Supporting Information for:

Improved Iterative Synthesis of Linearly Disassembling Dendrons

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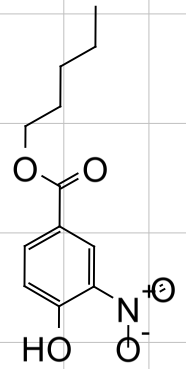
General: NMR spectra were recorded on commercial instrumentation at 300 MHz or 600 MHz for proton, and 75 or 125 MHz for carbon. All chemical shifts were reported as referenced from an internal TMS standard. All chemicals were purchased from chemical suppliers and used as received unless otherwise stated. All solvents used were freshly distilled prior to use or dried with 3 Å molecular sieves unless otherwise noted. Frechét type dendrons ([G-*n*]-CH_2OH) were prepared according to literature procedures.[1] Fréchet dendritic aldehydes [G-*n*]-CHO[2] were prepared via treatment of the respective [G-*n*]-CH_2OH with PCC in CH_2Cl_2. Flash chromatography was performed by the method of Still et al.[3] using silica gel (40-63 μm, Merck, Darmstadt, Germany). Thin-layer chromatography (TLC) was performed on precoated plates (silica gel 60 F_{254}, 250 μm, Merck, Darmstadt, Germany).

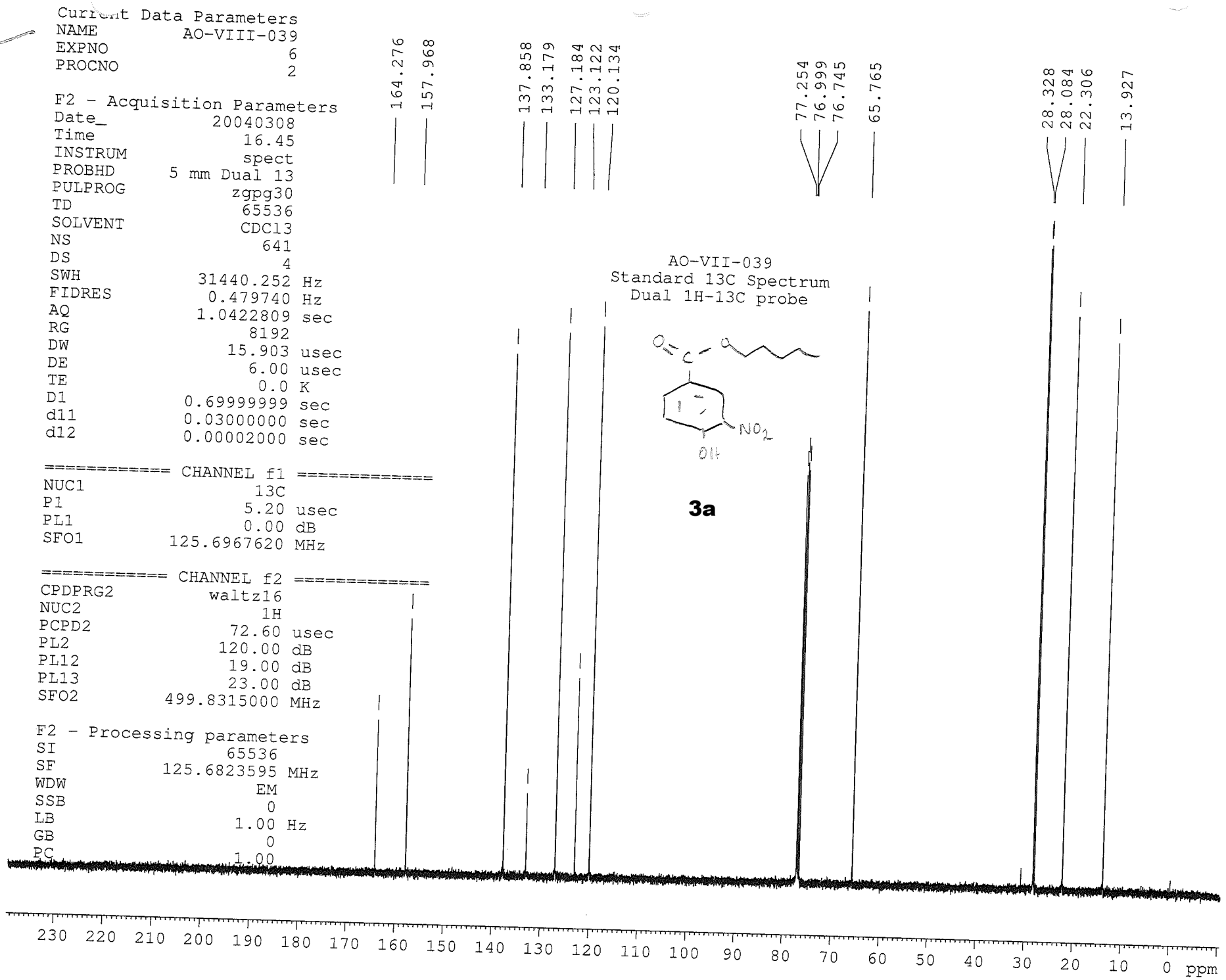
References Cited

(1) Hawker, C. J.; Fréchet, J. M. J. *J. Am. Chem. Soc.* **1990**, *112*, 7638-7647.
(2) Pollak, K. W.; Sanford, E. M.; Fréchet, J. M. J. *J. Mater. Chem.* **1998**, *8*, 519-527.
(3) Still, W. C.; Kahn, M.; Mitra, A. *J. Org. Chem* **1978**, 2923-2925.

Title: Ao-vii-039 (3a)
Date: 2010-06-23T10:35:00
Spectrometer: spect
Probe: 5 mm BBO BB-1H/D Z-GRD
Z8007/0116
Pulse Sequence: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: 4
SWH (Hz): 6250.000
FIDRES (Hz): 0.19073486
Acquisition Time (sec): 2.6215701
Receiver Gain: 20.2
DW (sec): 0.00008000
DE (usec): 6.00
Temperature (K): 298
D1 (sec): 0
TD0: 1
Nucleus: 1H
P1 (usec): 12.5
PL1 (dB): -2.00
SFO1 (MHz): 499.48294693
SI: 32768
SF (MHz): 499.48000000
WDW: 1
SSB: 0
LB (Hz): 0.20
GB: 0
PC: 1



3a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EXPNO 6
PROCNO 2
F2 - Acquisition Parameters
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Time 16.45
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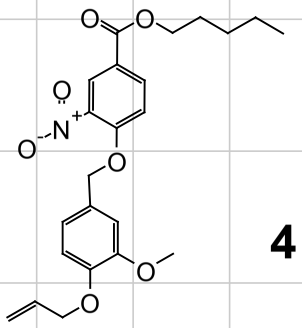
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 641
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823595 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
164.276
157.968
137.858
133.179
127.184
123.122
120.134
77.254
76.999
76.745
65.765
28.328
28.084
22.306
13.927
AO-VII-039
Standard 13C Spectrum
Dual 1H-13C probe
NO2
3a
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

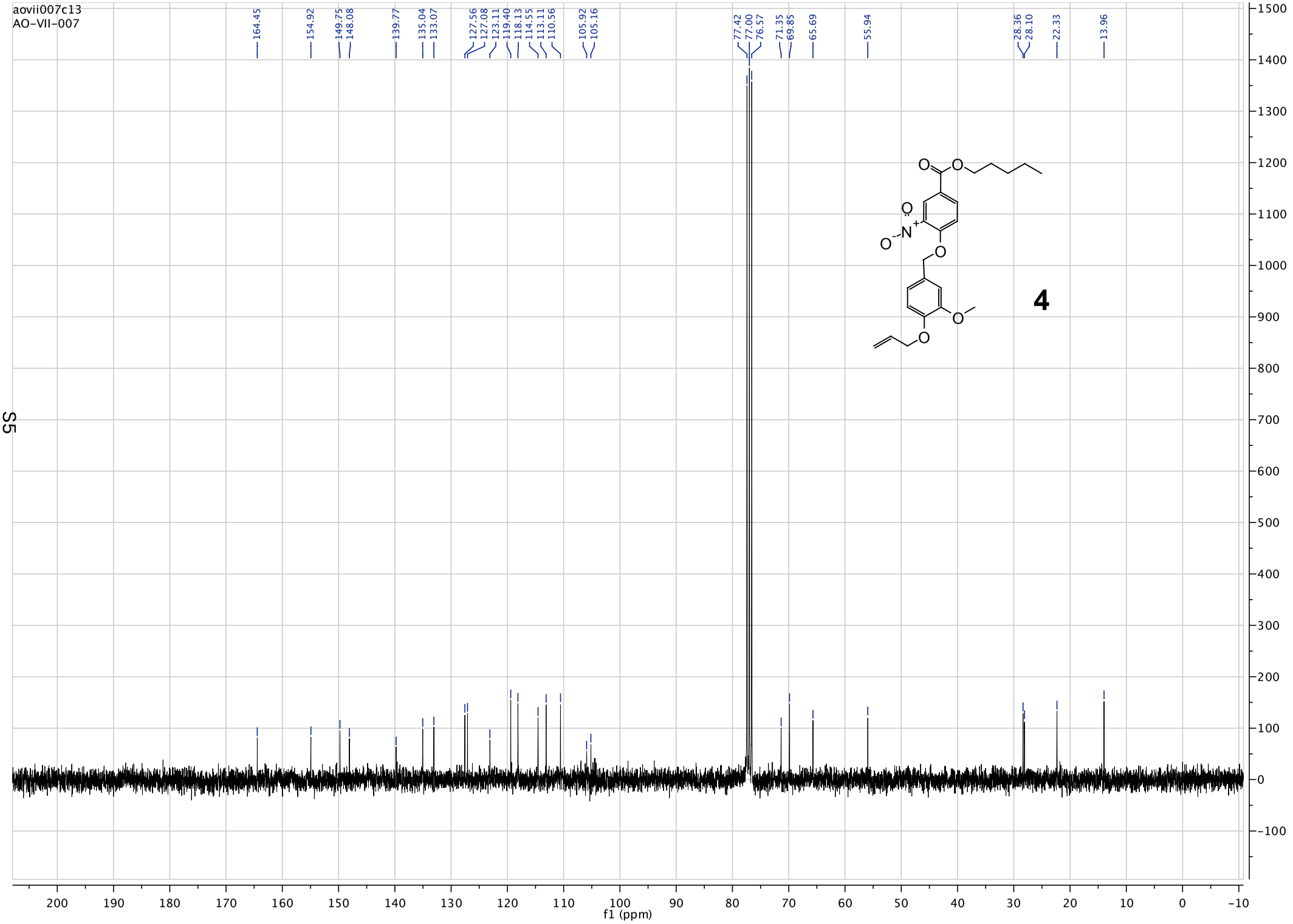
aovii007
STANDARD 1H OBSERVE

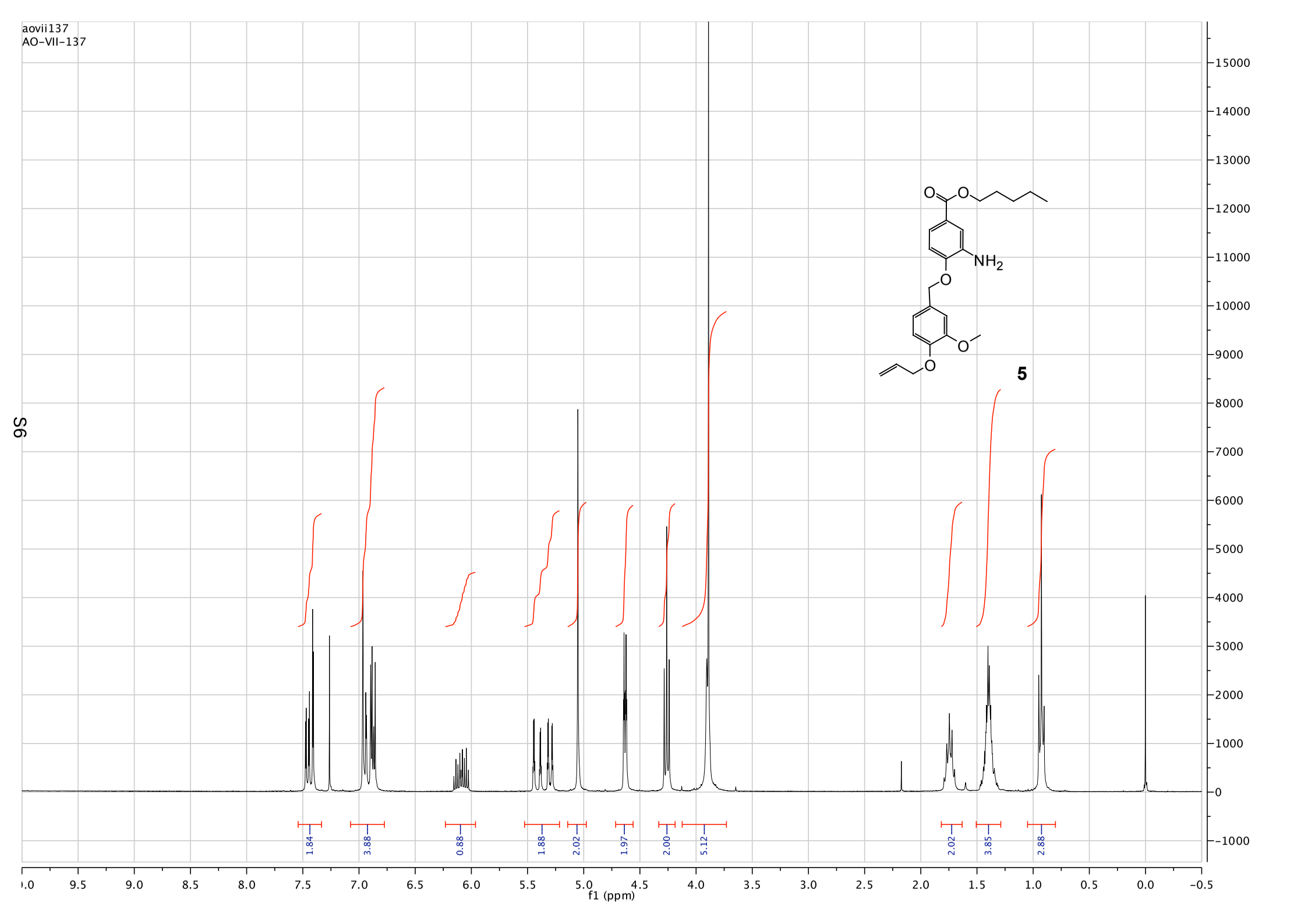
Parameters

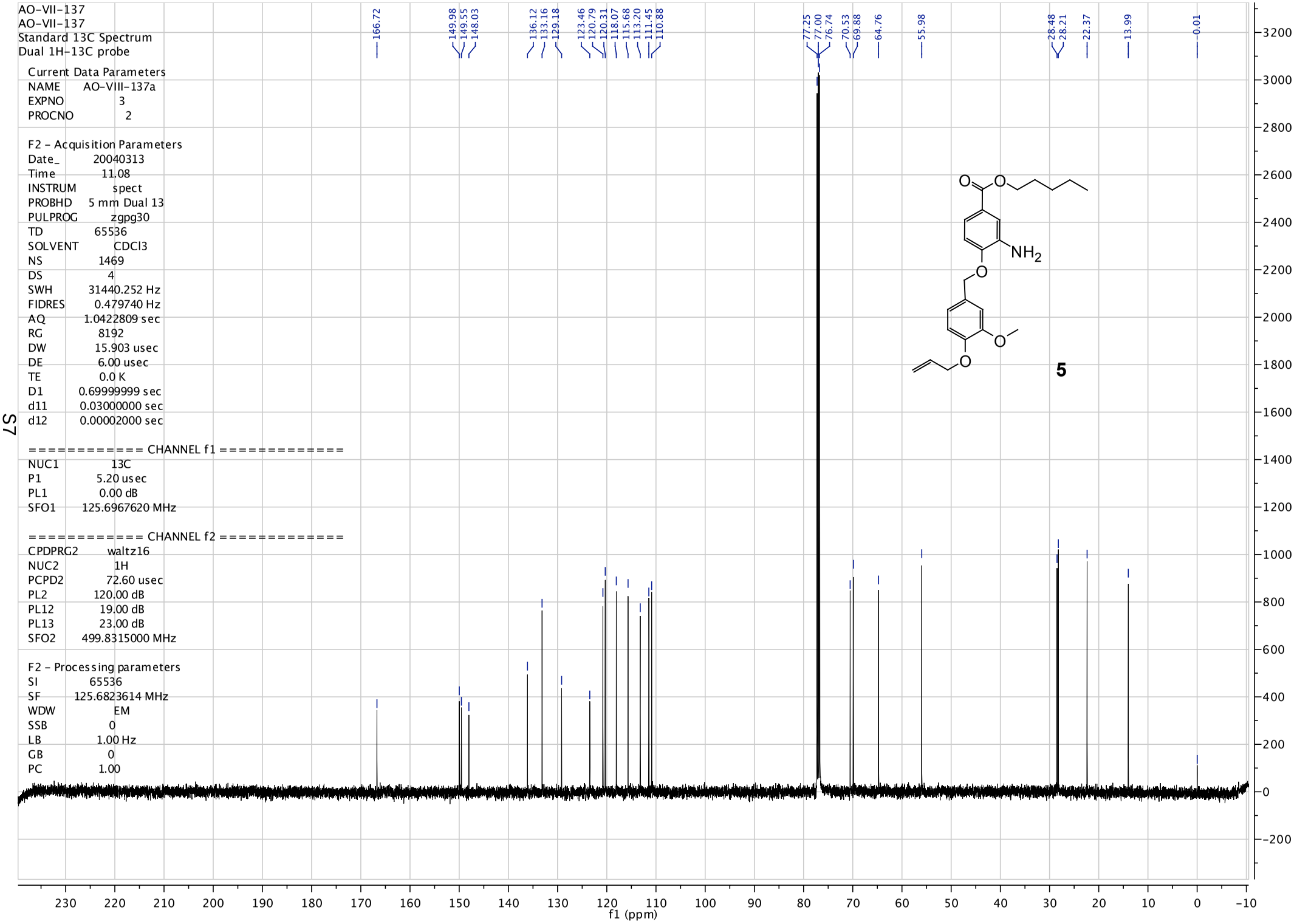
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aovii007.fid/ fid
Title	aovii007
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	16
Receiver Gain	50
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2003-11-05T07:51:01
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-923.6
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



4


aovii007c13
AO-VII-007
164.45
154.92
149.75
148.08
139.77
135.04
133.07
127.56
127.08
123.11
119.40
118.13
114.55
113.11
110.56
105.92
105.16
77.42
77.00
76.57
71.35
69.85
65.69
55.94
28.36
28.10
22.33
13.96
4
f1 (ppm)


aovii137
AO-VII-137
S6
5
NH2
O
O
O
O
O
f1 (ppm)
1.84
3.88
0.88
1.88
2.02
1.97
2.00
5.12
2.02
3.85
2.88

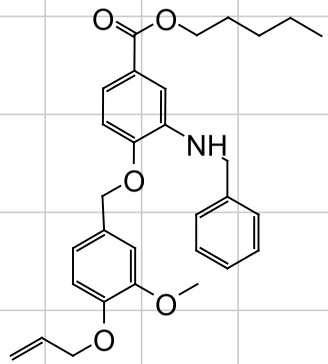

AO-VII-137
AO-VII-137
Standard 13C Spectrum
Dual 1H-13C probe
Current Data Parameters
NAME AO-VIII-137a
EXPNO 3
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040313
Time 11.08
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1469
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
166.72
149.98
149.55
148.03
136.12
133.16
129.18
123.46
120.79
120.31
118.07
115.68
113.20
111.45
110.88
77.25
77.00
76.74
70.53
69.88
64.76
55.98
28.48
28.21
22.37
13.99
0.01
NH2
5
S7
f1 (ppm)

aovii045
AO-VII-045

Parameters

Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aovii045.fid/ fid
Title	aovii045
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	55
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2003-11-15T07:51:07
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-923.5

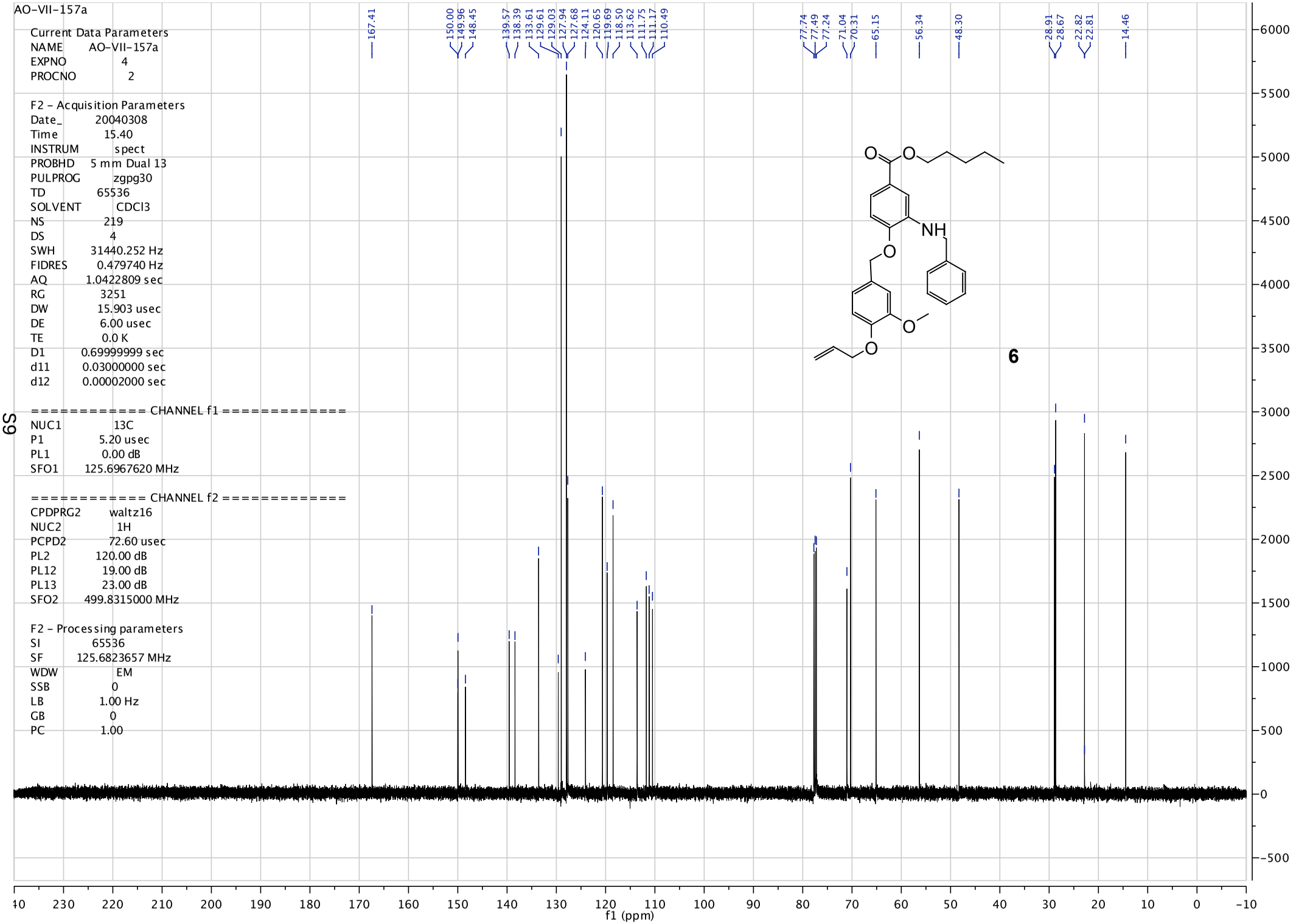
S8



6

8.17 4.08 1.36 2.09 2.05 3.21 2.17 2.17 2.93 2.26 3.97 3.00

f1 (ppm)


AO-VII-157a
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NAME AO-VII-157a
EXPNO 4
PROCNO 2
F2 - Acquisition Parameters
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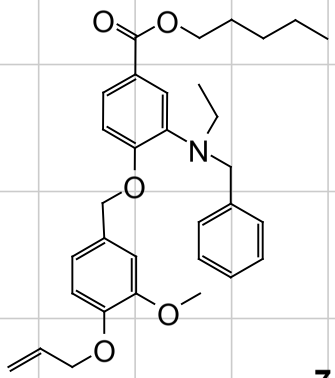
Time 15.40
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 219
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 3251
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
============ CHANNEL f1 ============
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
============ CHANNEL f2 ============
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823657 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
167.41
150.00
149.96
148.45
139.57
138.39
133.61
129.61
129.03
127.94
127.68
124.11
120.65
119.69
118.50
113.62
111.75
111.17
110.49
77.74
77.49
77.24
71.04
70.31
65.15
56.34
48.30
28.91
28.67
22.82
22.81
14.46
O
O
NH
O
O
O
6
S9
f1 (ppm)

aovii053
AO-VII-053

Parameters

Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aovii053.fid/ fid
Title	aovii053
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	49
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2003-11-18T16:56:34
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-923.5



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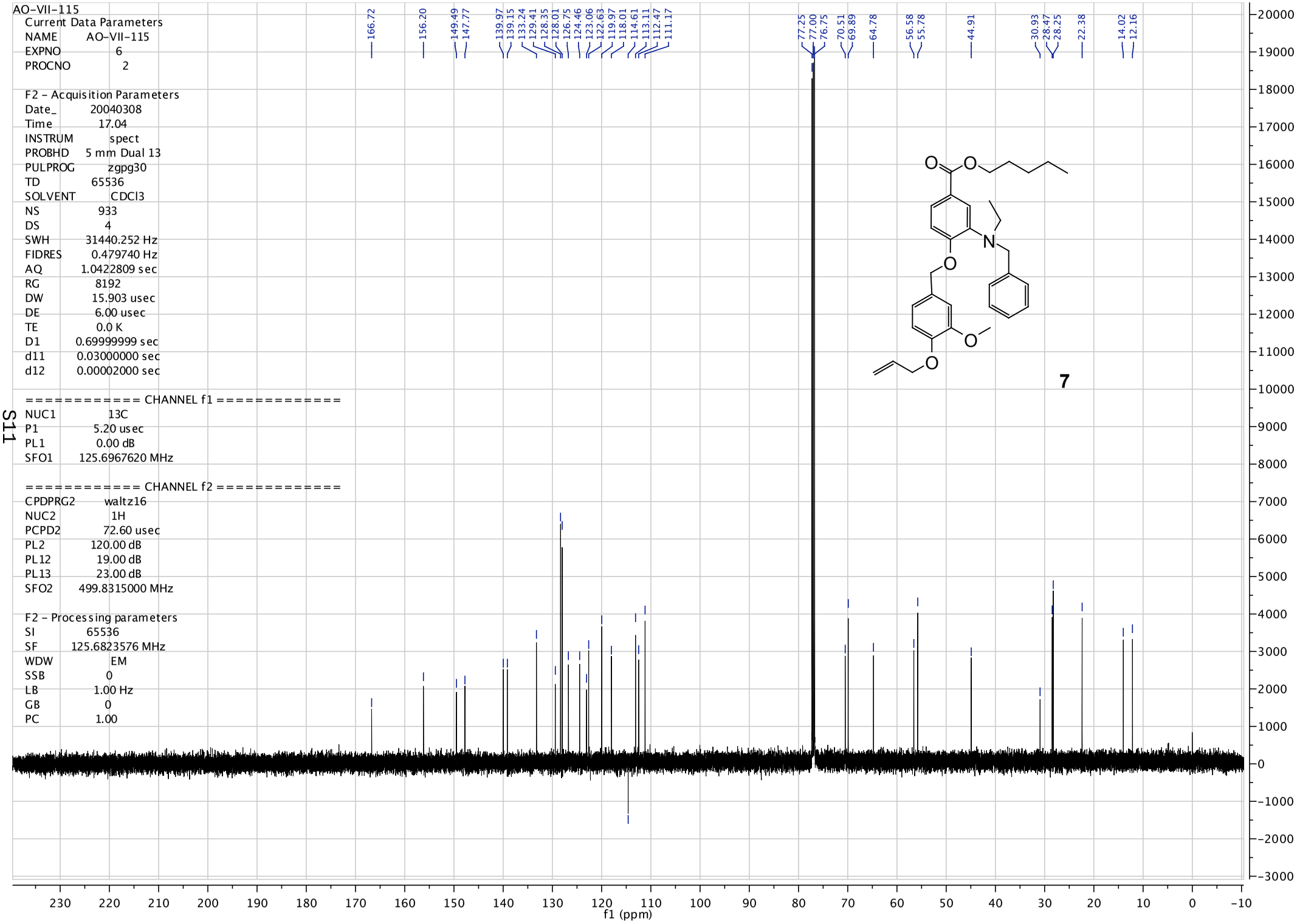
1.81 5.11 3.77 0.83 1.68 1.95 1.75 3.82 2.93 2.00 1.96 3.79 5.88

f1 (ppm)


AO-VII-115
Current Data Parameters
NAME AO-VII-115
EXPNO 6
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040308
Time 17.04
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 933
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
166.72
156.20
149.49
147.77
139.97
139.15
133.24
129.41
128.35
128.01
126.75
124.46
123.06
122.63
119.97
118.01
114.61
113.11
112.47
111.17
77.25
77.00
76.75
70.51
69.89
64.78
56.58
55.78
44.91
30.93
28.47
28.25
22.38
14.02
12.16
7
f1 (ppm)

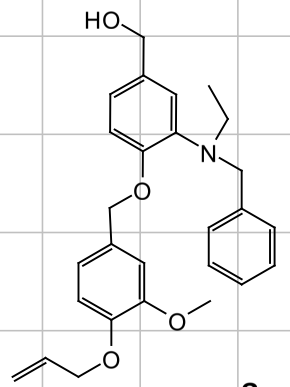
AO-VIII-175(8)
Ao-VIII-175(8)

Current Data Parameters
NAME AO-VIII-175(8)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100623
Time 10.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 6250.000 Hz
FIDRES 0.190735 Hz
AQ 2.6215701 sec
RG 12.7
DW 80.000 usec
DE 6.00 usec
TE 298.0 K
D1 0.00000000 sec
TD0 1

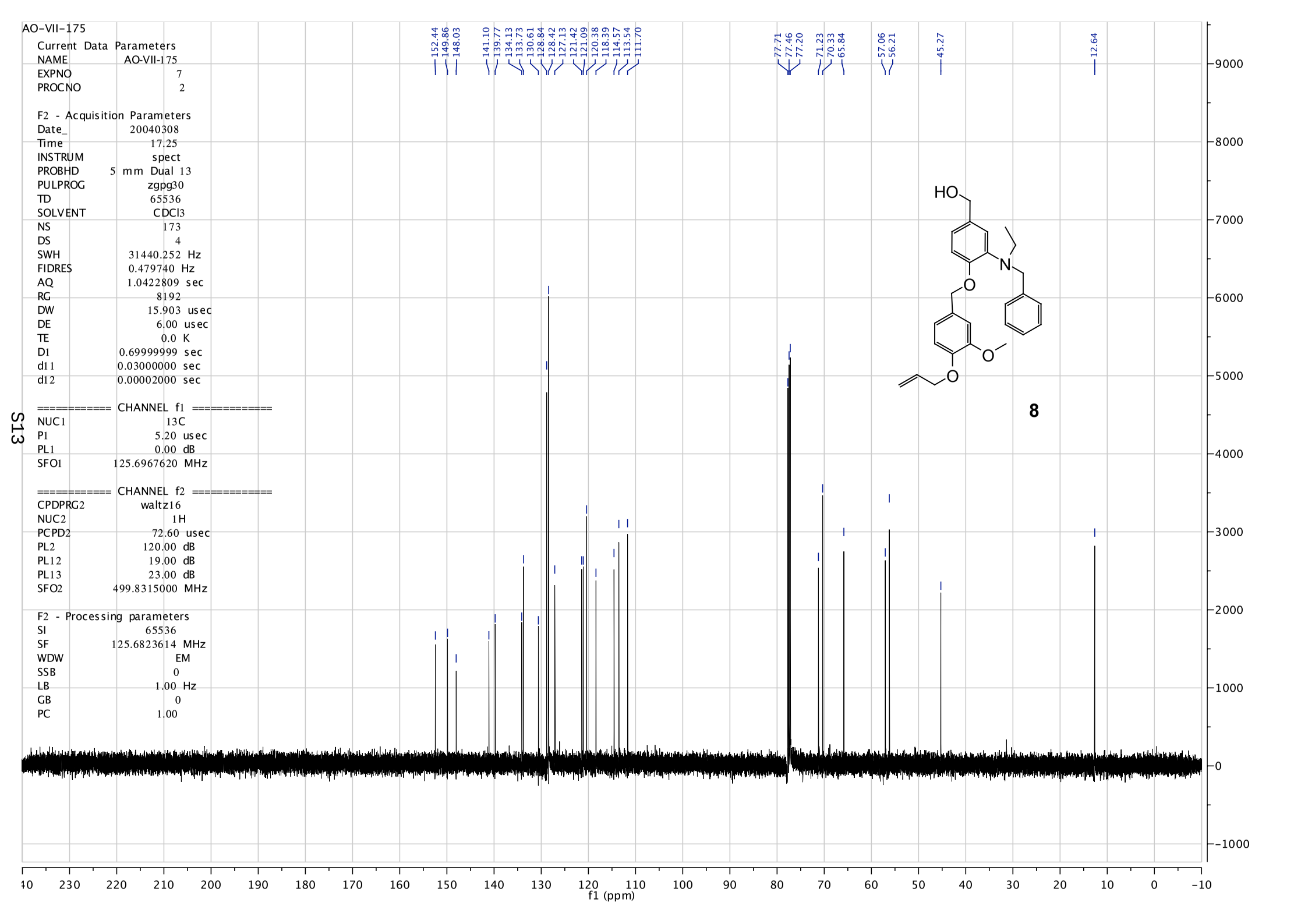
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
SFO1 499.4829469 MHz

F2 - Processing parameters
SI 32768
SF 499.4800000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



8

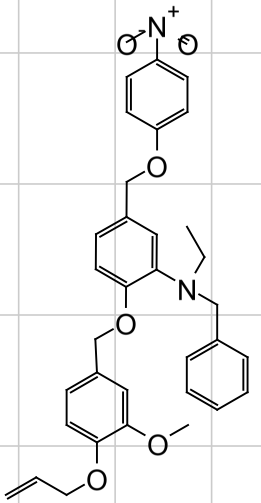
f1 (ppm)


AO-VII-175
Current Data Parameters
NAME AO-VII-175
EXPNO 7
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040308
Time 17.25
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 173
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
152.44
149.86
148.03
141.10
139.77
134.13
133.73
130.61
128.84
128.42
127.13
121.42
121.09
120.38
118.39
114.57
113.54
111.70
77.71
77.46
77.20
71.23
70.33
65.84
57.06
56.21
45.27
12.64
HO
N
O
O
O
8
f1 (ppm)

aovii143
AO-VII-143

Parameters

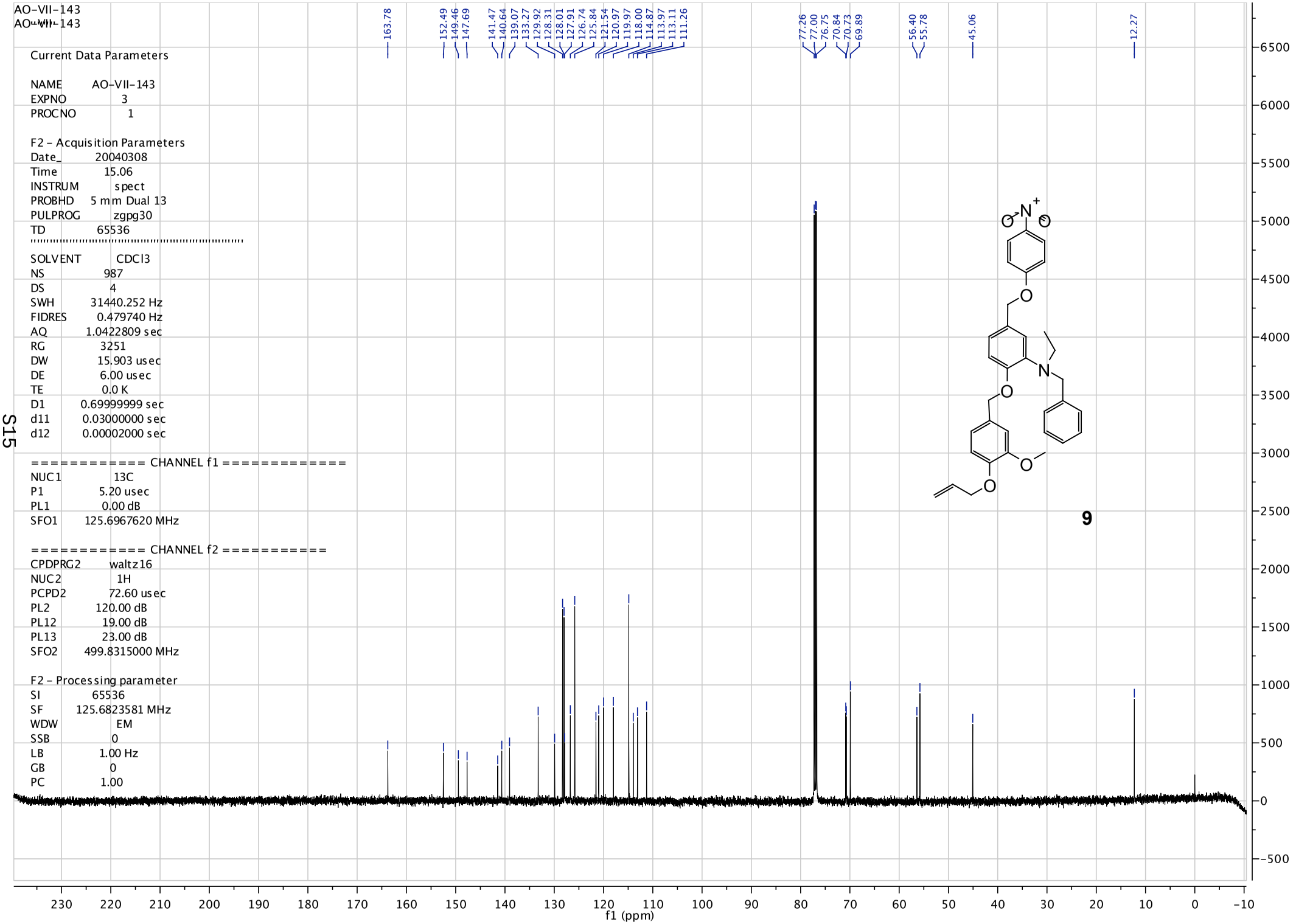
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aovii143.fid/ fid
Title	aovii143
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	55
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2003-12-23T12:14:36
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-923.3
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



9

2.11 6.65 7.21 1.19 2.18 3.72 2.03 2.00 2.82 2.13 2.96

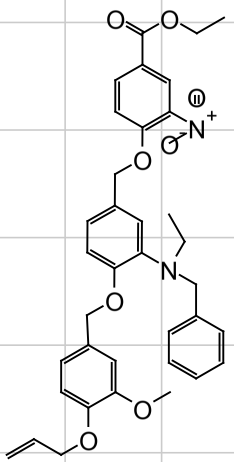
f1 (ppm)


AO-VII-143
AO-VII-143
Current Data Parameters
NAME AO-VII-143
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040308
Time 15.06
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 987
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 3251
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameter
SI 65536
SF 125.6823581 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
163.78
152.49
149.46
147.69
141.47
140.64
139.07
133.27
129.92
128.31
128.01
127.91
126.74
125.84
121.54
120.97
119.97
118.00
114.87
113.97
113.11
111.26
77.26
77.00
76.75
70.84
70.73
69.89
56.40
55.78
45.06
12.27
9
f1 (ppm)

aovii187b
AO-VII-187b

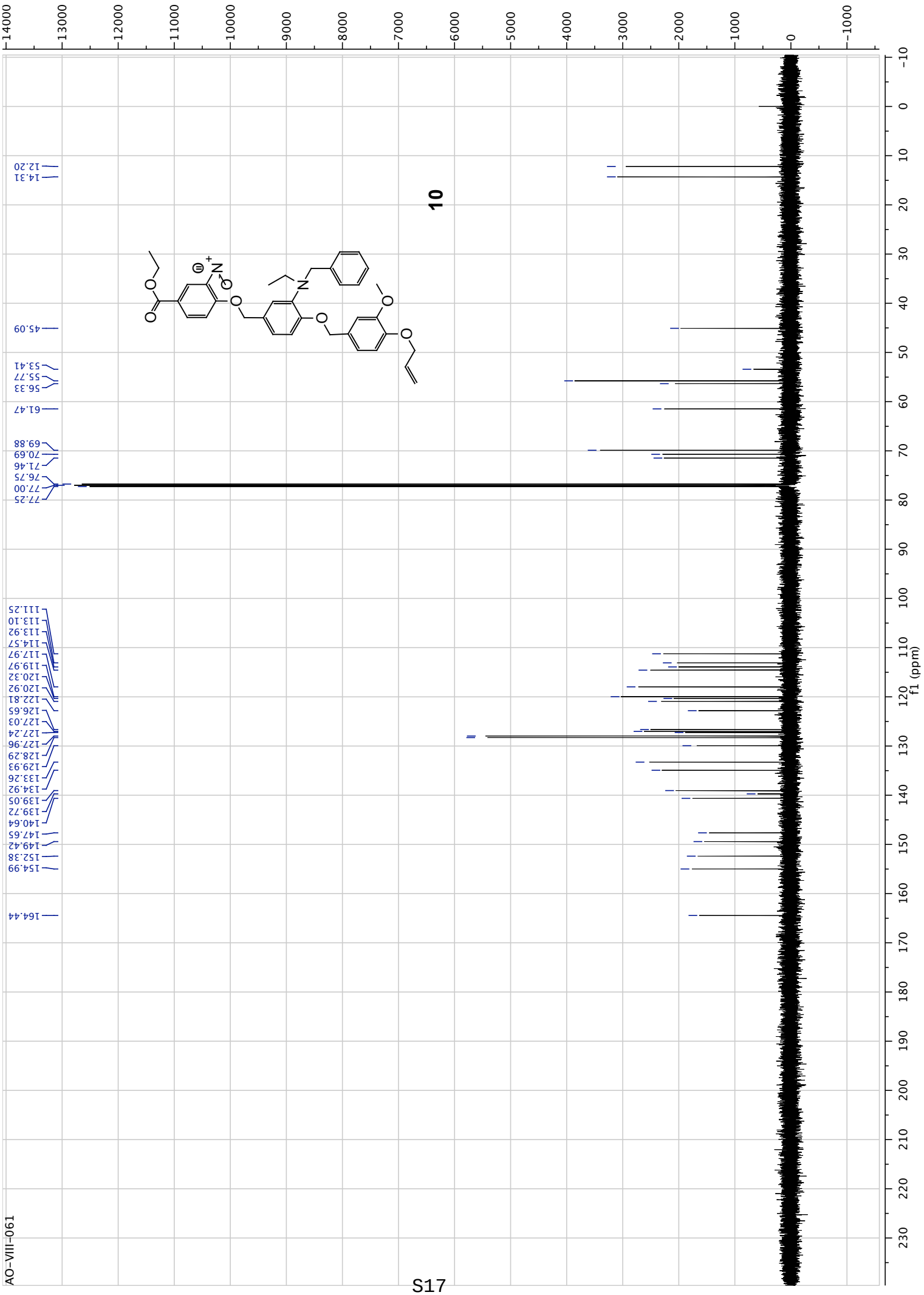
Parameters

Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aovii187b.fid/ fid
Title	aovii187b
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	48
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2004-01-09T13:05:20
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-921.1
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



10

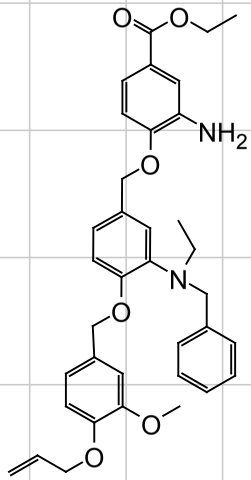
f1 (ppm)


10
AO-VIII-061
f1 (ppm)
12.20
14.31
45.09
53.41
55.77
56.33
61.47
69.88
70.69
71.46
76.75
77.00
77.25
111.25
113.10
113.92
114.57
117.97
119.97
120.32
120.92
122.81
126.65
127.03
127.24
127.96
128.29
129.93
133.26
134.92
139.05
139.72
140.64
147.65
149.42
152.38
154.99
164.44

aoviii093
AO-VIII-093

Parameters

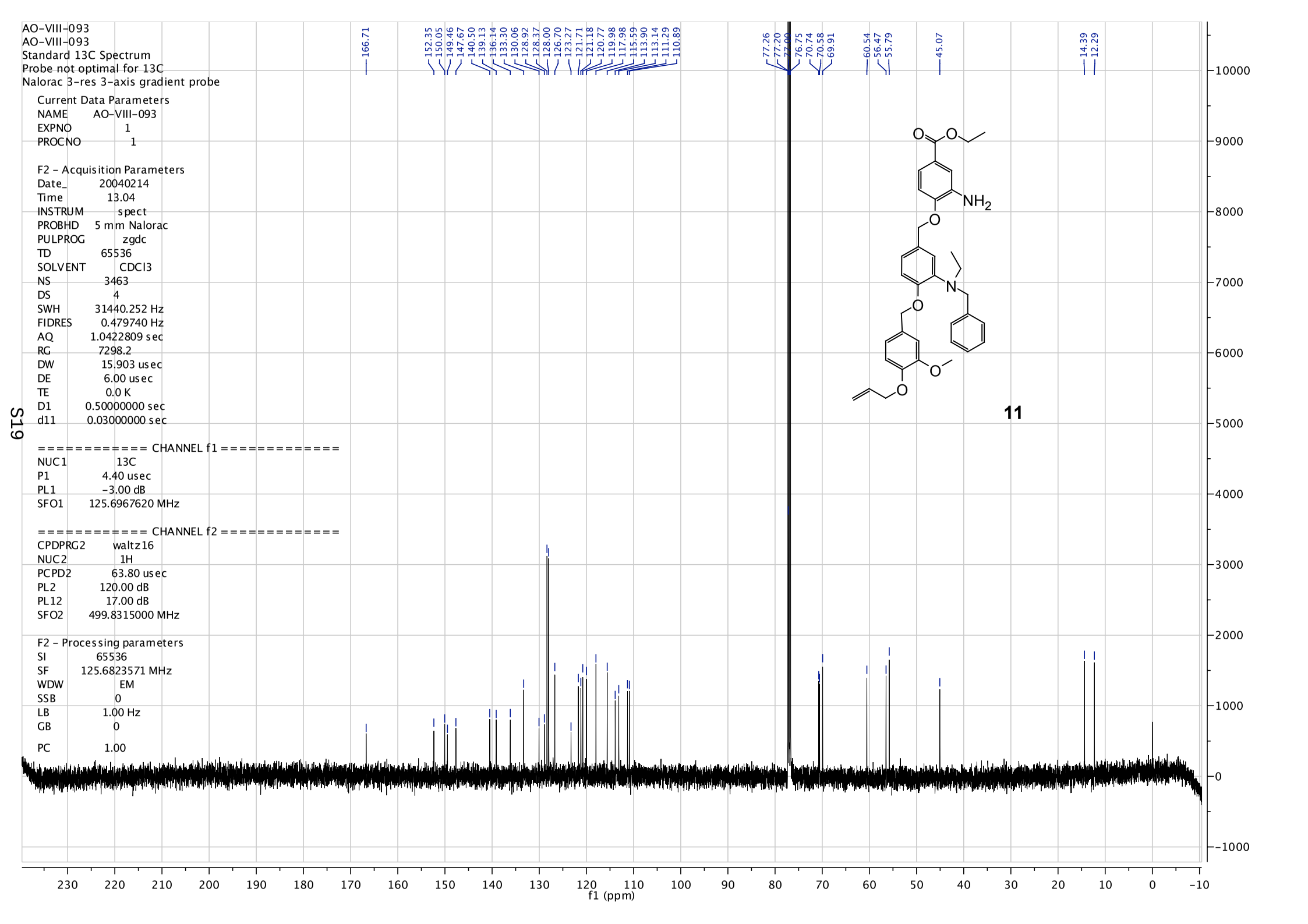
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aoviii093.fid/ fid
Title	aoviii093
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	64
Receiver Gain	20
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2004-02-13T16:38:25
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-922.0



11

11.61 6.79 0.78 1.85 4.06 2.00 4.00 4.96 2.04 2.88 3.00

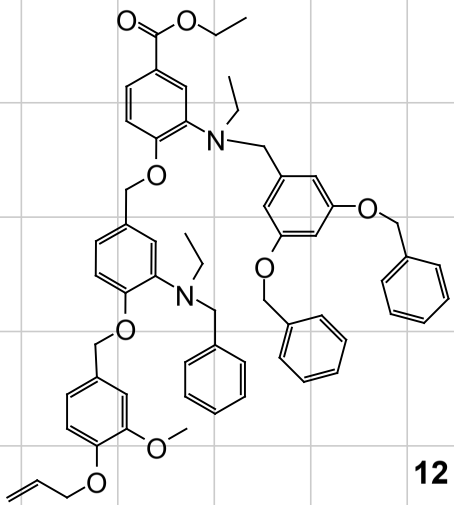
f1 (ppm)


AO-VIII-093
AO-VIII-093
Standard 13C Spectrum
Probe not optimal for 13C
Nalorac 3-res 3-axis gradient probe
Current Data Parameters
NAME AO-VIII-093
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040214
Time 13.04
INSTRUM spect
PROBHD 5 mm Nalorac
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 3463
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 7298.2
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.50000000 sec
d11 0.03000000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 4.40 usec
PL1 -3.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 63.80 usec
PL2 120.00 dB
PL12 17.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
166.71
152.35
150.05
149.46
147.67
140.50
139.13
136.14
133.30
130.06
128.92
128.37
128.00
126.70
123.27
121.71
121.18
120.77
119.98
117.98
115.59
113.90
113.14
111.29
110.89
77.26
77.20
77.00
76.75
70.74
70.58
69.91
60.54
56.47
55.79
45.07
14.39
12.29
NH2
11
S19
f1 (ppm)

aoviii105
AO-VIII-105

Parameters

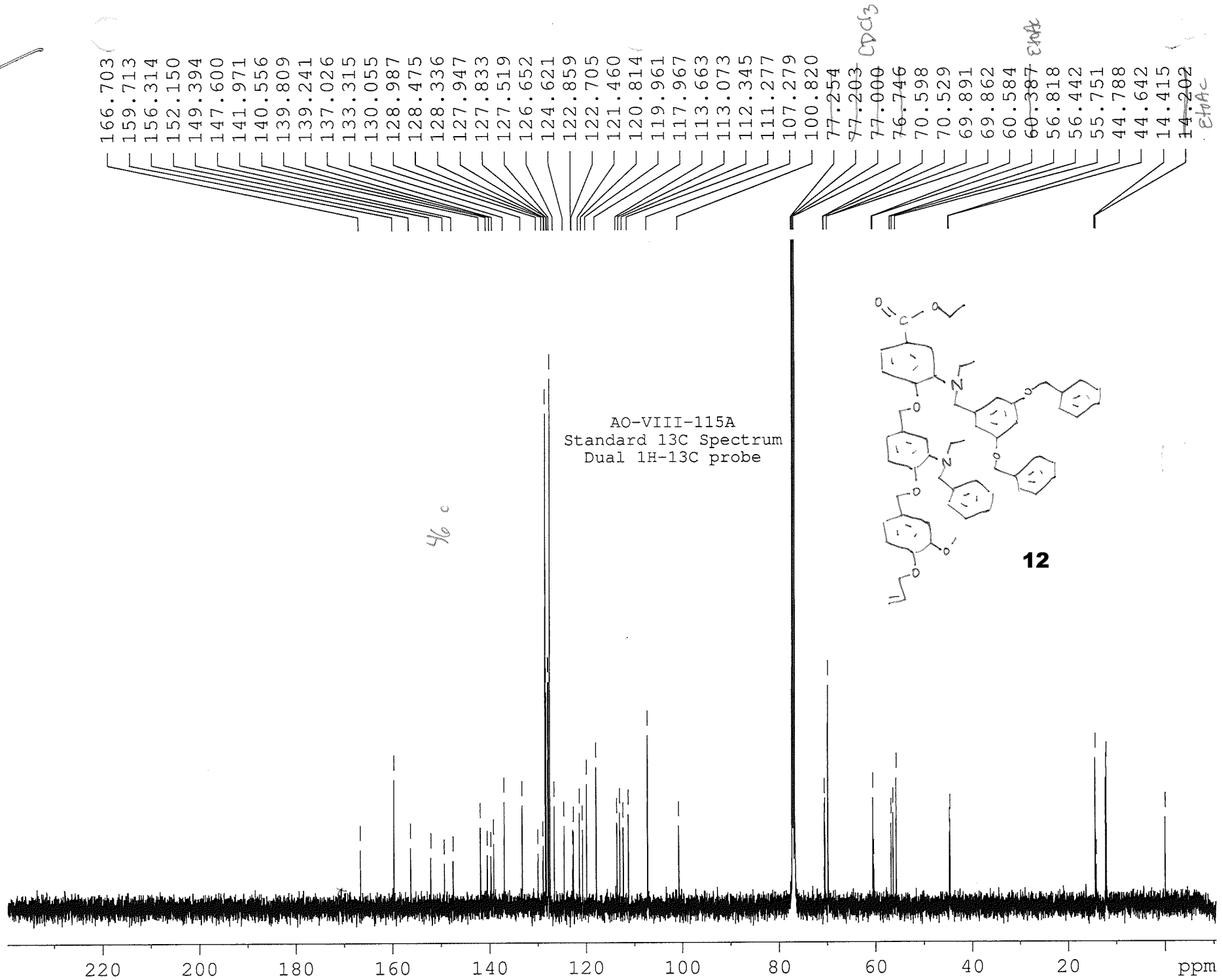
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aoviii105.fid/ fid
Title	aoviii105
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	30
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2004-02-18T13:41:01
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-929.6
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



12

1.88 15.73 6.95 2.03 0.98 0.77 1.80 8.38 2.02 6.18 3.01 4.00 2.99 6.07

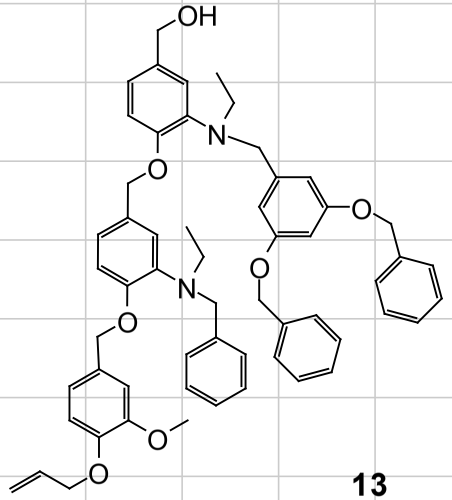
f1 (ppm)


166.703
159.713
156.314
152.150
149.394
147.600
141.971
140.556
139.809
139.241
137.026
133.315
130.055
128.987
128.475
128.336
127.947
127.833
127.519
126.652
124.621
122.859
122.705
121.460
120.814
119.961
117.967
113.663
113.073
112.345
111.277
107.279
100.820
77.254
77.203
77.000
76.746
70.598
70.529
69.891
69.862
60.584
60.387
56.818
56.442
55.751
44.788
44.642
14.415
14.202
CDCl3
EtOAc
AO-VIII-115A
Standard 13C Spectrum
Dual 1H-13C probe
12
220
200
180
160
140
120
100
80
60
40
20
ppm

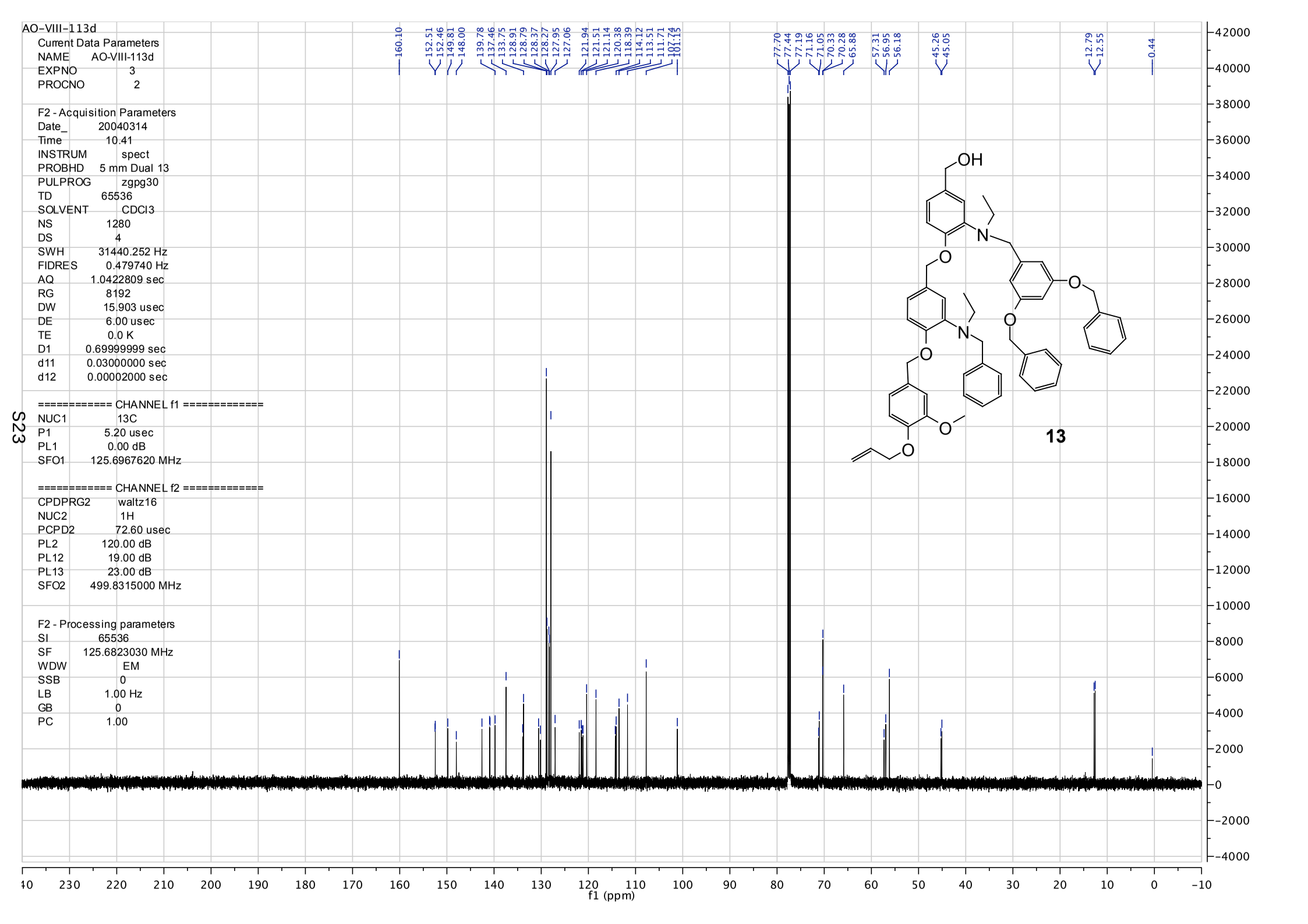
aoviii109
AO-VIII-109

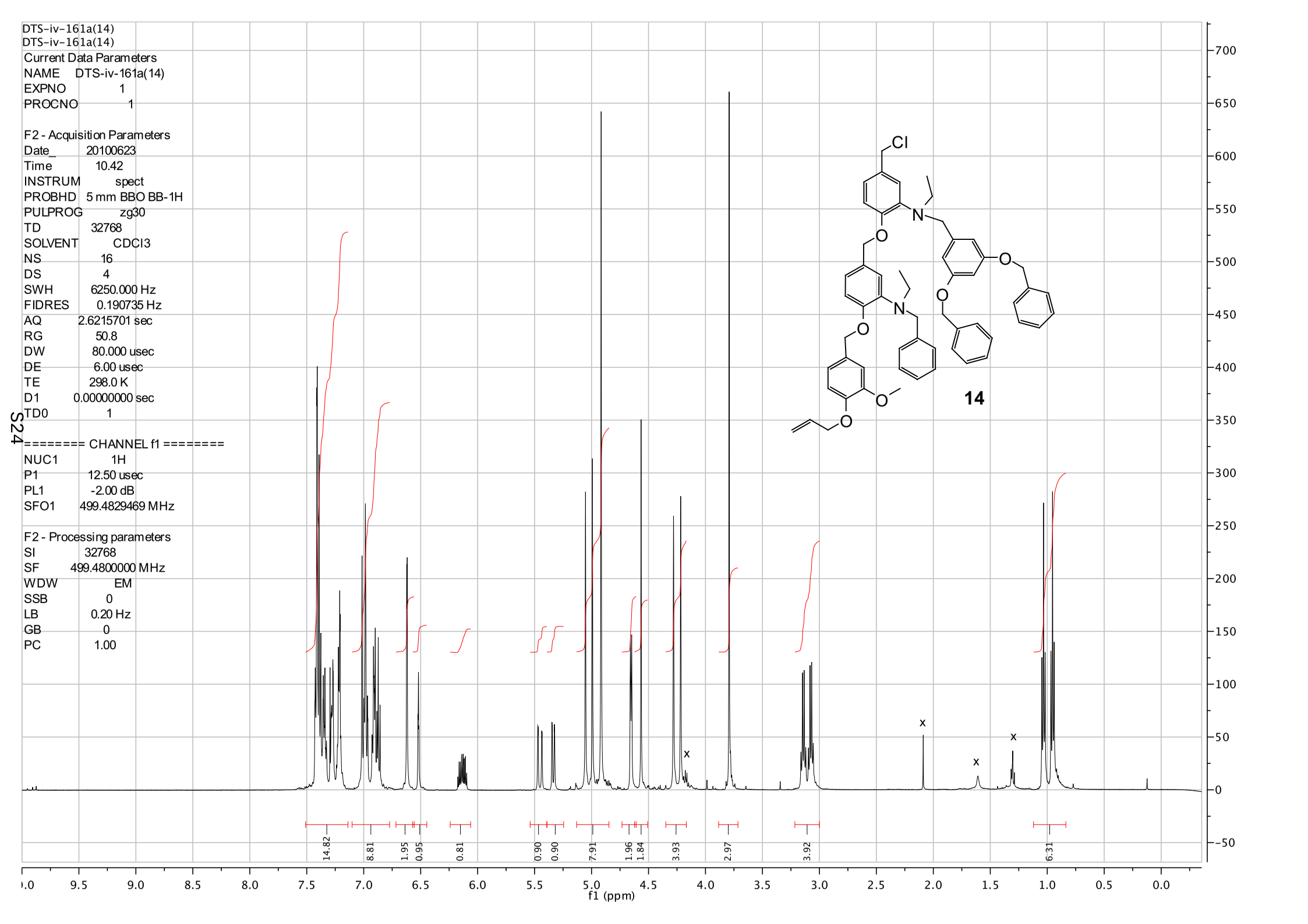
Parameters

Parameter	Value
Data File Name	/ Users/ mcgrath1/ McGrath/ Publications/ 1. IN PREPARATION/ Rapid Linear Synthesis (AO)/ NMR Spectra/ aoviii109 Folder/ aoviii109.fid/ fid
Title	aoviii109
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	41
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2004-02-22T12:59:16
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-924.4
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



13


AO-VIII-113d
Current Data Parameters
NAME AO-VIII-113d
EXPNO 3
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040314
Time 10.41
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1280
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823030 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
160.10
152.51
152.46
149.81
148.00
139.78
137.46
133.75
128.91
128.79
128.37
128.27
127.95
127.06
121.94
121.51
121.14
120.38
118.39
114.12
113.51
111.71
101.15
77.70
77.44
77.19
71.16
71.05
70.33
70.28
65.88
57.31
56.95
56.18
45.26
45.05
12.79
12.55
0.44
OH
N
O
N
O
O
O
O
O
13
S23
f1 (ppm)


DTS-iv-161a(14)
DTS-iv-161a(14)
Current Data Parameters
NAME DTS-iv-161a(14)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100623
Time 10.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 6250.000 Hz
FIDRES 0.190735 Hz
AQ 2.6215701 sec
RG 50.8
DW 80.000 usec
DE 6.00 usec
TE 298.0 K
D1 0.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
SFO1 499.4829469 MHz
F2 - Processing parameters
SI 32768
SF 499.4800000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
Cl
N
O
14
14.82
8.81
1.95
0.95
0.81
0.90
0.90
7.91
1.96
1.84
3.93
2.97
3.92
6.31
f1 (ppm)

DTS-iv-161a(14)
DTS-iv-161a(14)

Current Data Parameters
NAME DTS-iv-161a(14)
EXPNO 2
PROCNO 1

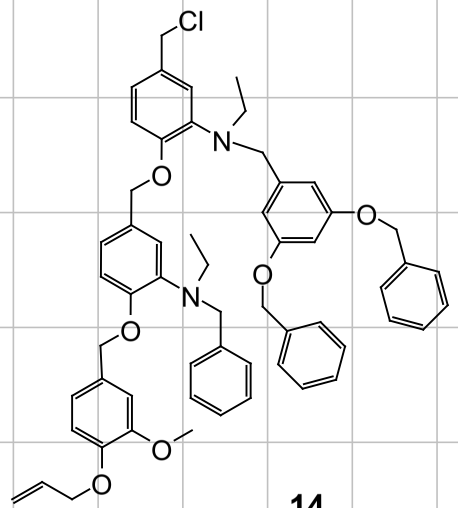
F2 - Acquisition Parameters
Date_ 20100623
Time 10.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 291
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 2896.3
DW 16.650 usec
DE 6.00 usec
TE 298.0 K
D1 0.69999999 sec
d11 0.03000000 sec
DELTA 0.59999996 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 125.6069050 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 499.4819980 MHz

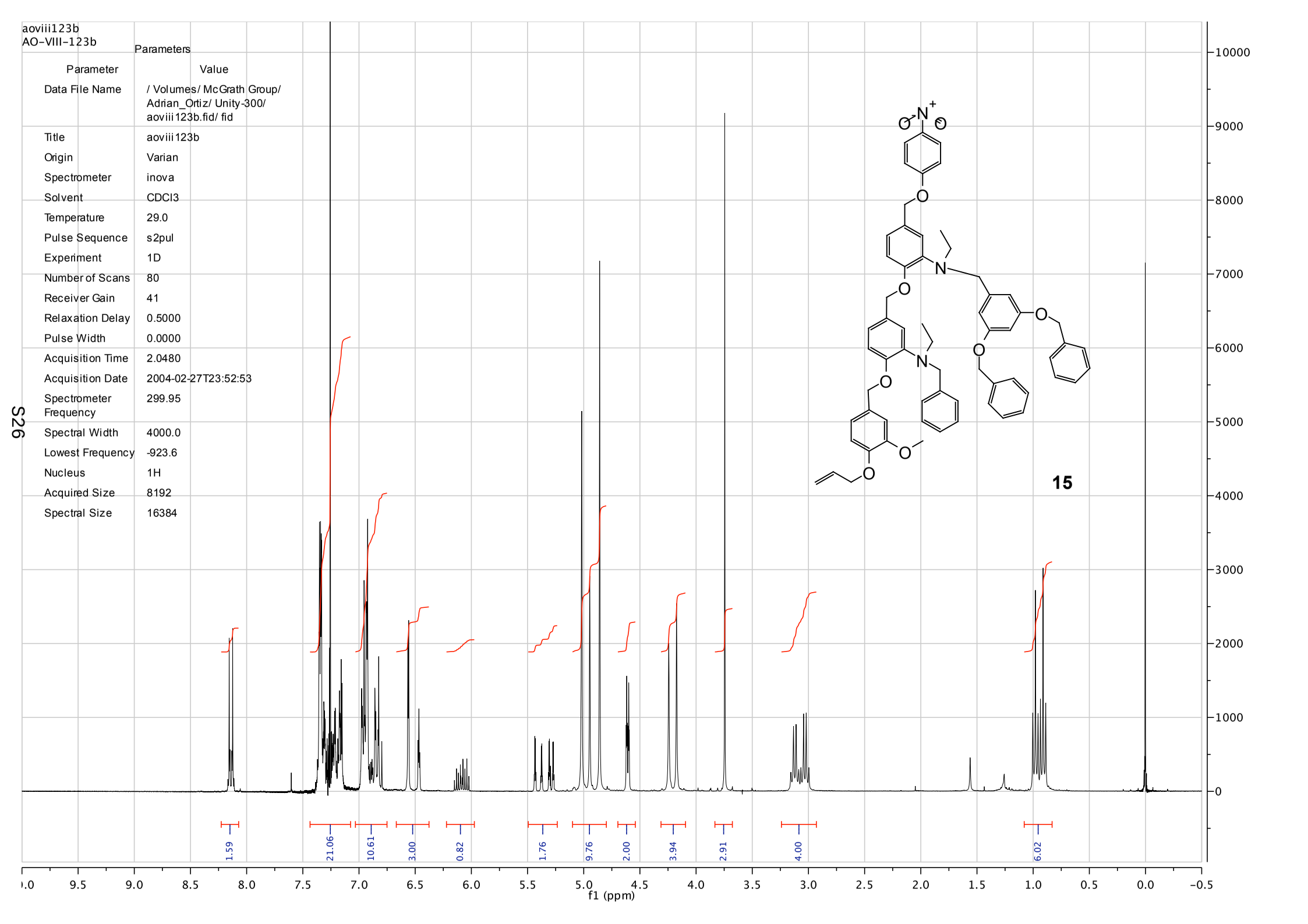
F2 - Processing parameters
SI 32768
SF 125.5943460 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

159.67
152.49
152.05
149.37
147.56
141.92
137.01
133.30
128.46
128.34
127.93
127.82
127.51
126.63
122.50
121.88
121.48
120.87
119.94
117.95
113.65
113.53
113.04
111.25
100.77
77.25
77.00
76.75
70.60
69.82
56.76
56.47
55.72
46.82
44.69
44.60
12.35
12.10



14

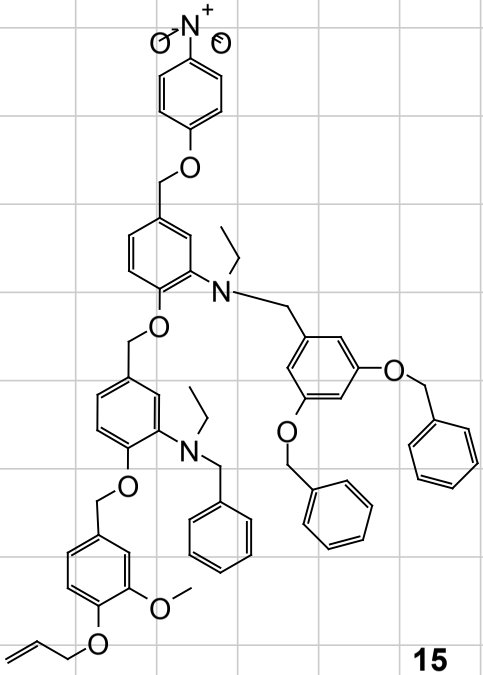
f1 (ppm)


aoviii123b
AO-VIII-123b
Parameters
Parameter Value
Data File Name / Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aoviii123b.fid/ fid
Title aoviii123b
Origin Varian
Spectrometer inova
Solvent CDCl3
Temperature 29.0
Pulse Sequence s2pul
Experiment 1D
Number of Scans 80
Receiver Gain 41
Relaxation Delay 0.5000
Pulse Width 0.0000
Acquisition Time 2.0480
Acquisition Date 2004-02-27T23:52:53
Spectrometer Frequency 299.95
Spectral Width 4000.0
Lowest Frequency -923.6
Nucleus 1H
Acquired Size 8192
Spectral Size 16384
S26
15
1.59
21.06
10.61
3.00
0.82
1.76
9.76
2.00
3.94
2.91
4.00
6.02
f1 (ppm)

AO-VIII-123b
AO-VIII-123b
Standard 13C Spectrum
Dual 1H-13C probe Parameters

Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ DRX-500/ AO-VIII-123b/ 2/ fid
Title	AO-VIII-123b
Comment	AO-VIII-123b Standard 13C Spectrum Dual 1H-13C probe
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	0.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	3011
Receiver Gain	3251
Relaxation Delay	0.7000
Pulse Width	5.2000
Acquisition Time	1.0423
Acquisition Date	2004-03-08T14:38:00
Modification Date	2004-07-26T09:42:10
Spectrometer Frequency	125.68
Spectral Width	31440.3
Lowest Frequency	-1317.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

163.78 159.69 152.53 152.08 149.39 147.59 136.96 133.30 128.48 128.35 127.95 127.86 127.48 126.64 125.82 121.51 120.91 119.95 117.96 114.83 113.70 113.67 113.07 111.26 100.61 77.26 77.00 76.75 70.89 70.68 70.61 69.89 69.83 56.57 56.49 55.75 45.12 44.63 12.39 12.12



15

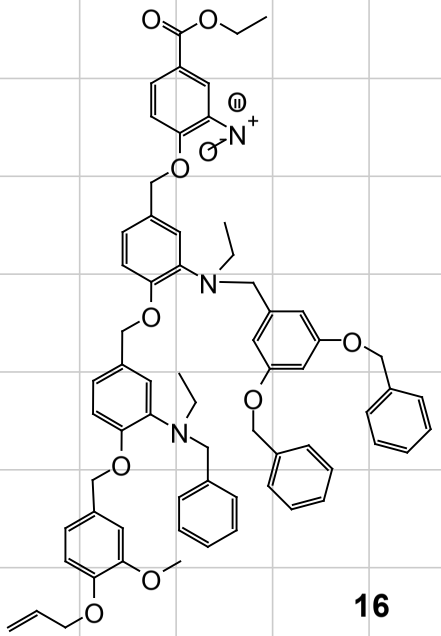
S27

f1 (ppm)

AO-VIII-17
Standard 13C Spectrum
Dual 1H-13C probe

Parameters

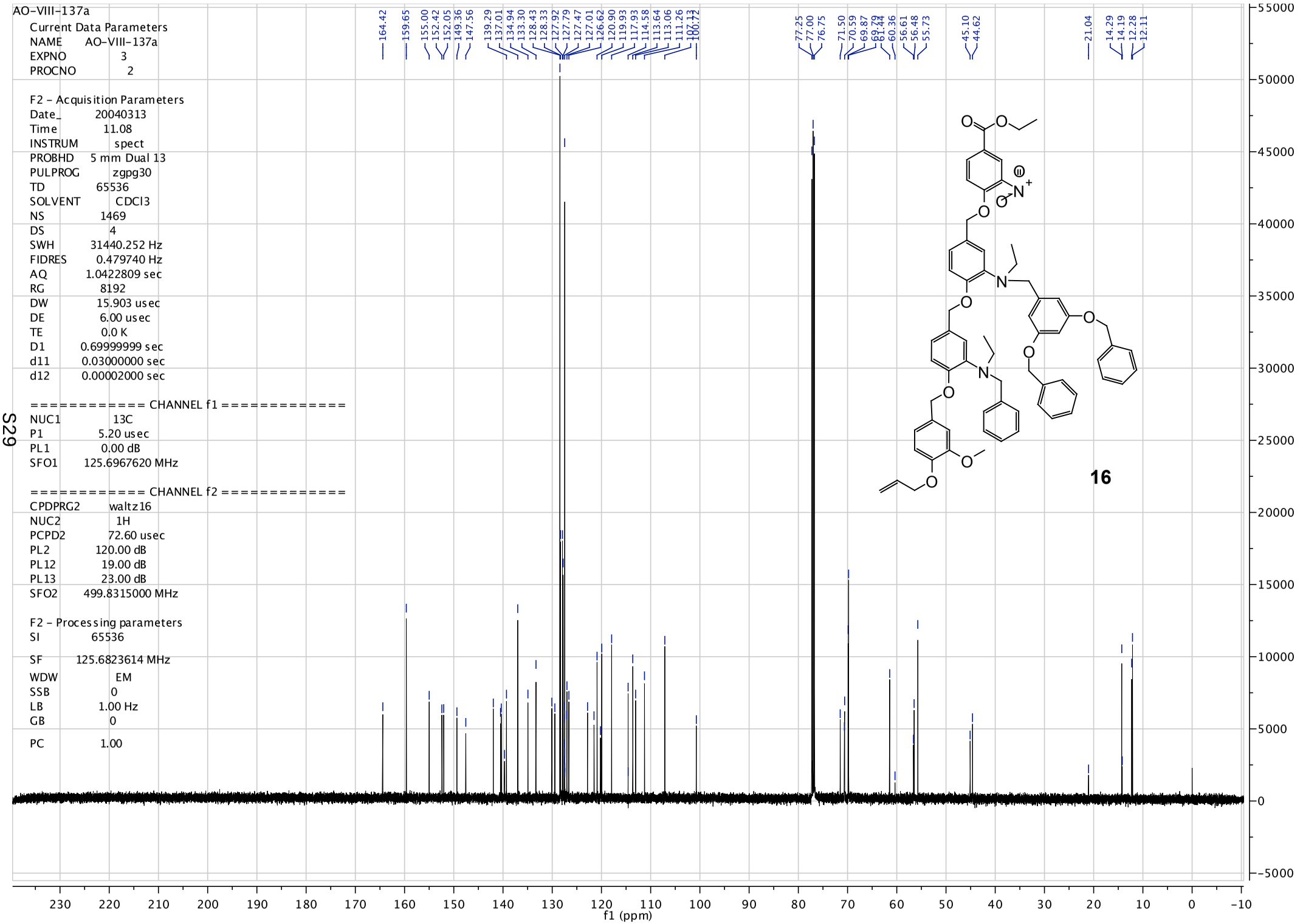
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ DRX-500/ AO-VIII-17/ 1/ fid
Title	AO-VIII-17
Comment	Standard 13C Spectrum Dual 1H-13C probe
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg30
Experiment	1D
Number of Scans	64
Receiver Gain	36
Relaxation Delay	2.0000
Pulse Width	13.4000
Acquisition Time	1.3080
Acquisition Date	2004-03-31T14:22:00
Modification Date	2004-07-26T09:42:42
Spectrometer Frequency	499.83
Spectral Width	6263.2
Lowest Frequency	-1331.4
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



16

0.67 0.72 16.71 10.28 3.00 0.92 2.02 1.92 8.22 1.96 2.09 4.00 2.98 4.00 3.05 6.03

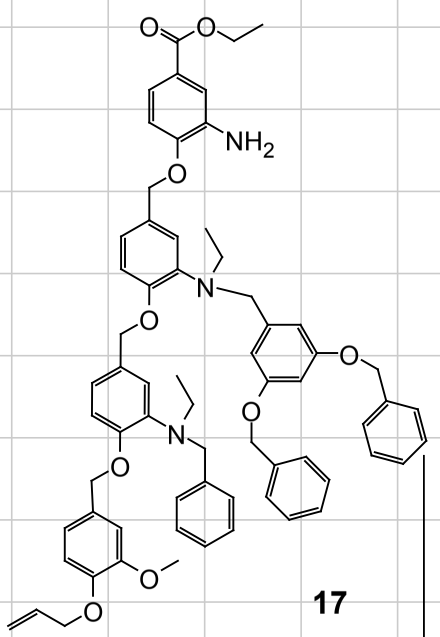
f1 (ppm)


AO-VIII-137a
Current Data Parameters
NAME AO-VIII-137a
EXPNO 3
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040313
Time 11.08
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1469
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
164.42
159.65
155.00
152.42
152.05
149.36
147.56
139.29
137.01
134.94
133.30
128.43
128.33
127.92
127.79
127.47
127.01
126.62
120.90
119.93
117.93
114.58
113.64
113.06
111.26
77.25
77.00
76.75
71.50
70.59
69.87
60.36
56.61
56.48
55.73
45.10
44.62
21.04
14.29
14.19
12.28
12.11
16
f1 (ppm)

aoviii145
AO-VIII-145

Parameters

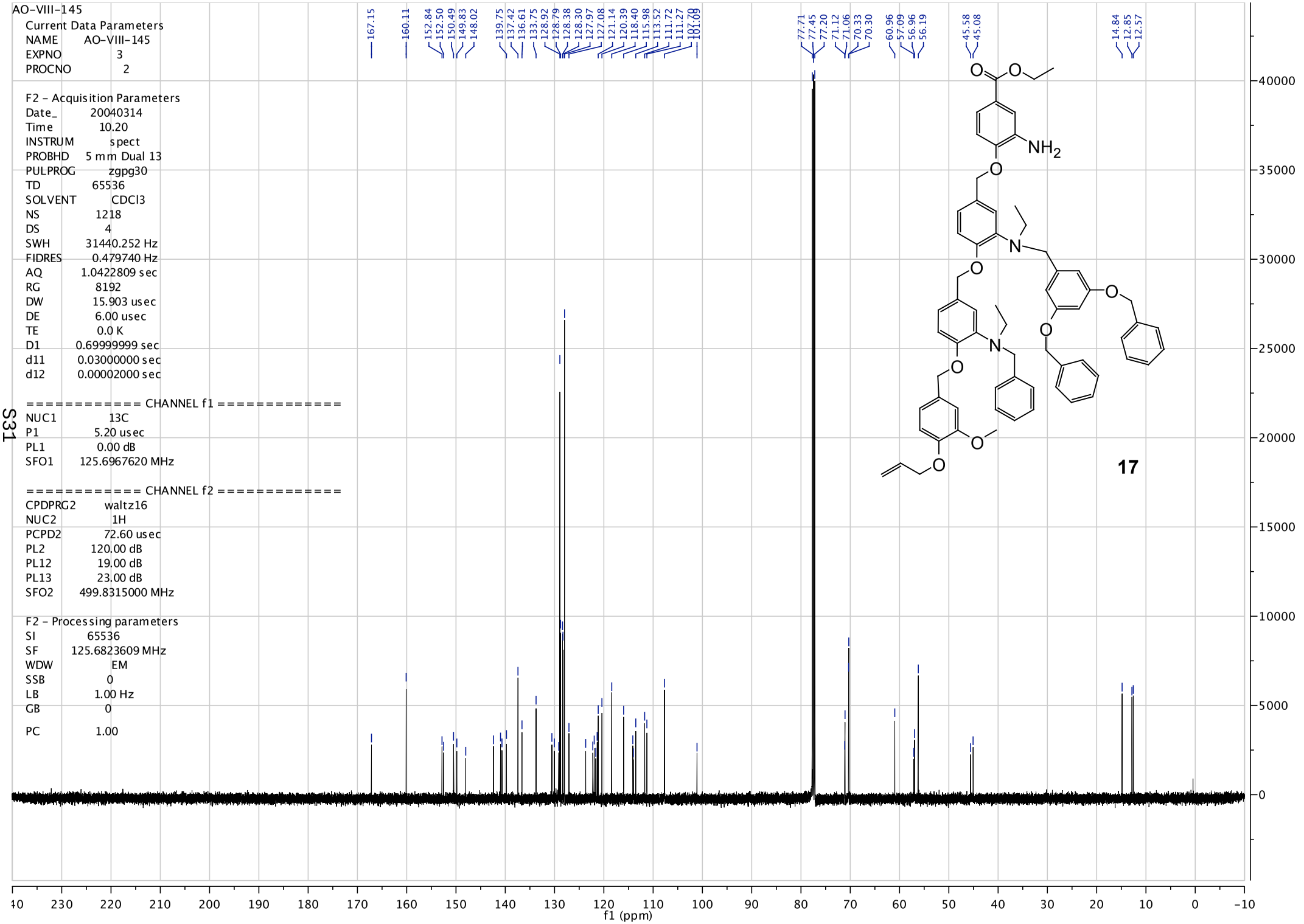
Parameter	Value
Data File Name	/ Volumes/ McGrath Group/ Adrian_Ortiz/ Unity-300/ aoviii145.fid/ fid
Title	aoviii145
Origin	Varian
Spectrometer	inova
Solvent	CDCl3
Temperature	29.0
Pulse Sequence	s2pul
Experiment	1D
Number of Scans	80
Receiver Gain	36
Relaxation Delay	0.5000
Pulse Width	0.0000
Acquisition Time	2.0480
Acquisition Date	2004-03-13T21:16:49
Spectrometer Frequency	299.95
Spectral Width	4000.0
Lowest Frequency	-925.4
Nucleus	1H
Acquired Size	8192
Spectral Size	16384



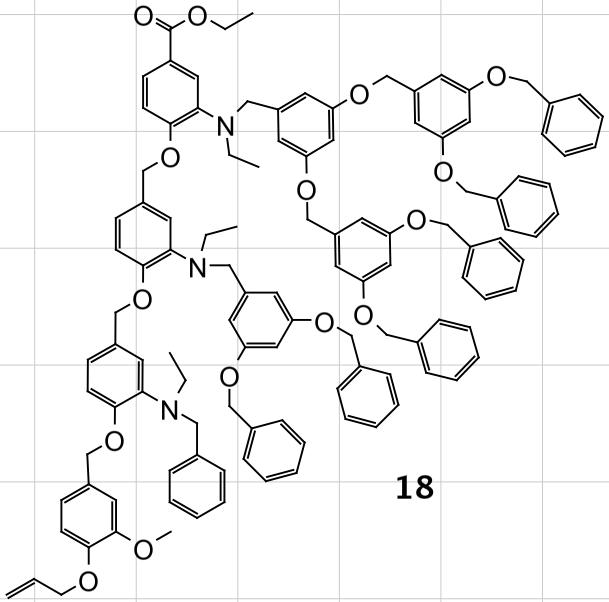
17

15.58 9.50 2.91 0.75 1.72 9.89 2.07 5.98 4.70 4.00 2.97 6.37

f1 (ppm)


AO-VIII-145
Current Data Parameters
NAME AO-VIII-145
EXPNO 3
PROCNO 2
F2 - Acquisition Parameters
Date_ 20040314
Time 10.20
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1218
DS 4
SWH 31440.252 Hz
FIDRES 0.479740 Hz
AQ 1.0422809 sec
RG 8192
DW 15.903 usec
DE 6.00 usec
TE 0.0 K
D1 0.69999999 sec
d11 0.03000000 sec
d12 0.00002000 sec
========== CHANNEL f1 ==========
NUC1 13C
P1 5.20 usec
PL1 0.00 dB
SFO1 125.6967620 MHz
========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.60 usec
PL2 120.00 dB
PL12 19.00 dB
PL13 23.00 dB
SFO2 499.8315000 MHz
F2 - Processing parameters
SI 65536
SF 125.6823609 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
167.15
160.11
152.84
152.50
150.49
149.83
148.02
139.75
137.42
136.61
133.75
128.92
128.79
128.38
128.30
127.97
127.08
121.14
120.39
118.40
115.98
113.52
111.72
111.27
101.69
77.71
77.45
77.20
71.12
71.06
70.33
70.30
60.96
57.09
56.96
56.19
45.58
45.08
14.84
12.85
12.57
NH2
17
f1 (ppm)

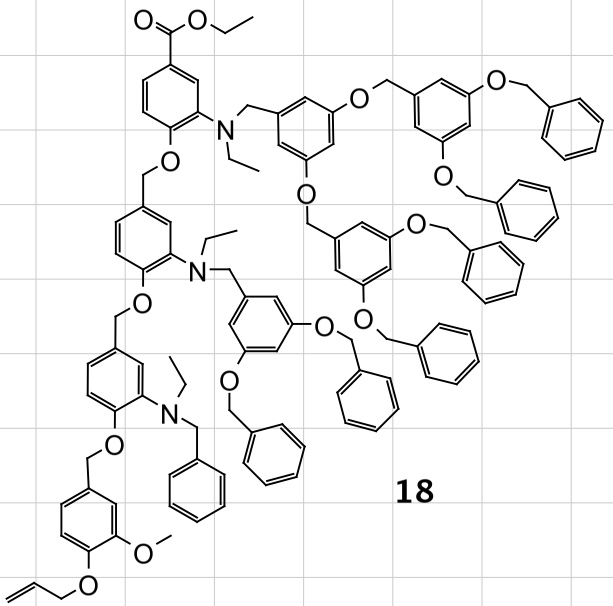
Title: PR-VI-114
Date: 2010-06-25T15:01:00
Spectrometer:
Probe:
Pulse Sequence:
TD:
Solvent:
NS: 0
DS:
SWH (Hz):
FIDRES (Hz): 0.00000000
Acquisition Time (sec): 3.9846387
Receiver Gain: 0
DW (sec): 0.00000000
DE (usec):
Temperature (K): 0
D1 (sec): 0
TD0:
Nucleus:
P1 (usec): 0
PL1 (dB):
SFO1 (MHz):
SI: 65536
SF (MHz): 400.13000000
WDW: 3
SSB: 4
LB (Hz): 0.00
GB: 0
PC: 1



18

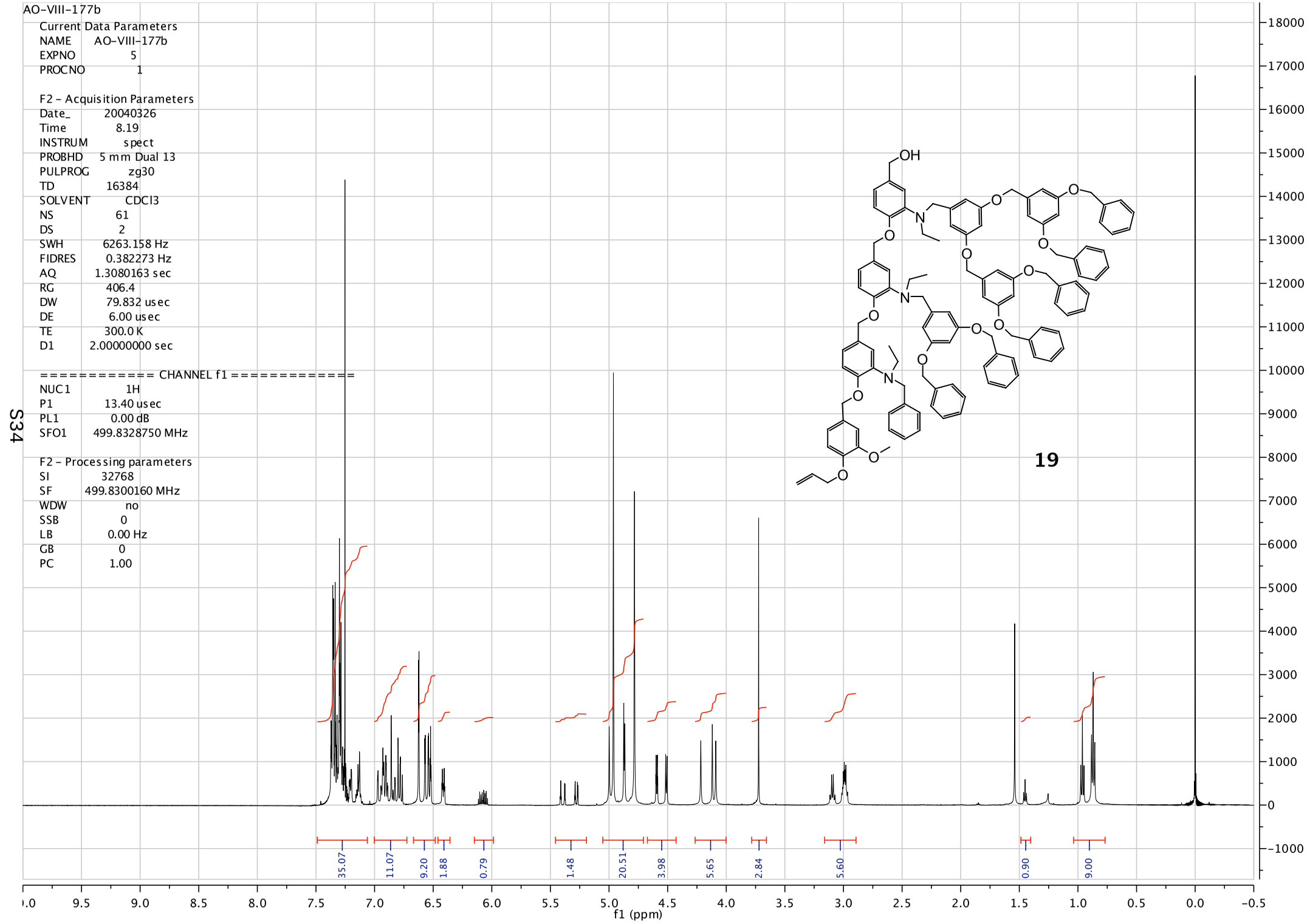
Title: PR-VI-114(18)
Date: 2010-06-26T18:46:00
Spectrometer: spect
Probe: 5 mm BBO BB-1H/D Z-GRD Z8007/0116
Pulse Sequence: zgpg30
TD: 65536
Solvent: CDCl3
NS: 301
DS: 4
SWH (Hz): 30030.030
FIDRES (Hz): 0.45822189
Acquisition Time (sec): 1.091241
Receiver Gain: 2896.3
DW (sec): 0.00001665
DE (usec): 6.00
Temperature (K): 298
D1 (sec): 0.7
D11 (sec): undefined
TD0: 1
Nucleus 1: 13C
P1 (usec): 5
PL1 (dB): 0.00
SFO1 (MHz): 125.60690500
CPDPRG: waltz16
Nucleus 2: 1H
PCPD2 (usec): 80.00
PL2 (dB): -2.00
PL12: 18.00
PL13 (dB): 18.00
SFO2 (MHz): undefined
SI: 32768
SF (MHz): 125.59434600
WDW: 1
SSB: 0
LB (Hz): 1.00
GB: 0
PC: 1.4

166.7817, 160.1671, 159.7535, 159.7207, 156.4446, 152.3503, 152.1177, 149.4607, 147.6545, 139.5956, 137.1216, 136.8772, 133.4166, 128.6144, 128.5263, 128.4424, 128.0246, 127.8738, 127.6186, 127.5940, 126.7069, 120.0397, 118.0397, 113.1294, 111.3607, 107.3538, 107.2423, 106.4289, 101.3501, 100.9234, 100.7253, 77.3786, 77.1233, 76.8680, 70.6147, 70.1011, 69.9482, 69.8166, 60.6597, 57.0023, 56.7234, 56.5688, 55.8036, 44.8214, 44.6963, 44.6272, 29.7750, 14.4890, 12.3495, 12.2479, 12.1718



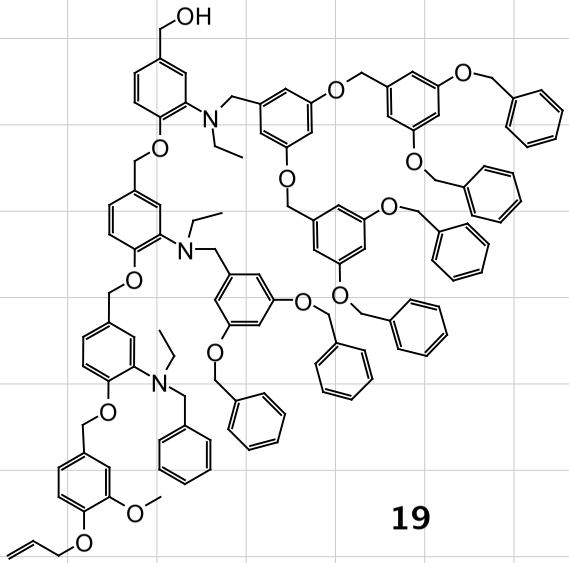
18

f1 (ppm)


AO-VIII-177b
Current Data Parameters
NAME AO-VIII-177b
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040326
Time 8.19
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 61
DS 2
SWH 6263.158 Hz
FIDRES 0.382273 Hz
AQ 1.3080163 sec
RG 406.4
DW 79.832 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
========== CHANNEL f1 ==========
NUC1 1H
P1 13.40 usec
PL1 0.00 dB
SFO1 499.8328750 MHz
F2 - Processing parameters
SI 32768
SF 499.8300160 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
N
O
19
35.07
11.07
9.20
1.88
0.79
1.48
20.51
3.98
5.65
2.84
5.60
0.90
9.00
f1 (ppm)

Title: PR-VI-117(19)
Date: 2010-06-27T19:47:00
Spectrometer: spect
Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0359
Pulse Sequence: zgpg30
TD: 65536
Solvent: CDCl3
NS: 4096
DS: 4
SWH (Hz): 24038.462
FIDRES (Hz): 0.36679781
Acquisition Time (sec): 1.3631988
Receiver Gain: 203
DW (sec): 0.00002080
DE (usec): 6.50
Temperature (K): 298
D1 (sec): 1.2
D11 (sec): undefined
TD0: 1
Nucleus 1: 13C
P1 (usec): 9.6
PL1 (dB): 3.00
SFO1 (MHz): 100.62282980
CPDPRG: waltz16
Nucleus 2: 1H
PCPD2 (usec): 90.00
PL2 (dB): 3.00
PL12: 18.74
PL13 (dB): 18.74
SFO2 (MHz): undefined
SI: 65536
SF (MHz): 100.61276900
WDW: 1
SSB: 0
LB (Hz): 1.00
GB: 0
PC: 1.4

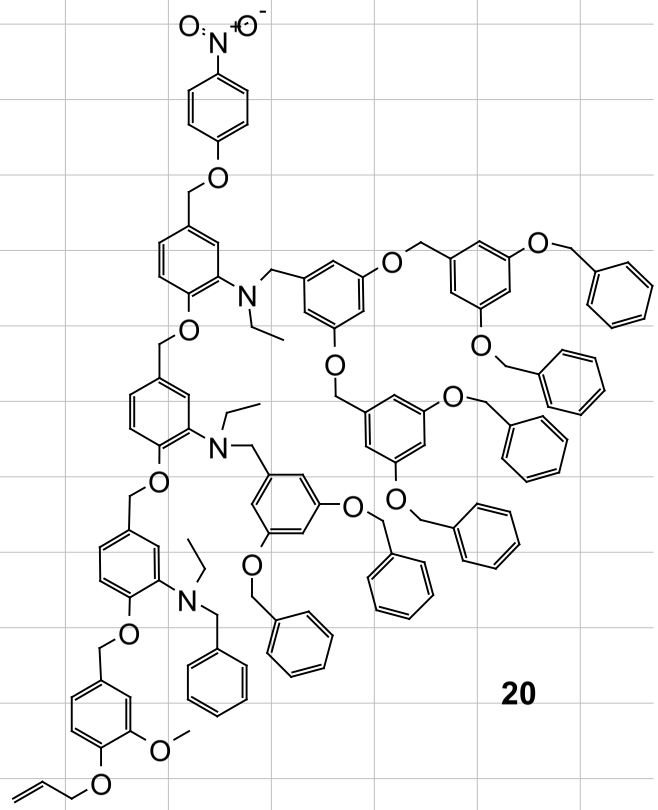
160.0603
159.6306
159.5644
152.1152
152.0603
152.0022
149.3591
147.5480
139.5027
137.0255
136.7668
128.5168
128.4212
128.3428
127.9300
127.7673
127.5222
127.4956
121.5931
120.8924
119.9341
117.9363
113.0354
111.2608
107.3187
107.1601
101.4407
100.7284
100.6536
77.3175
77.2035
76.9999
76.6823
70.0140
69.8562
69.7233
65.3389
56.9347
56.6584
56.4730
55.7047
44.8176
44.6281
44.5300
29.6707
12.3851
12.1695
12.0653



19

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Title: AO-ix-105a (20)
Date: 2010-06-23T10:17:00
Spectrometer: spect
Probe: 5 mm BBO BB-1H/D Z-GRD Z8007/0116
Pulse Sequence: zg30
TD: 32768
Solvent: CDCl3
NS: 16
DS: 4
SWH (Hz): 6250.000
FIDRES (Hz): 0.19073486
Acquisition Time (sec): 2.6215701
Receiver Gain: 28.5
DW (sec): 0.00008000
DE (usec): 6.00
Temperature (K): 298
D1 (sec): 0
TD0: 1
Nucleus: 1H
P1 (usec): 12.5
PL1 (dB): -2.00
SFO1 (MHz): 499.48294693
SI: 32768
SF (MHz): 499.48000000
WDW: 1
SSB: 0
LB (Hz): 0.20
GB: 0
PC: 1



20

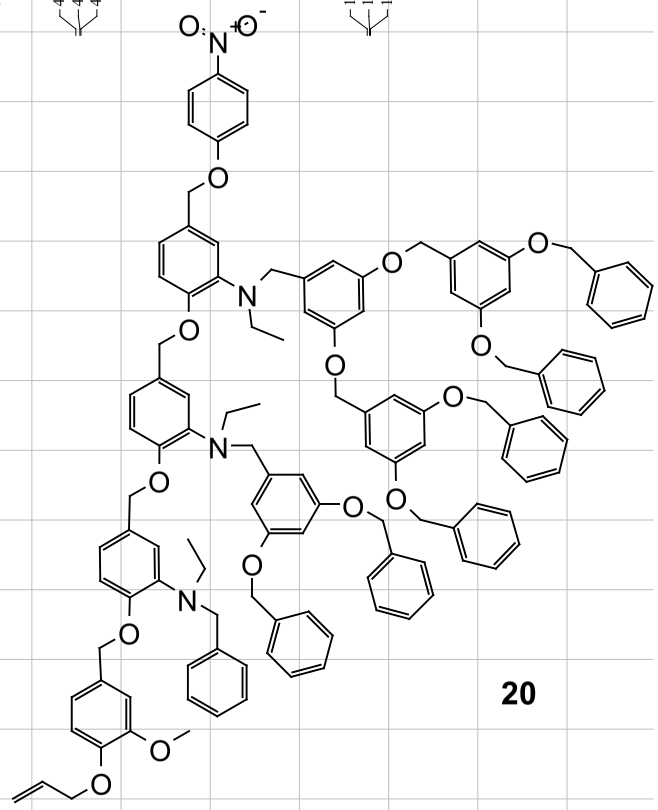
Title: AO-ix-105a (20)
Date: 2010-06-23T10:22:00
Spectrometer: spect
Probe: 5 mm BBO BB-1H/D Z-GRD Z8007/0116
Pulse Sequence: zgpg30
TD: 65536
Solvent: CDCl3
NS: 274
DS: 4
SWH (Hz): 30030.030
FIDRES (Hz): 0.45822189
Acquisition Time (sec): 1.091241
Receiver Gain: 2580.3
DW (sec): 0.00001665
DE (usec): 6.00
Temperature (K): 298
D1 (sec): 0.7
D11 (sec): undefined
TD0: 1
Nucleus 1: 13C
P1 (usec): 5
PL1 (dB): 0.00
SFO1 (MHz): 125.60690500
CPDPRG: waltz16
Nucleus 2: 1H
PCPD2 (usec): 80.00
PL2 (dB): -2.00
PL12: 18.00
PL13 (dB): 18.00
SFO2 (MHz): undefined
SI: 32768
SF (MHz): 125.59434600
WDW: 1
SSB: 0
LB (Hz): 1.00
GB: 0
PC: 1.4

163.7016 160.0363 159.6182 159.5314 152.5038 152.1324 151.9748 149.3214 147.5165 141.3396 139.4105 136.9763 136.6988 133.2718 128.4809 128.3896 128.3079 127.9051 127.7394 127.4762 127.4472 125.7403 119.9032 117.8961 114.7436 112.9920 111.2219 107.1175 100.6001

77.2545 77.0001 76.7453 70.7700 70.6664 70.4788 69.9579 69.8001 69.6798 69.6135 56.6214 56.4329 55.6623

45.0715 44.6124 44.4979

12.4015 12.1452 12.0379



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)