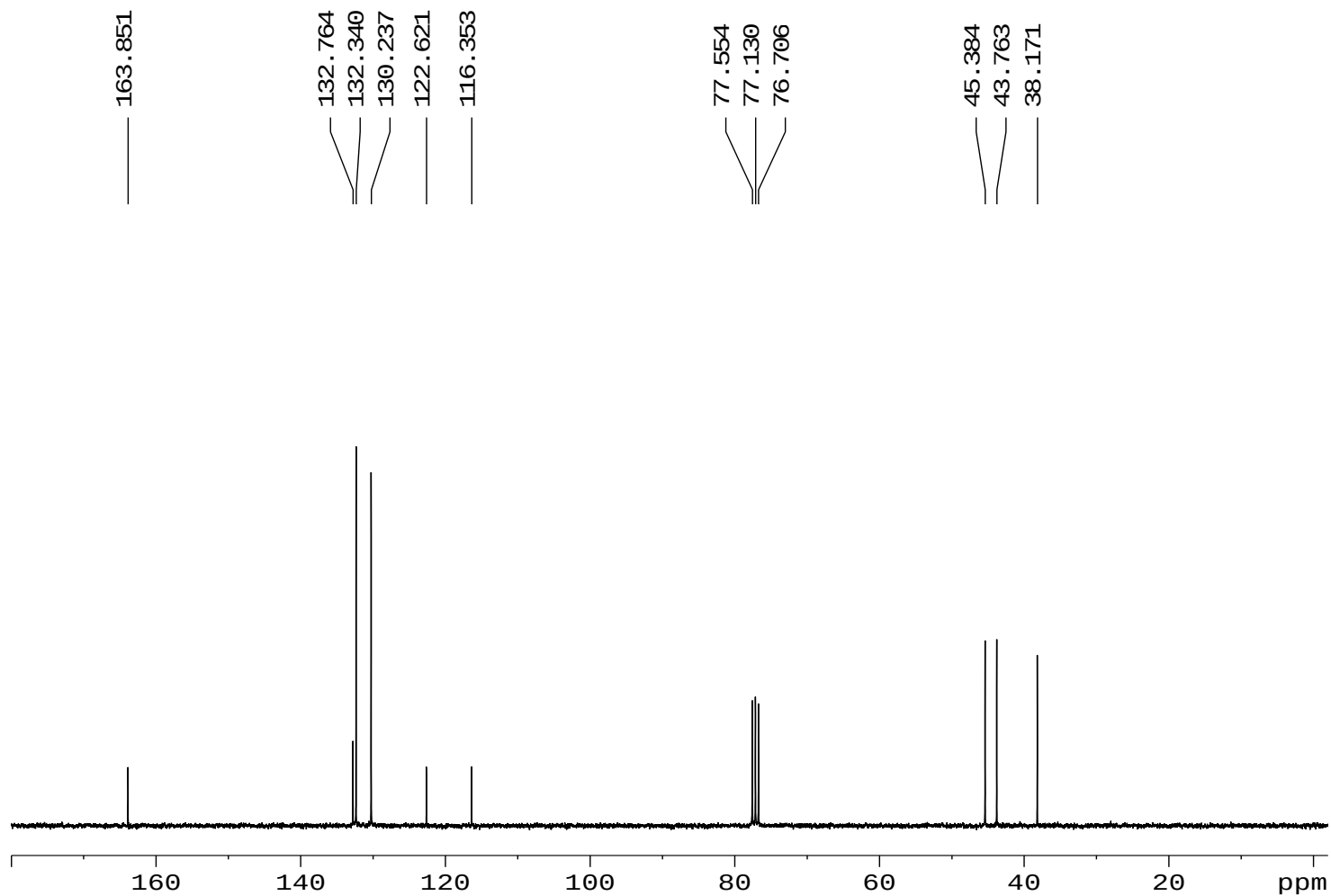
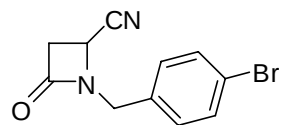
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1d-¹³C NMR



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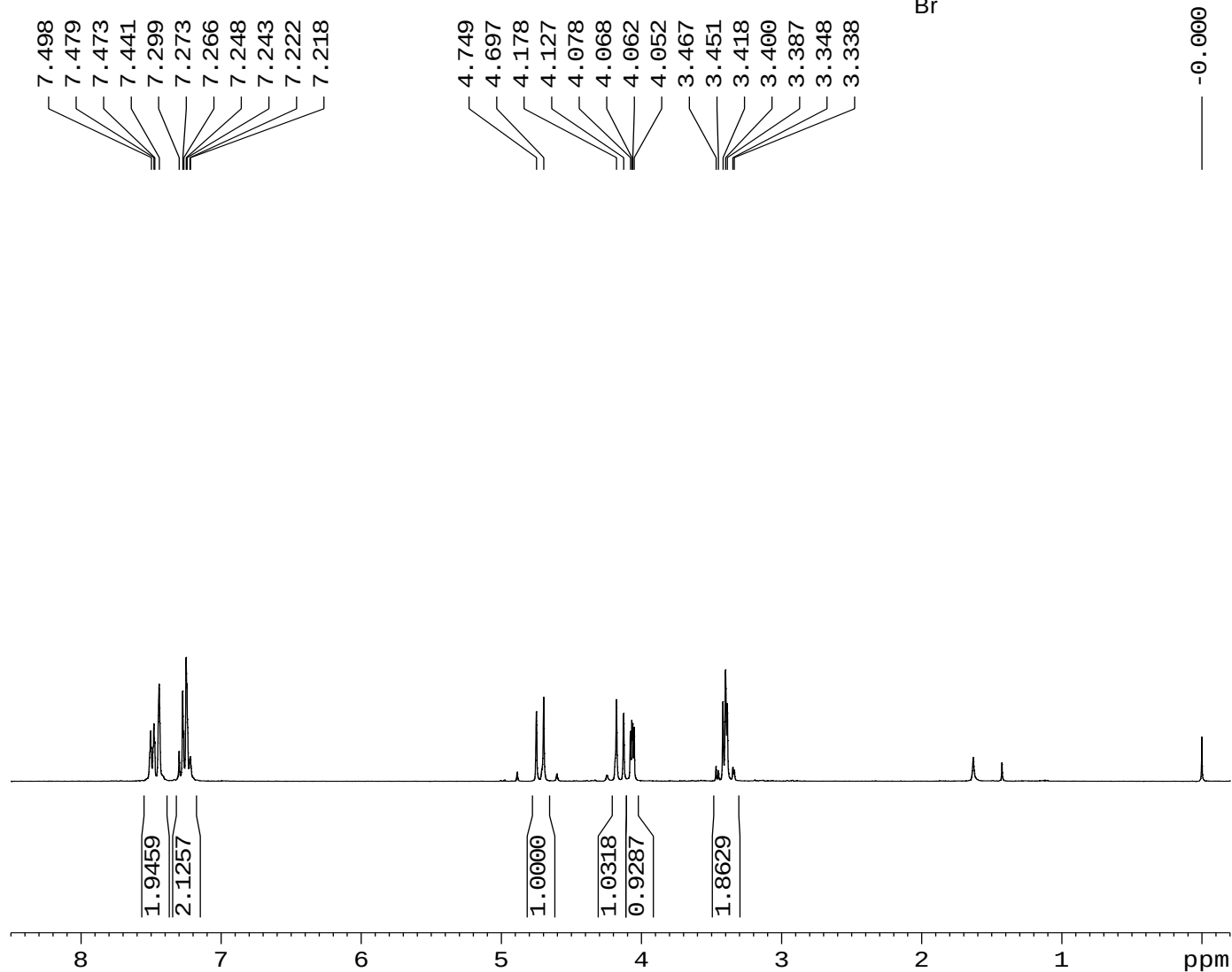
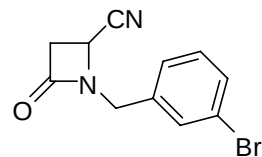
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FIDRES 0.274439 Hz
AQ 1.8219508 sec
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D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
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===== CHANNEL f2 =====
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1e-¹H NMR



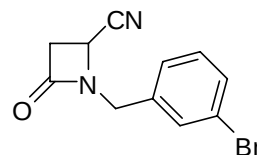
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AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
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TE 297.6 K
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===== CHANNEL f1 =====
NUC1 1H
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1e-¹³C NMR



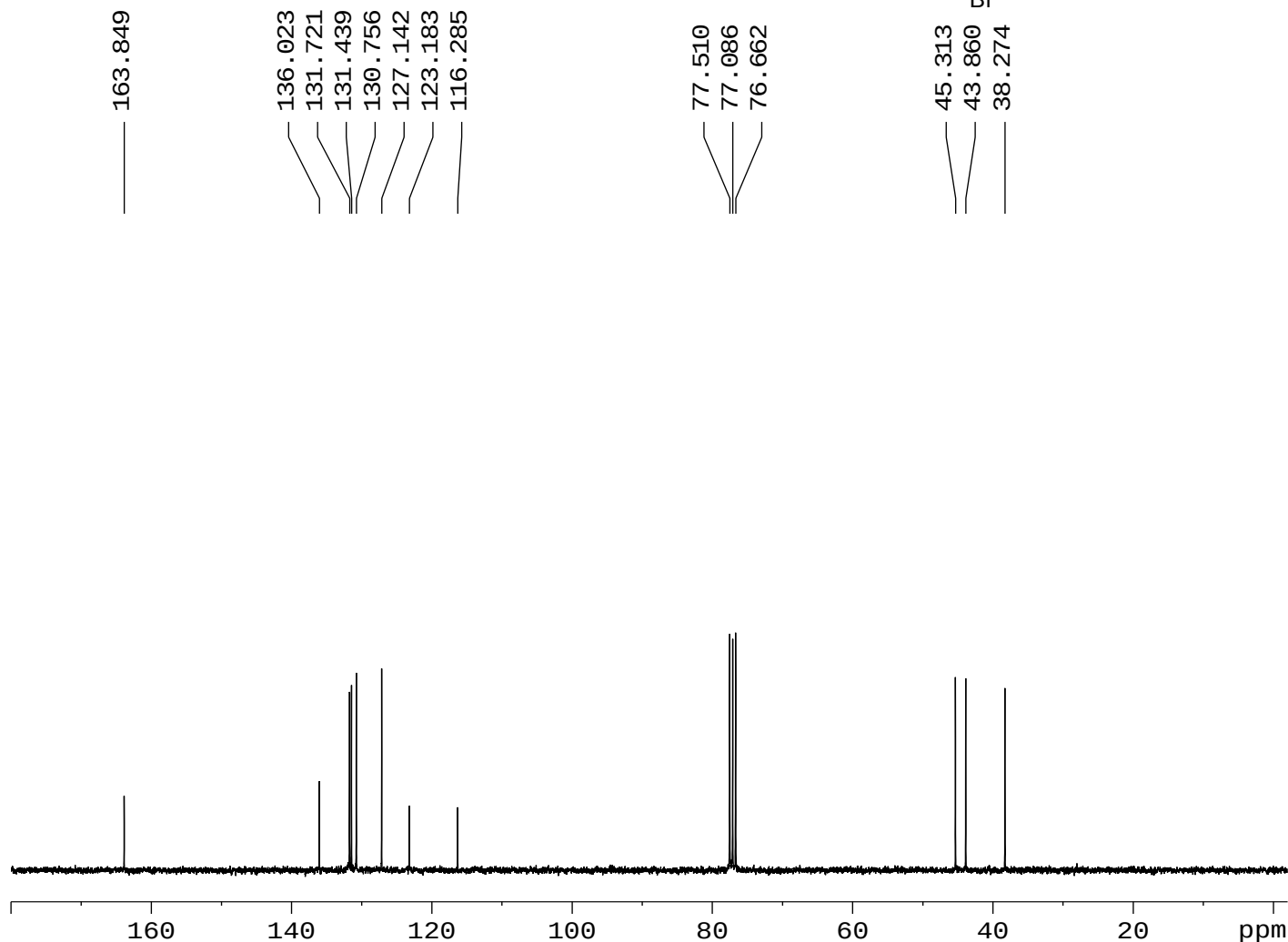
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DE 8.00 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

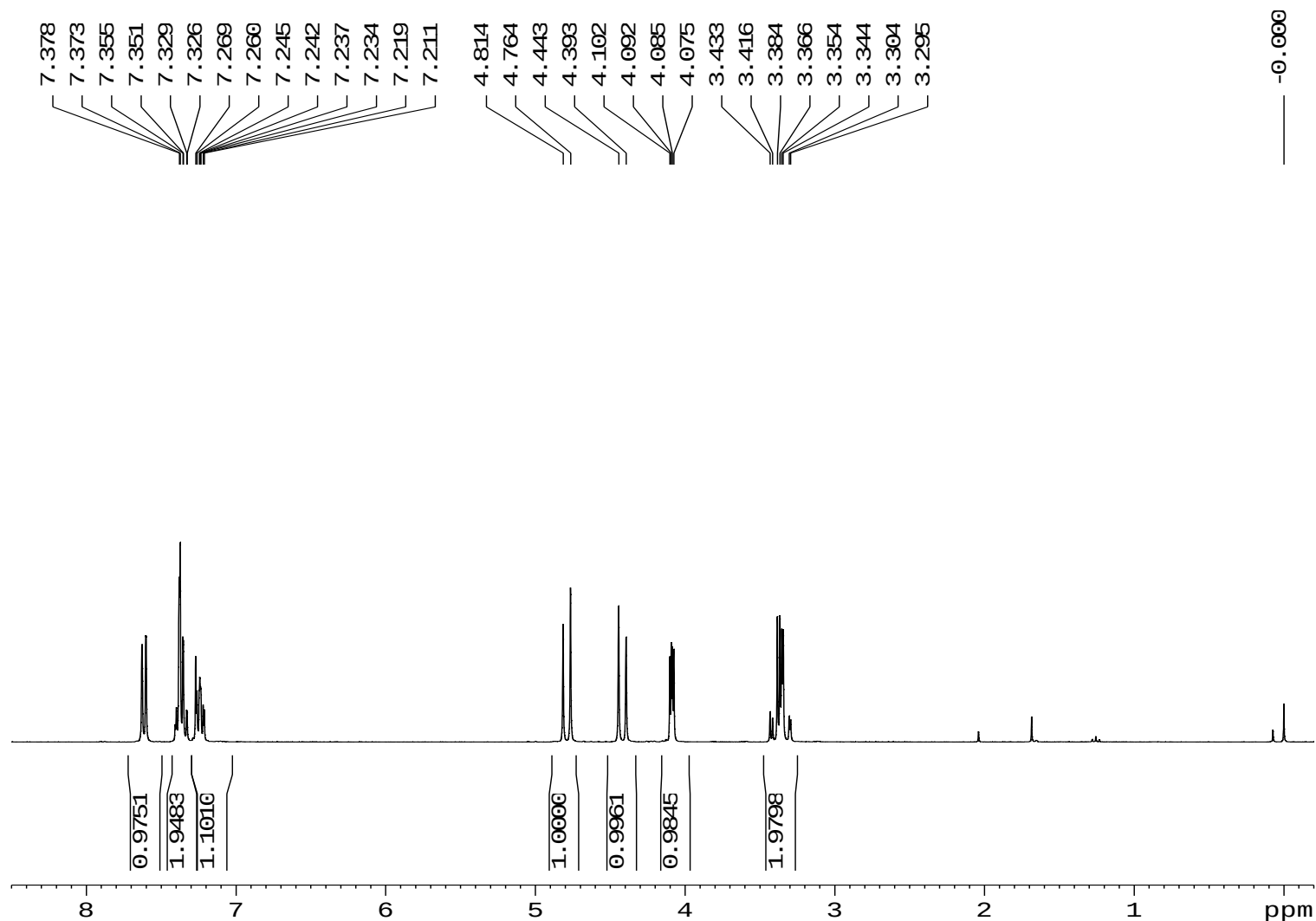
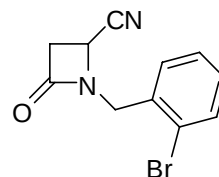
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4676374 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



1f-¹H NMR



-0.000



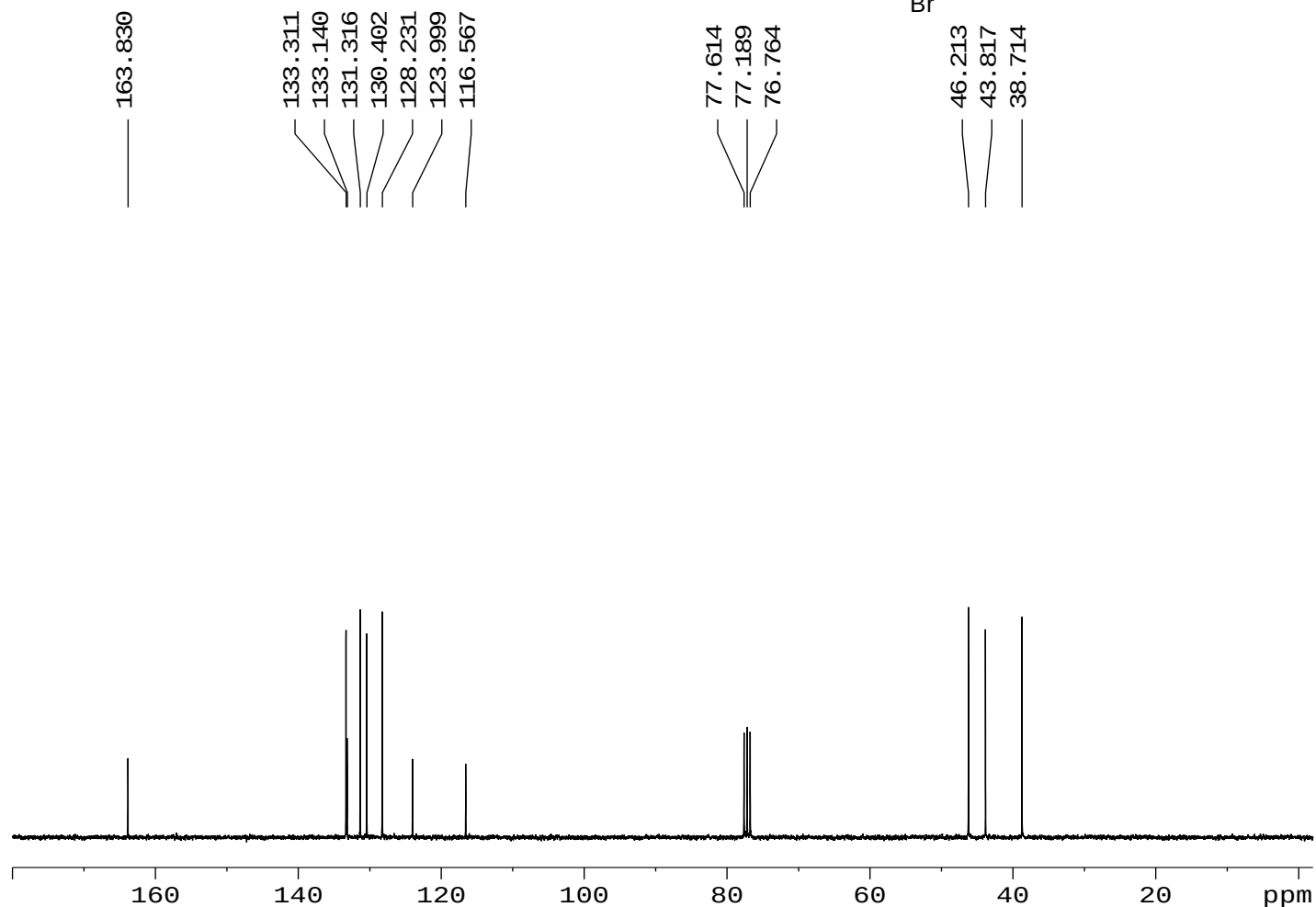
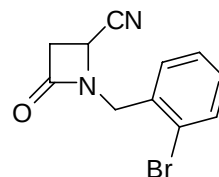
Current Data Parameters
NAME ldh-L-N-o-Br(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 13.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 8.00 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1f-¹³C NMR



Current Data Parameters
NAME ldh-L-N-o-Br(1)
EXPNO 20
PROCNO 1

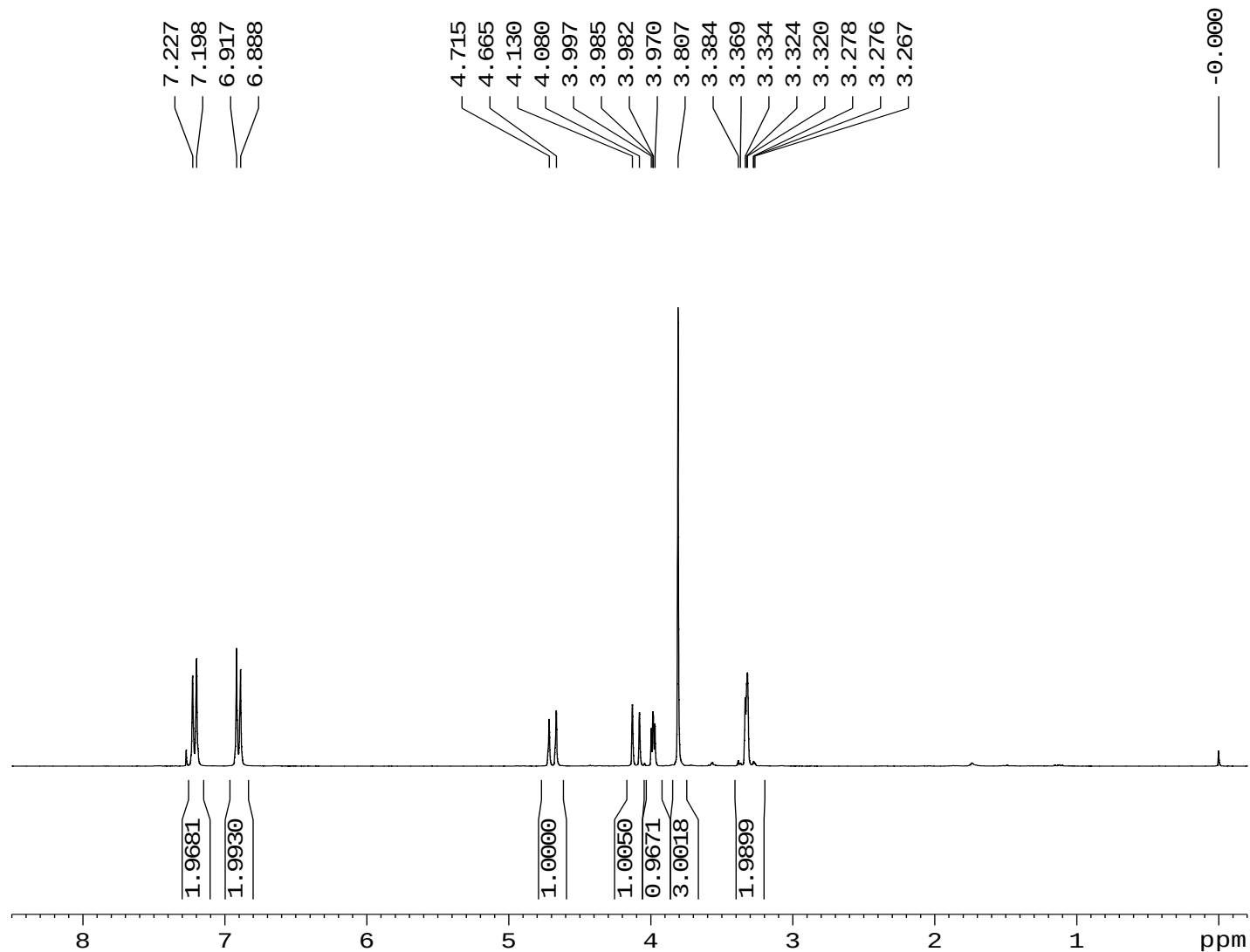
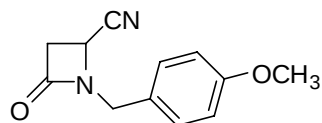
F2 - Acquisition Parameters
Date_ 20091211
Time 12.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 66
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1g-¹H NMR



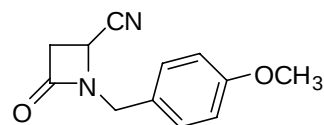
Current Data Parameters
NAME ldh-L-N-OCH3(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091208
Time 23.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 8.00 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1g-¹³C NMR



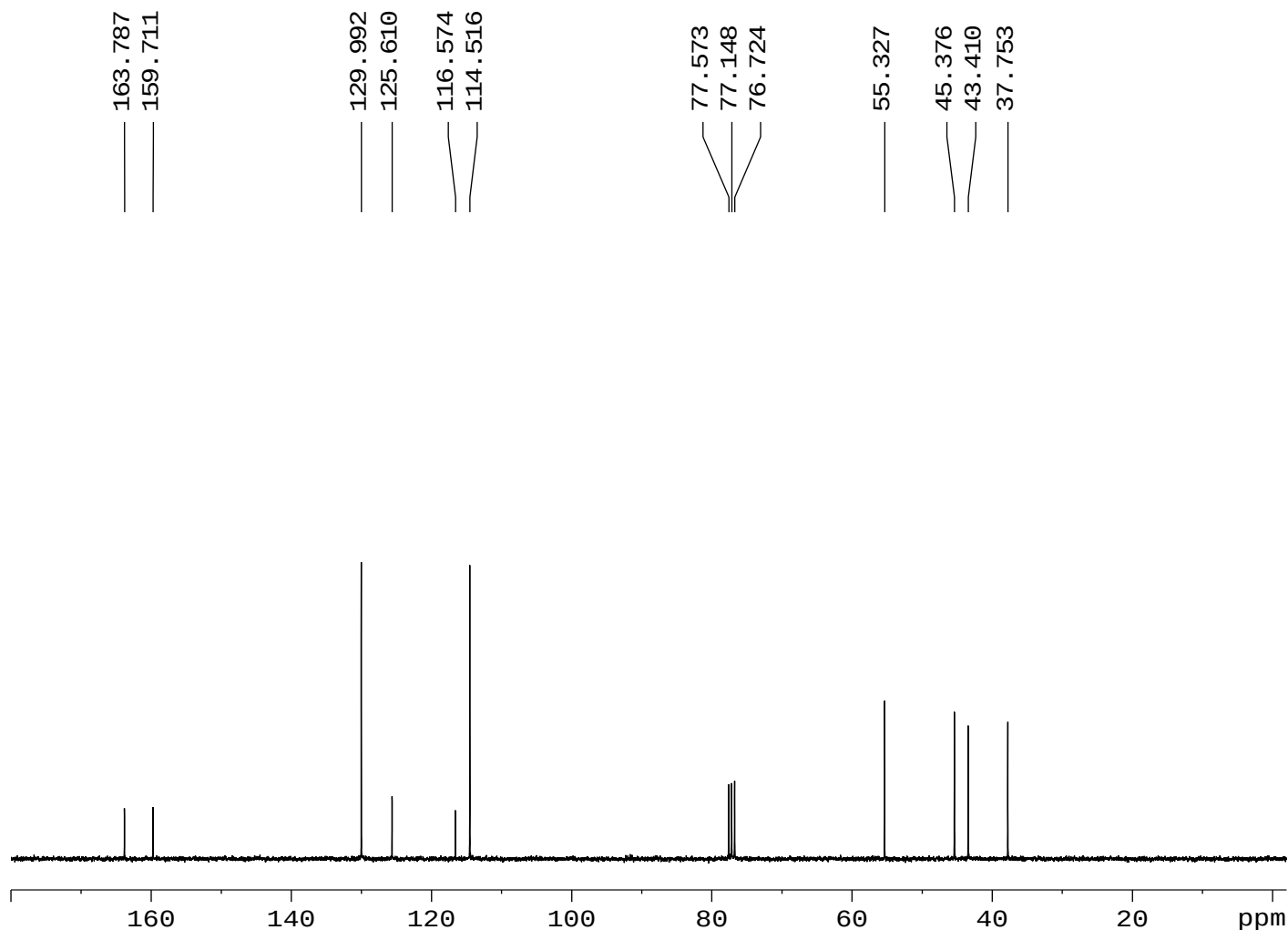
Current Data Parameters
NAME ldh-L-N-OCH3(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091211
Time 12.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 47
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

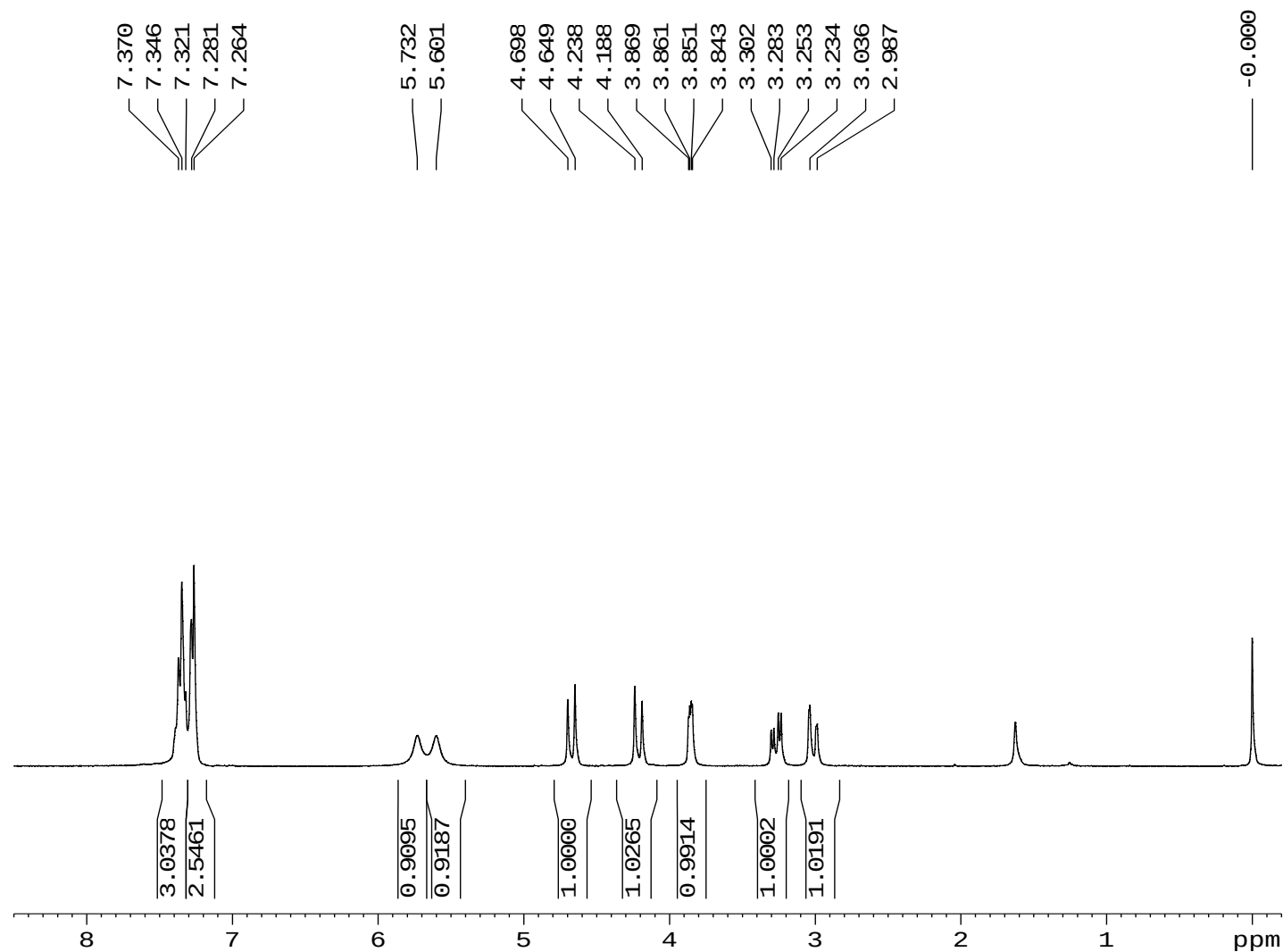
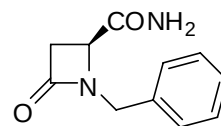
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2a-¹H NMR



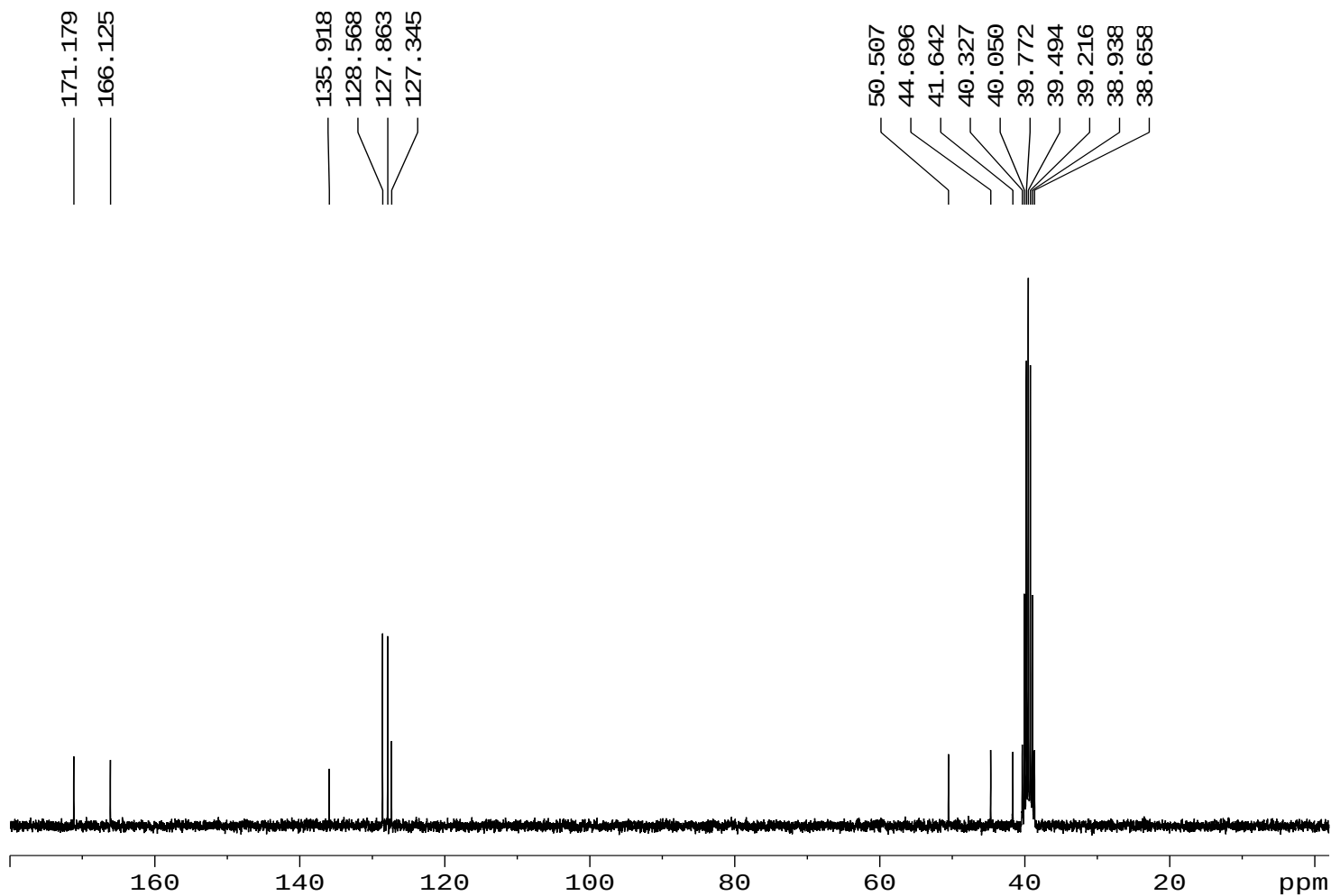
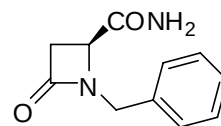
Current Data Parameters
NAME ldh-L-Am-H(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 15.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 8.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2a-¹³C NMR



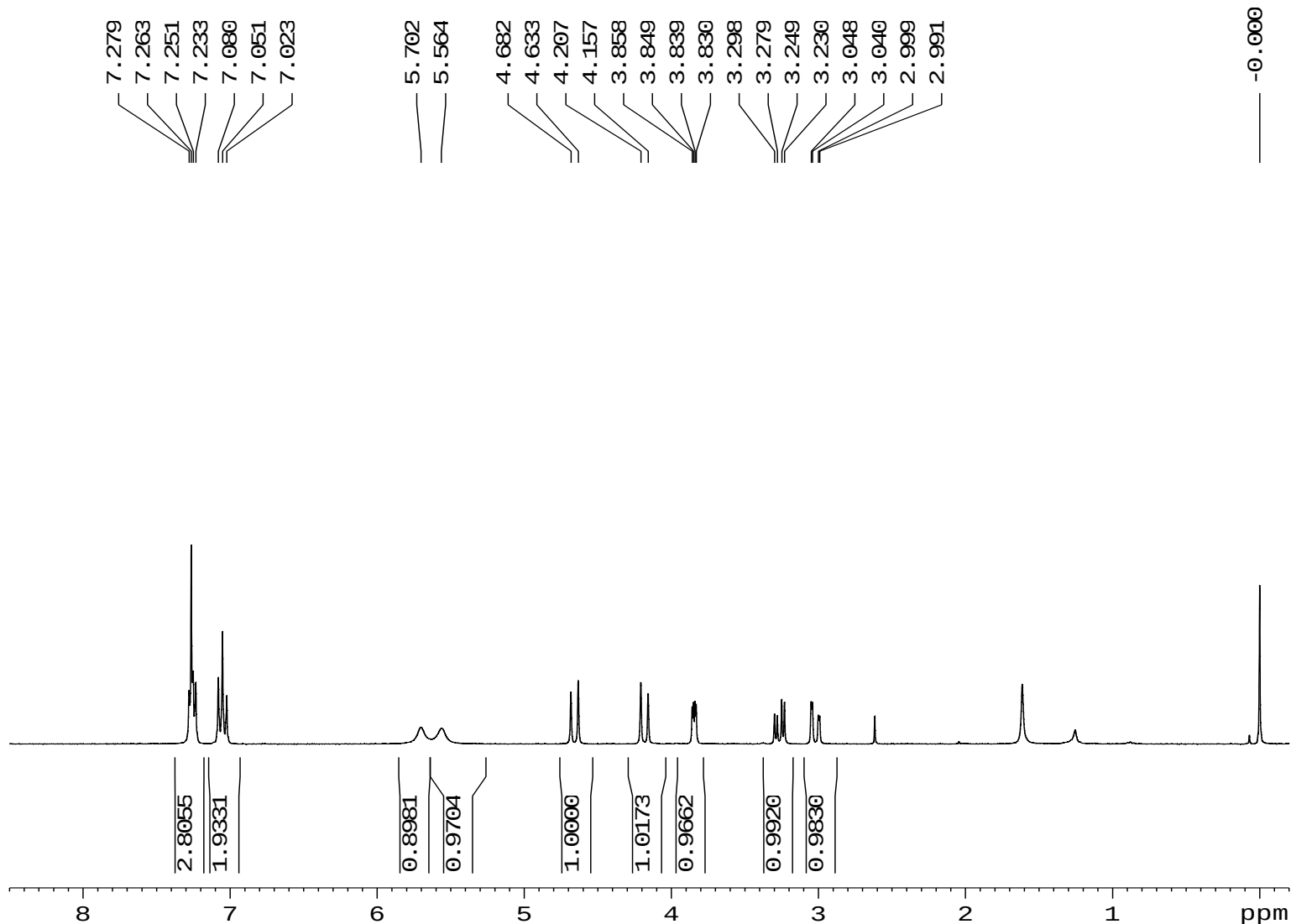
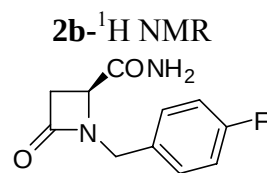
Current Data Parameters
NAME ldh-L-Am-H(1)
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091212
Time 12.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 107
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

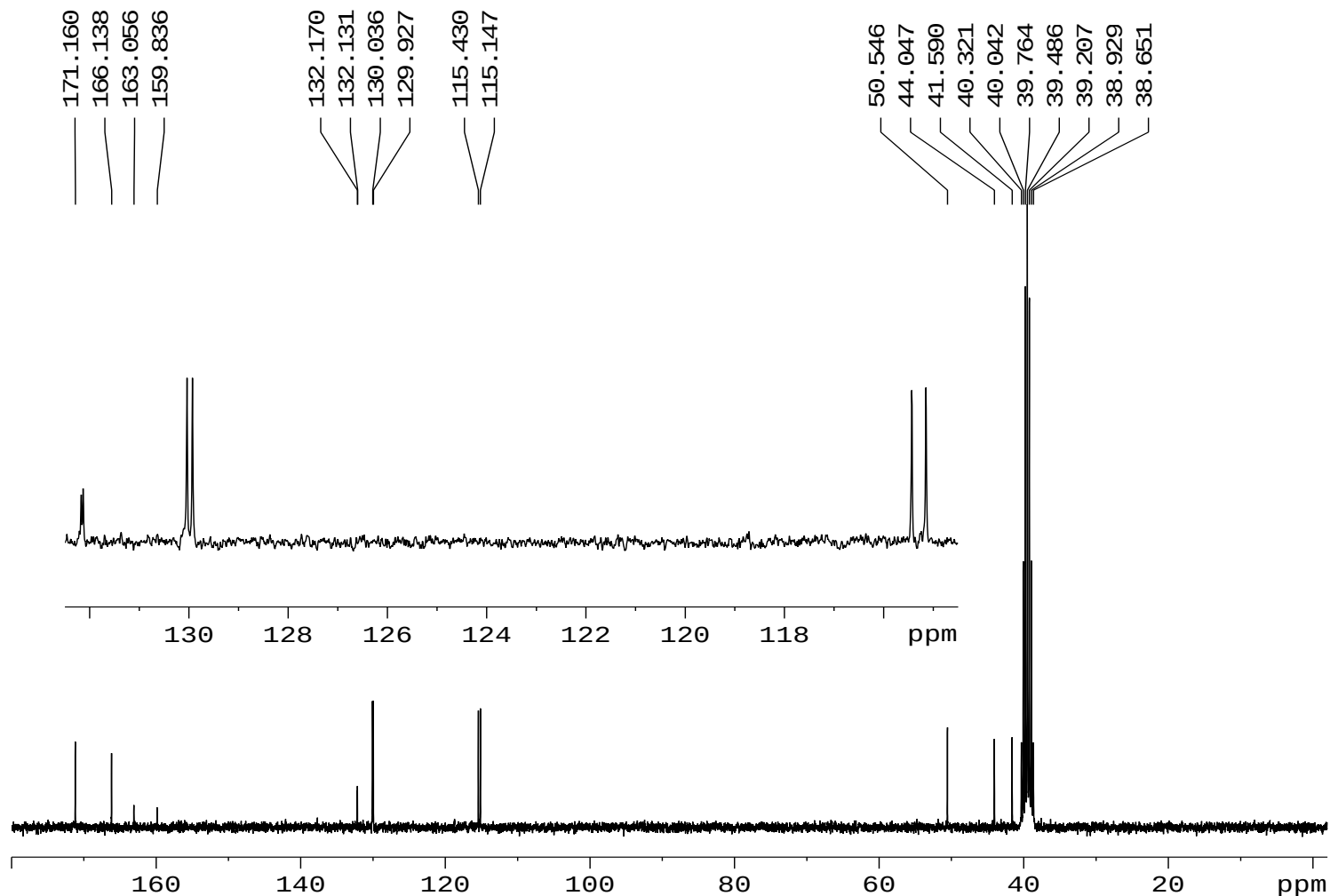
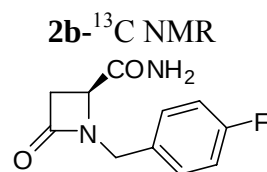


Current Data Parameters
NAME ldh-L-Am-F(1)
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091210
Time 11.30
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 8.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-F(1)
EXPNO 30
PROCNO 1

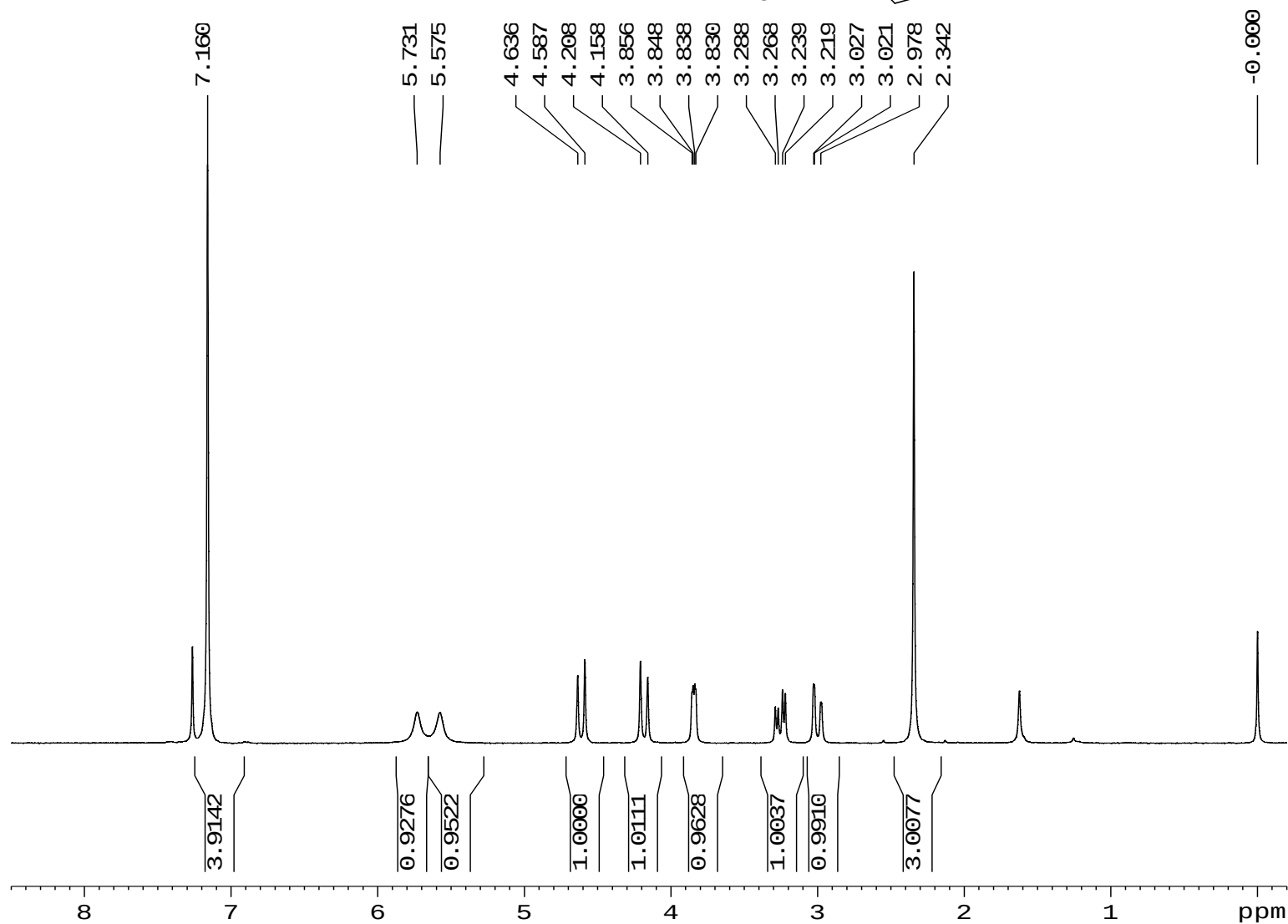
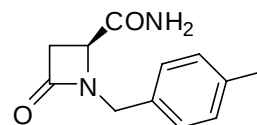
F2 - Acquisition Parameters
Date_ 20091212
Time 12.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 217
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 8.00 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2c-¹H NMR

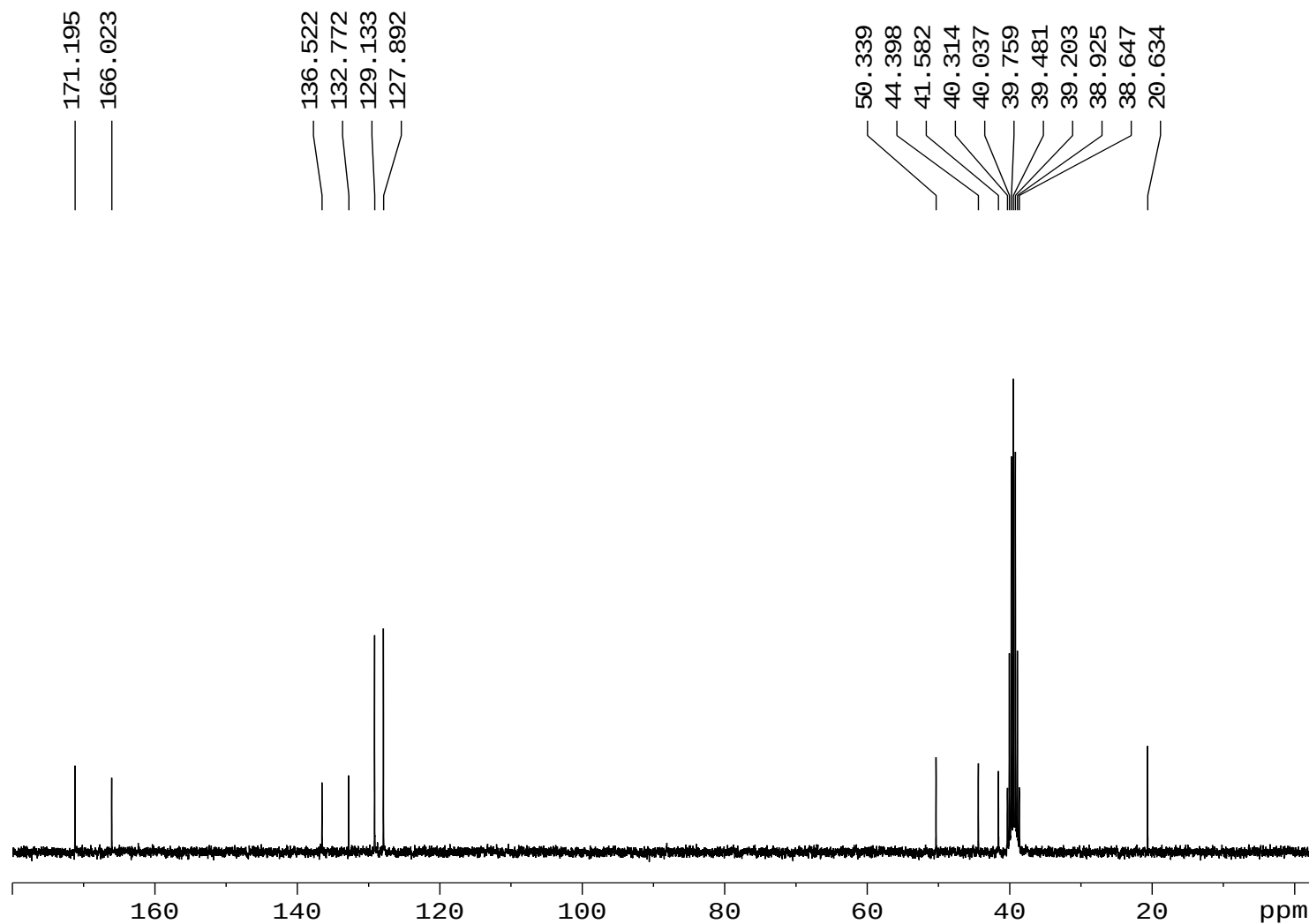
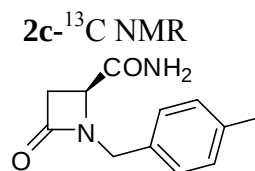


Current Data Parameters
NAME ldh-L-Am-CH3(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091210
Time 11.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 8.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-CH3(1)
EXPNO 40
PROCNO 1

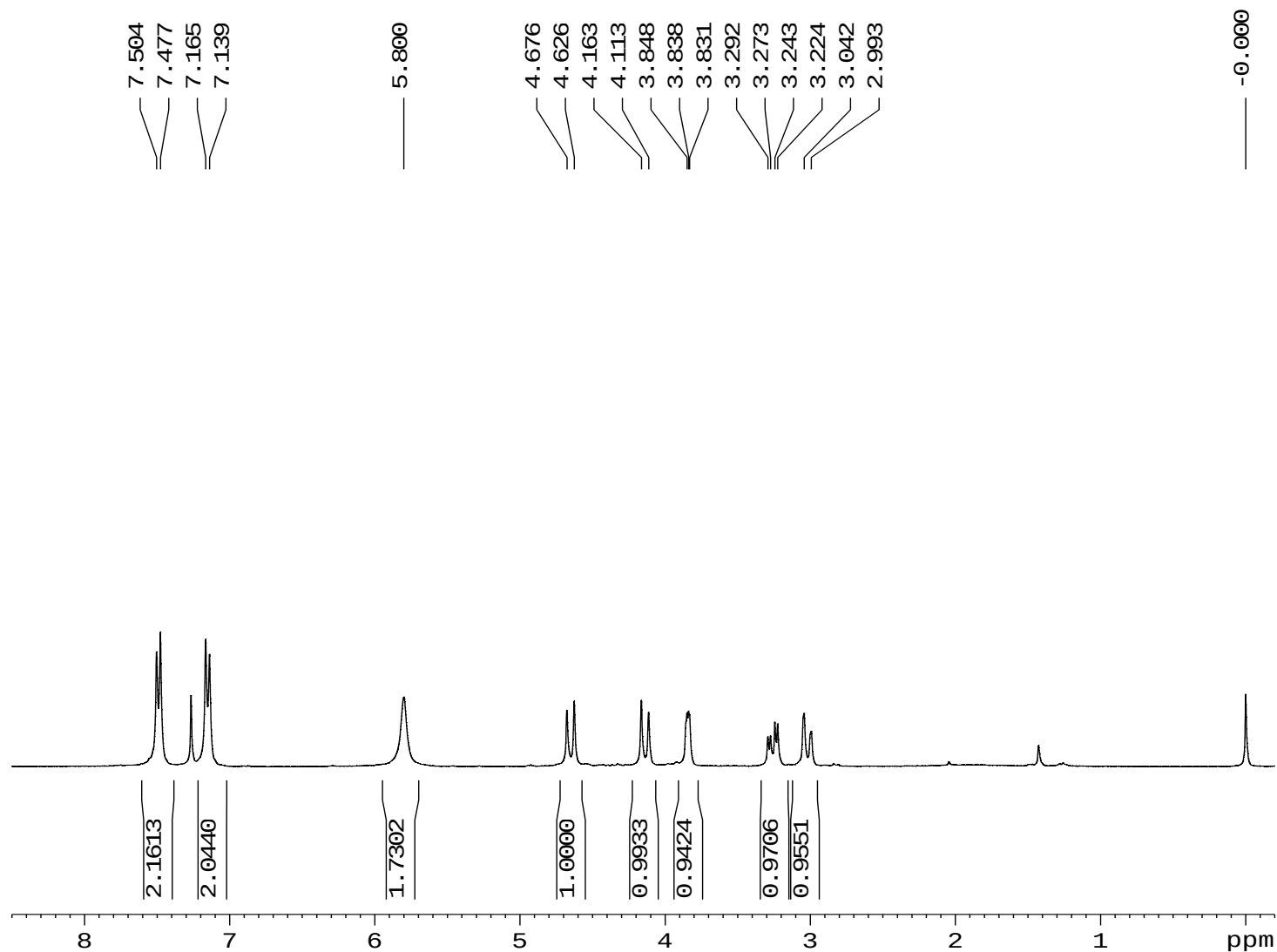
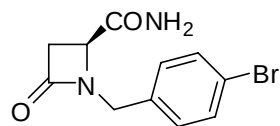
F2 - Acquisition Parameters
Date_ 20091212
Time 12.02
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 104
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DW 27.800 usec
DE 8.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2d-¹H NMR

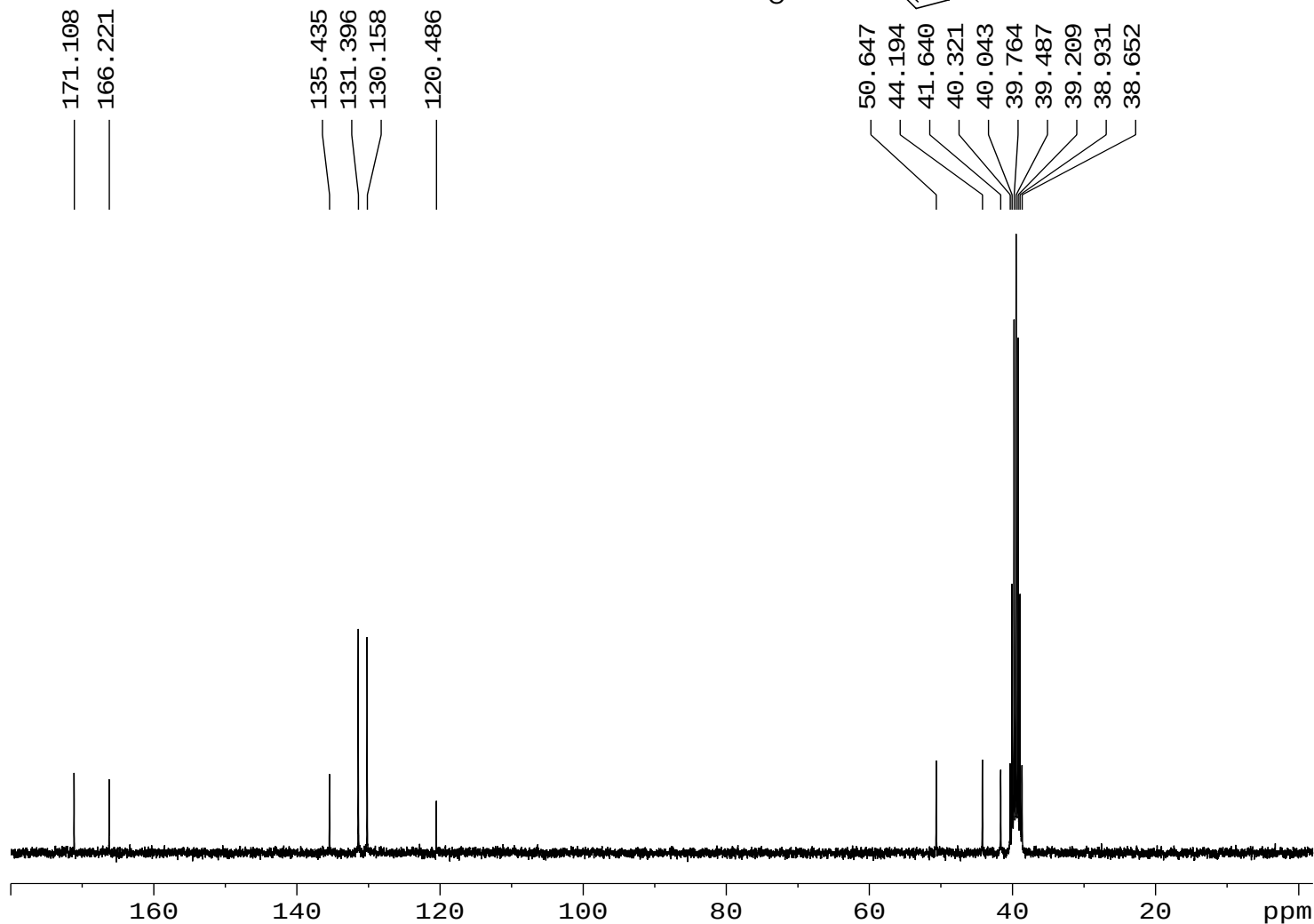
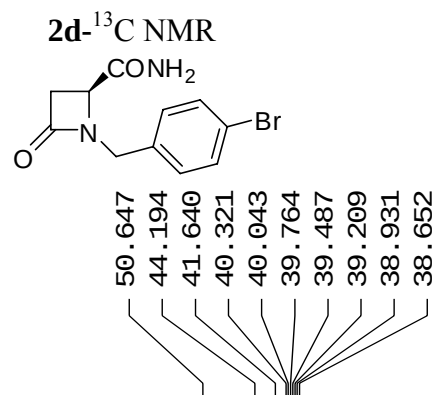


Current Data Parameters
NAME ldh-L-Am-p-Br(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 15.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 8.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-p-Br(1)
EXPNO 30
PROCNO 1

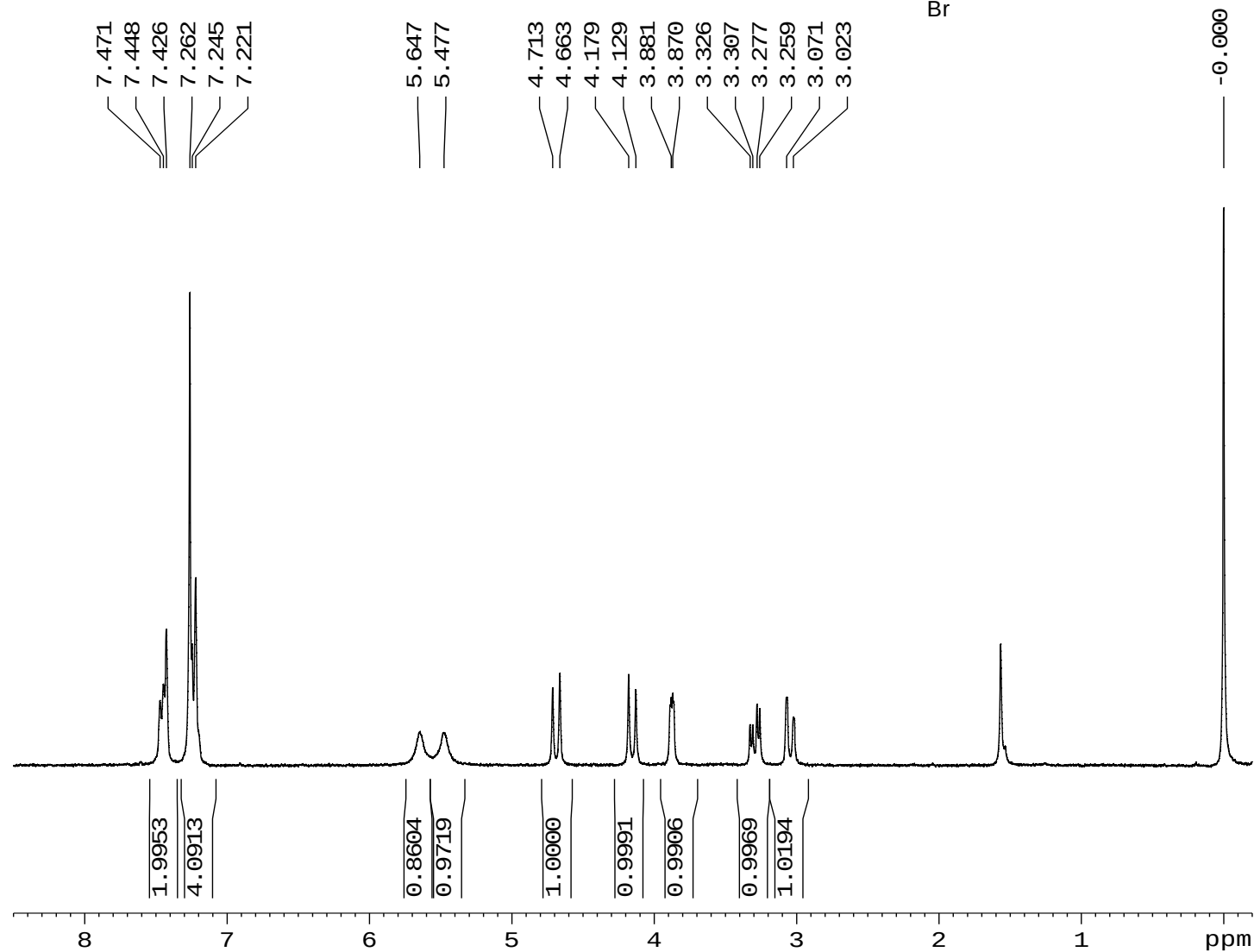
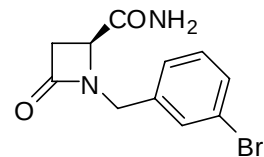
F2 - Acquisition Parameters
Date_ 20091212
Time 11.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 253
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2e-¹H NMR

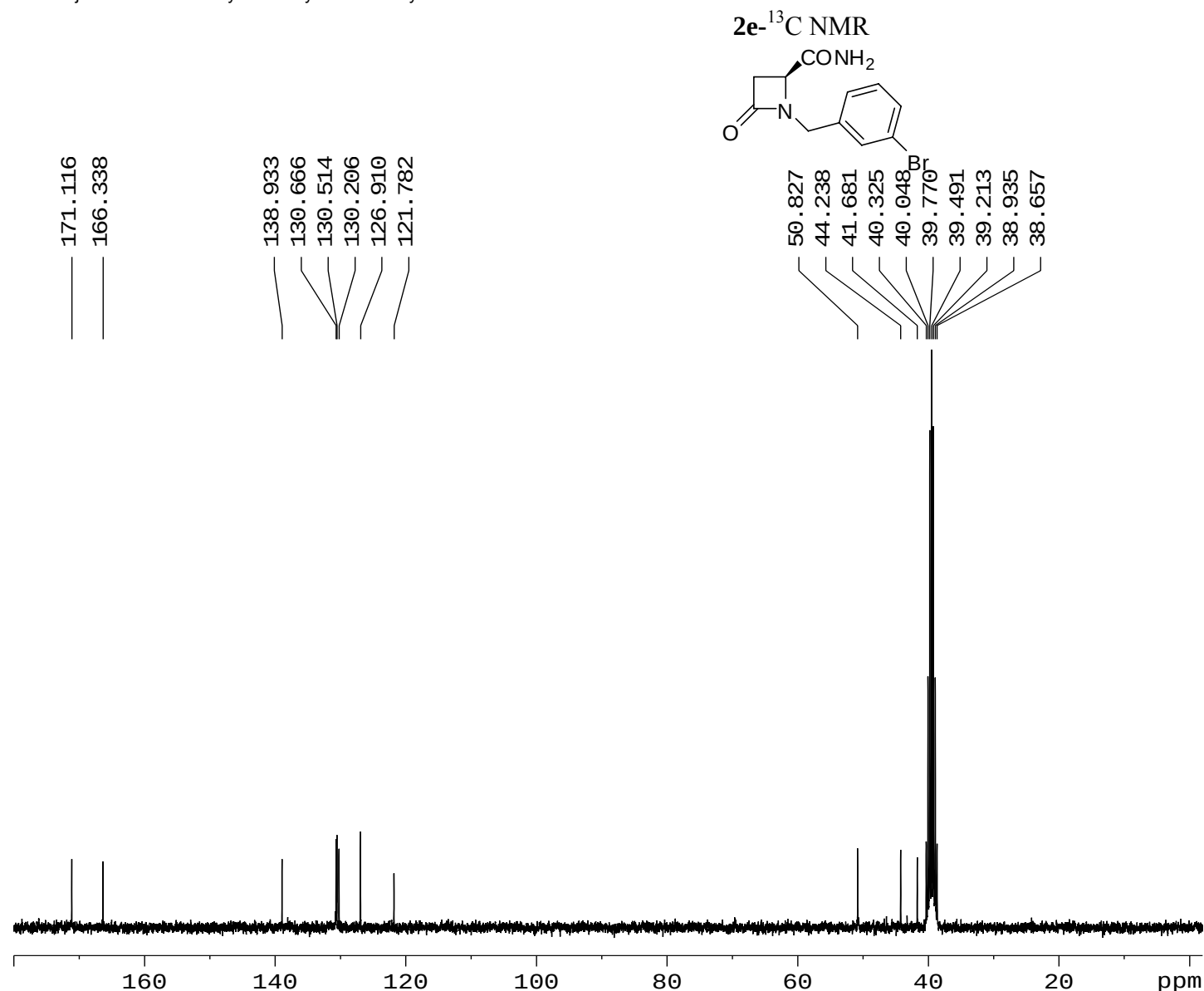


Current Data Parameters
NAME ldh-L-Am-m-Br
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100326
Time 11.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 574.7
DW 55.600 usec
DE 8.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-m-Br(1)
EXPNO 40
PROCNO 1

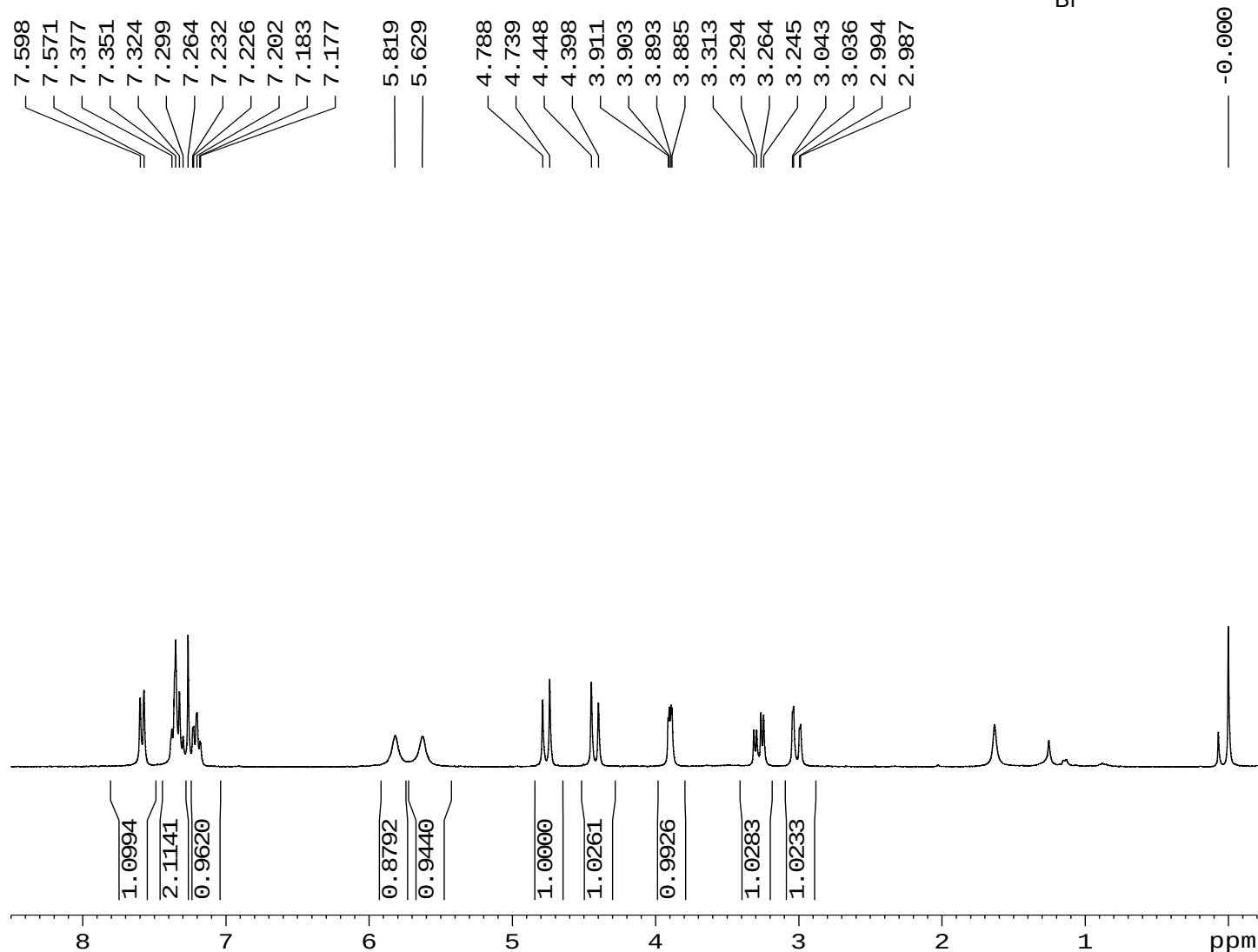
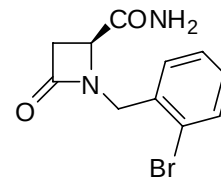
F2 - Acquisition Parameters
Date_ 20091212
Time 13.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 156
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2f-¹H NMR

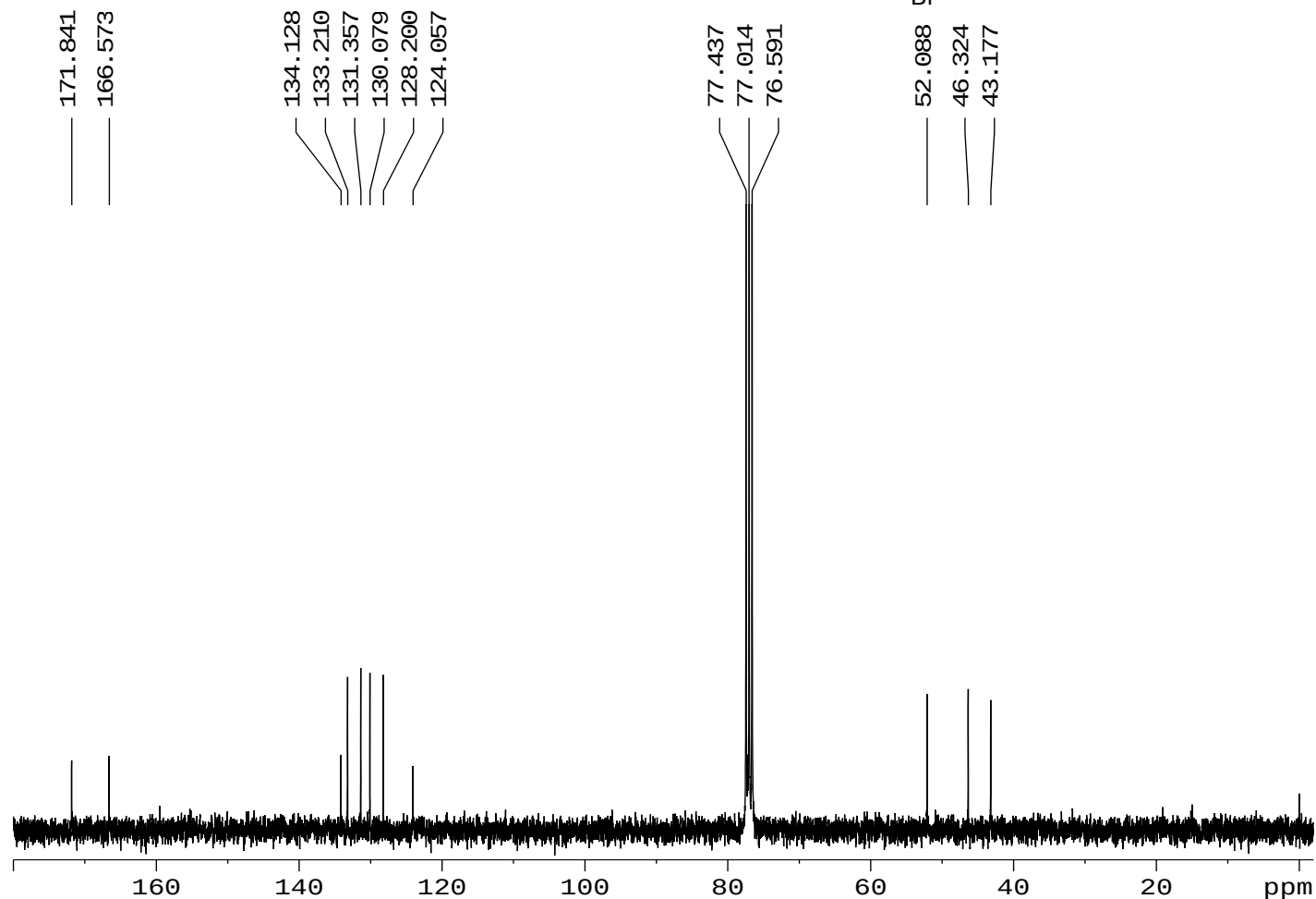
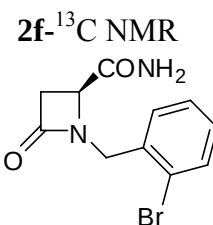


Current Data Parameters
NAME ldh-L-Am-o-Br(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 15.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 8.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



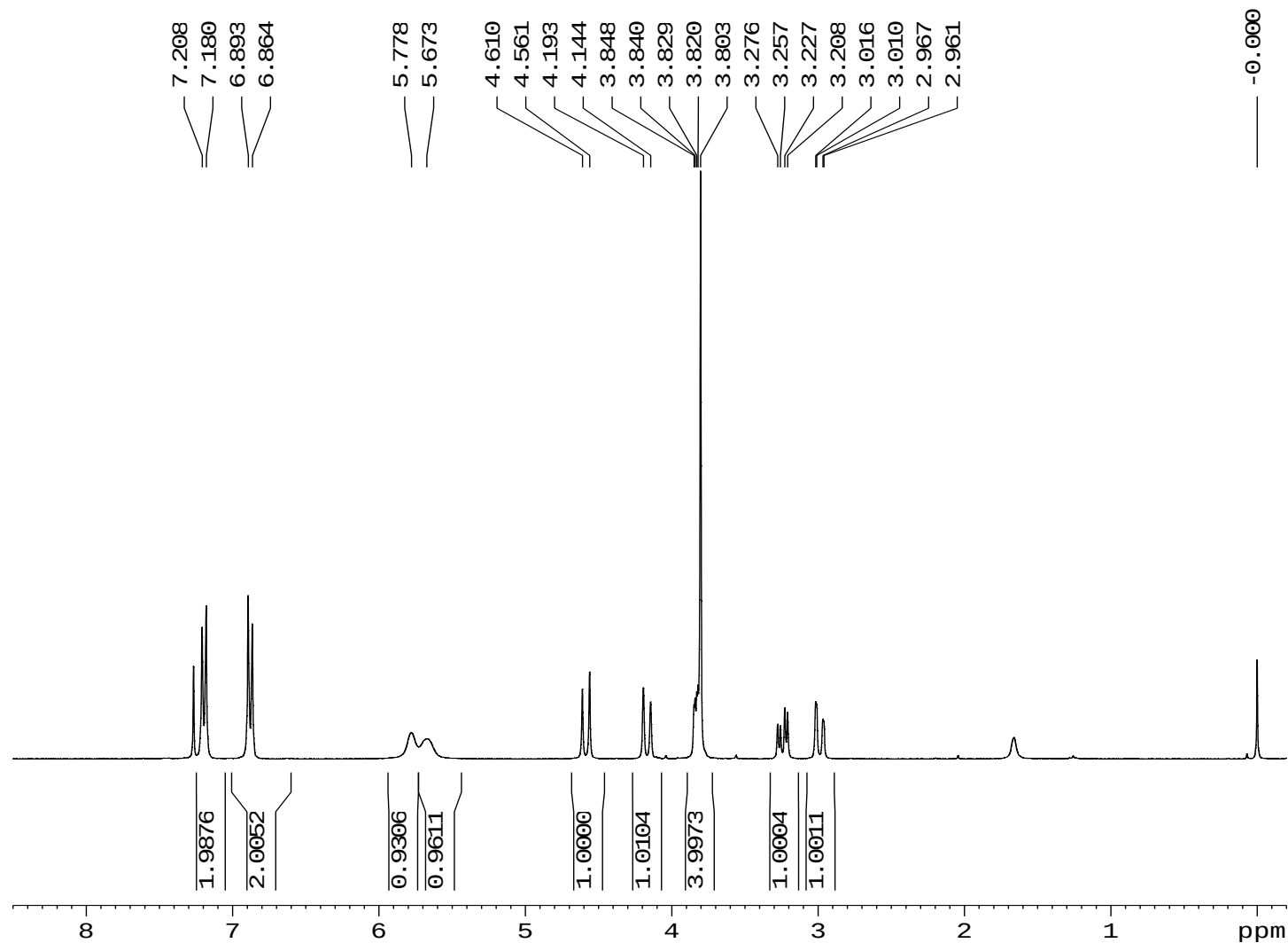
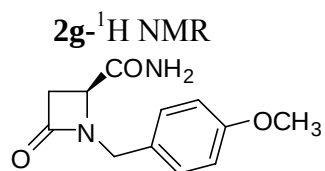
Current Data Parameters
NAME ldh-L-Am-o-Br
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100305
Time 11.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 519
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 8.00 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

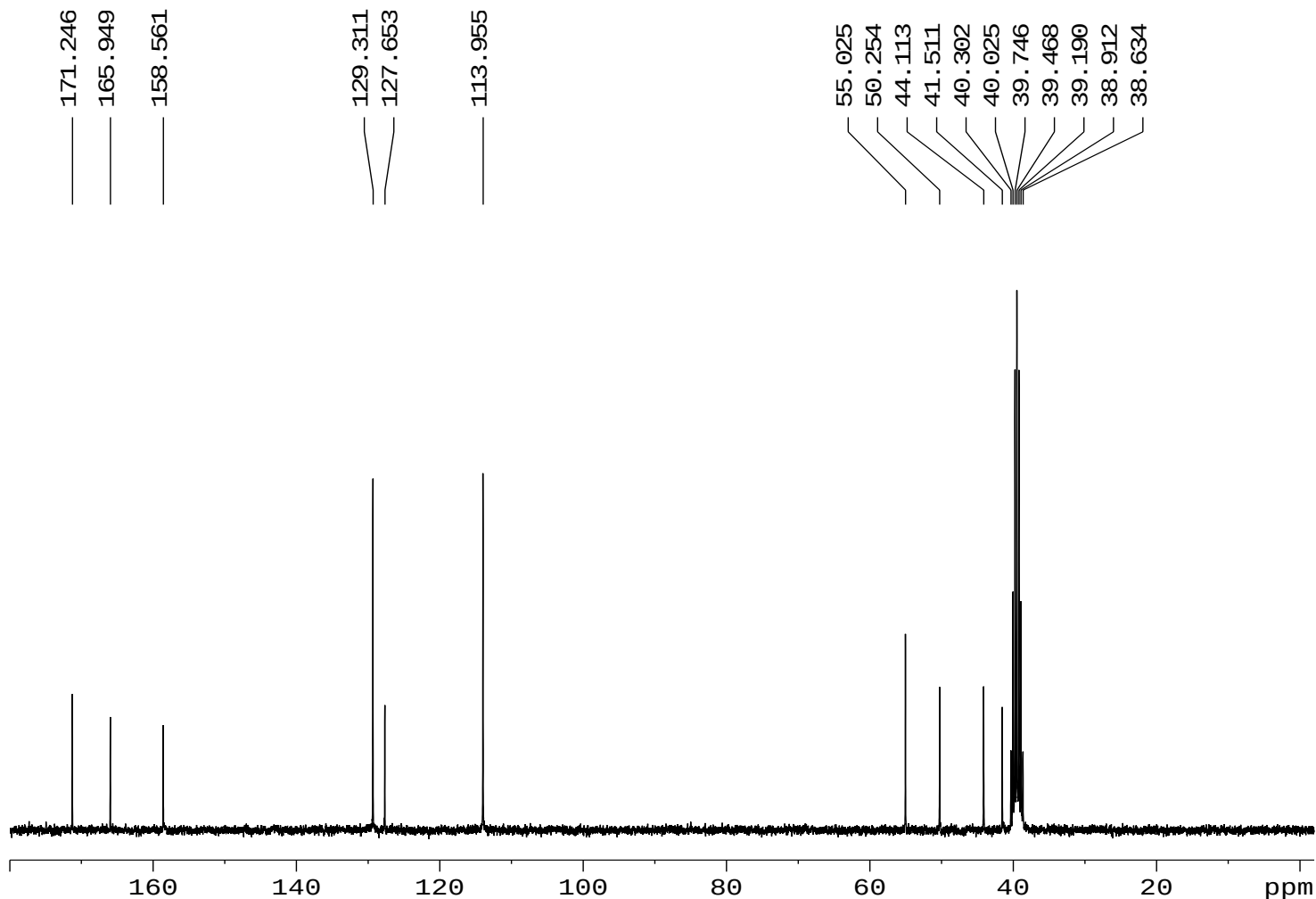
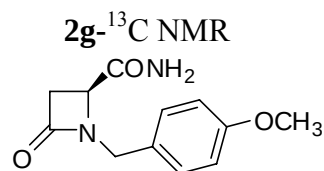


Current Data Parameters
NAME ldh-L-Am-OCH3(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091210
Time 11.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 8.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-OCH3(1)
EXPNO 30
PROCNO 1

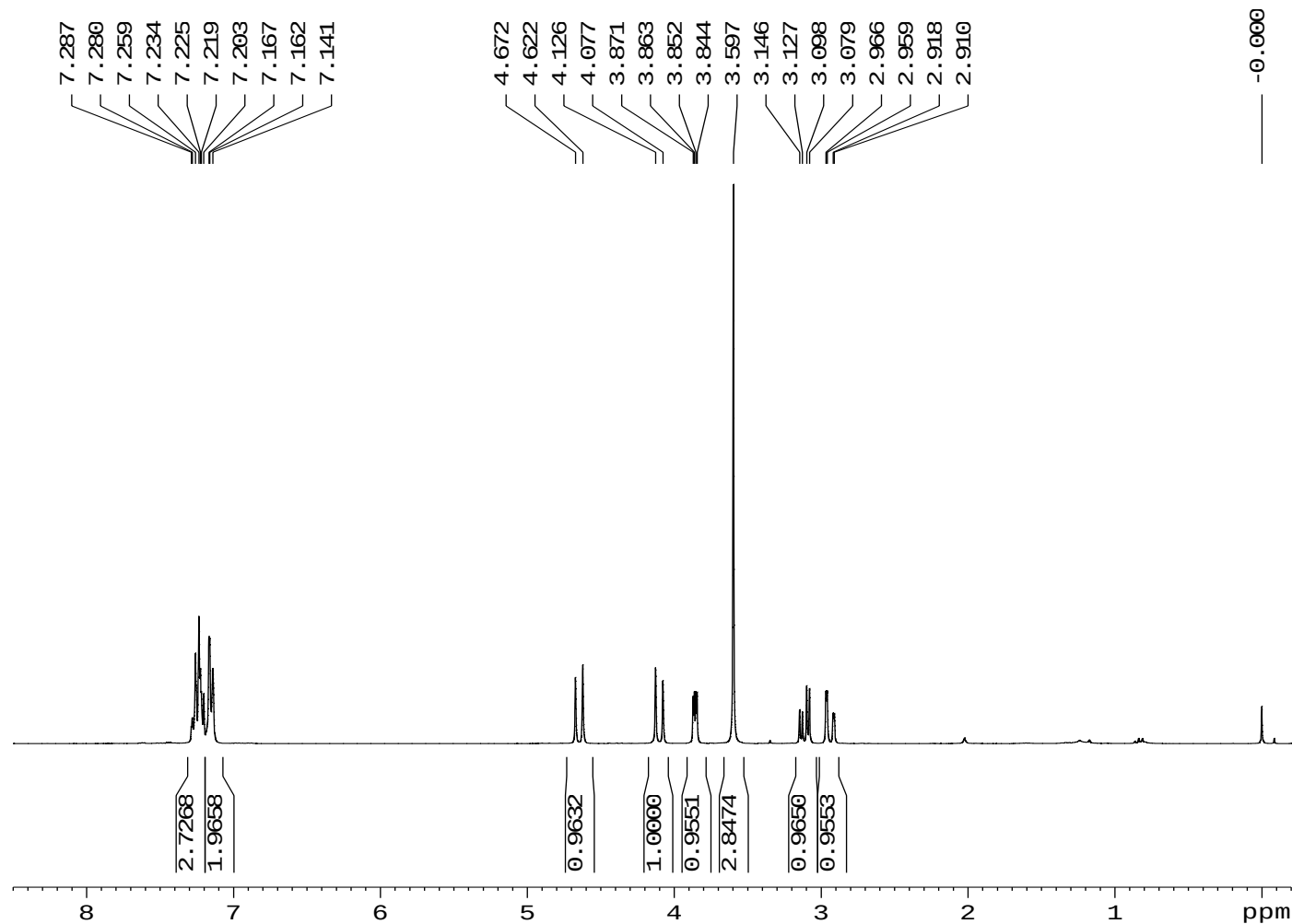
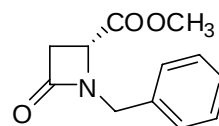
F2 - Acquisition Parameters
Date_ 20091212
Time 11.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 229
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4a-¹H NMR

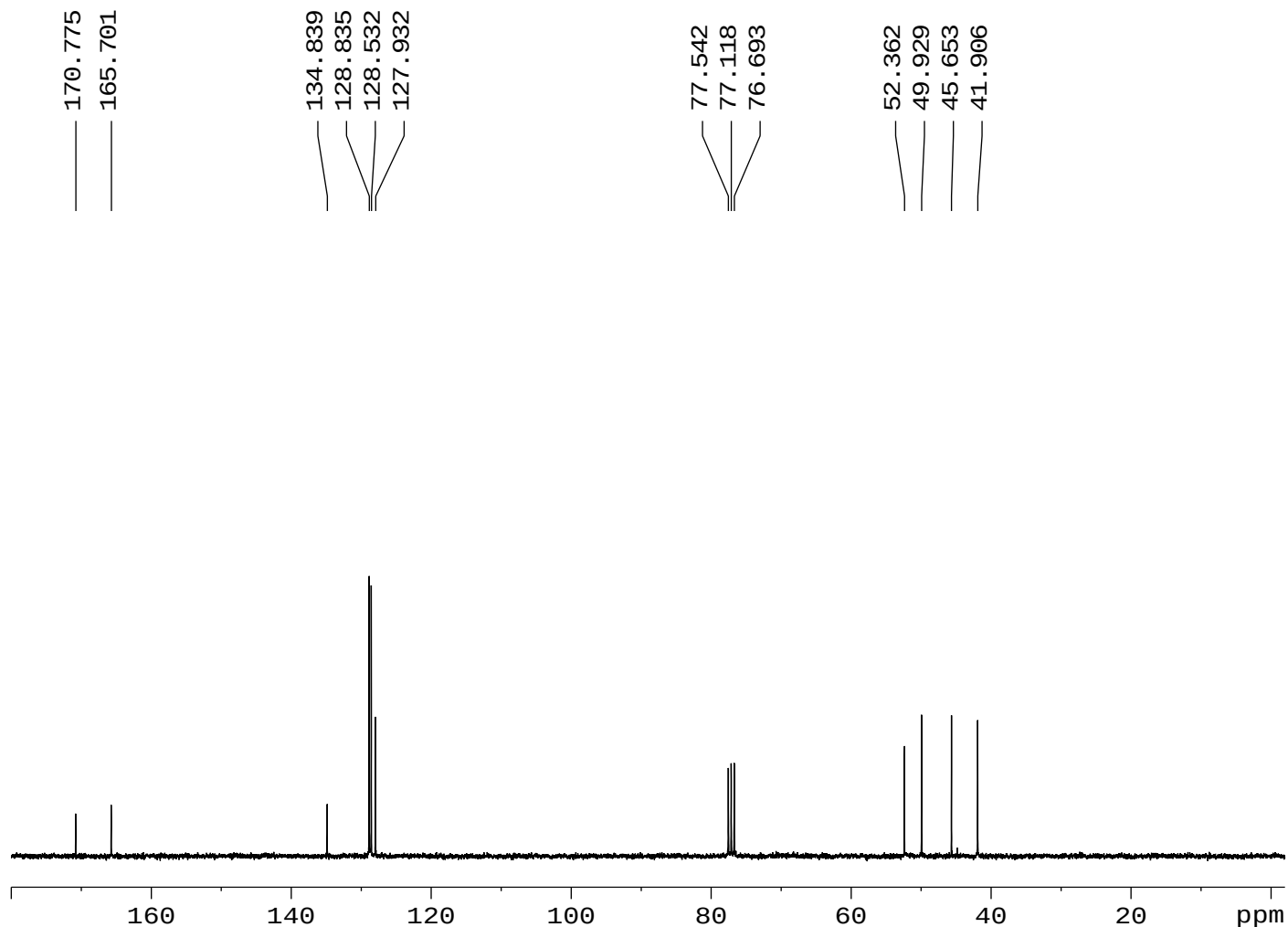
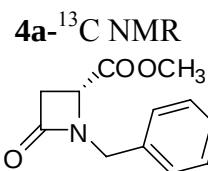


Current Data Parameters
NAME ldh-L-E-H
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100318
Time 12.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 45.3
DW 55.600 usec
DE 8.00 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300189 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-E-H(1)
EXPNO 20
PROCNO 1

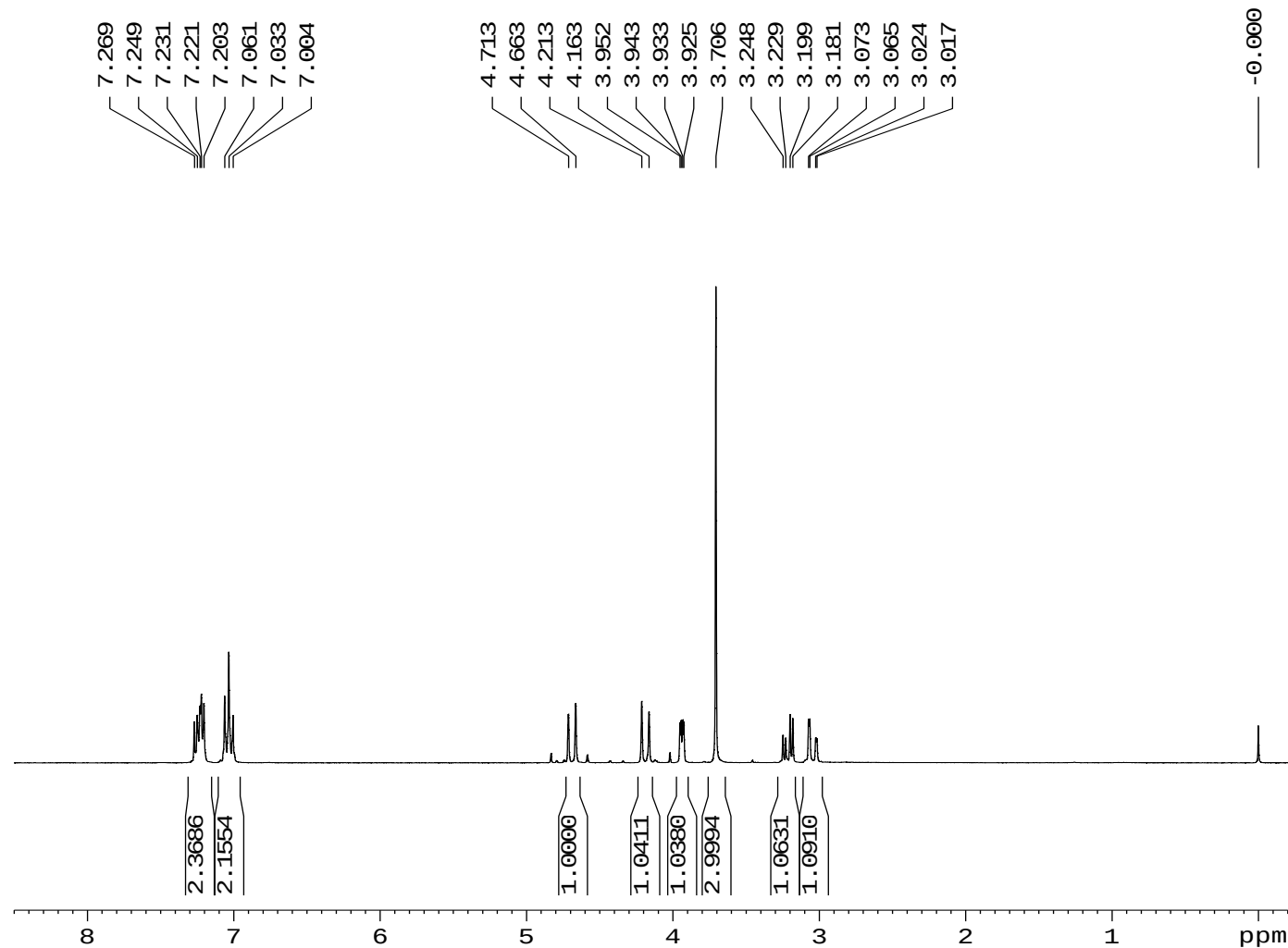
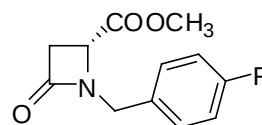
F2 - Acquisition Parameters
Date_ 20091211
Time 17.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4b-¹H NMR

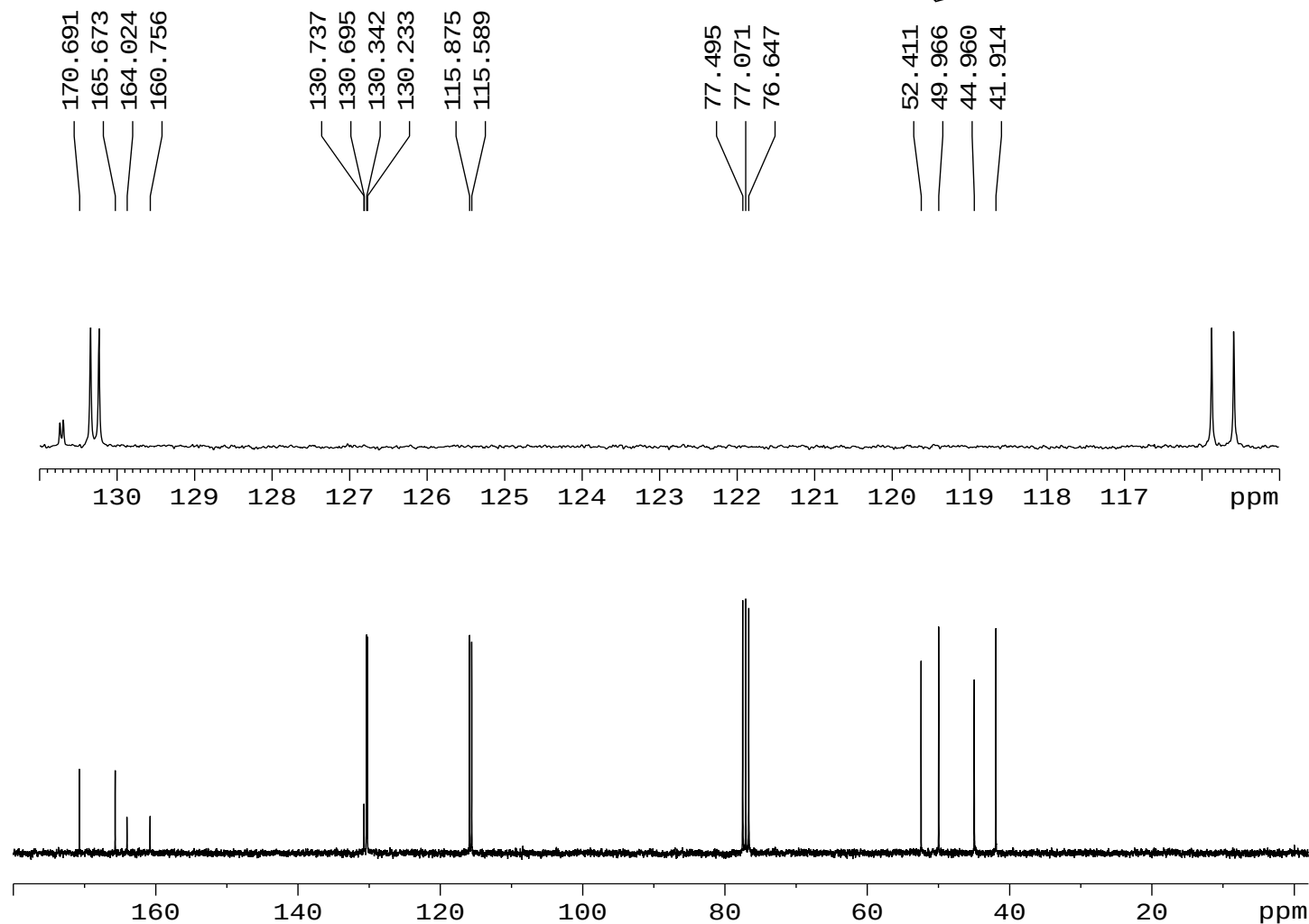
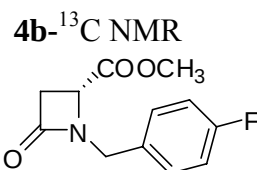


Current Data Parameters
NAME ldh-L-E-F(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091208
Time 23.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 8.00 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-E-F(1)
EXPNO 30
PROCNO 1

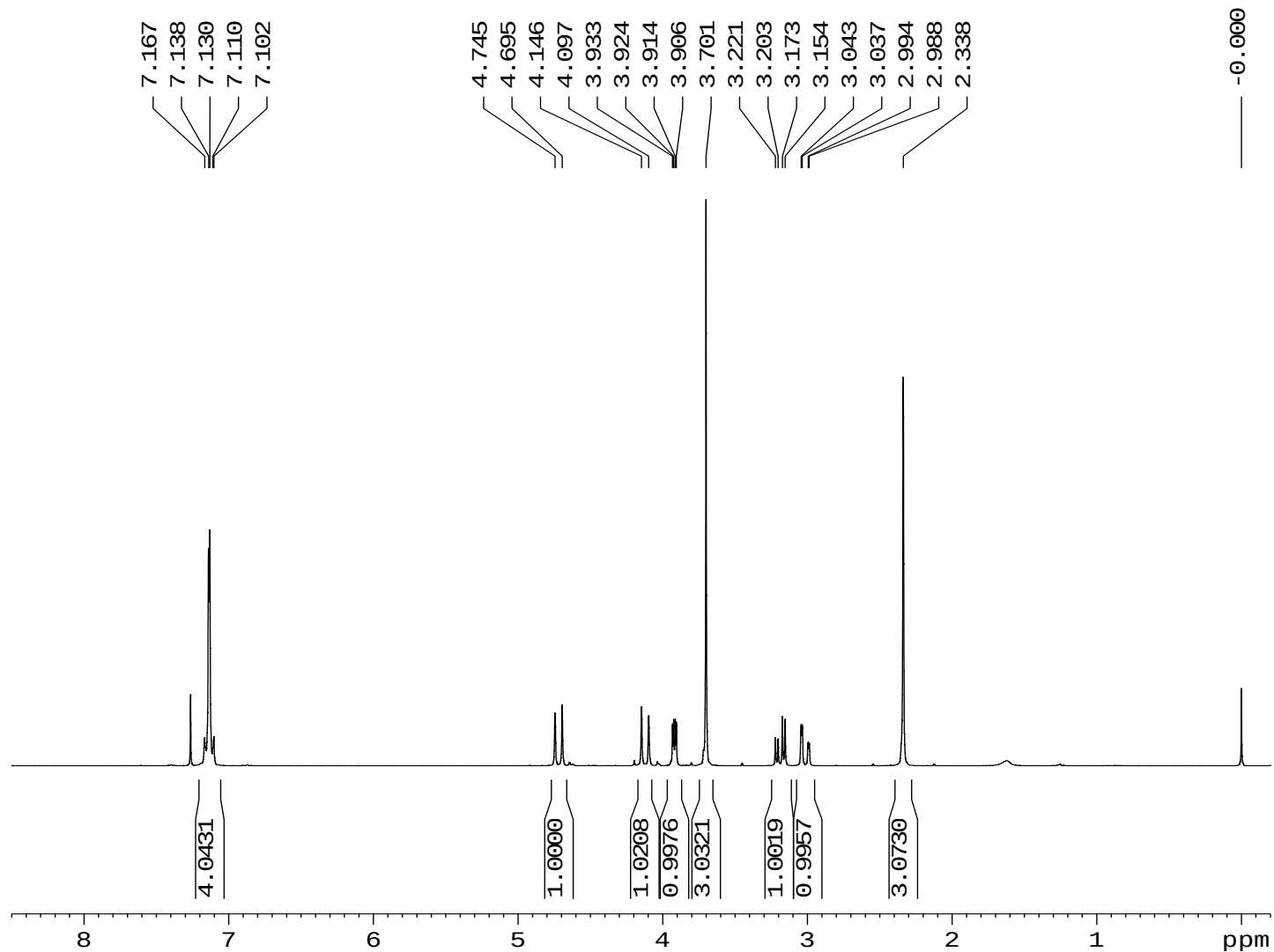
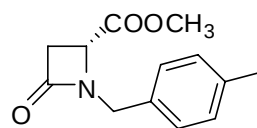
F2 - Acquisition Parameters
Date_ 20091211
Time 17.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4c-¹H NMR

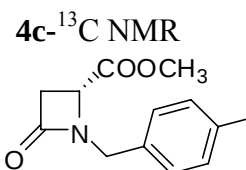


Current Data Parameters
NAME ldh-L-E-CH3(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 13.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 8.00 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



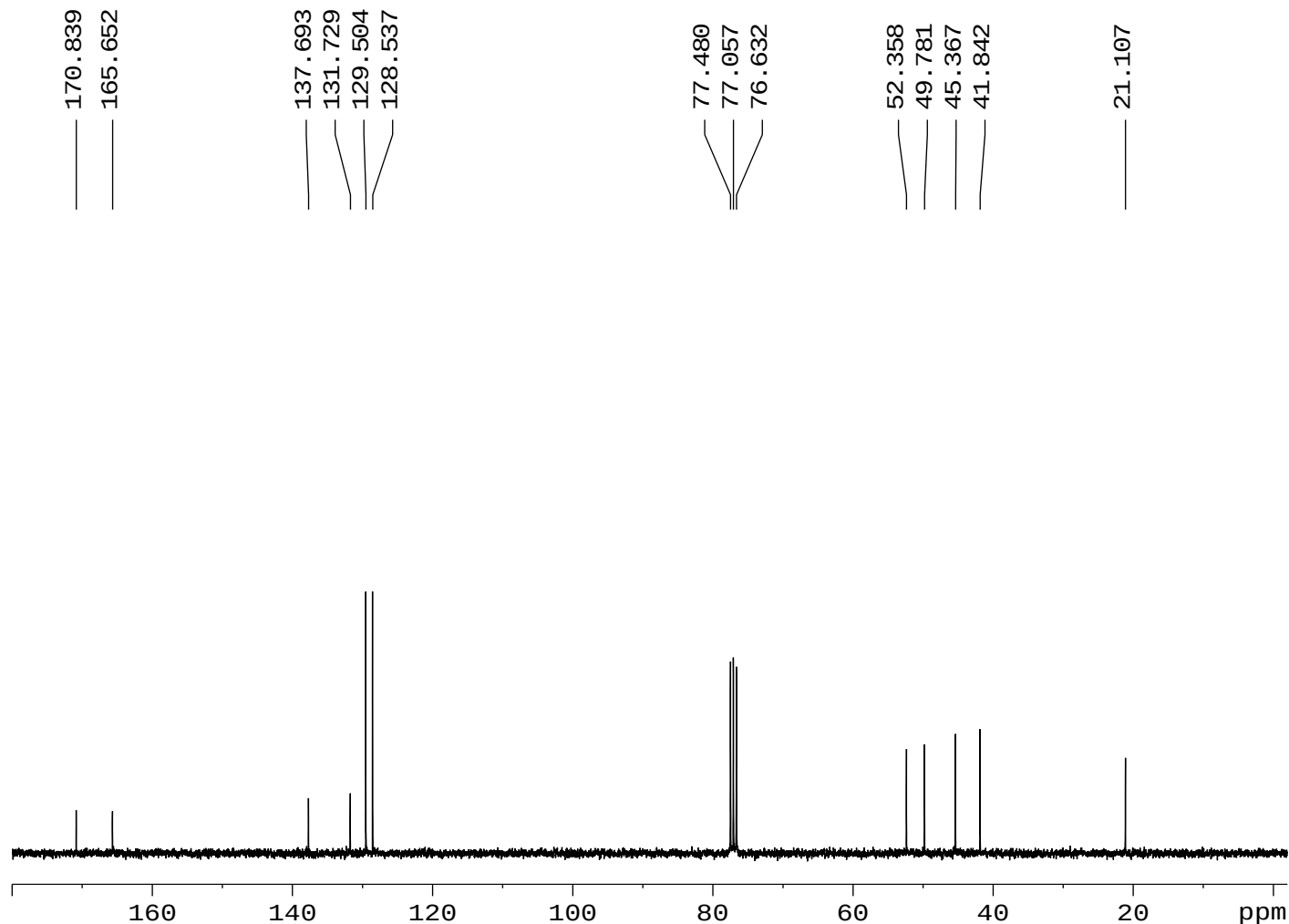
Current Data Parameters
NAME ldh-L-E-CH3(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091211
Time 18.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 56
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

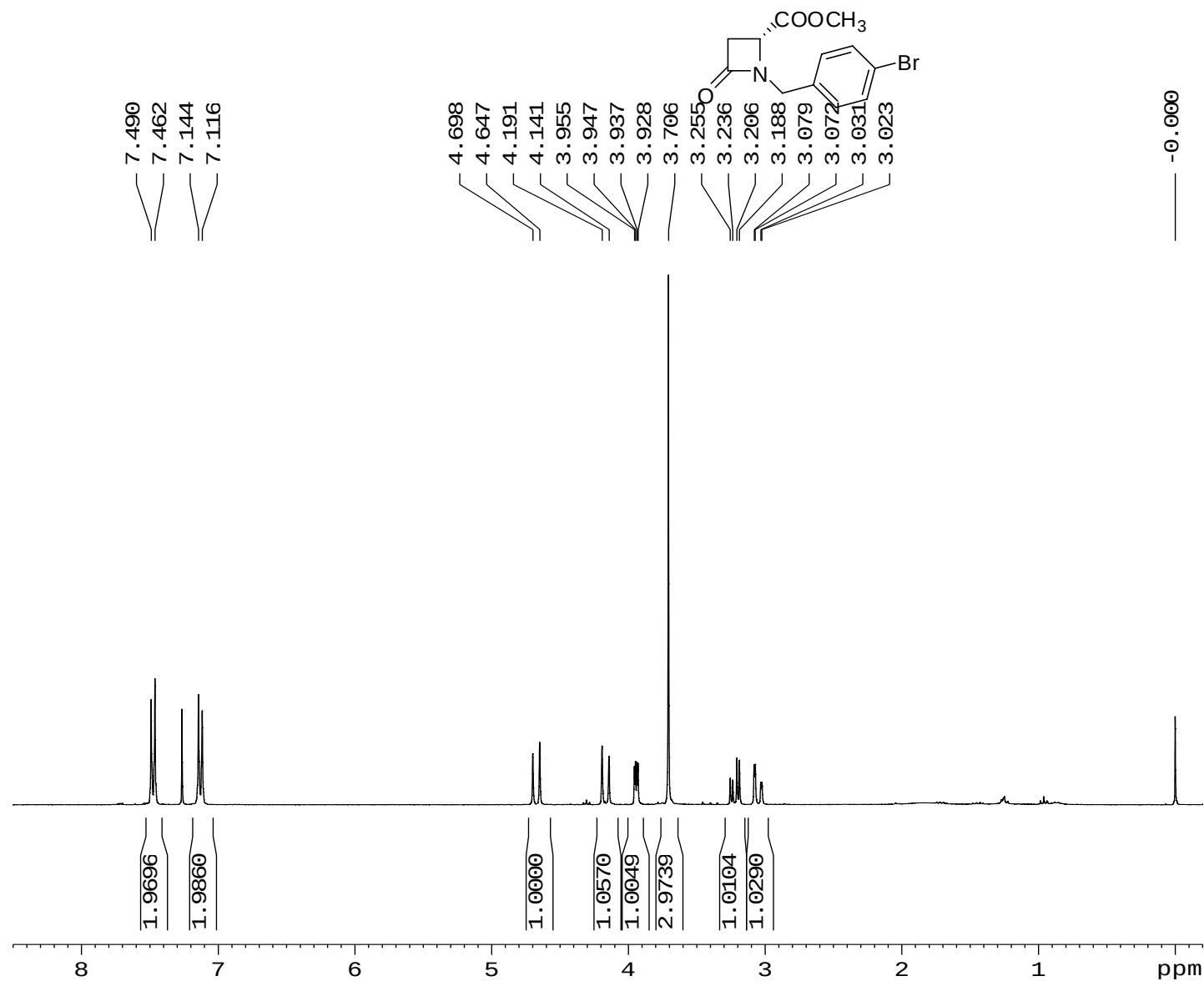
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4d-¹H NMR



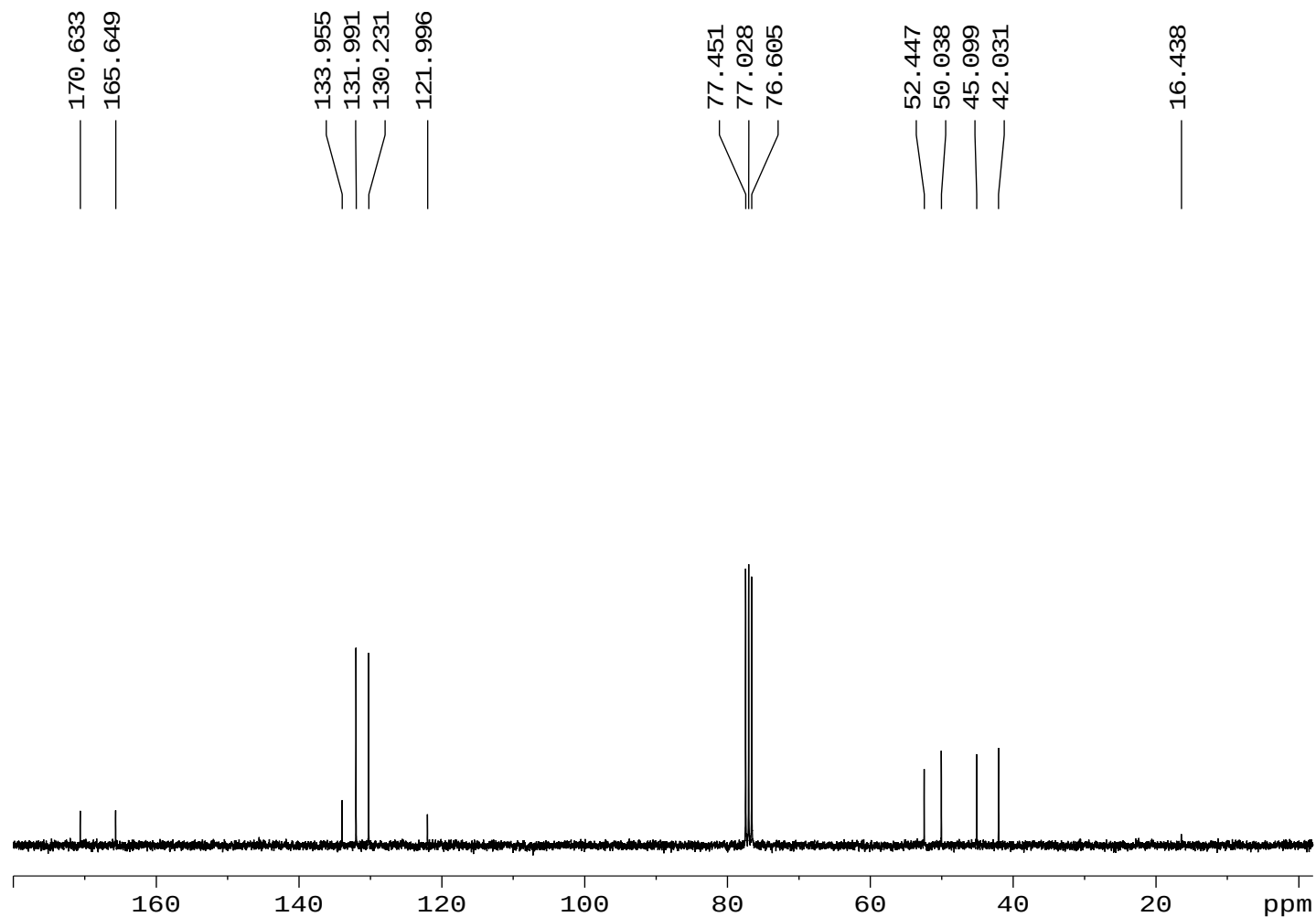
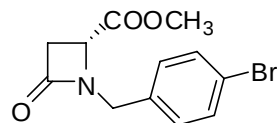
Current Data Parameters
NAME ldh-L-E-p-Br(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 13.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 8.00 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4d-¹³C NMR



Current Data Parameters
NAME ldh-L-E-p-Br
EXPNO 21
PROCNO 1

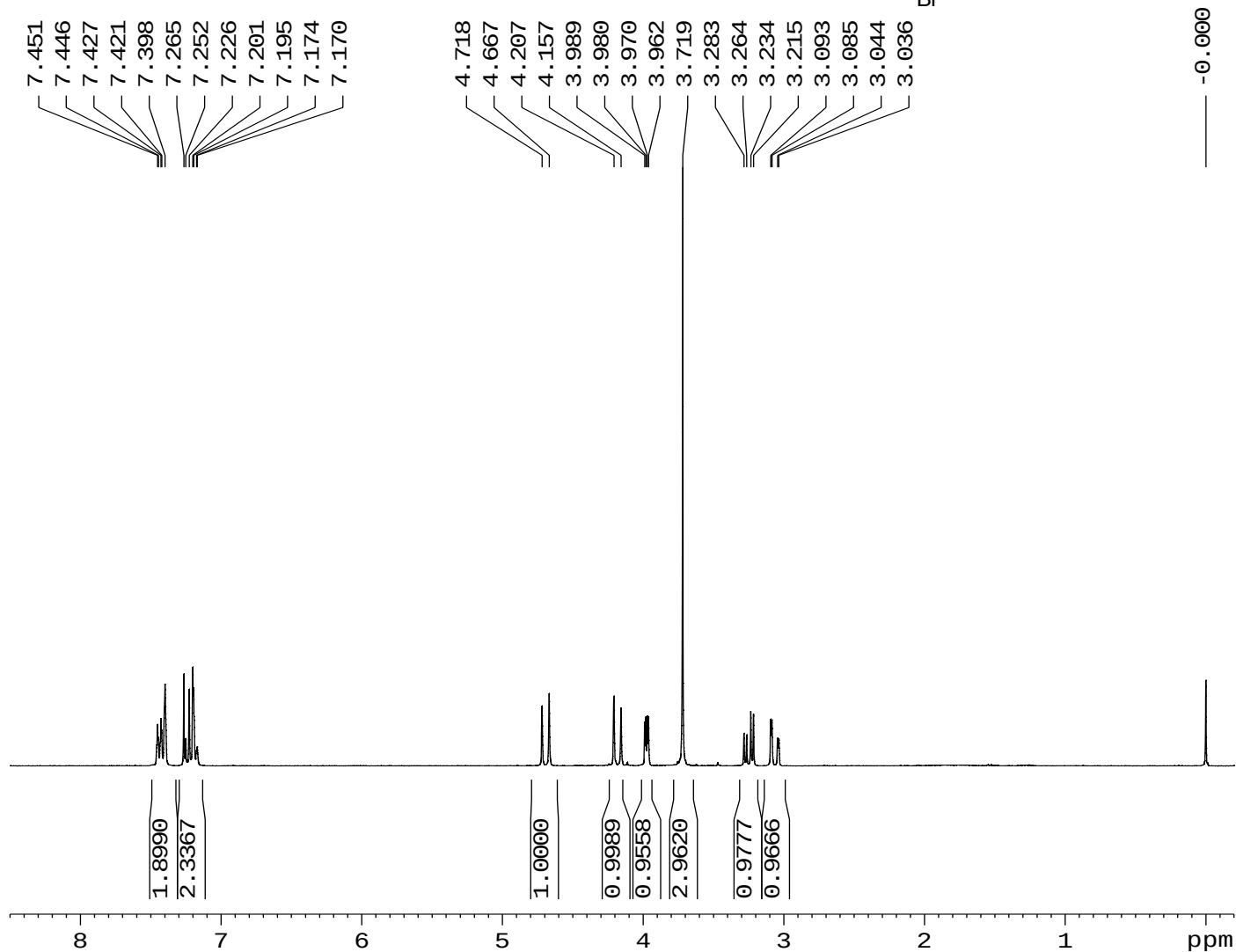
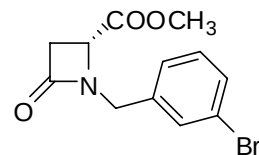
F2 - Acquisition Parameters
Date_ 20100316
Time 20.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 8.00 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4e-¹H NMR



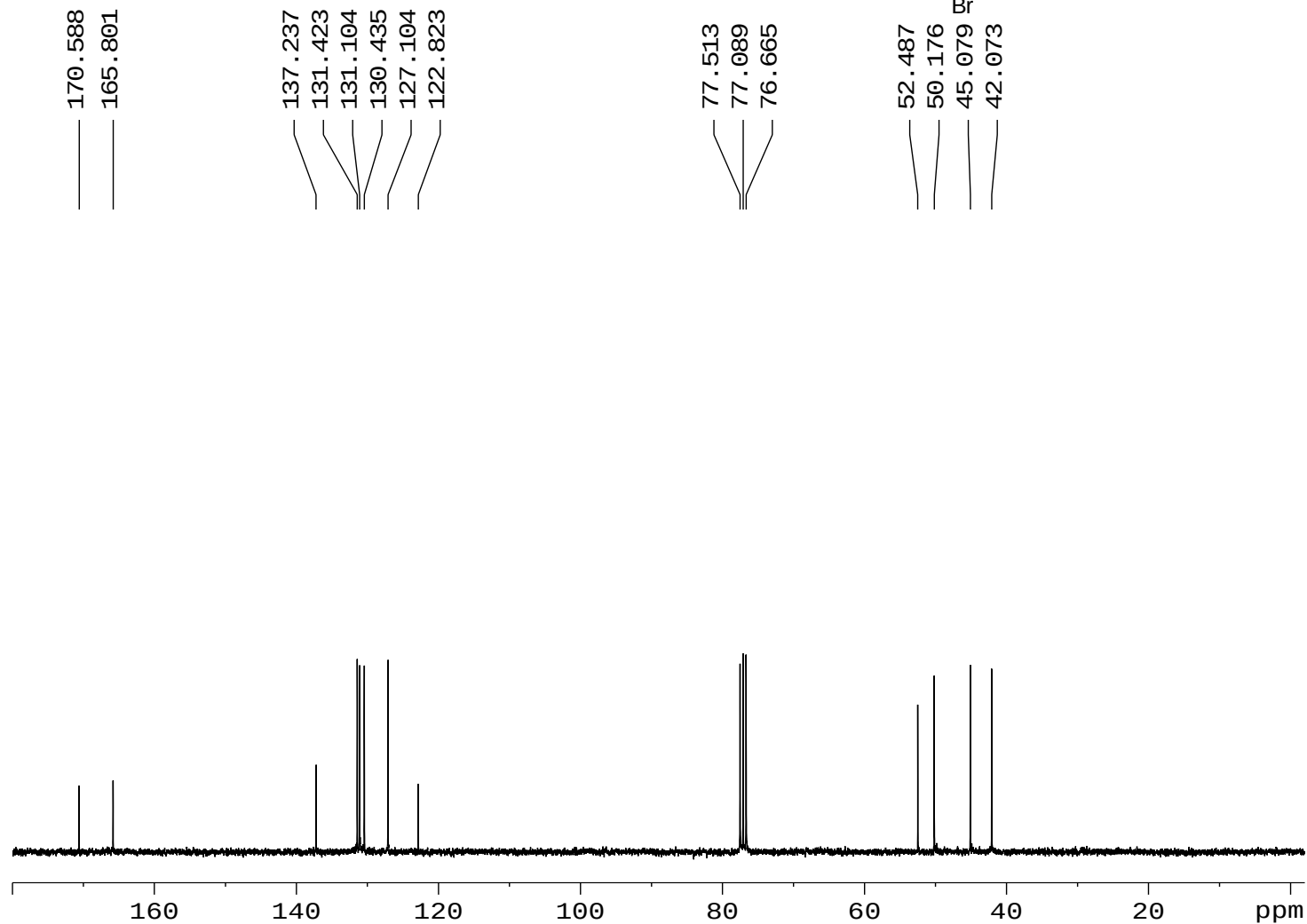
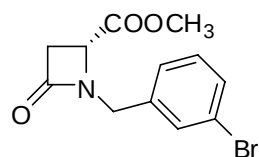
Current Data Parameters
NAME ldh-L-E-m-Br
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100316
Time 20.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 456.1
DW 55.600 usec
DE 8.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4e-¹³C NMR



Current Data Parameters
NAME ldh-L-E-m-Br(1)
EXPNO 30
PROCNO 1

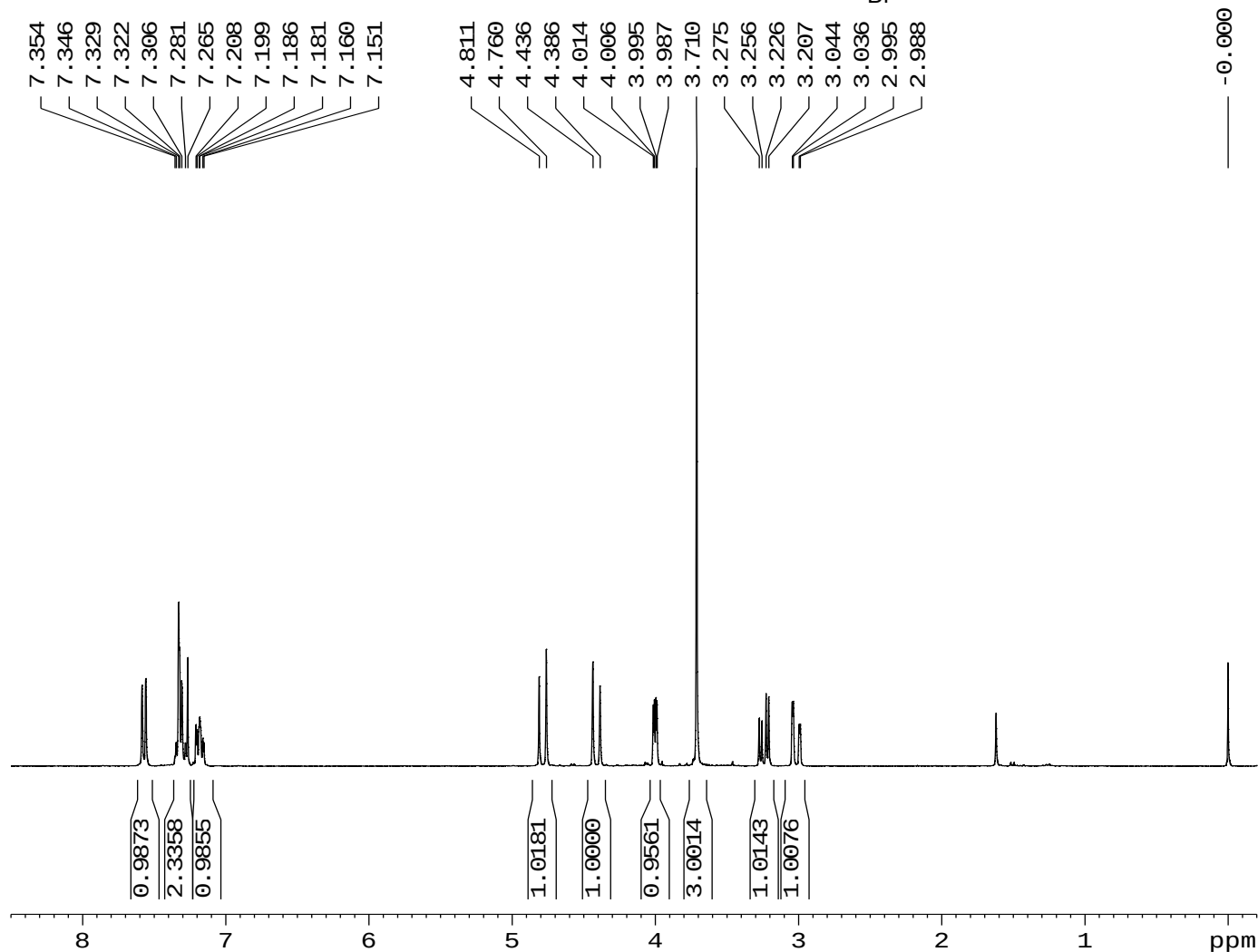
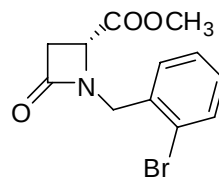
F2 - Acquisition Parameters
Date_ 20091212
Time 10.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 108
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4f-¹H NMR

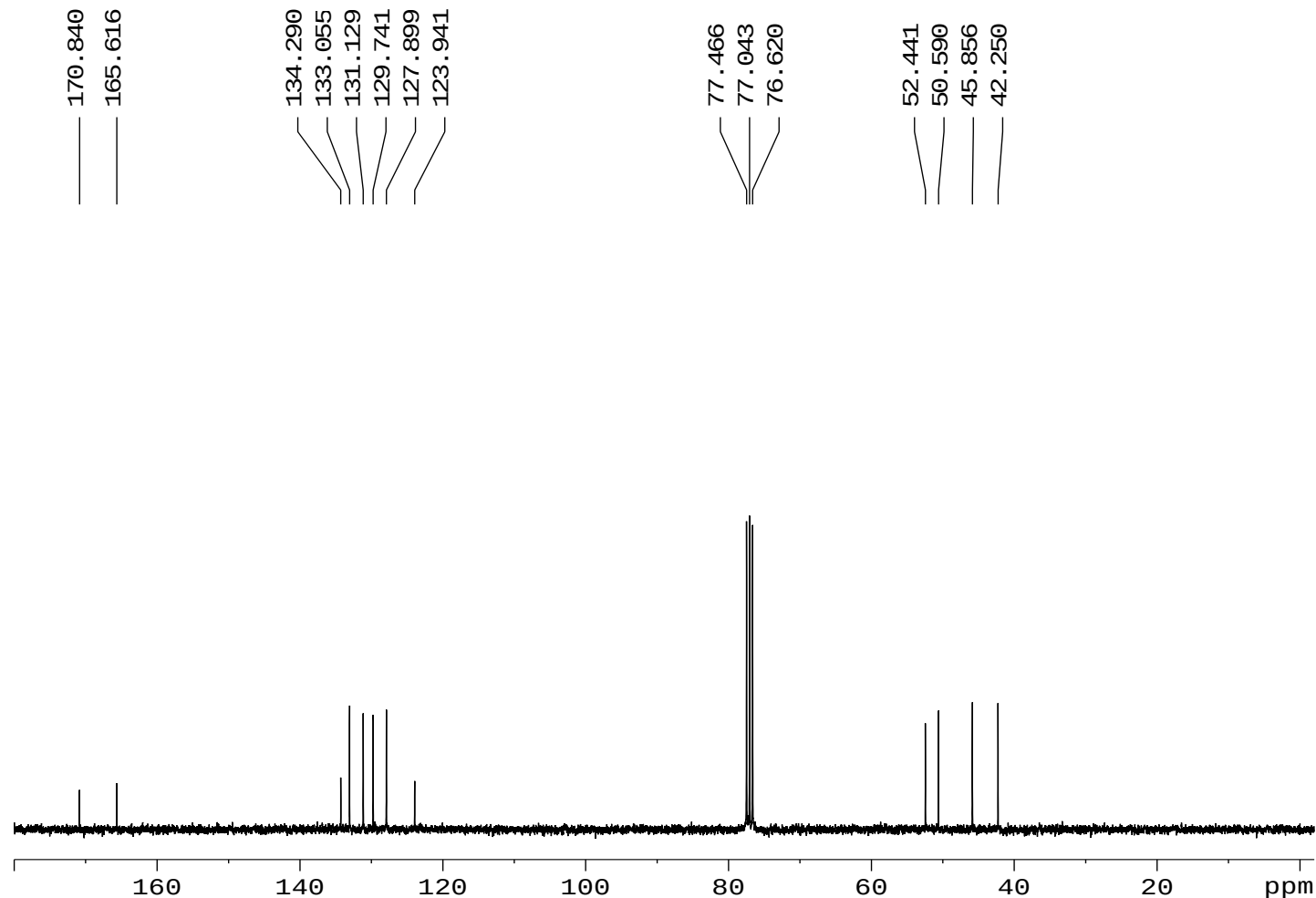
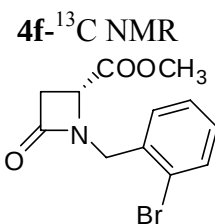


Current Data Parameters
NAME ldh-L-E-o-Br
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100316
Time 20.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 456.1
DW 55.600 usec
DE 8.00 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300044 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-E-o-Br(1)
EXPNO 10
PROCNO 1

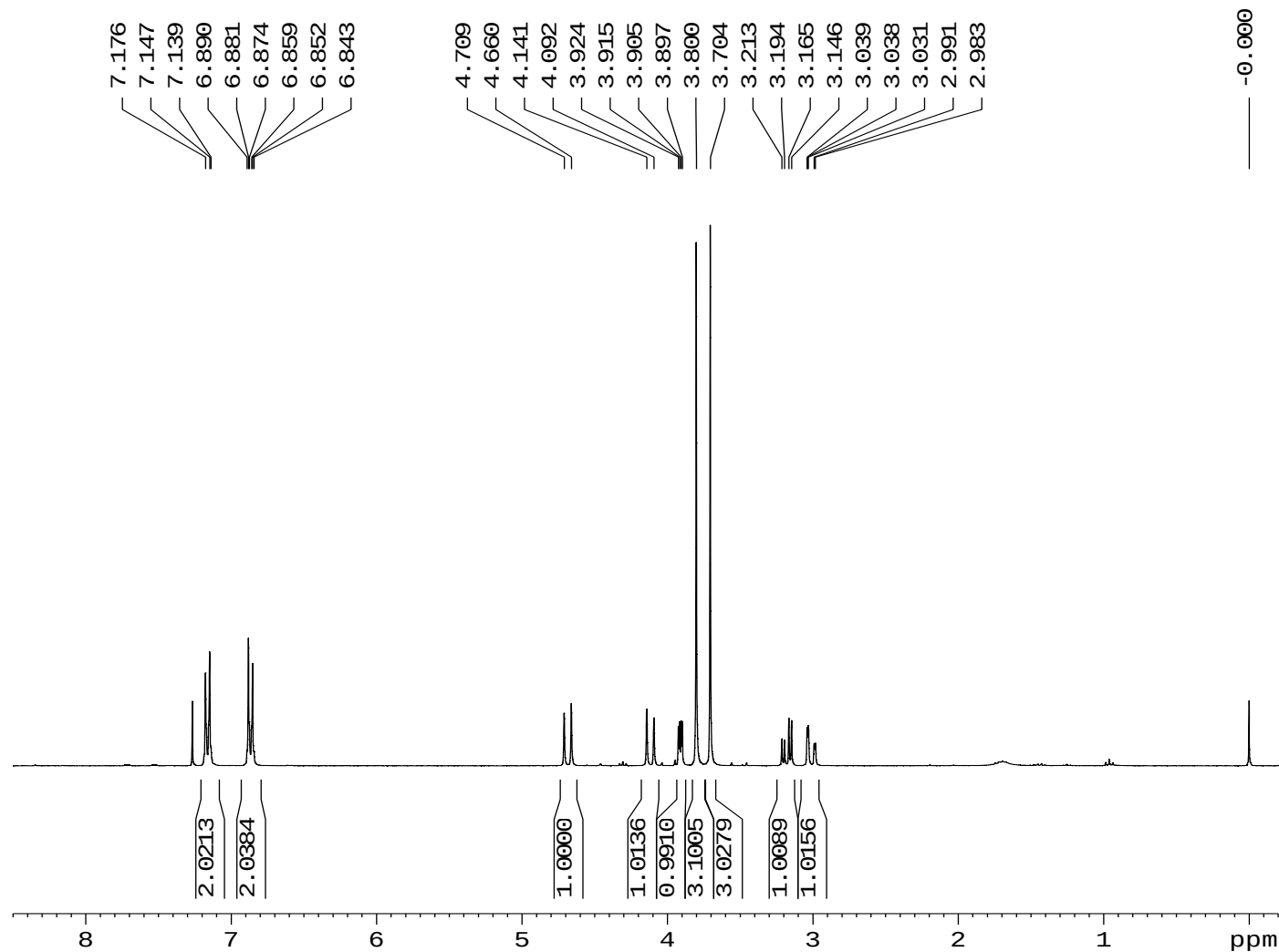
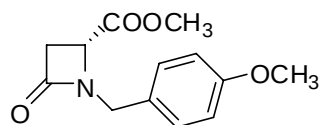
F2 - Acquisition Parameters
Date_ 20091211
Time 17.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4g-¹H NMR



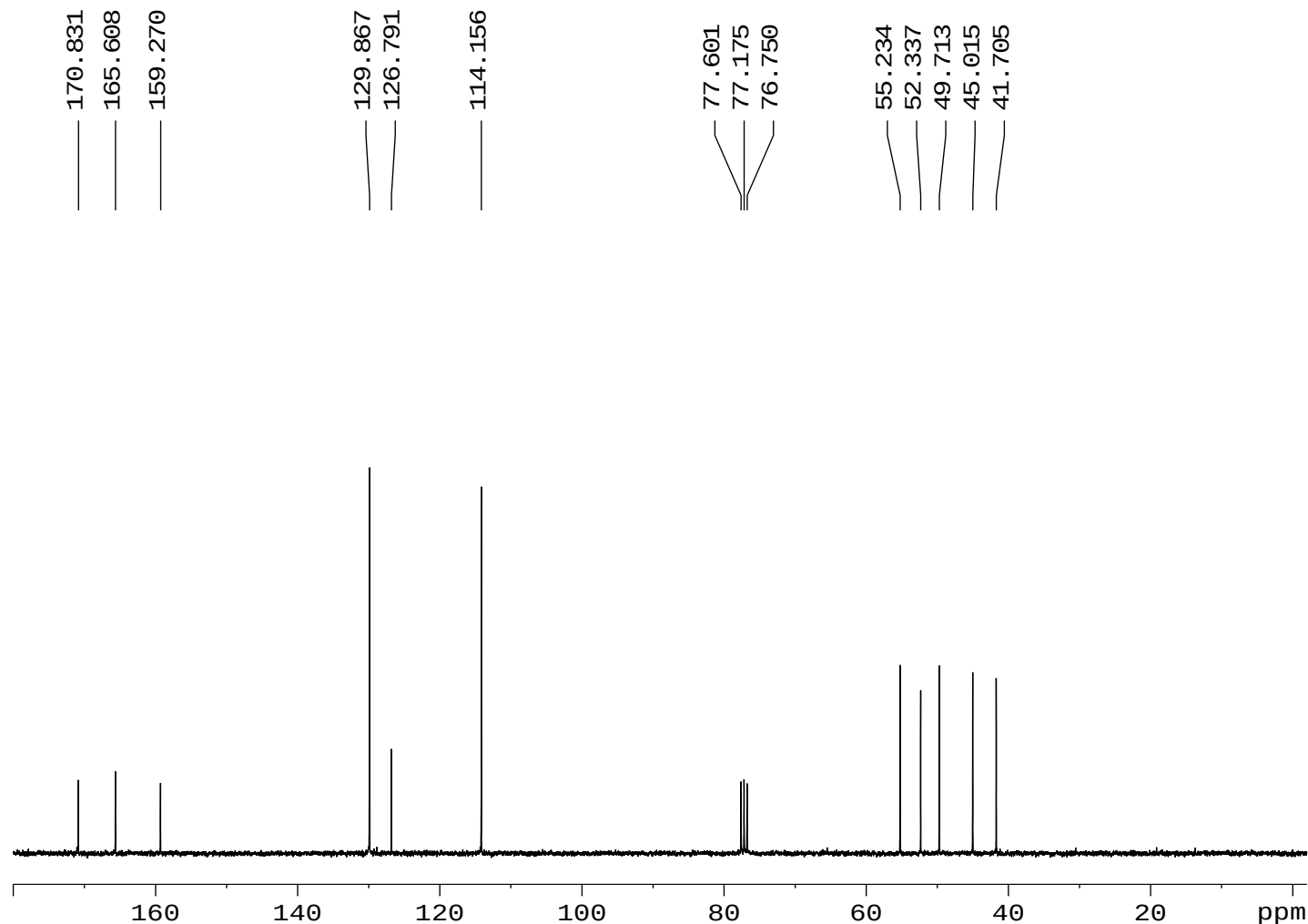
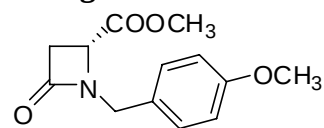
Current Data Parameters
NAME ldh-L-E-OCH3(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 13.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 8.00 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300041 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

4g-¹³C NMR



Current Data Parameters
NAME ldh-L-E-OCH3(1)
EXPNO 20
PROCNO 1

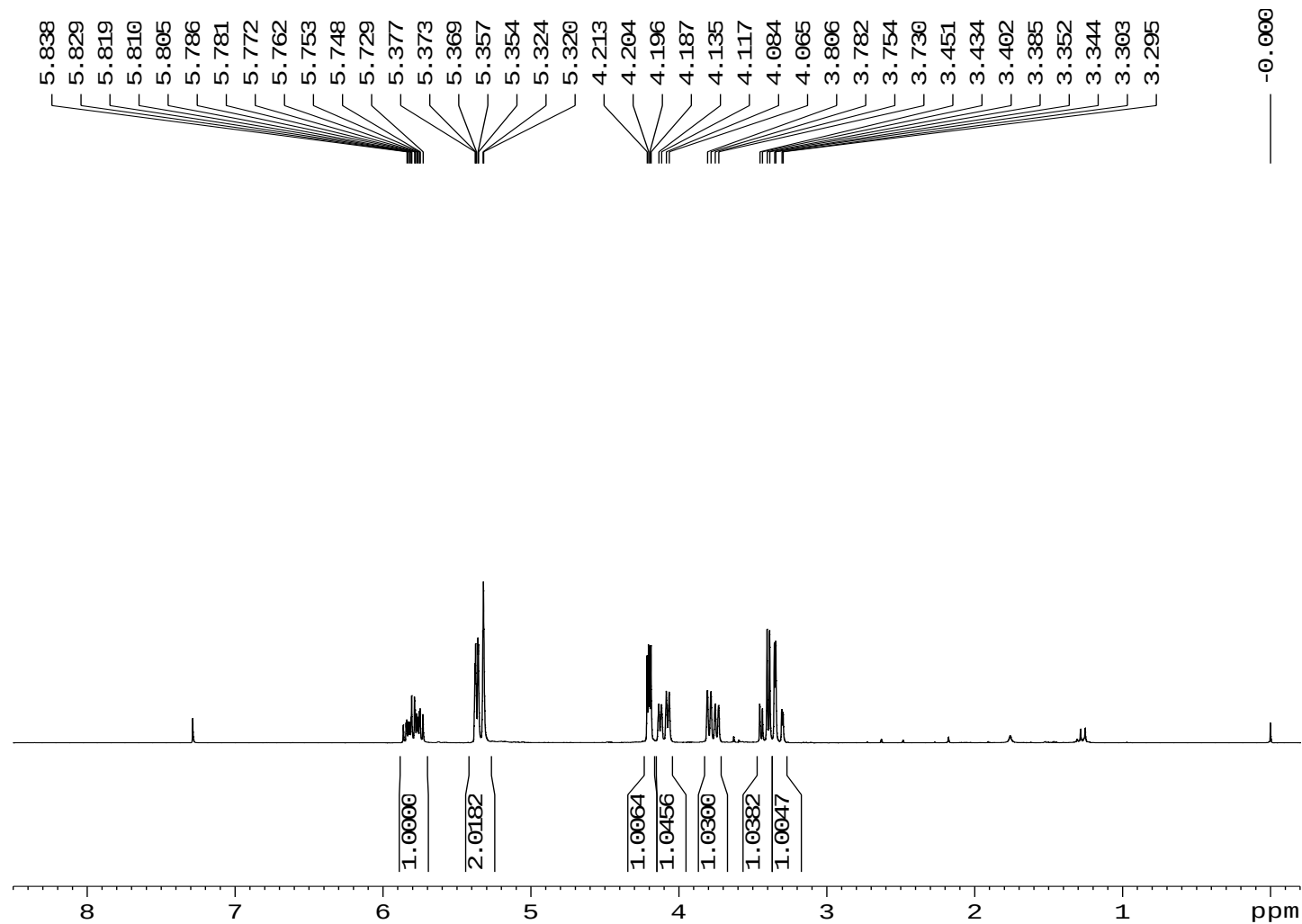
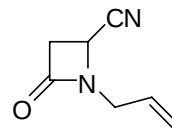
F2 - Acquisition Parameters
Date_ 20091211
Time 17.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 8.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5-¹H NMR



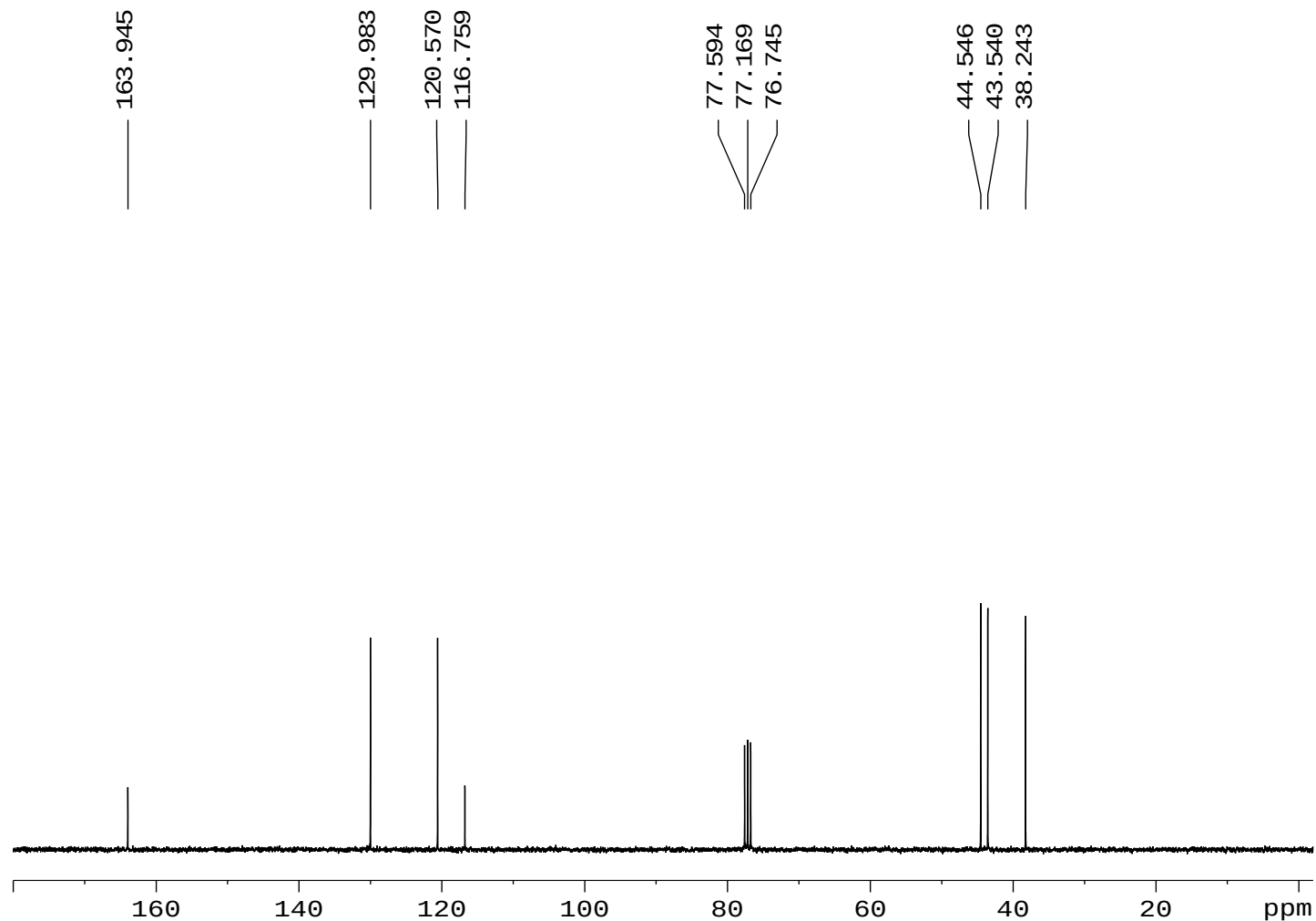
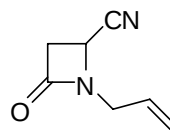
Current Data Parameters
NAME ldh-L-N-allyl(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091208
Time 20.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 8.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

5-¹³C NMR



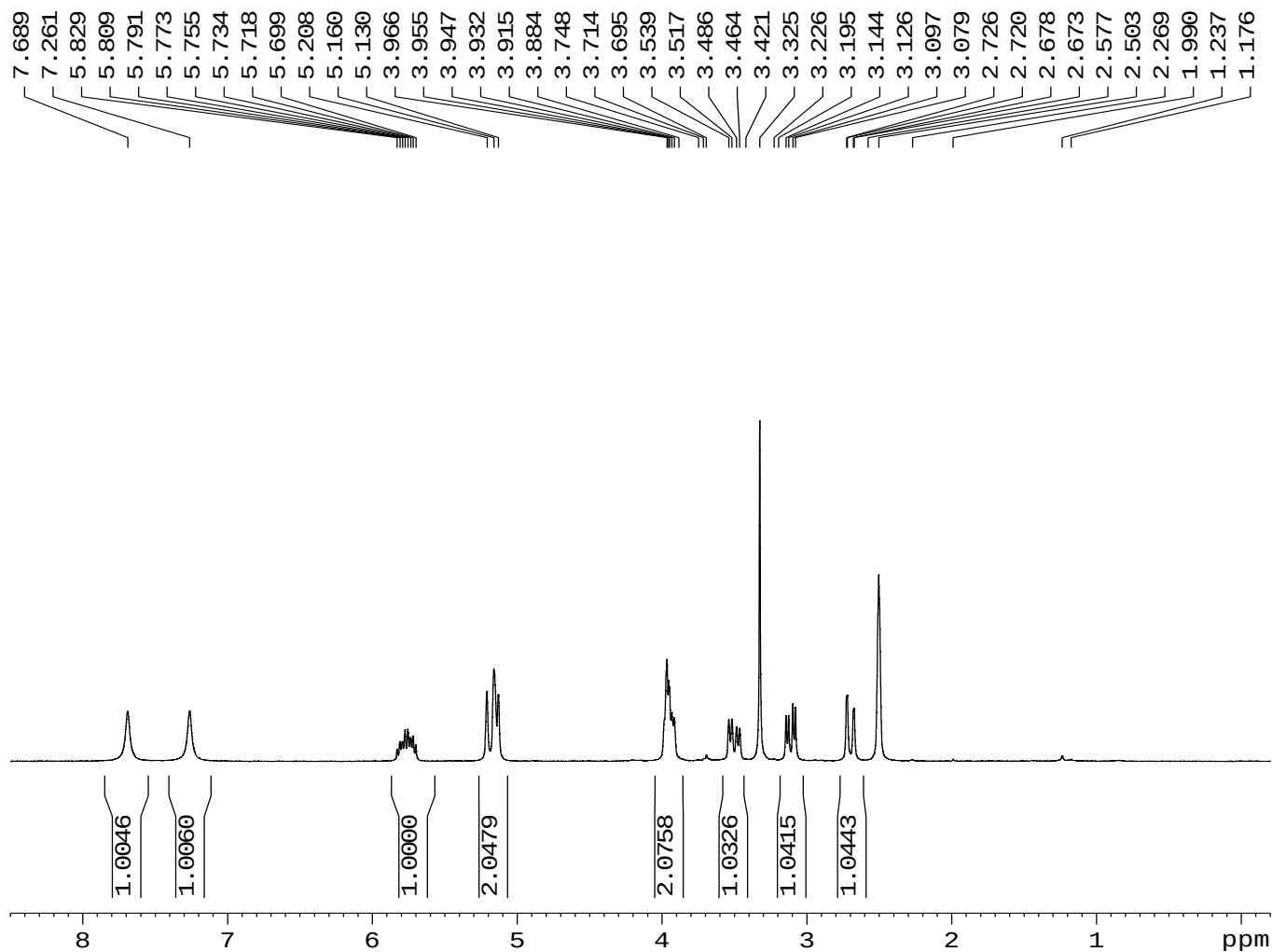
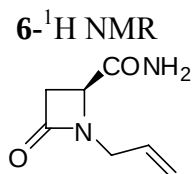
Current Data Parameters
NAME ldh-L-N-allyl(1)
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091211
Time 11.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 58
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

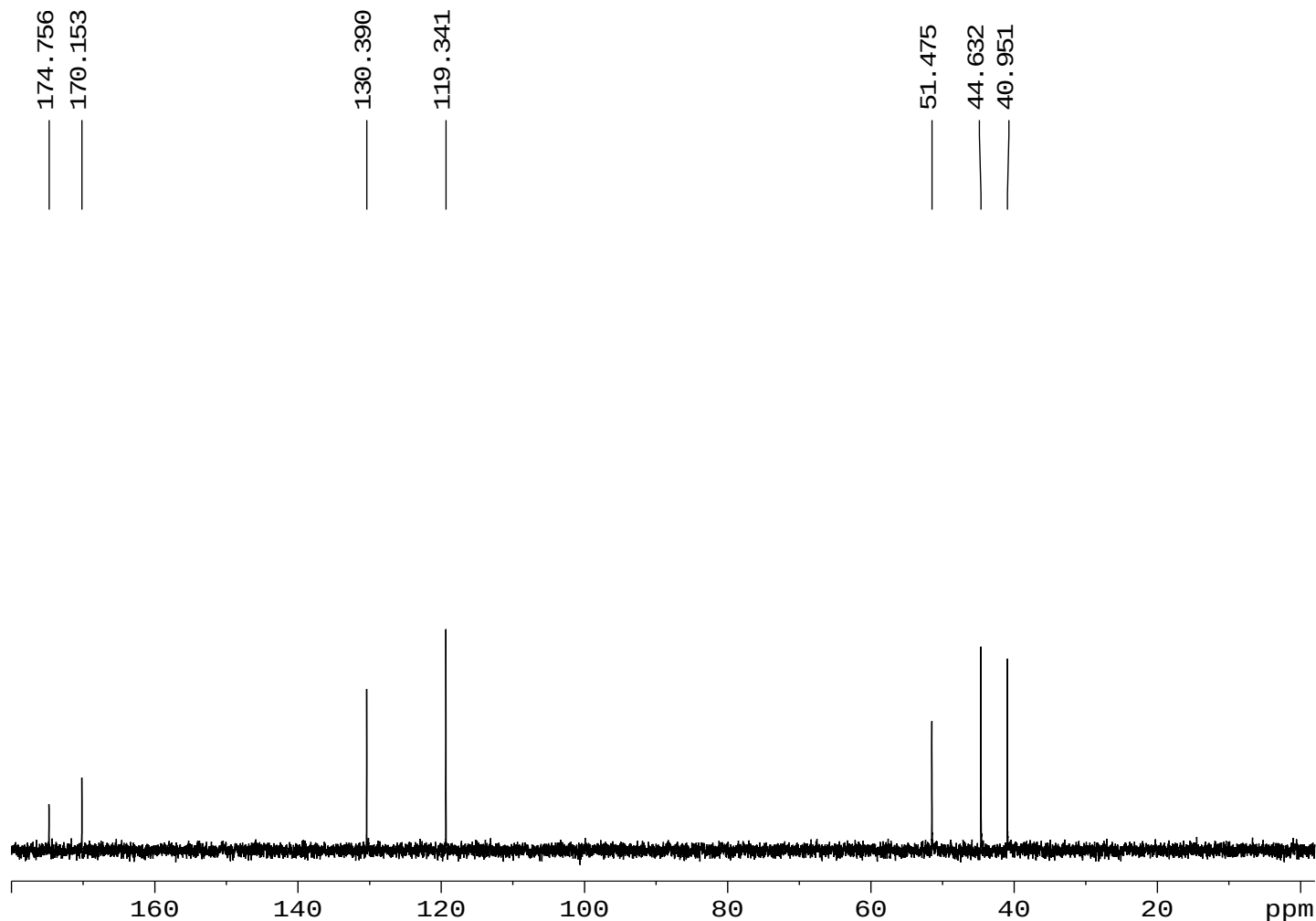
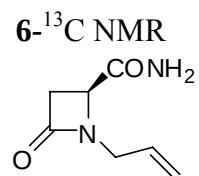


Current Data Parameters
NAME ldh-L-Am-allyl(1)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091209
Time 19.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 8.00 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-allyl
EXPNO 10
PROCNO 1

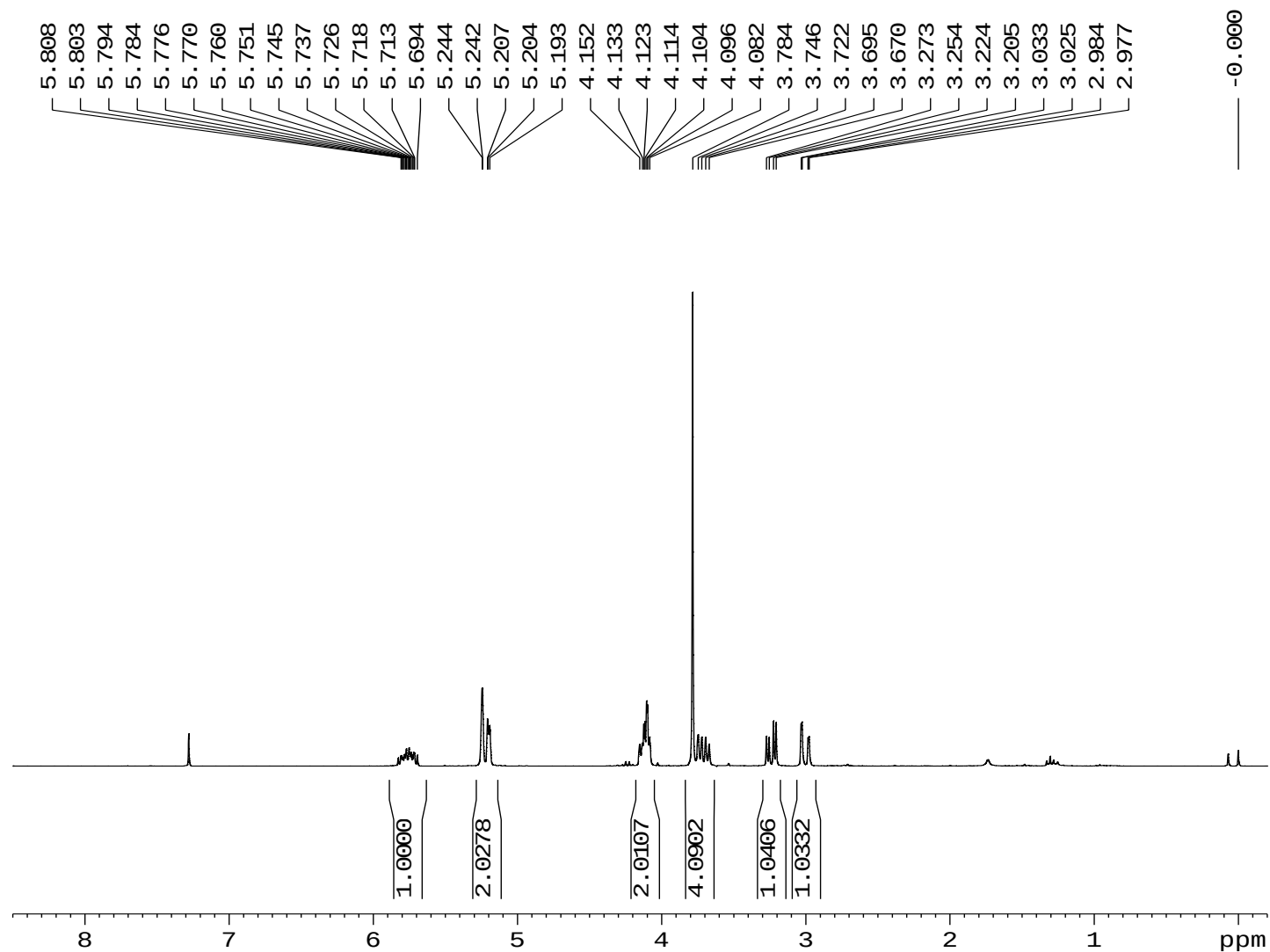
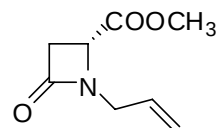
F2 - Acquisition Parameters
Date_ 20100317
Time 13.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 287
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 8.00 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7-¹H NMR

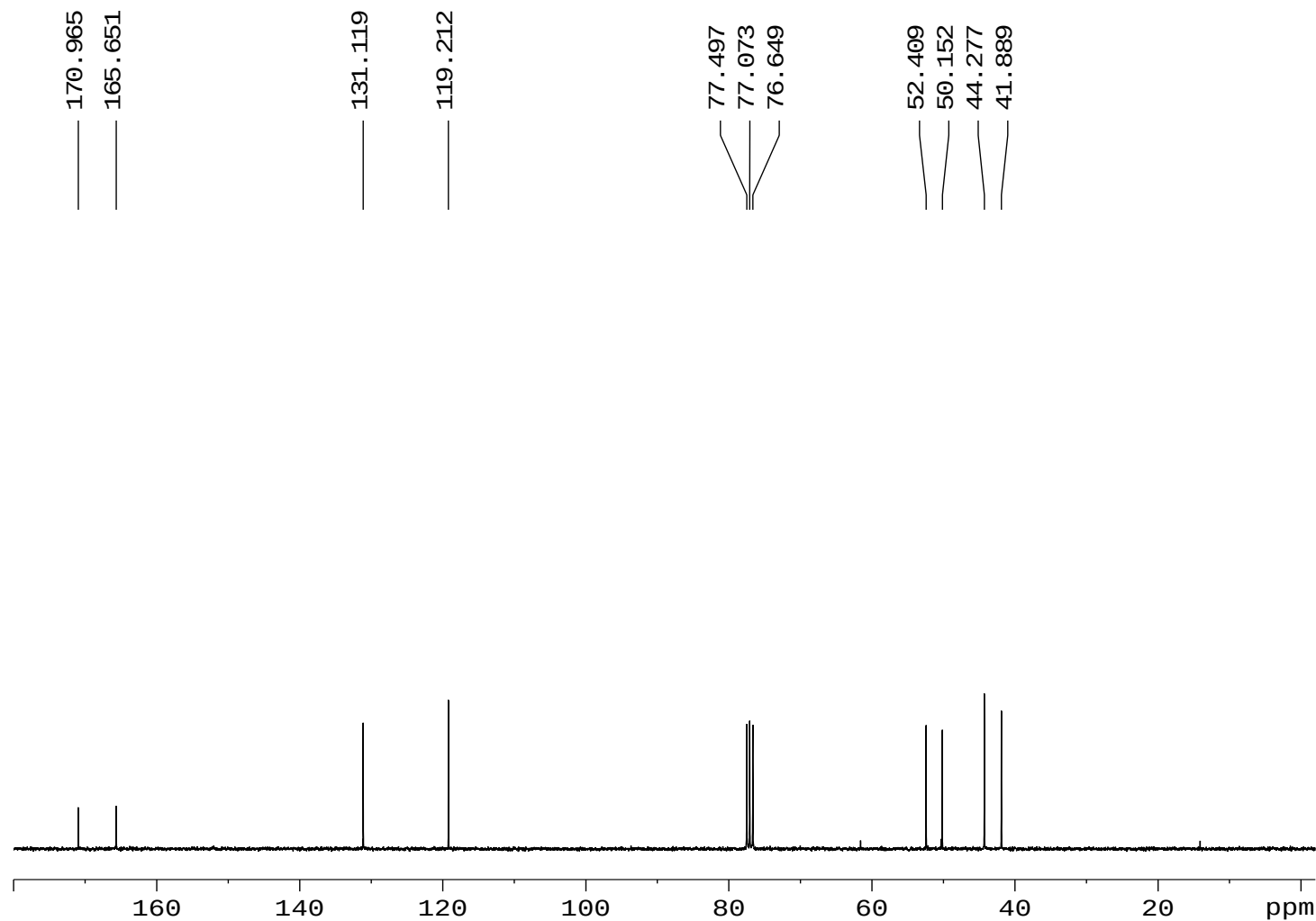
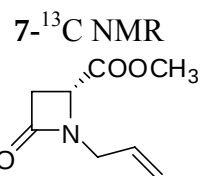


Current Data Parameters
NAME ldh-L-E-allyl
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100128
Time 11.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 256
DW 55.600 usec
DE 8.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300003 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-E-allyl(1)
EXPNO 20
PROCNO 1

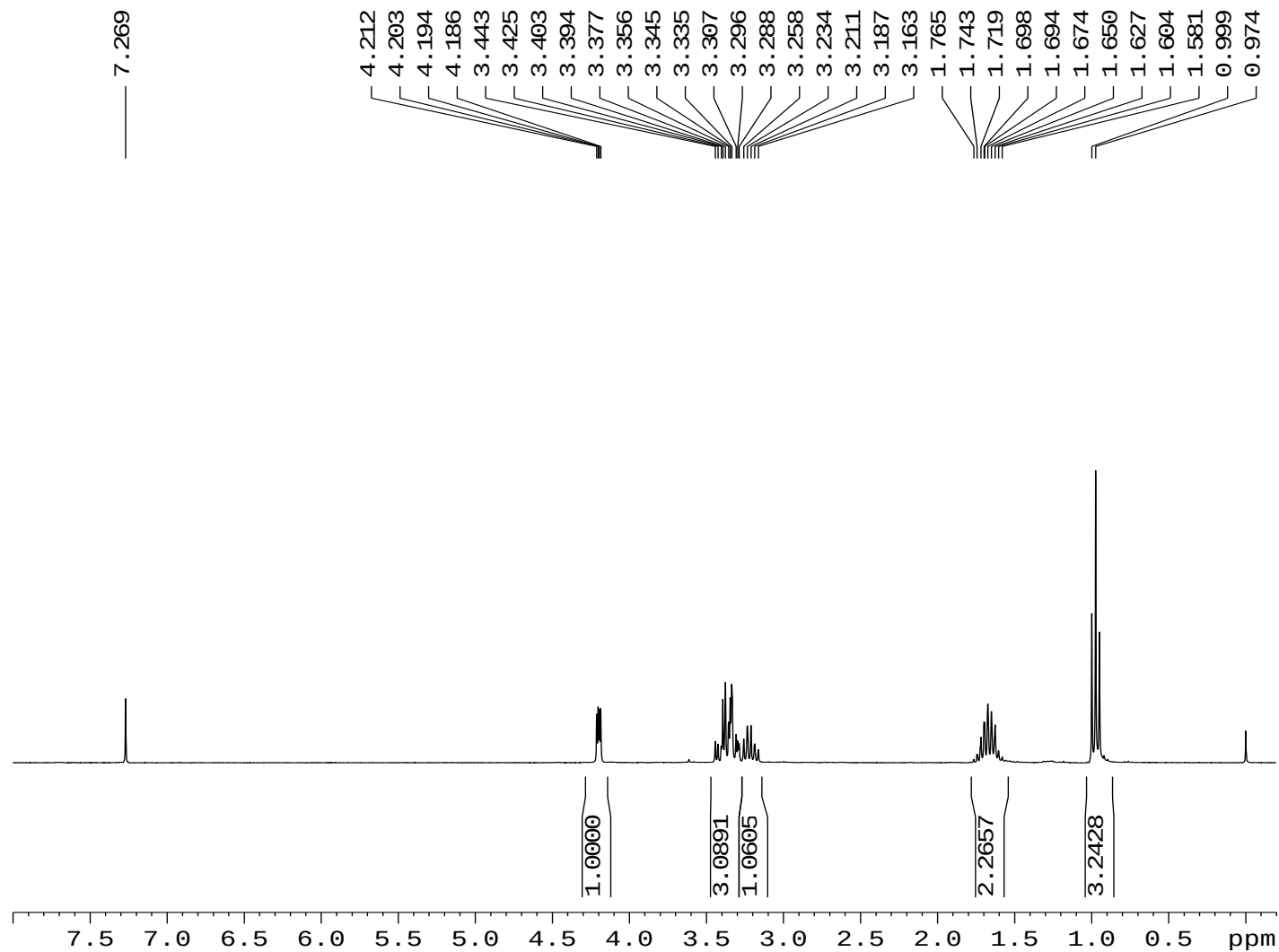
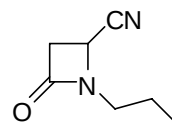
F2 - Acquisition Parameters
Date_ 20091211
Time 11.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 192
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

8-¹H NMR



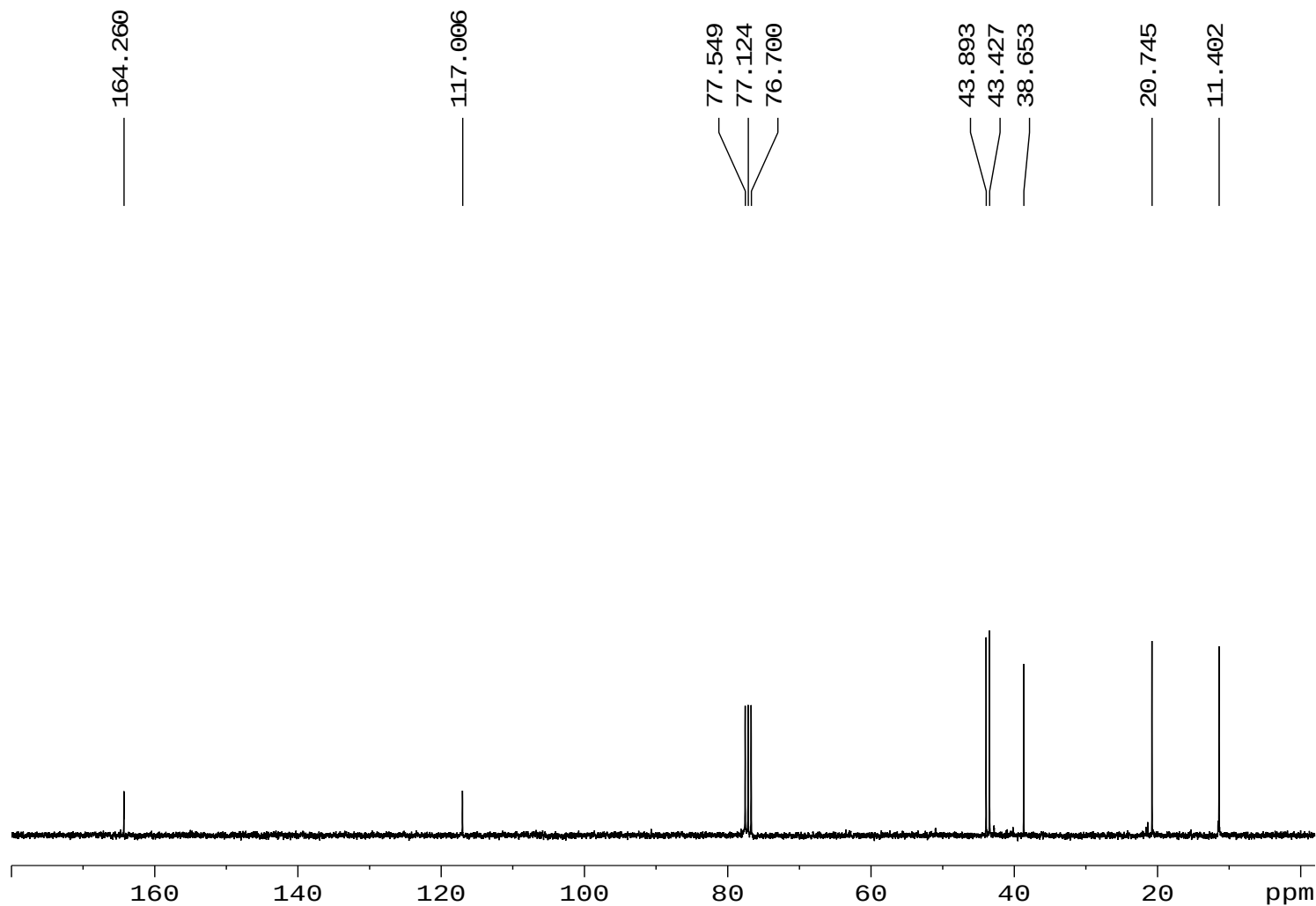
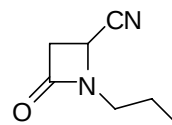
Current Data Parameters
NAME ldh-L-N-prog
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100130
Time 14.33
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 362
DW 55.600 usec
DE 8.00 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8-¹³C NMR



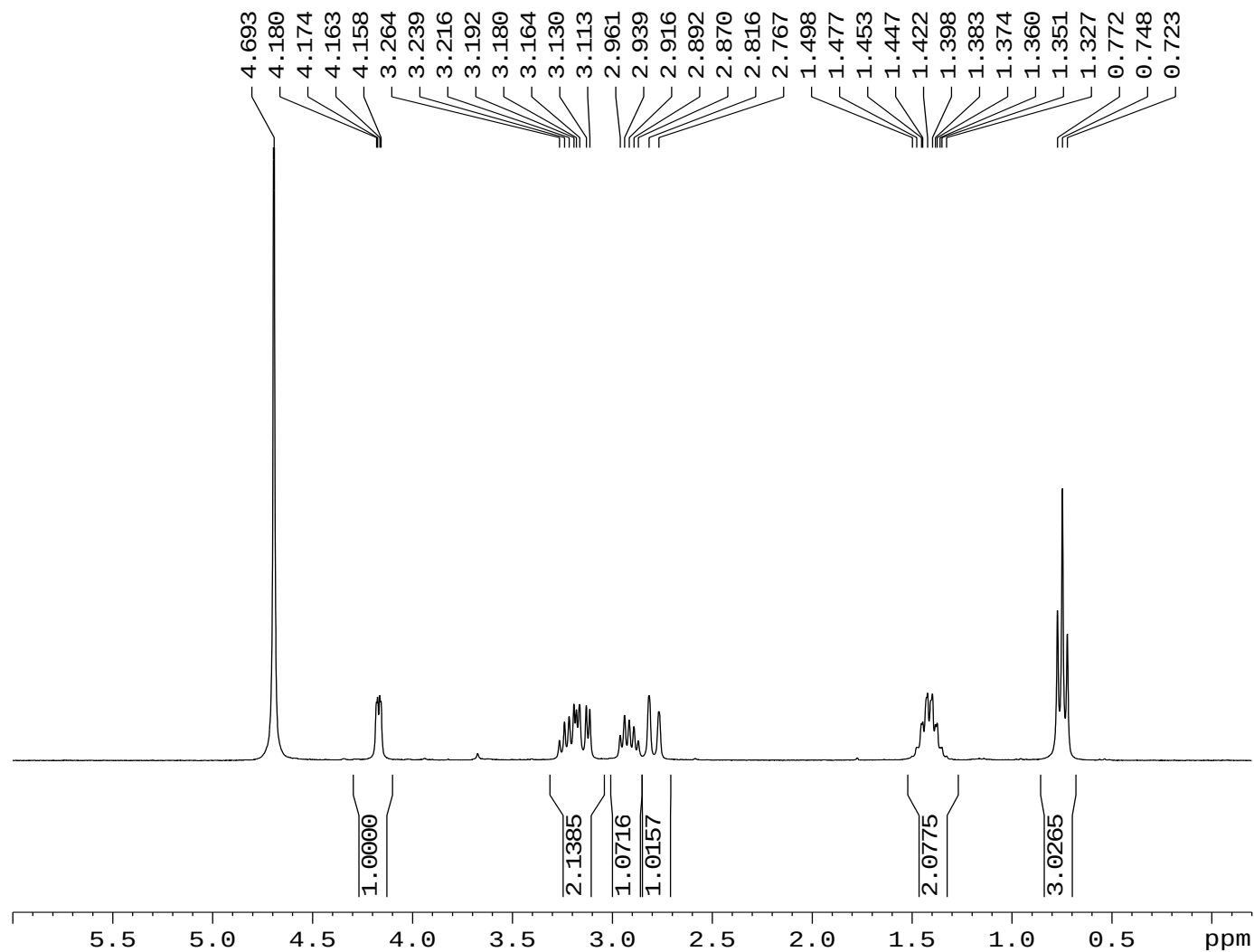
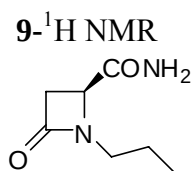
Current Data Parameters
NAME ldh-L-N-prog
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100201
Time 13.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 69
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 9195.2
DW 27.800 usec
DE 8.00 usec
TE 292.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

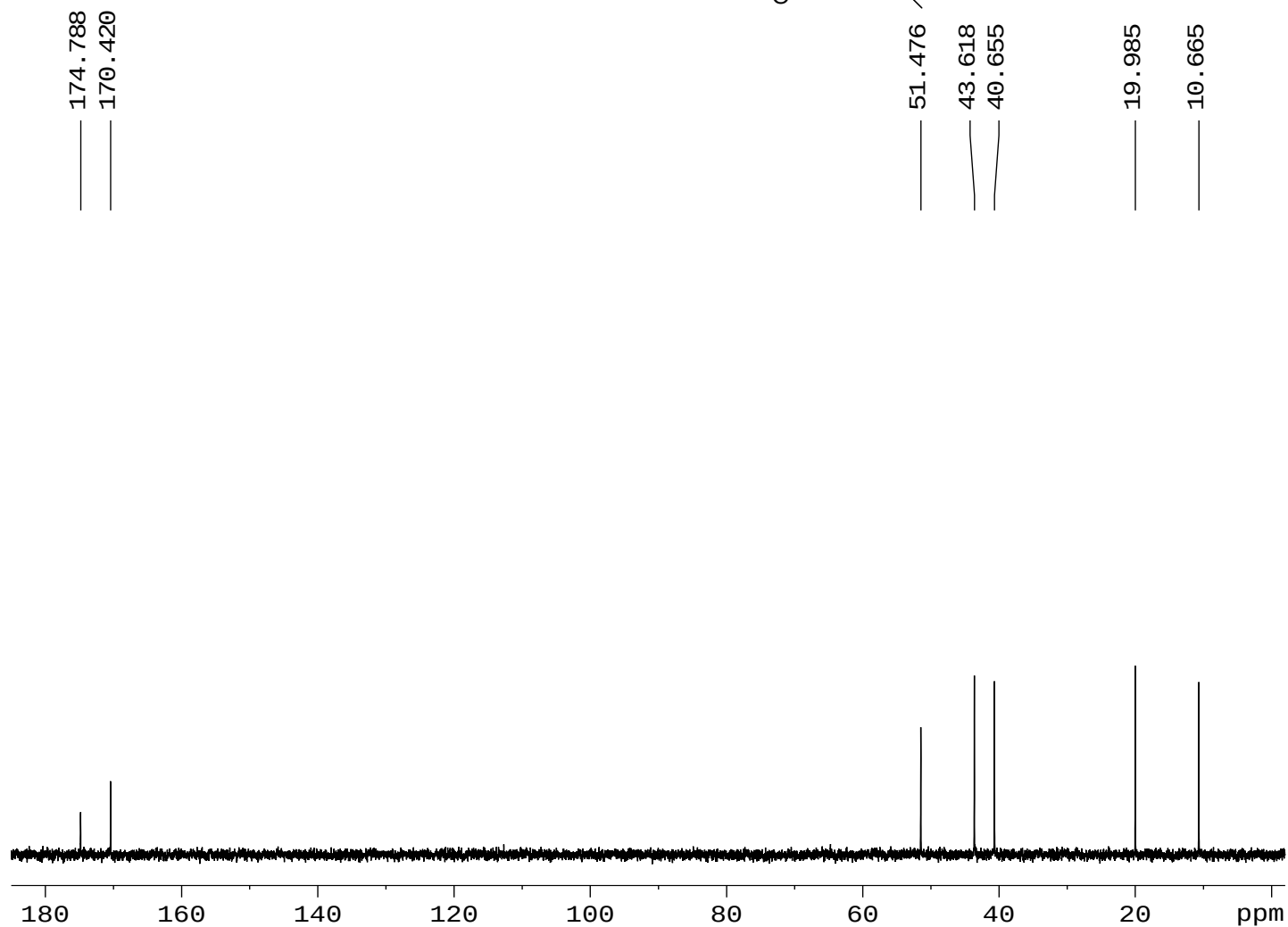
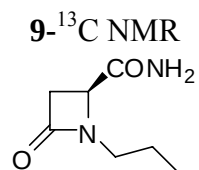


Current Data Parameters
NAME ldh-L-Am-arg-RE
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100128
Time 11.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 362
DW 55.600 usec
DE 8.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-Am-prog
EXPNO 10
PROCNO 1

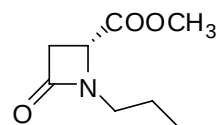
F2 - Acquisition Parameters
Date_ 20100129
Time 19.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 308
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

$^{10}\text{-}^1\text{H}$ NMR

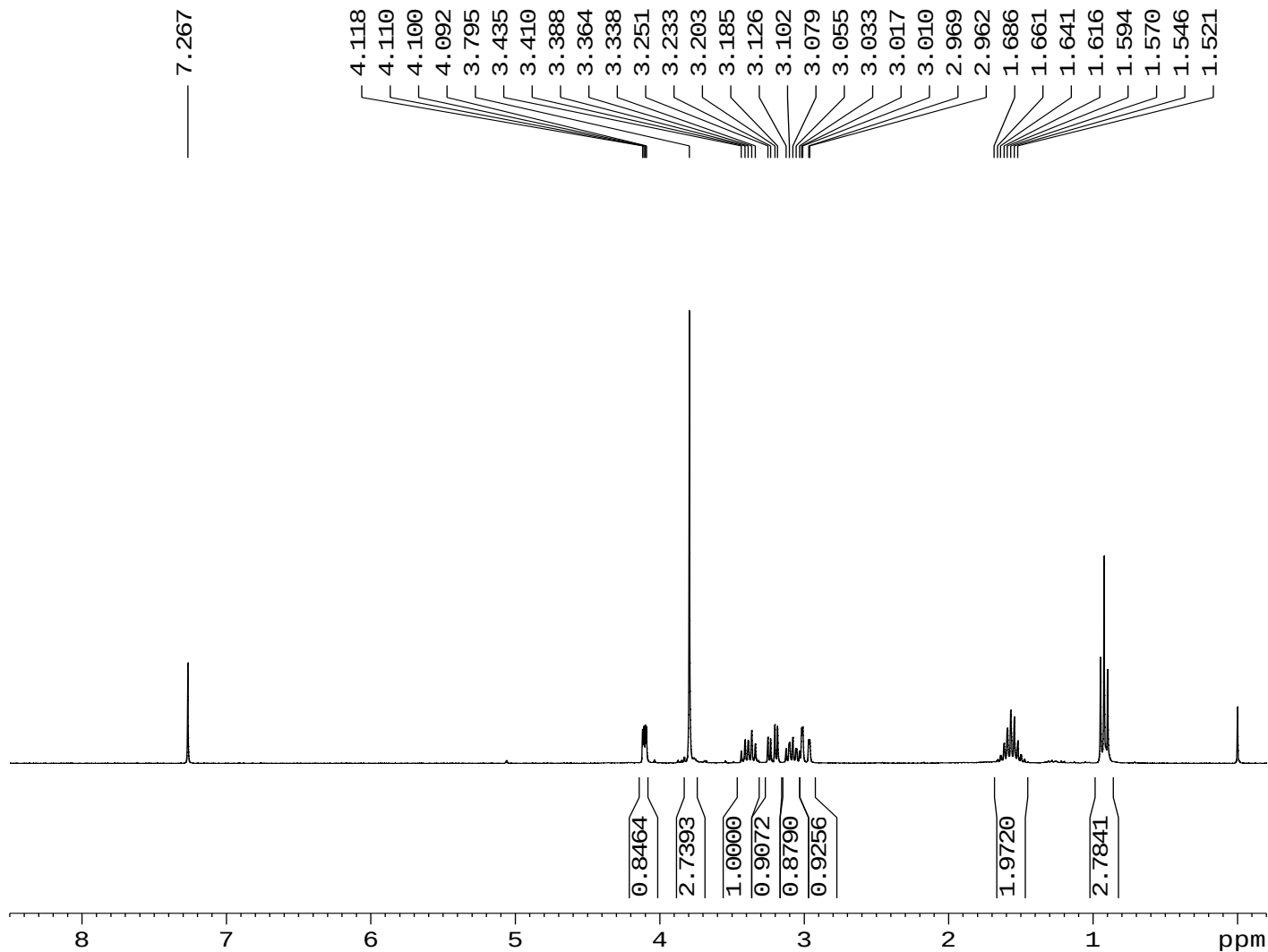


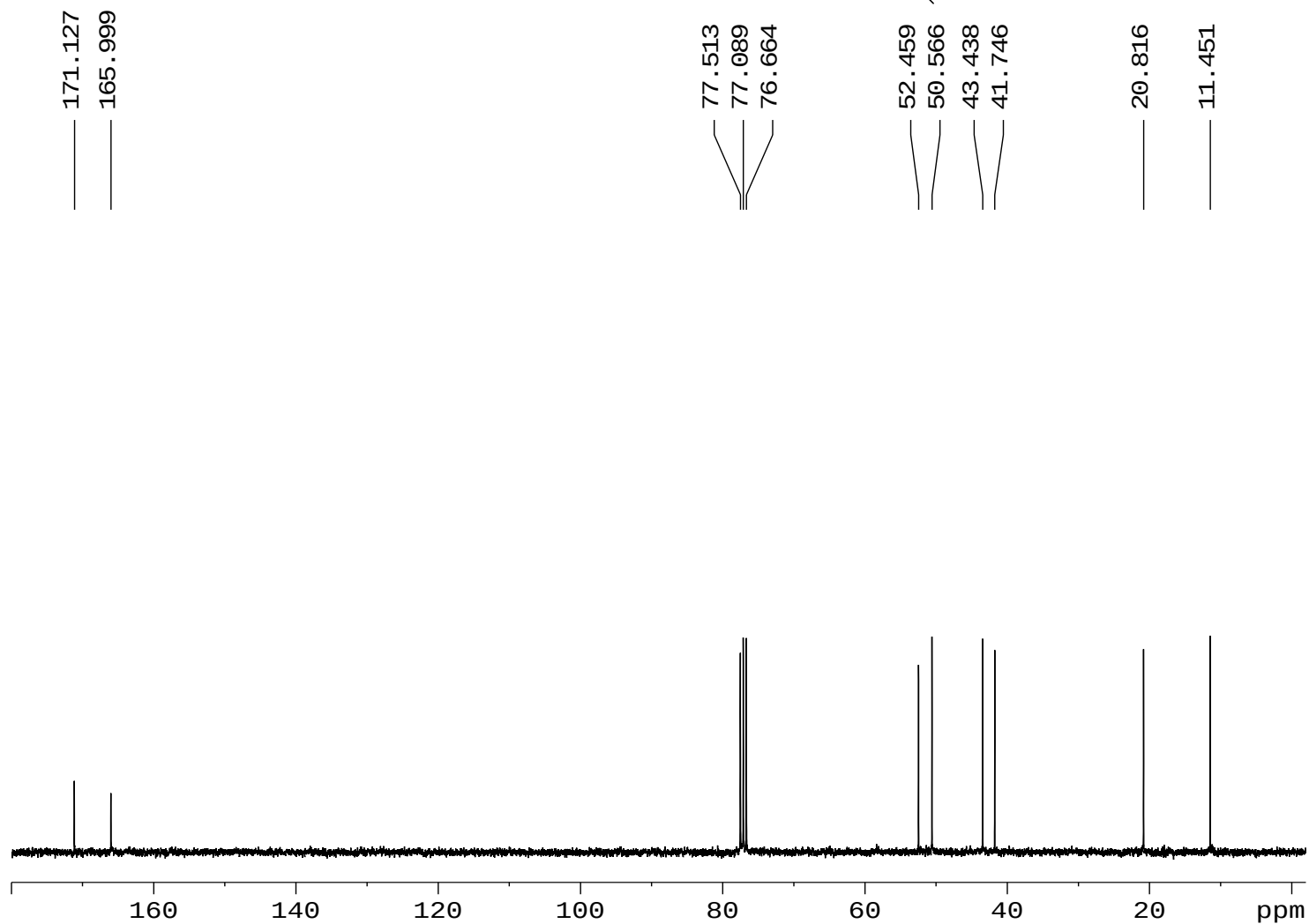
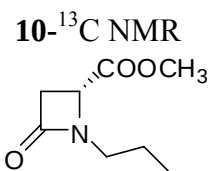
Current Data Parameters
NAME ldh-L-E-prog
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100129
Time 19.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 512
DW 55.600 usec
DE 8.00 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300038 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME ldh-L-E-prog
EXPNO 60
PROCNO 1

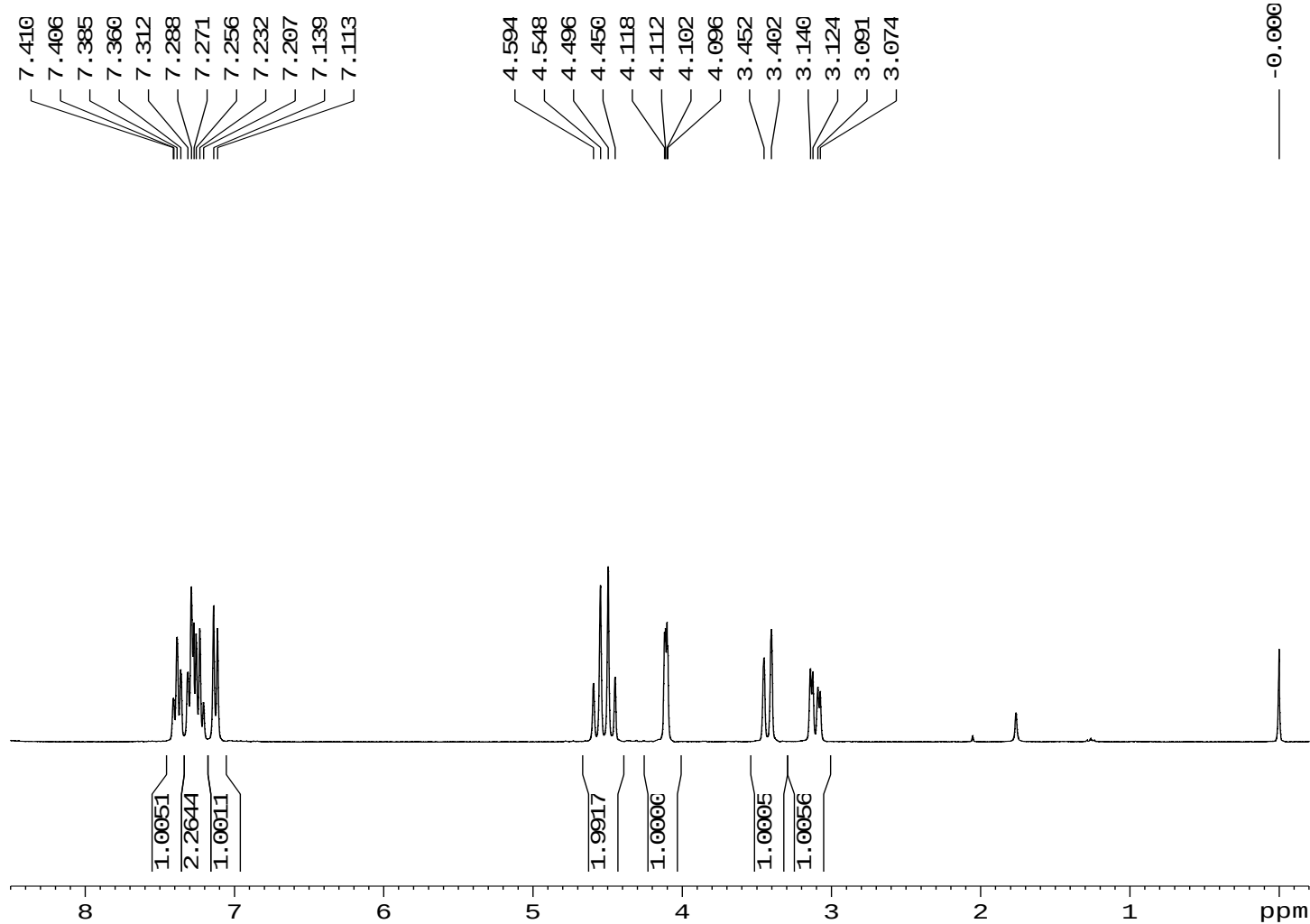
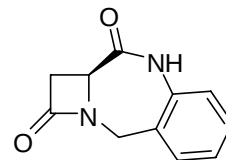
F2 - Acquisition Parameters
Date_ 20100129
Time 23.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgig30
TD 32768
SOLVENT CDCl3
NS 121
DS 0
SWH 18832.393 Hz
FIDRES 0.574719 Hz
AQ 0.8700404 sec
RG 16384
DW 26.550 usec
DE 8.00 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C - ^1H NMR



-0.000



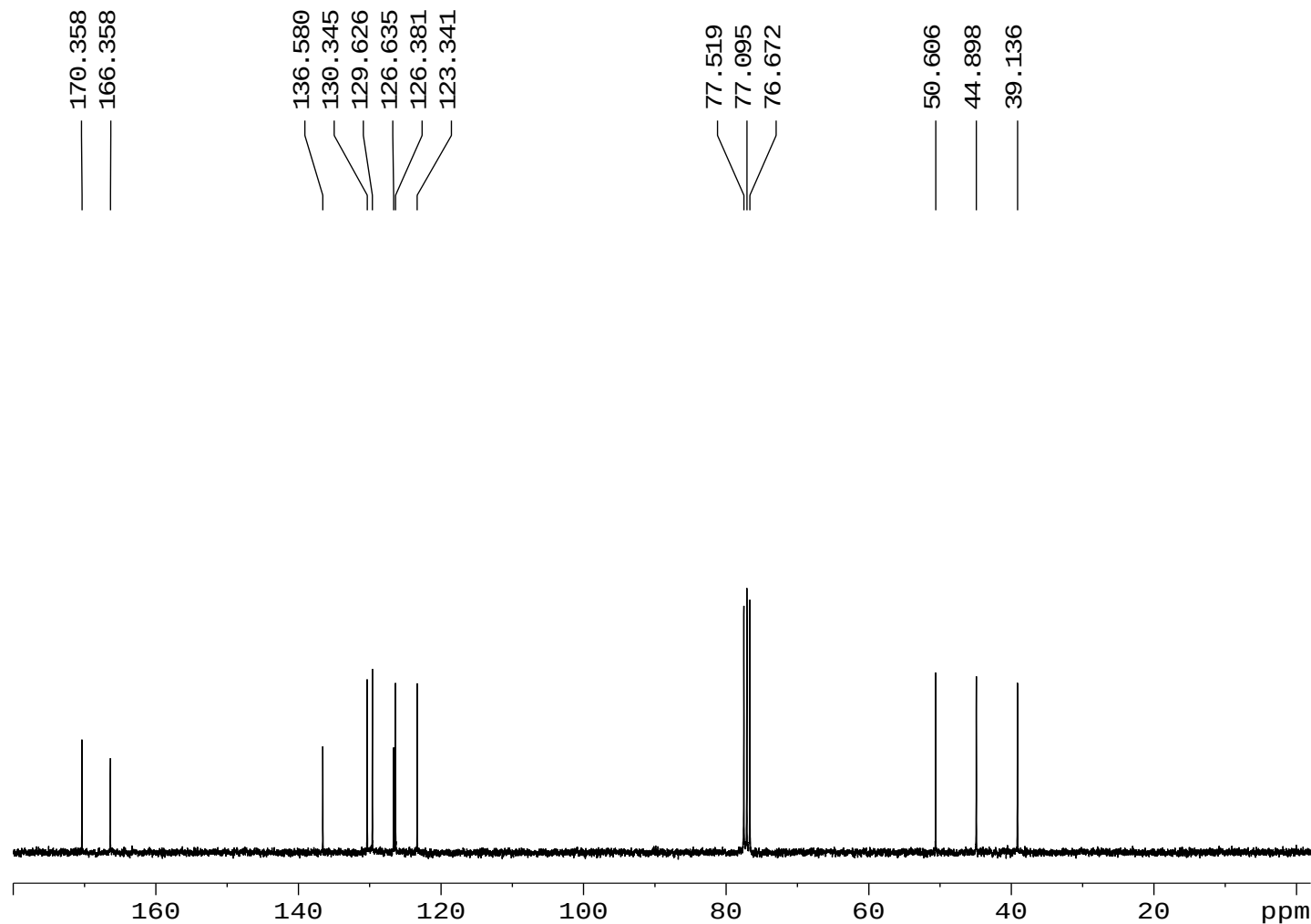
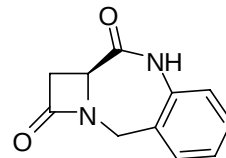
Current Data Parameters
NAME ldh-L-r47
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100107
Time 19.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 8.00 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR



Current Data Parameters
NAME ldh-L-r-47
EXPNO 20
PROCNO 1

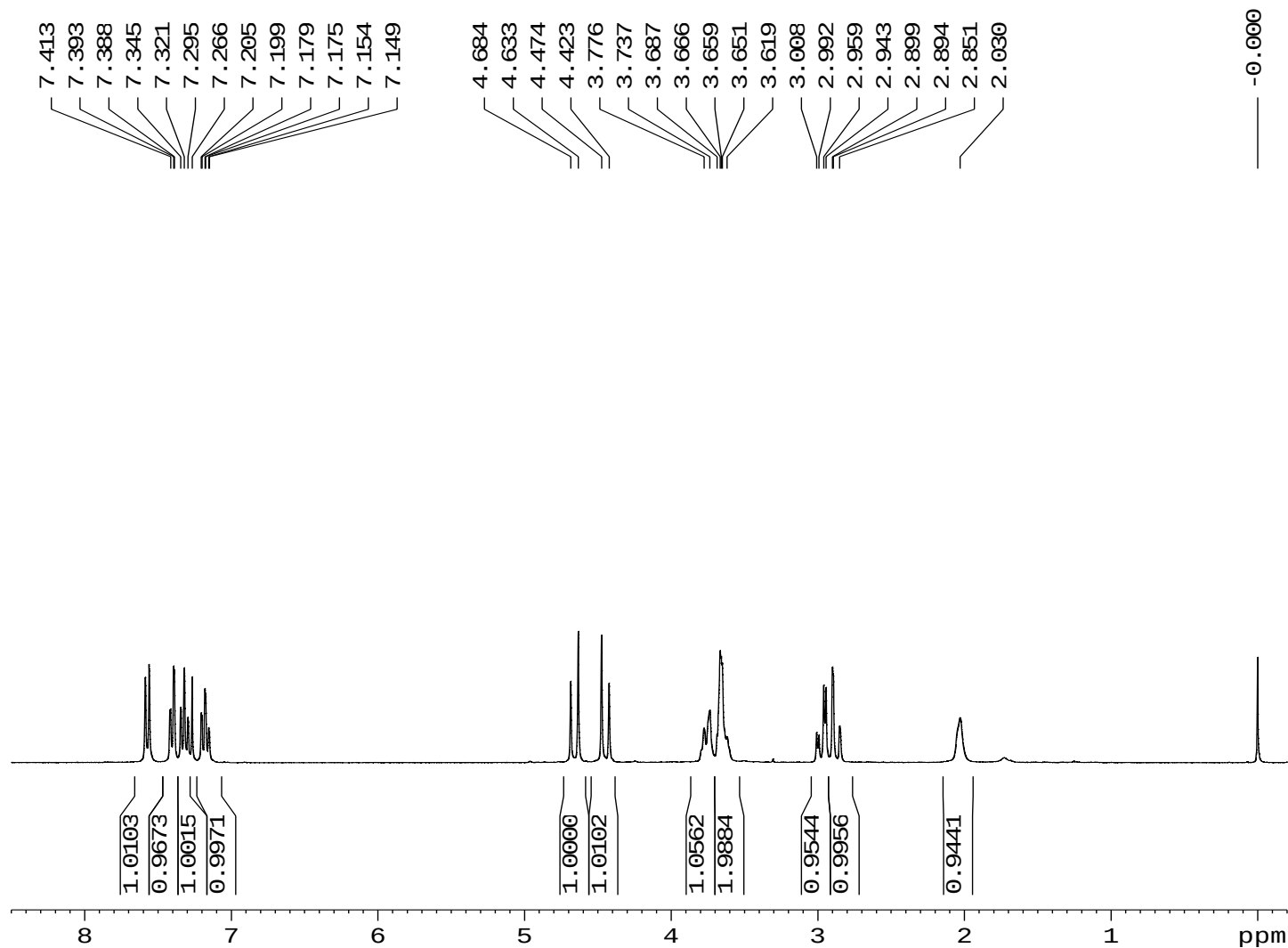
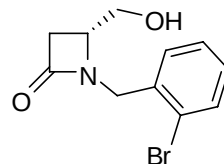
F2 - Acquisition Parameters
Date_ 20091231
Time 12.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 152
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 292.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

14-¹H NMR

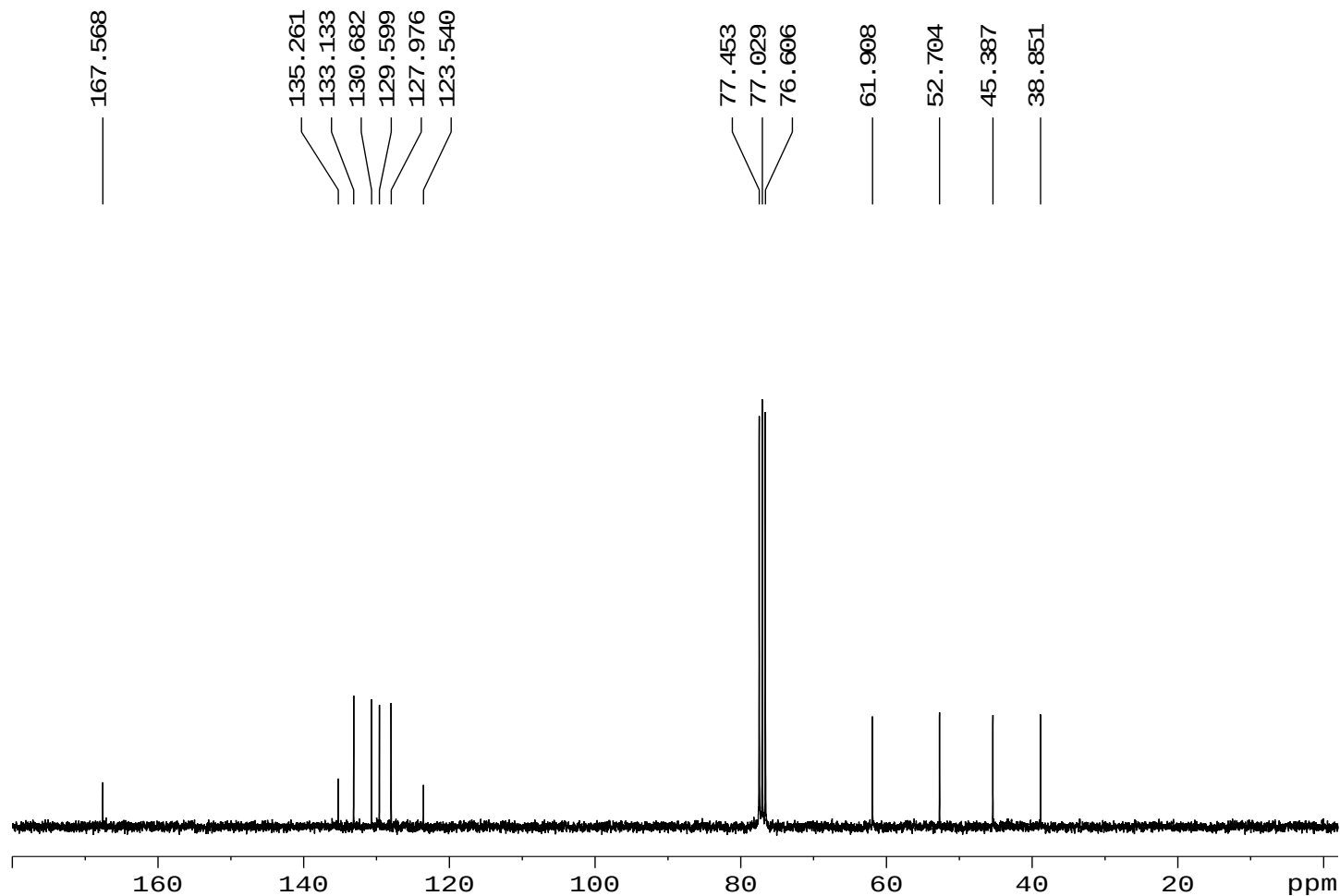
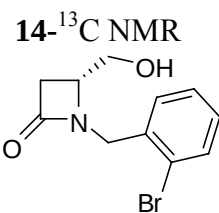


Current Data Parameters
NAME ldh-L-OH-o-Br
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100324
Time 21.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 362
DW 55.600 usec
DE 8.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300040 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME ldh-L-OH-o-Br
EXPNO 11
PROCNO 1

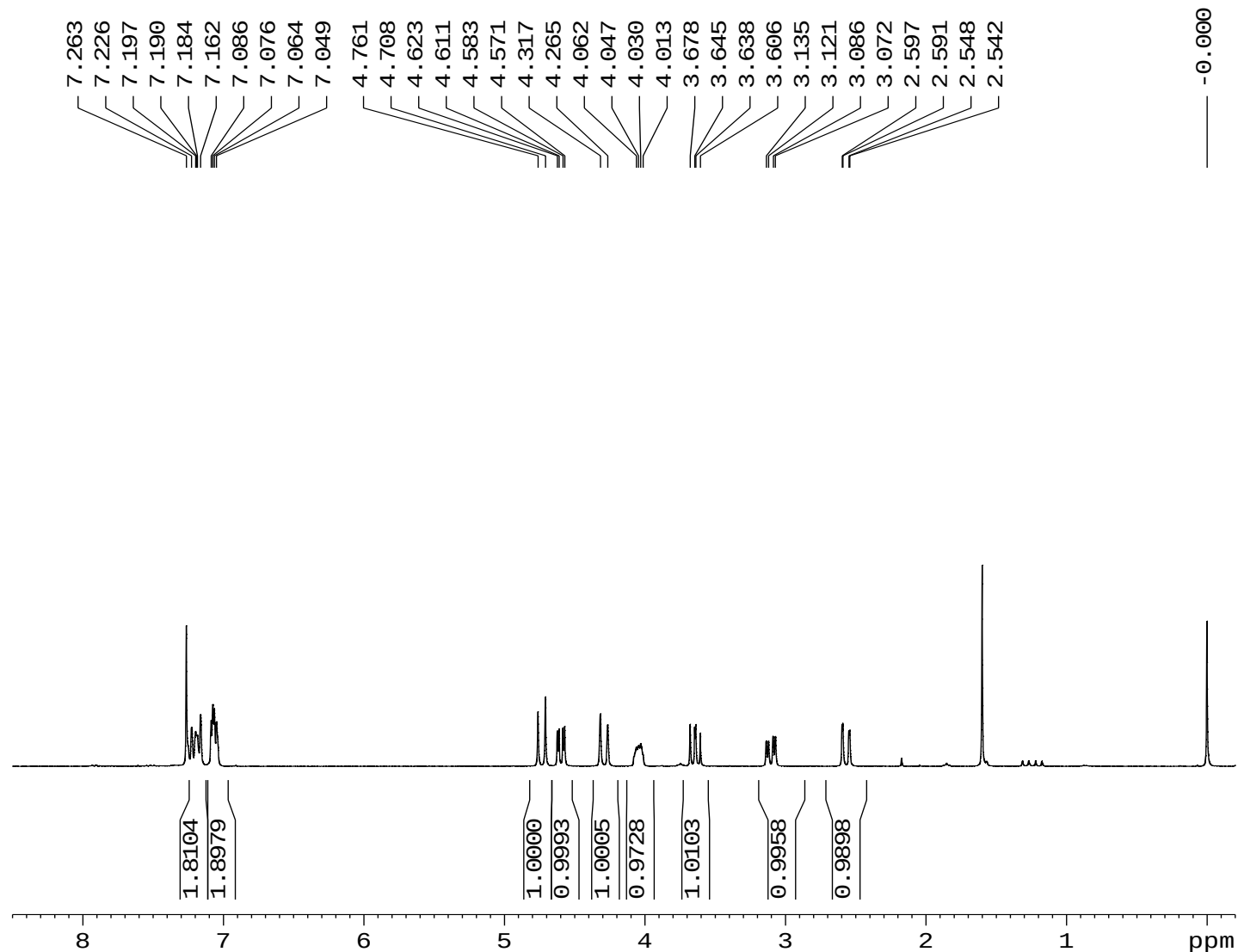
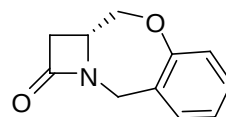
F2 - Acquisition Parameters
Date_ 20100324
Time 21.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 158
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 8.00 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

15-¹H NMR



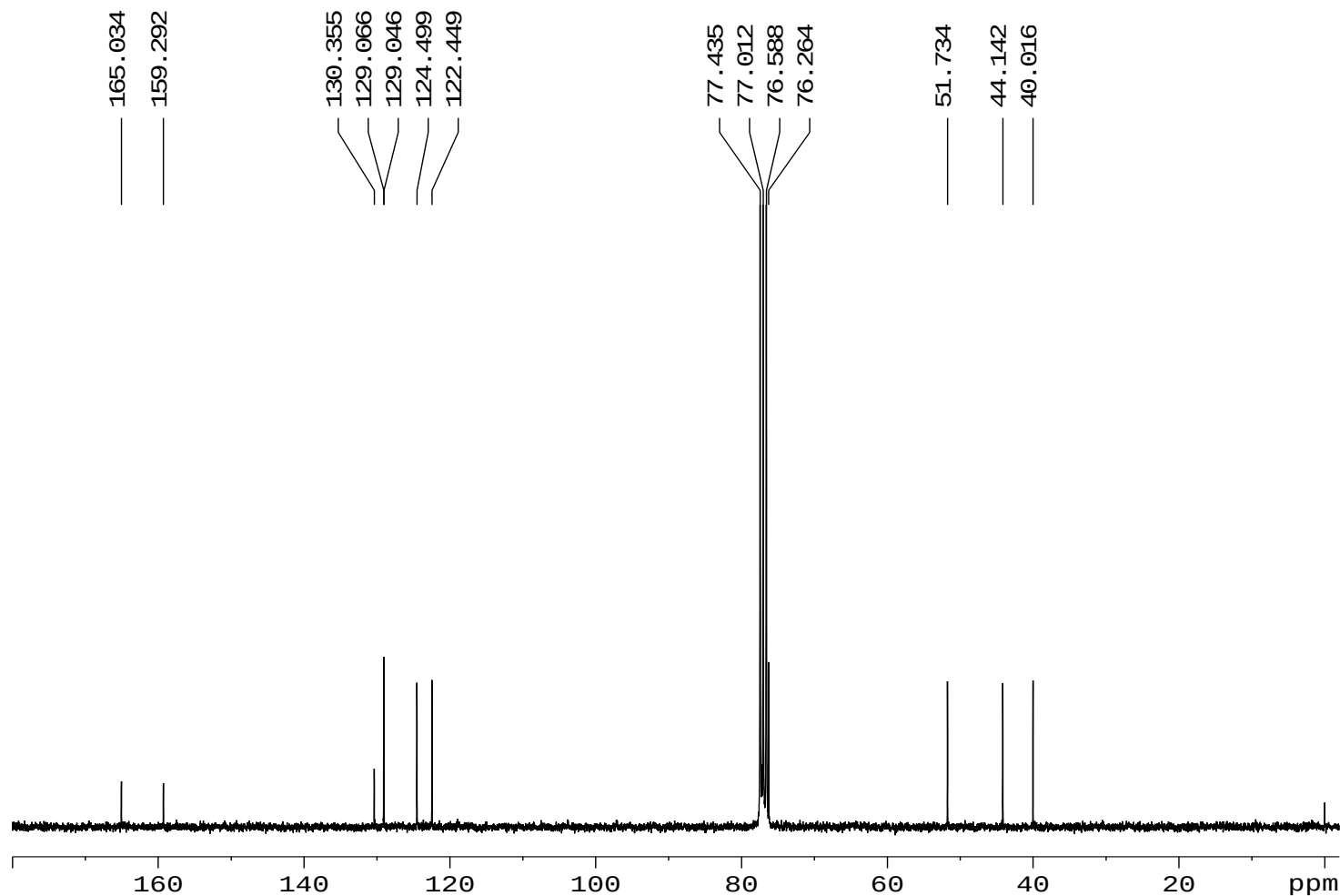
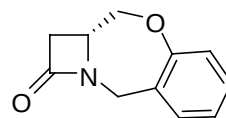
Current Data Parameters
NAME ldh-L-OH-coupl
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100330
Time 19.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 512
DW 55.600 usec
DE 8.00 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz

F2 - Processing parameters
SI 32768
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

$^{15}\text{-}^{13}\text{C}$ NMR



Current Data Parameters
NAME ldh-L-OH-coupl
EXPNO 30
PROCNO 1

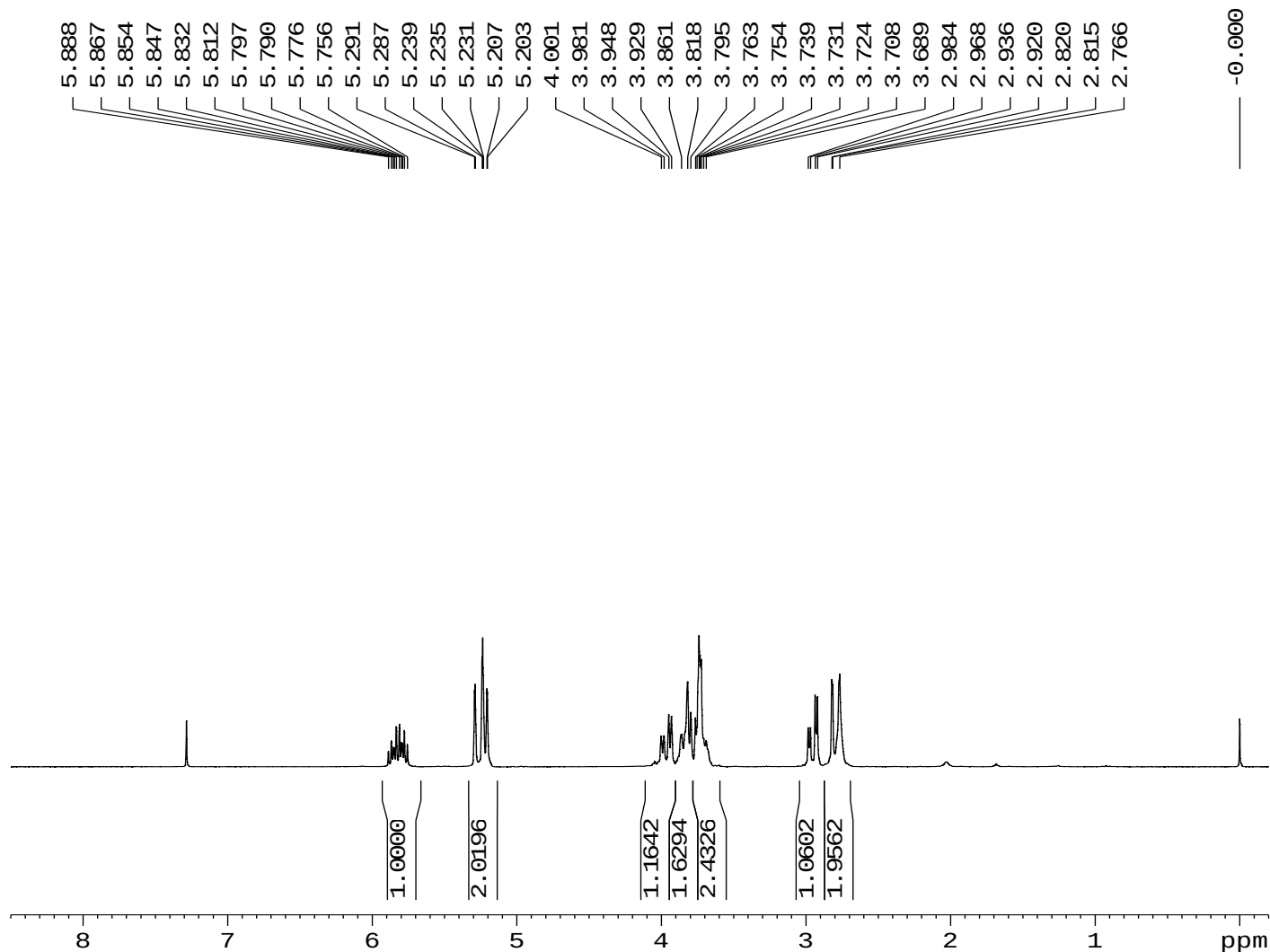
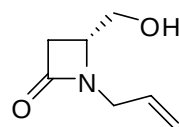
F2 - Acquisition Parameters
Date_ 20100331
Time 12.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2832
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DW 27.800 usec
DE 8.00 usec
TE 297.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

$^{16}\text{-}^1\text{H}$ NMR



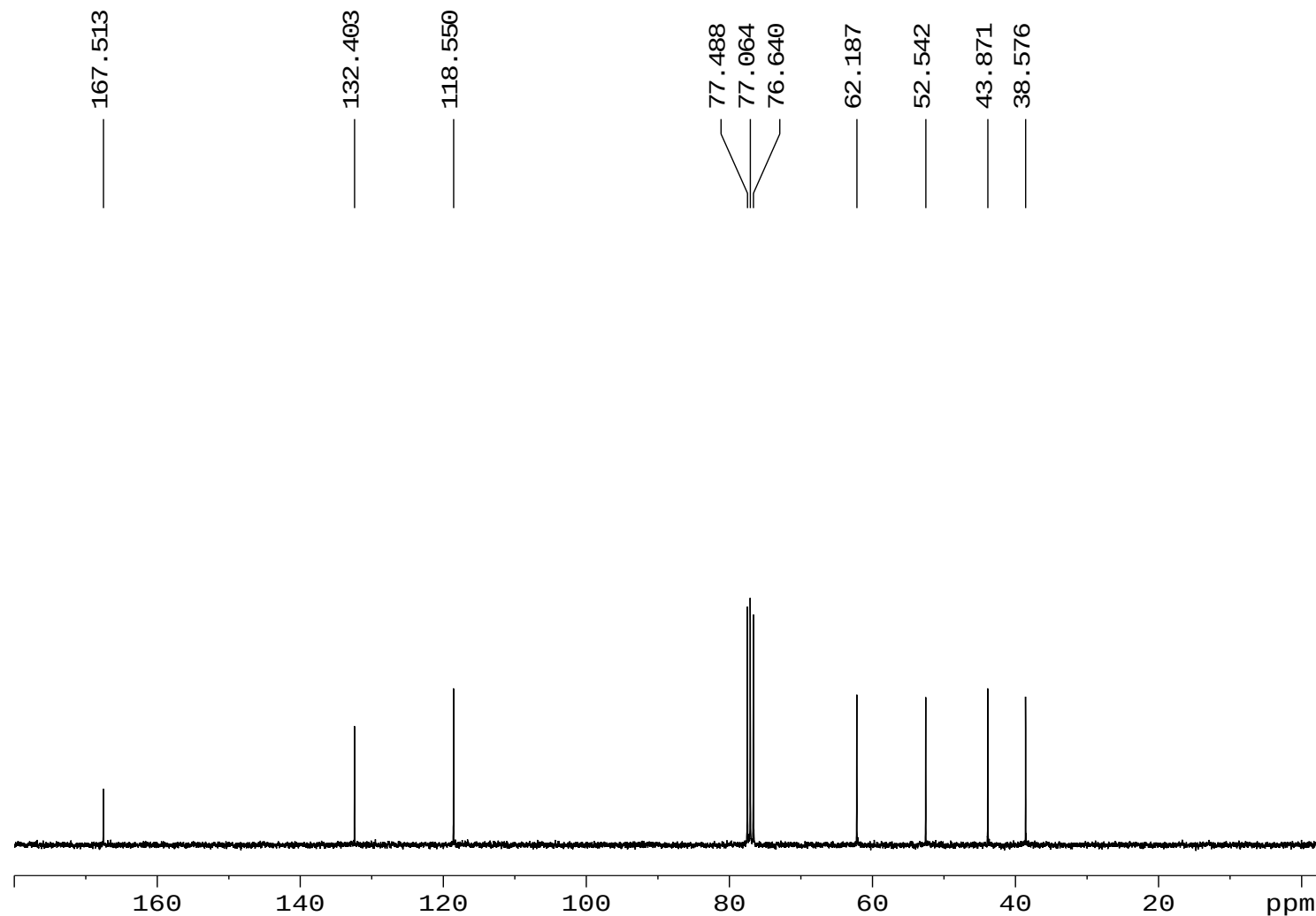
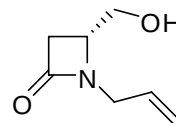
Current Data Parameters
NAME ldh-L-allyl-OH
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091231
Time 11.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 8.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299987 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

16-¹³C NMR



Current Data Parameters
NAME ldh-L-allyl-OH
EXPNO 11
PROCNO 1

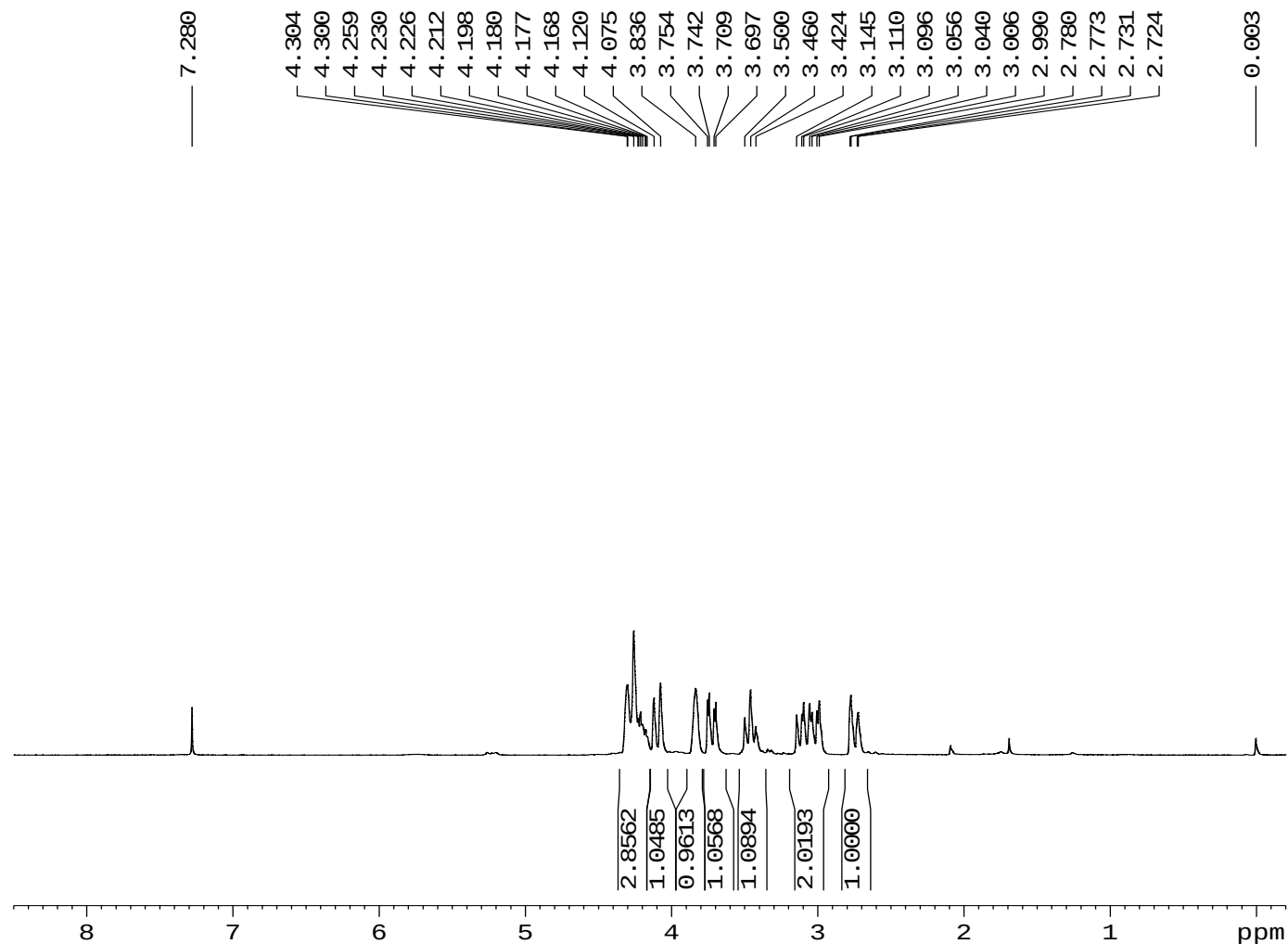
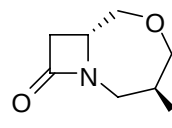
F2 - Acquisition Parameters
Date_ 20091231
Time 12.04
INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 130
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DW 27.800 usec
DE 8.00 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
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P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
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17-¹H NMR



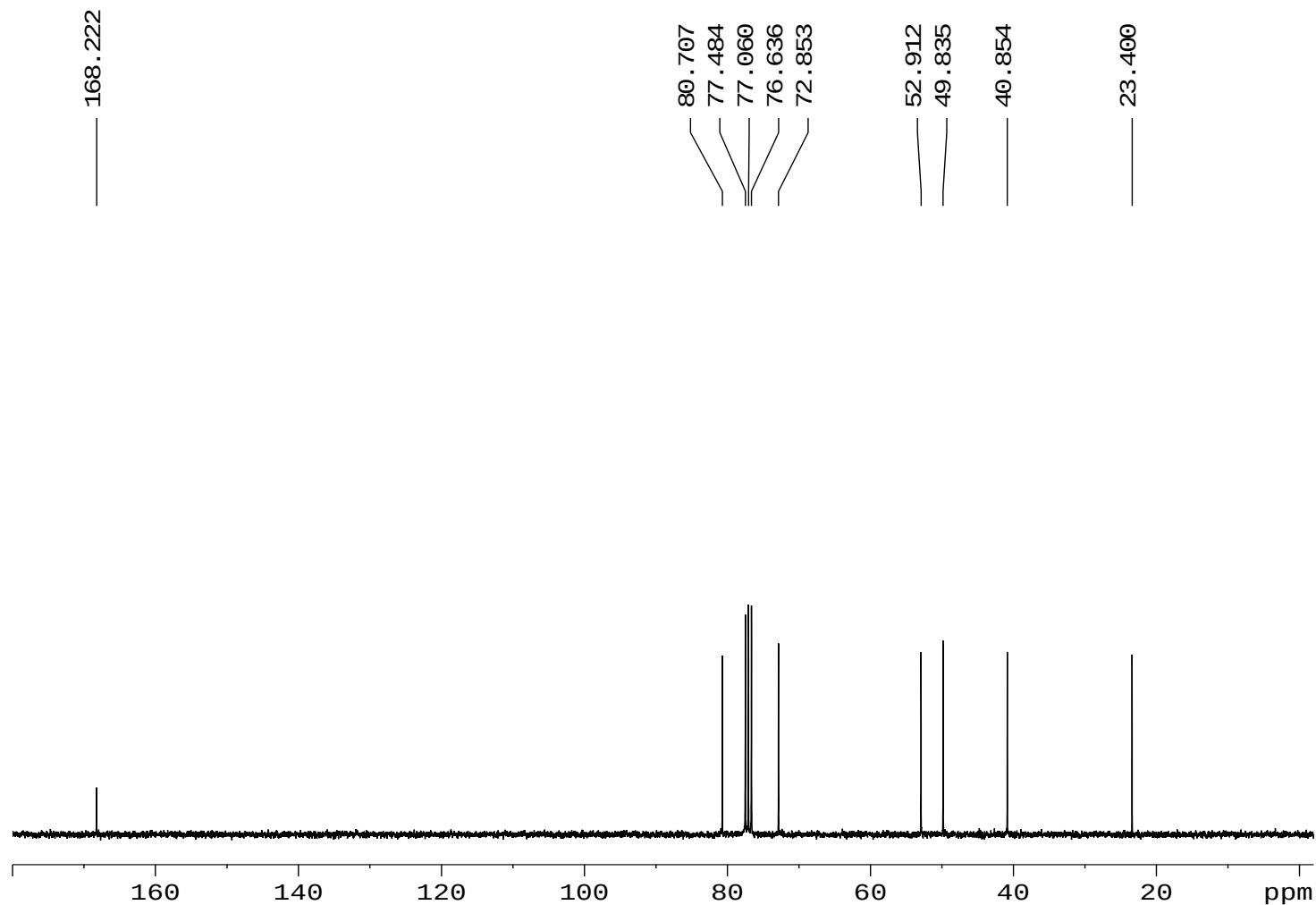
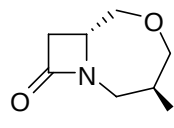
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PROCNO 1

F2 - Acquisition Parameters
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RG 228.1
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DE 8.00 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

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F2 - Processing parameters
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PC 1.00

17-¹³C NMR



Current Data Parameters
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EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
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Time 14.03
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TD 65536
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FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 13004
DW 27.800 usec
DE 8.00 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SF01 75.4752953 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 100.00 usec
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PL12 22.33 dB
PL13 23.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
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SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5. HPLC analysis of products. A Shimadzu LC-10AVP HPLC system was used to analyze enantiomeric excess values of all products.

Table S1: HPLC analysis of amides 2a-g, 6, 9 and methyl esters 4a-g, 7, 10.

Compound	T1(min)	T2(min)	Column
2a	45.7	53.4	Chiralcel ODH
2b	38.3	43.6	Chiralcel ODH
2c	36.2	39.0	Chiralcel ODH
2d	45.1	50.6	Chiralcel ODH
2e	45.1	49.6	Chiralcel ODH
2f	46.4	49.8	Chiralcel ODH
2g	57.9	62.6	Chiralcel ODH
4a	38.3	42.2	Chiralcel OJH
4b	46.6	50.3	Chiralcel OJH
4c	31.7	35.5	Chiralcel OJH
4d	66.7	88.9	Chiralcel OJH
4e	53.6	58.3	Chiralcel OJH
4f	39.8	50.4	Chiralcel OJH
4g	30.4	34.2	Chiralcel OJH
6	34.4	38.3	Chiralcel OD
7	17.5	21.4	Chiralcel ADH
9	16.4	18.3	Chiralcel ADH
10	16.3	21.8	Chiralcel ADH

Chiralcel ODH, OJH and ADH employed hexane : isopropanol = 9 : 1 as mobile phase; flow rate 0.5ml/min; 25°C.

Chiralcel OD employed hexane : isopropanol = 9 : 1 as mobile phase; flow rate 0.8ml/min; 25°C.

Table S2: HPLC analysis of compounds 13, 14, and 15.

Compound	T1(min)	T2(min)	Column
13	54.2	59.4	Chiralcel ADH
15	26.9	28.9	Chiralcel ADH
16	14.8	16.5	Chiralcel AD
17	72.4	78.8	Chiralcel ADH

Chiralcel ADH employed hexane : isopropanol = 9 : 1 as mobile phase; flow rate 0.5ml/min; 25°C.

Chiralcel AD employed hexane : isopropanol = 9 : 1 as mobile phase; flow rate 0.8ml/min; 25°C.

6. References

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- (2) Torracca, K. E.; Kuwabe, S.; Buchwald, S. L. *J.Am.Chem. Soc.* **2000**, 122, 12907-12908.
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