Supporting Information

For

Temperature Dependant Nuclearity in bis(Benzimidazoyl) Nickel Complexes and Their Catalysis Towards Conjugate Addition of Thiophenols to α,β- Enones

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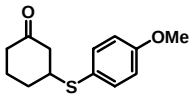
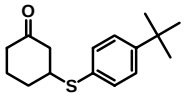
Analytical data for the products of thia-Michael addition

3-(4-methoxyphenylsulfanyl)-cyclohexan-1-one (1a)[1a, 1b]



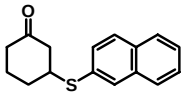
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.38 (d, *J* = 8.8, 2H), 6.84 (d, *J* = 8.8, 2H), 3.79 (s, 3H), 3.24-3.20 (m, 1H), 2.61 (dd, *J* = 14.2, 4.4, 1H), 2.34-2.28 (m, 3H), 2.12-2.09 (m, 2H), 1.69-1.65 (m, 2H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 209.20, 160.17, 136.64, 123.13, 114.77, 55.49, 47.94, 47.18, 40.99, 31.41, 24.20; TLC R_f 0.25 (EtOAc/hexanes, 1/10).

3-(4-tert-butylphenylsulfanyl)cyclohexan-1-one (1b)[1a]



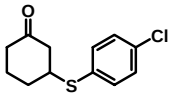
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.36 (d, J = 8.5, 2H), 7.33 (d, J = 8.5, 2H), 3.38-3.36 (m, 1H), 2.67 (dd, J = 14.3, 4.4, 1H), 2.40-2.31 (m, 3H), 2.17-2.13 (m, 2H), 1.75-1.70 (m, 2H), 1.31 (s, 9H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ = 209.17, 151.44, 133.68, 129.47, 126.31, 48.10, 46.55, 41.09, 34.80, 31.51, 31.44, 24.31; TLC R_f 0.29 (EtOAc/hexanes, 1/10).

3-(naphthalene- 2-ylsulfanyl)cyclohexan-1-one (1c)[1a, 1b]



^{1}H-NMR ($CDCl_3$, 400 MHz), δ 7.92 (s, 1H), 7.82-7.77 (m, 3H), 7.52-7.46 (m, 3H), 3.55-3.52 (m, 1H), 2.73 (dd, J = 14.3, 4.5, 1H), 2.46-2.30 (m, 3H), 2.17-2.13 (m, 2H), 1.79-1.74 (m, 2H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 208.74, 133.75, 132.69, 132.27, 130.56, 130.35, 128.79, 127.84, 127.61, 126.77, 126.59, 47.89, 46.21, 41.00, 31.42, 24.14; TLC R_f 0.28 (EtOAc/hexanes, 1/10).

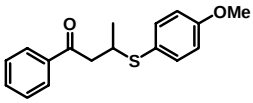
3-(4-chlorophenylsulfanyl)cyclohexan-1-one (1d)[1b]



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.29 (d, J = 8.4, 2H), 7.22 (d, J = 8.4,

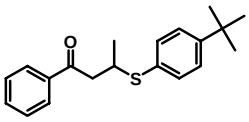
2H), 3.37-3.35 (m, 1H), 2.60 (dd, J = 14.3, 4.3, 1H), 2.33-2.24 (m, 3H), 2.09-2.07 (m, 2H), 1.68-1.64 (m, 2H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 208.25, 134.46, 133.93, 131.62, 129.22, 47.53, 46.27, 40.80, 31.05, 23.89; TLC R_f 0.63 (EtOAc/hexanes, 1/9).

3-(4-methoxyphenylsulfanyl)-1-phenylpropan-1-one (2a)



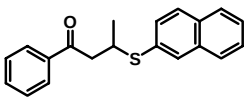
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.86 (d, J = 7.1, 2H), 7.51-7.49 (m, 1H), 7.42-7.38 (m, 4H), 6.83 (d, J = 6.8, 2H), 3.75 (s, 3H), 3.73-3.69 (m, 1H), 3.26 (dd, J = 16.6, 4.9, 1H), 3.04-2.98 (m, 1H), 1.31 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 198.08, 159.73, 136.86, 135.98, 133.19, 128.62, 128.07, 124.22, 114.54, 55.29, 45.46, 40.03, 21.05; TLC R_f 0.58 (EtOAc/hexanes, 1/9); IR (neat): 1684 cm^{-1} (ν_{co}); Anal. Calc. for $C_{17}H_{18}O_2S$: C, 71.30; S, 11.20; H, 6.34; Found: C, 71.73; S, 11.10; H, 6.15.

3-(4-tert-butylphenylsulfanyl)-1-phenylpropan-1-one (2b)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.90 (d, J = 7.4, 2H), 7.54 (t, J = 7.4, 1H), 7.47-7.41 (m, 4H), 7.34 (d, J = 8.4, 2H), 3.91-3.86 (m, 1H), 3.33 (dd, J = 16.8, 4.6, 1H), 3.13-3.07 (m, 1H), 1.39 (d, J = 6.7, 3H), 1.32 (s, 9H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 198.10, 150.64, 136.94, 133.24, 132.70, 130.80, 128.67, 128.15, 126.08, 45.68, 39.13, 34.59, 31.35, 21.14; TLC R_f 0.55 (EtOAc/hexanes, 1/9); IR (neat): 1682 cm^{-1} (ν_{co}); HR-MS (m/z, amu): 312.16.

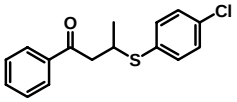
3-(naphthalene-2-ylsulfanyl)-1-phenylpropan-1-one (2c)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.90-7.88 (m, 3H), 7.79-7.75 (m, 3H), 7.55-7.41 (m, 6H), 4.07-4.02(m, 1H), 3.35 (dd, J = 16.8, 4.6, 1H), 3.18-3.12 (m, 1H), 1.43 (d, J = 6.7, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 198.30, 137.02, 133.86, 133.47, 132.52, 132.08, 130.98, 129.81, 128.83, 128.74, 128.28,

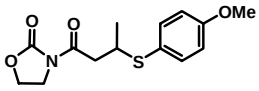
127.89, 127.59, 126.75, 126.36, 45.66, 38.93, 21.25; TLC R_f 0.35 (EtOAc/hexanes, 1/50); IR (neat): 1684 cm^{-1} (ν_{co}); HR-MS (m/z, amu): 306.11

3-(4-chlorophenylsulfanyl)-1-phenylpropan-1-one (2d)



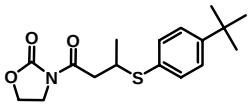
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.91 (d, J = 8.0, 2H), 7.60-7.56 (m, 1H), 7.47 (t, J = 7.6, 2H), 7.38 (d, J = 8.4, 2H), 7.28 (d, J = 8.4, 2H), 3.91-3.86 (m, 1H), 3.28 (dd, J = 16.9, 4.8, 1H), 3.15-3.09 (m, 1H), 1.37 (d, J = 6.7, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 198.00, 136.94, 133.82, 133.58, 133.54, 133.12, 129.31, 128.86, 128.24, 45.49, 39.25, 21.25; TLC R_f 0.40 (EtOAc/hexanes, 1/30); IR (neat): 1684 cm^{-1} (ν_{co}); HR-MS (m/z, amu): 290.05

3-(4-methoxyphenylsulfanyl)-2-oxazolidinone (3a)[2a, 2b]



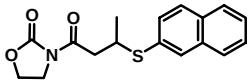
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.43 (d, J = 8.8, 2H), 6.84 (d, J = 8.8, 2H), 4.37 (t, J = 8.1, 2H), 3.98-3.94 (m, 2H), 3.79 (s, 3H), 3.59 (q, J = 6.9, 1H), 3.24 (dd, J = 17.0, 6.6, 1H), 3.05 (dd, J = 17.0, 7.3, 1H), 1.30 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 171.38, 159.99, 153.56, 136.57, 124.07, 114.63, 62.26, 55.52, 42.66, 42.49, 40.12, 21.36; TLC R_f 0.62 (EtOAc/hexanes, 1/9).

3-(4-tert-butylphenylsulfanyl)-2-oxazolidinone (3b)[2a]



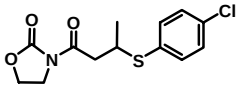
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.38 (d, J = 8.4, 2H), 7.31 (d, J = 8.4, 2H), 4.36 (t, J = 8.3, 2H), 3.97-3.92 (m, 2H), 3.71 (q, J = 6.8, 1H), 3.25 (dd, J = 17.0, 6.5, 1H), 3.12 (dd, J = 17.0, 7.4, 1H), 1.34 (d, J = 6.8, 3H), 1.30 (s, 9H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 171.80, 154.04, 151.41, 133.68, 130.99. 126.61, 62.74, 43.11, 43.06, 39.79, 35.23, 31.93, 22.00; TLC R_f 0.59 (EtOAc/hexanes, 1/9).

3-(naphthalene-2-ylsulfanyl)-2-oxazolidinone (3c)[2a, 2b]



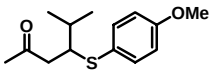
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.80 (s, 1H), 7.68-7.63 (m, 3H), 7.41-7.32 (m, 3H), 4.11 (t, J = 8.1, 2H), 3.79 (q, J = 6.8, 1H), 3.72-3.68 (m, 2H), 3.19 (dd, J = 17.0, 6.4, 1H), 3.01 (dd, J = 17.0, 7.4, 1H), 1.28 (d, J = 6.8, 3H).

3-(4-chlorophenylsulfanyl)-2-oxazolidinone (3d)[2b]



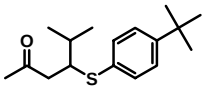
^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.39 (d, J = 8.5, 2H), 7.27 (d, J = 8.5, 2H), 4.41-4.37 (m, 2H), 3.99-3.95 (m, 2H), 3.73 (q, J = 6.8, 1H), 3.25 (dd, J = 17.0, 6.5, 1H), 3.11 (dd, J = 17.0, 7.3, 1H), 1.34 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 171.03, 153.53, 134.39, 133.75, 132.77, 129.22, 62.28, 42.61, 42.36, 39.44, 21.36; TLC R_f 0.81(EtOAc/hexanes, 1/3).

4-(4-methoxyphenylsulfanyl)-5-methylhexan-2-one (4a)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.38 (d, J = 8.6, 2H), 6.82 (d, J = 8.6, 2H), 3.78 (s, 3H), 3.44-3.39 (m, 1H), 2.62 (d, J = 6.8, 2H), 2.12 (s, 3H), 1.91-1.87 (m, 1H), 1.00 (d, J = 6.8, 3H), 0.95 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 207.27, 159.51, 135.32, 125.84, 114.66, 55.46, 52.49, 46.00, 31.89, 30.97, 19.50, 19.40; TLC R_f 0.45 (EtOAc/hexanes, 1/9); IR (neat): 1716 cm^{-1} (ν_{co}); Anal. Calc. for $C_{14}H_{20}O_2S$: C, 66.63; S, 12.71; H, 7.99; Found: C, 66.95; S, 12.54; H, 7.82.

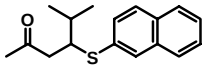
4-(4-tert-butylphenylsulfanyl)-5-methylhexan-2-one (4b)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.35 (d, J = 8.4, 2H), 7.29 (d, J = 8.3, 2H), 3.59-3.55 (m, 1H), 2.67 (d, J = 6.8, 2H), 2.13 (s, 3H), 1.99-1.91 (m, 1H), 1.30 (s, 9H), 1.02 (d, J = 6.8, 3H), 0.97 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 207.33, 150.31, 132.11, 131.95, 126.17, 51.10, 46.20, 34.70, 32.01, 31.46, 31.02, 19.64, 19.36; TLC R_f 0.5 (EtOAc/hexanes, 1/9); IR (neat): 1715

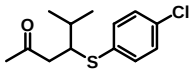
cm^{-1} (ν_{co}); HR-MS (m/z, amu): 278.17

4-(naphthalene-2-ylsulfanyl)-5-methylhexan-2-one (4c)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.89 (s, 1H), 7.80-7.75 (m, 3H), 7.53 (dd, J = 8.5, 1.7, 1H), 7.50-7.42 (m, 2H), 3.80-3.76 (m, 1H), 2.73 (d, J = 6.7, 2H), 2.15 (s, 3H), 2.04-1.97 (m, 1H), 1.06 (d, J = 6.7, 3H), 1.01 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 207.10, 133.85, 133.37, 132.30, 130.05, 129.37, 128.66, 127.85, 127.47, 126.65, 126.13, 50.69, 46.04, 32.13, 31.03, 19.69, 19.31; TLC R_f 0.46 (EtOAc/hexanes, 1/9); IR (neat): 1716 cm^{-1} (ν_{co}); Anal. Calc. for $C_{17}H_{20}OS$: C, 74.96; S, 11.77; H, 7.40; Found: C, 75.39; S, 11.58; H, 7.31.

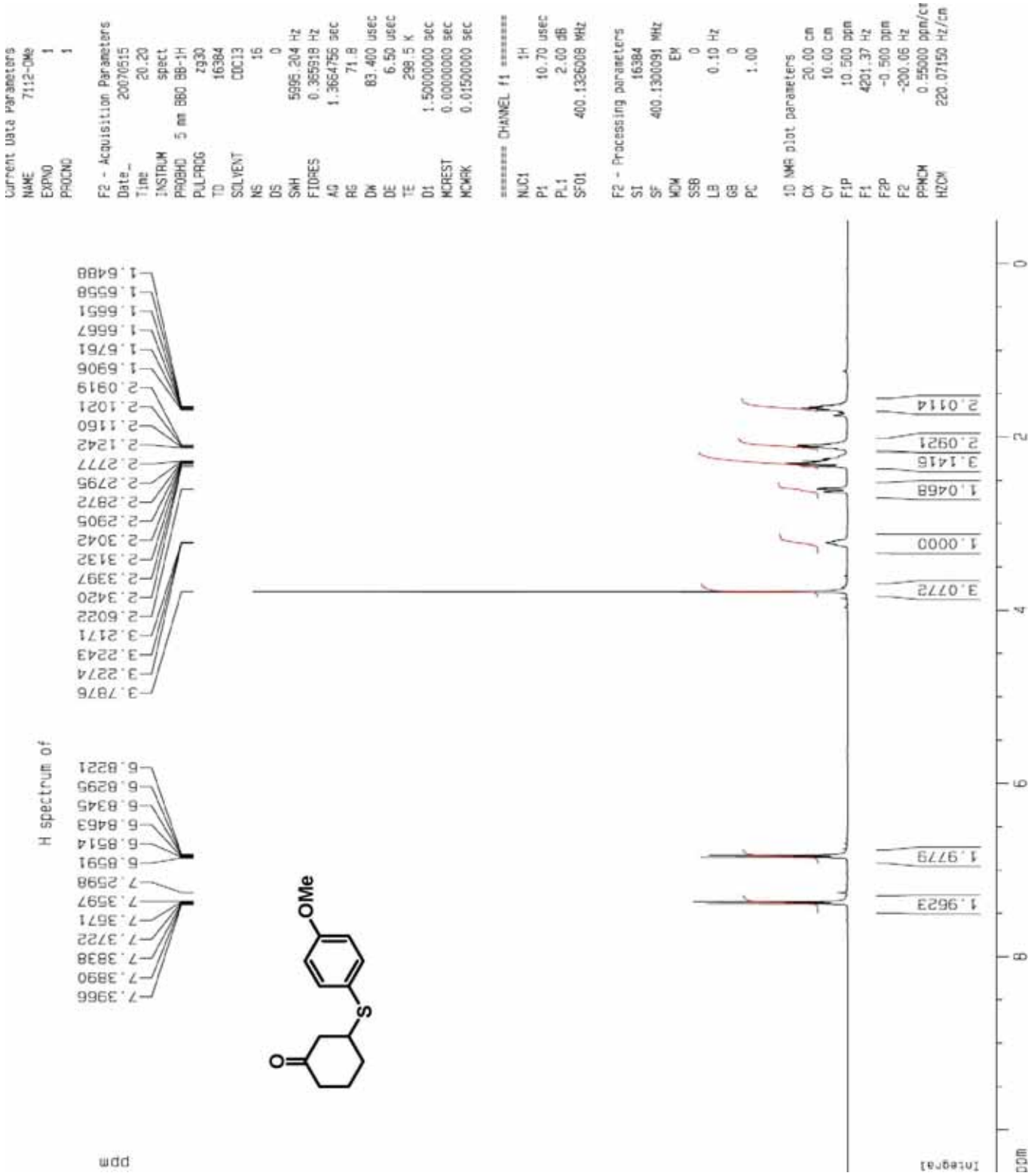
4-(4-chlorophenylsulfanyl)-5-methylhexan-2-one (4d)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ 7.36 (d, J = 8.5, 2H), 7.24 (d, J = 8.5, 2H), 3.60-3.55 (m, 1H), 2.66 (d, J = 6.76, 2H), 2.15 (s, 3H), 1.95-1.90 (m, 1H), 0.99 (d, J = 6.8, 3H), 0.95 (d, J = 6.8, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ 206.85, 134.65, 133.15, 133.07, 129.25, 51.41, 46.06, 32.30, 31.06, 19.66, 19.28; TLC R_f 0.38 (EtOAc/hexanes, 1/20); IR (neat): 1717 cm^{-1} (ν_{co}); Anal. Calc. for $C_{13}H_{17}ClOS$: C, 60.80; S, 12.49; H, 6.67; Found: C, 61.26; S, 12.60; H, 6.89.

Reference:

1. (a) McDaid, P.; Chen, Y.; Deng, L. *Angew. Chem. Int. Ed.* **2002**, *41*, 338. (b) Yadav, J. S.; Reddy, B. V. S.; Baishya, G.; *J. Org. Chem.* **2003**, *68*, 7098.
2. (a) Kanemasa, S.; Oderaotoshi, Y.; Wada, E. *J. Am. Chem. Soc.* **1999**, *121,* 8675. (b) Kawatsura, M.; Yuji Komatsu, Y.; Yamamoto, M.; Hayase, S.; Itoh T. *Tetrahedron Lett.* **2007**, *48*, 6480.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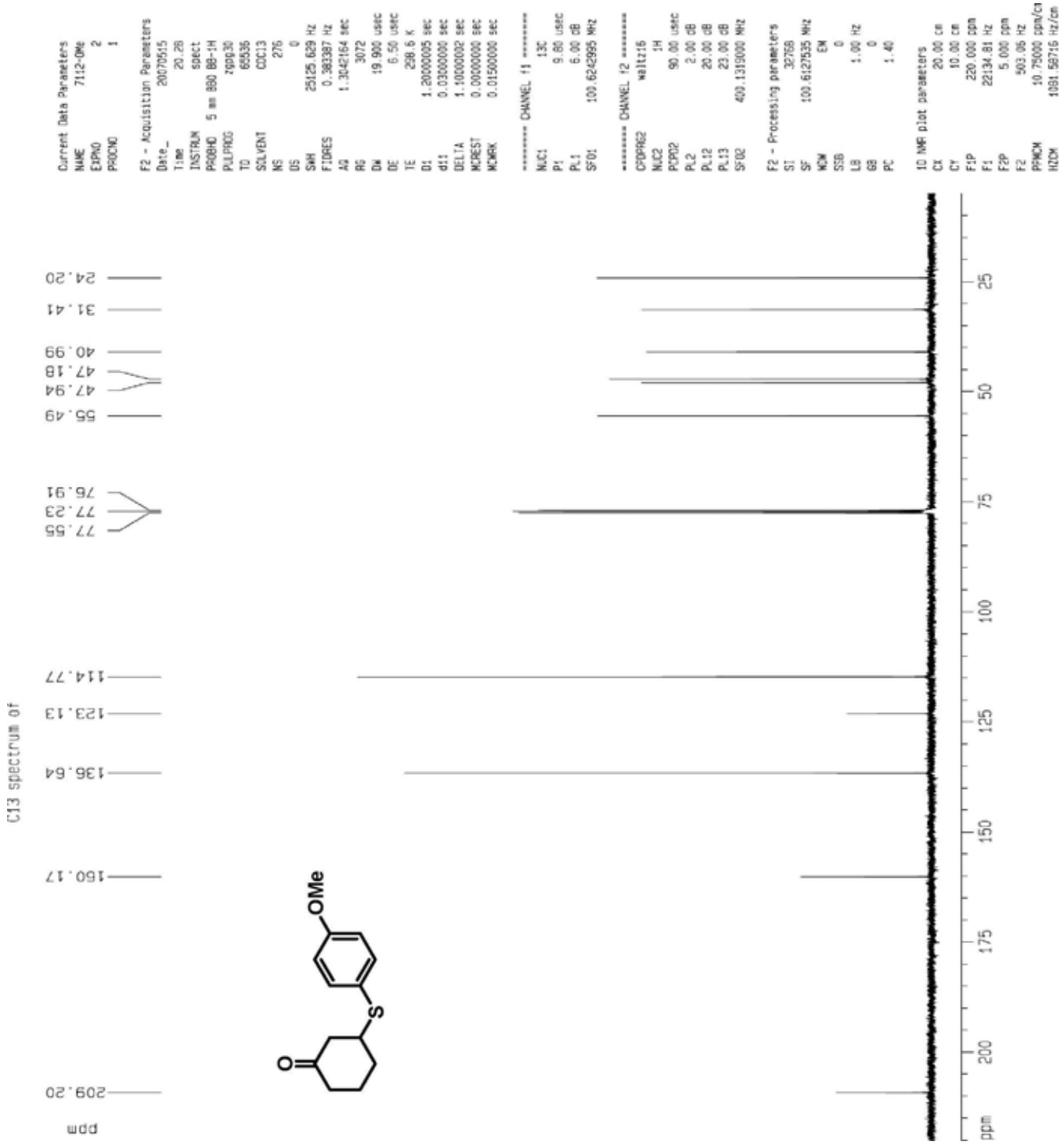
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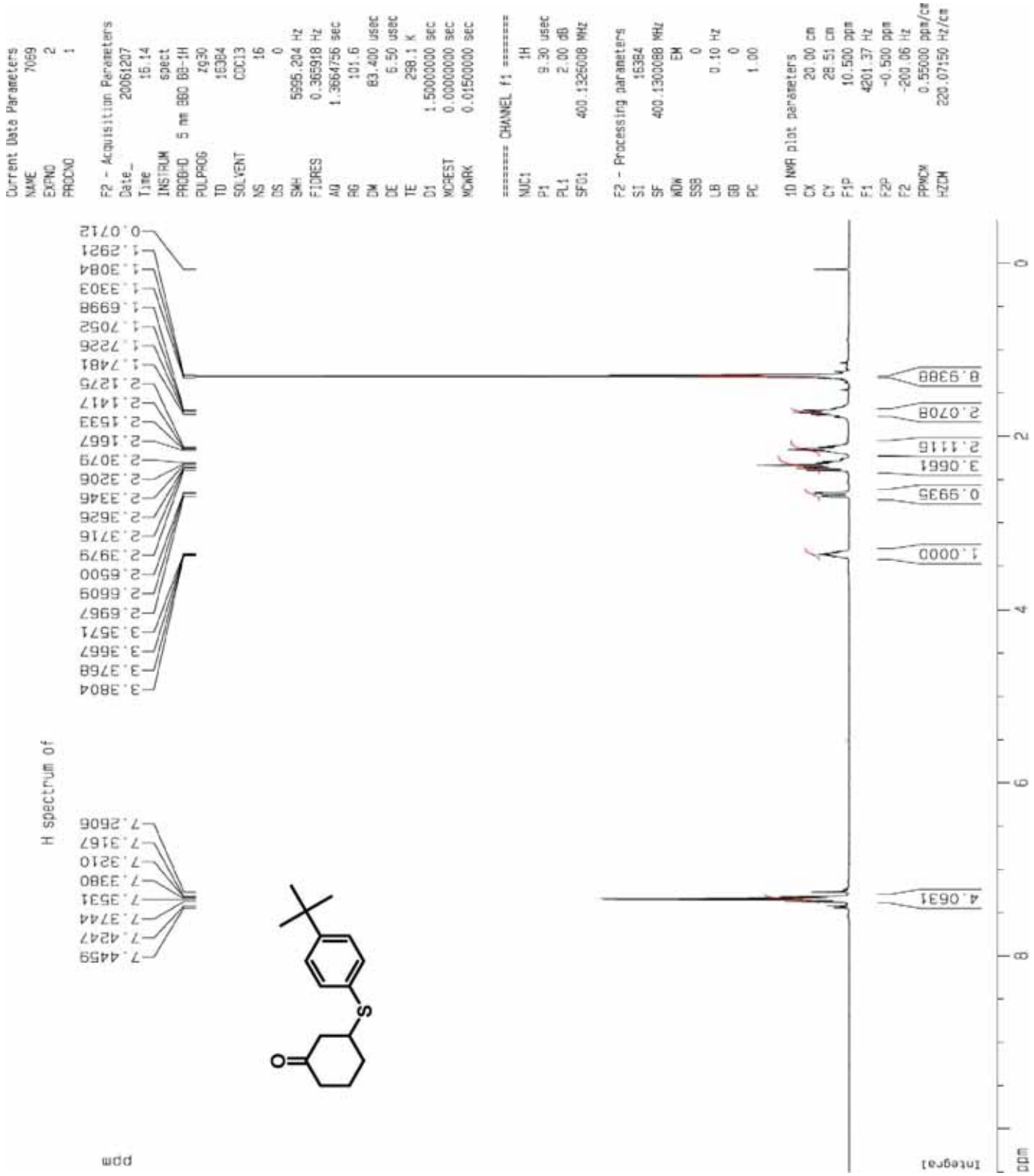
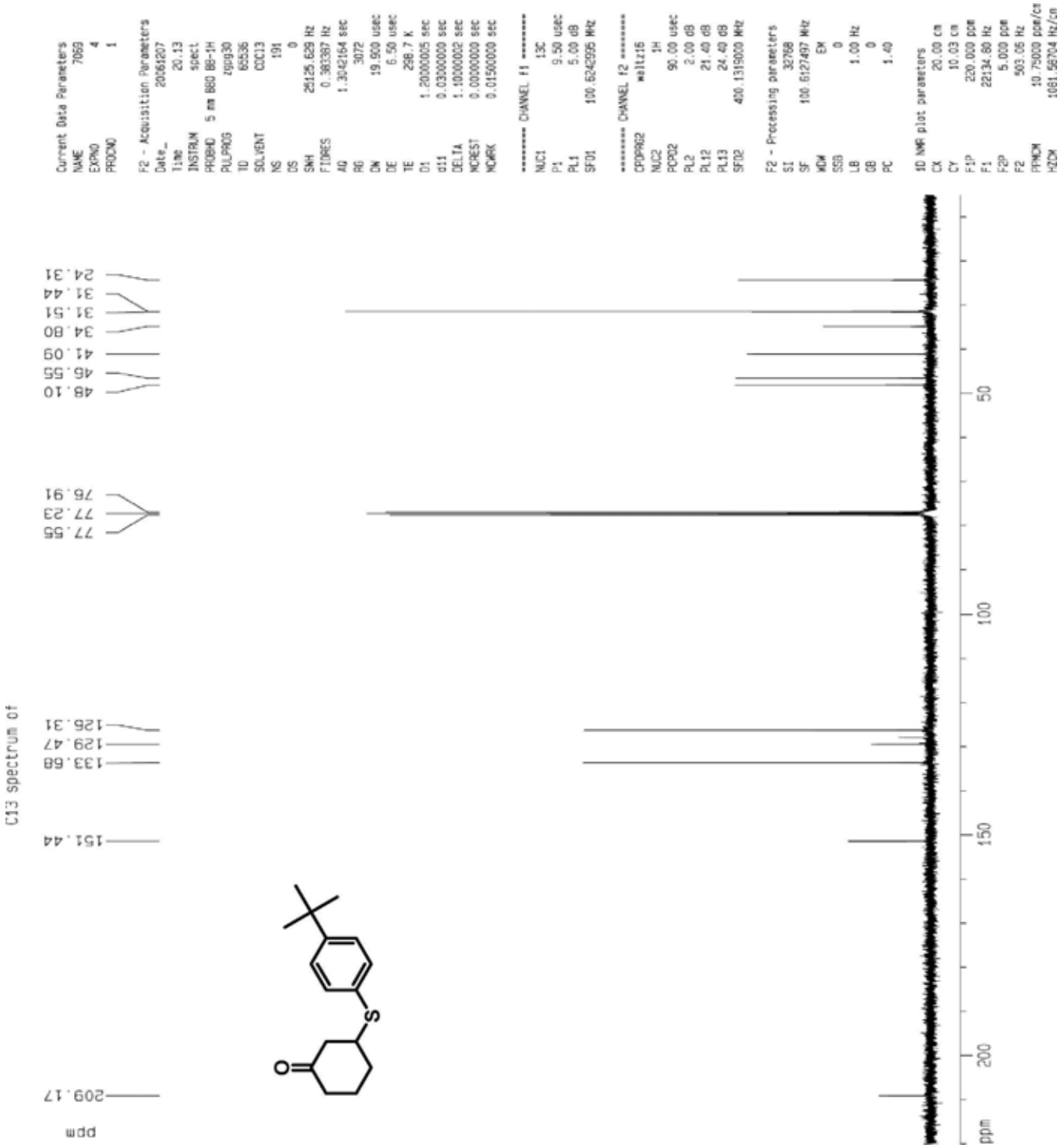
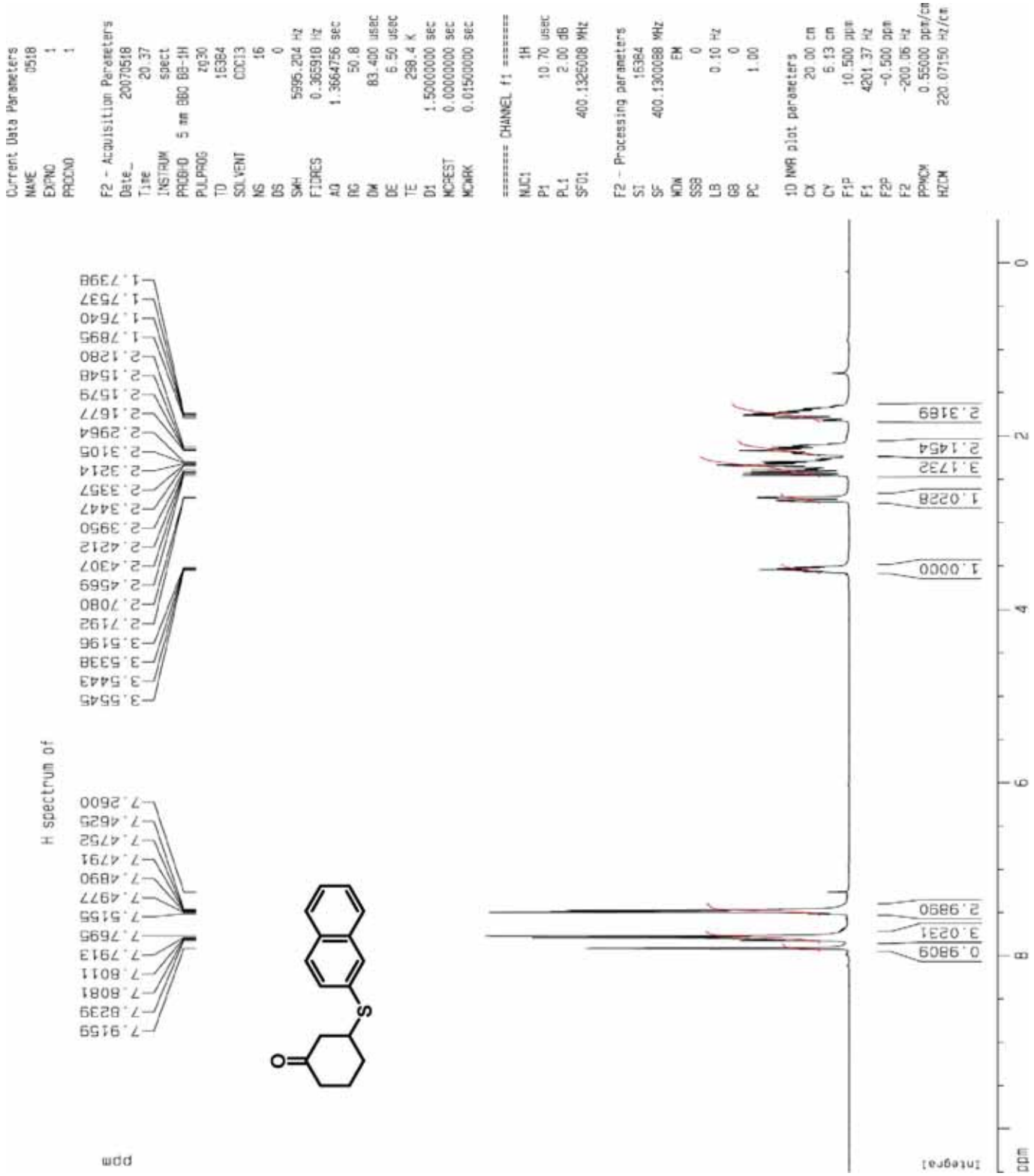
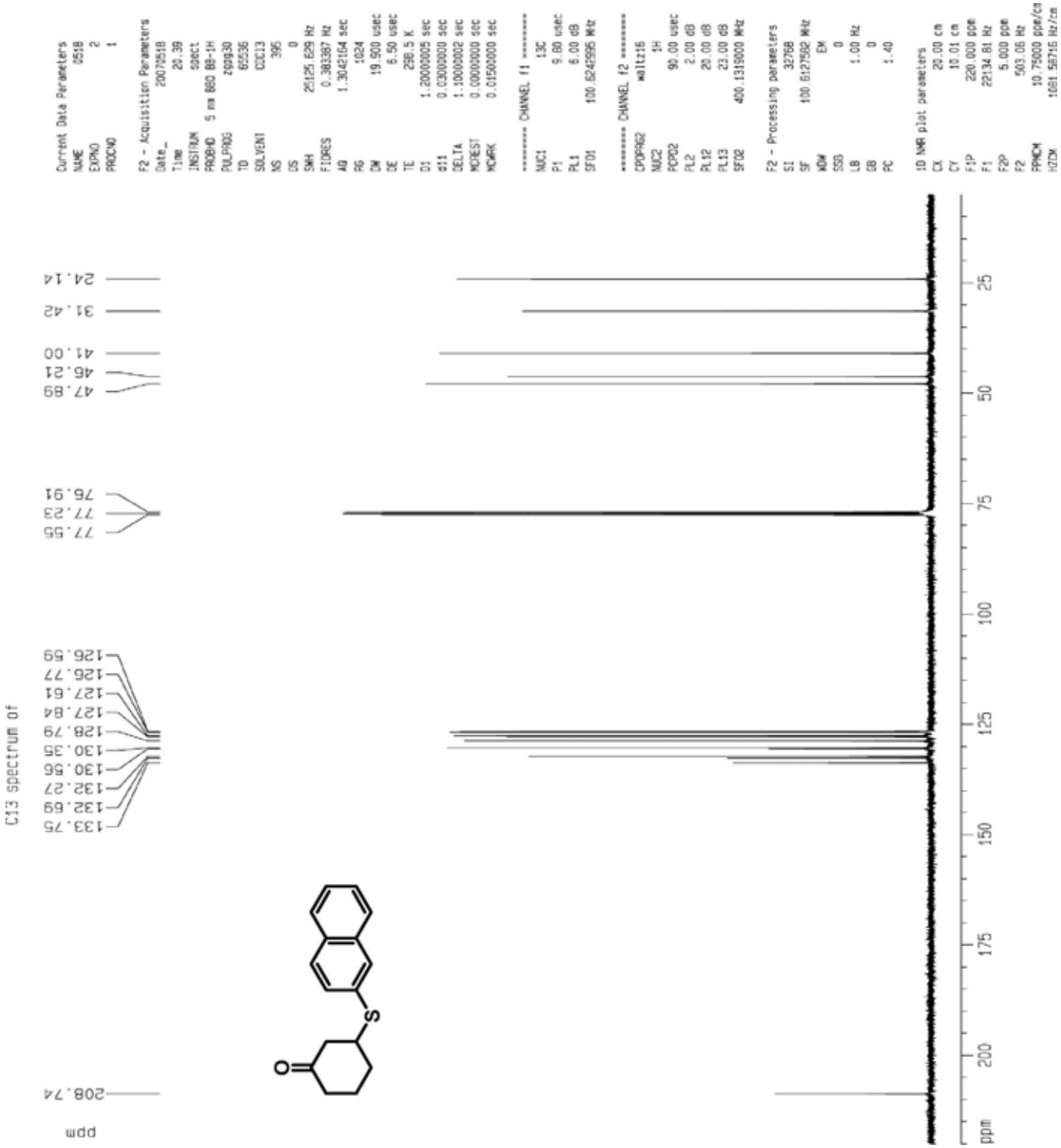
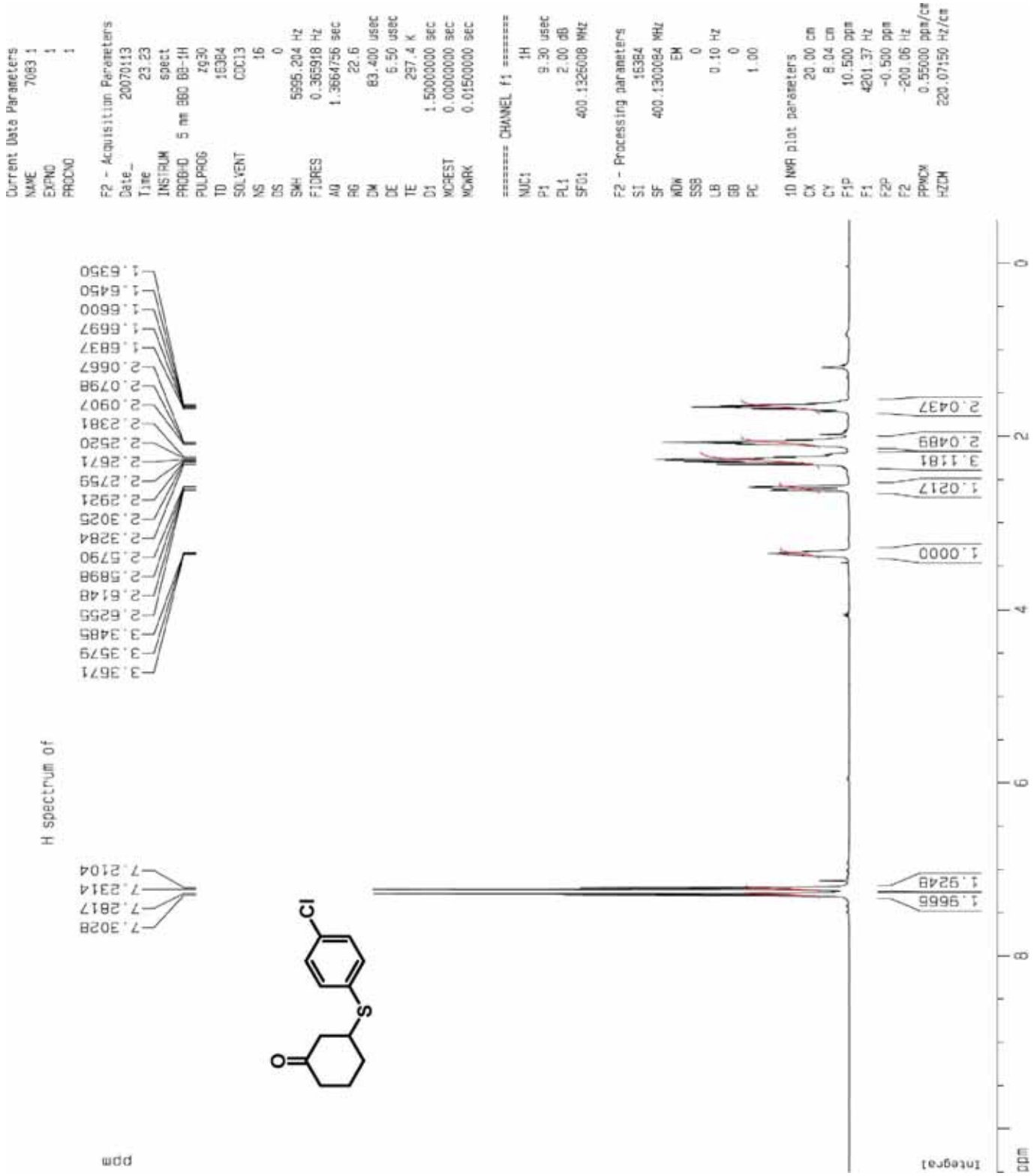
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58716 Hz/cm

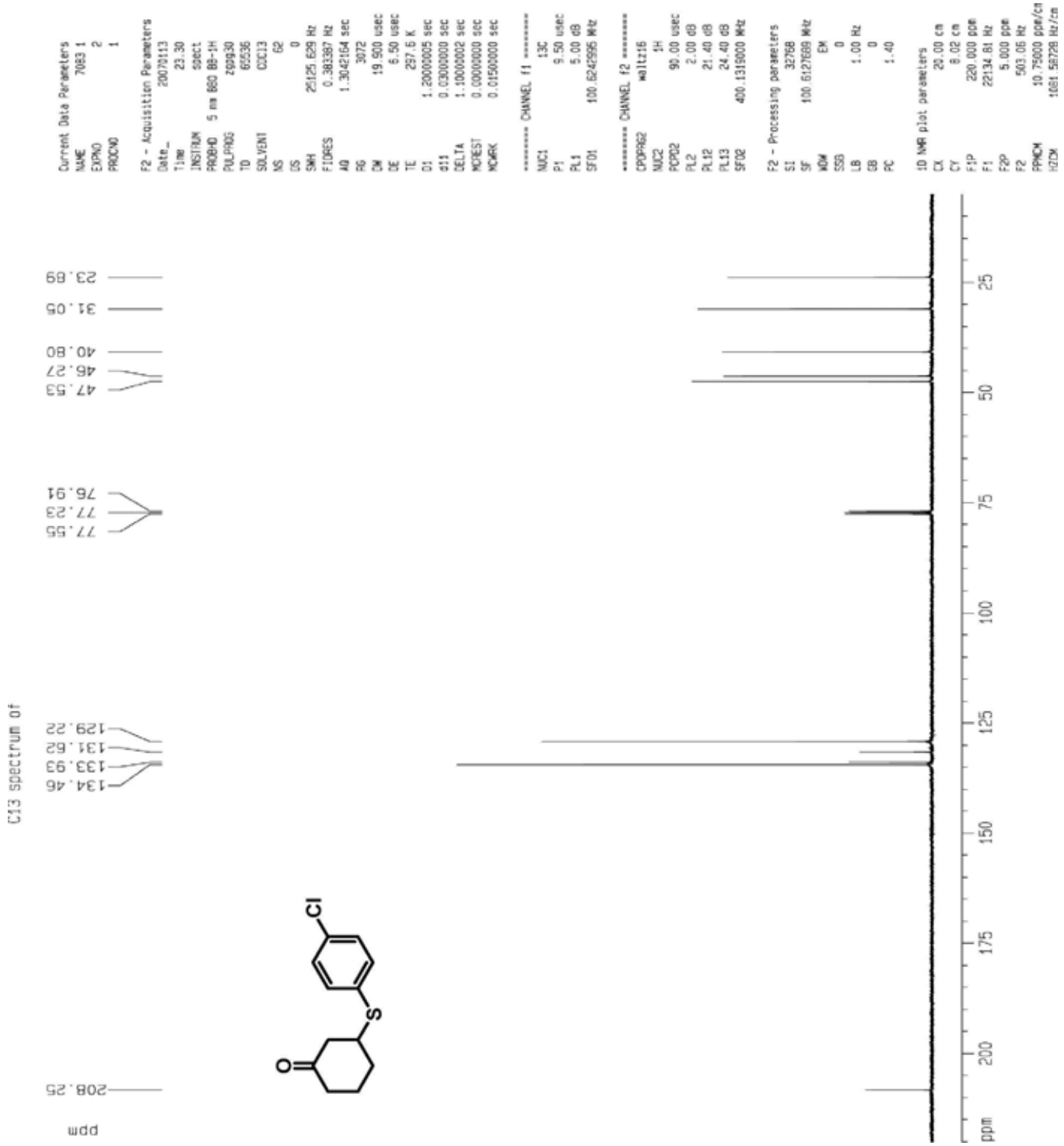

Current Data Parameters
NAME 7069
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061207
Time 16.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 101.6
DW 83.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 28.51 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
8.9388
2.0708
2.1115
3.0661
0.9935
1.0000
4.0631
0.0712
1.2921
1.3084
1.3303
1.6998
1.7052
1.7226
1.7481
2.1275
2.1417
2.1533
2.1667
2.3079
2.3206
2.3346
2.3626
2.3716
2.3979
2.6500
2.6609
2.6967
3.3571
3.3667
3.3768
3.3804
7.2606
7.3167
7.3210
7.3380
7.3531
7.3744
7.4247
7.4459
S
O

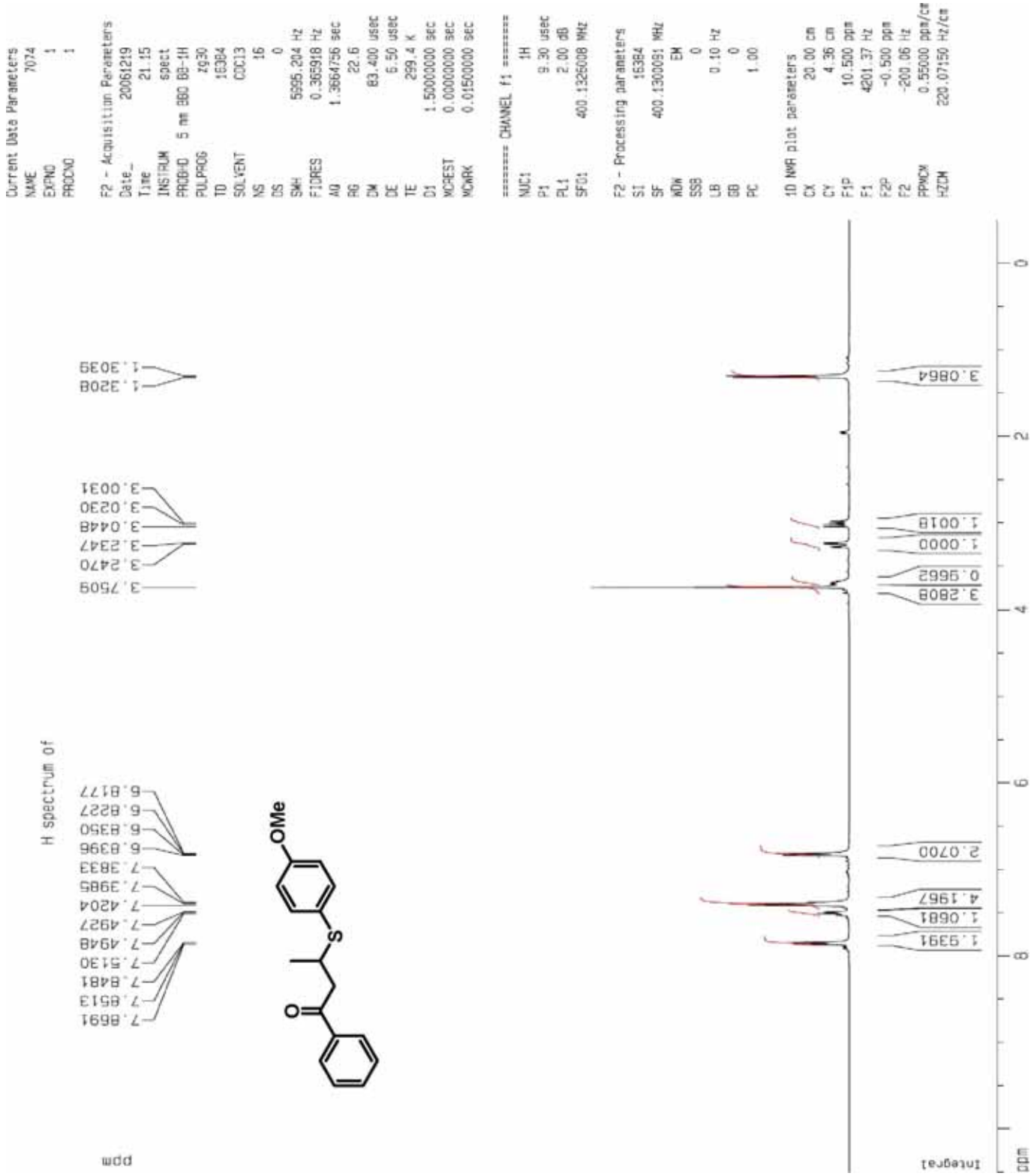

C13 spectrum of
ppm
209.17
151.44
133.68
129.47
125.31
77.55
77.23
76.91
48.10
46.55
41.09
34.80
31.51
31.44
24.31
S
O
Current Data Parameters
NAME 7069
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061207
Time 20.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 191
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 298.7 K
D1 1.20000025 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127497 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.03 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.56704 Hz/cm
ppm
50
100
150
200

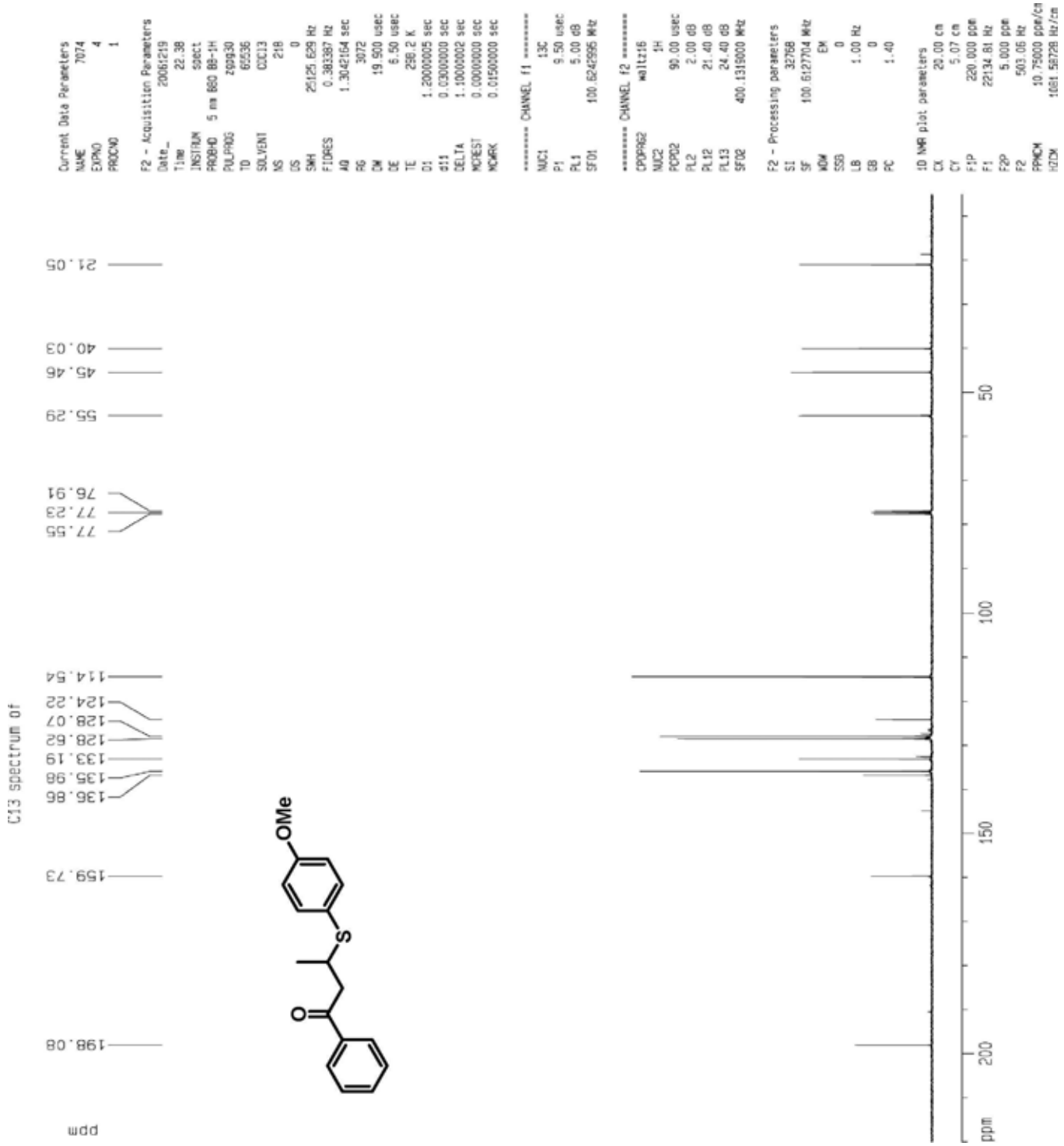

Current Data Parameters
NAME 0518
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070518
Time 20.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 50.8
DW 83.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.13 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
7.9159
7.8239
7.8081
7.8011
7.7913
7.7695
7.5155
7.4977
7.4890
7.4791
7.4752
7.4625
7.2600
3.5545
3.5443
3.5338
3.5196
2.7192
2.7080
2.4569
2.4307
2.4212
2.3950
2.3447
2.3357
2.3214
2.3105
2.2964
2.1677
2.1579
2.1548
2.1280
1.7895
1.7640
1.7537
1.7398
S
O
ppm
Integral
2.9890
3.0231
0.9809
1.0000
1.0228
3.1732
2.1454
2.3189
0
2
4
6
8
ppm

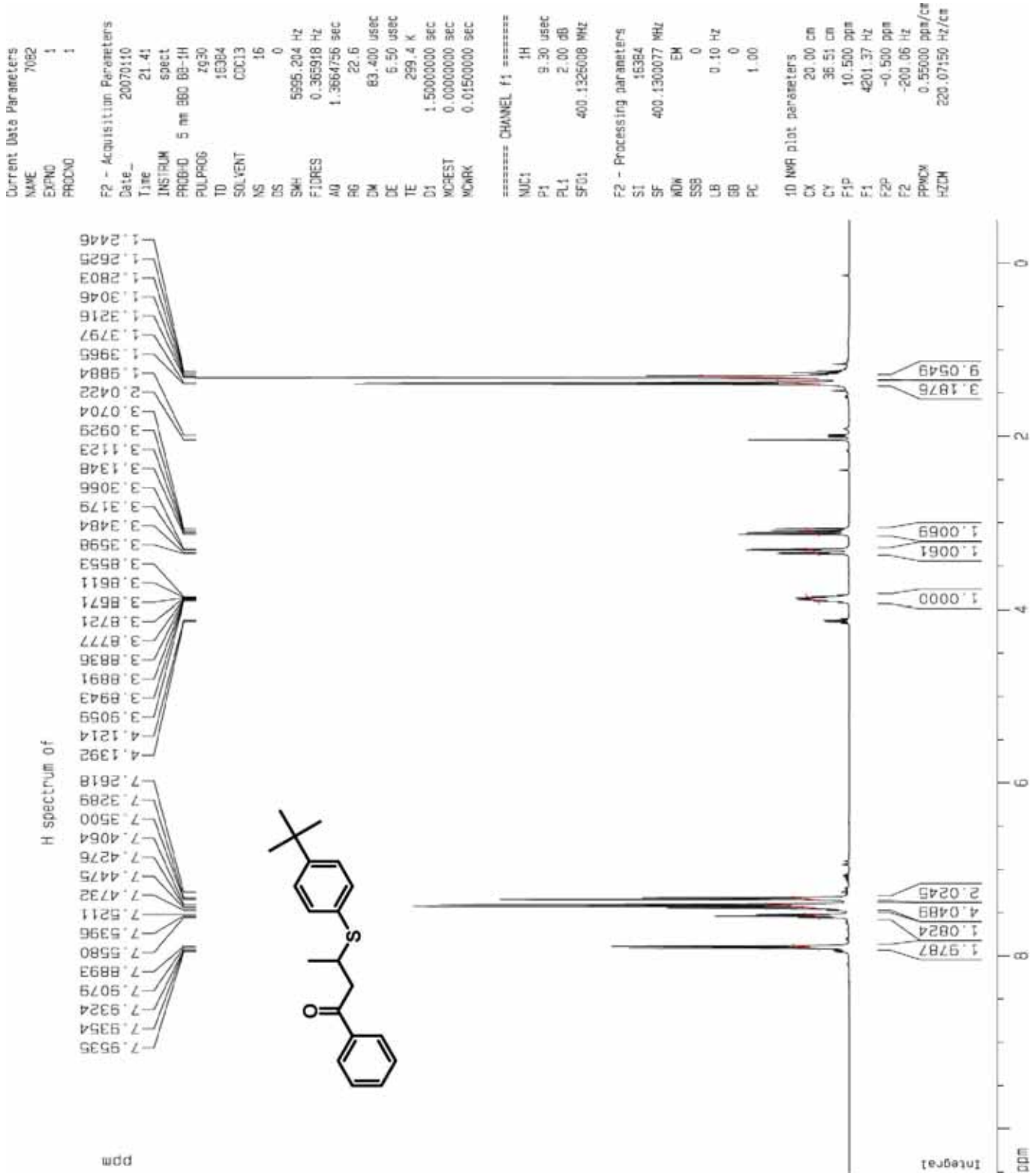

C13 spectrum of
ppm
208.74
133.75
132.69
132.27
130.56
130.35
128.79
127.84
127.61
126.77
126.59
77.55
77.23
76.91
47.89
46.21
41.00
31.42
24.14
S
O
Current Data Parameters
NAME 0518
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070518
Time 20.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 395
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 1024
DW 19.900 usec
DE 6.50 usec
TE 298.5 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127562 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.01 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58716 Hz/cm
ppm
25
50
75
100
125
150
175
200

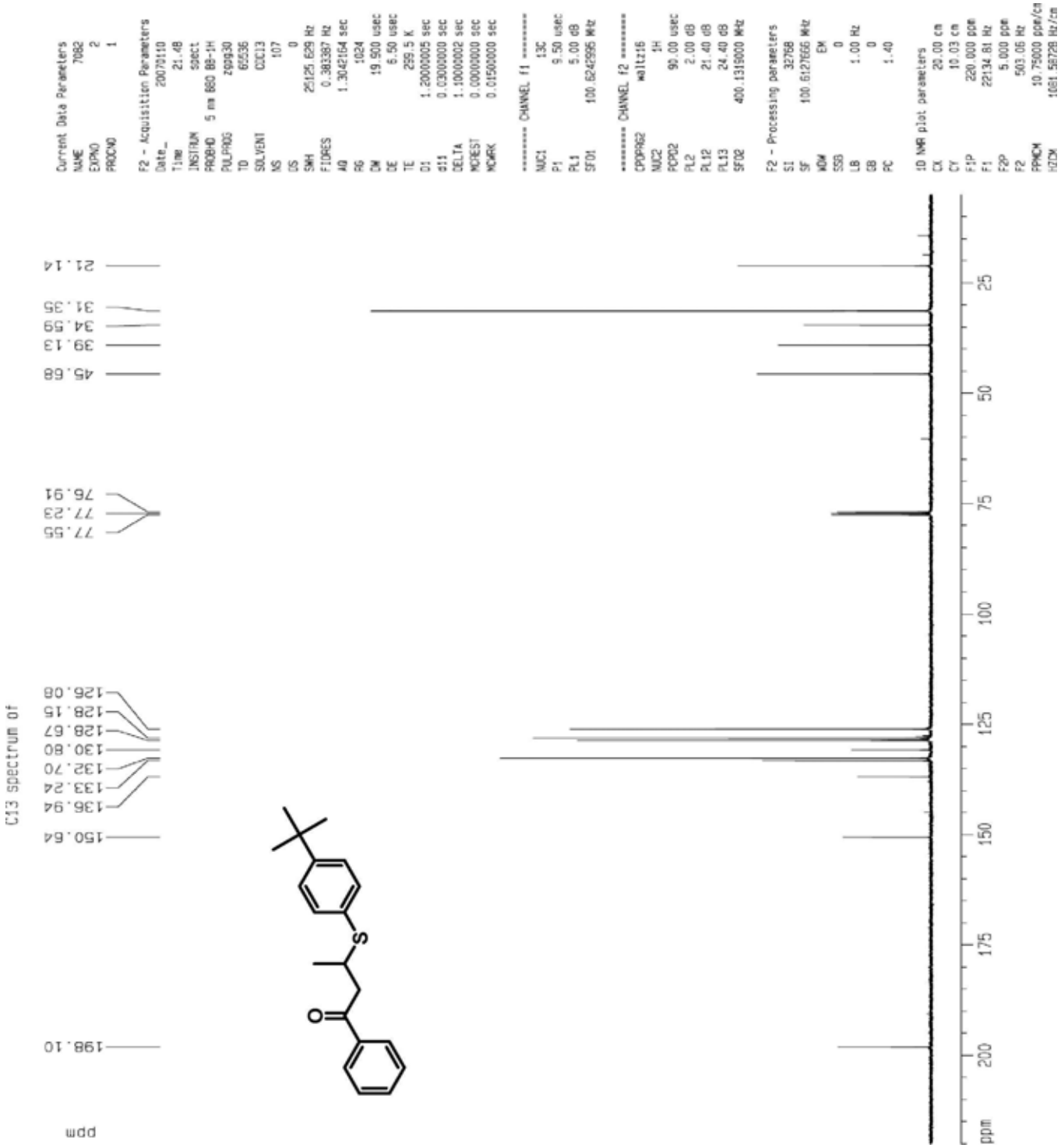

Current Data Parameters
NAME 7083 1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070113
Time 23.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.04 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
7.3028
7.2817
7.2314
7.2104
3.3671
3.3579
3.3485
2.6255
2.6148
2.5898
2.5790
2.3284
2.3025
2.2921
2.2759
2.2671
2.2520
2.2381
2.0907
2.0798
2.0667
1.6837
1.6697
1.6600
1.6450
1.6350
Cl
S
O
ppm
Integral
1.9248
1.9666
1.0000
1.0217
3.1181
2.0489
2.0437
0
2
4
6
8
ppm

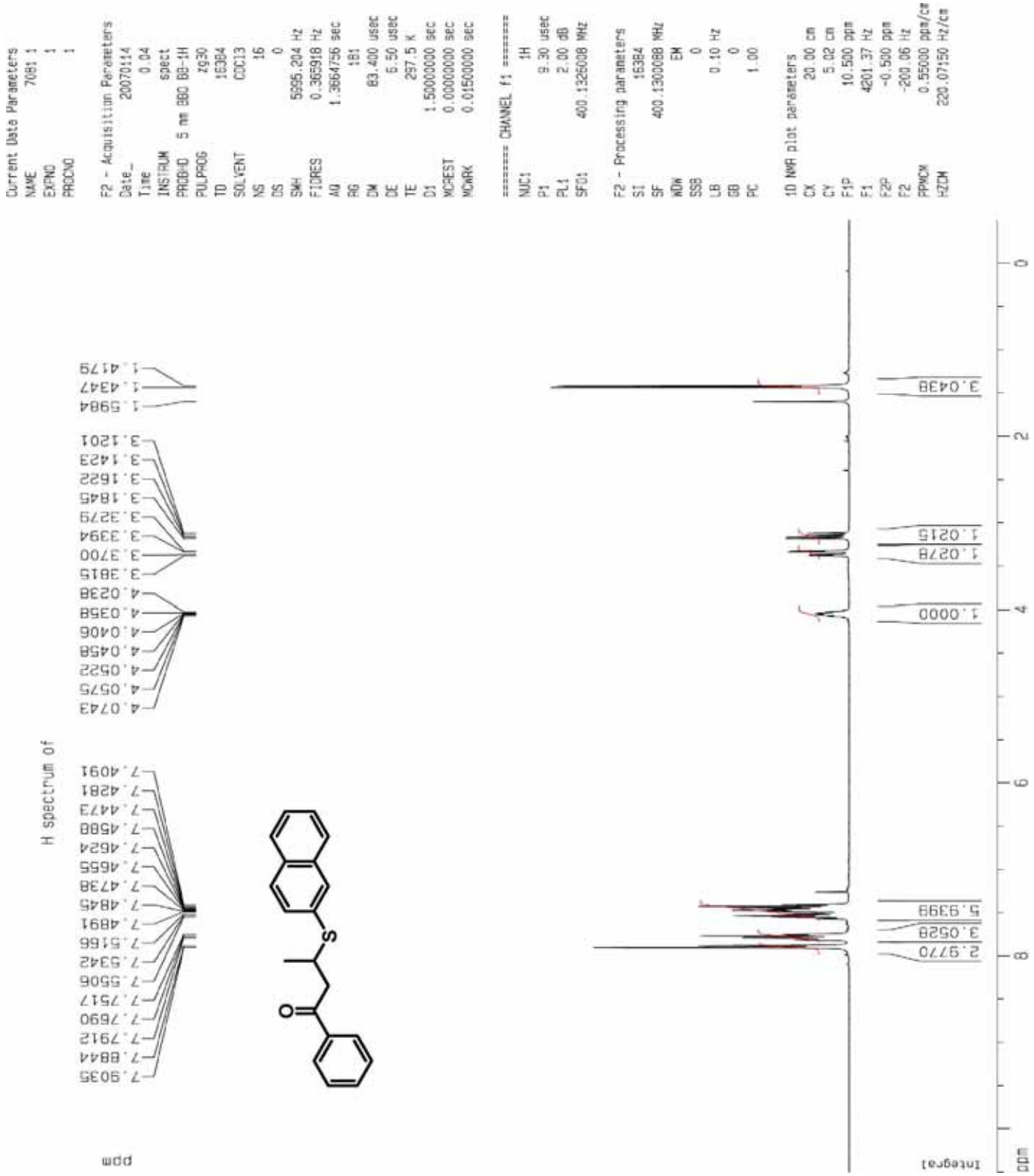

C13 spectrum of
Current Data Parameters
NAME 7083 1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070113
Time 23.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 62
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 297.6 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.02 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58728 Hz/cm
23.89
31.05
40.80
46.27
47.53
76.91
77.23
77.55
129.22
131.62
133.93
134.46
208.25
ppm
Cl
S
O
25
50
75
100
125
150
175
200
ppm


H spectrum of
Current Data Parameters
NAME 7074
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061219
Time 21.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.36 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
7.8691
7.8513
7.8481
7.5130
7.4948
7.4927
7.4204
7.3985
7.3833
6.8396
6.8350
6.8227
6.8177
3.7509
3.2470
3.2347
3.0448
3.0230
3.0031
1.3208
1.3039
OMe
S
O
ppm
Integral
3.0864
1.0018
1.0000
0.9662
3.2808
2.0700
4.1967
1.0681
1.9391
0
2
4
6
8


C13 spectrum of
ppm
198.08
159.73
136.86
135.98
133.19
128.62
128.07
124.22
114.54
77.55
77.23
76.91
55.29
45.46
40.03
21.05
OMe
S
O
Current Data Parameters
NAME 7074
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061219
Time 22.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 218
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 298.2 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.07 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58728 Hz/cm
ppm
200
150
100
50


Current Data Parameters
NAME 7082
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070110
Time 21.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 36.51 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
9.0549
3.1876
1.0069
1.0061
1.0000
2.0245
4.0489
1.0824
1.9787
S
O


C13 spectrum of
Current Data Parameters
NAME 7082
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070110
Time 21.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 107
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 1024
DW 19.900 usec
DE 6.50 usec
TE 299.5 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127666 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.03 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58728 Hz/cm
21.14
31.35
34.59
39.13
45.68
76.91
77.23
77.55
126.08
128.15
128.67
130.80
132.70
133.24
136.94
150.64
198.10
ppm
25
50
75
100
125
150
175
200
S
O


Current Data Parameters
NAME 7081 1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070114
Time 0.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 181
DW 83.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 5.02 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
7.9035
7.8844
7.7912
7.7690
7.7517
7.5506
7.5342
7.5166
7.4891
7.4845
7.4738
7.4655
7.4624
7.4588
7.4473
7.4281
7.4091
4.0743
4.0575
4.0522
4.0458
4.0406
4.0358
4.0238
3.3815
3.3700
3.3394
3.3279
3.1845
3.1622
3.1423
3.1201
1.5984
1.4347
1.4179
S
O
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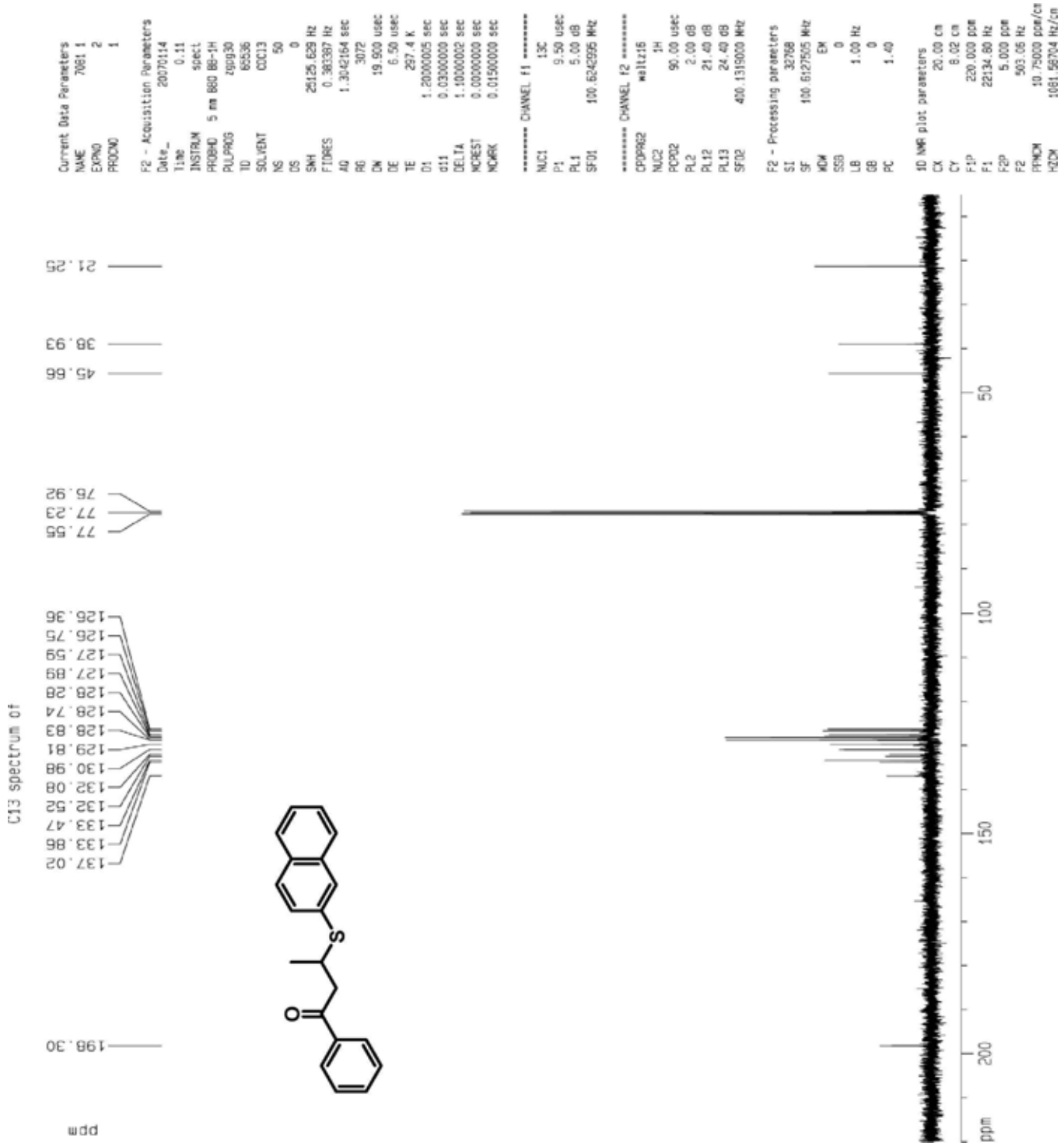
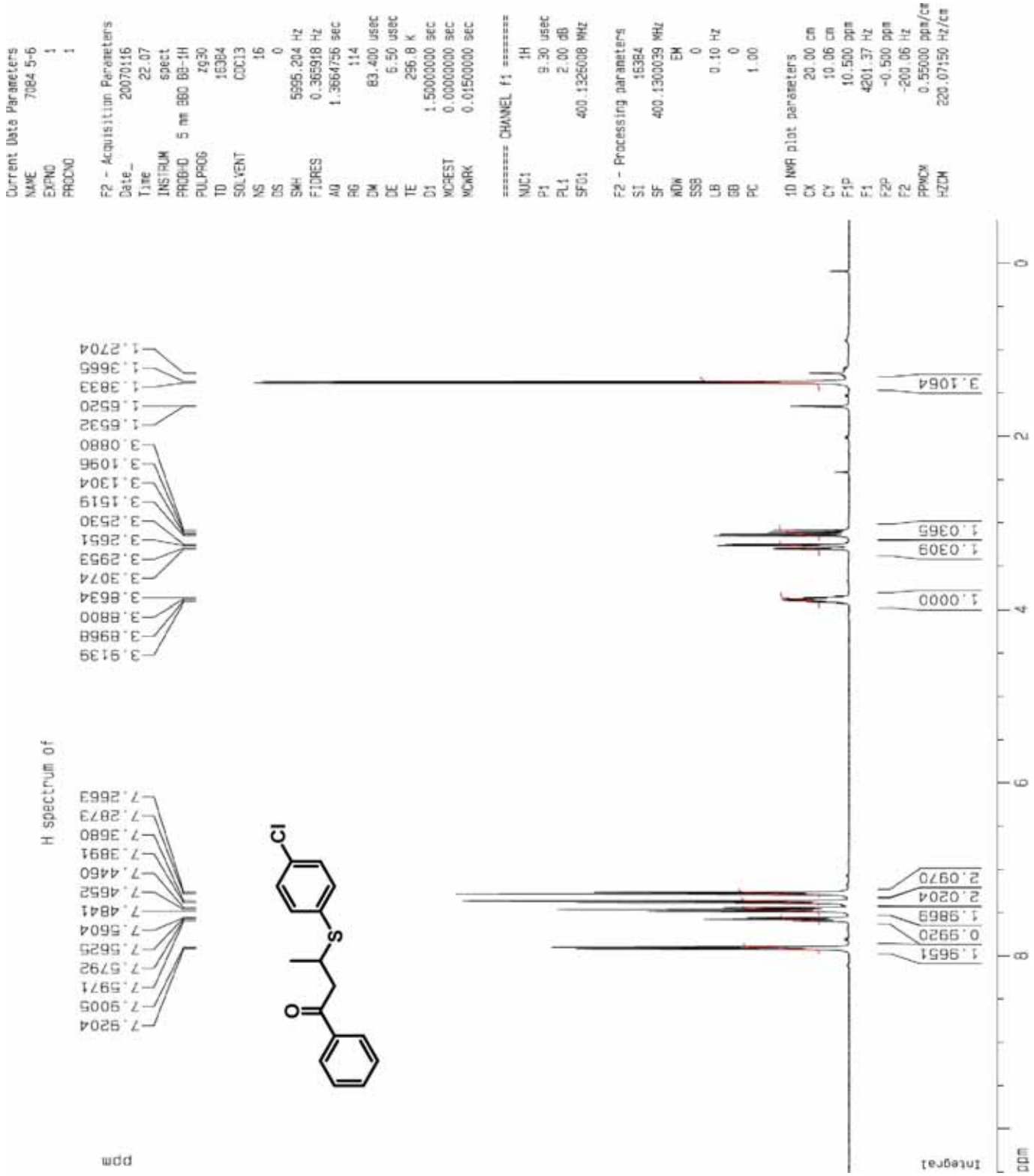
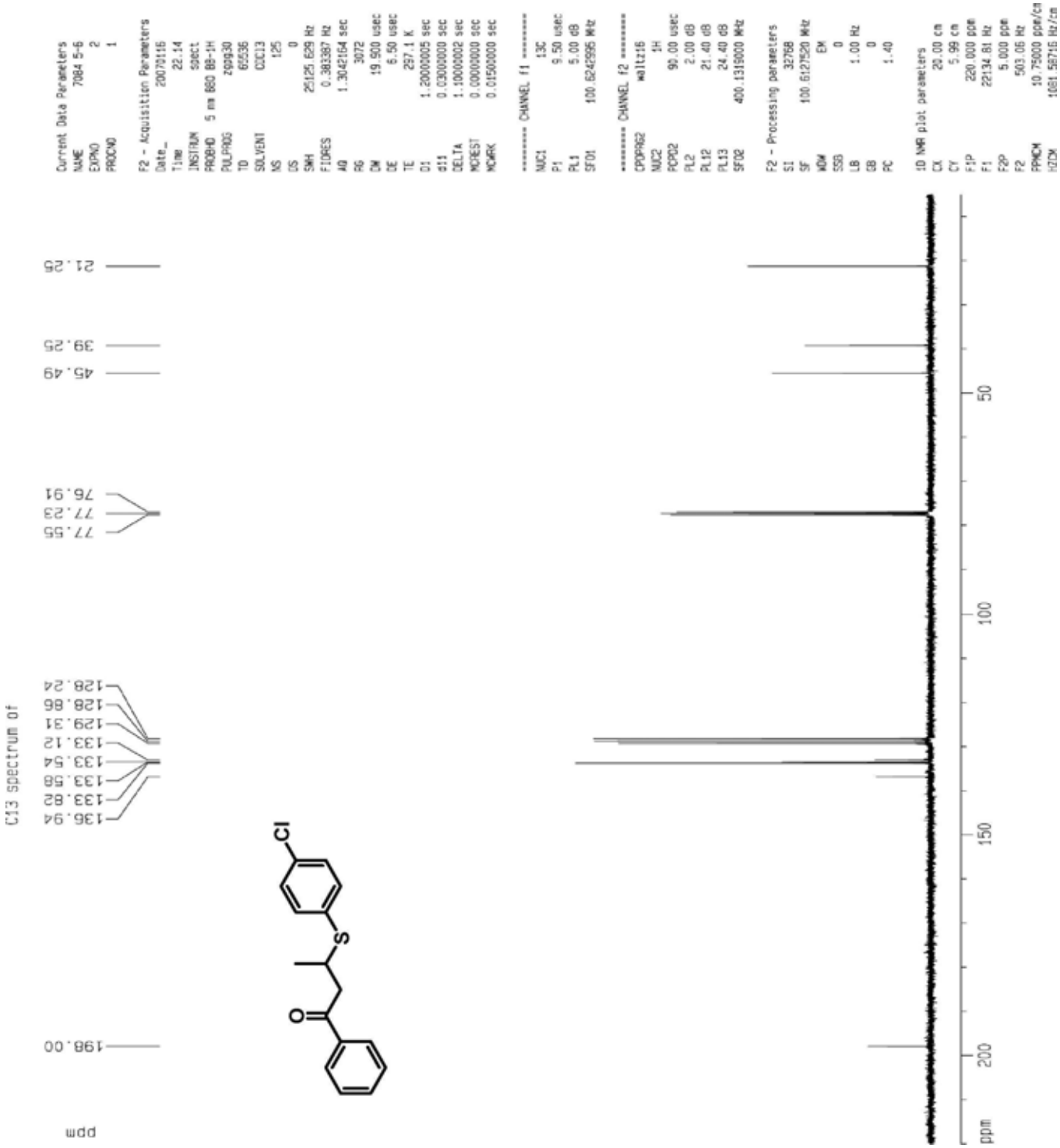
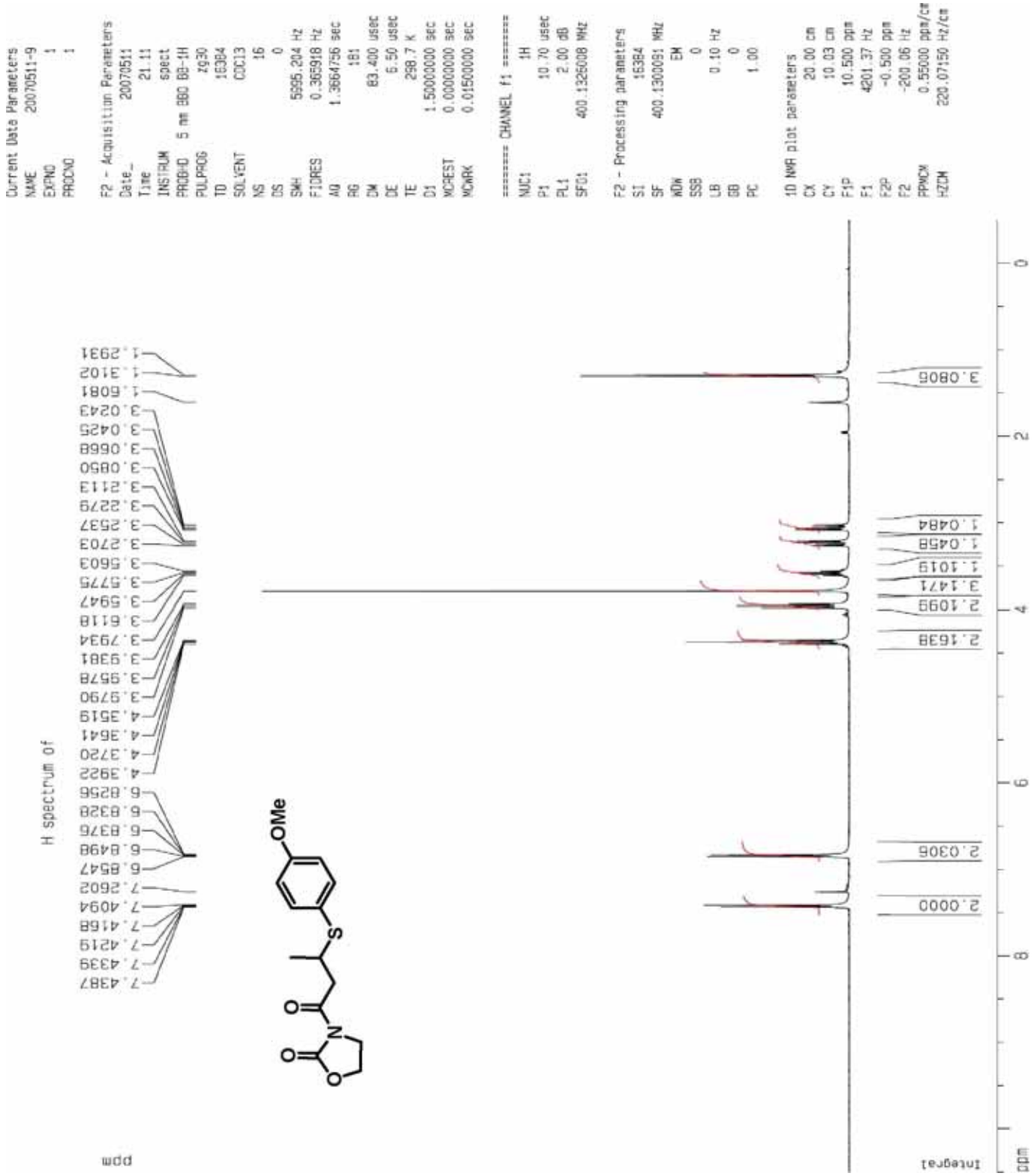
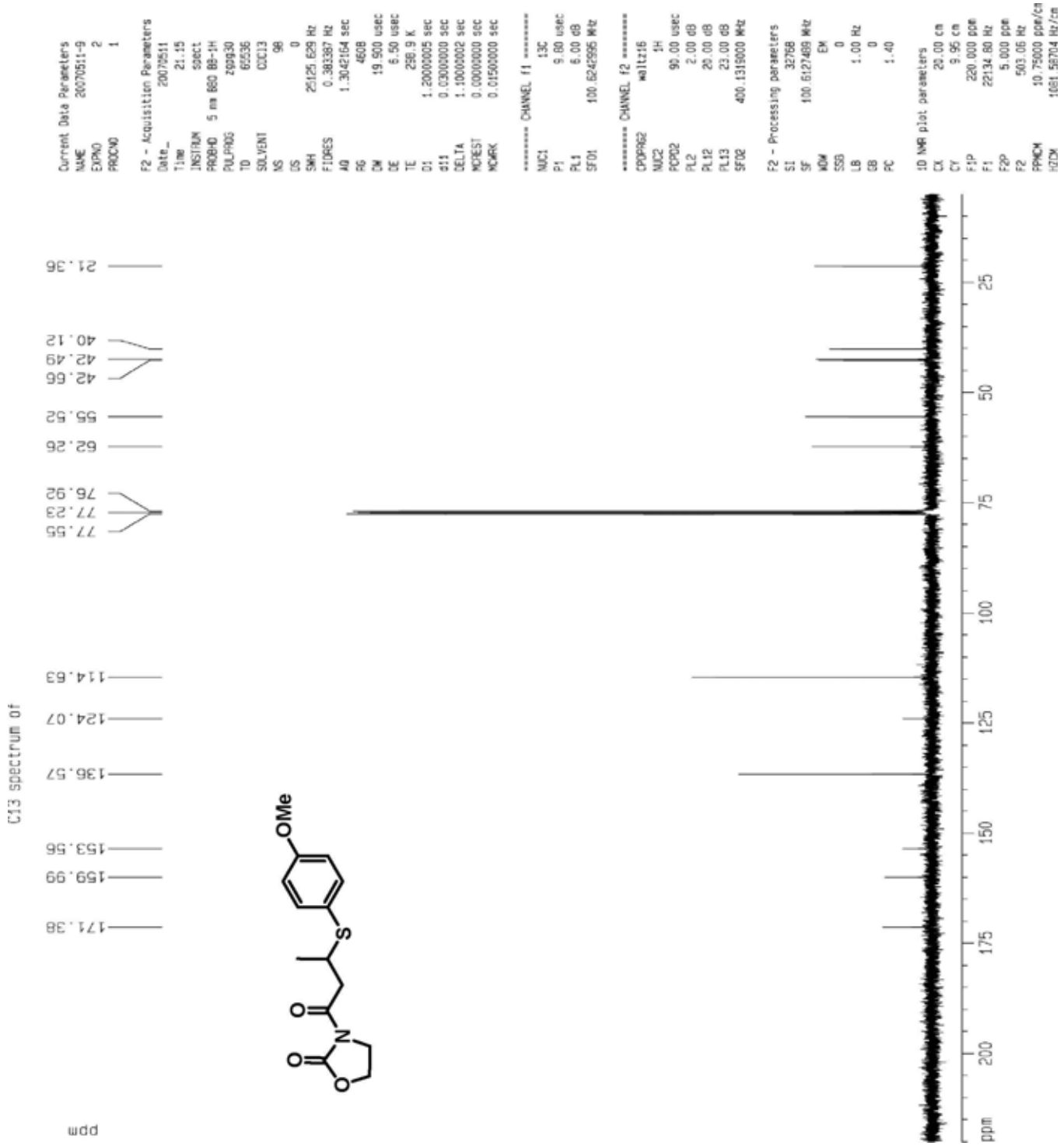
1.0000
5.9399
3.0528
2.9770
0
2
4
6
8

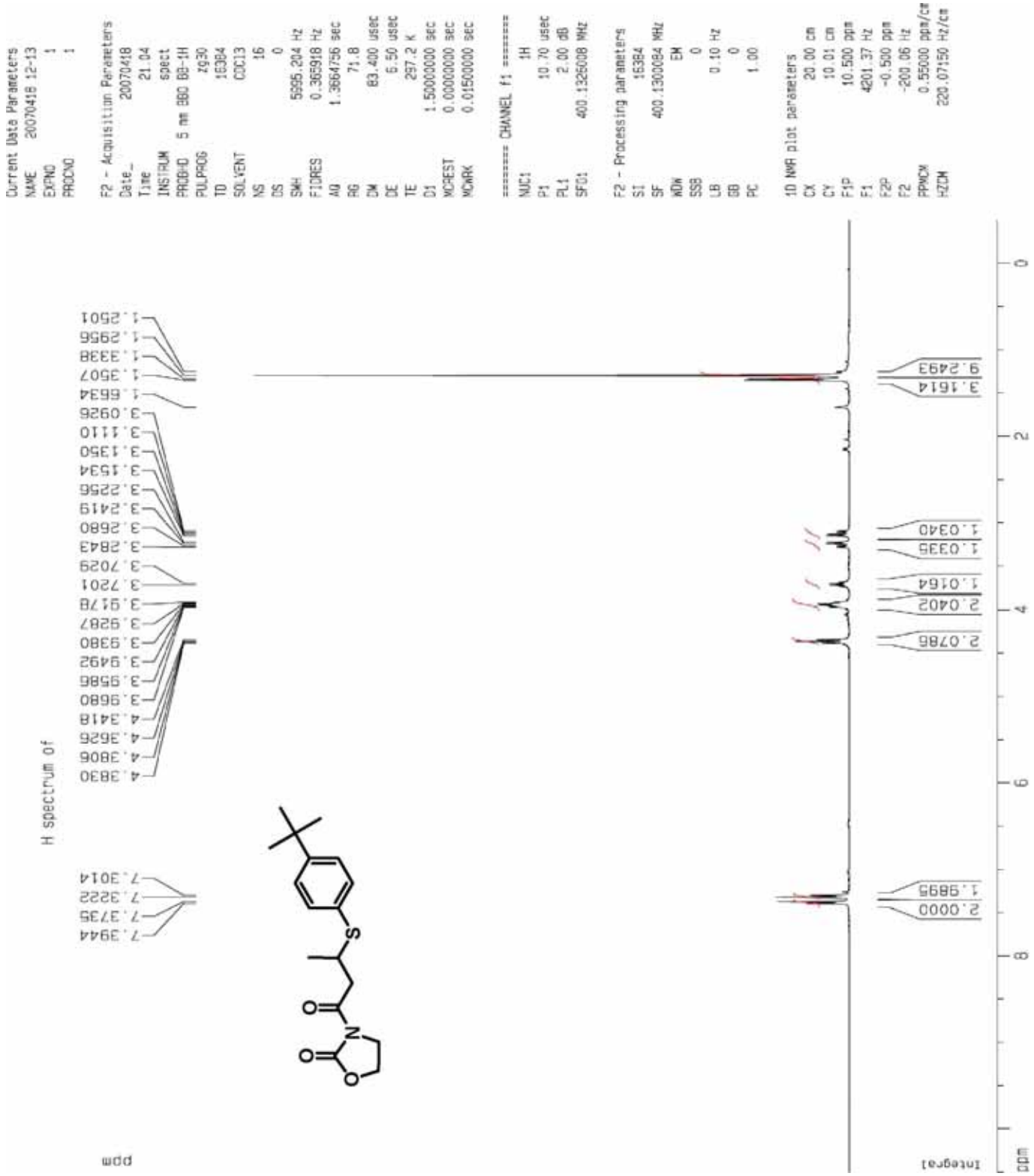

C13 spectrum of
ppm
198.30
137.02
133.86
133.47
132.52
130.98
129.81
128.83
128.74
128.28
127.89
127.59
126.75
126.36
77.55
77.23
76.92
45.66
38.93
21.25
S
O
Current Data Parameters
NAME 7061 1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070114
Time 0.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 50
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 297.4 K
D1 1.20000025 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127505 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.02 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.56704 Hz/cm
ppm
50
100
150
200

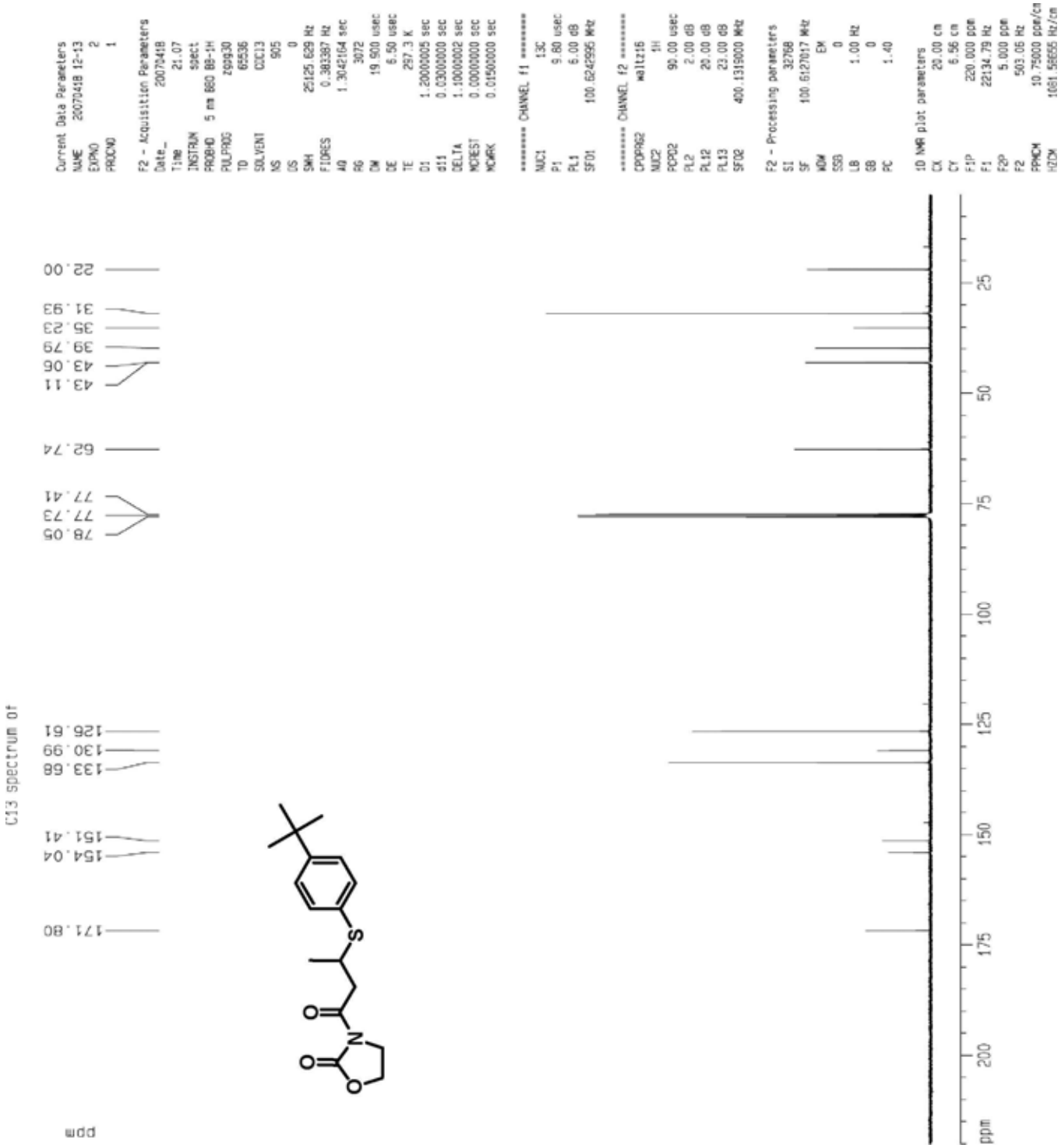

Current Data Parameters
NAME 7084 5-6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070116
Time 22.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 114
DW 83.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300039 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.06 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
7.9204
7.9005
7.5971
7.5792
7.5625
7.5504
7.4841
7.4652
7.4460
7.3891
7.3680
7.2873
7.2663
3.9139
3.8968
3.8800
3.8634
3.3074
3.2953
3.2651
3.2530
3.1519
3.1304
3.1096
3.0880
1.6532
1.6520
1.3833
1.3665
1.2704
Cl
S
O
3.1064
1.0365
1.0309
1.0000
2.0970
2.0204
1.9869
0.9920
1.9651
ppm
Integral
ppm

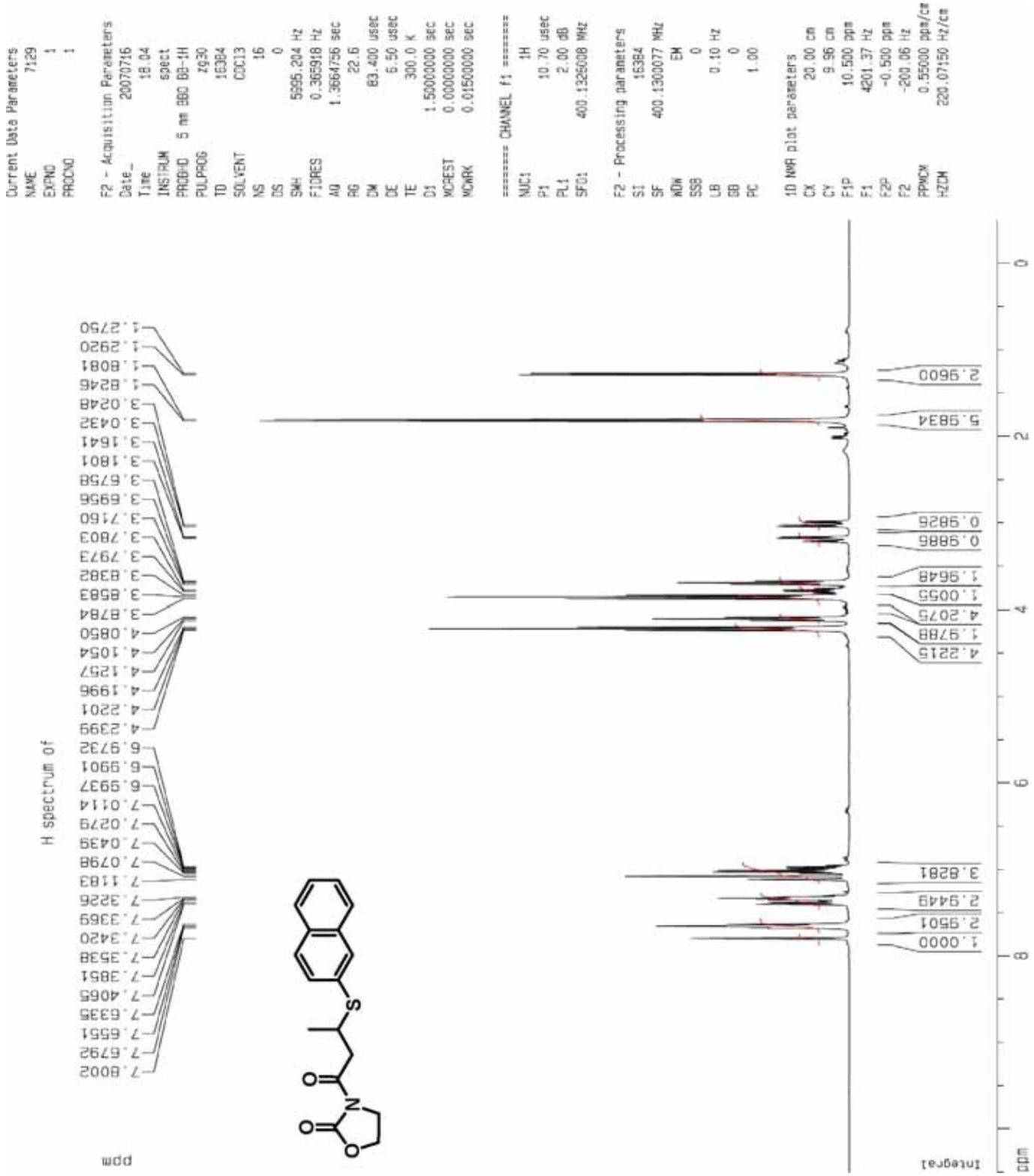

C13 spectrum of
Current Data Parameters
NAME 7084 5-6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070116
Time 22.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 125
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 297.1 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.99 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58716 Hz/cm
198.00
136.94
133.82
133.58
133.54
133.12
129.31
128.86
128.24
77.55
77.23
76.91
45.49
39.25
21.25
ppm
50
100
150
200
ppm
Cl
S
O

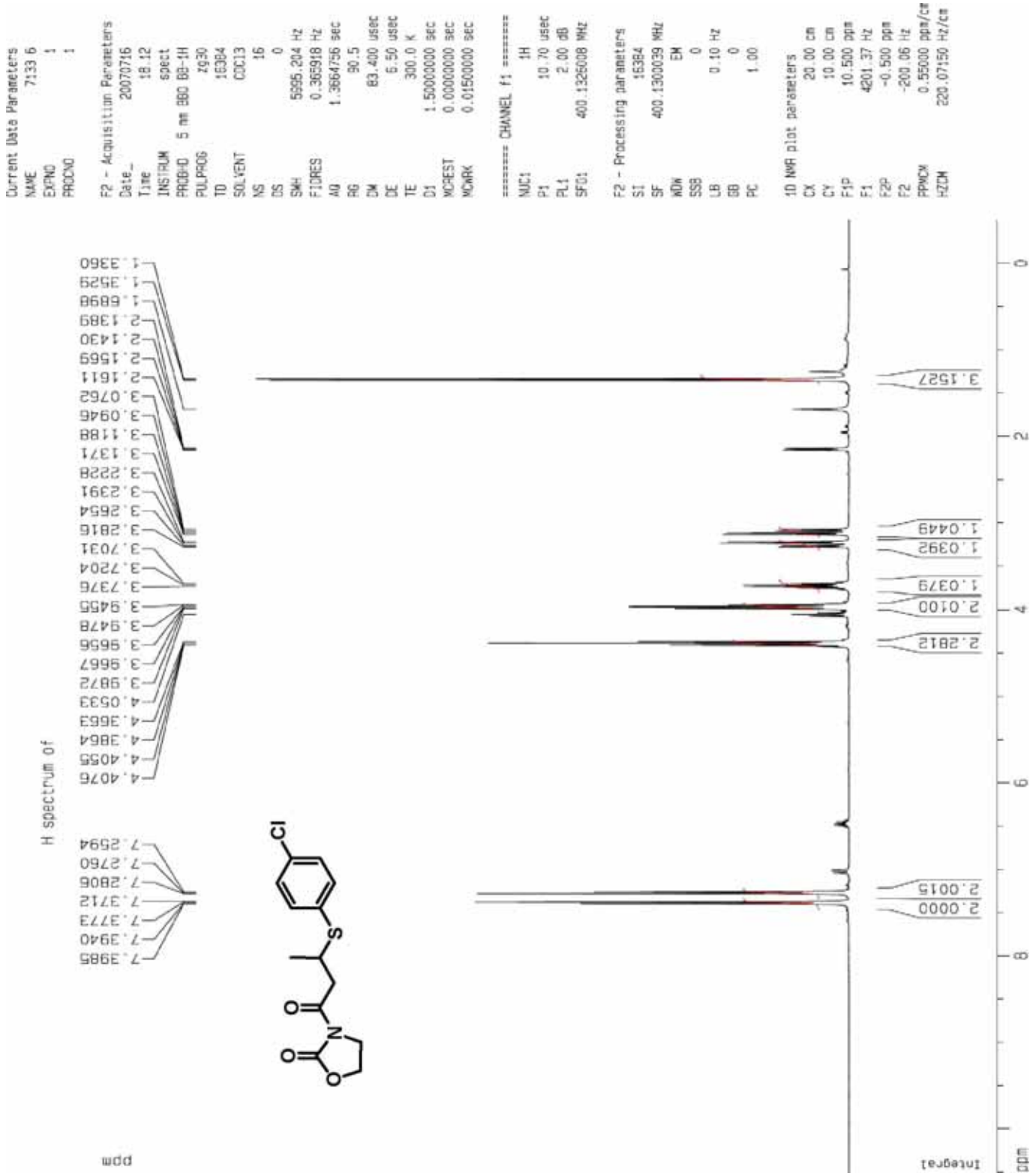

Current Data Parameters
NAME 20070511-9
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070511
Time 21.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 181
DW 83.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.03 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
OMe
S
O
N
O
O
7.4387
7.4339
7.4219
7.4168
7.4094
7.2602
6.8547
6.8498
6.8376
6.8328
6.8256
4.3922
4.3720
4.3641
4.3519
3.9790
3.9578
3.9381
3.7934
3.6118
3.5947
3.5775
3.5603
3.2703
3.2537
3.2279
3.2113
3.0850
3.0668
3.0425
3.0243
1.6081
1.3102
1.2931
3.0805
1.0484
1.0458
1.1019
3.1471
2.1099
2.1638
2.0306
2.0000
integral
ppm
0
2
4
6
8
ppm

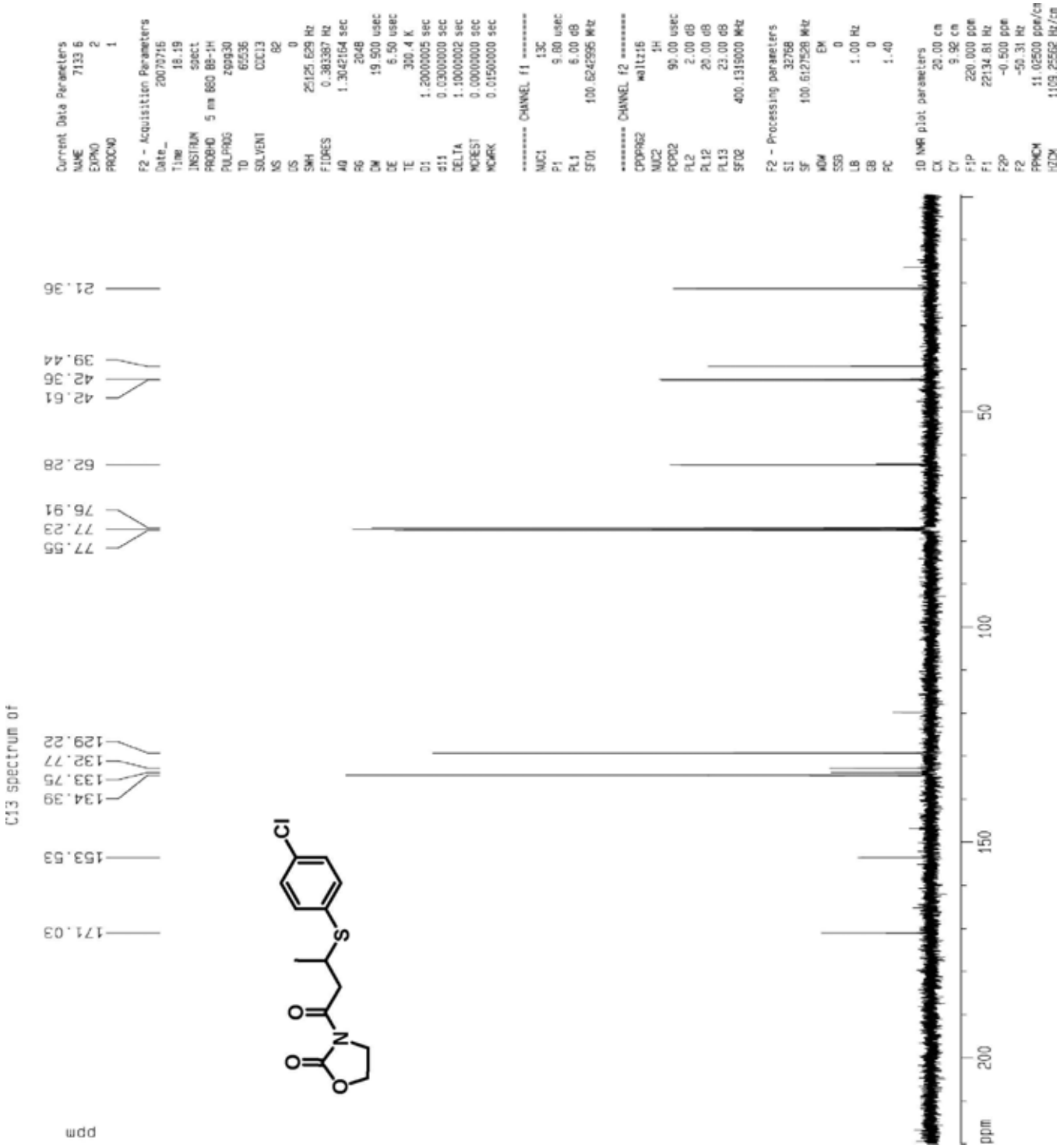

C13 spectrum of
ppm
171.38
159.99
153.56
136.57
124.07
114.63
77.55
77.23
76.92
62.26
55.52
42.66
42.49
40.12
21.36
OMe
S
O
N
O
O
Current Data Parameters
NAME 20070511-9
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070511
Time 21.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 98
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4608
DW 19.900 usec
DE 6.50 usec
TE 298.9 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127489 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 9.95 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58704 Hz/cm
ppm
25
50
75
100
125
150
175
200

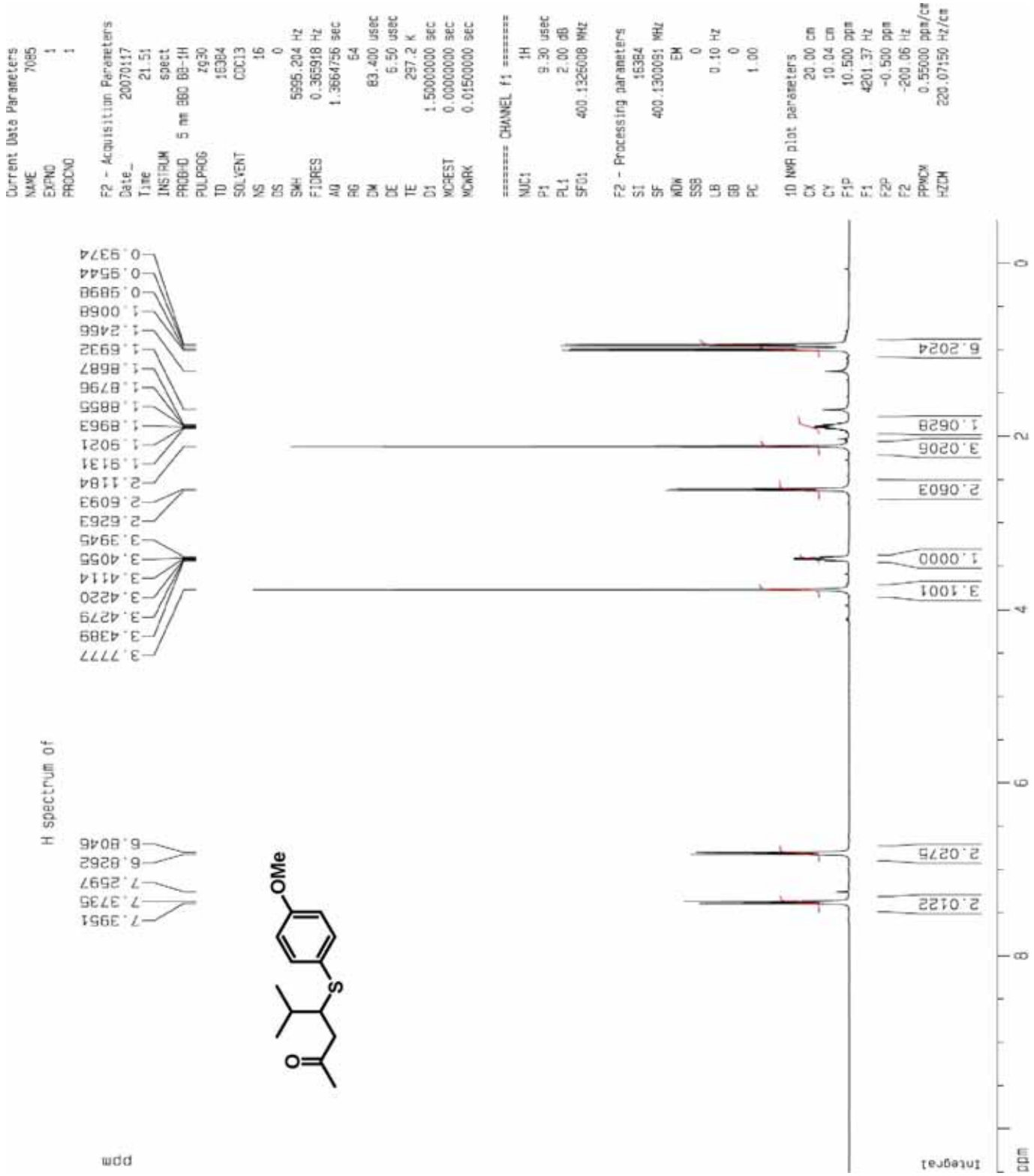

Current Data Parameters
NAME 20070418 12-13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070418
Time 21.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 71.8
DW 83.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.01 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
7.3944
7.3735
7.3222
7.3014
4.3830
4.3806
4.3626
4.3418
3.9680
3.9586
3.9492
3.9380
3.9287
3.9178
3.7201
3.7029
3.2843
3.2680
3.2419
3.2256
3.1534
3.1350
3.1110
3.0926
1.6534
1.3507
1.3338
1.2956
1.2501
9.2493
3.1614
1.0340
1.0335
1.0164
2.0402
2.0786
1.9895
2.0000
Integral
ppm
0
2
4
6
8

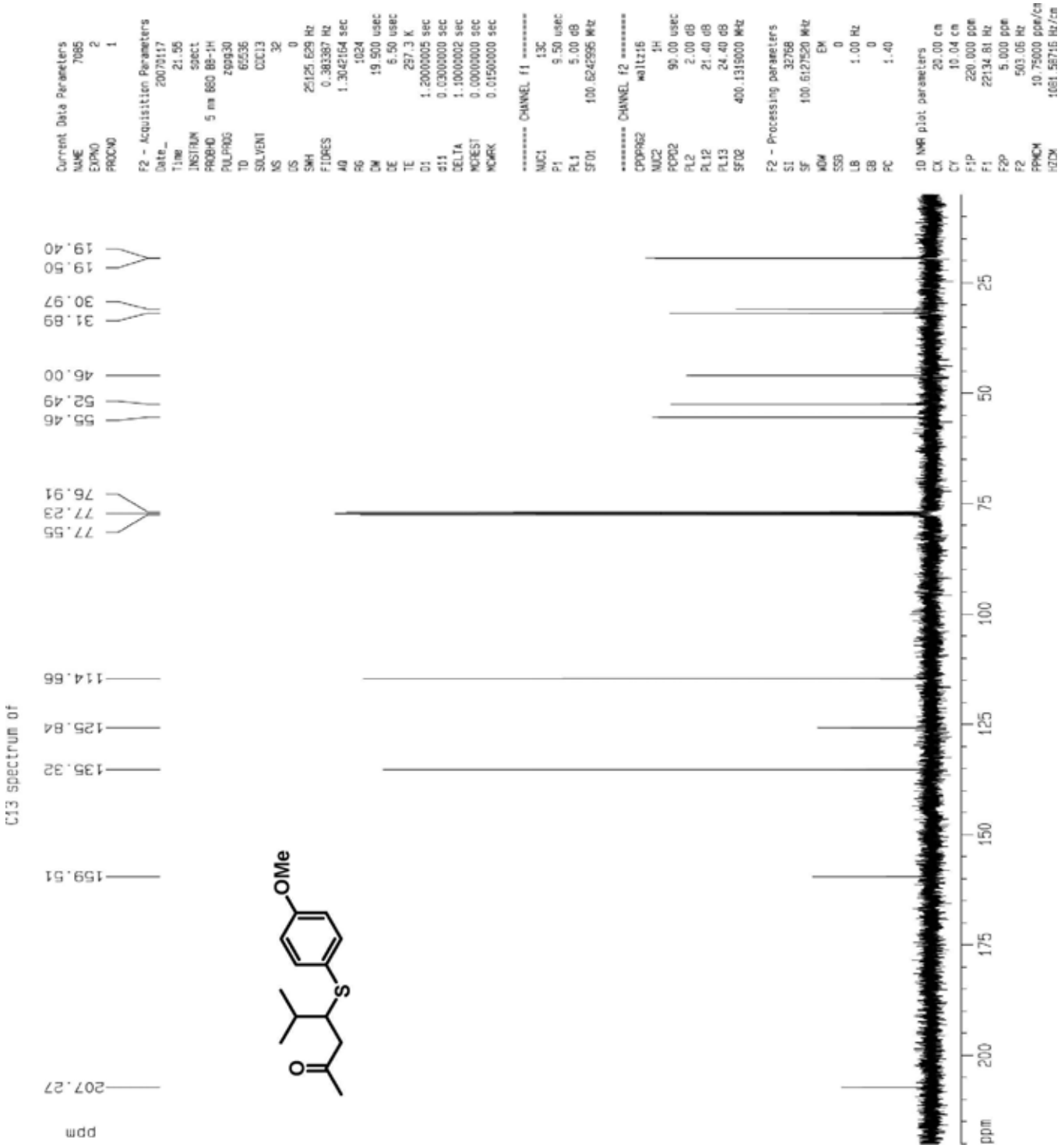

C13 spectrum of
Current Data Parameters
NAME 20070418 12-13
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070418
Time 21.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 905
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 3072
DW 19.900 usec
DE 6.50 usec
TE 297.3 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127017 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.56 cm
F1P 220.000 ppm
F1 22134.79 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58656 Hz/cm
22.00
31.93
35.23
39.79
43.06
43.11
62.74
77.41
77.73
78.05
126.61
130.99
133.68
151.41
154.04
171.80
ppm
25
50
75
100
125
150
175
200
ppm
S
O
O
N
O

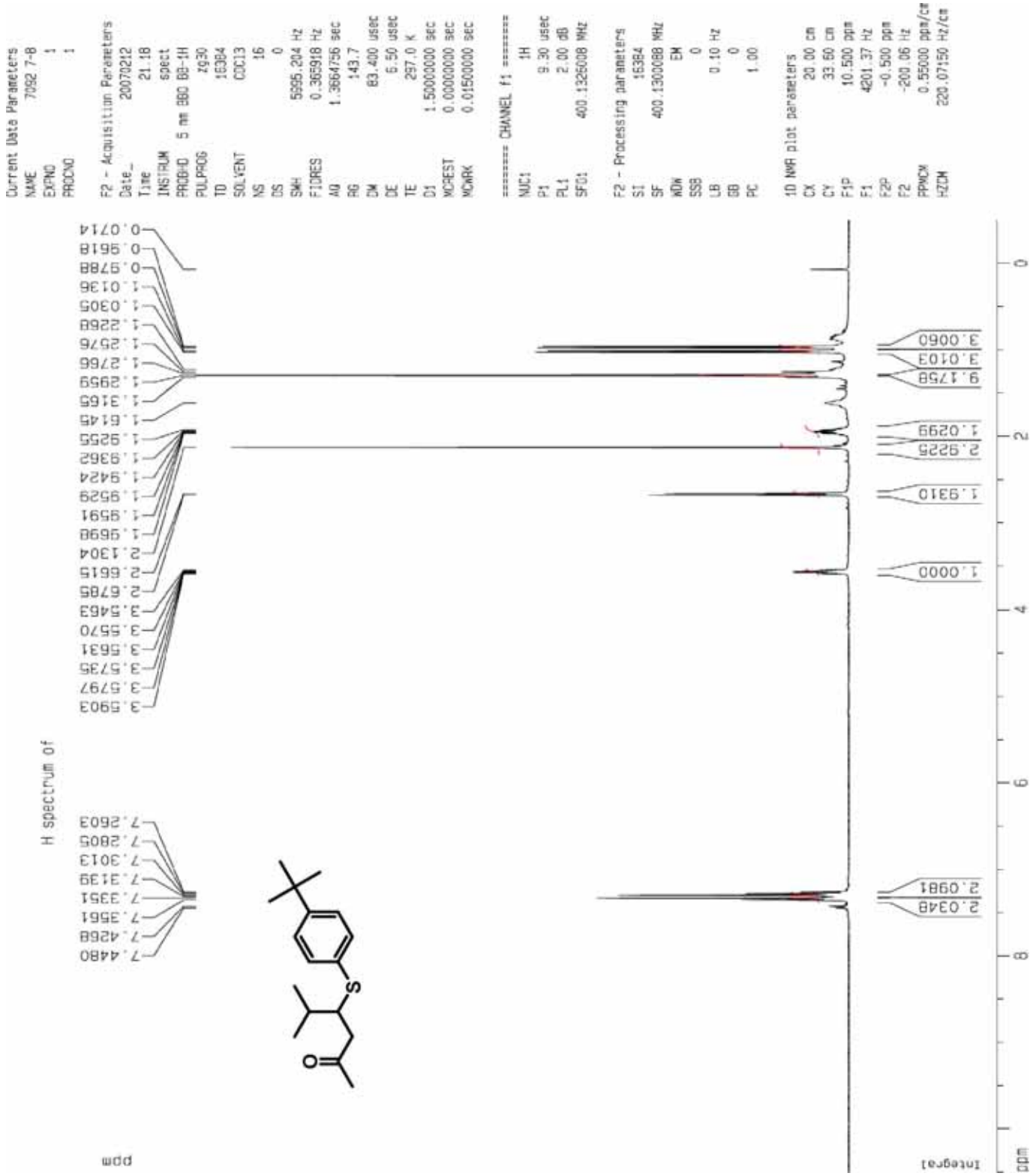

Current Data Parameters
NAME 7129
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 18.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 22.6
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.96 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
7.8002
7.6792
7.6551
7.6335
7.4065
7.3851
7.3538
7.3420
7.3369
7.3226
7.1183
7.0798
7.0439
7.0279
7.0114
6.9937
6.9901
6.9732
4.2399
4.2201
4.1996
4.1257
4.1054
4.0850
3.8784
3.8583
3.8382
3.7973
3.7803
3.7160
3.6956
3.6758
3.1801
3.1641
3.0432
3.0248
1.8246
1.8081
1.2920
1.2750
2.9600
5.9834
0.9826
0.9886
1.9648
1.0055
4.2075
1.9788
4.2215
3.8281
2.9449
2.9501
1.0000
S
O
N
O
O

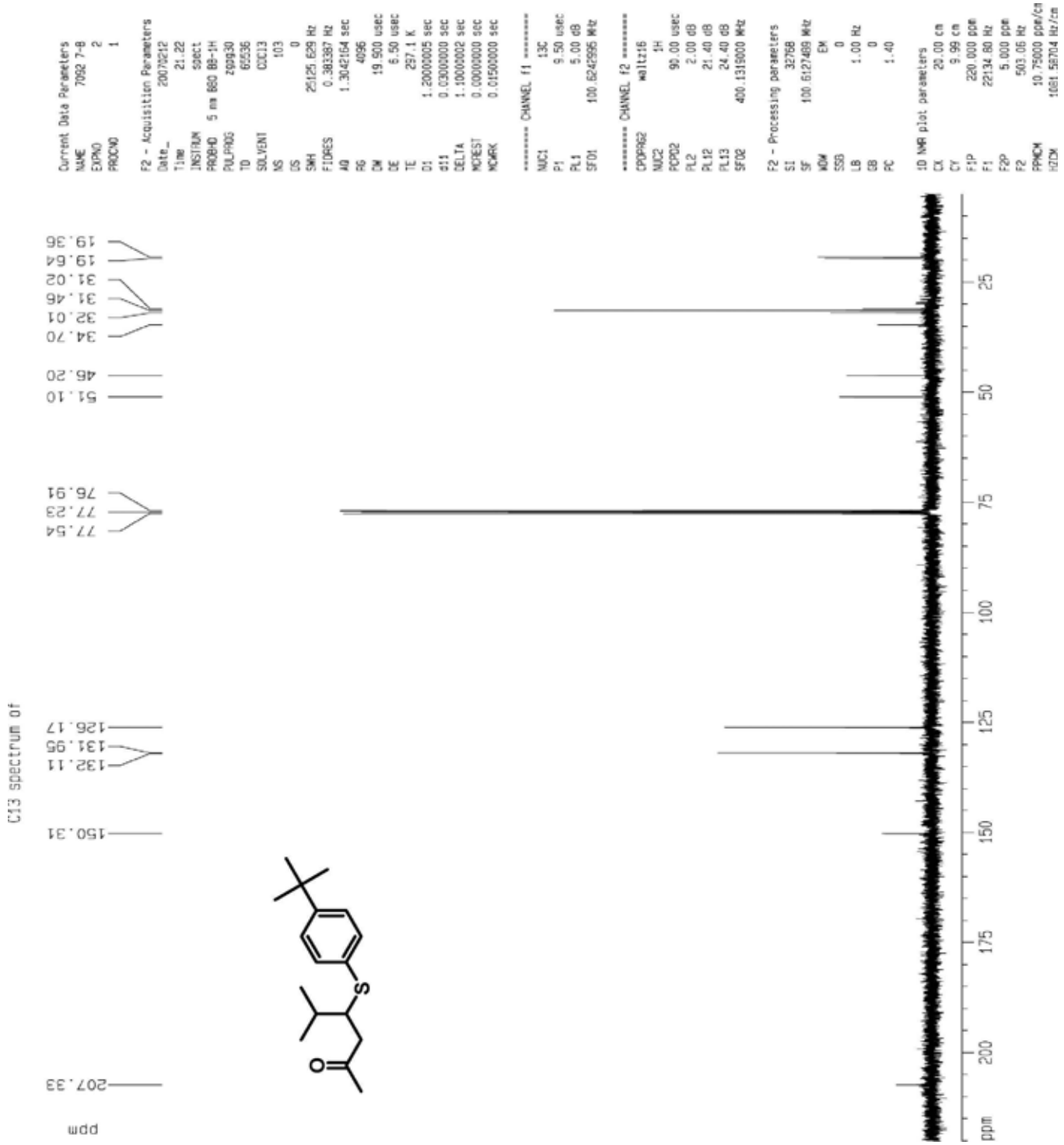

Current Data Parameters
NAME 7133 6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 18.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 90.5
DW 83.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300039 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
7.3985
7.3940
7.3773
7.3712
7.2806
7.2760
7.2594
4.4076
4.4055
4.3864
4.3653
4.0533
3.9872
3.9667
3.9656
3.9478
3.9455
3.7376
3.7204
3.7031
3.2816
3.2654
3.2391
3.2228
3.1371
3.1188
3.0946
3.0762
2.1611
2.1569
2.1430
2.1389
1.6898
1.3529
1.3360
Cl
S
O
N
O
O
3.1527
1.0449
1.0392
1.0379
2.0100
2.2812
2.0015
2.0000
ppm
Integral
0
2
4
6
8

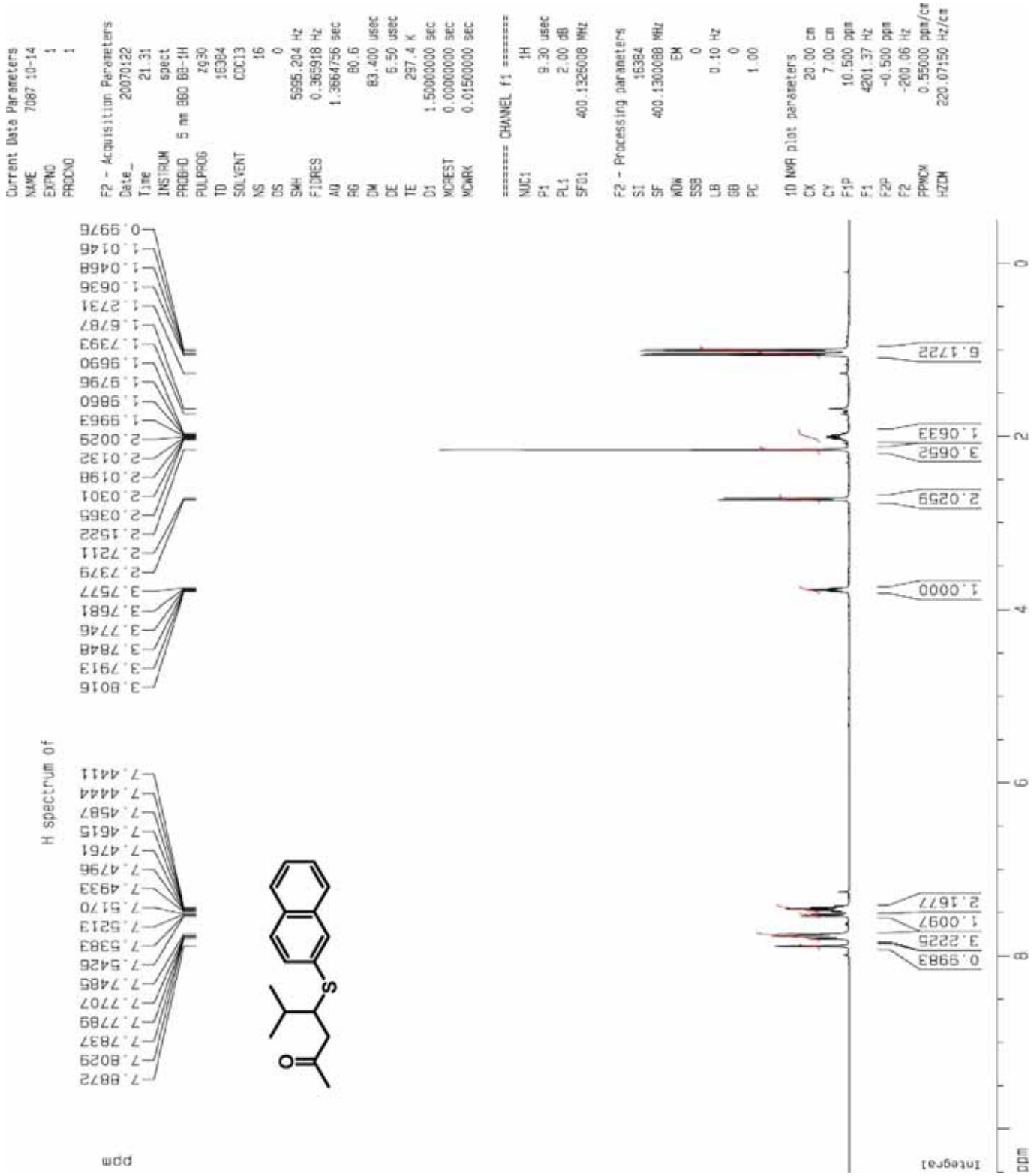

C13 spectrum of
171.03
153.53
134.39
133.75
132.77
129.22
77.55
77.23
76.91
62.28
42.61
42.36
39.44
21.36
ppm
200
150
100
50
Current Data Parameters
NAME 7133 6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 18.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 82
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042154 sec
RG 2048
DW 19.900 usec
DE 6.50 usec
TE 300.4 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127528 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 9.92 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -0.500 ppm
F2 -50.31 Hz
PPMCM 11.02500 ppm/cm
HZCM 1109.25552 Hz/cm

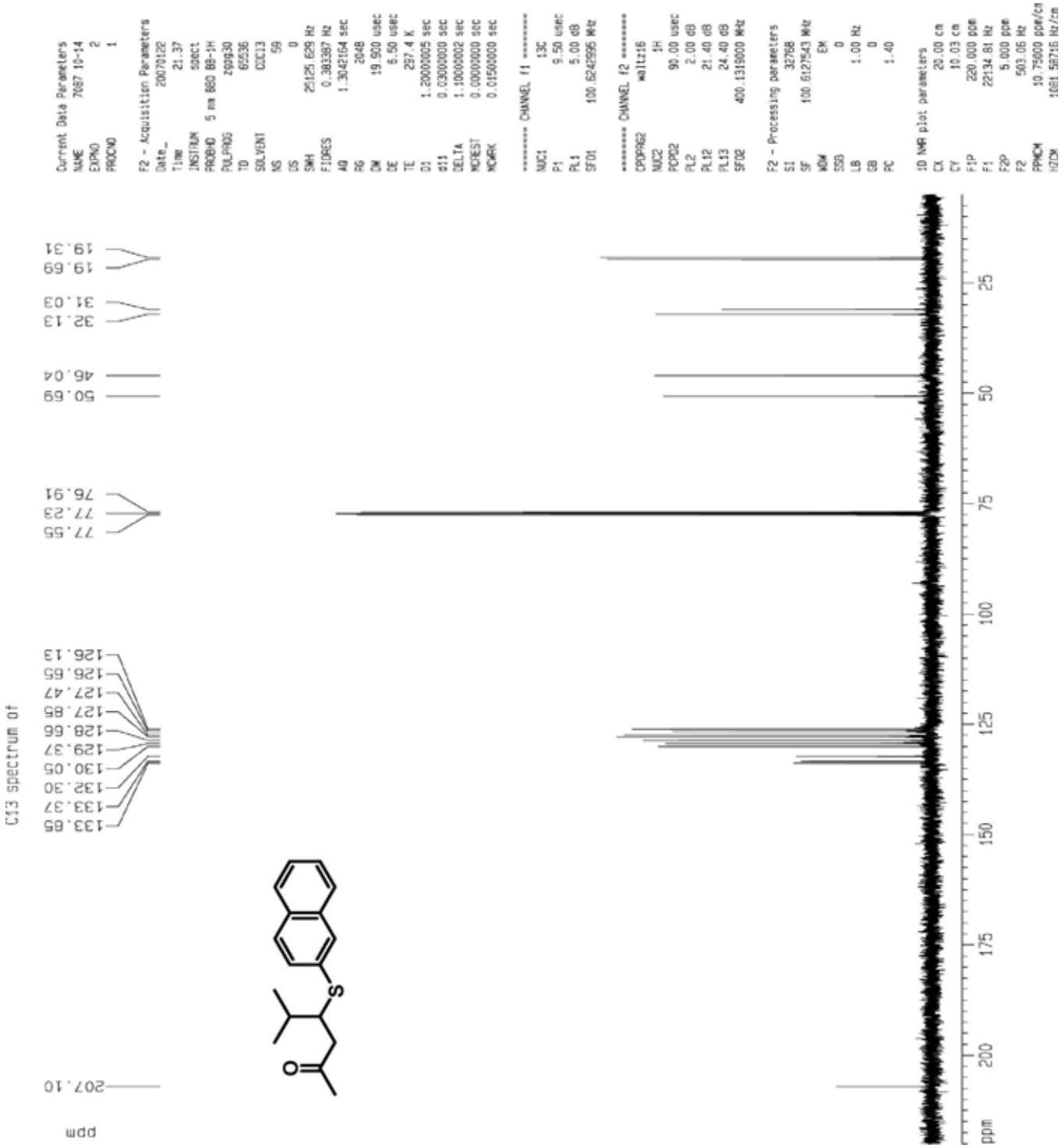

Current Data Parameters
NAME 7085
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070117
Time 21.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 64
DW 83.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.04 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
OMe
S
O
ppm
Integral

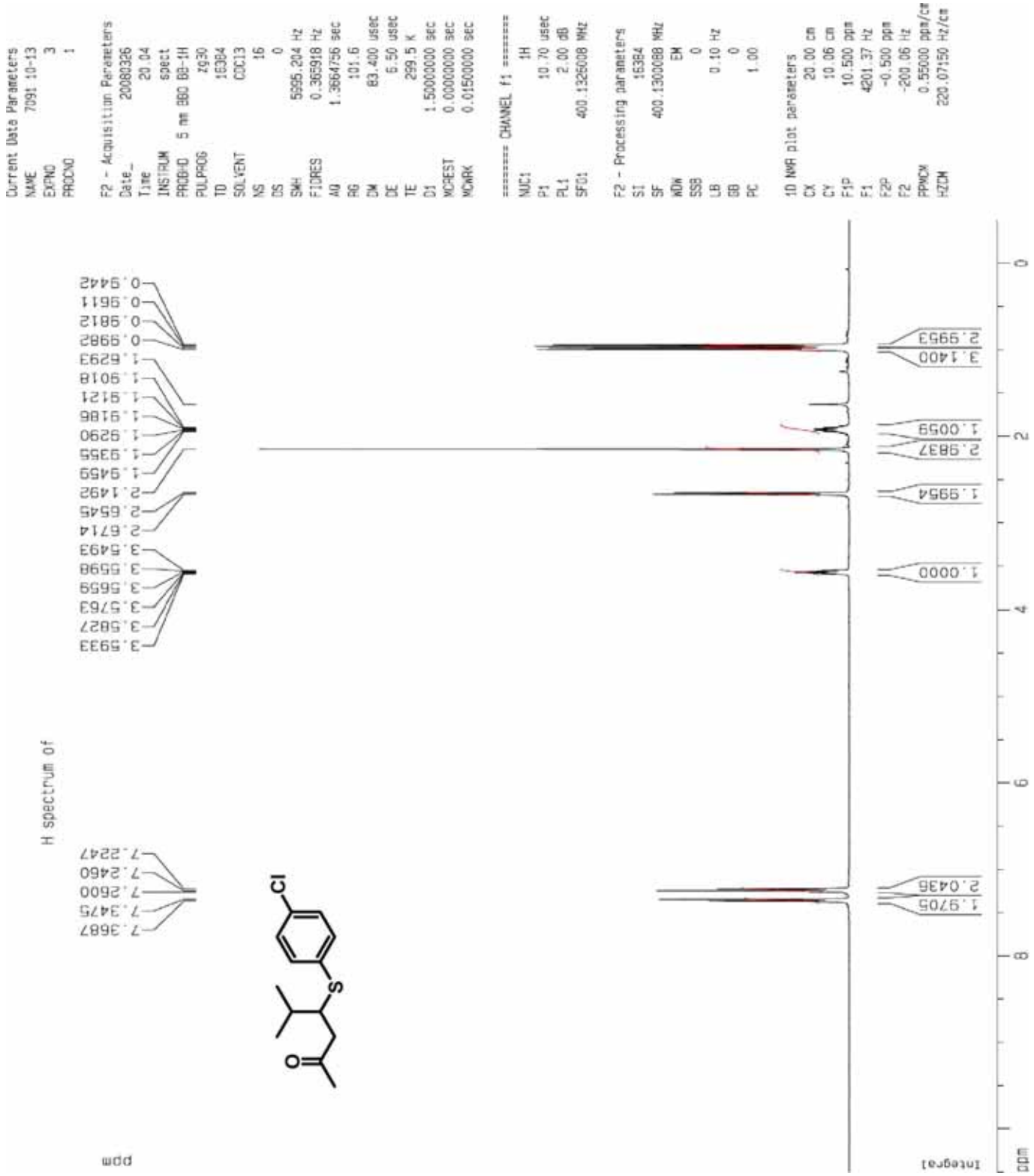

C13 spectrum of
ppm
207.27
159.51
135.32
125.84
114.66
77.55
77.23
76.91
55.46
52.49
46.00
31.89
30.97
19.50
19.40
OMe
S
O
Current Data Parameters
NAME 7085
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070117
Time 21.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 1024
DW 19.900 usec
DE 6.50 usec
TE 297.3 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.04 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58716 Hz/cm
25
50
75
100
125
150
175
200
ppm

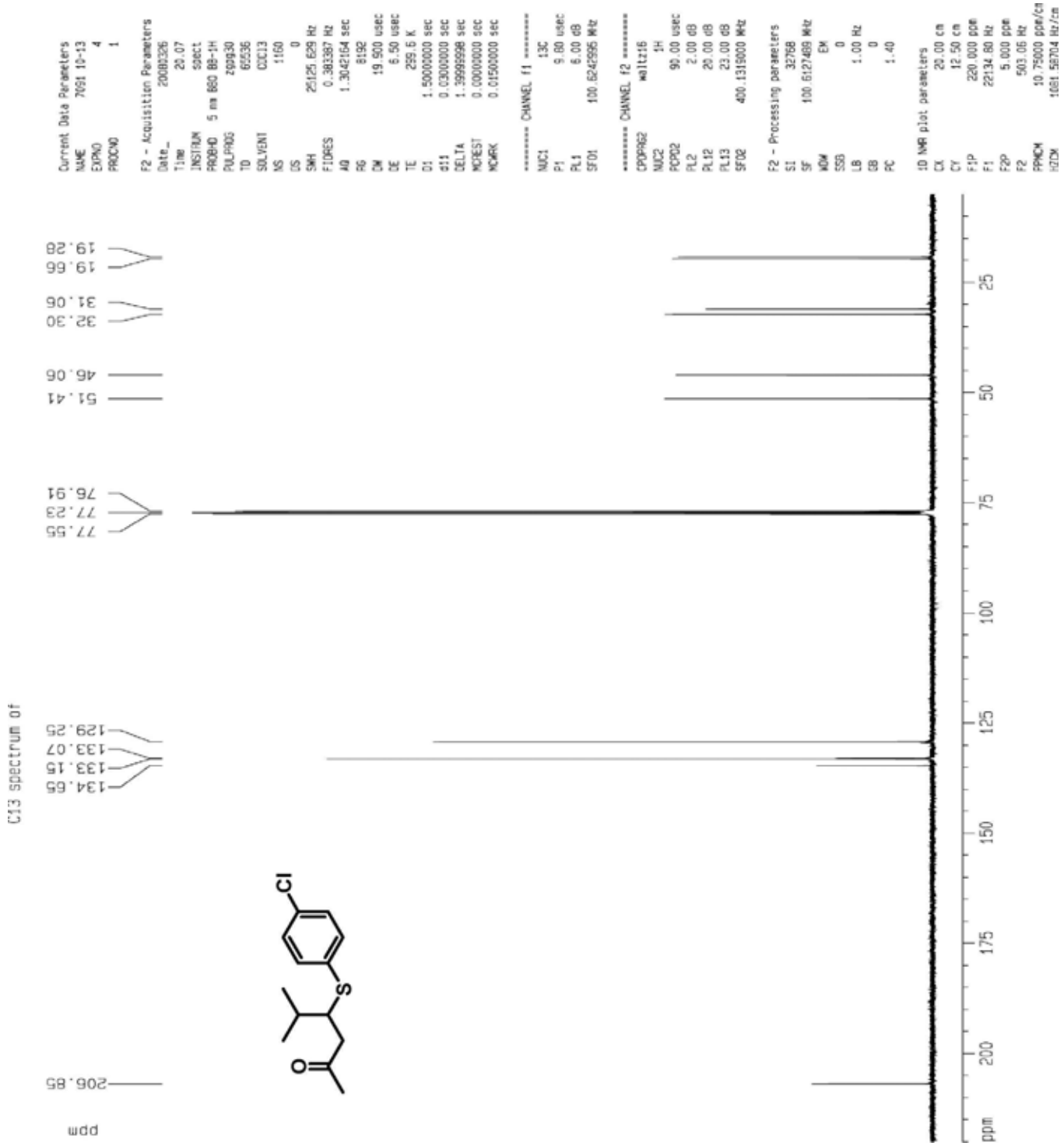

Current Data Parameters
NAME 7092 7-8
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070212
Time 21.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 143.7
DW 83.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 33.60 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
7.4480
7.4268
7.3561
7.3351
7.3139
7.3013
7.2805
7.2603
3.5903
3.5797
3.5735
3.5631
3.5570
3.5463
2.6785
2.6615
2.1304
1.9698
1.9591
1.9529
1.9424
1.9362
1.9255
1.6145
1.3165
1.2959
1.2766
1.2576
1.2268
1.0305
1.0136
0.9788
0.9618
0.0714
2.0348
2.0981
1.0000
1.9310
2.9225
1.0299
9.1758
3.0103
3.0060
0
2
4
6
8


C13 spectrum of
ppm
207.33
150.31
132.11
131.95
126.17
77.54
77.23
76.91
51.10
46.20
34.70
32.01
31.46
31.02
19.64
19.36
S
O
Current Data Parameters
NAME 7092 7-8
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070212
Time 21.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 4096
DW 19.900 usec
DE 6.50 usec
TE 297.1 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127489 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 9.99 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58704 Hz/cm
ppm
25
50
75
100
125
150
175
200


Current Data Parameters
NAME 7087 10-14
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070122
Time 21.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 80.6
DW 83.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
7.8872
7.8029
7.7837
7.7789
7.7707
7.7485
7.5426
7.5383
7.5213
7.5170
7.4933
7.4796
7.4761
7.4615
7.4587
7.4444
7.4411
3.8016
3.7913
3.7848
3.7746
3.7681
3.7577
2.7379
2.7211
2.1522
2.0365
2.0301
2.0198
2.0132
2.0029
1.9963
1.9860
1.9796
1.9690
1.7393
1.6787
1.2731
1.0636
1.0468
1.0146
0.9976
6.1722
1.0633
3.0652
2.0259
1.0000
2.1677
1.0097
3.2225
0.9983
S
O


C13 spectrum of
ppm
207.10
133.85
133.37
132.30
130.05
129.37
128.66
127.85
127.47
126.65
126.13
77.55
77.23
76.91
50.69
46.04
32.13
31.03
19.69
19.31
S
O
Current Data Parameters
NAME 7087 10-14
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070122
Time 21.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 59
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042154 sec
RG 2048
DW 19.900 usec
DE 6.50 usec
TE 297.4 K
D1 1.20000005 sec
d11 0.03000000 sec
DELTA 1.10000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 5.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 21.40 dB
PL13 24.40 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127543 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.03 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58716 Hz/cm
ppm
25
50
75
100
125
150
175
200


Current Data Parameters
NAME 7091 10-13
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080326
Time 20.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 101.6
DW 83.400 usec
DE 6.50 usec
TE 299.5 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 2.00 dB
SFO1 400.1325008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.06 cm
F1P 10.500 ppm
F1 4201.37 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.55000 ppm/cm
HZCM 220.07150 Hz/cm
H spectrum of
ppm
Integral
7.3687
7.3475
7.2600
7.2460
7.2247
3.5933
3.5827
3.5763
3.5659
3.5598
3.5493
2.6714
2.6545
2.1492
1.9459
1.9355
1.9290
1.9186
1.9121
1.9018
1.6293
0.9982
0.9812
0.9611
0.9442
Cl
S
O
1.9705
2.0436
1.0000
1.9954
2.9837
1.0059
3.1400
2.9953
0
2
4
6
8


C13 spectrum of
Current Data Parameters
NAME 7091 10-13
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080326
Time 20.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1160
DS 0
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 8192
DW 19.900 usec
DE 6.50 usec
TE 299.6 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PL1 6.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 2.00 dB
PL12 20.00 dB
PL13 23.00 dB
SFO2 400.1315000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127489 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 220.000 ppm
F1 22134.80 Hz
F2P 5.000 ppm
F2 503.06 Hz
PPMCM 10.75000 ppm/cm
HZCM 1081.58704 Hz/cm
206.85
134.65
133.15
133.07
129.25
77.55
77.23
76.91
51.41
46.06
32.30
31.06
19.66
19.28
ppm
25
50
75
100
125
150
175
200
Cl
S
O