The Iptycene Chemistry: New Pentiptycene Building Blocks Derived from Pentiptycene Quinones

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Supporting Information Available. Experimental procedures and characterization data for compounds **17-24** and ^{1}H and ^{13}C NMR spectra of **13**, **14**, and **17-24**.

Contents:

Synthesis of Compound 17. A mixture of **13** (2.0 g, 4.5 mmol), K_2CO_3 (0.9 g, 6.5 mmol), KI (1.1 g, 6.6 mmol), 1-bromooctane (1.3 g, 6.7 mmol), and 100 mL of acetone in a 250-mL flask was heated to reflux for 16 h. The acetone was removed under reduced pressure and the residue was then dissolved in CH_2Cl_2 and washed with 20% $HCl_{(aq)}$. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:1) as eluent afforded the white solid of **17** with a yield of 91%.

M.P. 278-279 ^oC; ^1H-NMR (500 MHz, $CDCl_3$) δ: 0.98 (t, J = 6.8 Hz, 3H), 1.39-1.55 (m, 8H), 1.69 (quin, J = 7.6 Hz, 2H), 2.03 (tt, J = 6.8 and 7.6 Hz, 2 H), 3.96 (t, J = 6.8 Hz, 2H), 5.32 (s, 2H), 5.69 (s, 2H), 6.93-6.99 (m, 8H), 7.26 (s, 1H), 7.31-7.34 (m, 8H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.2, 22.7, 26.4, 29.4, 29.6, 30.6, 31.9, 48.1, 54.2, 76.0, 115.8, 123.4 (2C), 125.0, 125.1, 134.8, 144.3, 145.1, 145.7, 149.8 ppm; IR (KBr) 1221 cm^{-1}; FAB-HRMS calcd for $C_{42}H_{38}O$ (M^+) 558.2923, found 558.2927.

Synthesis of Compound 18. A mixture of **17** (0.3 g, 0.54 mmol), Ag_2SO_4 (0.8 g, 2.57 mmol), I_2 (0.7 g, 2.76 mmol), and 30 mL of ethanol in a 50-mL flask was heated to reflux for 3 h. The resulting precipitate was filtered off and the filtrate was concentrated under reduced pressure. The residue was then dissolved in CH_2Cl_2 and washed with 0.1 M $Na_2SO_{3(aq)}$ and brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:3) as eluent afforded the white solid of **18** with a yield of 94%. M.P. 267-268 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ: 0.95 (t, J = 6.9 Hz, 3H), 1.38-1.51 (m, 8H), 1.66 (quin, J = 7.6 Hz, 2H), 2.01 (tt, J = 6.9 and 7.6 Hz, 2H), 3.91 (t, J = 6.9 Hz, 2H), 5.67 (s, 2H), 5.80 (s, 2H), 6.93-6.99 (m, 8H), 7.31-7.40 (m, 8H) ppm; ^{13}C NMR (100

MHz, $CDCl_3$) δ: 14.2, 22.7, 26.4, 29.4, 29.6, 30.5, 31.9, 48.6, 58.6, 76.1, 88.7, 123.4, 123.9, 125.3, 125.4, 137.1, 144.9, 145.0, 147.0, 149.9 ppm; IR (KBr) 1219 cm^{-1}; FAB-HRMS calcd for $C_{42}H_{37}IO$ (M^+) 684.1889, found 684.1897.

Synthesis of Compound 19. A mixture of **17** (0.5 g, 0.9 mmol), NBS (0.3 g, 1.7 mmol), and 10 mL of DMF in a 25-mL flask was heated to reflux for 48 h. The DMF was removed under reduced pressure and the residue was then dissolved in CH_2Cl_2 and washed with brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:1) as eluent afforded the white solid of **19** with a yield of 90%. M.P. 271-272 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ: 0.99 (t, *J* = 6.6 Hz, 3H), 1.42-1.57 (m, 8H), 1.70 (quin, *J* = 7.4 Hz, 2H), 2.04 (tt, *J* = 6.6 and 7.4 Hz, 2H), 3.95 (t, *J* = 6.6 Hz, 2H), 5.71 (s, 2H), 5.88 (s, 2H), 6.97-7.01 (m, 8H), 7.35-7.41 (m, 8H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.5, 23.1, 26.7, 29.7, 29.9, 30.9, 32.3, 48.9, 54.0, 76.5, 111.8, 123.8, 124.3, 125.6, 125.7, 137.9, 143.7, 145.2, 145.3, 149.2 ppm; IR (KBr) 1221 cm^{-1}; FAB-HRMS calcd for $C_{42}H_{37}BrO$ (M^+) 636.2028, found 636.2040.

Synthesis of Compound 20. A mixture of **18** (0.2 g, 0.29 mmol), $Pd(PPh_3)_4$ (0.04 g, 0.03 mmol), trimethylsilyl acetylene (0.05 mL, 0.35 mmol), 3 mL of benzene, and 3 mL of diisopropylamine was heated to 90 ^oC for 16 h under argon. The precipitate was filtered off and the filtrate was concentrated under reduced pressure. The residue was then dissolved in CH_2Cl_2 and washed with brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:6) as eluent afforded the white solid of **20** with a

yield of 90%. M.P. 257-258 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.50 (s, 9H), 0.97 (t, *J* = 6.9 Hz, 3H), 1.38-1.49 (m, 8H), 1.65 (quin, *J* = 7.6 Hz, 2H), 2.00 (tt, *J* = 6.9 and 7.6 Hz, 2H), 3.95 (t, *J* = 6.8 Hz, 2H), 5.67 (s, 2H), 5.81 (s, 2H), 6.92-6.97 (m, 8H), 7.31-7.37 (m, 8H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$), δ: 0.4, 14.2, 22.8, 26.4, 29.4, 29.6, 30.5, 32.0, 48.2, 52.3, 76.1, 100.1, 101.0, 111.1, 123.4, 124.0, 125.2 (2C), 135.2, 145.0, 145.2, 146.1, 149.7 ppm; IR (KBr) 1264, 2147 cm^{-1}; FAB-HRMS calcd for $C_{47}H_{46}OSi$ (M^+) 654.3318, found 654.3337.

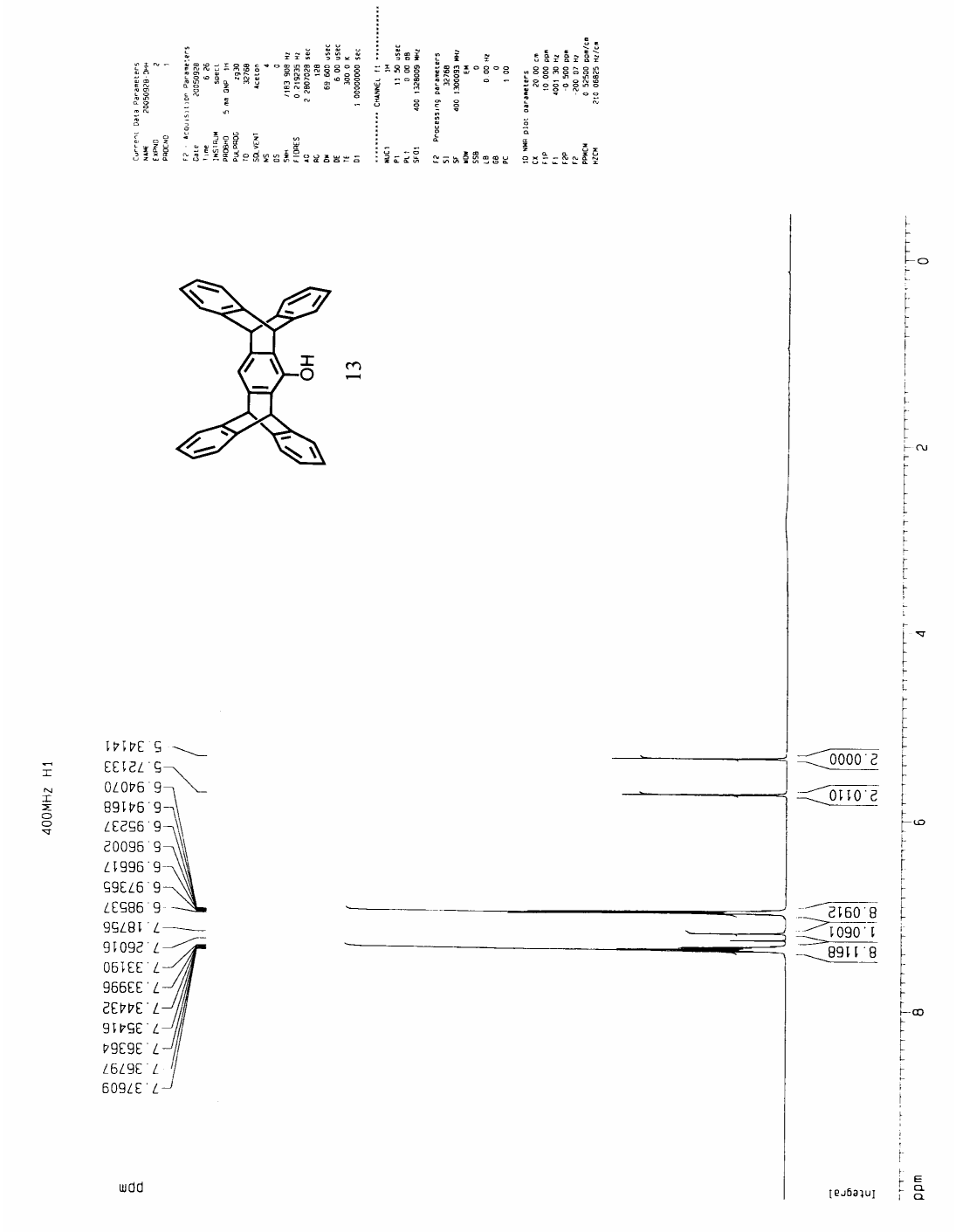
Synthesis of Compound 21. A mixture of **18** (0.2 g, 0.29 mmol), $Pd(OAc)_2$ (0.01 g, 0.04 mmol), P(*o*-tolyl)$_3$ (0.02 g, 0.07 mmol), styrene (0.04 mL, 0.35 mmol), 2mL of anhydrous DMF, and 2 mL of triethylamine was heated to 90 ^{o}C for 16 h under argon. The precipitate was filtered off and the filtrate was concentrated under reduced pressure. The residue was then dissolved in CH_2Cl_2 and washed with brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:5) as eluent afforded the white solid of **21** with a yield of 83%. M.P. 256-257 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 0.96 (t, *J* = 6.7 Hz, 3H), 1.39-1.54 (m, 8H), 1.68 (quin, *J* = 7.5 Hz, 2H), 2.03 (tt, *J* = 6.7 and 7.5 Hz, 2 H), 3.95 (t, *J* = 6.7 Hz, 2H), 5.71 (s, 2H), 5.72 (s, 2H), 6.72, (d, *J* = 16.4 Hz, 1H), 6.93-6.95 (m, 8H), 7.28-7.33, (m, 8H), 7.42-7.56 (m, 4H), 7.73, (d, *J* = 7.4 Hz, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.2, 22.7, 26.5, 29.4, 29.6, 30.6, 32.0, 48.3, 51.1, 76.0, 123.5, 123.6, 124.1, 125.1 (2C), 126.3, 126.7, 128.1, 129.0, 135.0, 136.2, 137.3, 142.3, 145.3, 145.6, 149.0 ppm; IR (KBr) 972, 1266 cm^{-1}; FAB-HRMS calcd for $C_{50}H_{44}O$ (M^+) 660.3392, found 660.3394.

Synthesis of Compound 22. A mixture of **18** (0.2 g, 0.29 mmol), $Pd(dba)_2$ (0.02 g, 0.03 mmol), PPh_3 (0.02 g, 0.08 mmol), phenylboronic acid (0.05 g, 0.40 mmol), Cs_2CO_3 (0.4 g, 1.23 mmol), and 5 mL of anhydrous dioxane was heated to 100 ^oC for 16 h under argon. The precipitate was filtered off and the filtrate was concentrated under reduced pressure. The residue was then dissolved in CH_2Cl_2 and washed with brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:6) as eluent afforded the white solid of **22** with a yield of 83%. M.P. 160-161 ^oC; ^1H NMR (500 MHz, $CDCl_3$ δ: 0.97 (t, J = 6.6 Hz, 3H), 1.40-1.56 (m, 8H), 1.71 (quin, J = 7.5 Hz, 2H), 2.06 (tt, J = 6.7 and 7.5 Hz, 2H), 3.99 (t, J = 6.7 Hz, 2H), 5.30 (s, 2H), 5.74 (s, 2H), 6.89-6.96 (m, 8H), 7.12-7.13 (m, 4H), 7.26-7.35 (m, 6H), 7.58-7.66 (m, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.5, 23.1, 26.8, 29.8, 30.0, 31.0, 32.3, 48.6, 51.6, 76.5, 123.8, 123.9, 125.4, 125.5, 127.7, 128.9, 130.2, 130.6, 134.9, 138.6, 142.6, 145.7, 146.0, 149.5 ppm; IR (KBr) 1266 cm^{-1}; FAB-HRMS calcd for $C_{48}H_{42}O$ (M^+) 634.3236, found 634.3230.

Synthesis of Compound 23. A mixture of **19** (1.0 g, 1.6 mmol), CuCN (0.3 g, 3.3 mmol), and 15 mL of anhydrous NMP (*N*-methylpyrrolidone) was heated to 200 ^oC for 16 h under argon. After the reaction mixture was cooled to rt, CH_2Cl_2 and water were added to dissolve the solids. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:1) as eluent afforded the white solid of **23** with a yield of 87%. M.P. 281-282 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ: 0.95 (t, J = 6.7 Hz, 3H), 1.38-1.54 (m, 8H), 1.66 (quin, J = 7.4 Hz, 2H), 2.01 (tt, J = 6.7 and 7.4 Hz, 2H), 4.00 (t, J = 6.7 Hz, 2H), 5.70 (s, 2H), 5.74 (s, 2H), 6.97-7.01 (m, 8H), 7.33-7.43 (m, 8H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$), δ: 14.5,

23.0, 26.6, 29.7, 29.9, 30.9, 32.3, 48.4, 52.8, 76.6, 100.6, 116.7, 123.9, 124.5, 126.0 (2C), 137.4, 144.4, 144.6, 148.3, 153.1 ppm; IR (KBr) 1260, 2224 cm^{-1}; FAB-HRMS calcd for $C_{42}H_{37}NO$ (M^+) 583.2875, found 583.2878.

Synthesis of Compound 24. To a solution of **23** (1.0 g, 1.7 mmol) in 20 mL of CH_2Cl_2 at -20 ^oC was added 3.4 mL of 1.0 M DIBAL-H (diisobutylaluminum hydride (3.4 mmol) in hexane under argon. The mixture was stirred and kept at -20 ^oC for 16 h. The reaction was quenched by slowly adding 2 mL of concentrated $HCl_{(aq)}$. The solution was then washed with brine. The organic layer was dried over anhydrous $MgSO_4$ and the filtrate was concentrated under reduced pressure. Column chromatography with CH_2Cl_2/hexane (1:2) as eluent afforded the white solid of **24** with a yield of 91%. M.P. 253-254 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ: 0.96 (t, *J* = 6.2 Hz, 3H), 1.39-1.54 (m, 8H), 1.69 (quin, *J* = 7.4 Hz, 2H), 2.04 (tt, *J* = 6.7 and 7.4 Hz, 2H), 4.00 (t, *J* = 6.7 Hz, 2H), 5.74 (s, 2H), 6.57 (s, 2H), 6.96-6.98 (m, 8H), 7.33-7.39 (m, 8H), 10.95 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ: 14.5, 23.1, 26.7, 29.7, 29.9, 30.9, 32.3, 48.2, 49.0, 76.3, 123.6, 123.8, 124.5, 125.8 (2C), 137.3, 145.0 (2C C), 147.9, 153.8, 190.7 ppm; IR (KBr) 1275, 1688 cm^{-1}; FAB-HRMS calcd for $C_{43}H_{38}O_2$ (M^+) 586.2872, found 586.2870.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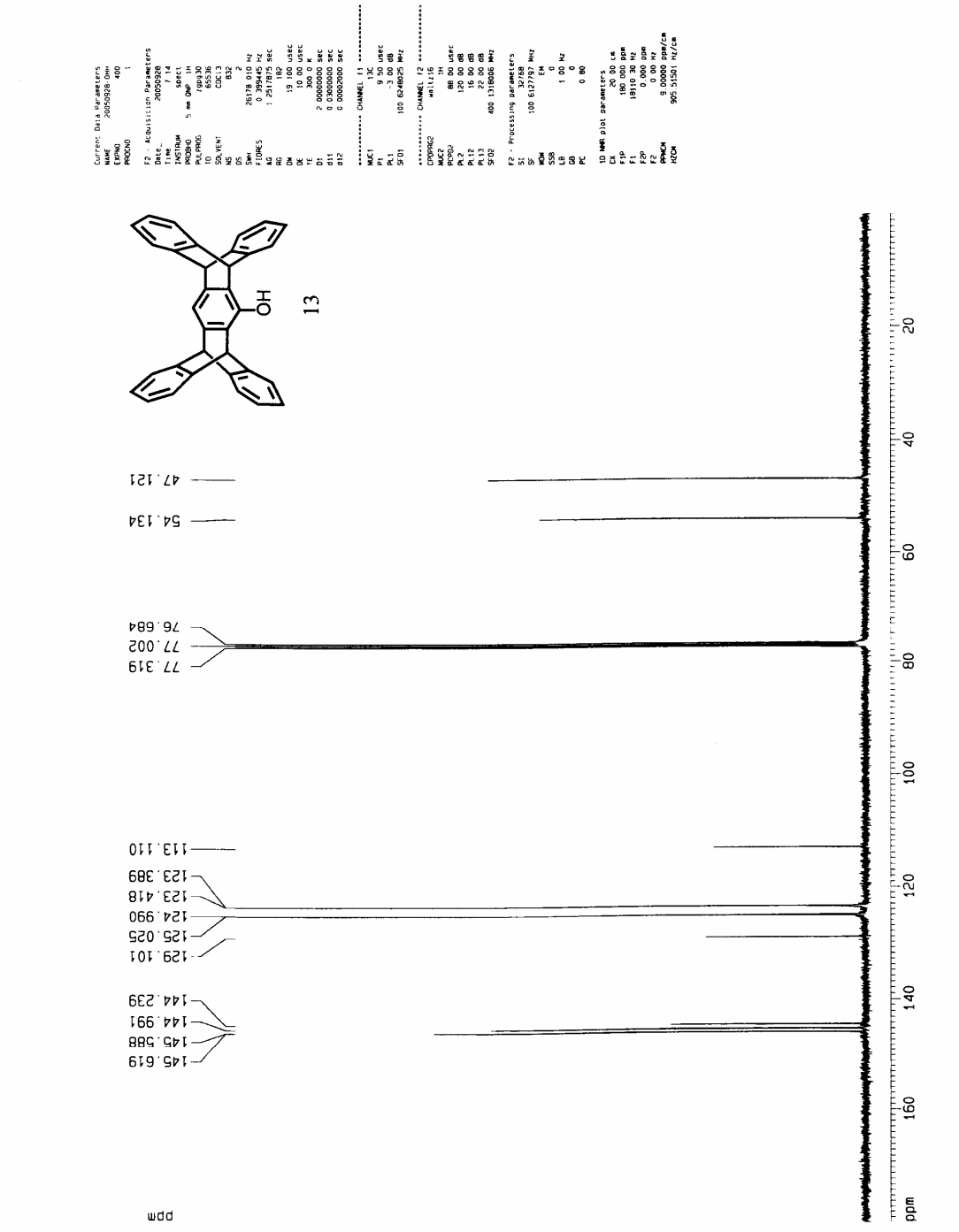
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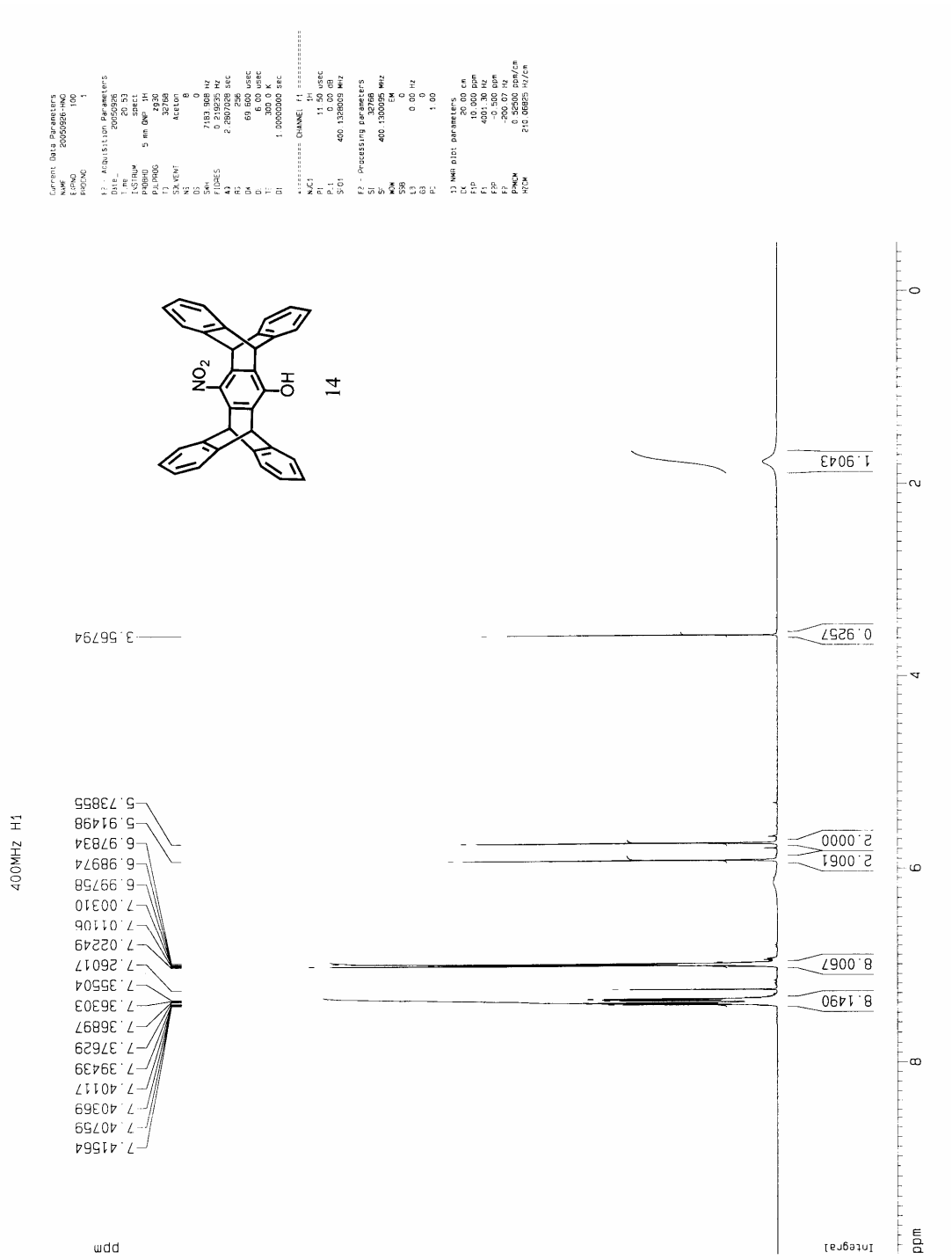
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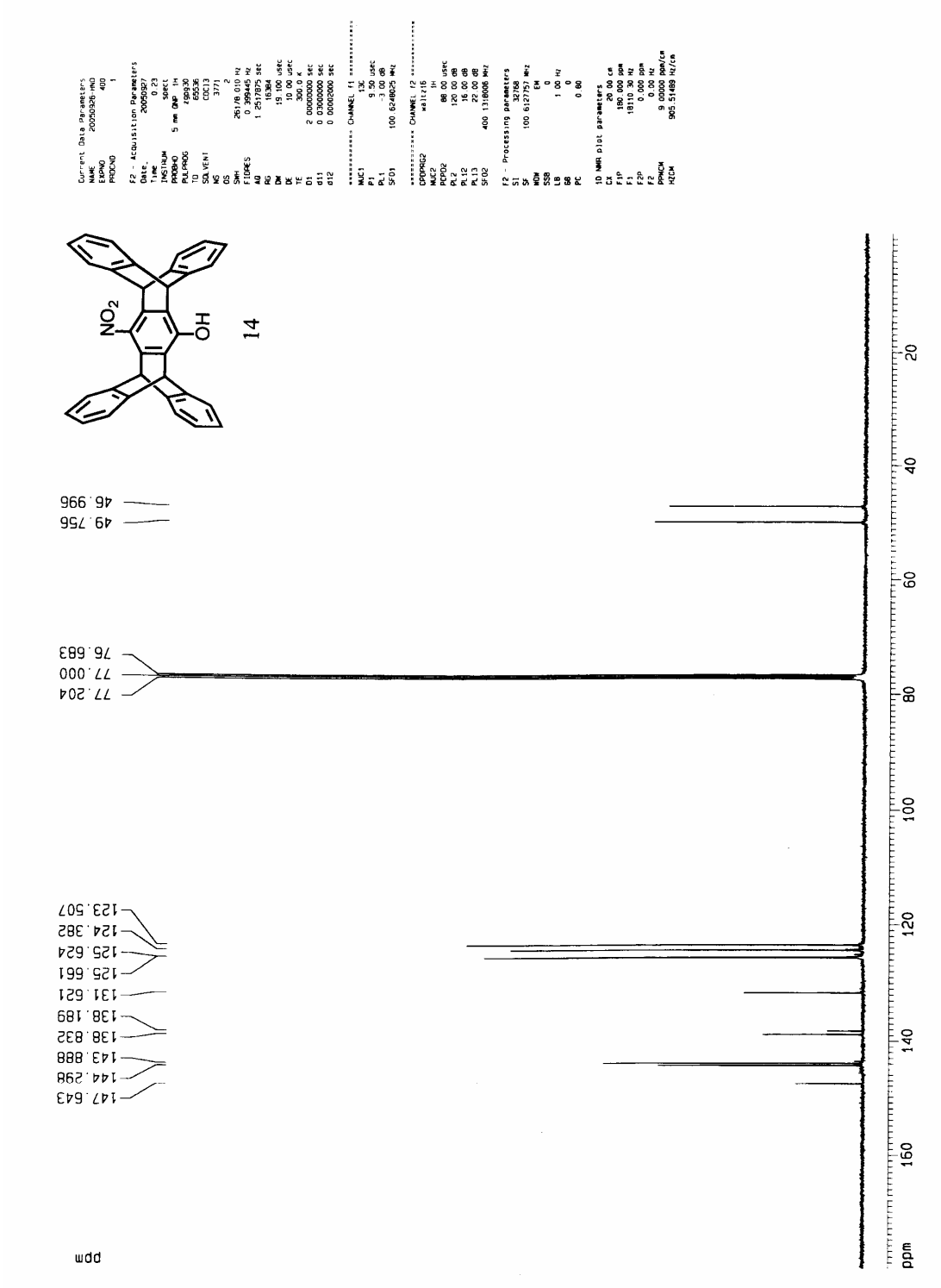
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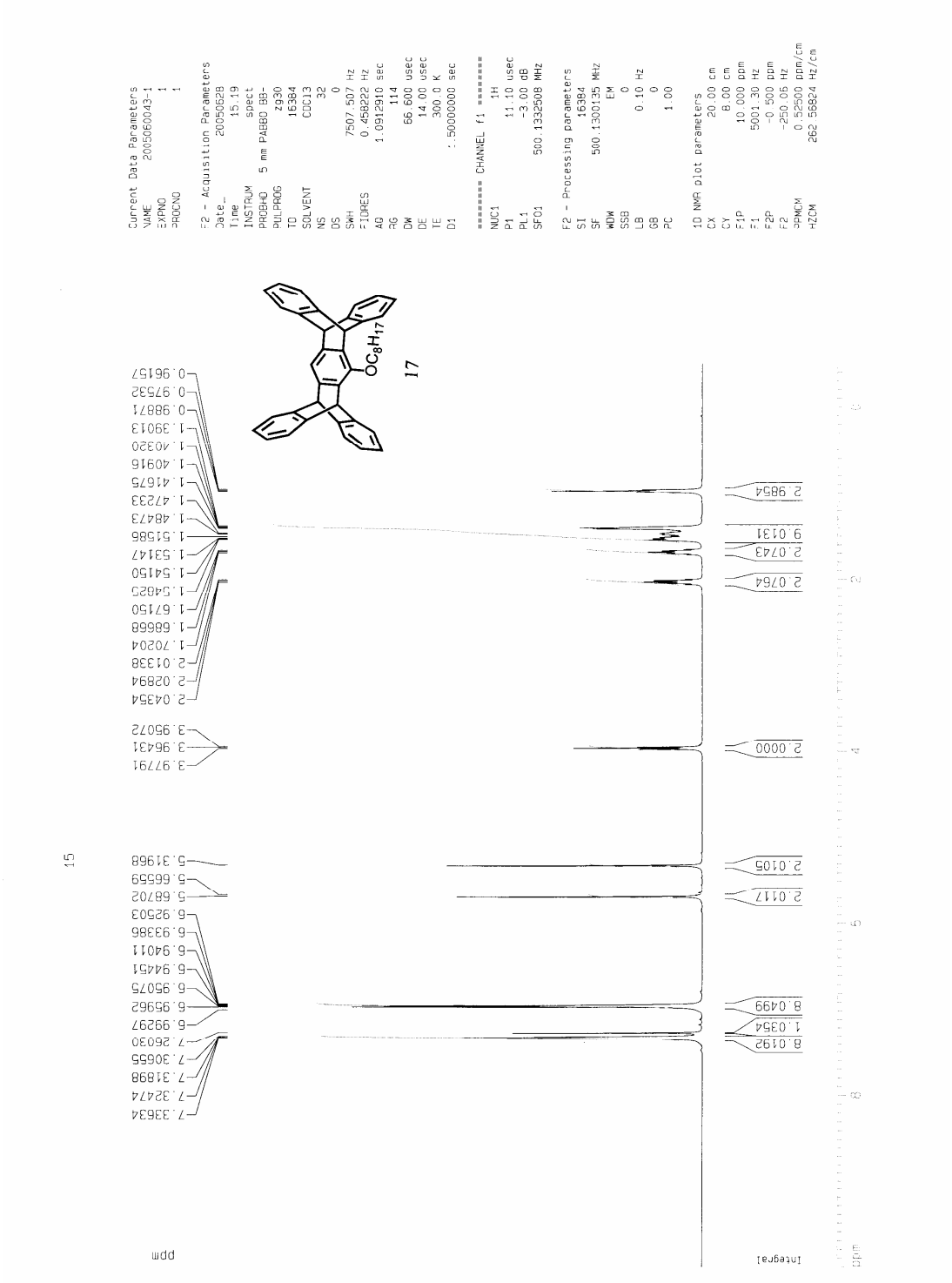
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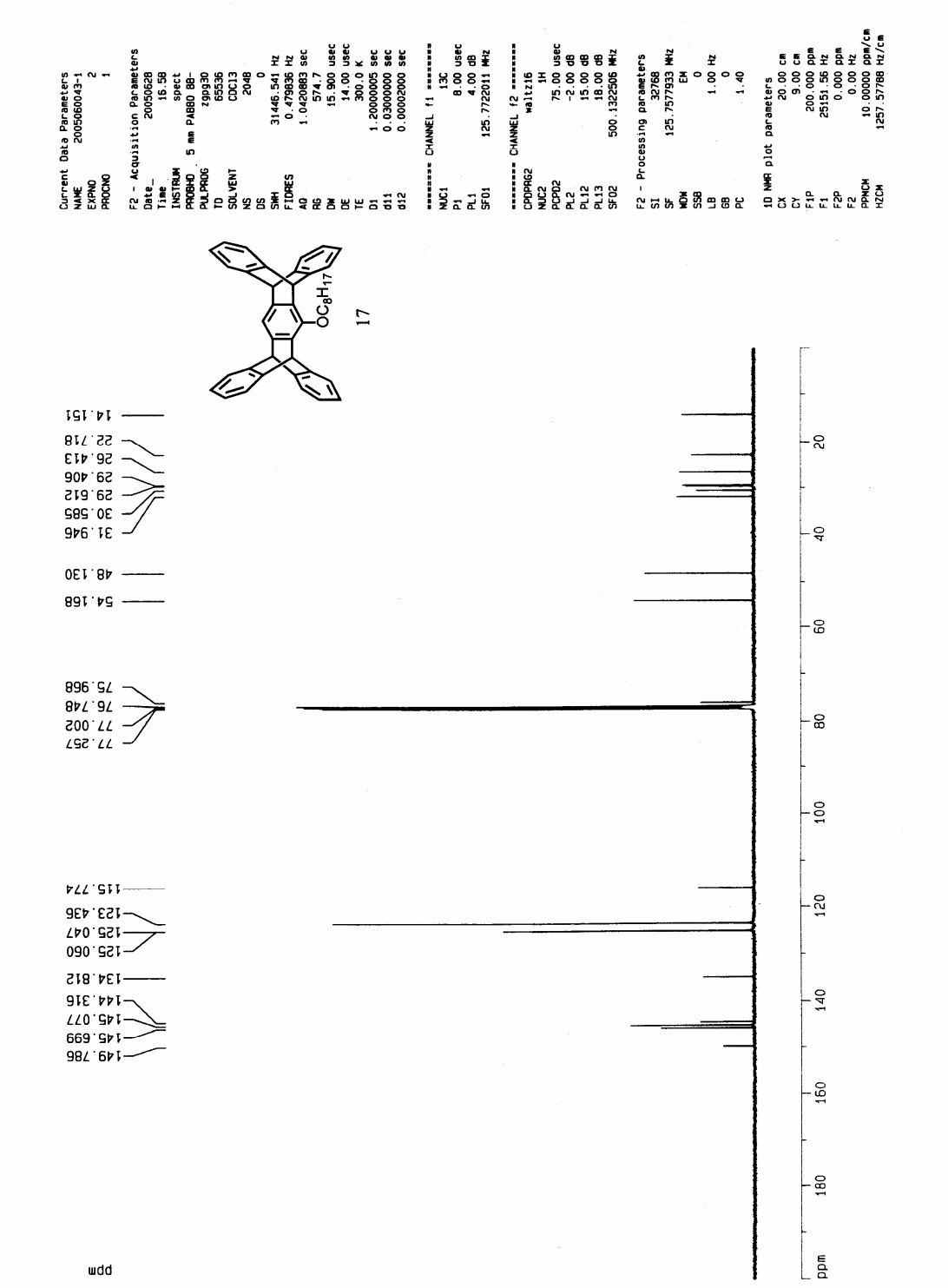
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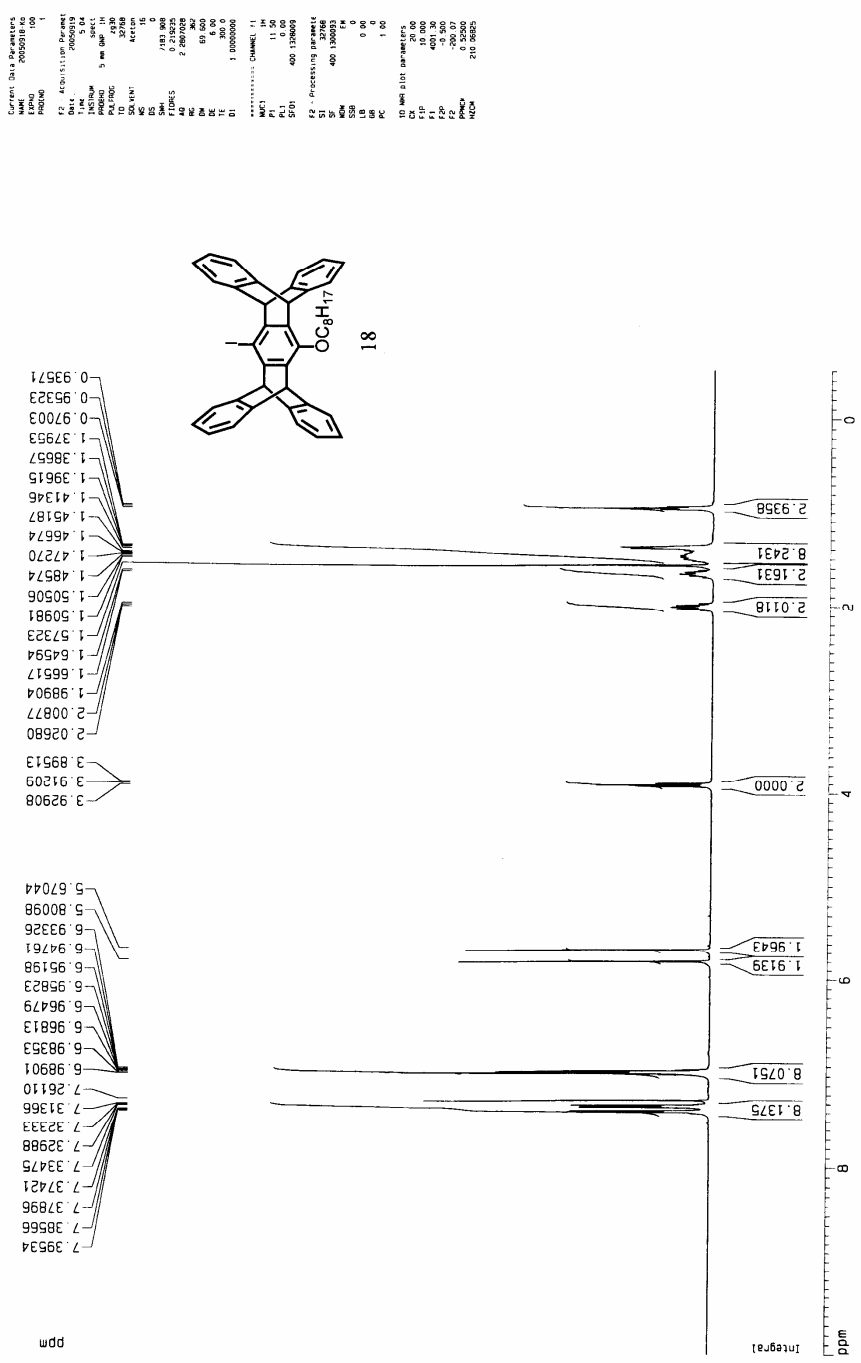
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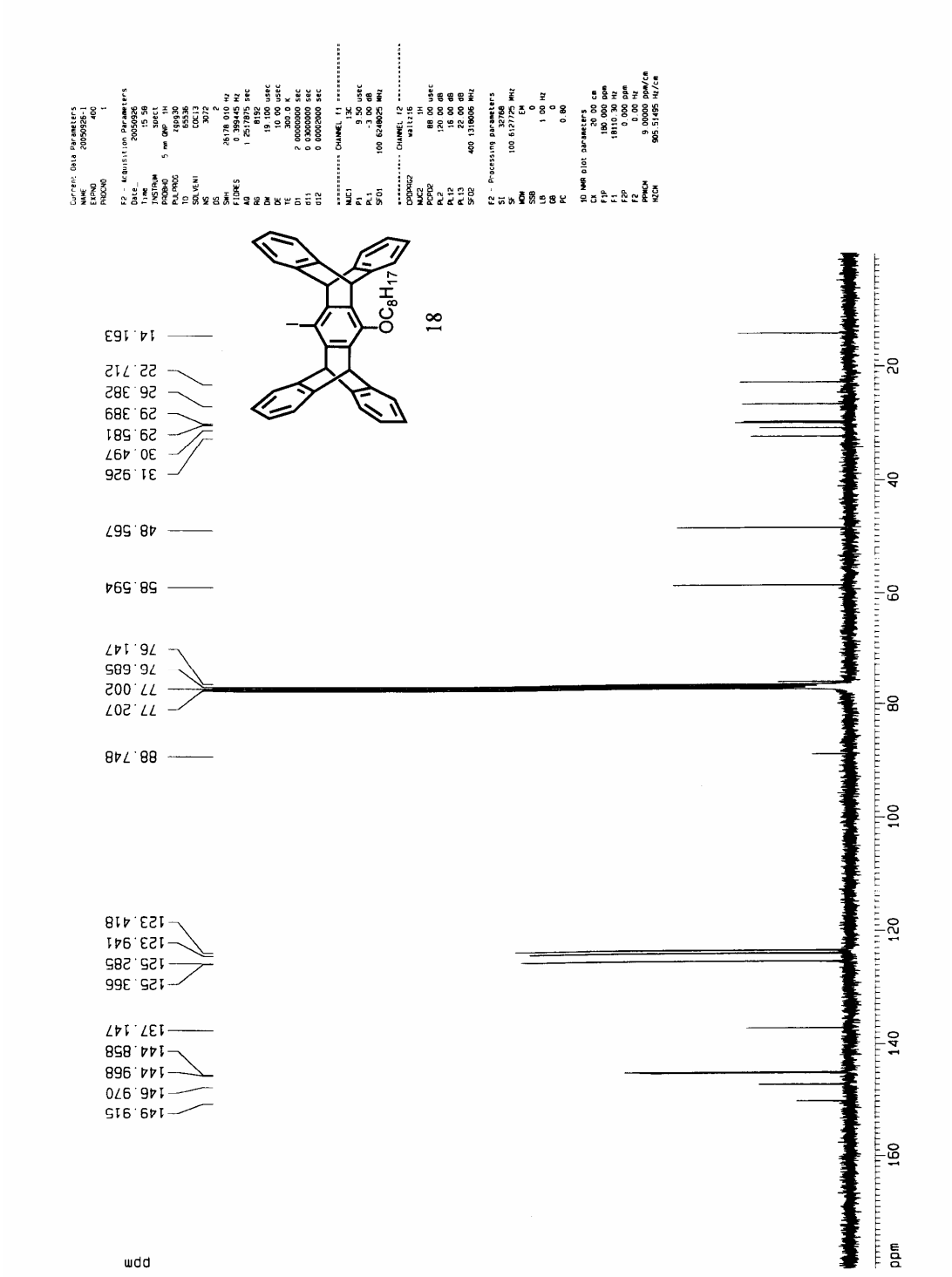
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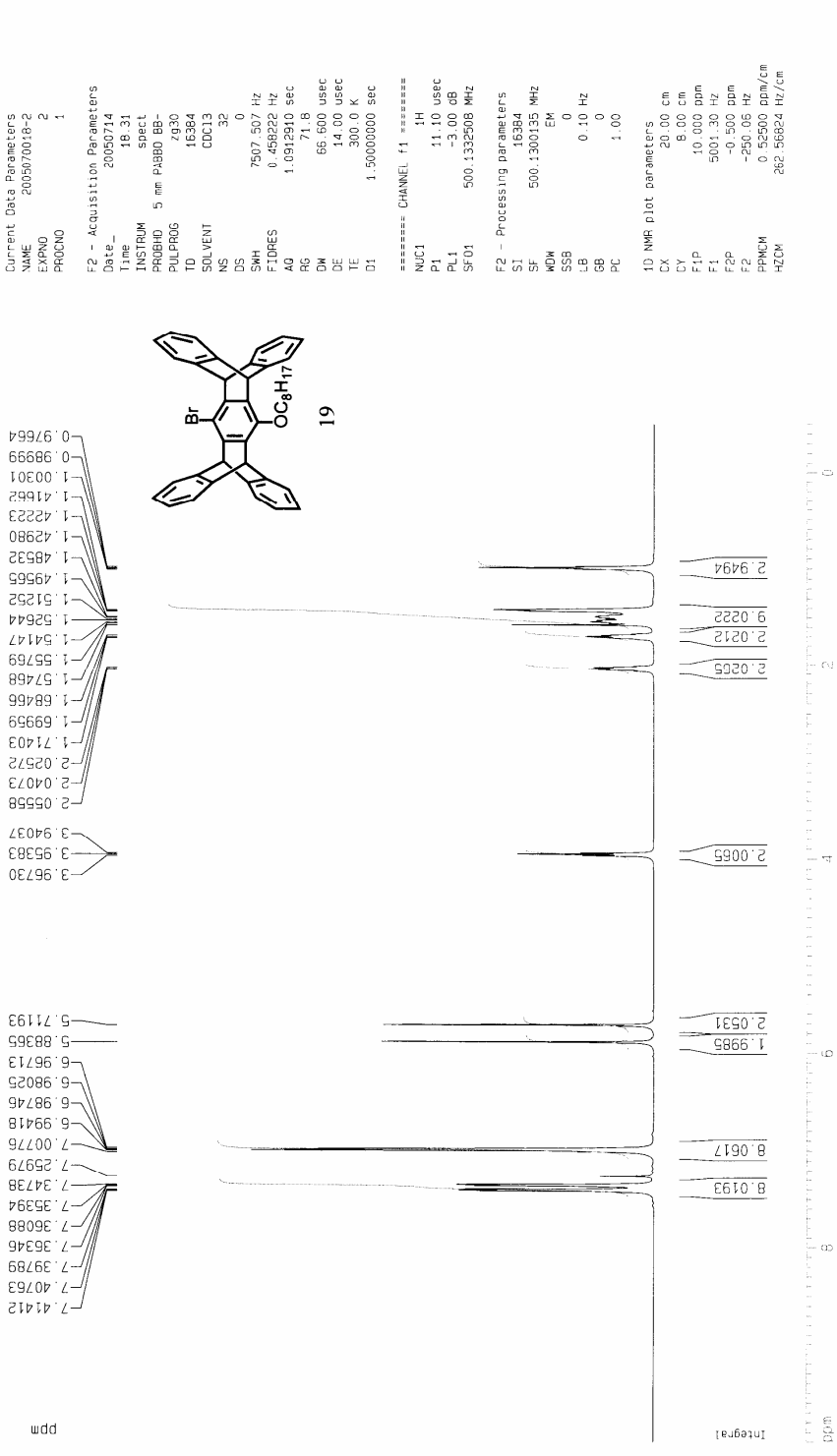
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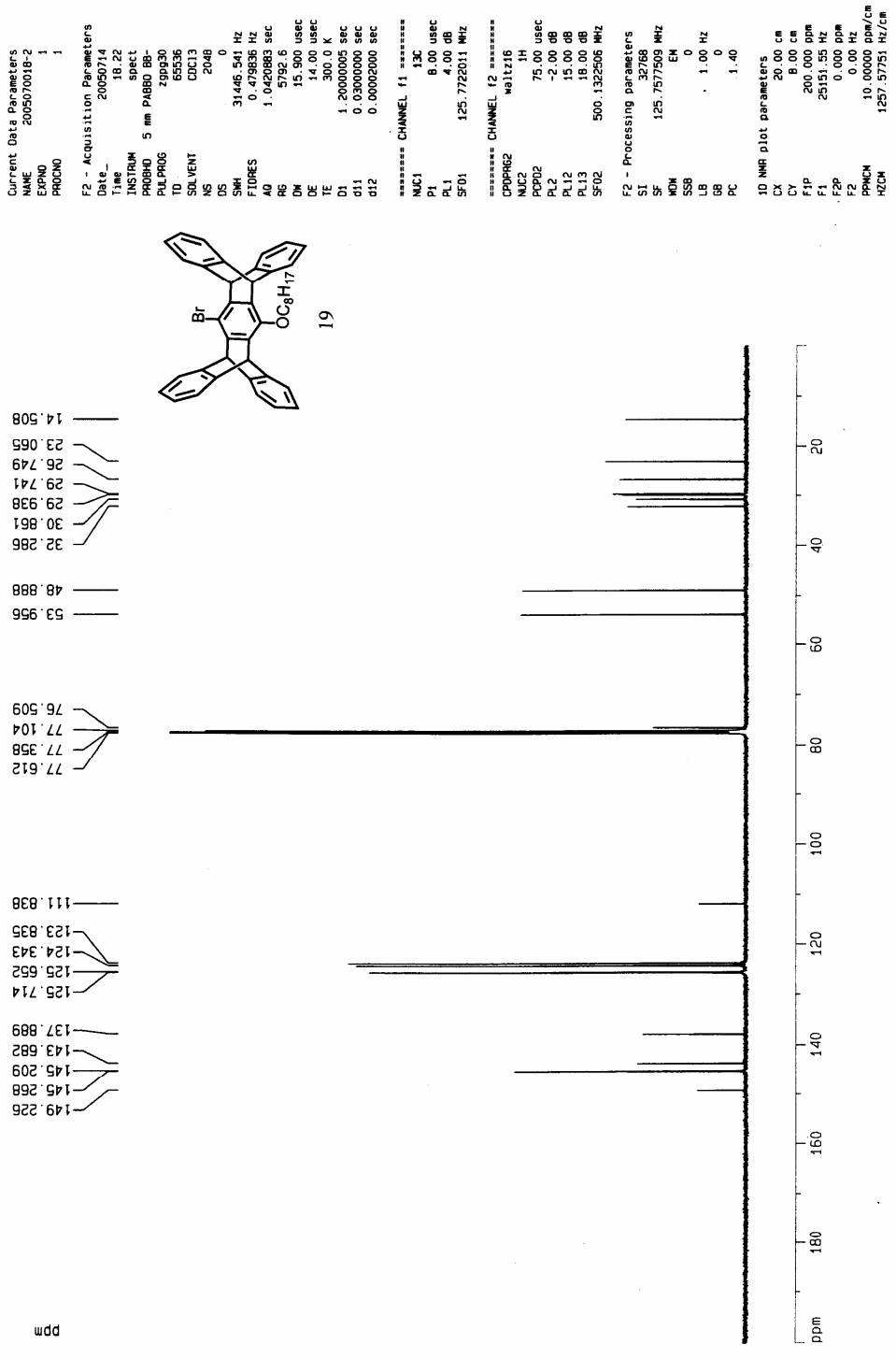
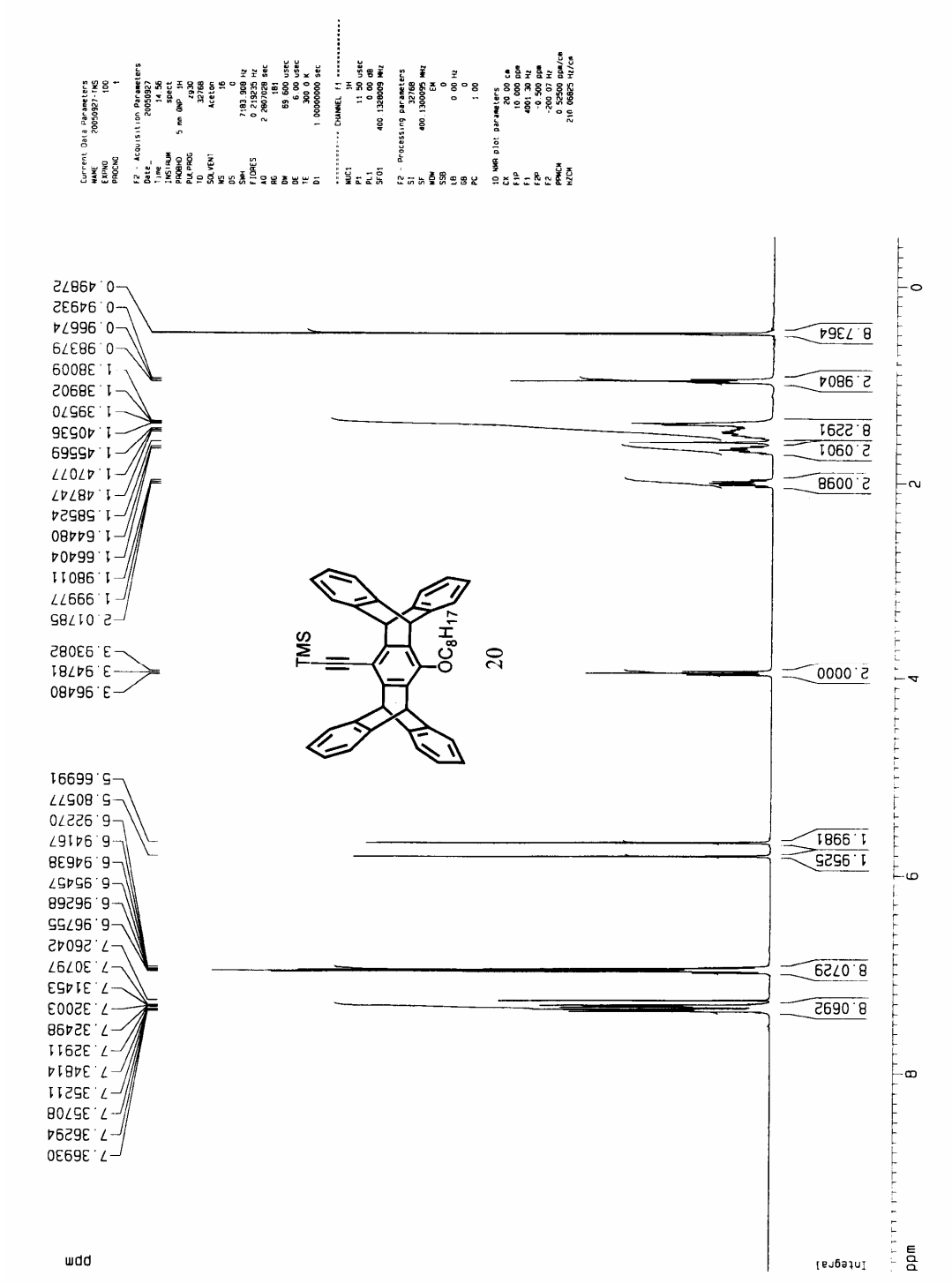
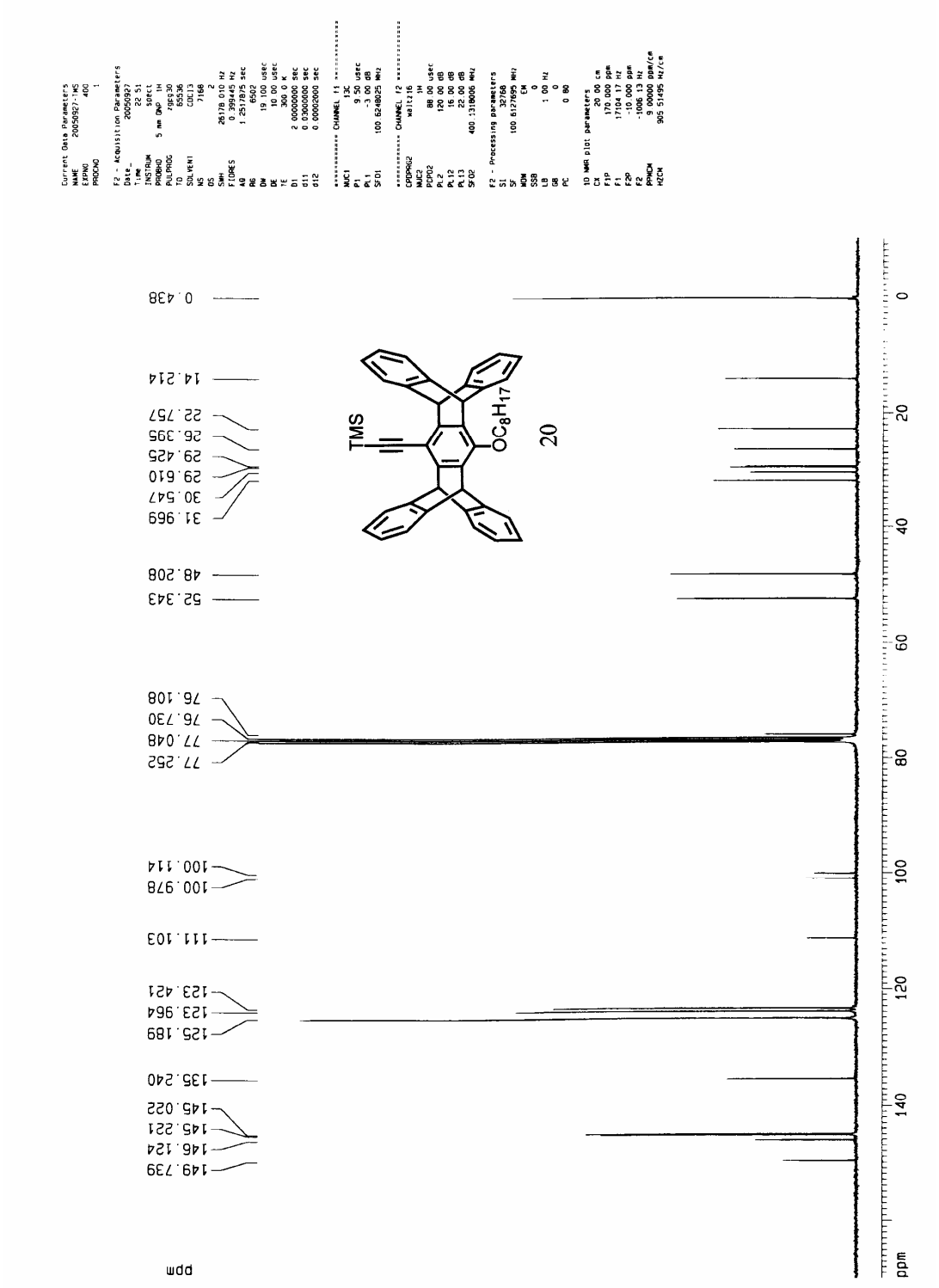
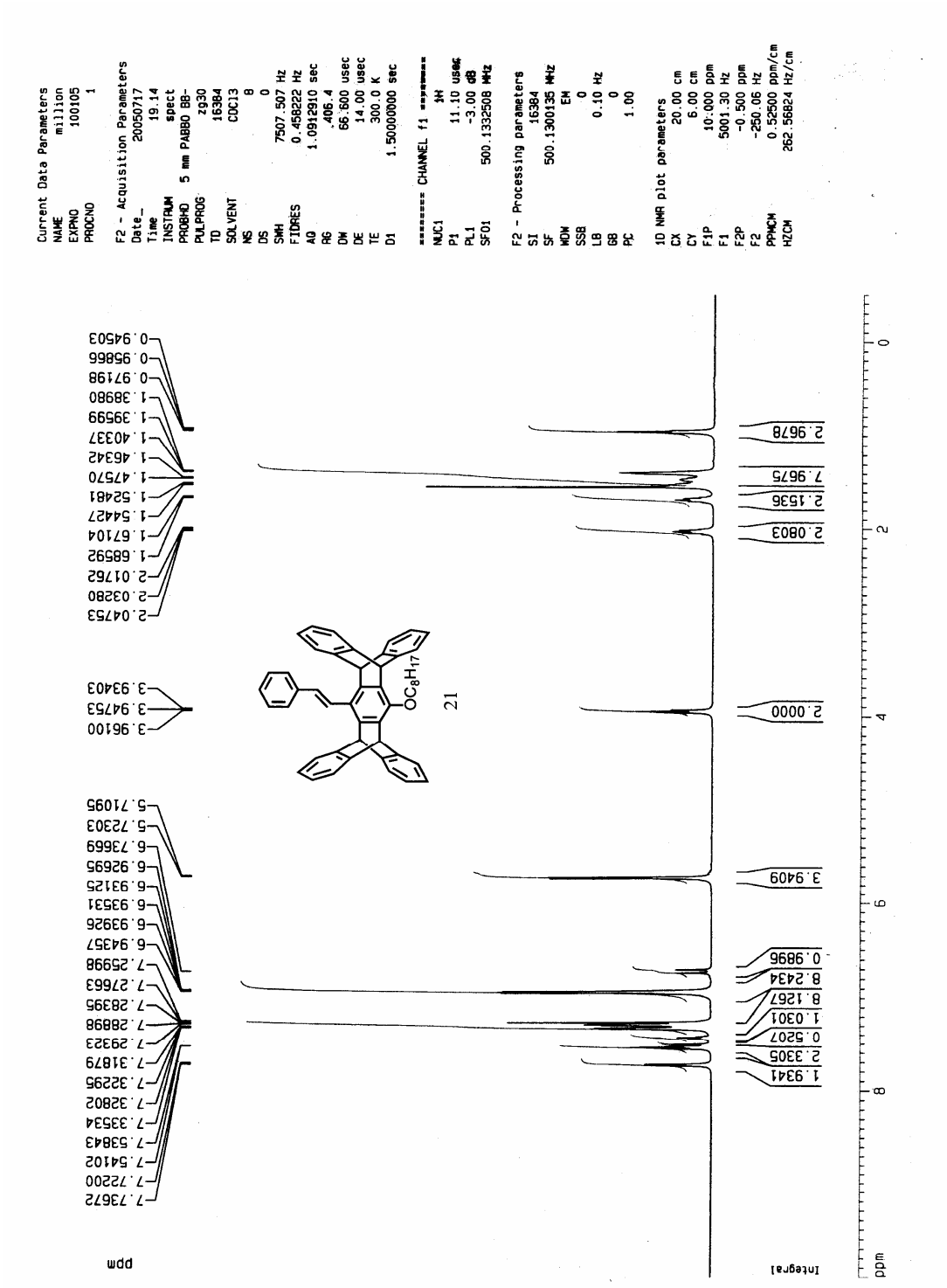
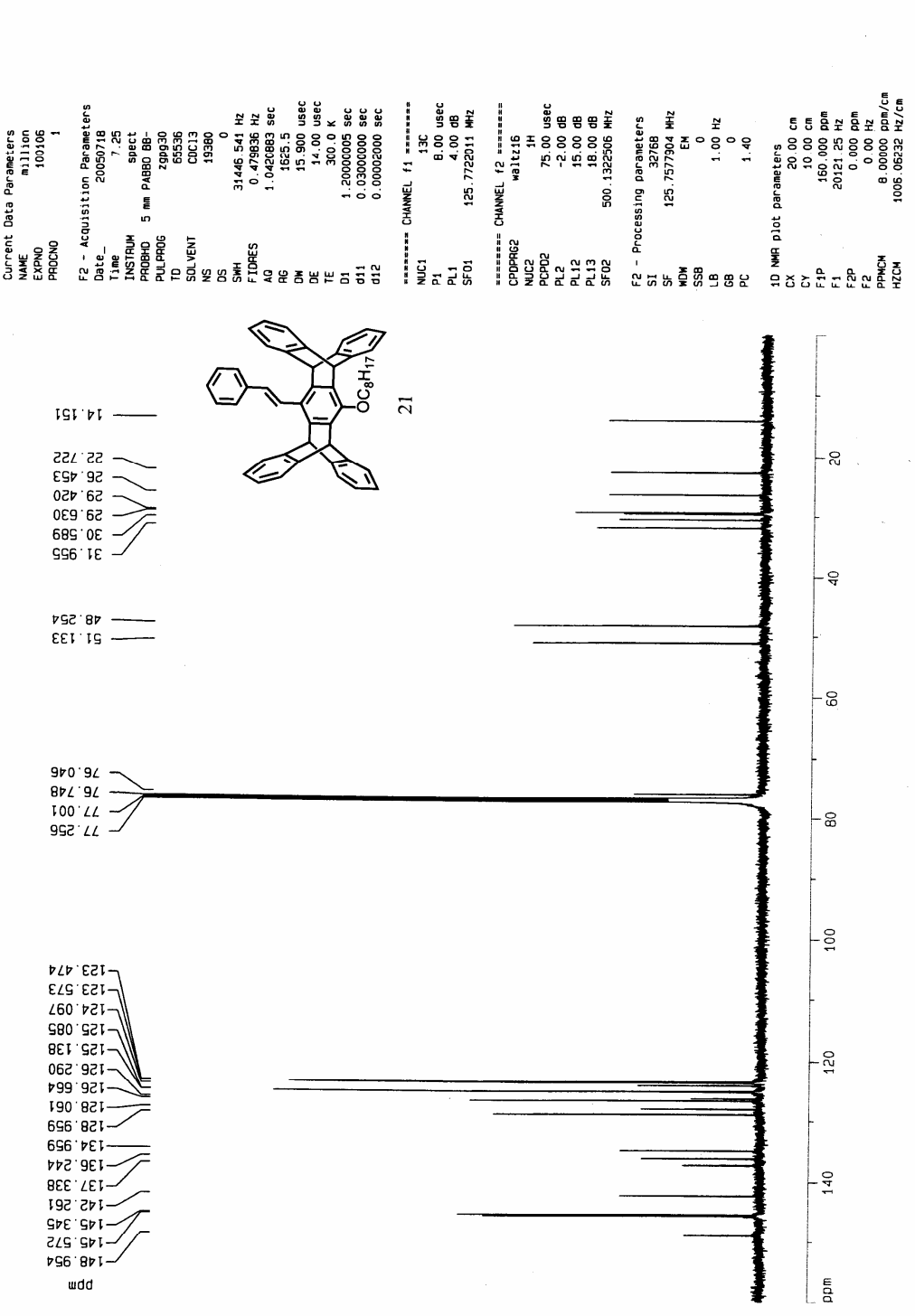
6.98746
6.99418
7.00776
7.25979
7.34738
7.35394
7.36088
7.36346
7.39789
7.40763
7.41412
2.9494
9.0222
2.0212
2.0205
2.0065
2.0531
1.9985
8.0617
8.0193
Integral
ppm

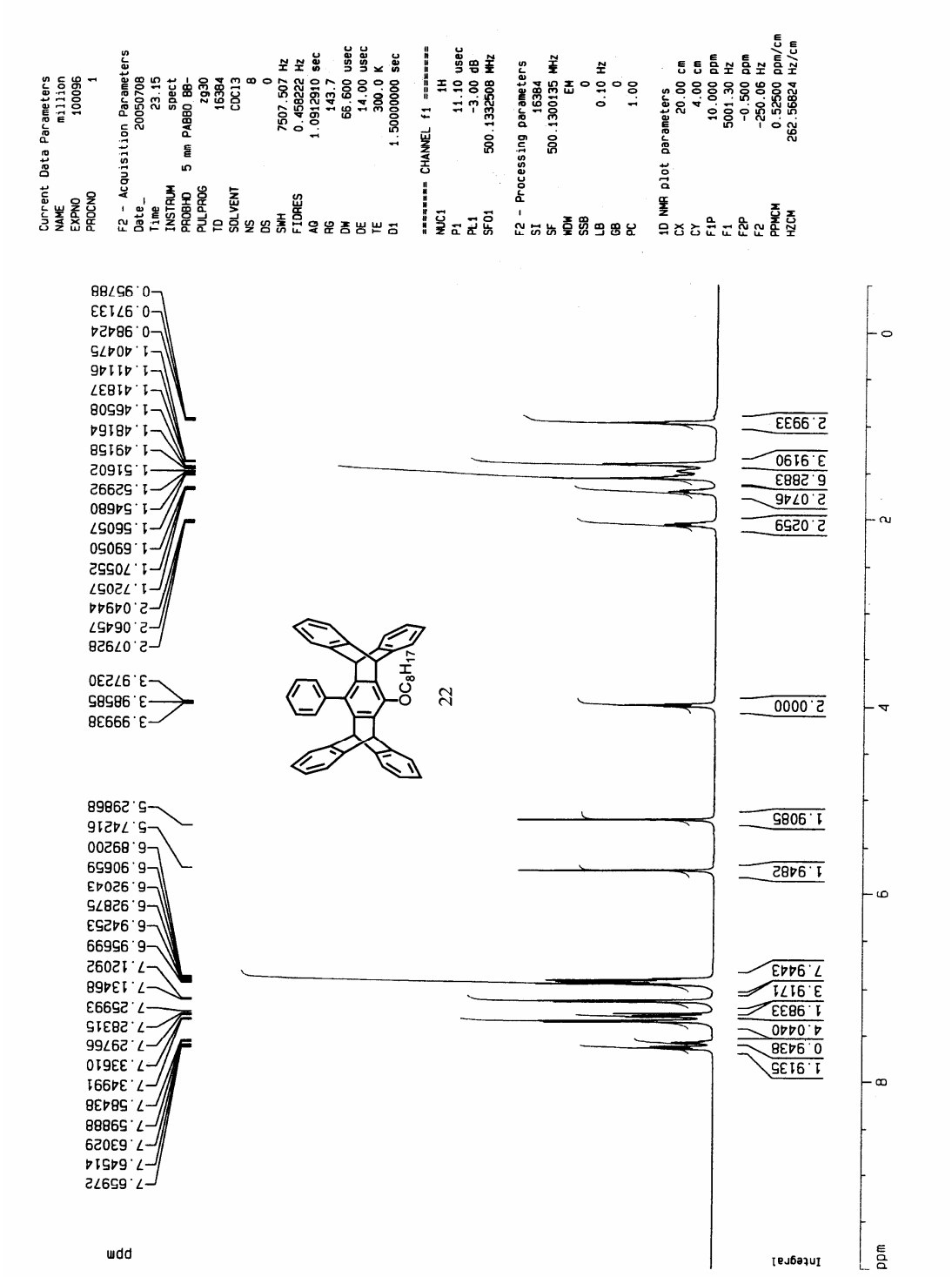

Current Data Parameters
NAME 20050700018-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050714
Time 18.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 5792.6
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SF01 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SF02 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577509 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 25151.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1257.57751 Hz/cm
Br
OC8H17
19
14.508
23.065
26.749
29.741
29.938
30.861
32.286
48.888
53.956
76.509
77.104
77.358
77.612
111.838
123.835
124.343
125.652
125.714
137.889
143.682
145.209
145.268
149.226
ppm
20
40
60
80
100
120
140
160
180

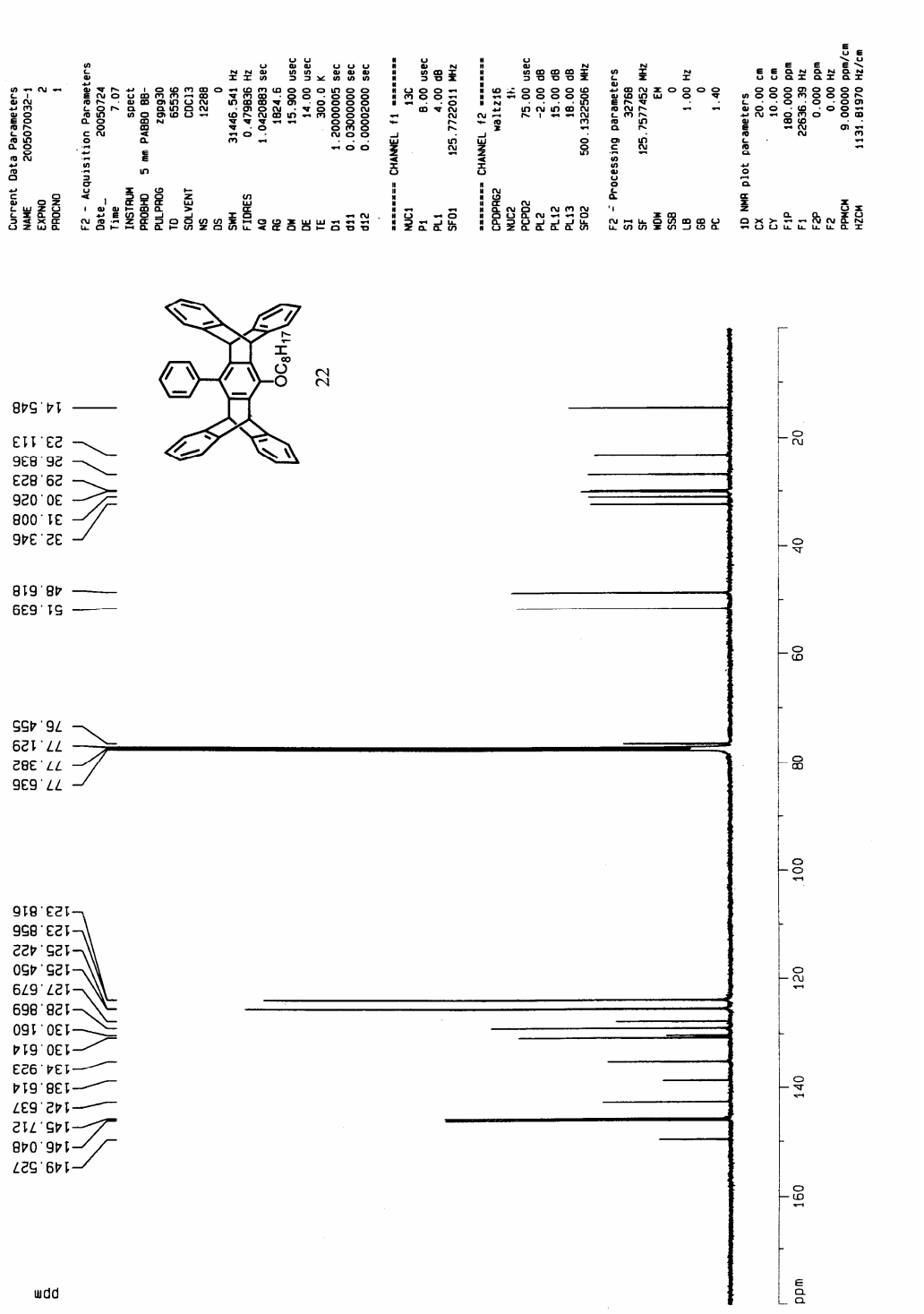

TMS
OC_8H_{17}
20
ppm
Integral

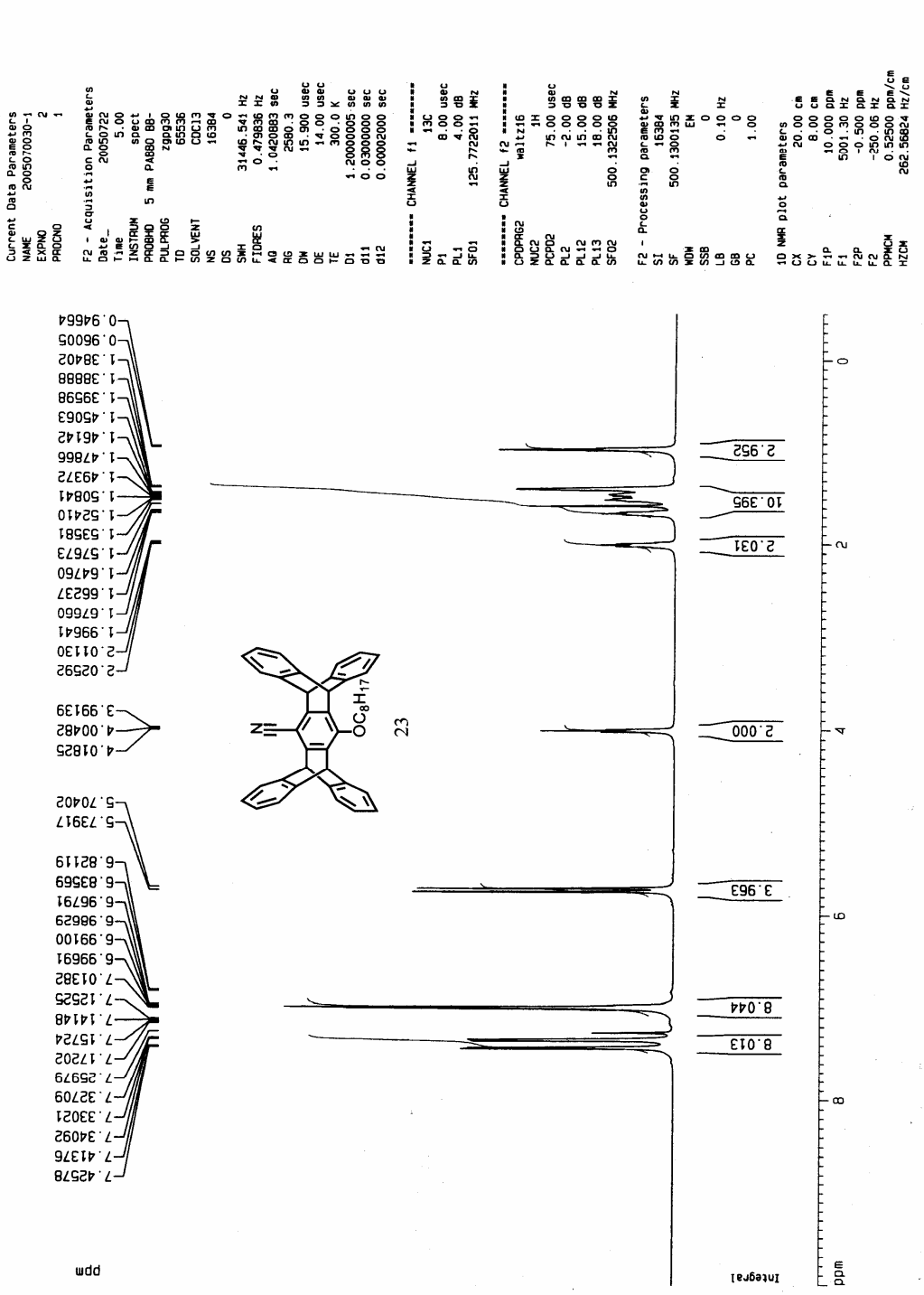

TMS
OC8H17
20
ppm

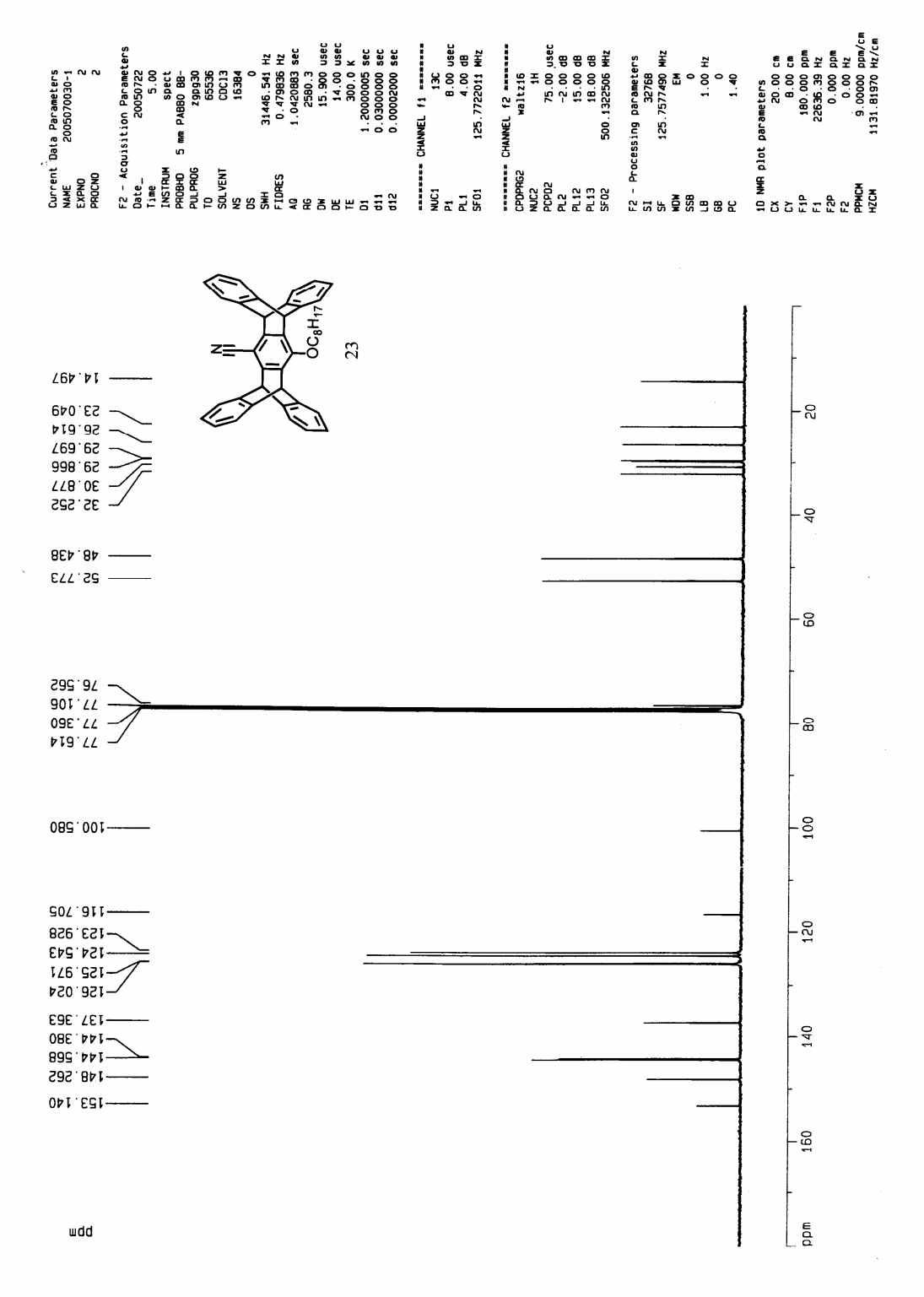

Current Data Parameters
NAME million
EXPNO 100105
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050717
Time 19.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 406.4
DW 66.600 usec
DE 14.00 usec
TE 300.0 K
D1 1.50000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.10 usec
PL1 -3.00 dB
SFO1 500.1332508 MHz
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 262.56824 Hz/cm
OC8H17
21
ppm
Integral

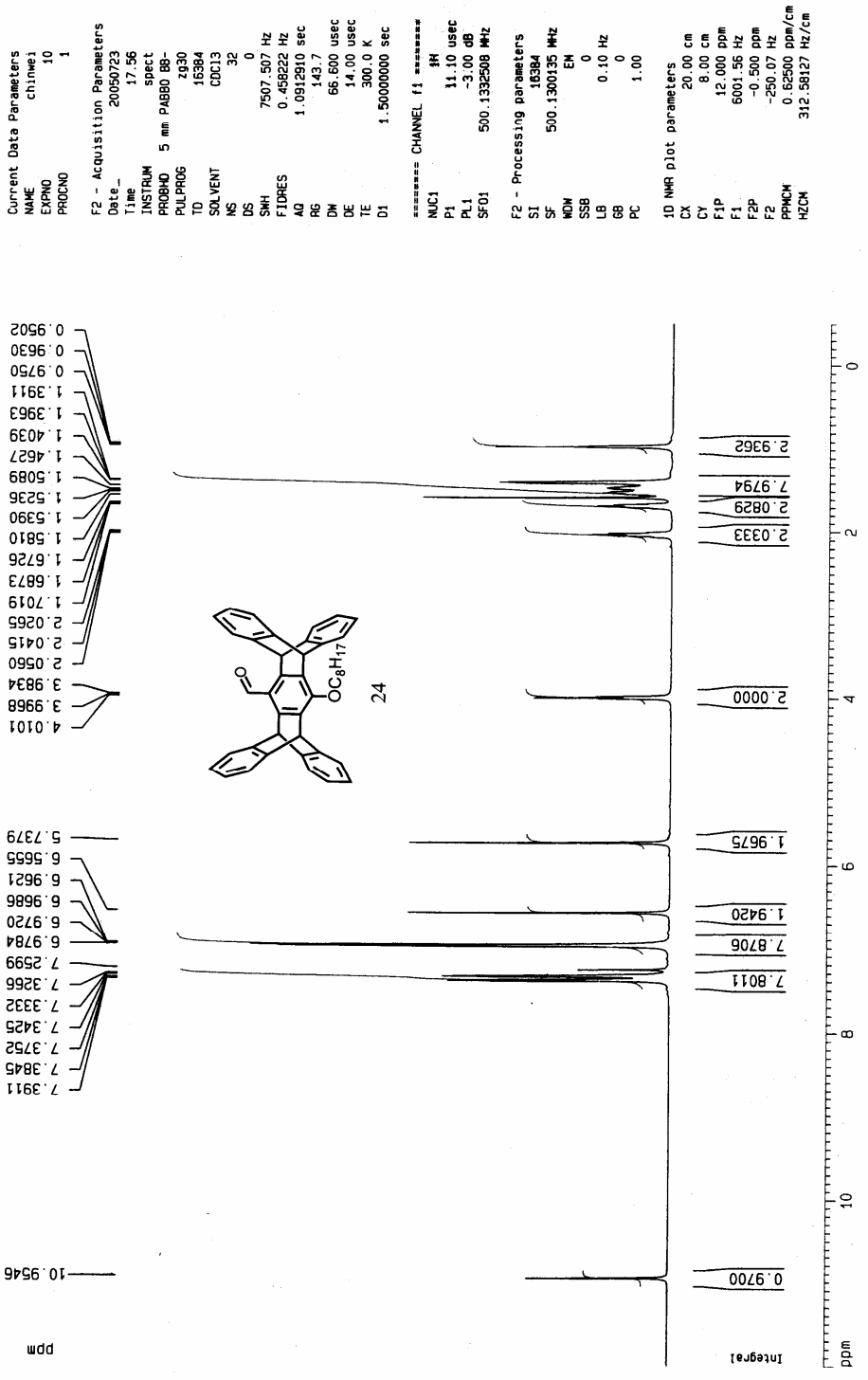

Current Data Parameters
NAME million
EXPNO 100106
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050718
Time 7.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 19380
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 1625.5
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577904 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 160.000 ppm
F1 20121.25 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.00000 ppm/cm
HZCM 1006.06232 Hz/cm
OC8H17
21
14.151
22.722
26.453
29.420
29.630
30.589
31.955
48.254
51.133
76.046
76.748
77.001
77.256
123.474
123.573
124.097
125.085
125.138
126.290
126.664
128.061
128.959
134.959
136.244
137.338
142.261
145.345
145.572
148.954
ppm
20
40
60
80
100
120
140
ppm


Current Data Parameters
NAME million
EXPNO 100096
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050708
Time 23.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 143.7
DW 66.600 usec
DE 14.00 usec
TE 300.0 K
D1 1.50000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.10 usec
PL1 -3.00 dB
SF01 500.1332508 MHz
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 262.56824 Hz/cm
OC8H17
22
ppm
Integral


Current Data Parameters
NAME 20050703Z-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050724
Time 7.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12288
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 1824.6
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SF01 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SF02 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577452 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 180.000 ppm
F1 22636.39 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.00000 ppm/cm
HZCM 1131.81970 Hz/cm
OC8H17
22
14.548
23.113
26.836
29.823
30.026
31.008
32.346
48.618
51.639
76.455
77.129
77.382
77.636
123.816
123.856
125.422
125.450
127.679
128.869
130.160
130.614
134.923
138.614
142.637
145.712
146.048
149.527
ppm
20
40
60
80
100
120
140
160


Current Data Parameters
NAME 20050730-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050722
Time 5.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16384
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2580.3
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322505 MHz
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.06 Hz
PPMCM 0.52500 ppm/cm
HZCM 262.36824 Hz/cm
0.94664
0.96005
1.38402
1.38888
1.39598
1.45063
1.46142
1.47866
1.49372
1.50841
1.52410
1.53581
1.57573
1.64760
1.66237
1.67660
1.99641
2.01130
2.02592
3.99139
4.00482
4.01825
5.70402
5.73917
6.82119
6.83569
6.96791
6.98629
6.99100
6.99691
7.01382
7.12525
7.14148
7.15724
7.17202
7.25979
7.32709
7.33021
7.34092
7.41376
7.42578
ppm
2.952
10.395
2.031
2.000
3.963
8.044
8.013
Integral
ppm
0
2
4
6
8
23
OC_8H_{17}
N


Current Data Parameters
NAME 20050700301
EXPNO 2
PROCNO 2
F2 - Acquisition Parameters
Date_ 20050722
Time 5.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16384
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2580.3
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SF01 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SF02 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 180.000 ppm
F1 22636.39 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.00000 ppm/cm
HZCM 1131.81970 Hz/cm
N
OC8H17
23
14.497
23.049
26.614
29.697
29.866
30.877
32.252
48.438
52.773
76.562
77.106
77.360
77.614
100.580
116.705
123.928
124.543
125.971
126.024
137.363
144.380
144.568
148.262
153.140
ppm
20
40
60
80
100
120
140
160
ppm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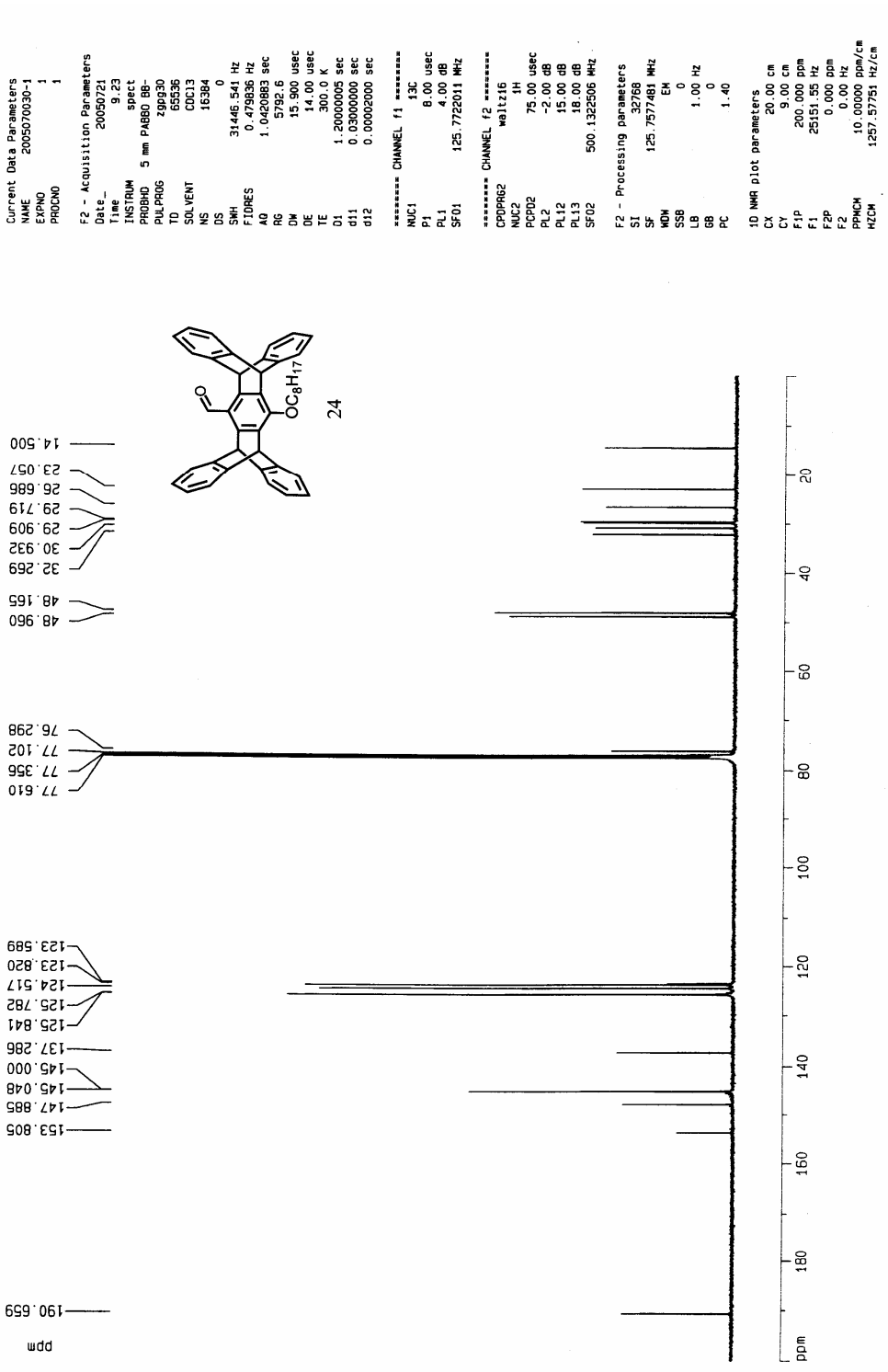
NAME chinwei
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050723
Time 17.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 32
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 143.7
DW 66.600 usec
DE 14.00 usec
TE 300.0 K
D1 1.50000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.10 usec
PL1 -3.00 dB
SFO1 500.1332508 MHz
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 12.000 ppm
F1 6001.56 Hz
F2P -0.500 ppm
F2 -250.07 Hz
PPMCM 0.62500 ppm/cm
HZCM 312.58127 Hz/cm
10.9546
7.9911
7.3845
7.3752
7.3425
7.3332
7.3266
7.2599
6.9784
6.9720
6.9686
6.9621
6.5655
5.7379
4.0101
3.9968
3.9834
2.0560
2.0415
2.0265
1.7019
1.6873
1.6726
1.5810
1.5390
1.5236
1.5089
1.4627
1.4039
1.3963
1.3911
0.9750
0.9630
0.9502
OC8H17
O
24
0.9700
1.9420
7.8706
7.8011
1.9675
2.0000
2.9362
7.9794
2.0829
2.0333
Integral
ppm
ppm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NAME 20050700301
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20050721
Time 9.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16384
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 5792.6
DW 15.900 usec
DE 14.00 usec
TE 300.0 K
D1 1.20000005 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 4.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577481 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 9.00 cm
F1P 200.000 ppm
F1 25151.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1257.57751 Hz/cm
OC8H17
O
24
14.500
23.057
26.686
29.719
29.909
30.932
32.269
48.165
48.960
76.298
77.102
77.356
77.610
123.589
123.820
124.517
125.782
125.841
137.286
145.000
145.048
147.885
153.805
190.659
ppm
20
40
60
80
100
120
140
160
180
ppm