

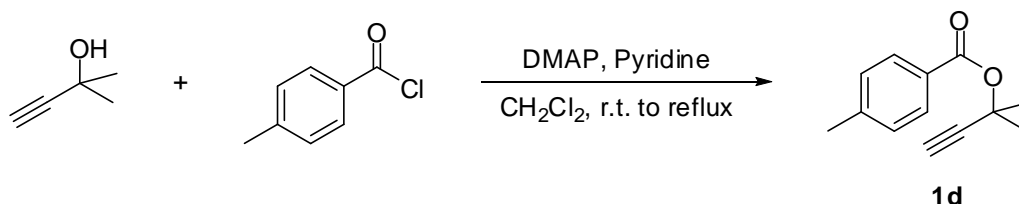
Supplementary Information for

Gold-catalyzed Intermolecular [4+3] Cycloaddition Reactions

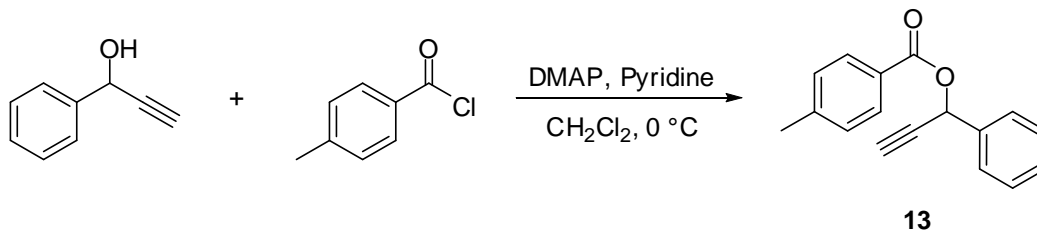
Benjamin W. Gung,* Lauren N. Bailey, and Josh Wonser

General procedures. Unless otherwise stated, all reactions were carried out under an inert nitrogen atmosphere with dry solvents under anhydrous conditions. Dry tetrahydrofuran (THF) and toluene (PhCH₃) were distilled over sodium benzophenone, dichloromethane (CH₂Cl₂), dichloroethane (DCE), and pentane (C₅H₁₂) were distilled over calcium hydride. Reagents were purchased and used without further purification unless otherwise stated. Yields refer to chromatographically and spectroscopically (¹H NMR) homogeneous materials, unless otherwise stated. Reactions were monitored by thin layer chromatography (TLC) carried out on 0.25 mm Merck silica gel plates (60F-254) using UV light as the visualizing agent and an acidic mixture of anisaldehyde, phosphomolybdic acid, or ceric ammonium molybdate, or basic aqueous potassium permanganate (KMnO₄), and heat as developing agents. Merck silica gel (60, particle size 0.043–0.063 mm) was used for flash column chromatography. NMR spectra were recorded on Bruker Av-500, and Av-300 instruments and calibrated using residual undeuterated solvent as an internal reference (CHCl₃ @ 7.26 ppm ¹H NMR, 77.0 ppm ¹³C NMR). The following abbreviations (or combinations thereof) were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad. IR spectra were recorded on a Perkin Elmer Spectrum 2000 FTIR spectrometer. Melting points were recorded on a Thomas-Hoover melting point apparatus.

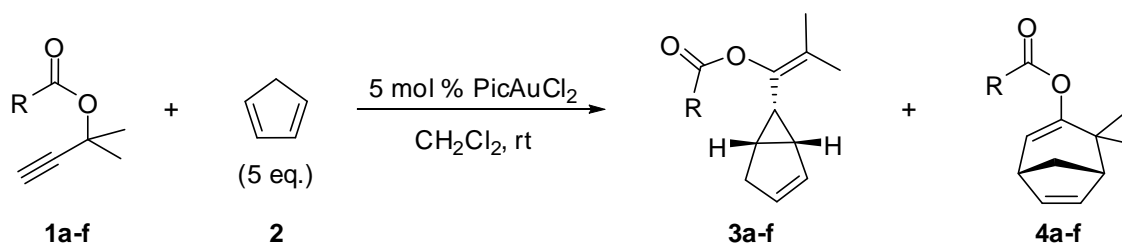
Synthesis of Propargyl Esters.



Propargyl Ester 1d. 2-methyl-3-butyn-2-ol (200 mg, 2.4 mmol) was added to a solution of DMAP (15 mg, 0.119 mmol), pyridine (1.9 mL, 24.0 mmol) and CH₂Cl₂ (2.4 mL) under a nitrogen atmosphere. The mixture was stirred 15 min. at room temperature. The acid chloride (0.94 mL, 7.2 mmol) was added by syringe at the same temperature and the reaction was heated to reflux (45–50°C) and stirred overnight. The reaction was cooled to room temperature, diluted with Et₂O, and quenched with 1N HCl. The aqueous layer was extracted with Et₂O, and the combined organic extracts were washed with 10% aq. NaOH, and brine. The organic extracts were dried over MgSO₄, filtered, concentrated, and purified via silica gel chromatography (5–10–20% EtOAc/hexanes) to yield 460 mg (95 %) of a colorless oil. ¹H NMR (300 MHz, CDCl₃): δ 1.81 (6H, s), 2.39 (3H, s), 2.57 (1H, s), 7.21 (2H, d, J = 8.1 Hz), 7.92 (2H, 8.1 Hz). ¹³C NMR (75 MHz, CDCl₃): δ 21.6, 29.0, 71.9, 72.4, 84.8, 128.0, 128.9, 129.6, 143.4, 164.8. LCMS calcd for C₁₃H₁₄O₂Na 225.1, found 225.0.



Propargyl Ester 13. 1-phenylprop-2-yn-1-ol (250 mg, 1.9 mmol) was added to a solution of DMAP (12 mg, 0.095 mmol), pyridine (1.53 mL, 24.0 mmol) and CH₂Cl₂ (3.8 mL) under a nitrogen atmosphere. The mixture was stirred 15 min. at 0 °C. The acid chloride (0.75 mL, 5.67 mmol) was added by syringe at the same temperature. After 2h and completion by TLC, the reaction was warmed to room temperature, diluted with Et₂O, and quenched with 1N HCl. The aqueous layer was extracted with Et₂O, and the combined organic extracts were washed with 10% aq. NaOH, and brine. The organic extracts were dried over MgSO₄, filtered, concentrated, and purified via silica gel chromatography (5-10-20% EtOAc/hexanes) to yield 384 mg (81 %) of a colorless oil. ¹H NMR (300 MHz, CDCl₃): δ 2.39 (3H, s), 2.67-2.69 (1H, m), 6.69 (1H, d, J = 2.1 Hz), 7.22 (2H, d, J = 8.1 Hz), 7.36-7.42 (3H, m), 7.60-7.63 (2H, m), 7.96 (2H, d, J = 8.4 Hz). ¹³C NMR (75 MHz, CDCl₃): δ 21.6, 65.6, 75.5, 80.4, 126.8, 127.6, 128.7, 129.0, 129.1, 129.9, 136.7, 144.0, 165.4.



Typical Procedure for Intermolecular Cyclopropanation/Formal [4C + 3C] Cycloaddition.

Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (2 μmol) and AgSbF₆ (5 μmol) were added to CH₂Cl₂ (0.6 mL) under a nitrogen atmosphere at room temperature and this mixture was allowed to stir for 15 min. A solution of propargyl ester (0.247 mmol) and cyclopentadiene (1.24 mmol) in CH₂Cl₂ (0.6 mL) were added to the flask by syringe. The reaction was permitted to stir overnight and monitored by TLC. The reaction was diluted with EtOAc and filtered through a pad of silica and Celite. The filtrate was concentrated and purified via silica gel chromatography (1% EtOAc/hexanes).

Vinylcyclopropane 3a. A colorless oil (31 mg, 0.16 mmol, 23% yield). Data was consistent with previously reported values.¹

Formal [4C + 3C] Cycloadduct 4a. A colorless oil (47 mg, 0.024 mmol, 34 % yield). Data was consistent with previously reported values.¹

Vinylcyclopropane 3b. A colorless oil (23 mg, 0.10 mmol, 17% yield). ¹H NMR (500 MHz, CDCl₃): δ 1.26 (9H, s), 1.51 (3H, s), 1.74 (3H, s), 1.82-1.86 (1H, m), 1.95-1.99 (1H, m), 2.12-2.16 (1H, m), 2.23-2.27 (1H, m), 2.48-2.53 (1H, m), 5.44-5.46 (1H, m), 5.66-5.68 (1H, m). ¹³C

NMR (125 MHz, CDCl₃): δ 17.1, 18.7, 22.5, 23.2, 27.3, 30.1, 32.9, 38.8, 122.9, 129.3, 129.7, 138.7, 176.8.

Formal [4C + 3C] Cycloadduct 4b. A colorless oil (56 mg, 0.24 mmol, 40 % yield). ¹H NMR (500 MHz, CDCl₃): δ 0.92 (3H, s), 1.17 (3H, s), 1.23 (9H, s), 1.83-1.86 (1H, m), 1.97-1.99 (1H, m), 2.47-2.49 (1H, m), 2.77-2.80 (1H, m), 5.69 (1H, d, J = 6.80 Hz), 5.83-5.85 (1H, m), 6.36-6.38 (1H, m). ¹³C NMR (125 MHz, CDCl₃): δ 21.5, 27.2, 27.4, 38.2, 39.2, 40.3, 51.3, 119.5, 131.1, 141.0, 151.0, 177.1.

Vinylcyclopropane 3c. A colorless oil (39 mg, 0.15 mmol, 29% yield). Data was consistent with previously reported values.¹

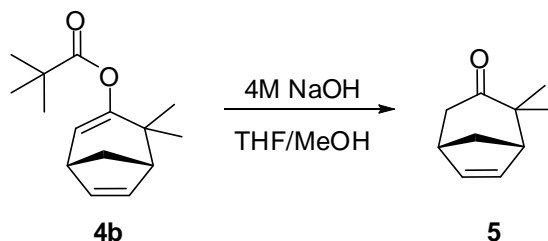
Formal [4C + 3C] Cycloadduct 4c. A colorless oil (83 mg, 0.33 mmol, 61% yield). Data was consistent with previously reported values.¹

Vinylcyclopropane 3d. A colorless oil (40 mg, 0.15 mmol, 30% yield). ¹H NMR (500 MHz, CDCl₃): δ 1.58 (3H, s), 1.80 (3H, s), 1.86-1.91 (1H, m), 2.08-2.11 (1H, m), 2.16-2.19 (1H, m), 2.28-2.31 (1H, m), 2.43 (3H, s), 2.50-2.55 (1H, m), 5.50-5.51 (1H, m), 5.65-5.67 (1H, m), 7.26 (2H, d, J = 6.95 Hz), 7.96 (2H, d, J = 8.05 Hz). ¹³C NMR (125 MHz, CDCl₃): δ 17.4, 18.6, 21.7, 22.9, 23.5, 30.4, 33.11, 118.0, 123.3, 127.6, 129.1, 129.6, 129.9, 138.9, 143.6, 164.8. LCMS calcd for C₁₈H₂₀O₂Na 291.1, found 291.1.

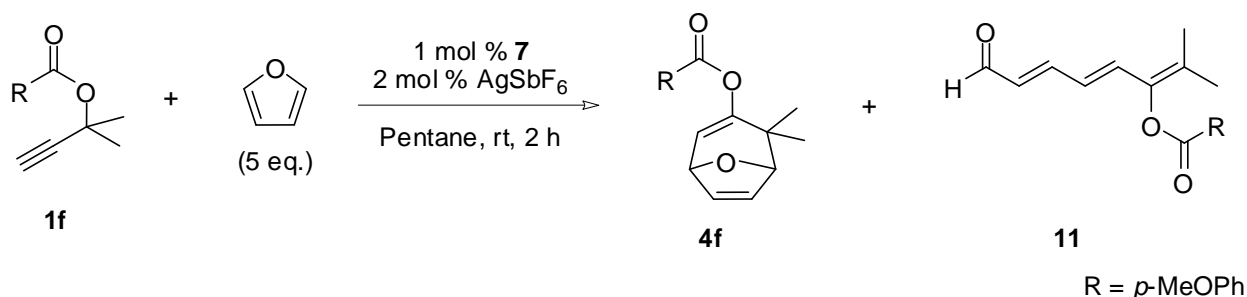
Formal [4C + 3C] Cycloadduct 4d. A colorless oil (83 mg, 0.31 mmol, 62 % yield). ¹H NMR (500 MHz, CDCl₃): δ 1.00 (3H, s), 1.25 (3H, s), 1.87-1.91 (1H, m), 2.04-2.06 (1H, m), 2.41 (3H, s), 2.53 (1H, s), 2.85 (1H, s), 5.87-5.90 (2H, m), 6.41-6.42 (1H, m), 7.25 (2H, d, J = 8.20 Hz), 7.94 (2H, d, J = 8.05 Hz). ¹³C NMR (125 MHz, CDCl₃): δ 21.7, 27.5, 38.4, 39.4, 40.3, 51.3, 120.1, 127.5, 129.1, 129.9, 131.2, 141.0, 143.8, 151.1, 165.3. LCMS calcd for C₁₈H₂₀O₂Na 291.1, found 291.1.

Vinylcyclopropane 3e. A white solid (36 mg, 0.12 mmol, 28 % yield). ¹H NMR (500 MHz, CDCl₃): δ 1.59 (3H, s), 1.82, (3H, s), 1.91-1.95 (1H, m), 2.09-2.12 (1H, m), 2.18-2.28 (2H, m), 2.53-2.58 (1H, m), 5.52-5.53 (1H, m), 5.62-5.64 (1H, m), 8.21-8.25 (2H, m), 8.28-8.33 (2H, m).

Formal [4C + 3C] Cycloadduct 4e. A white solid (45 mg, 0.15 mmol, 35 % yield). ¹H NMR (500 MHz, CDCl₃): δ 1.01 (3H, s), 1.26 (3H, s), 1.90-1.94 (1H, m), 2.04-2.06 (1H, m), 2.57-2.58 (1H, m), 2.87-2.88 (1H, m), 5.90-5.95 (2H, m), 6.42-6.44 (1H, m), 8.21-8.25 (2H, m), 8.30-8.33 (2H, m). ¹³C NMR (125 MHz, CDCl₃): δ 21.6, 27.5, 38.3, 39.1, 40.2, 51.3, 120.7, 123.6, 130.9, 131.3, 135.6, 141.0, 150.6, 151.2, 163.4.



Ketone 5. A solution of 4M NaOH (aq.) (4.0 mL) was added to a mixture of **4b** (170 mg, 0.72 mmol) in THF (16 mL) and MeOH (8 mL) under a nitrogen atmosphere at 0° C. The reaction stirred at this temperature 1 h, then was warmed to room temperature and stirred for 2 h. The solution was concentrated, then diluted with CH₂Cl₂ and quenched with 1N HCl. The aqueous layer was extracted with CH₂Cl₂, and the combined organic layers were washed with sat. NaHCO₃ and brine. Organic extracts were dried over MgSO₄, filtered, and concentrated. The residue was purified via column chromatography (5-10% EtOAc/hexanes) to give 62 mg (57%) of ketone as a colorless oil. Data was consistent with reported values.²



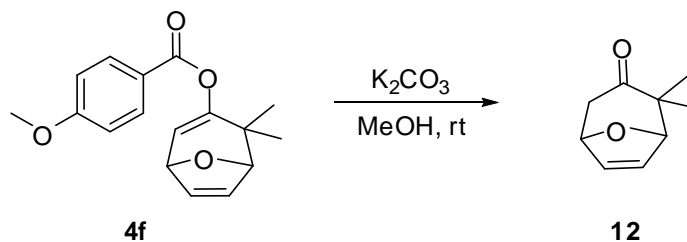
Typical Procedure for Intermolecular Formal [4C + 3C] Cycloaddition with Furan.

Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (2 μmol) and AgSbF₆ (5 μmol) were added to solvent (CH₂Cl₂ or pentane) (0.6 mL) under a nitrogen atmosphere at room temperature and this mixture was allowed to stir for 15 min. A solution of propargyl ester (0.247 mmol) and furan (1.24 mmol) in solvent (CH₂Cl₂ or pentane) (0.6 mL) were added to the flask by syringe. The reaction was permitted to stir 2 hours, or until completion as monitored by TLC. The reaction was diluted with EtOAc and filtered through a pad of silica and Celite. The filtrate was concentrated and purified via silica gel chromatography (1% EtOAc/hexanes).

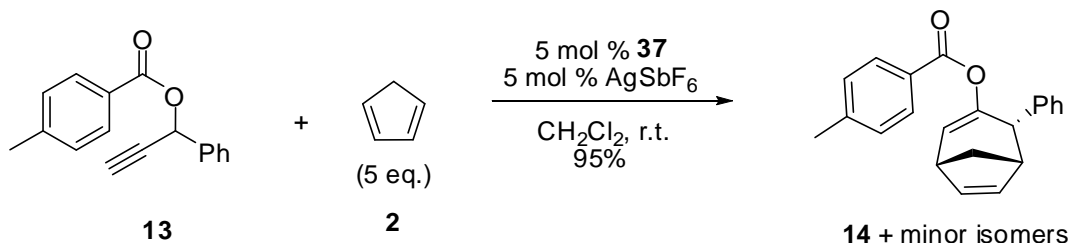
Formal [4C + 3C] Cycloadduct 4f. A colorless oil (12 mg, 40 μmol, 18 % yield). ¹HNMR (500 MHz, CDCl₃): δ 0.93 (3H, s), 1.41 (3H, s), 3.87 (3H, s), 4.56 (1H, d, J = 2.00 Hz), 4.85-4.86 (1H, m), 6.04 (1H, d, J = 4.50 Hz), 6.07-6.09 (1H, m), 6.70-6.72 (1H, m), 6.94 (2H, d, J = 9.0 Hz), 8.00 (2H, d, J = 9.0 Hz). ¹³C NMR (125 MHz, CDCl₃): δ 18.2, 26.7, 39.6, 55.5, 75.9, 87.3, 113.8, 117.1, 122.1, 127.4, 131.9, 139.8, 150.2, 163.7. LCMS calcd for C₁₇H₁₈O₄Na 309.1, found 309.1.

Triene Aldehyde 11. A yellow solid (34 mg, 0.12 mmol, 52 % yield, mixture of *cis* and *trans* isomers). Data is given for the major product, the *trans* isomer. ¹HNMR (300 MHz, CDCl₃): δ 1.78 (3H, s), 2.03 (3H, s), 3.90 (3H, s), 6.09 (1H, dd, J = 15.2, 8.1 Hz), 6.31 (1H, dd, J = 15.0,

11.4 Hz), 6.92-7.04 (3H, m), 7.18 (1H, dd, $J = 15.2, 11.4$ Hz), 8.15 (2H, d, $J = 8.7$ Hz), 9.54 (1H, d, $J = 7.8$ Hz).

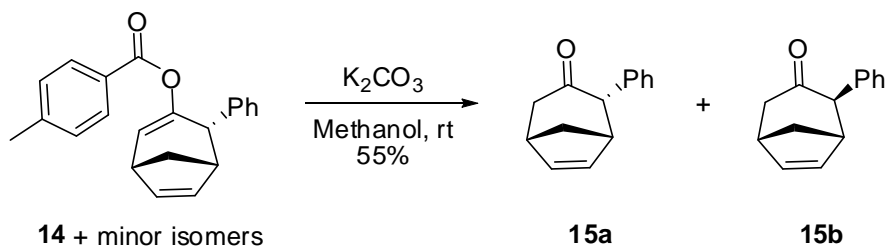


Ketone 12. The formal [4C + 3C] cycloadduct **4f** (53 mg, 0.19 mmol) was dissolved in methanol (2 ml) and potassium carbonate (64 mg, 0.46 mmol) was then added. After stirring overnight, TLC indicated that the starting ester had disappeared and the reaction mixture was diluted with ether and quenched with 1M HCl. The layers were separated and the aqueous phase was extracted with ether. The combined organic extracts were washed with brine and dried over MgSO_4 . The solution was concentrated and the residue was purified via column chromatography (10-20% EtOAc/hexanes) to give 12 mg (43%) of ketone. Data was consistent with reported values.²

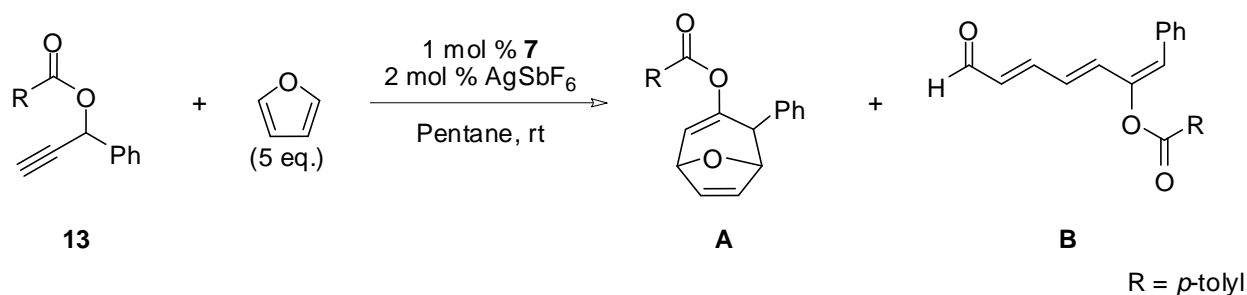


The same procedure used to prepare vinyl cyclopropanes **3a-e** and the formal [4C + 3C] cycloaddition products **4a-e** were used to prepare **14**.

Formal [4C + 3C] Cycloadduct 14. A colorless oil (60mg, 0.19 mol, 95 % yield, with minor impurities). Data is given for the major product. $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 2.07-2.10 (1H, m), 2.18-2.19 (1H, m), 2.30 (3H, s), 2.95-2.96 (1H, m), 3.08-3.09 (1H, m), 4.19 (1H, d, $J = 5$ Hz), 5.38-5.39 (1H, m), 6.20-6.21 (1H, d, $J = 7.5$ Hz), 6.42-6.43 (1H, m), 7.07 (2H, d, $J = 8$ Hz), 7.11-7.14 (3H, m) 7.21 (2H, t, $J = 7.3$ Hz), 7.62 (2H, d, $J = 8$ Hz).



Ketones 15a and 15b. The formal [4 + 3] cycloaddition product **14** (60 mg, 0.19 mmol) was dissolved in methanol (2 ml) and potassium carbonate (66 mg, 0.47 mmol) was then added. After stirring overnight, TLC indicated that the starting material had disappeared and the reaction mixture was diluted with Et₂O and quenched with 1M HCl. The layers were separated and the aqueous phase was extracted with Et₂O. The combined organic extracts were washed with brine and dried over MgSO₄. The solution was concentrated and the residue was purified via column chromatography (5-10% EtOAc/hexanes) to give 21 mg (55%) of ketones **15a** and **15b**. Data was consistent with reported values.³



The same procedure used to prepare the formal [4C+ 3C] cycloaddition product **4f** and triene aldehyde **11** was used to prepare **A** and **B**.

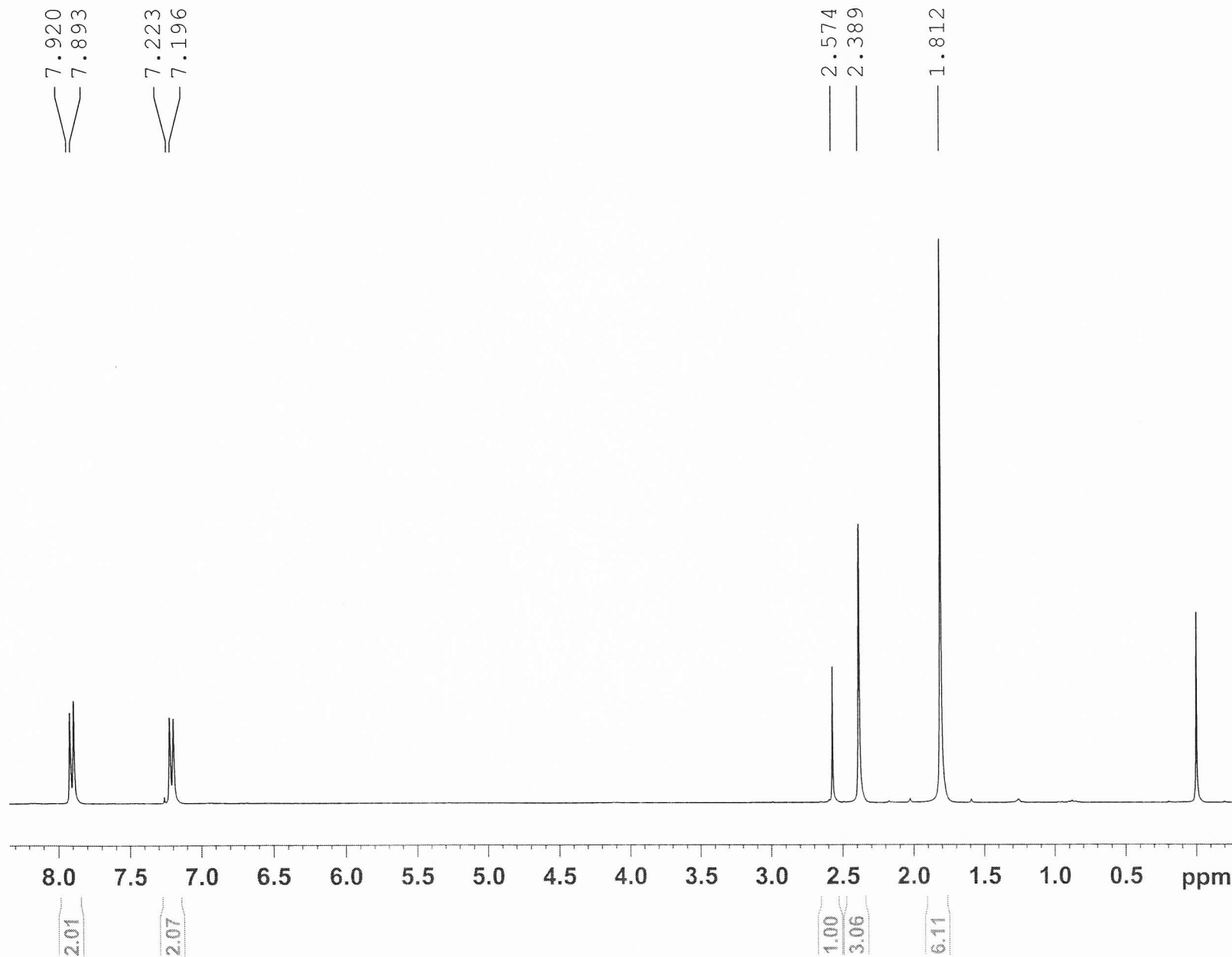
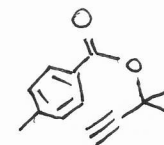
Formal [4C + 3C] Cycloadduct A. A colorless oil (13 mg, 41 μmol , 20 % yield). ¹HNMR (500 MHz, CDCl₃): δ 2.33 (3H, s), 4.48 (1H, d, J = 6.0 Hz), 5.01 (1H, d, J = 4.5 Hz), 5.13 (1H, d, J = 6.0 Hz), 5.60 (1H, d, J = 5.5 Hz), 6.35 (1H, d, J = 4.5 Hz), 6.70 (1H, d, J = 5.5 Hz), 7.10 (2H, d, J = 8.0 Hz), 7.13-7.26 (5H, m), 7.63 (2H, d, J = 8.0 Hz). ¹³C NMR (125 MHz, CDCl₃): δ 21.6, 47.6, 75.9, 82.5, 119.1, 126.8, 127.0, 127.1, 128.3, 128.9, 129.0, 129.8, 134.0, 139.2, 143.9, 146.5, 164.5.

Triene Aldehyde B. A yellow solid (38 mg, 0.12 mmol, 60 % yield, a mixture of *cis* and *trans* isomers). Data is given for the major product, the *trans* isomer. ¹HNMR (300 MHz, CDCl₃): δ 2.49 (3H, s), 6.13 (1H, dd, J = 15.0, 7.8 Hz), 6.45 (1H, dd, J = 15.0, 11.1 Hz), 6.56 (1H, s), 6.79 (1H, d, J = 15.0 Hz), 7.24-7.28 (4H, m), 7.37 (2H, d, J = 7.8 Hz), 7.49-7.52 (2H, m), 8.13 (2H, d, J = 8.1 Hz), 9.58 (1H, d, J = 8.1 Hz).

References

1. K. Miki, K. Ohe, S. Uemura, *J. Org. Chem.*, 2003, **68**, 8505.
2. N.J. Turro, S.S. Edelson, J.R. Williams, T.R. Darling, W.B. Hammond, *J. Am. Chem. Soc.*, 1969, **91**, 2283.
3. T.H. Chan, M. P. Li, W. Mychajlowskij, D.N.Harpp, *Tetrahedron Lett.*, 1974, **39**, 3511.

2-112 Pure



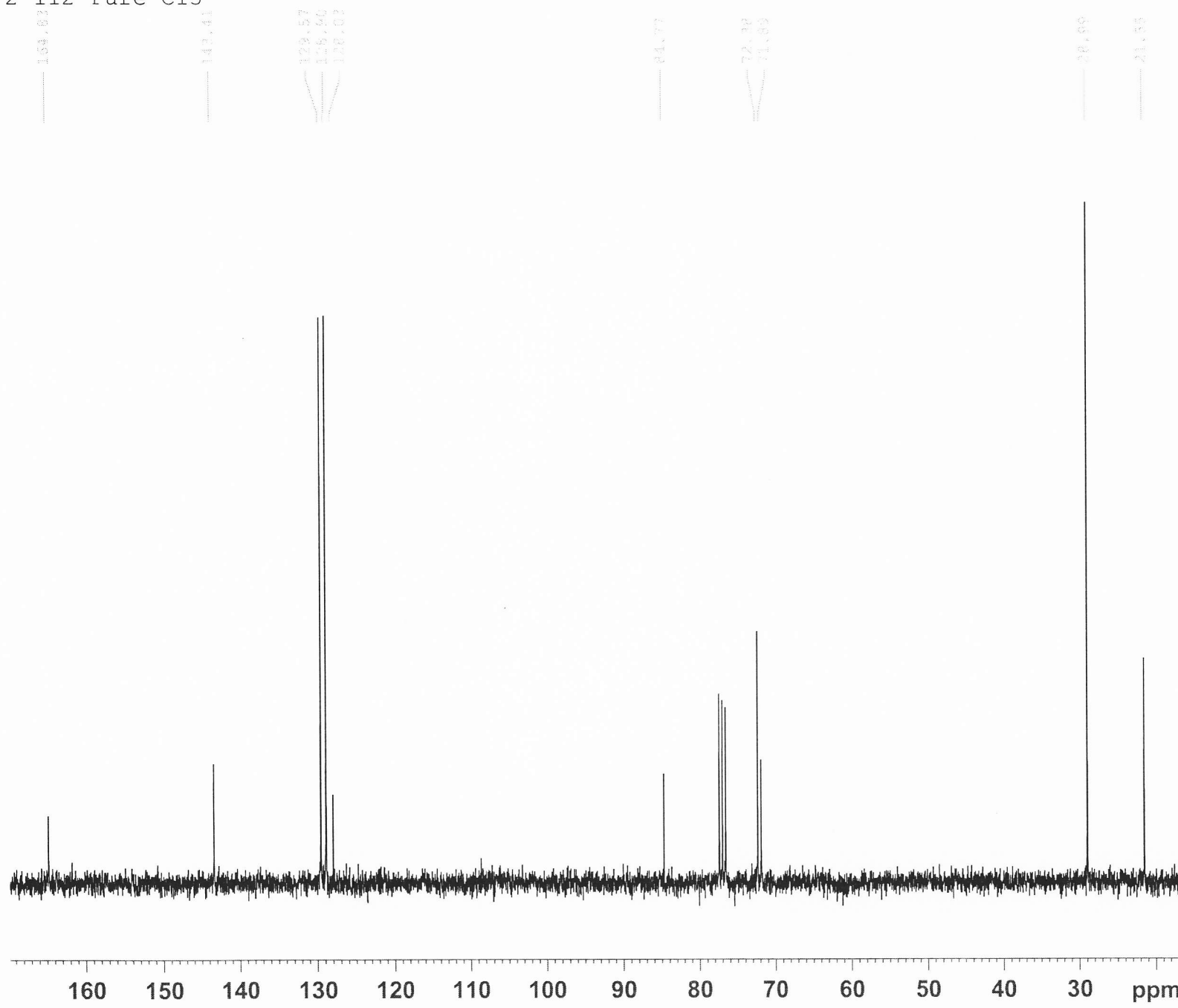
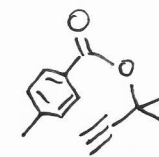
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2-112 Pure C13



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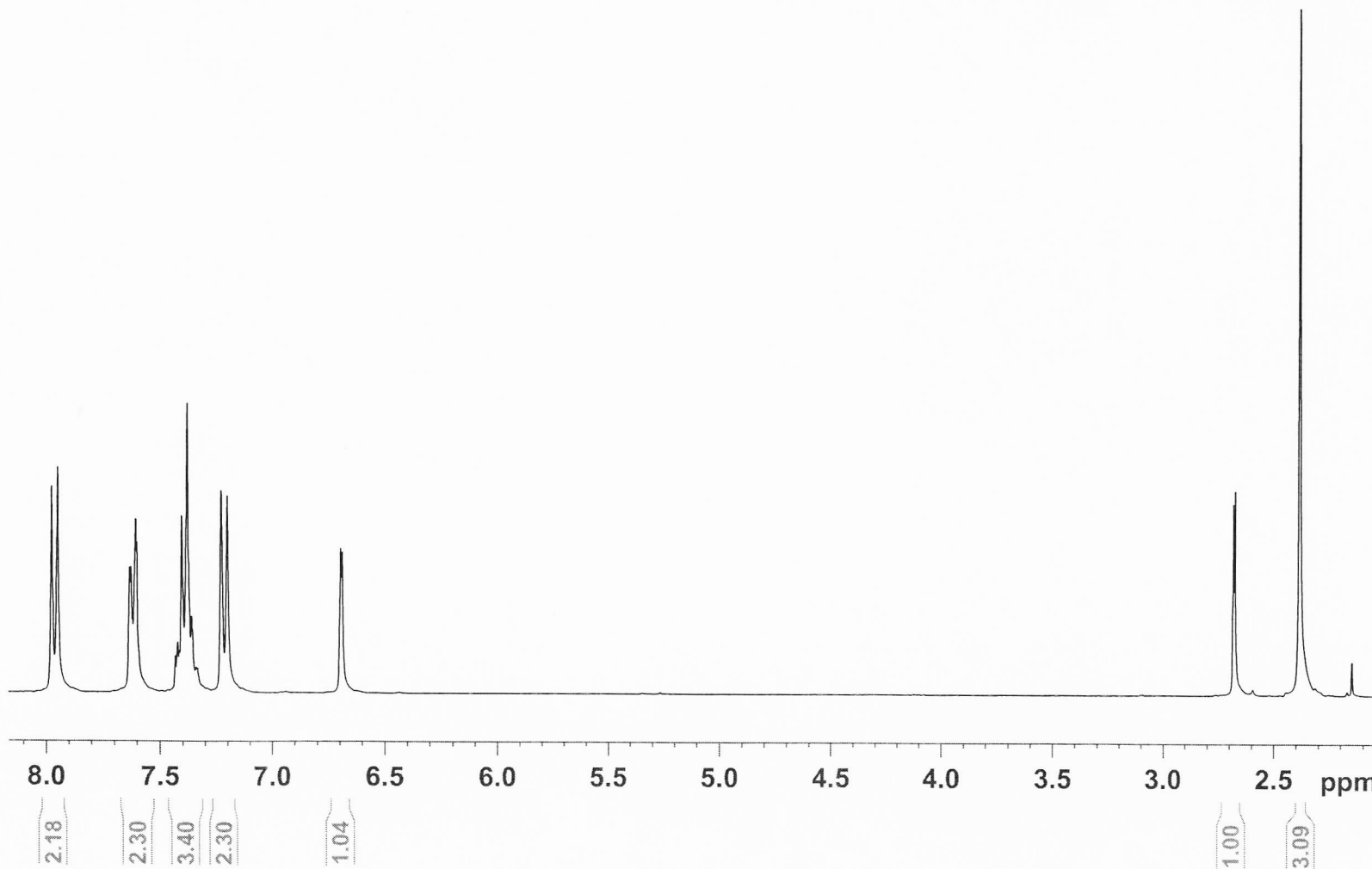
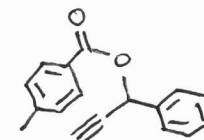
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3-2ndary tolyl derivative

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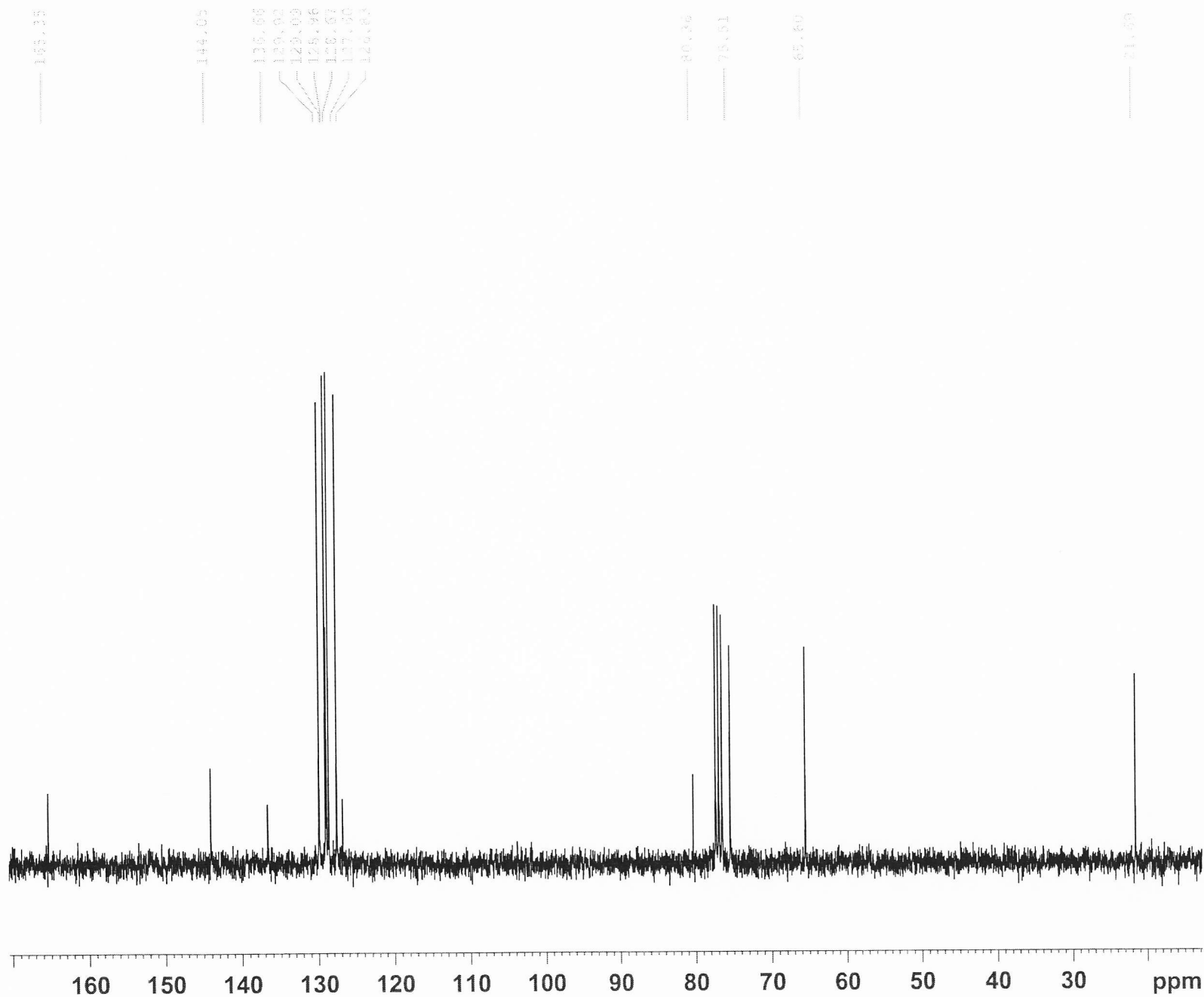
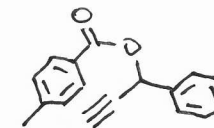
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2ndary tolyl derivative



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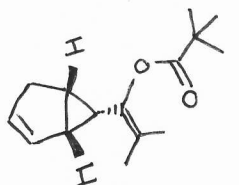
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PL13       26.00 dB
SFO2       300.1312005 MHz

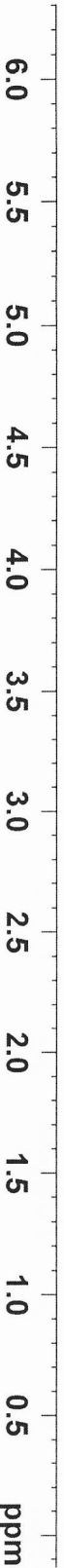
F2 - Processing parameters
SI         16384
SF         75.4677533 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

2-99 Pure B



5.681
5.677
5.672
5.666
5.661
5.657
5.455
5.449
5.444

2.529
2.519
2.515
2.493
2.479
2.270
2.267
2.234
2.231
2.159
2.154
2.148
2.142
2.139
2.133
2.127
2.123
1.985
1.969
1.954
1.861
1.847
1.833
1.818
1.788
1.737
1.735
1.584
1.510
1.506
1.265



1.00
1.02

1.02

1.02

1.00

1.02

1.02

3.04

0.71

3.06

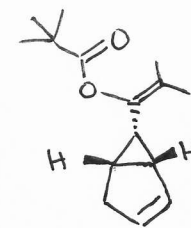
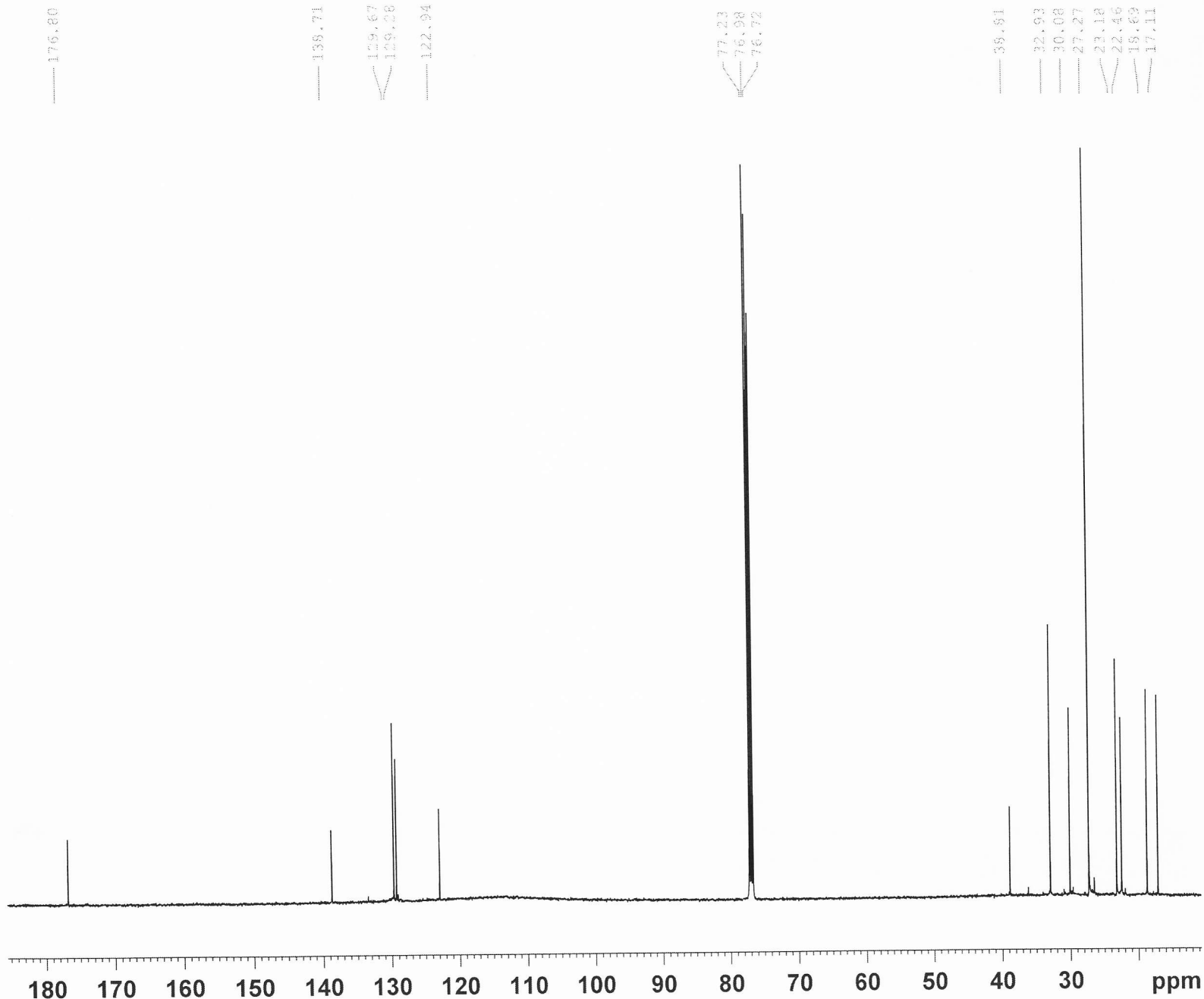
9.78

```

NAME          1mb2-99pureB
EXPNO         1
PROCNO       20090513
Date_        16-02-2009
INSTRUM      spect
PROBHD       5 mm TXI 1H-13
PULPROG      zg30
TD           32768
SOLVENT      CDCl3
NS           16
DS           2
SWH          6510.417 Hz
FIDRESS      0.130682 Hz
RG           2.514718 sec
AQ           77.18 sec
DE           76.800 usec
TE           7.50 usec
TD0          296.2 K
D1           1.00000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1           6.70 usec
PL1          0.00 dB
PL1M         15.07131863 W
SFO1         500.130008 MHz
SI           16384
SF           500.1300115 MHz
WDW          EM
SSB          0
GB           0.30 Hz
PC           1.00
  
```

2-99 Pure B C13

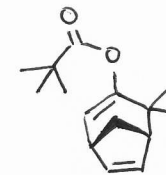


```
NAME      lnb2-99pureB
EXPNO     2
PROCNO    1
Date_     20090516
Time      9.02
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS        21000
DS        4
SWH       30303.031 Hz
FIDRES    0.924775 Hz
AQ        0.5407385 sec
RG        3649.1
DW        16.500 usec
DE        7.50 usec
TE        296.8 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
```

```
===== CHANNEL f1 =====
NUC1      13C
P1        12.20 usec
PL1       -3.00 dB
PL1W      190.45114136 W
SF01      125.7726284 MHz
```

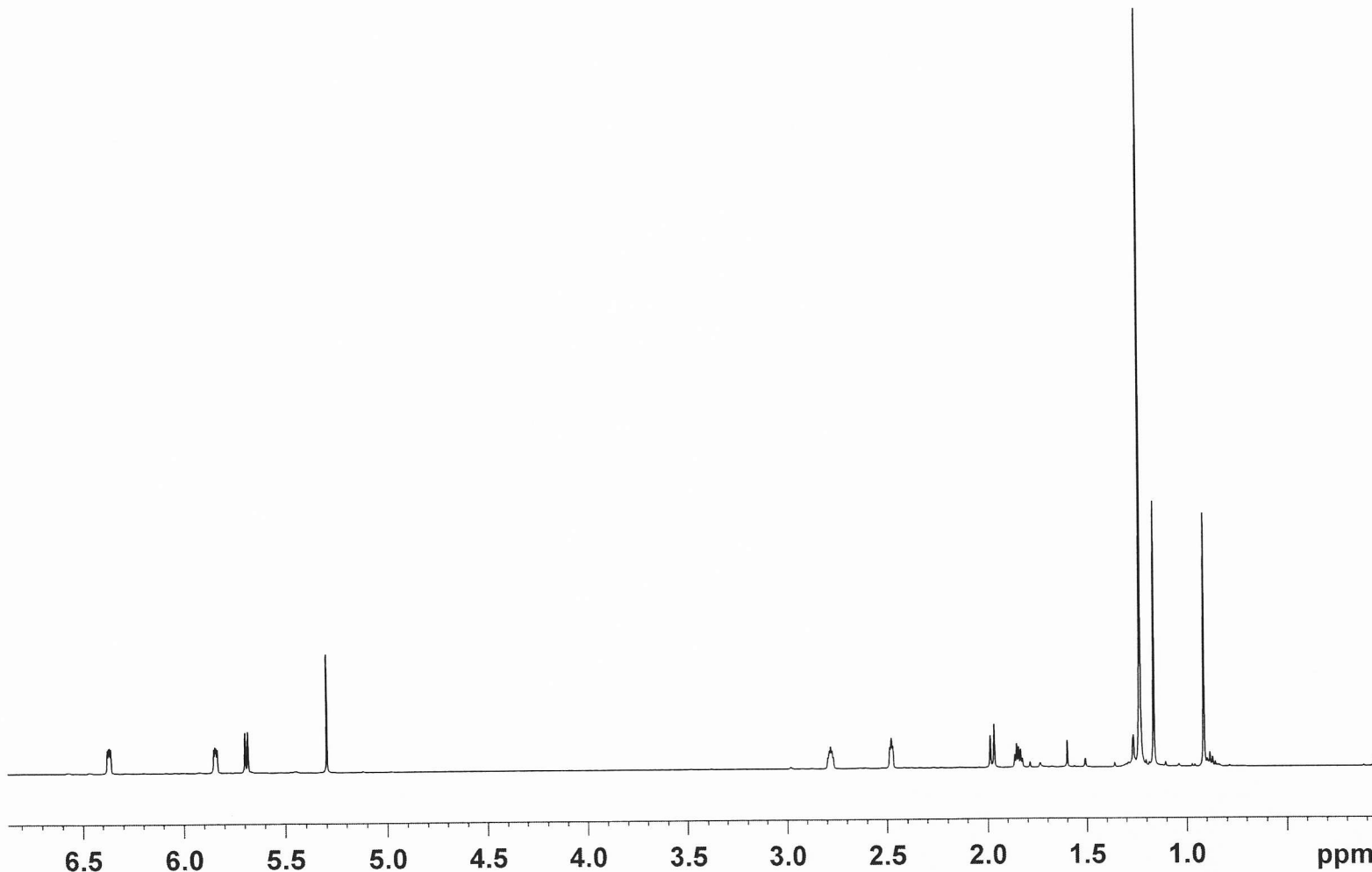
```
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        0.00 dB
PL12       23.48 dB
PL13       25.00 dB
PL2W      15.07131863 W
PL12W     0.06763186 W
PL13W     0.04765970 W
SFO2      500.1320005 MHz
SI        16384
SF        125.7577920 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

2-101 B Pure



6.377
6.371
6.365
6.360
5.851
5.845
5.840
5.834
5.697
5.684
5.299

2.796
2.789
2.782
2.775
2.769
2.486
2.478
2.471
1.987
1.968
1.863
1.854
1.844
1.834
1.825
1.600
1.508
1.269
1.265
1.235
1.166
0.915
0.898
0.884



1.00

1.02

1.03

1.02

1.05

1.11

1.09

9.18

3.09

3.06

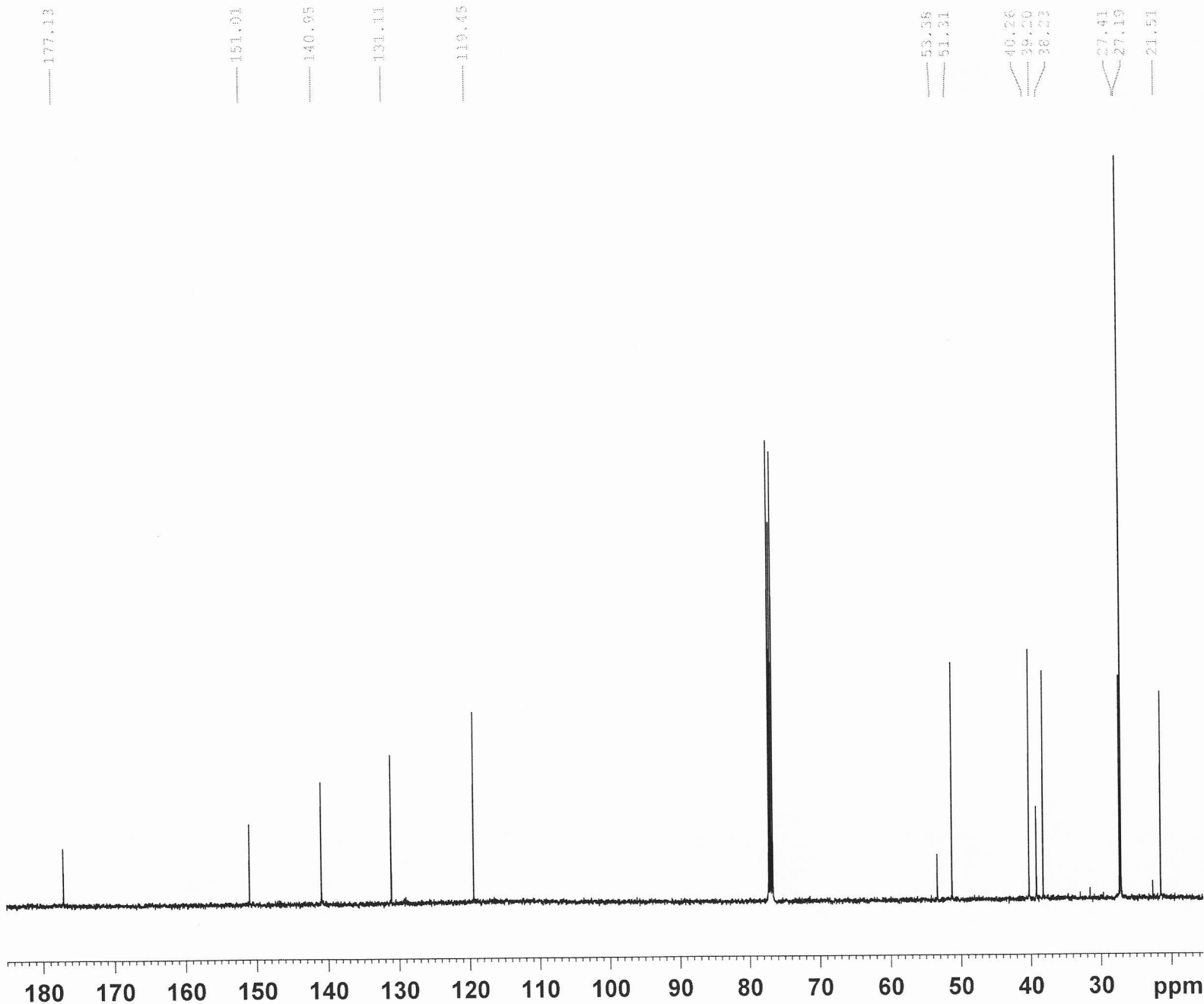
```

NAME      lnb2-101B Pure
EXPNO     1
PROCNO    1
Date_     20090520
Time      14.57
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        6510.417 Hz
FIDRES     0.198682 Hz
AQ         2.5167091 sec
RG         40.3
DW         76.800 usec
DE         7.50 usec
TE         298.1 K
D1         1.00000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        6.70 usec
PL1       0.00 dB
PL1W      15.07131863 W
SF01      500.1330008 MHz
SI        16384
SF        500.1300110 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

2-101 B Pure C13

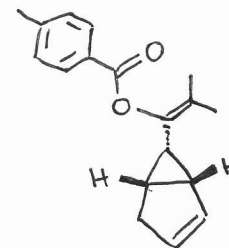


NAME lnb2-101B Pure
EXPNO 2
PROCNO 1
Date_ 20090520
Time_ 15.55
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 1023
DS 4
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 812.7
DW 16.500 usec
DE 7.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

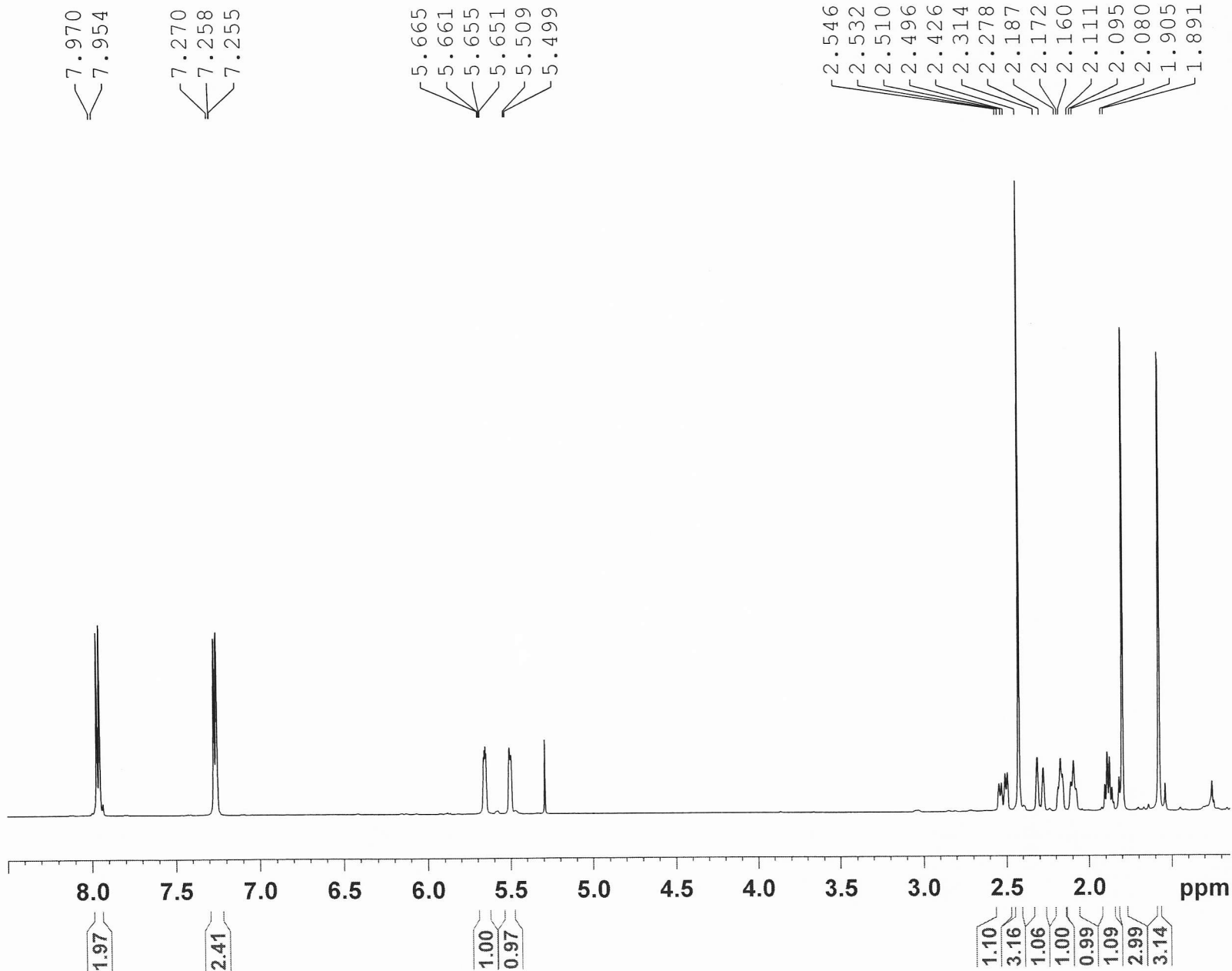
===== CHANNEL f1 =====
NUC1 13C
P1 12.20 usec
PL1 -3.00 dB
PL1W 190.45114136 W
SFO1 125.7726284 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 23.48 dB
PL13 25.00 dB
PL2W 15.07131863 W
PL12W 0.06763186 W
PL13W 0.04765970 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577909 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

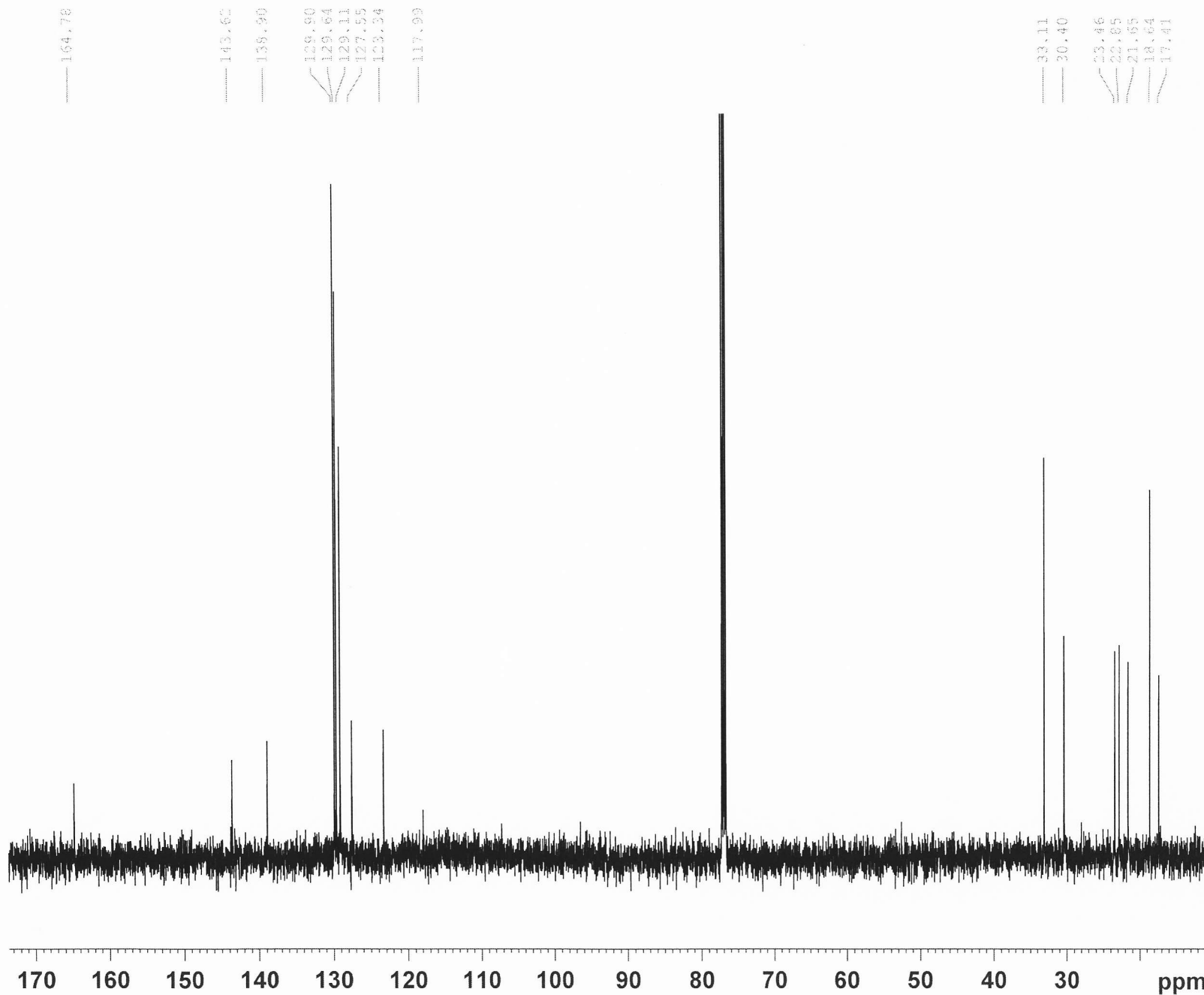
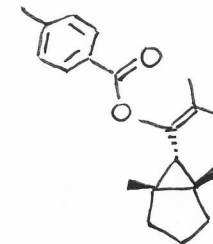
3-23 Pure B



```
NAME      lnb3-23pureB
EXPNO     1
PROCNO    1
Date_     20091026
Time_     9.47
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
NS        16
DS        2
SWH       6510.417 Hz
FIDRES    0.198682 Hz
AQ        2.5167091 sec
RG        71.8
DW        76.800 usec
DE        7.50 usec
TE        296.9 K
D1        1.0000000 sec
TDO       1
===== CHANNEL f1 =====
NUC1      1H
P1        6.70 usec
PL1       0.00 dB
PL1W      15.07131863 W
SFO1      500.1330008 MHz
SI        16384
SF        500.1300142 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



3-23 Pure B C13



NAME lnb3-23pureB
EXPNO 2
PROCNO 1
Date_ 20091026
Time 10.00
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 203
DS 4
SWH 30303.031 Hz
FIDRES 0.924775 Hz
AQ 0.5407385 sec
RG 14596.5
DW 16.500 usec
DE 7.50 usec
TE 297.7 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 12.20 usec
PL1 -3.00 dB
PL1W 190.45114136 W
SFO1 125.7726284 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 23.48 dB
PL13 25.00 dB
PL2W 15.07131863 W
PL12W 0.06763186 W
PL13W 0.04765970 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577913 MHz
WDSB 0
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

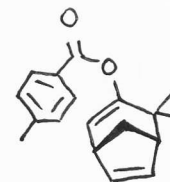
3-37 Pure A

7.950
7.934

7.250
7.234

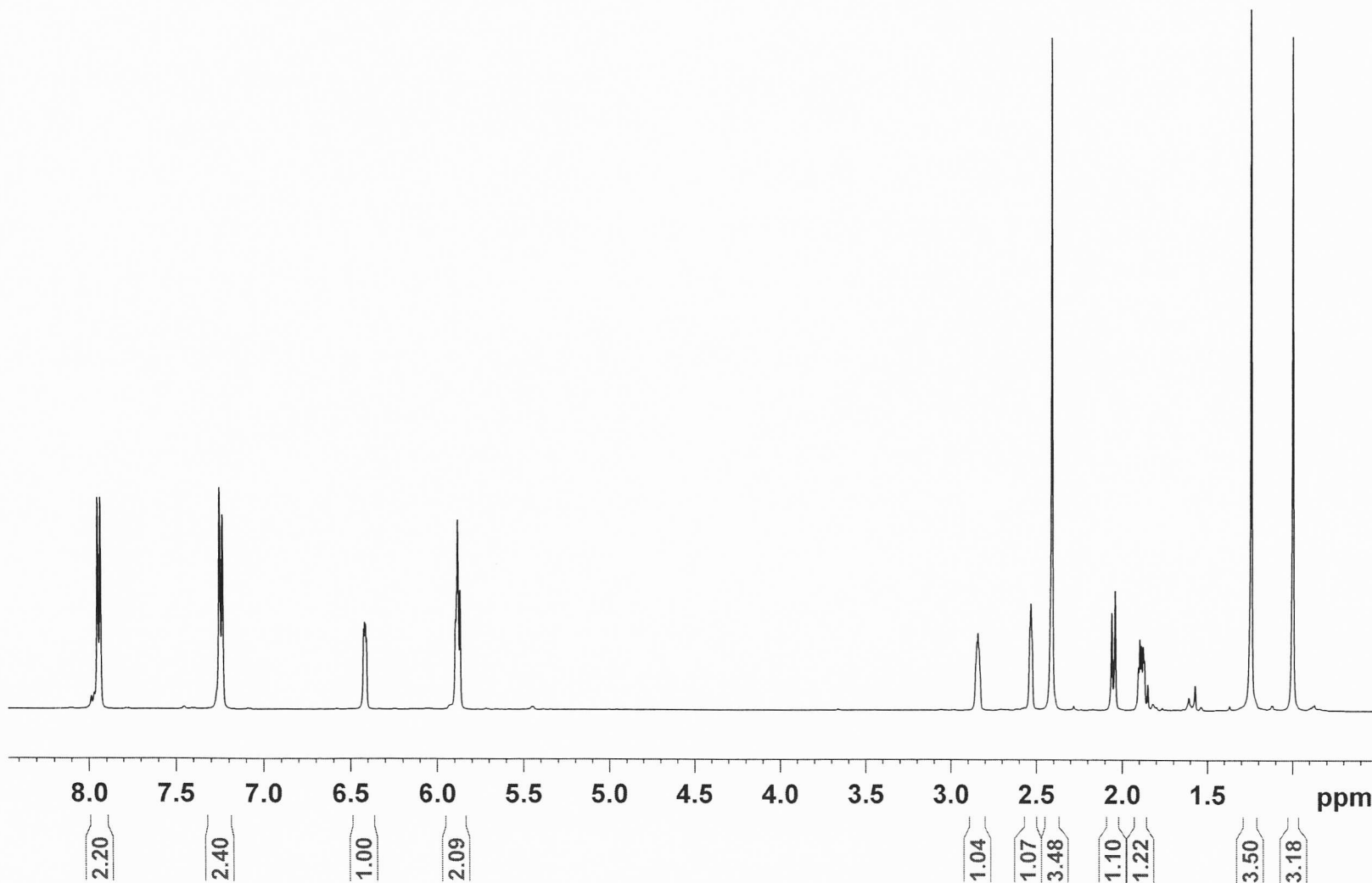
6.423
6.418
6.412
6.407
5.894
5.882
5.868

2.843
2.533
2.410
2.061
2.042
1.907
1.898
1.889
1.878
1.245
0.999

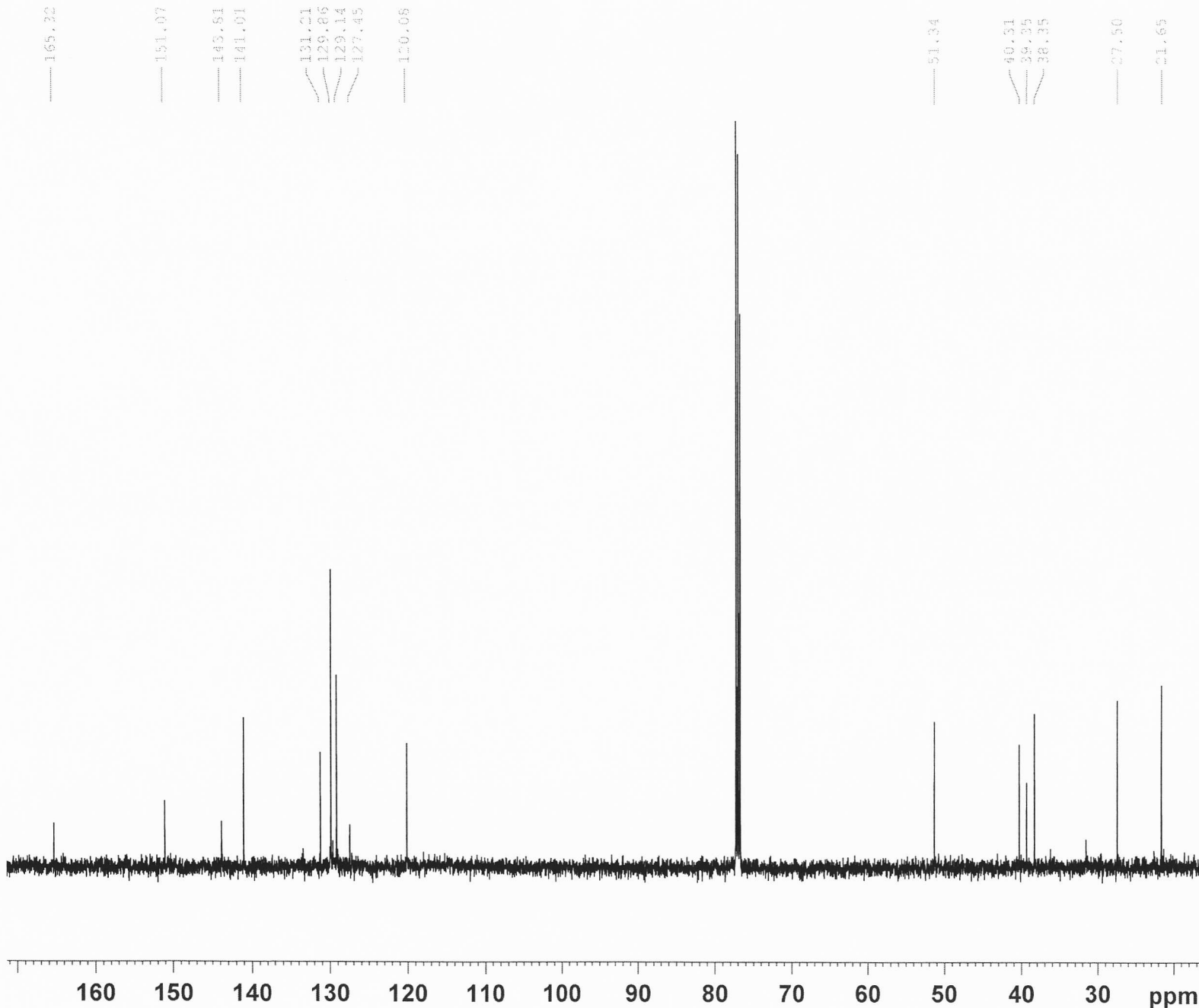
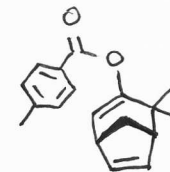


NAME lnb3-37pureA
EXPNO 1
PROCNO 1
Date_ 20091112
Time_ 16.35
INSTRUM spect
PROBHD 5 mm TXI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6510.417 Hz
FIDRES 0.198682 Hz
AQ 2.5167091 sec
RG 40.3
DW 76.800 usec
DE 7.50 usec
TE 297.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.70 usec
PL1 0.00 dB
PL1W 15.07131863 W
SF01 500.1330008 MHz
SI 16384
SF 500.1300158 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3-23 Pure A C13



```

NAME      lnb3-23pureA
EXPNO     2
PROCNO    1
Date_     20091026
Time      9.38
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         199
DS         4
SWH       30303.031 Hz
FIDRES    0.924775 Hz
AQ         0.5407385 sec
RG         8192
DW         16.500 usec
DE         7.50 usec
TE         297.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
    
```

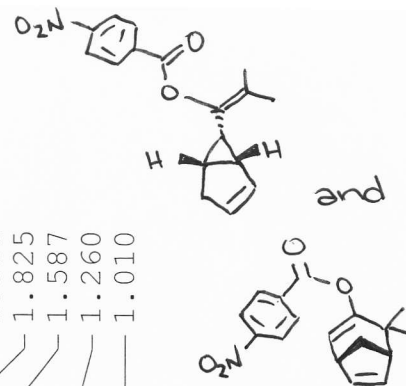
```

===== CHANNEL f1 =====
NUC1      13C
P1        12.20 usec
PL1       -3.00 dB
PL1W      190.45114136 W
SFO1      125.7726284 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        0.00 dB
PL12       23.48 dB
PL13       25.00 dB
PL2W       15.07131863 W
PL12W      0.06763186 W
PL13W      0.04765970 W
SFO2       500.1320005 MHz
SI         16384
SF         125.7577909 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

3-51 B Pure



8.349
8.305
8.259
8.214

7.265

6.423

5.957
5.922
5.613
5.539

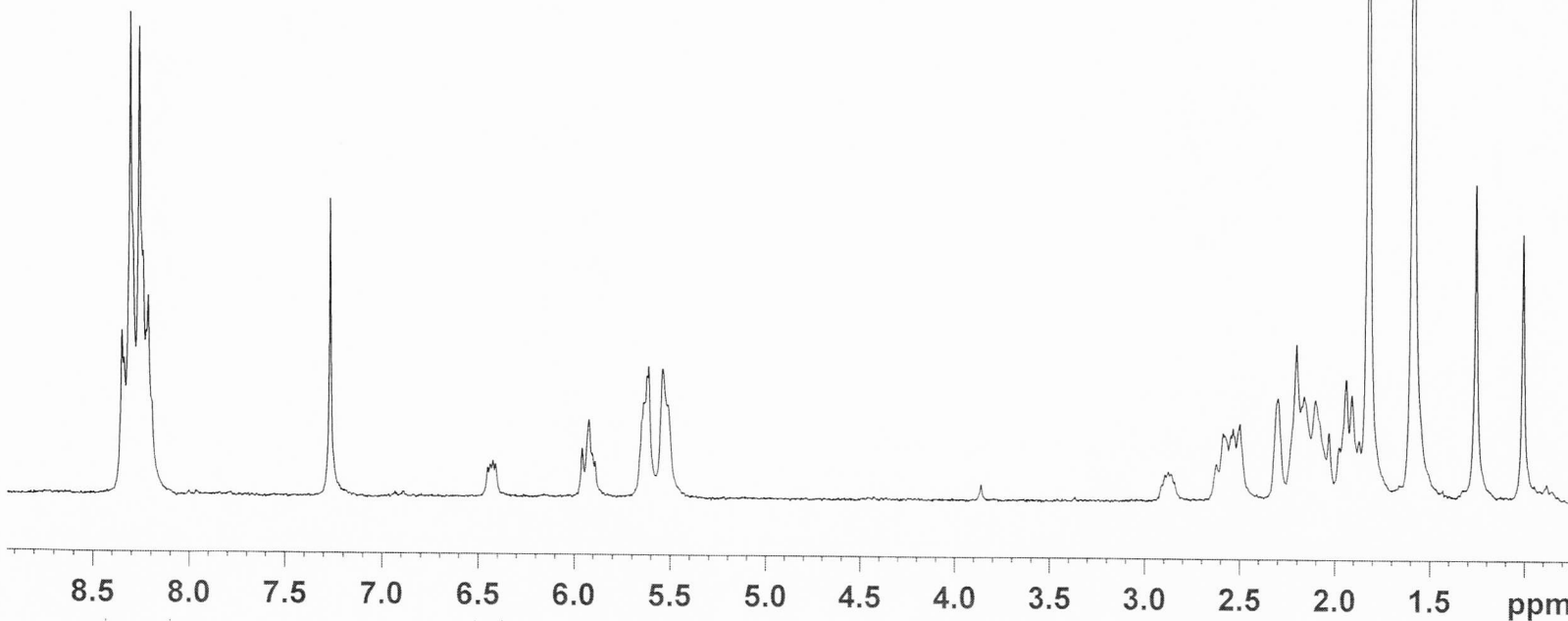
2.877
2.501
2.299
2.205
2.103
2.031
1.942
1.911
1.825
1.587
1.260
1.010

Current Data Parameters
NAME lnb3-51Bpure
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091215
Time 17.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 2604.167 Hz
FIDRES 0.079473 Hz
AQ 6.2915058 sec
RG 1824.6
DW 192.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.30 usec
PL1 -6.00 dB
SF01 200.1312008 MHz

F2 - Processing parameters
SI 16384
SF 200.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



19.10

1.00

2.15

3.32

4.02

1.13

4.79

12.13

4.77

11.80

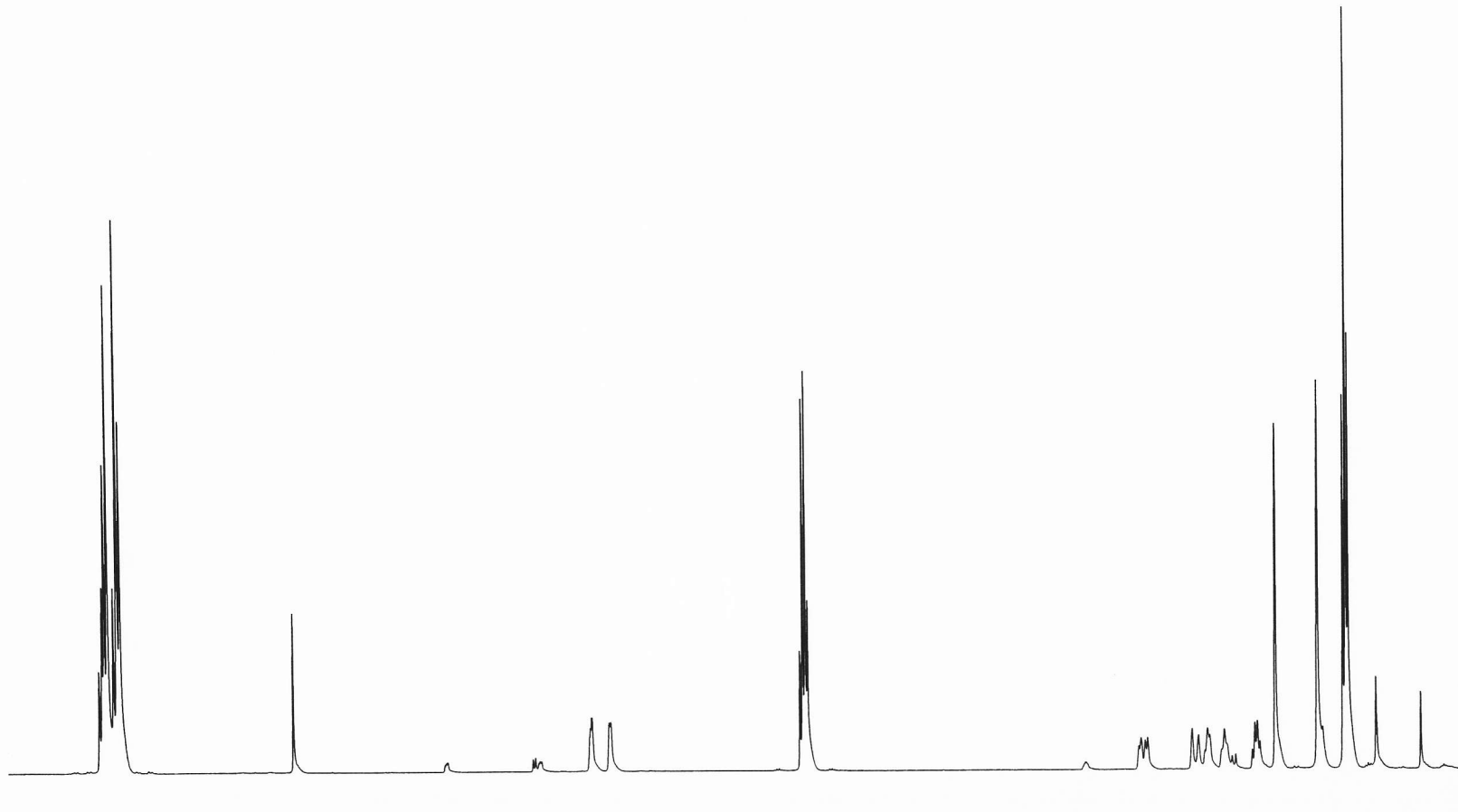
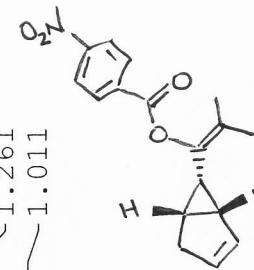
13.67

4.45

3.39

2-116 Pure AB

8.326
8.309
8.298
8.280
8.247
8.227
8.209
5.949
5.936
5.901
5.636
5.632
5.625
5.621
5.528
5.518
4.462
4.448
4.434
4.420
2.876
2.578
2.565
2.543
2.529
2.282
2.245
2.210
2.195
2.183
2.117
2.103
2.089
2.061
2.041
1.948
1.934
1.919
1.906
1.822
1.589
1.559
1.447
1.433
1.419
1.261
1.011



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

7.15
8.43
0.16
0.35
0.98
1.00
5.64
0.15
1.18
0.94
1.06
1.17
1.21
3.02
4.09
8.55
0.72
0.53

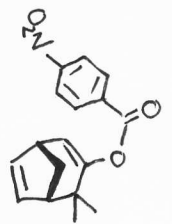
```

NAME      lnb2-116pureAB
EXPNO     1
PROCNO    1
Date_     20090612
Time      12.05
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zg30
TD         32768
SOLVENT   CDC13
NS         16
DS         2
SWH        6510.417 Hz
FIDRES     0.198682 Hz
AQ         2.5167091 sec
RG         90.5
DW         76.800 usec
DE         7.50 usec
TE         297.7 K
D1         1.0000000 sec
TDD        1
  
```

```

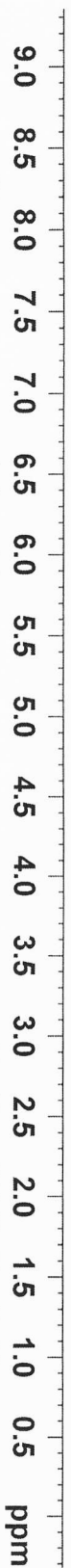
===== CHANNEL f1 =====
NUC1      1H
P1        6.70 usec
PL1       0.00 dB
PL1W      15.07131863 W
SFO1      500.1330008 MHz
SI        16384
SF        500.1300102 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

3-57 Pure



- 8.313
- 8.296
- 8.277
- 8.273
- 8.267
- 8.259
- 8.248
- 8.242
- 8.228
- 8.211
- 7.267
- 6.436
- 6.431
- 6.425
- 6.420
- 5.951
- 5.937
- 5.918
- 5.912
- 5.907
- 5.902

- 2.889
- 2.883
- 2.876
- 2.870
- 2.577
- 2.570
- 2.174
- 2.062
- 2.042
- 1.936
- 1.927
- 1.918
- 1.908
- 1.899
- 1.873
- 1.838
- 1.825
- 1.606
- 1.593
- 1.584
- 1.550
- 1.262
- 1.012



1.94
1.98

1.00

2.04

0.93

1.08

0.60

1.01

1.44

0.86

1.06

2.89

2.96

```

NAME          Inb3-57pure
EXNO          1
PROCNO       20100104
Date         17.13
Time         17.13
INSTRUM      spect
PROBHD       5 mm TXI 1H-13
PULPROG      zg30
TD           32768
SOLVENT      CDCl3
NS           16
DS           2
SWH          6510.417 Hz
FIDRES       0.198682 Hz
AQ           2.5167091 sec
RG           71.8
DM           76.800 usec
DE           23.30 usec
TE           298.2 K
DT           1.00000000 sec
TDO          1
===== CHANNEL F1 =====
NUC1          1H
PI           6.70 usec
PL1          0.00 dB
PL1W         15.07131863 W
SFO1         500.1330008 MHz
SI           16384
SF           500.1300092 MHz
WDW          EM
SSB          0
LB           0
GB           0
PC           1.00
  
```

3-42 E Pure

8.010
7.992

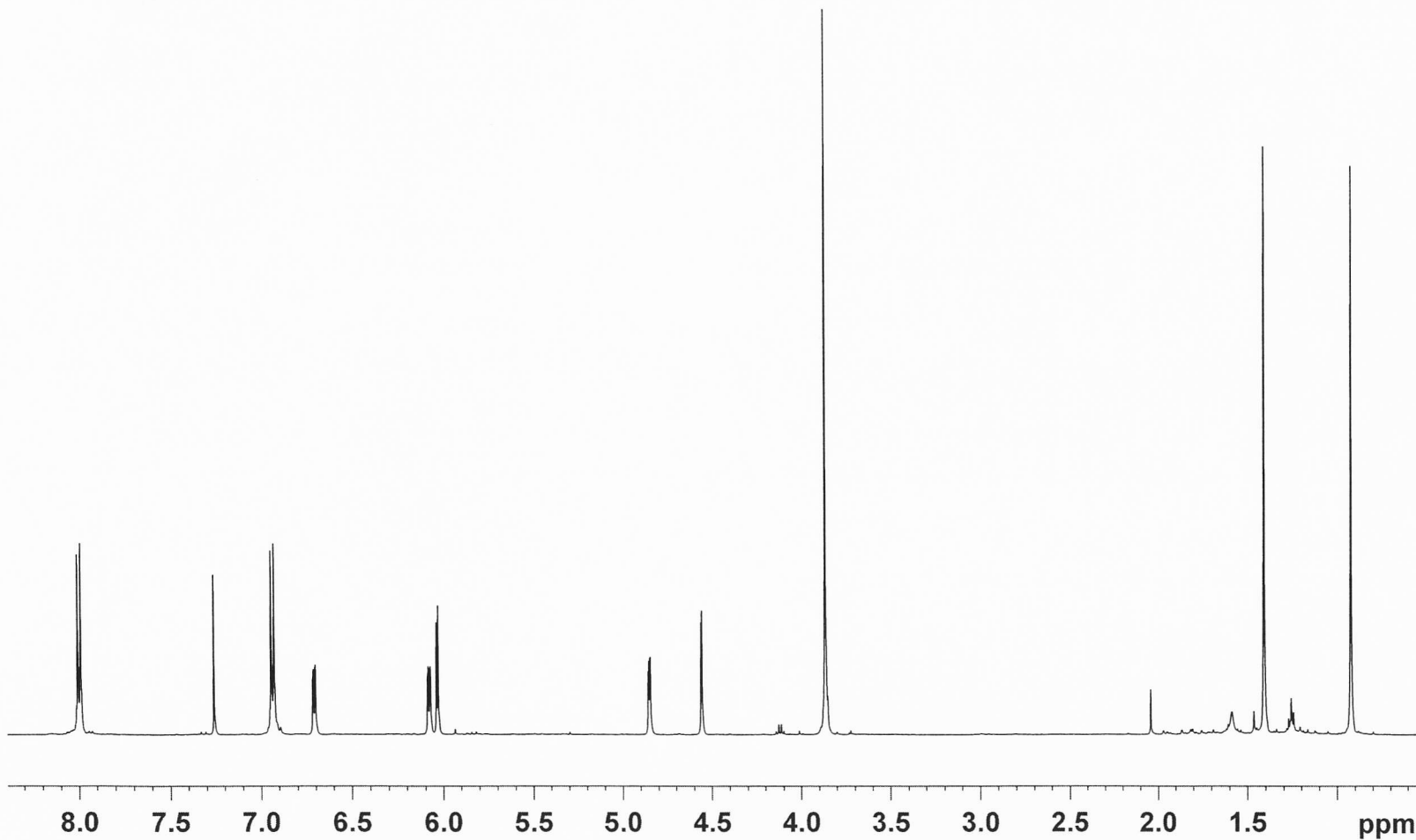
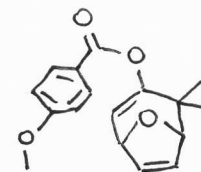
6.947
6.929
6.719
6.716
6.707
6.704
6.090
6.086
6.078
6.074
6.040
6.031

4.859
4.856
4.850
4.847
4.564
4.560

3.871

1.412

0.927



2.18

2.29

0.97

1.02

1.00

1.00

0.99

3.24

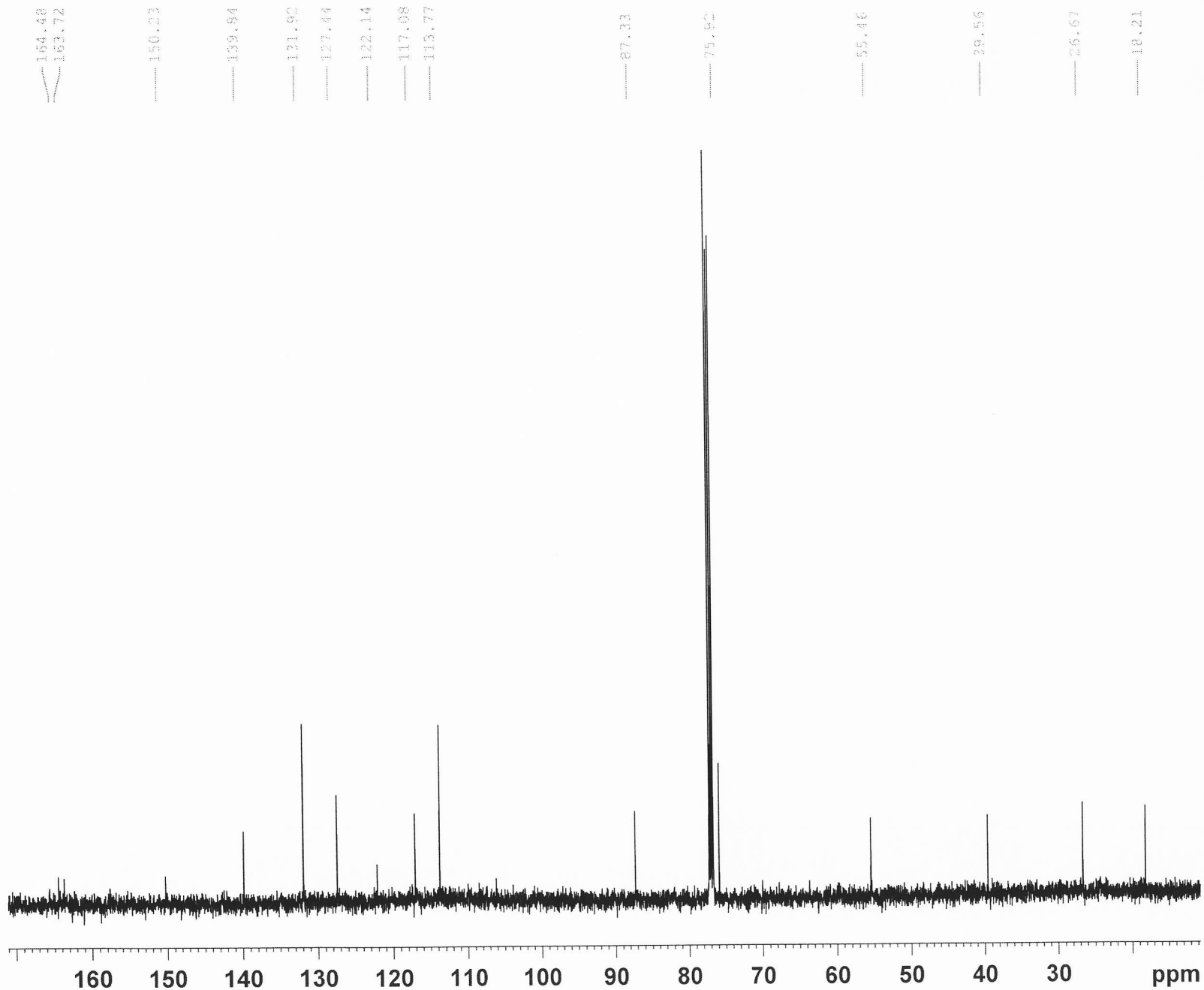
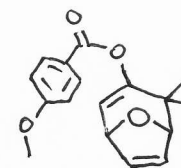
3.18

```

NAME      lnb3-42Epure
EXPNO     1
PROCNO    1
Date_     20091201
Time      9.26
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        6510.417 Hz
FIDRES     0.198682 Hz
AQ         2.5167091 sec
RG         90.5
DW         76.800 usec
DE         7.50 usec
TE         296.8 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1         6.70 usec
PL1        0.00 dB
PL1W      15.07131863 W
SFO1      500.1330008 MHz
SI         16384
SF         500.1300127 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

3-42 E Pure C13



```

NAME      lnb3-42Epure
EXPNO     2
PROCNO    1
Date_     20091201
Time      9.51
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zgpg30
TD        32768
SOLVENT   CDCl3
NS        224
DS        4
SWH       30303.031 Hz
FIDRES    0.924775 Hz
AQ        0.5407385 sec
RG        8192
DW        16.500 usec
DE        7.50 usec
TE        297.3 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
    
```

```

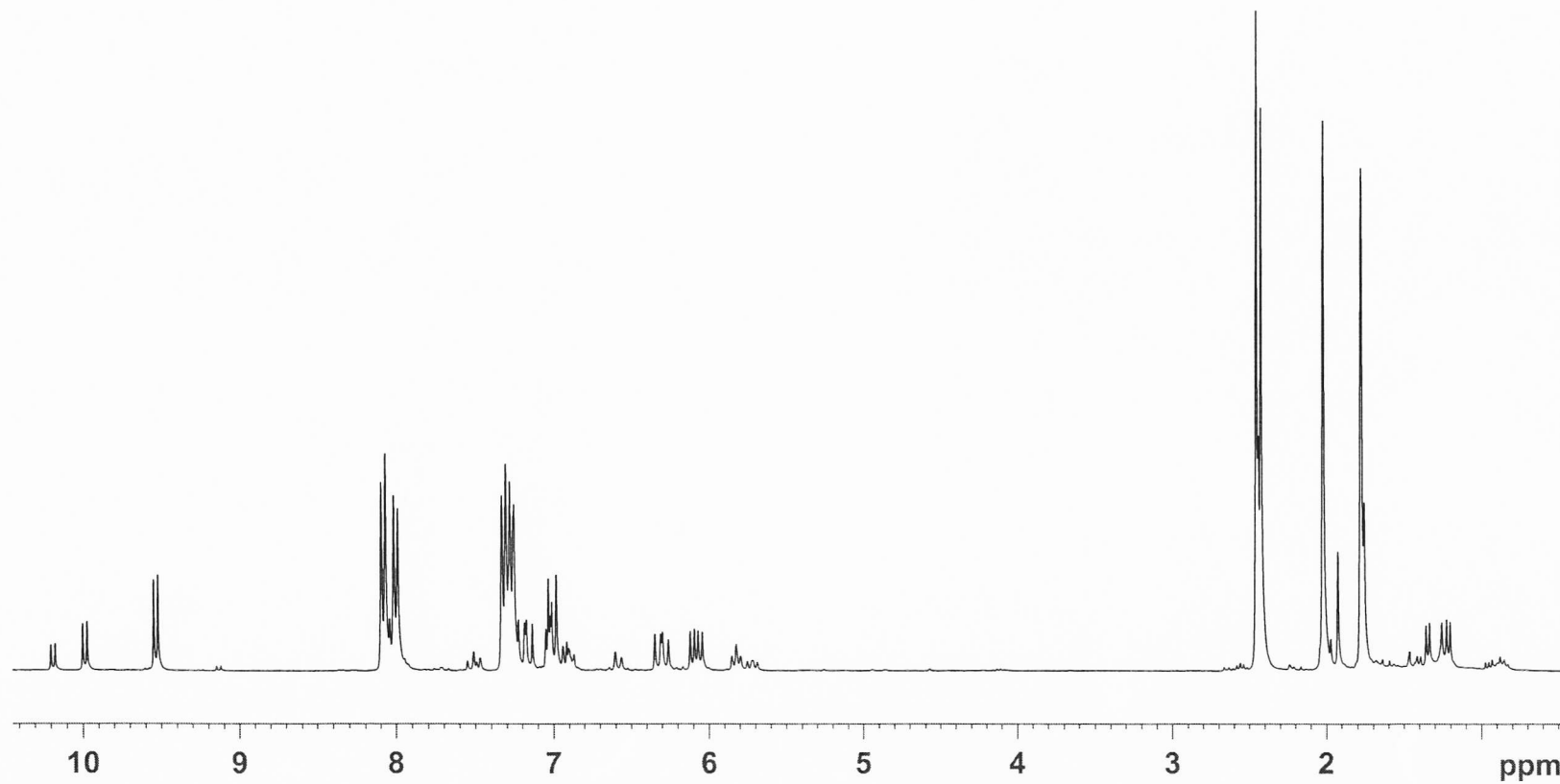
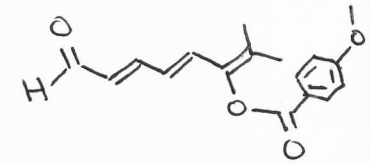
===== CHANNEL f1 =====
NUC1      13C
P1        12.20 usec
PL1       -3.00 dB
PL1W      190.45114136 W
SFO1      125.7726284 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        0.00 dB
PL12       23.48 dB
PL13       25.00 dB
PL2W      15.07131863 W
PL12W     0.06763186 W
PL13W     0.04765970 W
SFO2      500.1320005 MHz
SI        16384
SF        125.7577907 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

3-55 Pure DEF

10.173
10.002
9.975
9.551
9.525
8.098
8.071
8.043
8.018
7.991
7.335
7.309
7.282
7.261
7.255
7.226
7.188
7.175
7.138
7.051
7.035
7.022
7.013
6.985
6.918
6.349
6.311
6.300
6.262
6.122
6.095
6.071
6.045
5.826
2.456
2.442
2.426
2.026
1.974
1.927
1.780
1.760
1.359
1.336
1.257
1.227
1.204



0.28
0.50
1.00
3.01
3.18
0.38
6.55
1.51
2.10
0.80
0.31
1.03
1.12
0.50
0.30
9.65
4.84
0.88
5.50
0.69
1.33

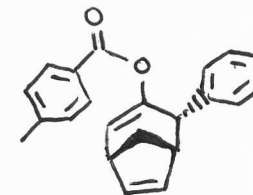
Current Data Parameters
NAME lnb3-55pureDEF
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091221
Time 10.39
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 3894.061 Hz
FIDRES 0.118838 Hz
AQ 4.2075896 sec
RG 80.6
DW 128.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

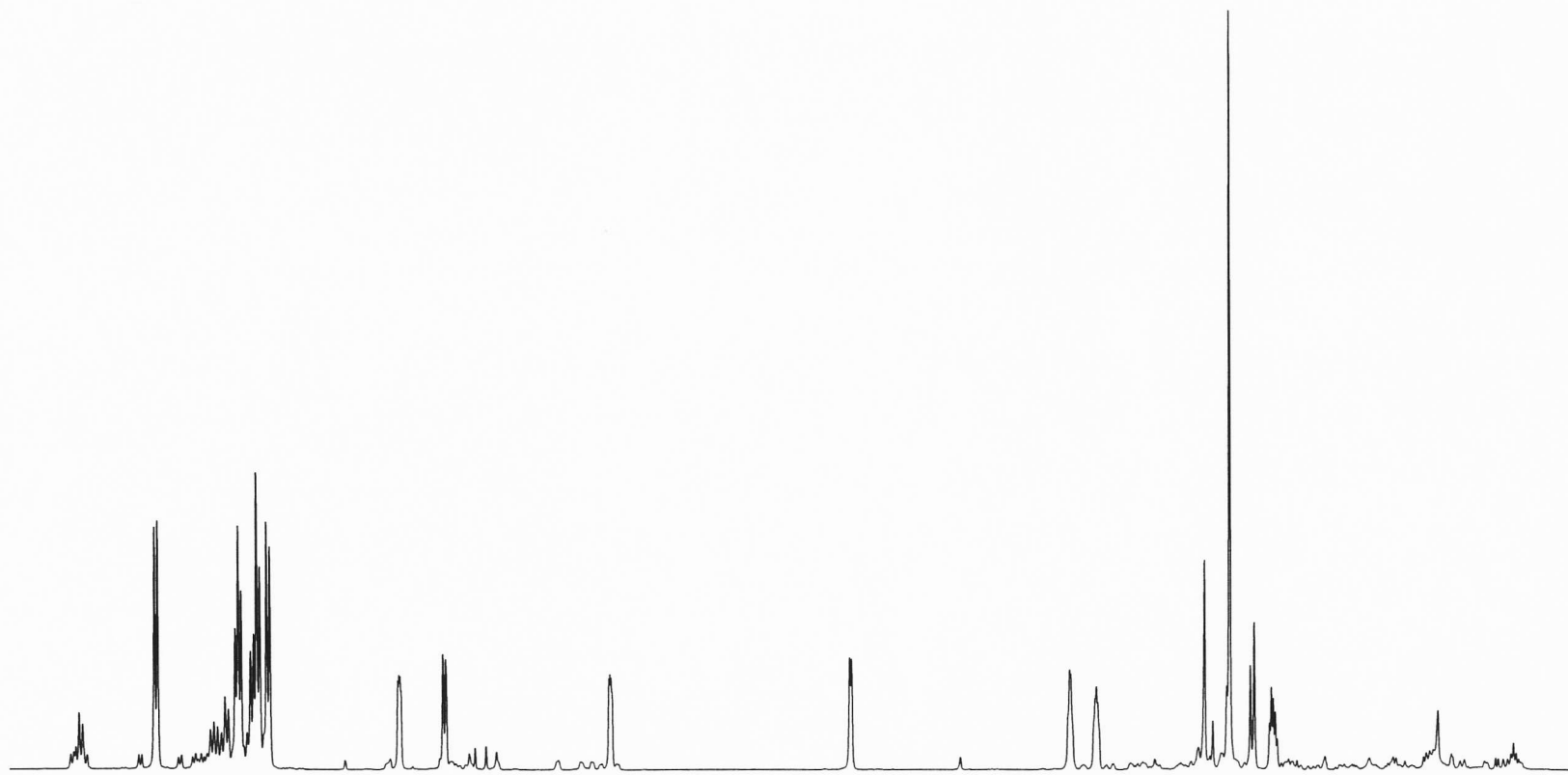
===== CHANNEL f1 =====
NUC1 1H
P1 6.40 usec
PL1 4.00 dB
SFO1 300.1318006 MHz

F2 - Processing parameters
SI 16384
SF 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3-46 Pure



8.020
8.010
7.993
7.976
7.624
7.608
7.228
7.213
7.199
7.139
7.125
7.109
7.076
7.060
6.434
6.429
6.424
6.419
6.214
6.199
5.394
5.389
5.384
5.379
4.196
4.186
3.092
3.087
2.964
2.958
2.952
2.421
2.380
2.310
2.296
2.194
2.175
2.098
2.090
2.080
2.071
1.316
1.299
1.281
1.258
0.880
0.867



8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm

0.83
0.14
2.08
0.13
2.04
2.60
3.56
2.27
1.00
1.05
1.00
1.03
1.14
1.03
1.12
3.40
1.14
1.05
1.01
0.59

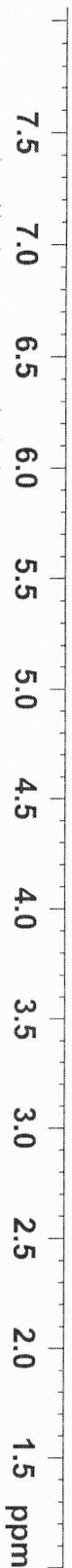
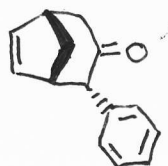
```
NAME      lnb3-46pure
EXPNO     1
PROCNO    1
Date_     20091208
Time      14.14
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zg30
TD         32768
SOLVENT   CDC13
NS         16
DS         2
SWH        6510.417 Hz
FIDRES     0.198682 Hz
AQ         2.5167091 sec
RG         32
DW         76.800 usec
DE         7.50 usec
TE         297.0 K
D1         1.00000000 sec
TD0        1
```

```
===== CHANNEL f1 =====
NUC1       1H
P1         6.70 usec
PL1        0.00 dB
PL1W       15.071331863 W
SFO1       500.1330008 MHz
SI         16384
SF         500.1300287 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

3-50c Pure

7.327
7.305
7.279
7.260
7.253
7.237
7.213
7.078
7.054
6.213
6.204
6.194
6.186
6.088
6.079
6.069
6.061

3.751
3.741
2.994
2.986
2.977
2.602
2.590
2.546
2.534
2.472
2.416
2.273
2.256
2.247
2.238
2.229
2.220
2.211
2.194
2.035
1.999



```

Current Data Parameters
NAME      Imb3-50cPure
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20091217
Time      6.40
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        3894.081 Hz
FIDRES     0.118838 Hz
AQ         4.2075826 sec
RG         312
DE         128.400 usec
TE         300.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         6.40 usec
PL1        4.00 dB
SFO1       300.1318008 MHz

F2 - Processing parameters
SI         32768
SF         300.130000 MHz
WDW        EM
SSB        0
GB         0
PC         1.00
  
```

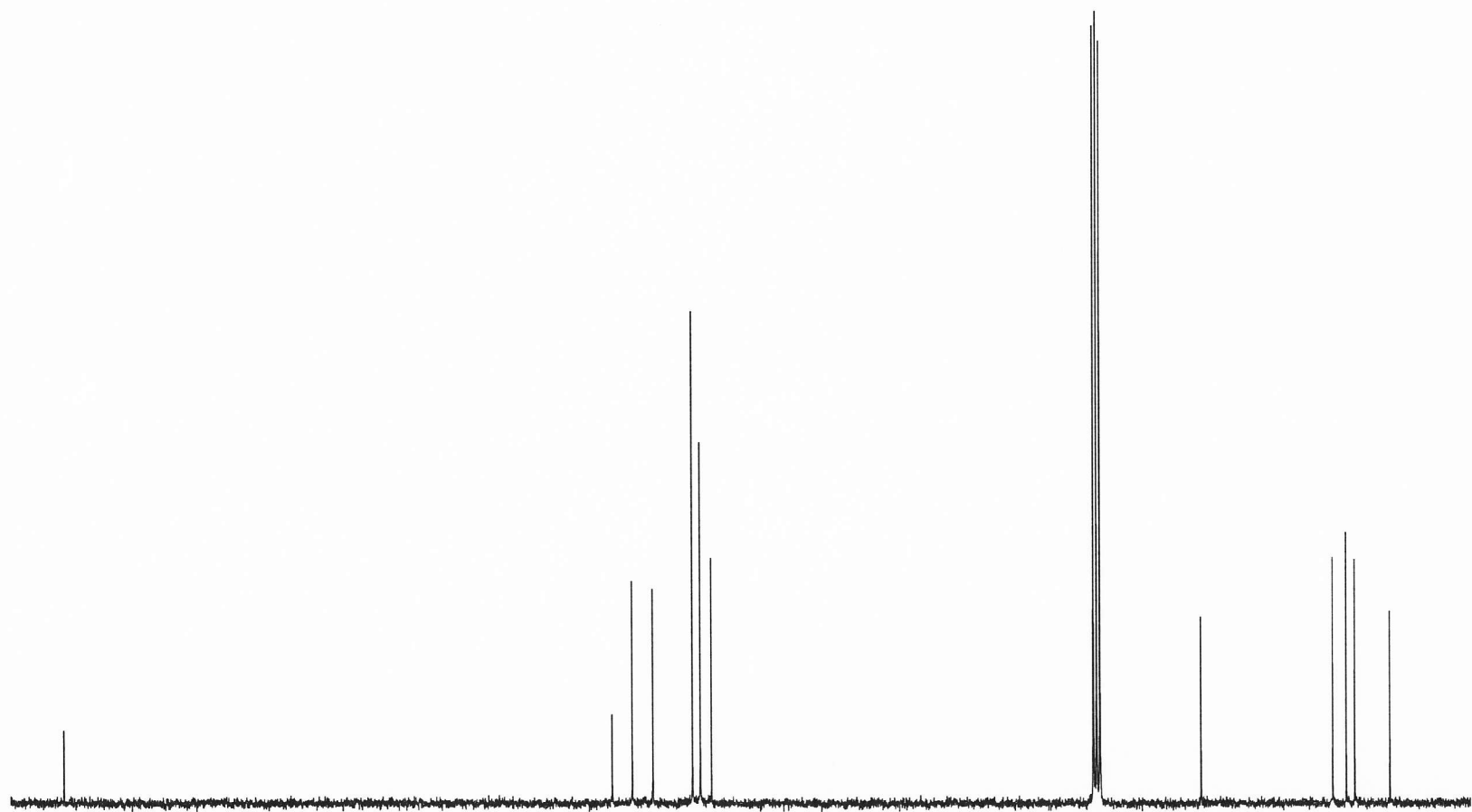
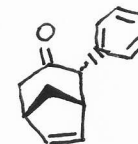
3-50 C Pure

209.26

135.58
135.96
134.32
128.07
128.21
126.75

63.61

48.56
48.73
42.71
35.14



```
Current Data Parameters
NAME      lnb3-50Cpure
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20091217
Time      17.11
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         3904
DS         4
SWH       18115.941 Hz
FIDRES    0.552855 Hz
AQ         0.9044744 sec
RG         10321.3
DW         27.600 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TDO        1

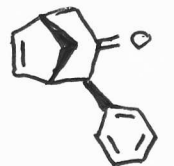
===== CHANNEL f1 =====
NUC1       13C
P1         23.00 usec
PL1        5.00 dB
SFO1       75.4766542 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     32.54 usec
PL2        5.00 dB
PL12      19.40 dB
PL13      26.00 dB
SFO2      300.1312005 MHz

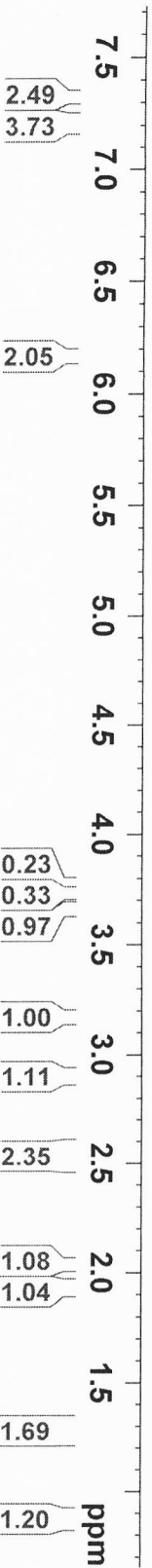
F2 - Processing parameters
SI         16384
SF         75.4677498 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 ppm

3-50 B2 Pure



- 7.333
- 7.318
- 7.303
- 7.258
- 7.248
- 7.233
- 7.219
- 7.204
- 6.169
- 6.155
- 5.295
- 3.784
- 3.744
- 3.727
- 3.661
- 3.172
- 3.168
- 3.162
- 2.905
- 2.900
- 2.590
- 2.583
- 2.556
- 2.549
- 2.513
- 2.511
- 2.479
- 2.478
- 2.042
- 2.019
- 1.952
- 1.946
- 1.942
- 1.937
- 1.931
- 1.925
- 1.919
- 1.915
- 1.561
- 1.313
- 1.287
- 1.267
- 1.259
- 0.897
- 0.884
- 0.870
- 0.857



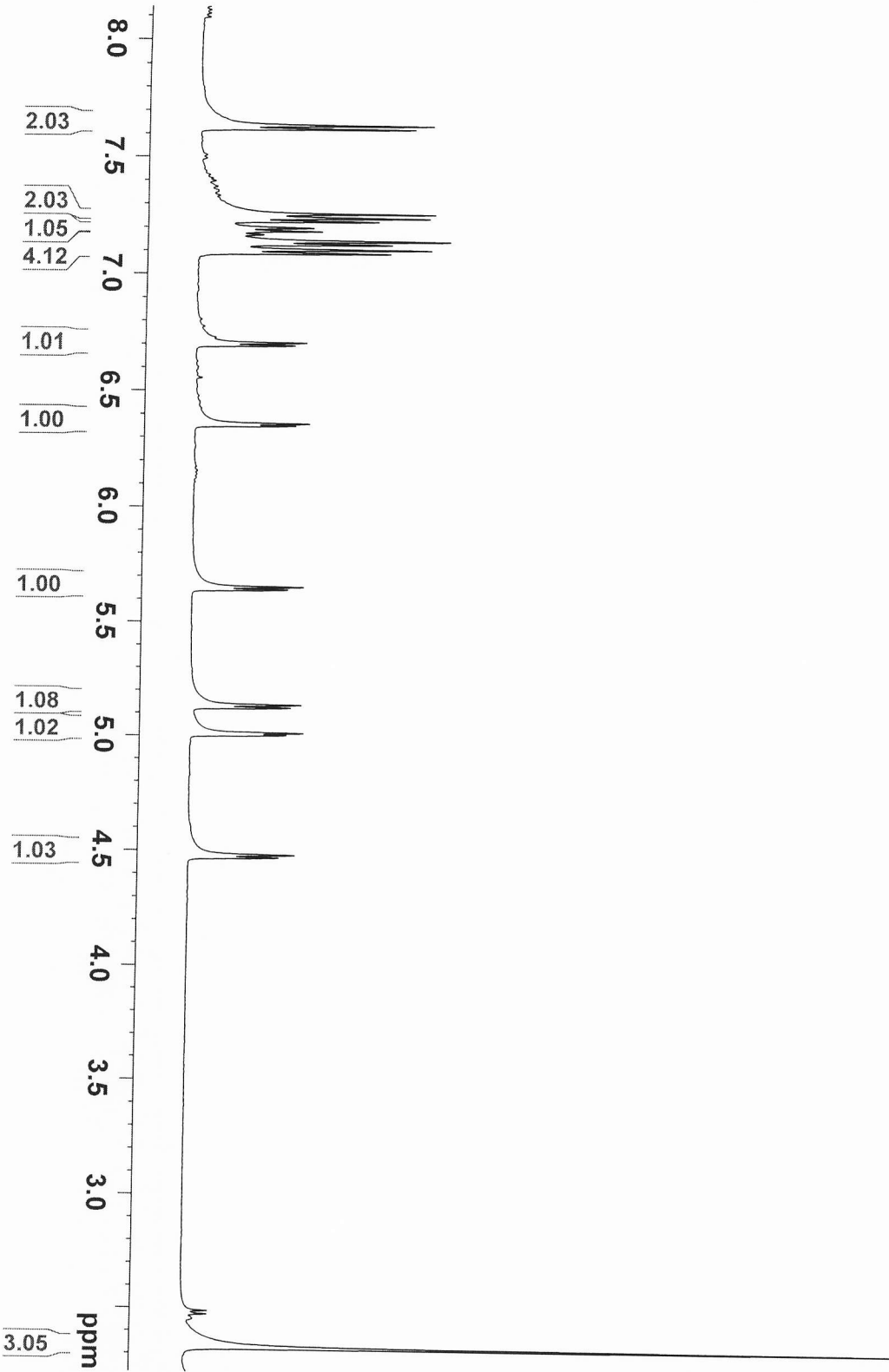
```

NAME                               1mb3-50B2pure
EXPNO                               1
PROCNO                               1
Date_                               20091215
Time_                               11.04
INSTRUM                             spect
PROBHD                               5 mm TXI 1H-13
PULPROG                             zgpg30
TD                                   32768
SOLVENT                             CDCl3
DS                                   19
SWH                                   6510.417 Hz
FIDRES                               0.139662 Hz
AQ                                   2.5167091 sec
RG                                   114
DW                                   76.800 usec
DE                                   7.50 usec
TE                                   298.0 K
D1                                   1.00000000 sec
TD0                                  1

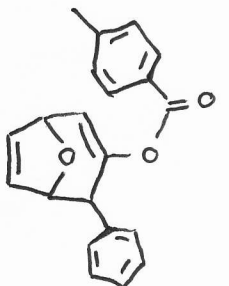
===== CHANNEL f1 =====
NUC1                                 1H
P1                                  6.70 usec
PL1                                 0.00 dB
PL12                                15.07131963 dB
SFO1                                500.1330008 MHz
SI                                   16384
SE                                   EM
WDW                                   EM
SSB                                   0
LB                                   0.30 Hz
GB                                   0
PC                                   1.00
  
```

3-59 C Pure

- 7.636
- 7.620
- 7.257
- 7.240
- 7.225
- 7.198
- 7.184
- 7.169
- 7.141
- 7.126
- 7.103
- 7.087
- 6.705
- 6.694
- 6.359
- 6.350
- 5.654
- 5.643
- 5.136
- 5.124
- 5.013
- 5.004
- 4.482
- 4.470



2.324

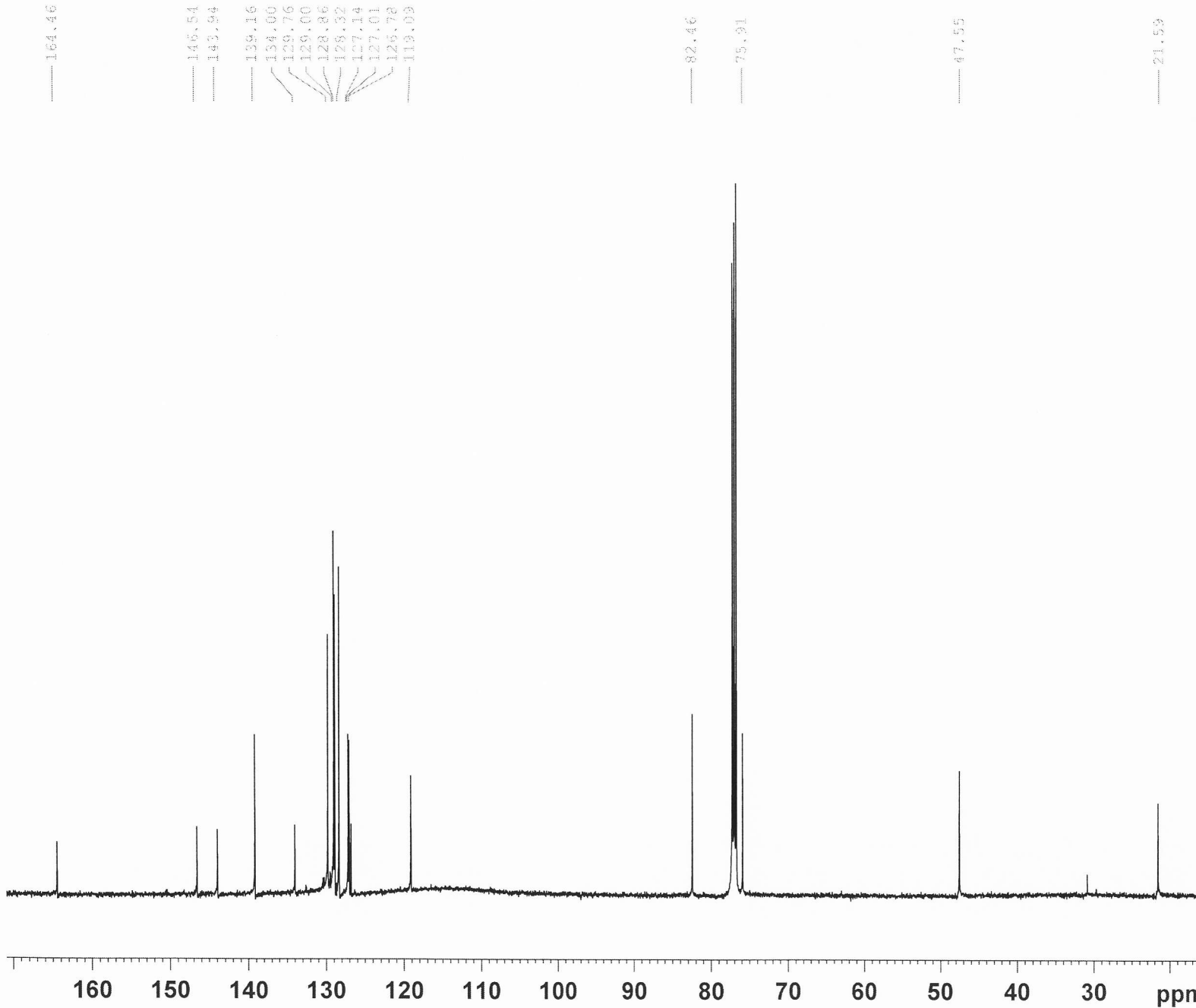
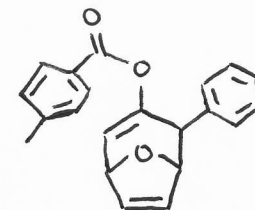


```

NAME          1nb3-59cure
EXPNO         1
PROCNO        1
Date_         20100104
Time_         20.52
INSTRUM       spect
PROBHD        5 mm TXI 1H-13
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            12
SMH           6510.417 Hz
FIDRES        0.198682 Hz
AQ            2.5167091 sec
RG            328
DM            76.800 usec
DE            7.50 usec
TE            298.0 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            6.70 usec
PL1           0.00 dB
ELI1          15.07131863 W
SE01          500.1330008 MHz
SI            16384
SF            500.1300143 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

3-59 C Pure C13



```

NAME      lnb3-59cpure
EXPNO     2
PROCNO    1
Date_     20100105
Time_     8.35
INSTRUM   spect
PROBHD    5 mm TXI 1H-13
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         15784
DS         4
SWH       30303.031 Hz
FIDRES    0.924775 Hz
AQ         0.5407385 sec
RG         812.7
DW         16.500 usec
DE         7.50 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
    
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        12.20 usec
PL1       -3.00 dB
PL1W      190.45114136 W
SFO1      125.7726284 MHz
    
```

```

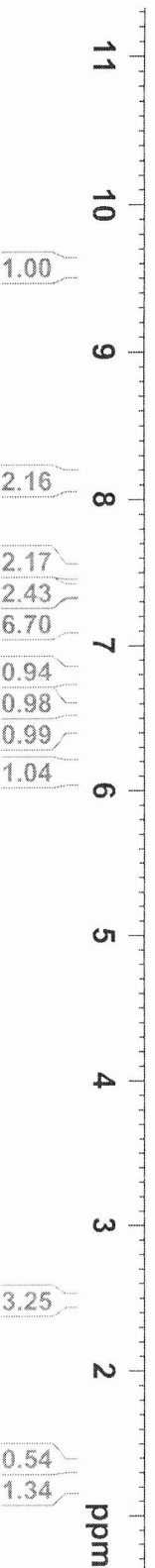
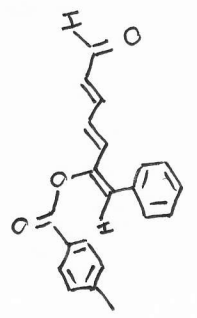
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        0.00 dB
PL12       23.48 dB
PL13       25.00 dB
PL2W       15.07131863 W
PL12W      0.06763186 W
PL13W      0.04765970 W
SFO2      500.1320005 MHz
SI         16384
SF         125.7577890 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```

3-59 G Pure

- 9.590
- 9.563
- 8.148
- 8.121
- 7.518
- 7.510
- 7.491
- 7.486
- 7.405
- 7.399
- 7.380
- 7.354
- 7.295
- 7.282
- 7.276
- 7.259
- 7.252
- 7.244
- 7.241
- 7.229
- 7.222
- 7.184
- 7.170
- 7.133
- 6.818
- 6.768
- 6.557
- 6.494
- 6.457
- 6.444
- 6.407
- 6.170
- 6.144
- 6.120
- 6.094

- 2.490
- 2.427
- 2.045

- 1.360
- 1.337
- 1.258
- 1.231
- 1.208



Current Data Parameters
 NAME Ind3-59gpure
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091230
 Time 8.36
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 3894.081 Hz
 FIDRES 0.118838 Hz
 AQ 4.2075896 sec
 RG 256
 DM 128.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUCL1 1H
 P1 6.40 usec
 PL1 4.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300066 MHz
 MDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00