Influence of Alkoxy Groups on Rates of Acetal Hydrolysis and Tosylate Solvolysis: Electrostatic Stabilization of Developing Oxocarbenium Ion Intermediates and Neighboring-Group Participation to Form Oxonium Ions

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Supporting Information

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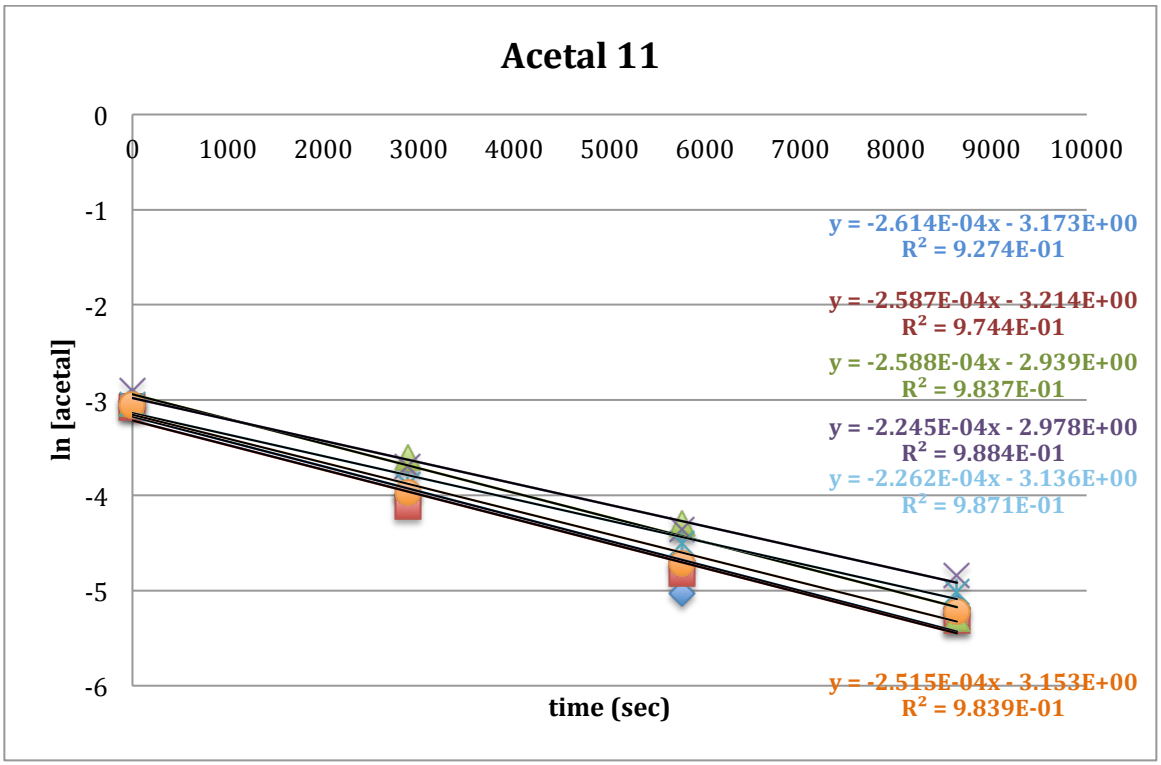
I. General Experimental

Infrared (IR) spectra were obtained by a FT-IR spectrometer using either attenuated total reflectance (ATR) or a thin film on a salt plate, as indicated. High-resolution mass spectra (HRMS) were acquired on an Accurate-Mass time-of-flight spectrometer. At ambient temperature, ^{1}H and ^{13}C NMR spectra were obtained utilizing AV–400 (400 and 100 MHz, respectively), AV–500 (500 and 125 MHz, respectively), or AVIII–600 (600 and 150 MHz, respectively) spectrometers, as indicated. The experimental data is listed as follows: chemical shift in ppm from internal tetramethylsilane or referenced to residual solvent (^{1}H NMR: C_6D_6 δ 7.16; $CDCl_3$ δ 7.26. ^{13}C NMR: C_6D_6 δ 128.06; $CDCl_3$ δ 77.16) on the δ scale, multiplicity (appar = apparent, br = broad, s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, m = multiplet), coupling constants (Hz), and integration. Microanalyses were performed by an independent facility in GA. Analytical thin layer chromatography was performed on silica gel 60 Å F_{254} plates. Liquid chromatography was performed using forced flow (flash chromatography) of the indicated solvent system on silica gel (SiO_2) 60 (230-400 mesh). THF, CH_2Cl_2, and Et_2O were dried by filtration through alumina following the method by Grubbs.[1] Reactions using solvents THF, CH_2Cl_2, and Et_2O were run under an atmosphere of nitrogen with glassware that was flame-dried under vacuum and cooled under a stream of nitrogen.

II. Hydrolysis of Acetal 11

The procedure for the hydrolysis of acetal **11** followed methods previously reported.[2] The hydrolysis of acetals **5**, **6**, *trans*-**7**, *trans*-**8**, **9**, **10**, **12**, and **13** have also previously been reported.[2]

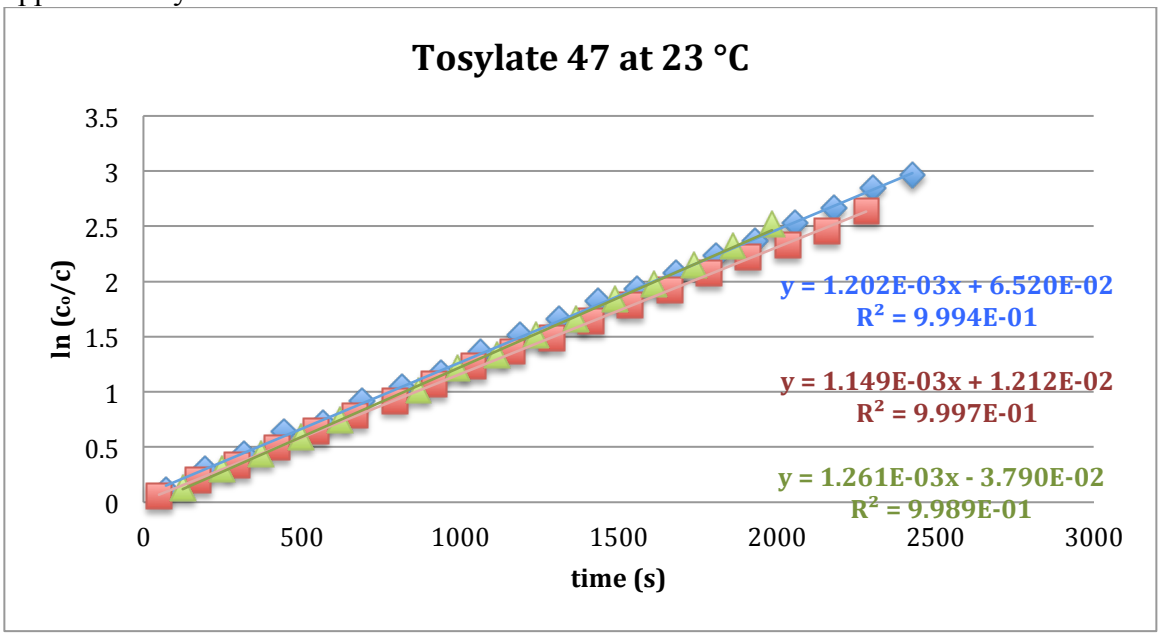
Graph S1. Rate of hydrolysis of acetal **11** plotted as ln [acetal] versus t (s) over approximately three half-lives, resulting in $k = 4.0 \times 10^{-3}$.



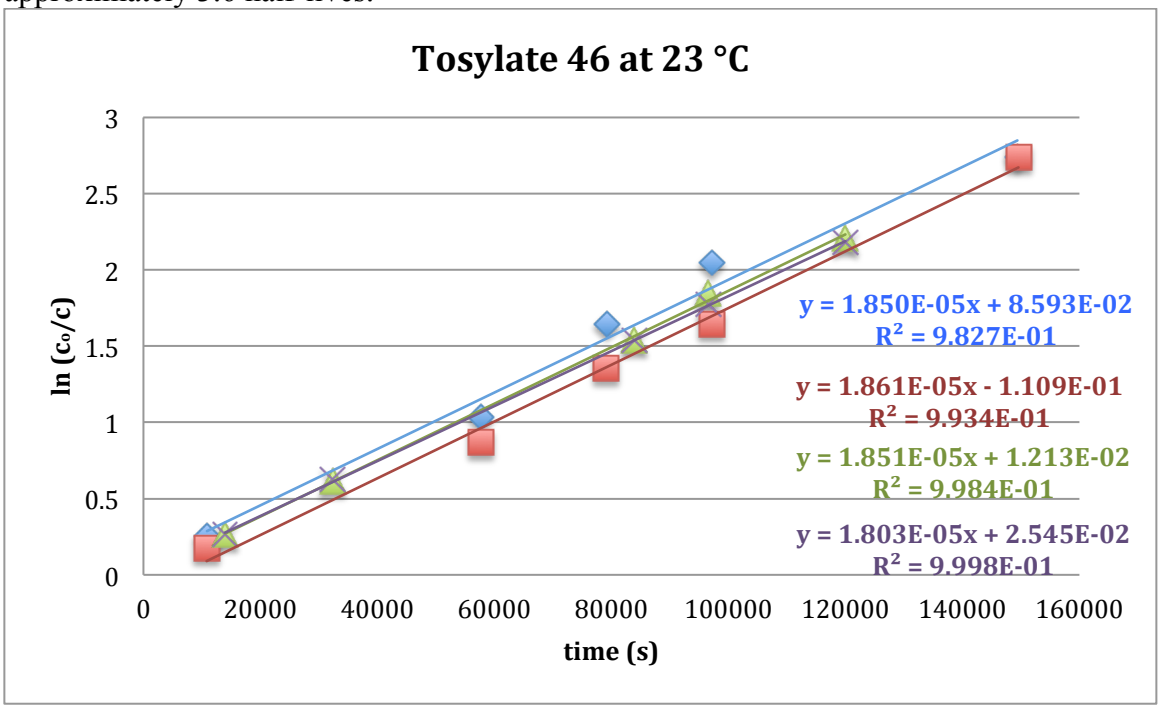
III. Solvolysis Studies

General Procedure: The tosylate was added to a standard NMR tube equipped with 1,4-dimethoxybenzene as an internal standard. Anisole was used for tosylate **45** due to stability issues over long periods of time. The NMR tube was inverted after addition of acetic acid-d_4. An NMR spectrum was obtained at 25 °C during given time points, depending on the tosylate substrate. The decrease of starting material/tosylate was measured to determine the rate, by plotting ln (c_0/c) versus time (s). The solvolysis rate of tosylate **45** was determined at three different temperatures (100, 110, and 125 °C) using a J. Young NMR tube, and the Arrhenius equation was applied to determine the relative rate of tosylate **45** at 23 °C.

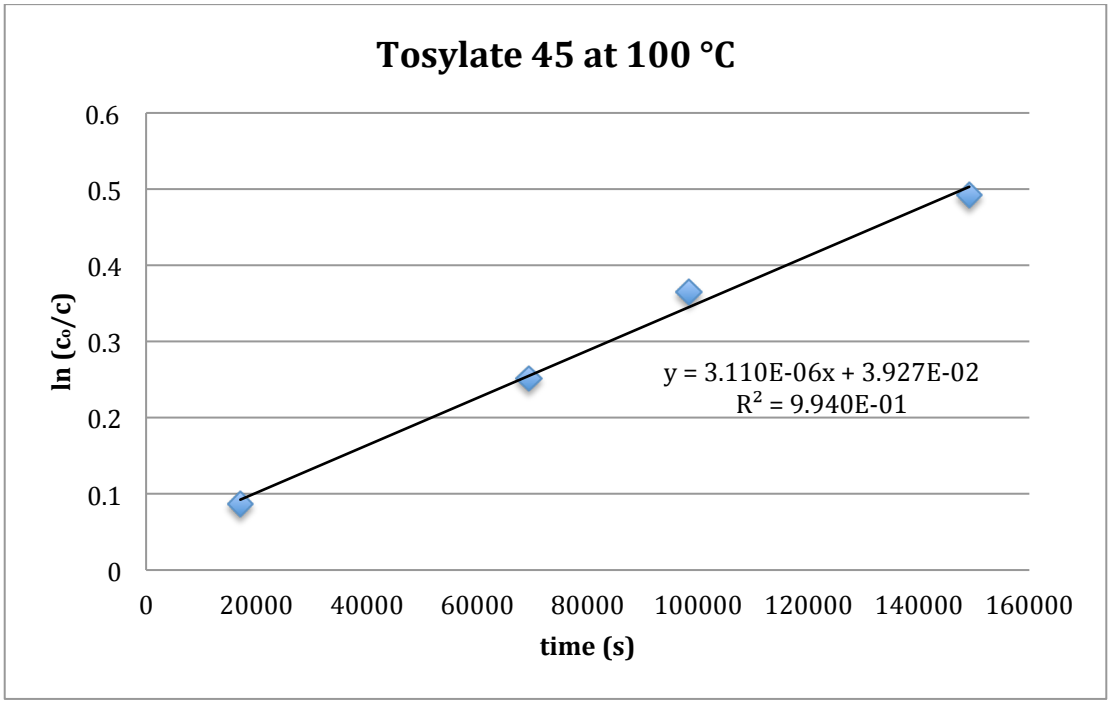
Graph S2. Solvolysis of tosylate **47** plotted as ln (c_o /c) versus time (s) at 23 °C, over approximately 4 half-lives.



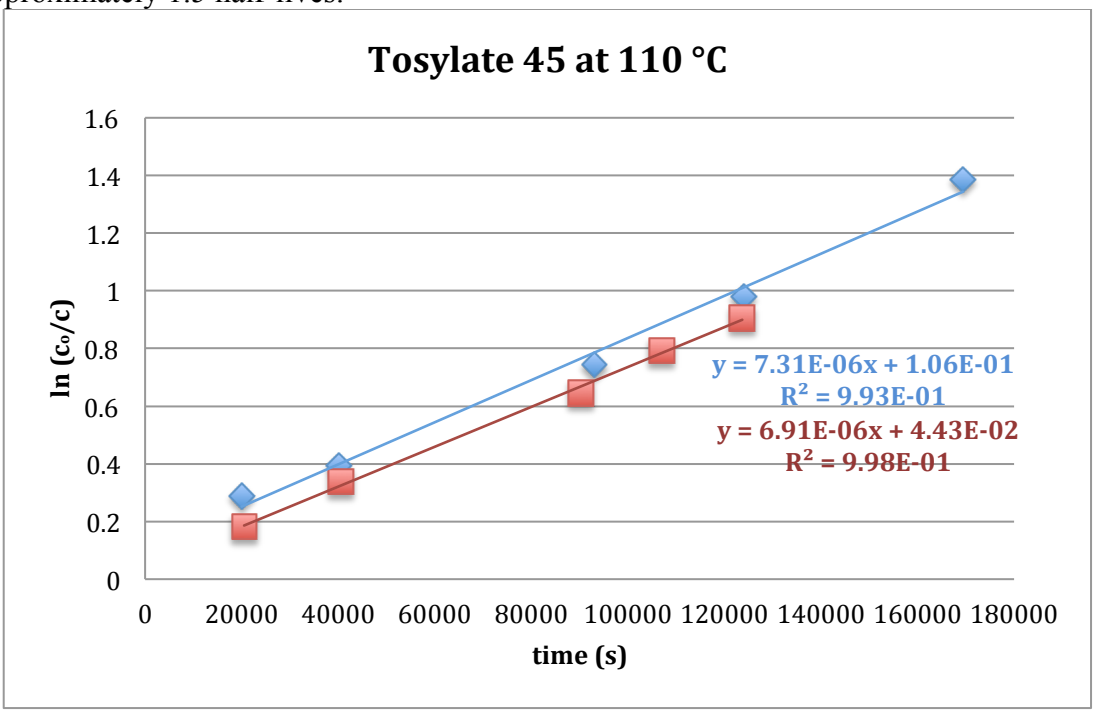
Graph S3. Solvolysis of tosylate **46** plotted as ln (c_o /c) versus time (s) at 23 °C, over approximately 3.6 half-lives.



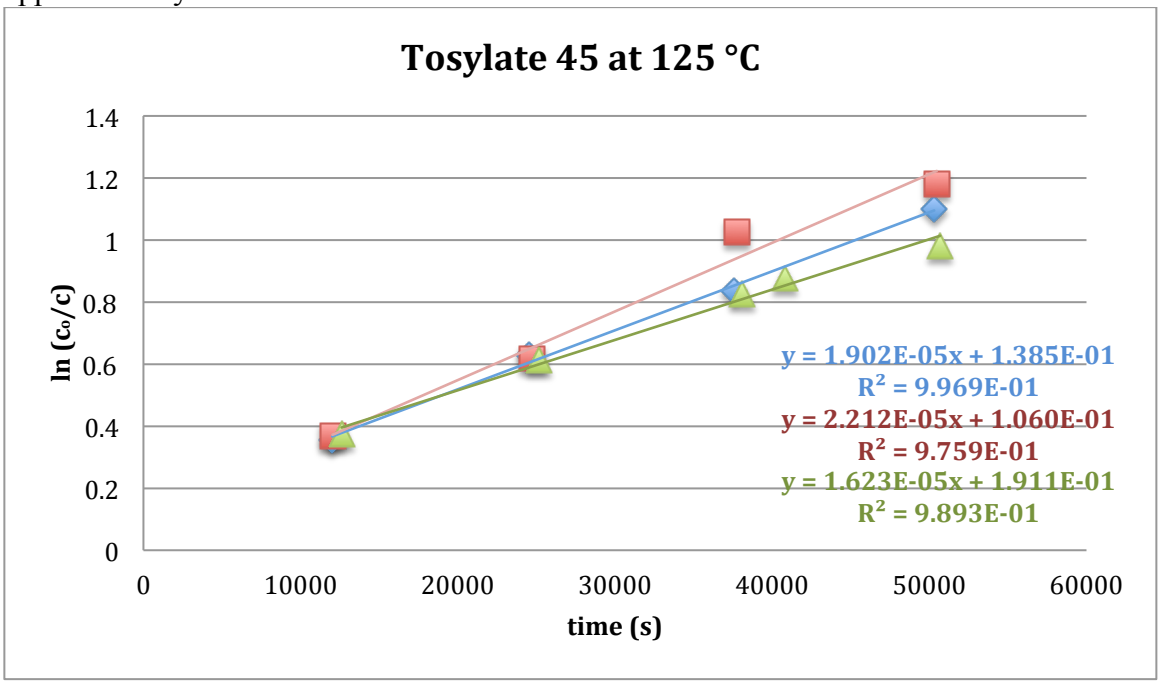
Graph S4. Solvolysis of tosylate **45** plotted as ln (c_o /c) versus time (s) at 100 °C, over less than one half-life.



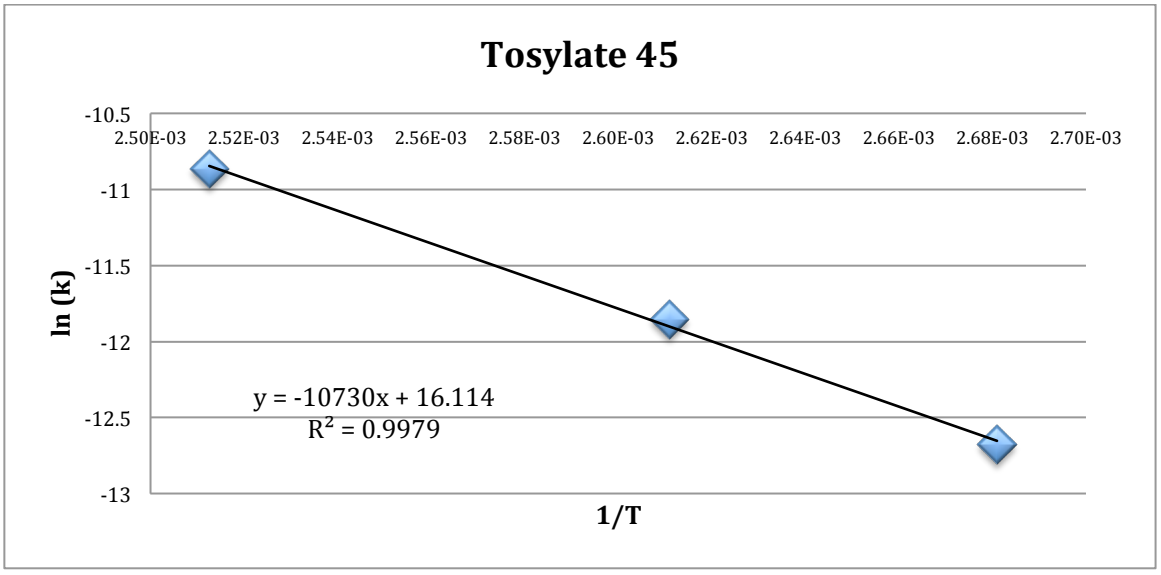
Graph S5. Solvolysis of tosylate **45** plotted as ln (c_o /c) versus time (s) at 110 °C, over approximately 1.5 half-lives.



Graph S6. Solvolysis of tosylate **45** plotted as ln (c_o /c) versus time (s) at 125 °C, over approximately 1.4 half-lives.



Graph S7. Arrhenius plot for tosylate **45**. ln (k) versus 1/T plotted to determine activation energy and pre-exponential factor to apply the Arrhenius equation and determine the rate at 23 °C.



IV. Computational Methods

The oxocarbenium ion intermediates derived from acetals were calculated using Spartan'10 (Wavefunction, Inc., Irvine, CA). An input structure was subjected to a search for low-energy conformers using the conformational search package using semi-empirical methods (AM1). The 35 lowest-energy structures (within 10 kcal/mol) were then minimized using Density Functional methods (B3LYP/6-31G*) with the Gaussian Software Package.

Oxocarbenium ion from acetal *trans*-**8**
Energy = -536760.45 kcal/mol

ATOM				
1	H1	-4.8382	-2.5601	0.7514 H
2	C2	-4.1739	-1.6942	0.6522 C
3	H3	-4.1524	-1.2290	1.6480 H
4	C4	-4.8352	-0.7356	-0.3590 C
5	H5	-5.9185	-0.8419	-0.2320 H
6	H6	-4.6296	-1.0788	-1.3837 H
7	C7	-4.5344	0.7698	-0.2455 C
8	H8	-5.3510	1.3005	-0.7489 H
9	H9	-4.5909	1.0776	0.8081 H
10	C10	-3.2333	1.3096	-0.8640 C
11	H11	-3.3537	2.3950	-0.9650 H
12	H12	-3.1177	0.9276	-1.8886 H
13	C13	-1.9198	1.0958	-0.0823 C
14	H14	-2.1109	1.2280	0.9888 H
15	C15	-1.5400	-1.4138	0.6516 C
16	H16	-0.6755	-2.0878	0.6286 H
17	C17	-2.7830	-2.2625	0.3145 C
18	H18	-2.7516	-2.5556	-0.7446 H
19	H19	-2.6628	-3.1938	0.8792 H
20	C20	-1.2395	-0.2626	-0.2986 C
21	H21	-1.3318	-0.5691	-1.3466 H
22	H22	-1.6043	-1.0282	1.6760 H
23	O23	0.2607	0.0491	-0.1338 O
24	C24	1.1478	-0.6372	-1.1426 C
25	H25	0.7349	-1.6456	-1.1892 H
26	H26	0.9924	-0.1322	-2.0999 H
27	C27	2.5786	-0.6341	-0.7096 C
28	C28	5.2728	-0.6772	0.0590 C
29	C29	3.5139	0.1854	-1.3593 C
30	C30	3.0077	-1.4869	0.3210 C
31	C31	4.3475	-1.5039	0.7067 C
32	C32	4.8572	0.1634	-0.9767 C
33	H33	3.1998	0.8258	-2.1805 H

34	H34	2.2949	-2.1423	0.8150 H
35	H35	4.6739	-2.1691	1.4998 H
36	H36	5.5764	0.7925	-1.4914 H
37	H37	6.3174	-0.6990	0.3533 H
38	C38	-0.8498	2.1209	-0.5123 C
39	H39	-1.0754	3.1272	-0.1523 H
40	H40	-0.7683	2.1567	-1.6050 H
41	C41	0.4480	1.6358	0.0793 C
42	H42	1.3729	1.8291	-0.4699 H
43	O43	0.5231	1.8728	1.3965 O
44	C44	1.8003	1.6853	2.0472 C
45	H45	2.5814	2.2326	1.5107 H
46	H46	2.0482	0.6228	2.0981 H
47	H47	1.6808	2.0938	3.0493 H

Oxocarbenium ion from acetal *trans*-**7**
Energy = -512012.10 kcal/mol

ATOM				
1	C1	-4.2782	-1.4622	-0.1459 C
2	H2	-5.2018	-2.0090	0.0720 H
3	H3	-3.9022	-1.8858	-1.0885 H
4	C4	-4.6506	0.0219	-0.3272 C
5	H5	-5.5090	0.0939	-1.0047 H
6	H6	-4.9960	0.4112	0.6400 H
7	C7	-3.5496	0.9446	-0.8756 C
8	H8	-3.9278	1.9736	-0.8815 H
9	H9	-3.3414	0.6896	-1.9250 H
10	C10	-2.2212	0.9264	-0.0965 C
11	H11	-2.4110	1.1038	0.9686 H
12	C12	-1.7835	-1.5293	0.7090 C
13	H13	-1.3653	-2.4609	0.3099 H
14	C14	-3.2908	-1.7262	1.0099 C
15	H15	-3.4104	-2.7552	1.3636 H
16	H16	-3.5745	-1.0870	1.8547 H
17	C17	-1.4803	-0.4012	-0.2711 C
18	H18	-1.5790	-0.7286	-1.3114 H
19	H19	-1.2565	-1.3193	1.6460 H
20	O20	-0.0046	-0.0398	-0.1316 O
21	C21	0.9019	-0.7449	-1.1084 C
22	H22	0.5258	-1.7687	-1.1011 H
23	H23	0.7271	-0.2961	-2.0902 H
24	C24	2.3322	-0.6661	-0.6811 C
25	C25	5.0246	-0.5611	0.0875 C
26	C26	3.2346	0.1570	-1.3717 C

27	C27	2.7940	-1.4488	0.3902 C
28	C28	4.1328	-1.3918	0.7757 C
29	C29	4.5770	0.2090	-0.9890 C
30	H30	2.8958	0.7421	-2.2238 H
31	H31	2.1077	-2.1088	0.9148 H
32	H32	4.4850	-2.0035	1.6003 H
33	H33	5.2710	0.8402	-1.5348 H
34	H34	6.0688	-0.5257	0.3821 H
35	C35	-1.2164	1.9804	-0.5986 C
36	H36	-1.4789	2.9931	-0.2838 H
37	H37	-1.1548	1.9648	-1.6928 H
38	C38	0.1164	1.5881	-0.0104 C
39	H39	1.0213	1.7774	-0.5929 H
40	O40	0.2107	1.8955	1.2864 O
41	C41	1.5088	1.7978	1.9179 C
42	H42	1.3934	2.2626	2.8955 H
43	H43	2.2558	2.3396	1.3303 H
44	H44	1.7975	0.7502	2.0263 H

Oxocarbenium ion from acetal *trans*-**6**
Energy = -487264.08 kcal/mol

ATOM				
1	H1	0.0000	0.0000	0.0000 H
2	C2	0.0000	0.0000	1.0968 C
3	C3	2.5587	0.0000	1.2943 C
4	C4	1.2956	2.1629	1.1412 C
5	C5	2.5374	1.4802	1.7269 C
6	C6	0.0351	1.4397	1.5976 C
7	C7	1.2491	-0.7309	1.6405 C
8	H8	3.4037	-0.5098	1.7681 H
9	H9	3.4453	1.9903	1.3871 H
10	H10	1.2698	-1.7497	1.2414 H
11	H11	-0.9082	-0.5149	1.4277 H
12	H12	2.7314	-0.0531	0.2111 H
13	H13	1.3498	2.0962	0.0463 H
14	H14	2.5208	1.5537	2.8232 H
15	H15	-0.0193	1.4569	2.6964 H
16	H16	1.1609	-0.8287	2.7310 H
17	O17	-1.0651	2.2739	1.1020 O
18	C18	-2.3165	2.1354	1.8649 C
19	H19	-2.5176	1.0617	1.9159 H
20	H20	-2.1447	2.5092	2.8809 H
21	C21	-3.4361	2.8684	1.1851 C
22	C22	-5.5495	4.2209	-0.0708 C

23	C23	-3.9879	2.3711	-0.0068 C
24	C24	-3.9628	4.0402	1.7469 C
25	C25	-5.0164	4.7147	1.1224 C
26	C26	-5.0356	3.0467	-0.6338 C
27	H27	-3.6035	1.4499	-0.4371 H
28	H28	-3.5687	4.4156	2.6889 H
29	H29	-5.4263	5.6133	1.5728 H
30	H30	-5.4629	2.6509	-1.5500 H
31	H31	-6.3732	4.7384	-0.5528 H
32	C32	1.0738	3.6458	1.5090 C
33	H33	1.8649	4.2814	1.0975 H
34	H34	1.0463	3.7807	2.5949 H
35	C35	-0.2311	4.0736	0.9145 C
36	H36	-1.0087	4.5561	1.5075 H
37	O37	-0.2205	4.3092	-0.3560 O
38	C38	-1.3982	4.8662	-1.0127 C
39	H39	-1.8929	5.5777	-0.3490 H
40	H40	-2.0665	4.0442	-1.2693 H
41	H41	-1.0219	5.3606	-1.9058 H

Oxocarbenium ion from acetal *trans*-**5**
Energy = -462498.62 kcal/mol

ATOM	X	Y	Z
1	H1	0.0000	0.0000	0.0000 H
2	C2	0.0000	0.0000	1.0955 C
3	C3	1.4566	0.0000	1.6596 C
4	C4	1.7712	1.4704	2.0966 C
5	C5	0.6256	2.2773	1.4723 C
6	C6	-0.5671	1.3359	1.5933 C
7	H7	-0.5759	-0.8670	1.4285 H
8	H8	2.1609	-0.3450	0.8989 H
9	H9	1.5542	-0.6802	2.5092 H
10	H10	1.7507	1.5610	3.1891 H
11	H11	2.7552	1.8076	1.7615 H
12	H12	0.8245	2.4114	0.3998 H
13	H13	-0.8602	1.2504	2.6516 H
14	O14	-1.6300	1.9421	0.8572 O
15	C15	-2.9490	1.3258	0.9736 C
16	H16	-2.8104	0.2405	1.0076 H
17	H17	-3.4506	1.5774	0.0372 H
18	C18	-3.7484	1.8168	2.1566 C
19	C19	-5.2623	2.7505	4.3380 C
20	C20	-3.6189	1.2238	3.4235 C
21	C21	-4.6600	2.8723	1.9958 C

22	C22	-5.4145	3.3356	3.0767 C
23	C23	-4.3640	1.6927	4.5099 C
24	H24	-2.9601	0.3696	3.5584 H
25	H25	-4.7957	3.3188	1.0137 H
26	H26	-6.1330	4.1368	2.9312 H
27	H27	-4.2639	1.2158	5.4802 H
28	H28	-5.8576	3.0999	5.1762 H
29	C29	0.2650	3.6488	2.0712 C
30	H30	0.1065	3.5917	3.1511 H
31	H31	1.0857	4.3641	1.8872 H
32	C32	-0.9023	4.2147	1.3575 C
33	H33	-0.9095	4.2361	0.2693 H
34	O34	-1.8661	4.8727	1.8620 O
35	C35	-2.0723	5.0135	3.3119 C
36	H36	-1.1869	5.4643	3.7601 H
37	H37	-2.2986	4.0300	3.7245 H
38	H38	-2.9314	5.6732	3.3950 H

Oxocarbenium ion from acetal *cis*-**5**
Energy = -462507.04 kcal/mol

ATOM				
1	H1	0.0000	0.0000	0.0000 H
2	C2	0.0000	0.0000	1.0932 C
3	C3	1.4168	0.0000	1.7111 C
4	C4	1.2017	0.5872	3.1173 C
5	C5	0.1880	1.7288	2.8745 C
6	C6	-0.6693	1.2528	1.6797 C
7	H7	-0.5552	-0.8834	1.4252 H
8	H8	2.0861	0.6429	1.1273 H
9	H9	1.8588	-0.9993	1.7259 H
10	H10	0.7731	-0.1700	3.7817 H
11	H11	2.1239	0.9520	3.5772 H
12	H12	0.7309	2.6327	2.5794 H
13	H13	-0.8661	2.0417	0.9523 H
14	O14	-2.0295	0.9197	2.2616 O
15	C15	-3.1979	1.5263	1.5160 C
16	H16	-3.1667	2.6042	1.6961 H
17	H17	-2.9546	1.3175	0.4735 H
18	C18	-4.4933	0.9057	1.9261 C
19	C19	-6.9512	-0.2342	2.6400 C
20	C20	-4.8372	-0.3784	1.4714 C
21	C21	-5.3989	1.6181	2.7276 C
22	C22	-6.6240	1.0499	3.0835 C
23	C23	-6.0583	-0.9474	1.8319 C

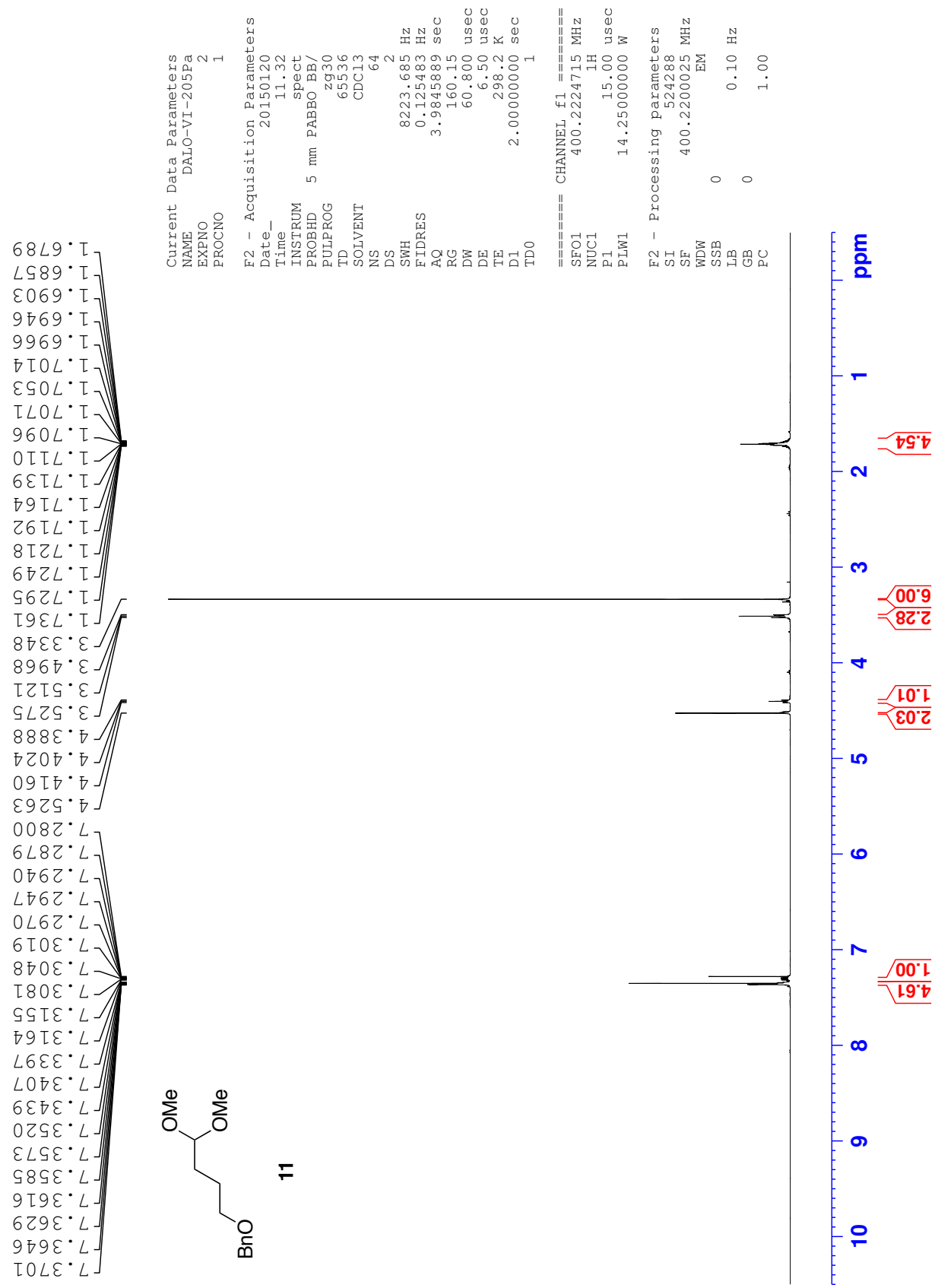
24	H24	-4.1549	-0.9265	0.8265 H
25	H25	-5.1588	2.6267	3.0563 H
26	H26	-7.3237	1.6111	3.6946 H
27	H27	-6.3214	-1.9369	1.4718 H
28	H28	-7.9061	-0.6740	2.9106 H
29	C29	-0.8026	2.0702	4.0022 C
30	H30	-1.1810	3.0909	3.8888 H
31	H31	-0.3539	1.9853	4.9951 H
32	C32	-1.9620	1.1044	3.8872 C
33	H33	-2.9651	1.4848	4.0944 H
34	O34	-1.7027	-0.0921	4.4241 O
35	C35	-2.8093	-1.0059	4.6124 C
36	H36	-2.4210	-1.8109	5.2340 H
37	H37	-3.1437	-1.3967	3.6491 H
38	H38	-3.6331	-0.4997	5.1240 H

V. References

(1) Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518.

(2) Garcia, A.; Otte, D. A. L.; Salamant, W. A.; Sanzone, J. R.; Woerpel, K. A. *Angew. Chem. Int. Ed.* **2015**, in press.

VI. Analytical Data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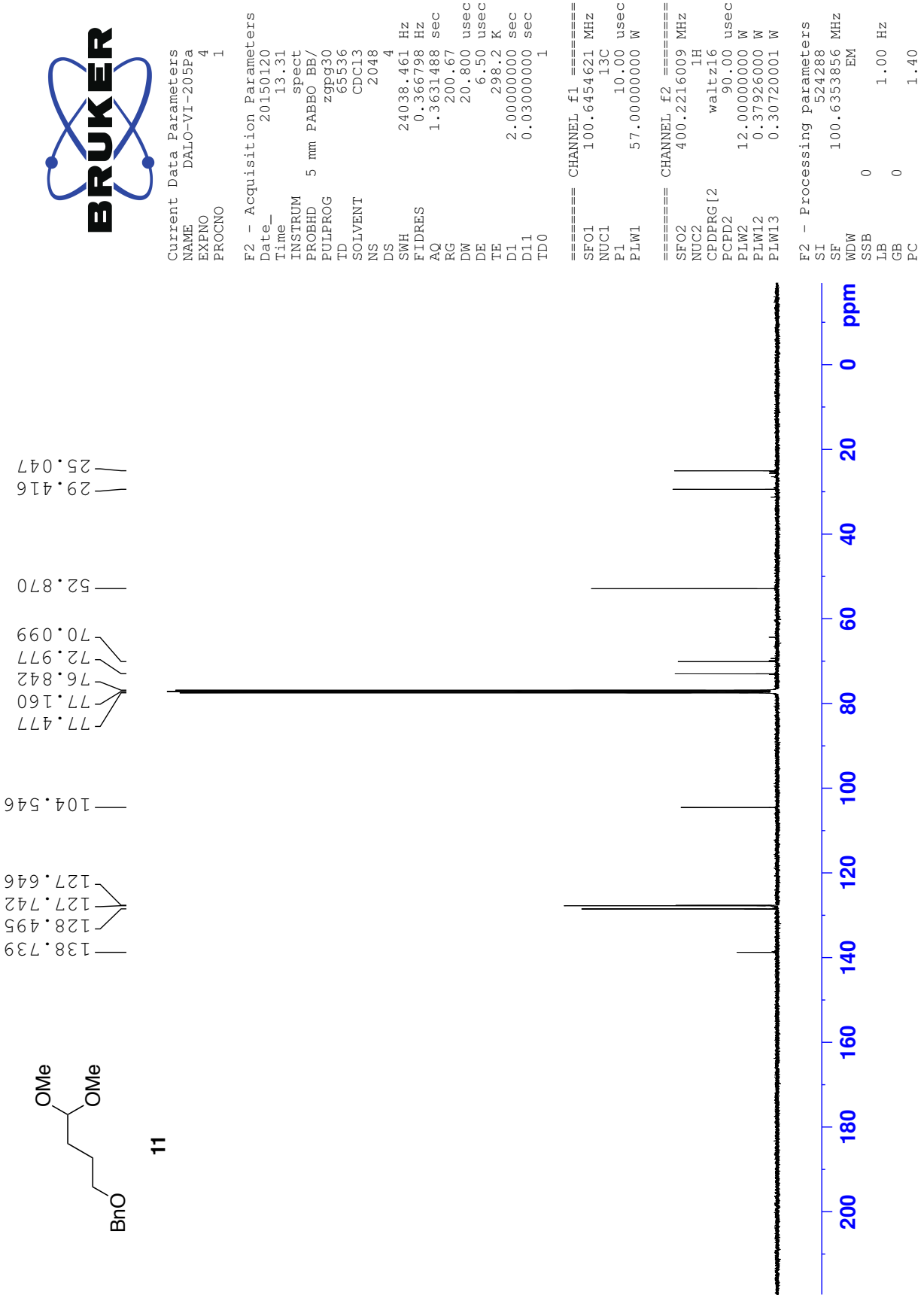
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DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
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NUC1 13C
P1 10.00 usec
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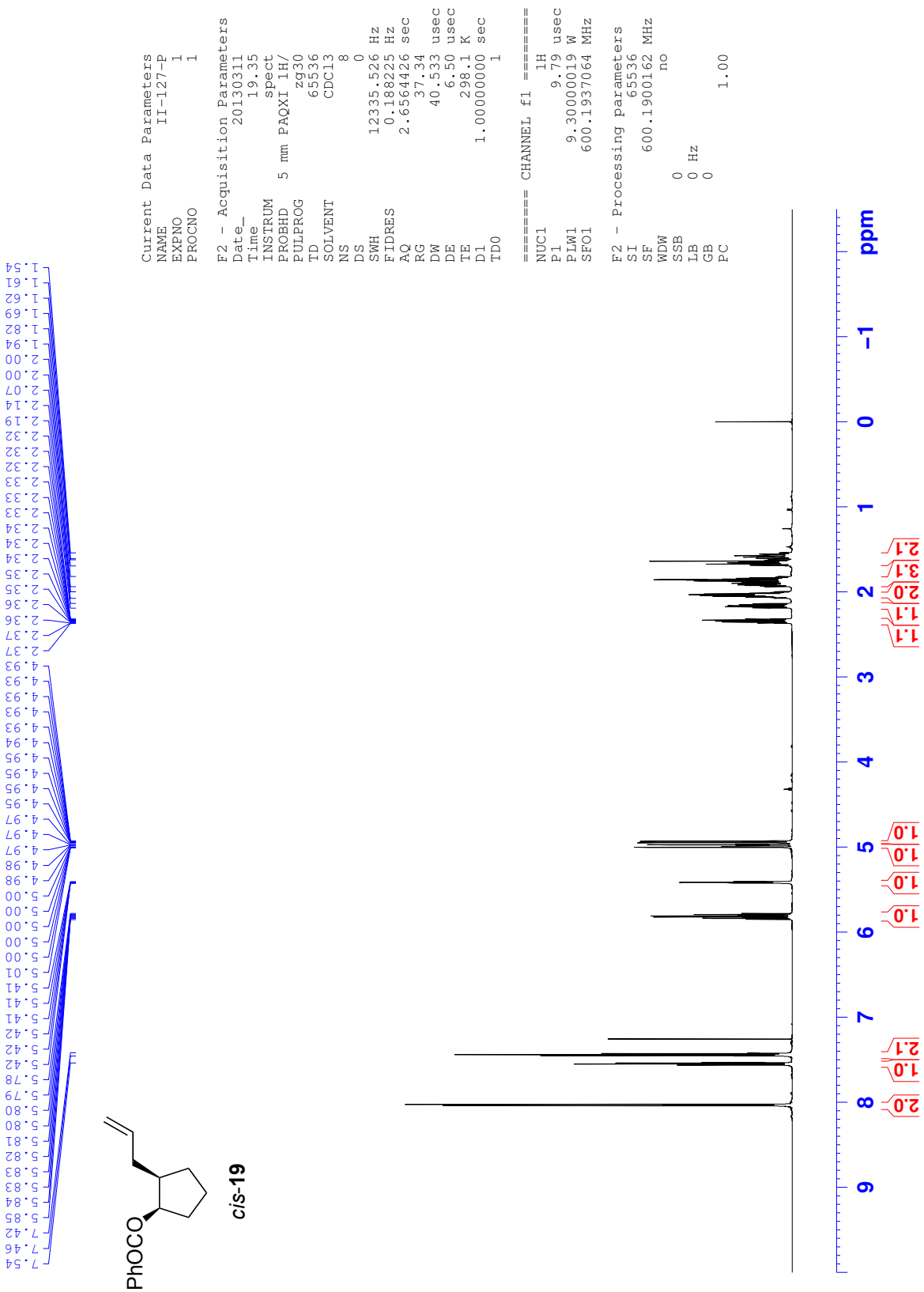
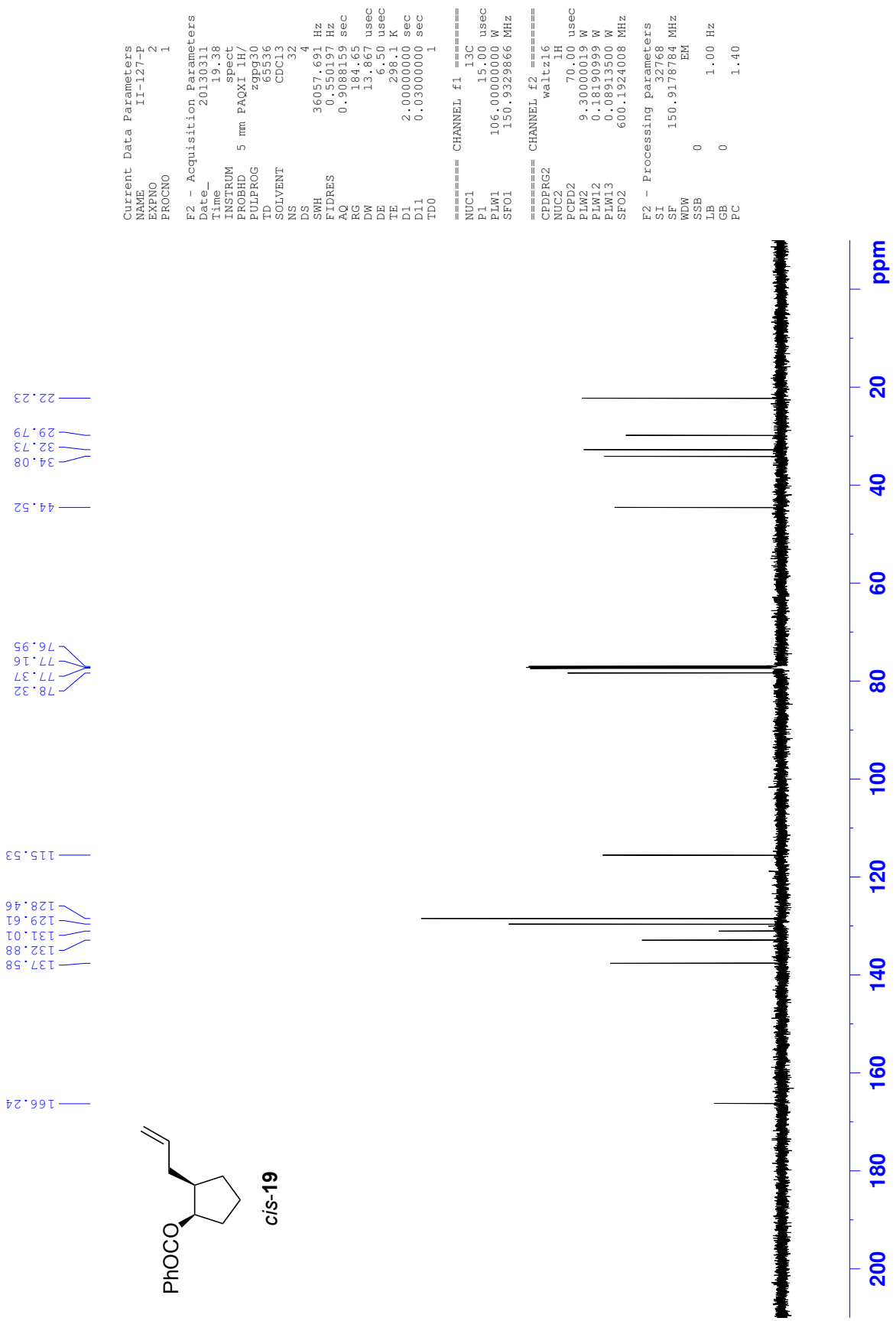
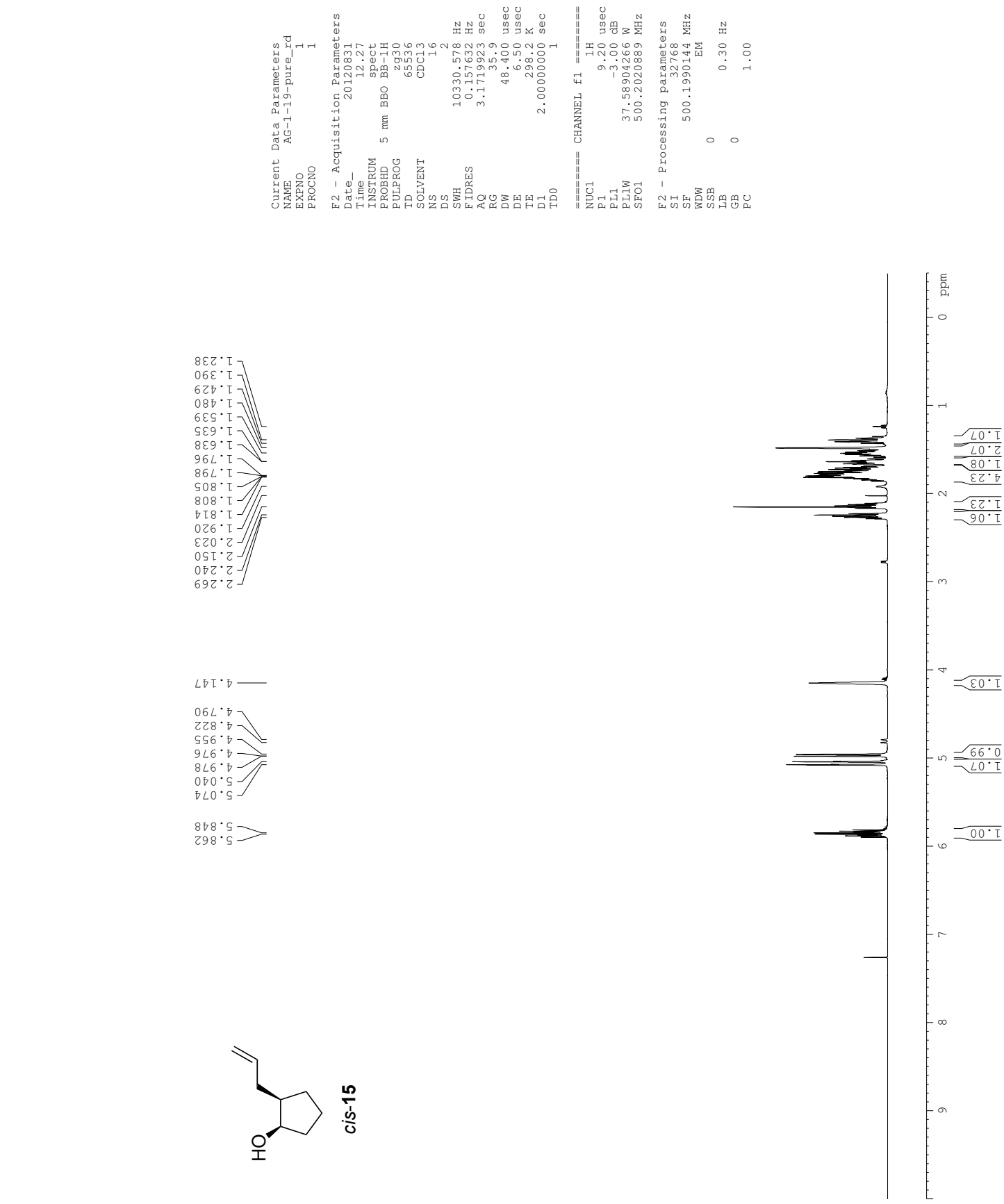
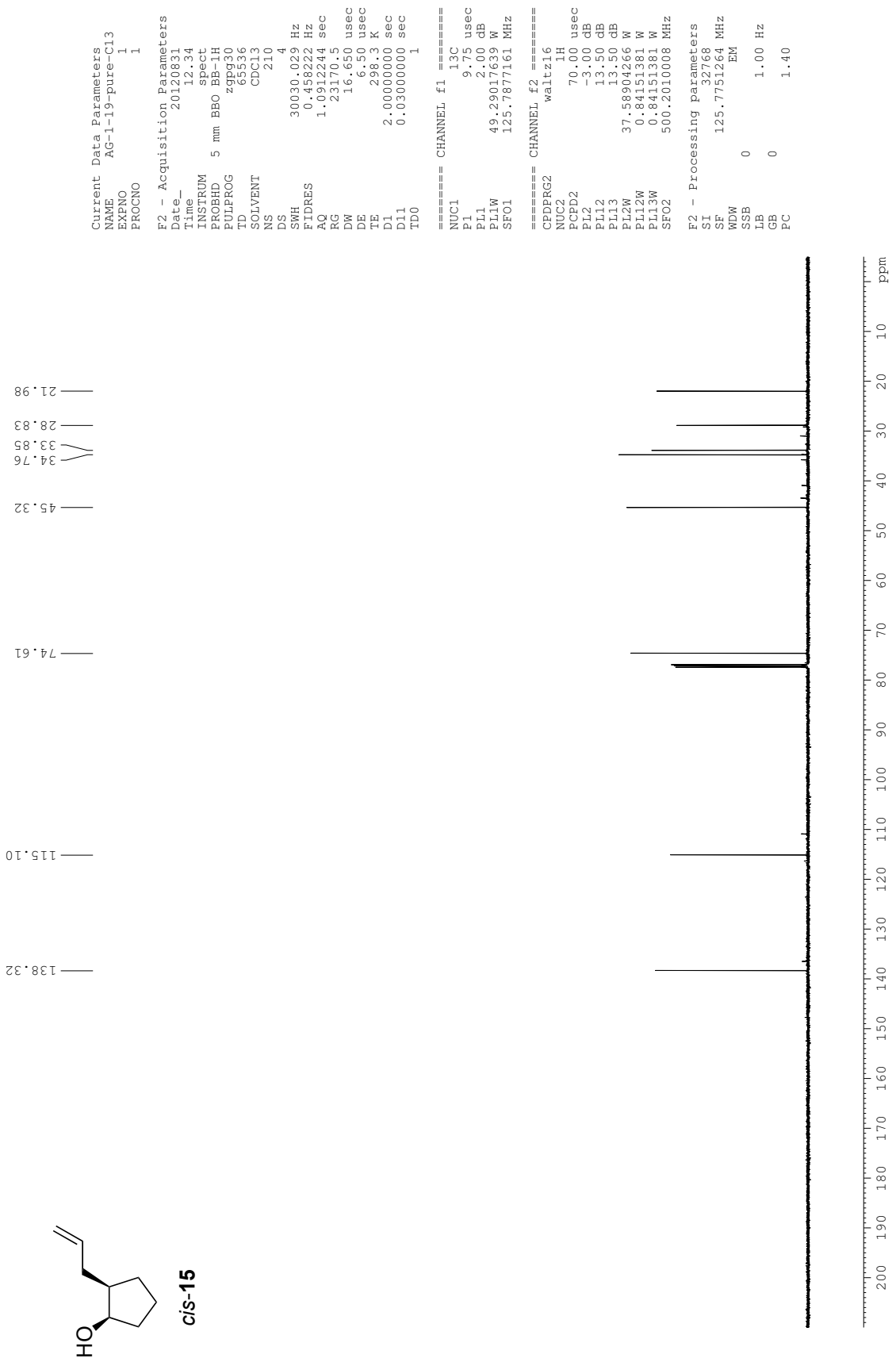
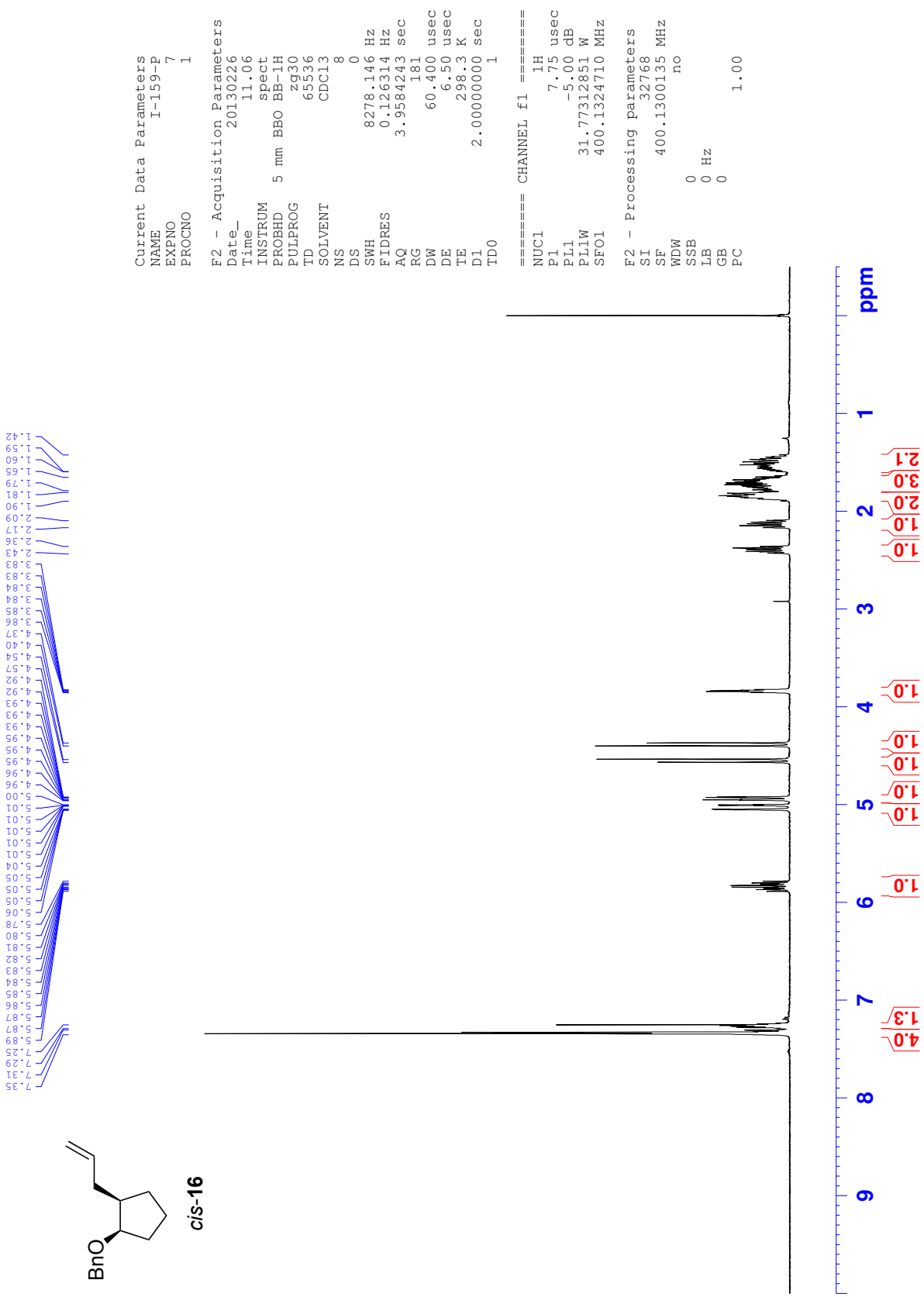
SFO2 400.2216009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.37926000 W
PLW13 0.30720001 W
F2 - Processing parameters
SI 524288
SF 100.6353856 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.047
29.416
52.870
70.099
72.977
76.842
77.160
77.477
104.546
127.646
127.742
128.495
138.739
ppm
0
20
40
60
80
100
120
140
160
180
200
OMe
OMe
BnO
11

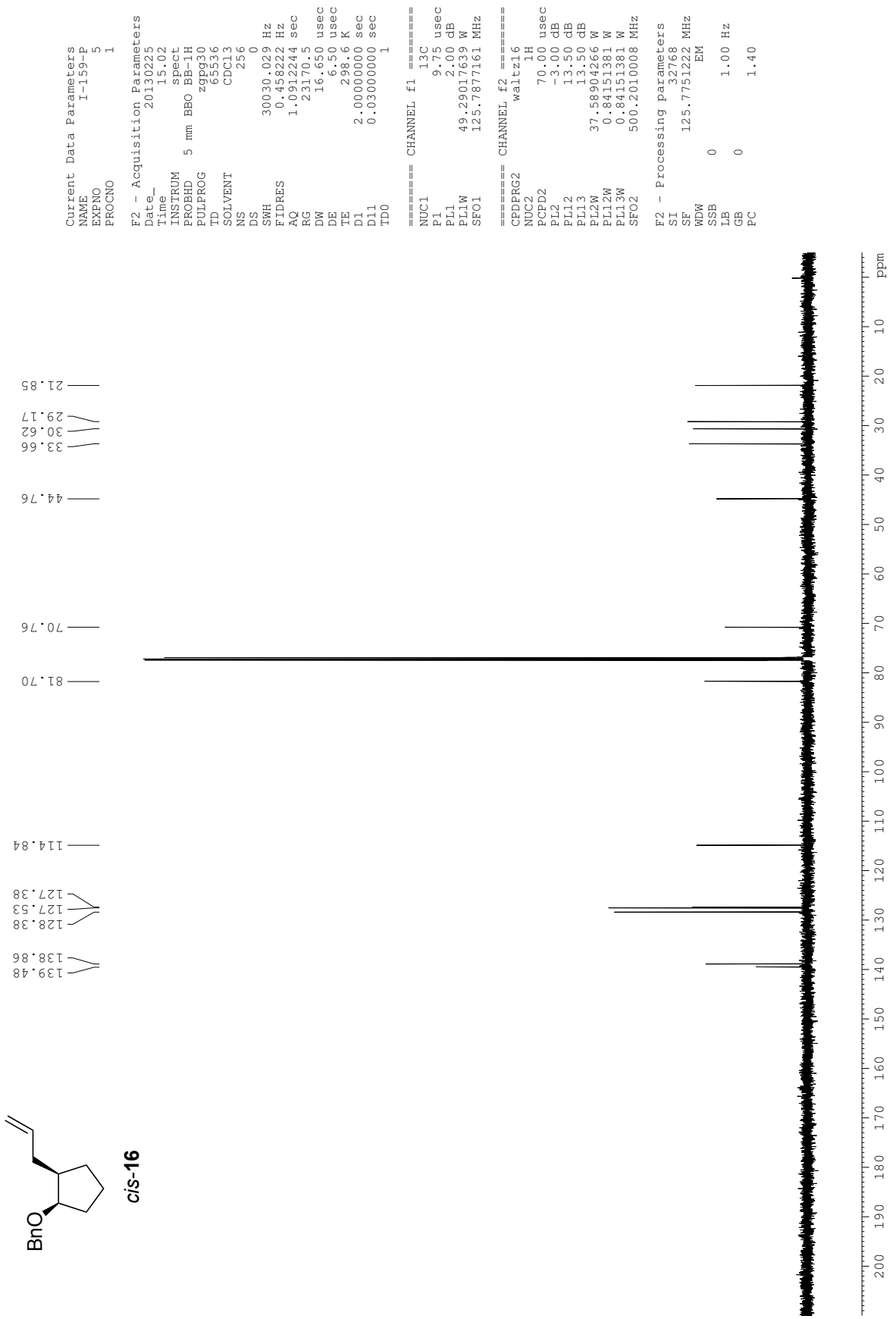

Current Data Parameters
NAME II-127-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130311
Time 19.35
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 37.34
DW 40.533 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.79 usec
PLW1 9.30000019 W
SFO1 600.1937064 MHz
F2 - Processing parameters
SI 65536
SF 600.1900162 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
PhOCO
cis-19
ppm
9
8
7
6
5
4
3
2
1
0
−1
2.0
1.0
2.1
1.0
1.0
1.0
1.0
1.1
1.1
2.0
3.1
2.1

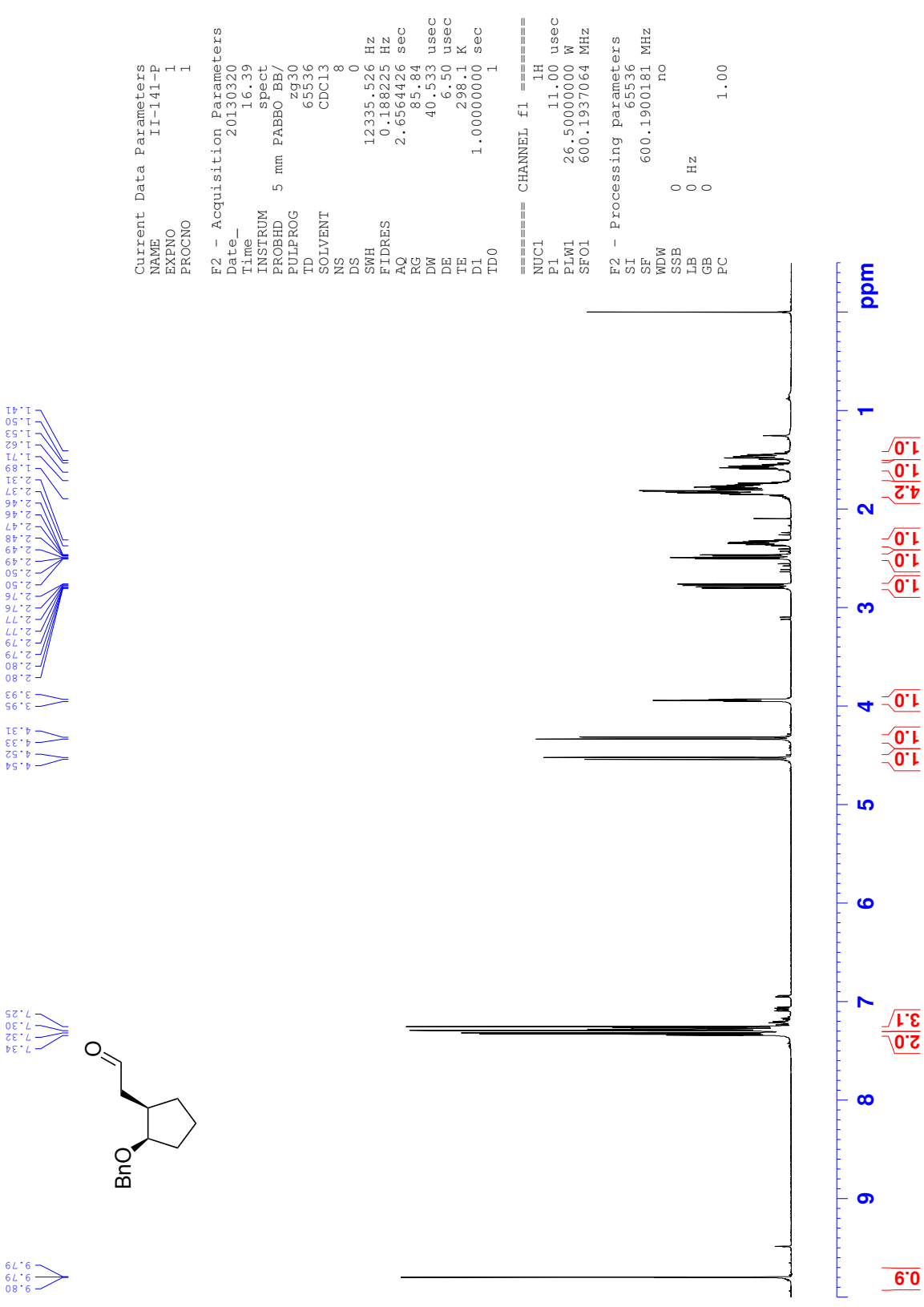

Current Data Parameters
NAME II-127-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130311
Time 19.38
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 184.65
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.00 usec
PLW1 106.00000000 W
SFO1 150.9329866 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 9.30000019 W
PLW12 0.18190999 W
PLW13 0.08913500 W
SFO2 600.1924008 MHz
F2 - Processing parameters
SI 32768
SF 150.9178784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.23
29.79
32.73
34.08
44.52
76.95
77.16
77.37
78.32
115.53
128.46
129.61
131.01
132.88
137.58
166.24
PhOCO
cis-19
ppm
200
180
160
140
120
100
80
60
40
20

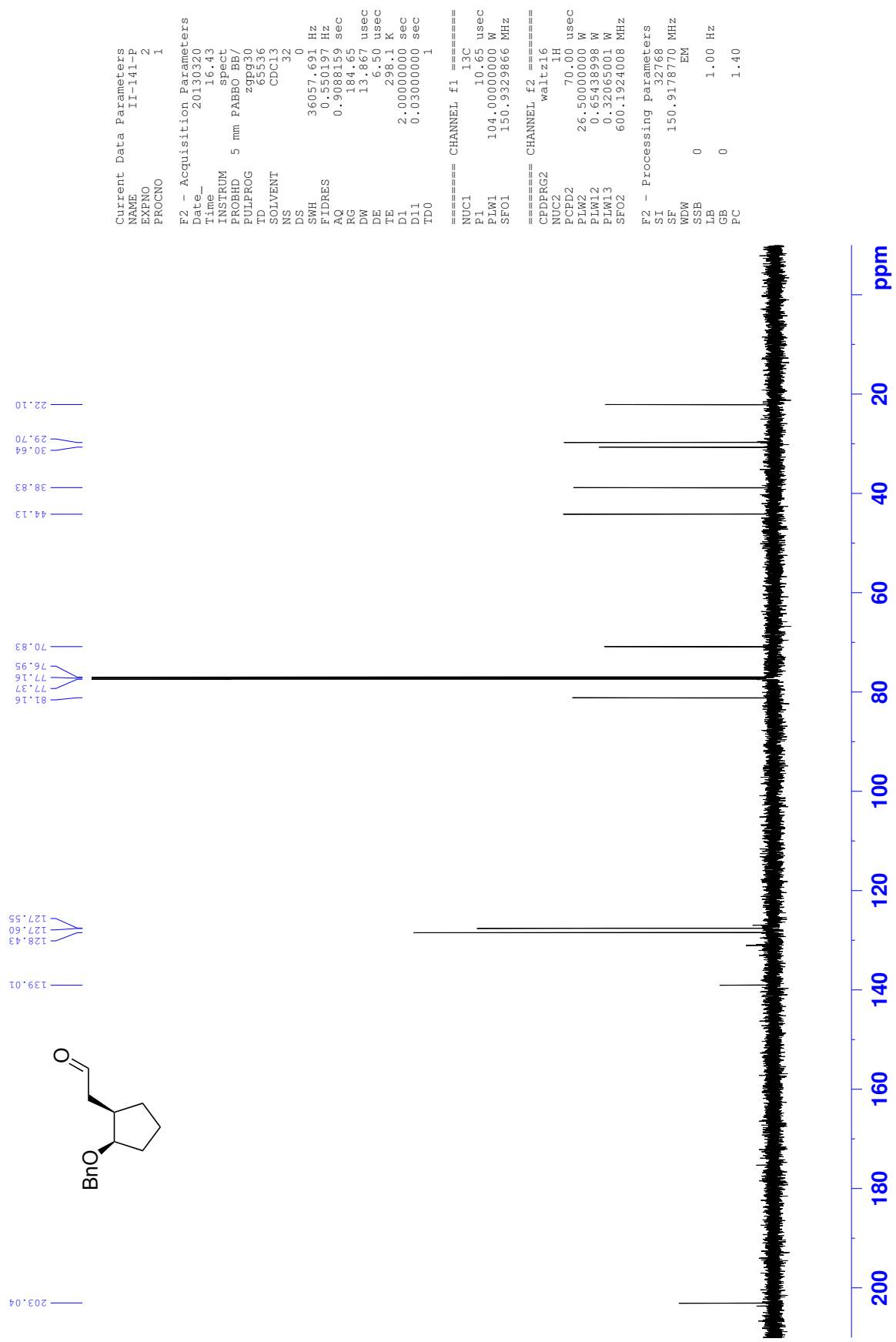

Current Data Parameters
NAME AG-1-19-pure_rd
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 12.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 35.9
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 32768
SF 500.1990144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.238
1.390
1.429
1.480
1.539
1.635
1.638
1.796
1.798
1.805
1.808
1.814
1.920
2.023
2.150
2.240
2.269
4.147
4.790
4.822
4.955
4.976
4.978
5.040
5.074
5.848
5.862
1.06
1.23
4.23
1.08
2.07
1.07
1.03
1.07
0.99
1.00
HO
cis-15
ppm

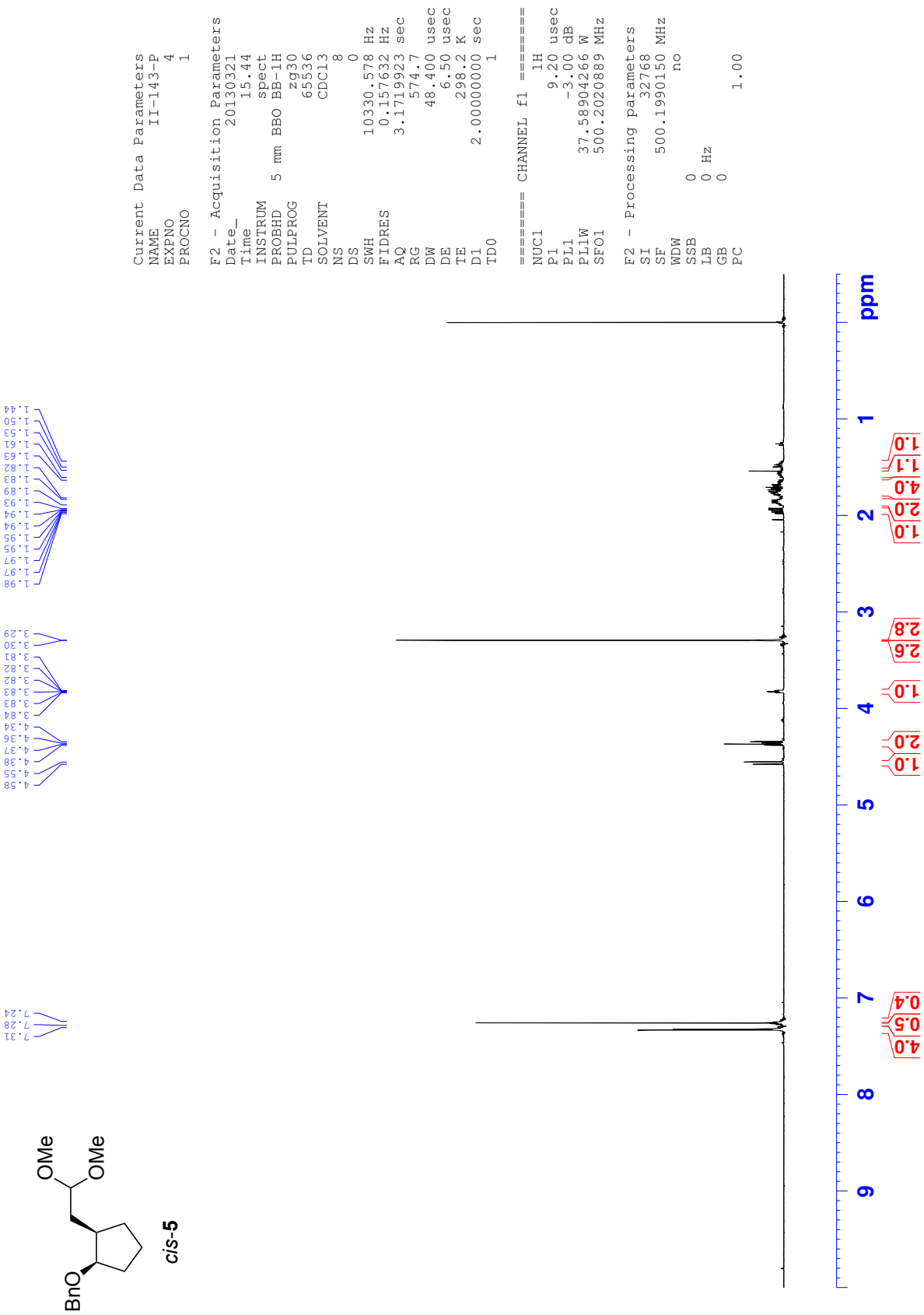

Current Data Parameters
NAME AG-1-19-pure-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 12.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 210
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 23170.5
DW 16.650 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 13.50 dB
PL13 13.50 dB
PL2W 37.58904266 W
PL12W 0.84151381 W
PL13W 0.84151381 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751264 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.98
28.83
33.85
34.76
45.32
74.61
115.10
138.32
ppm
HO
cis-15

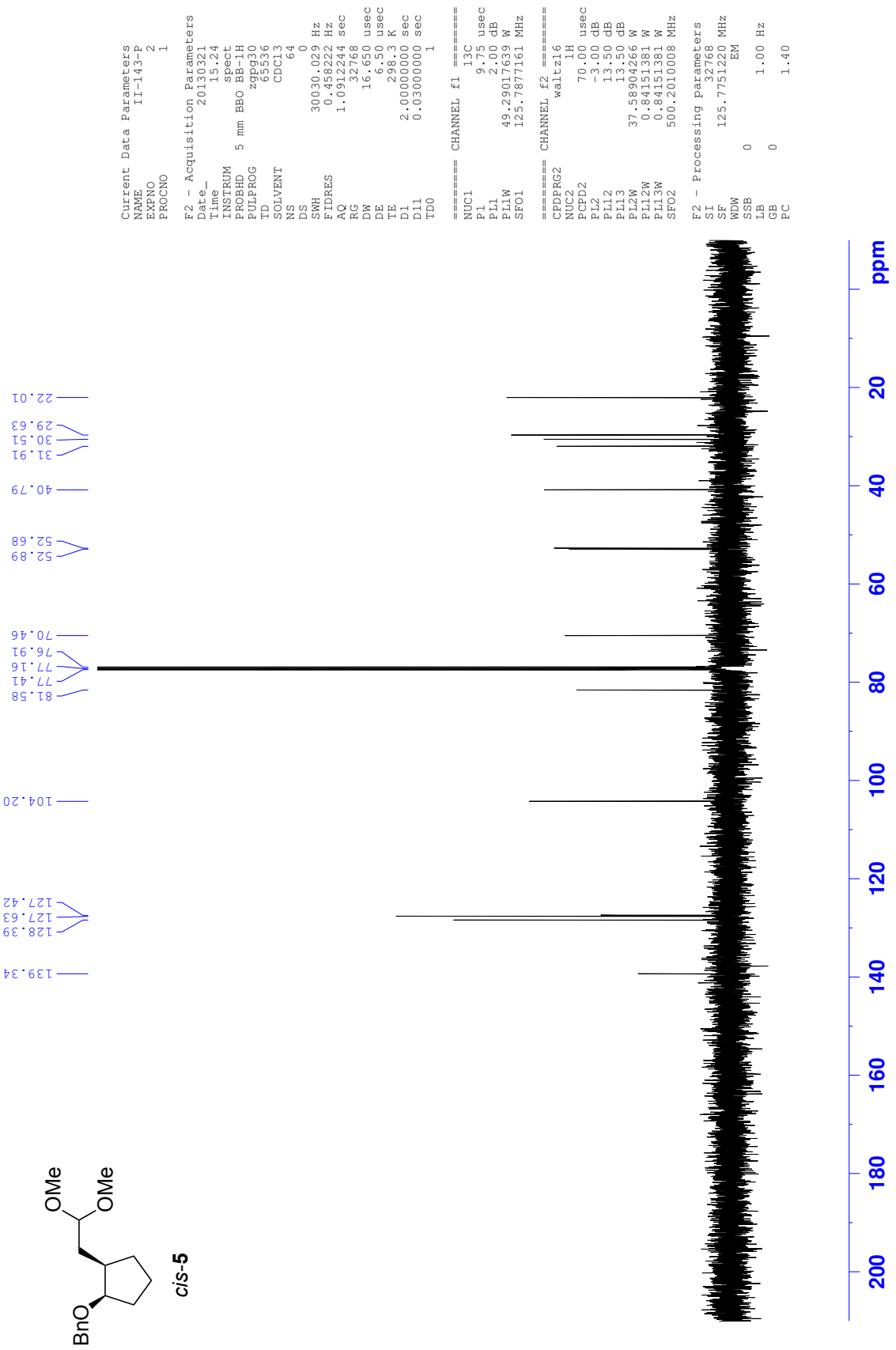

Current Data Parameters
NAME I-159-P
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130226
Time 11.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300135 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
BnO
cis-16

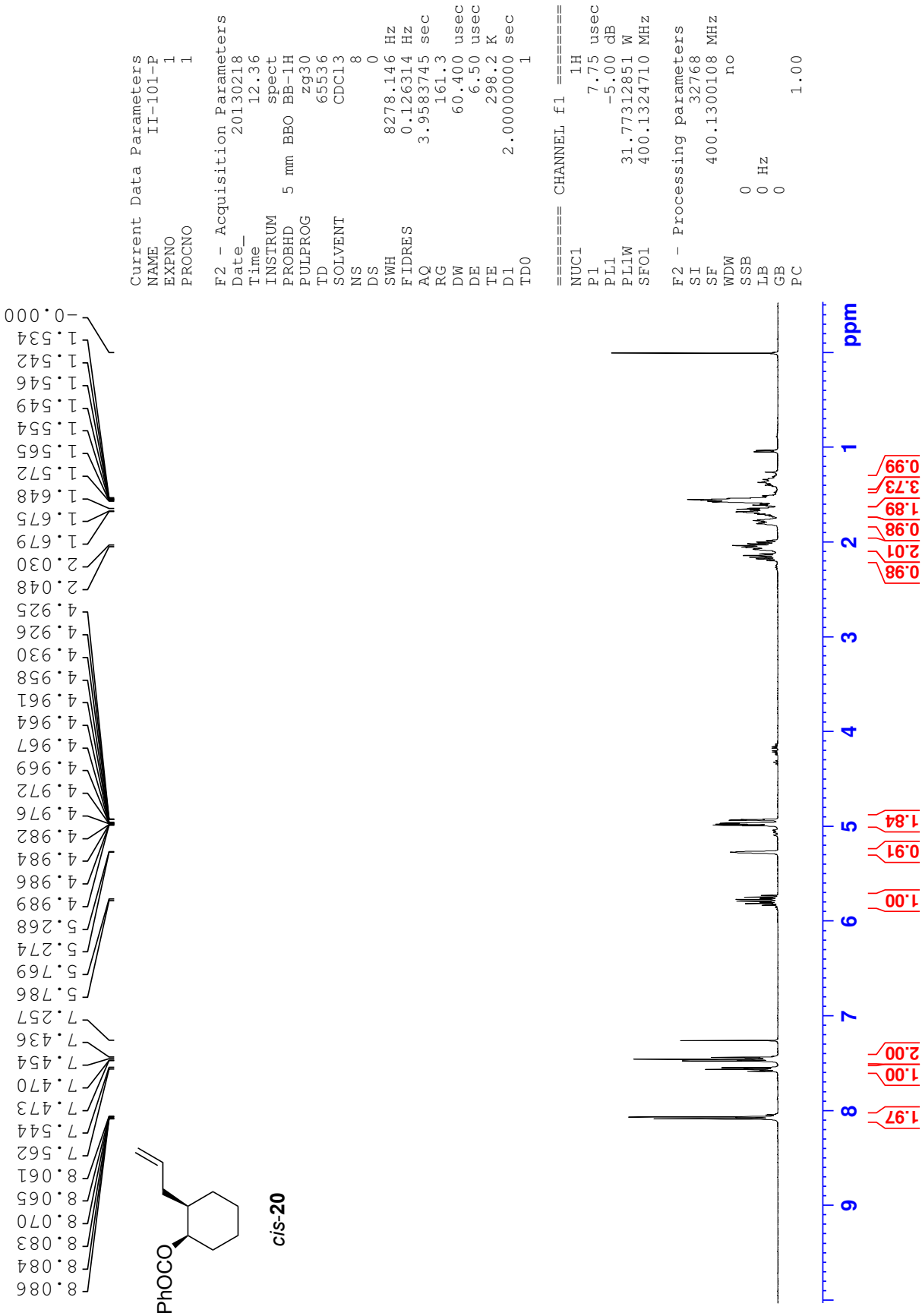

Current Data Parameters
NAME I-159-P
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130225
Time 15.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 23170.5
DW 16.650 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 13.50 dB
PL13 13.50 dB
PL2W 37.58904266 W
PL12W 0.84151381 W
PL13W 0.84151381 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751222 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.85
29.17
30.62
33.66
44.76
70.76
81.70
114.84
127.38
127.53
128.38
138.86
139.48
BnO
cis-16
ppm

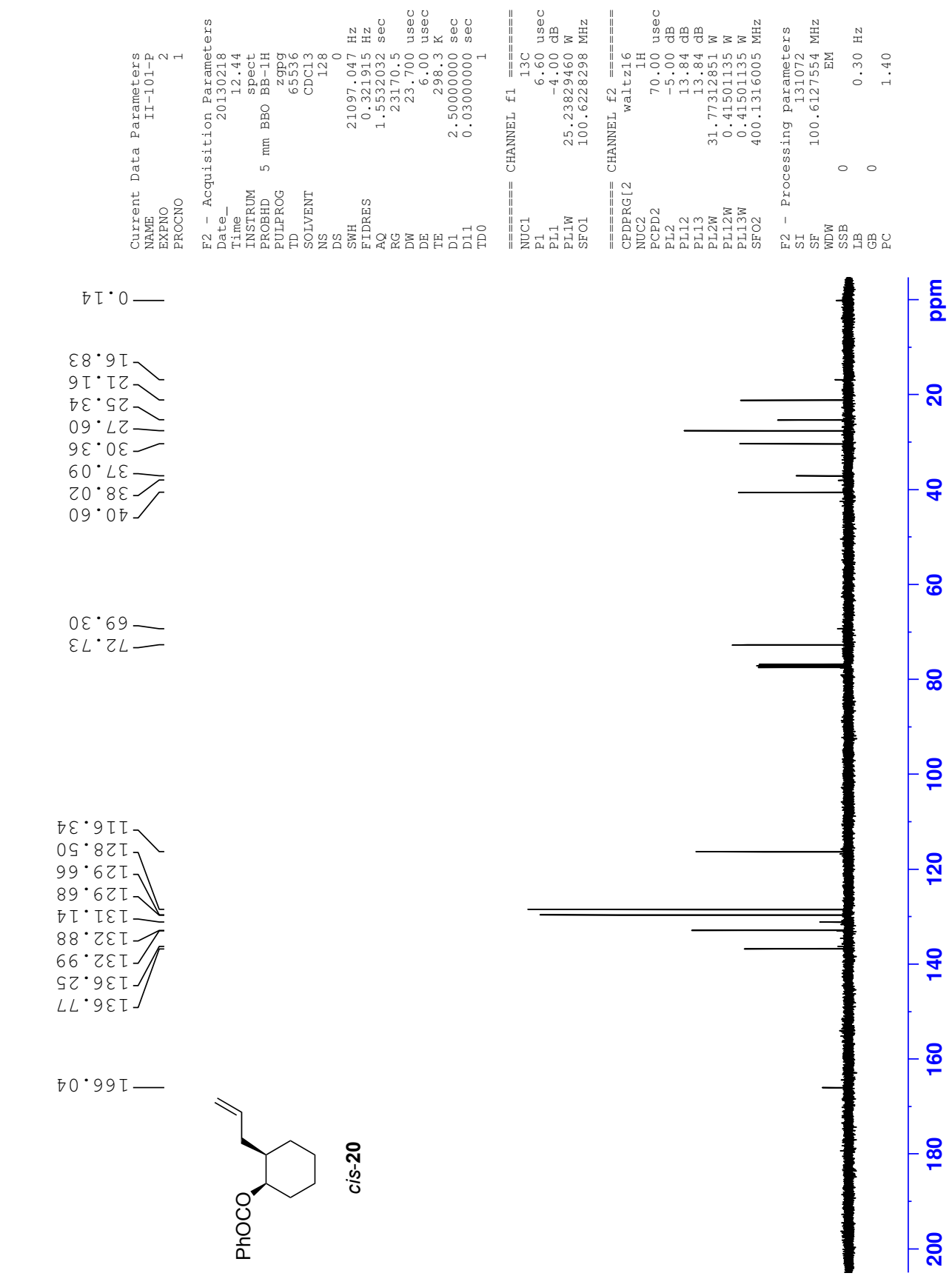

Current Data Parameters
NAME 11-141-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130320
Time 16.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 85.84
DW 40.533 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PLW1 26.50000000 W
SFO1 600.1937064 MHz
F2 - Processing parameters
SI 65536
SF 600.1900181 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
BnO
O

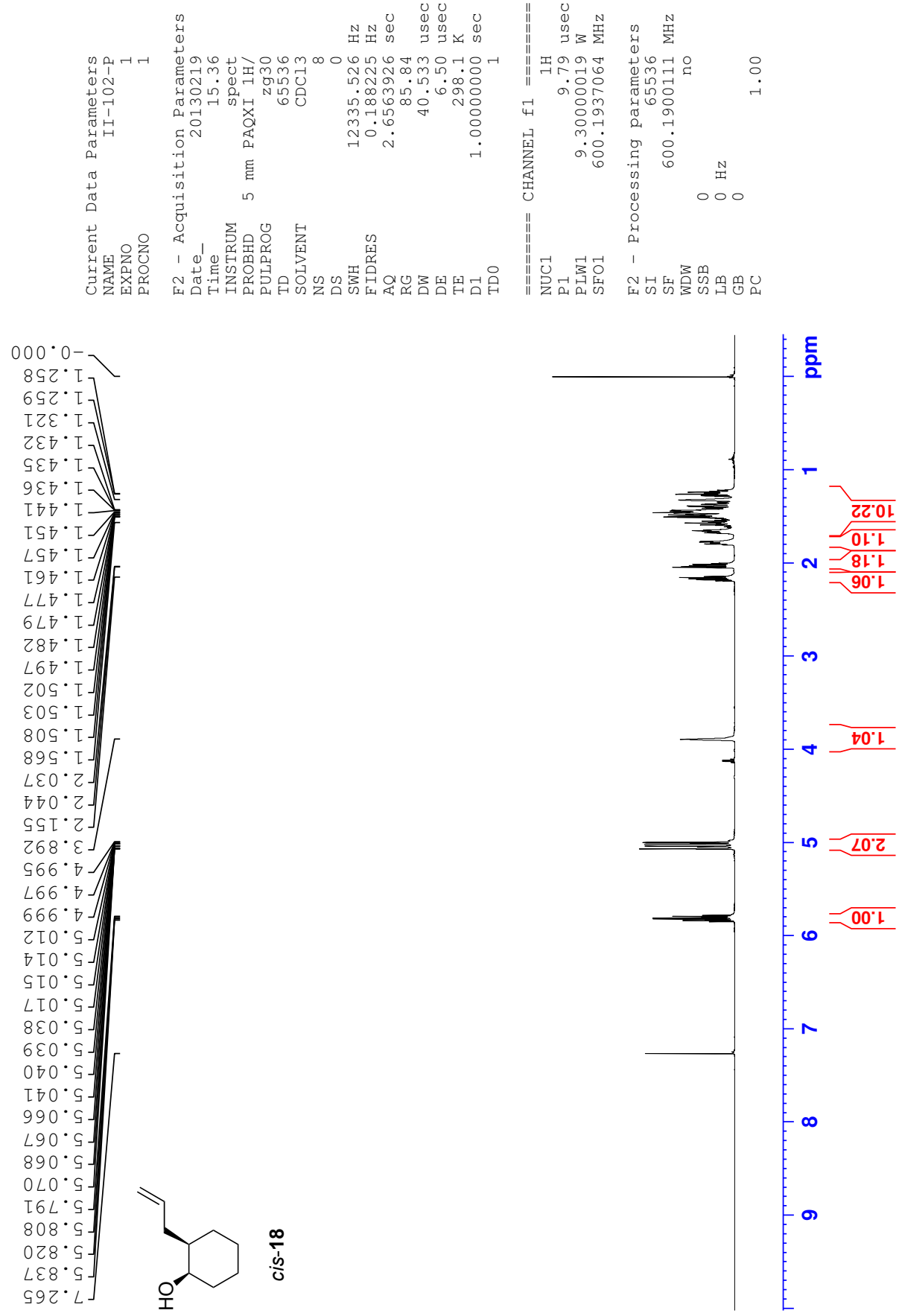

Current Data Parameters
NAME II-141-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130320
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 184.65
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.65 usec
PLW1 104.00000000 W
SFO1 150.9329866 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 26.50000000 W
PLW12 0.65438998 W
PLW13 0.32065001 W
SFO2 600.1924008 MHz
F2 - Processing parameters
SI 32768
SF 150.9178770 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.10
29.70
30.64
38.83
44.13
70.83
76.95
77.16
77.37
81.16
127.55
127.60
128.43
139.01
203.04
O
BnO
ppm
200
180
160
140
120
100
80
60
40
20

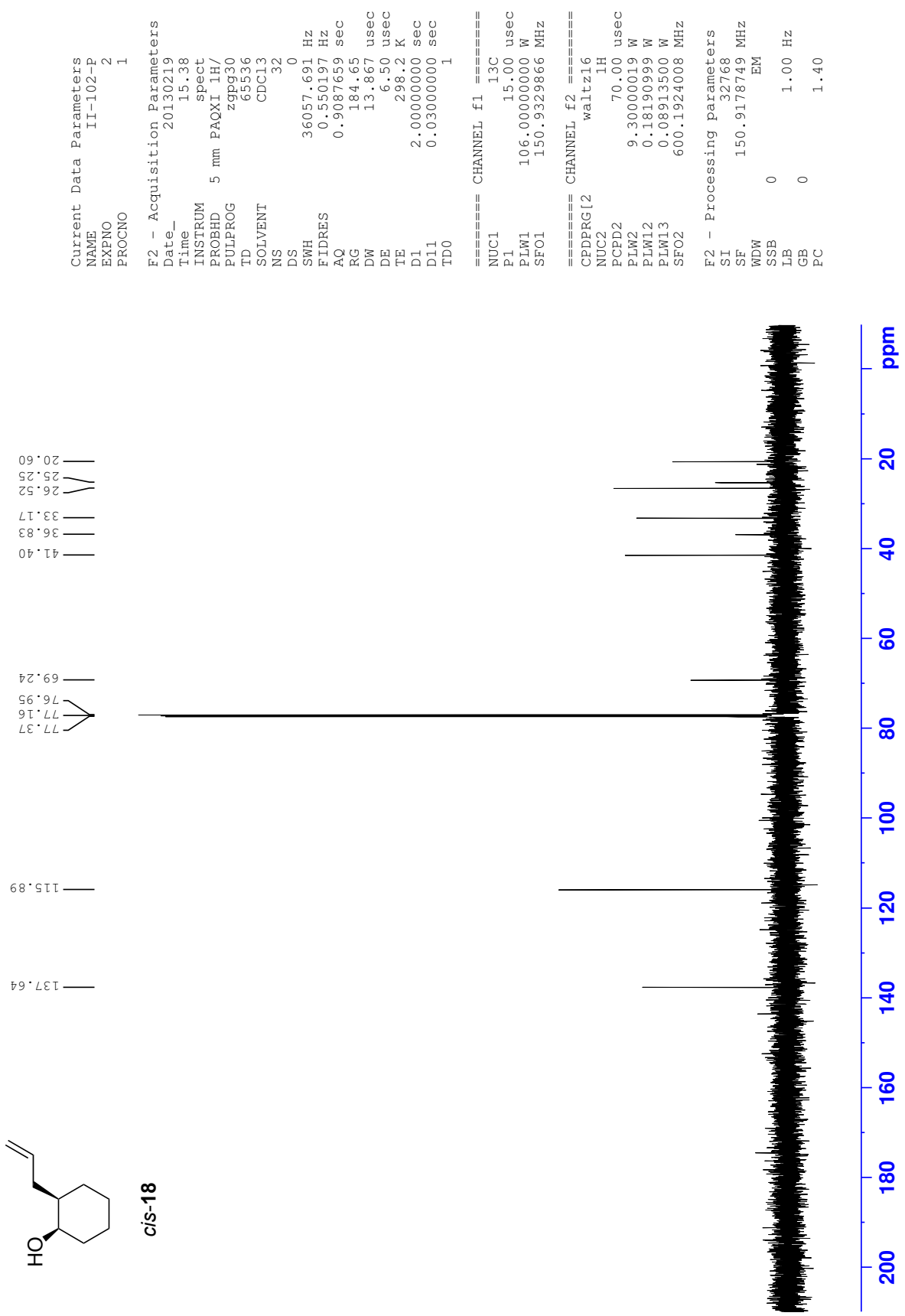

Current Data Parameters
NAME II-143-P
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130321
Time 15.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 574.7
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
F2 - Processing parameters
SI 32768
SF 500.1990150 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.31
7.28
7.24
4.58
4.55
4.38
4.37
4.36
4.34
3.84
3.83
3.83
3.82
3.82
3.81
3.30
3.29
1.98
1.97
1.97
1.95
1.95
1.94
1.94
1.93
1.89
1.83
1.82
1.63
1.61
1.53
1.50
1.44
OMe
OMe
BnO
cis-5
ppm
1
2
3
4
5
6
7
8
9
1.0
2.0
4.0
1.1
1.0
2.6
2.8
1.0
1.0
2.0
4.0
0.5
0.4

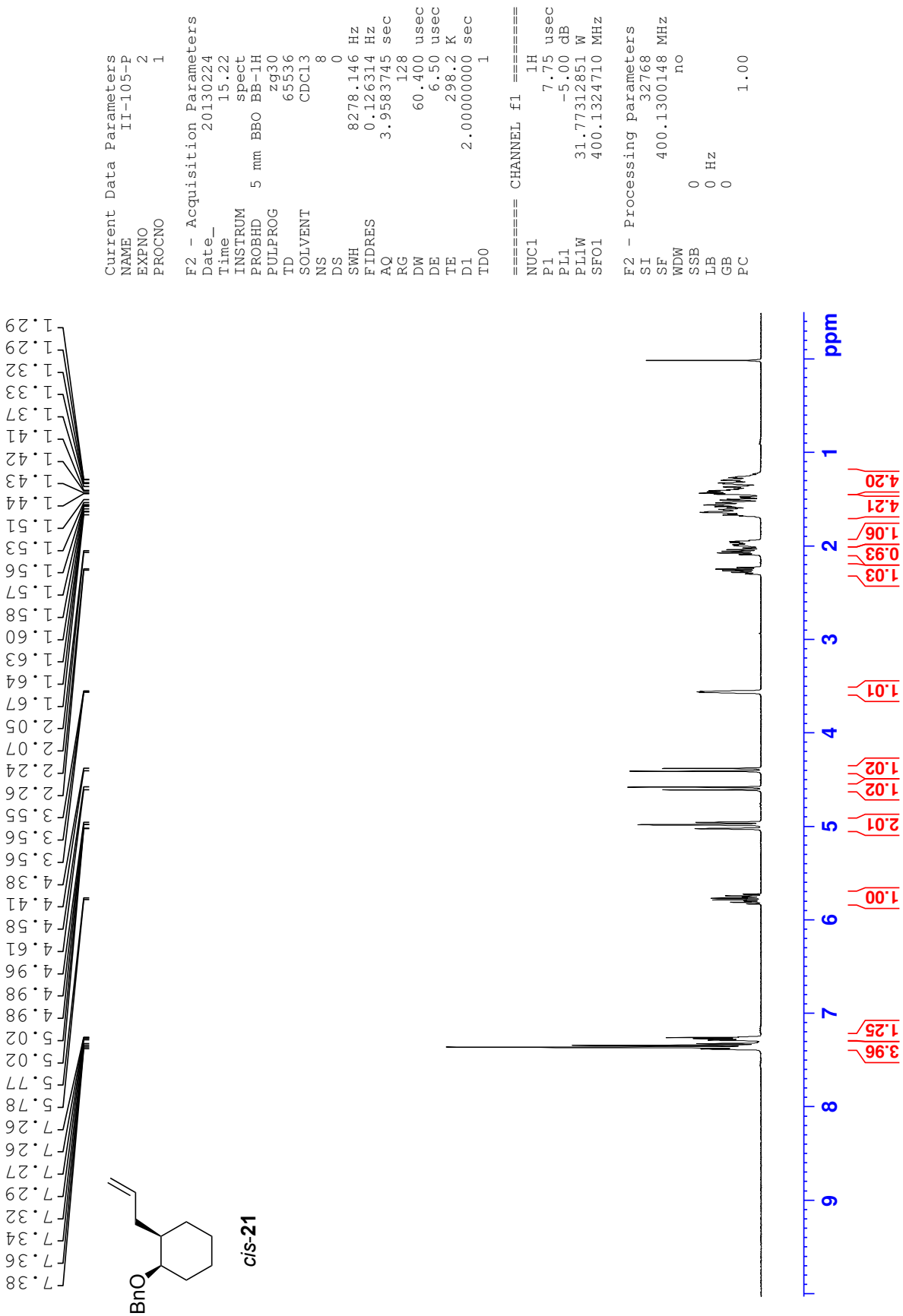

Current Data Parameters
NAME 11-143-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130321
Time 15.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.75 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -3.00 dB
PL12 13.50 dB
PL13 13.50 dB
PL2W 37.58904266 W
PL12W 0.84151381 W
PL13W 0.84151381 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751220 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
22.01
29.63
30.51
31.91
40.79
52.68
52.89
70.46
76.91
77.16
77.41
81.58
104.20
127.42
127.63
128.39
139.34
OMe
OMe
BnO
cis-5
ppm
20
40
60
80
100
120
140
160
180
200

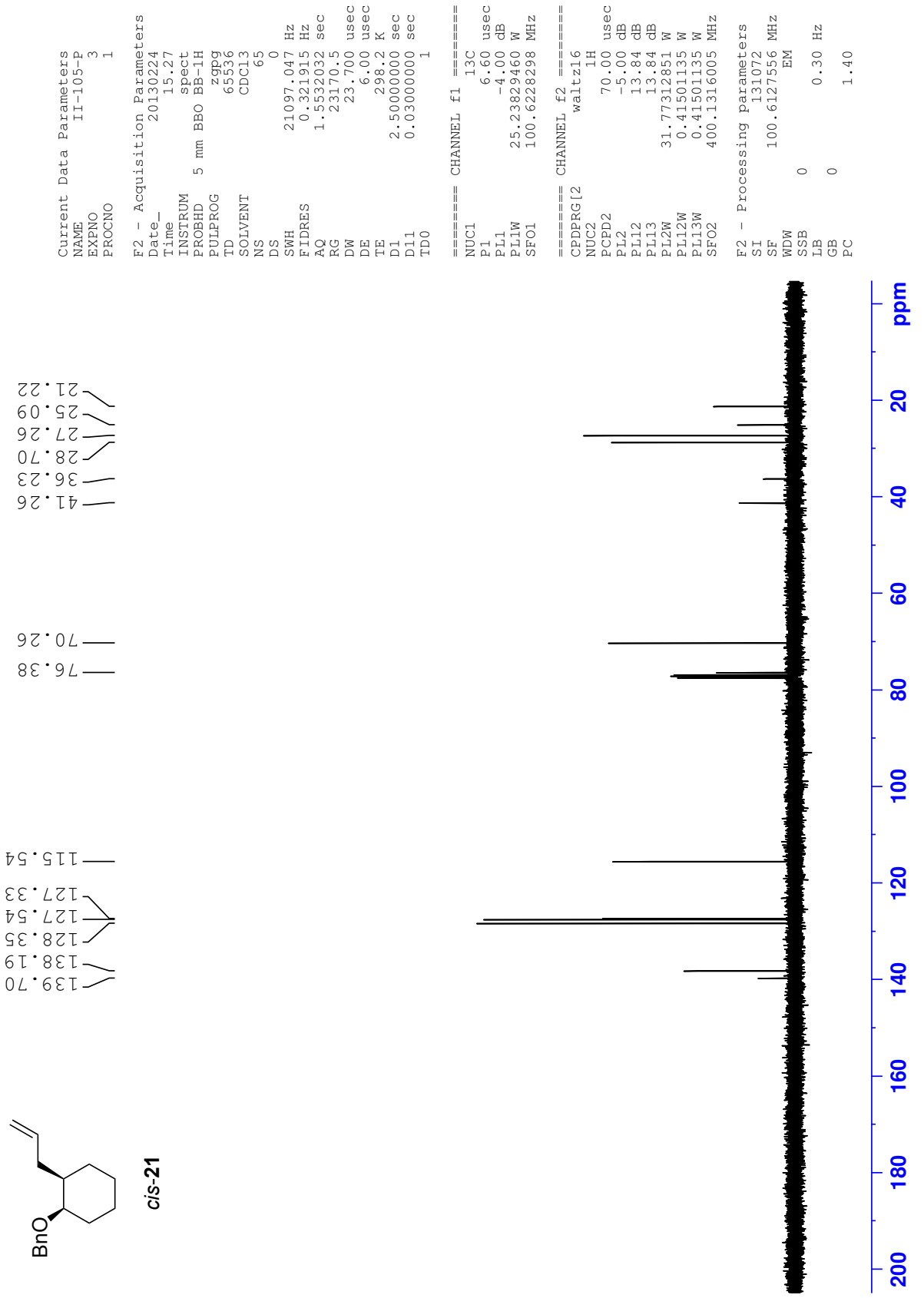

Current Data Parameters
NAME II-101-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130218
Time 12.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 161.3
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300108 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
8.086
8.084
8.083
8.070
8.065
8.061
7.562
7.544
7.473
7.470
7.454
7.436
7.257
5.786
5.769
5.274
5.268
4.989
4.986
4.984
4.982
4.976
4.972
4.969
4.967
4.964
4.961
4.958
4.930
4.926
4.925
2.048
2.030
1.679
1.675
1.648
1.572
1.565
1.554
1.549
1.546
1.542
1.534
0.000
PhOCO
cis-20
ppm
1
2
3
4
5
6
7
8
9
1.97
2.00
1.00
0.91
1.84
1.00
0.98
2.01
0.98
1.89
3.73
0.99

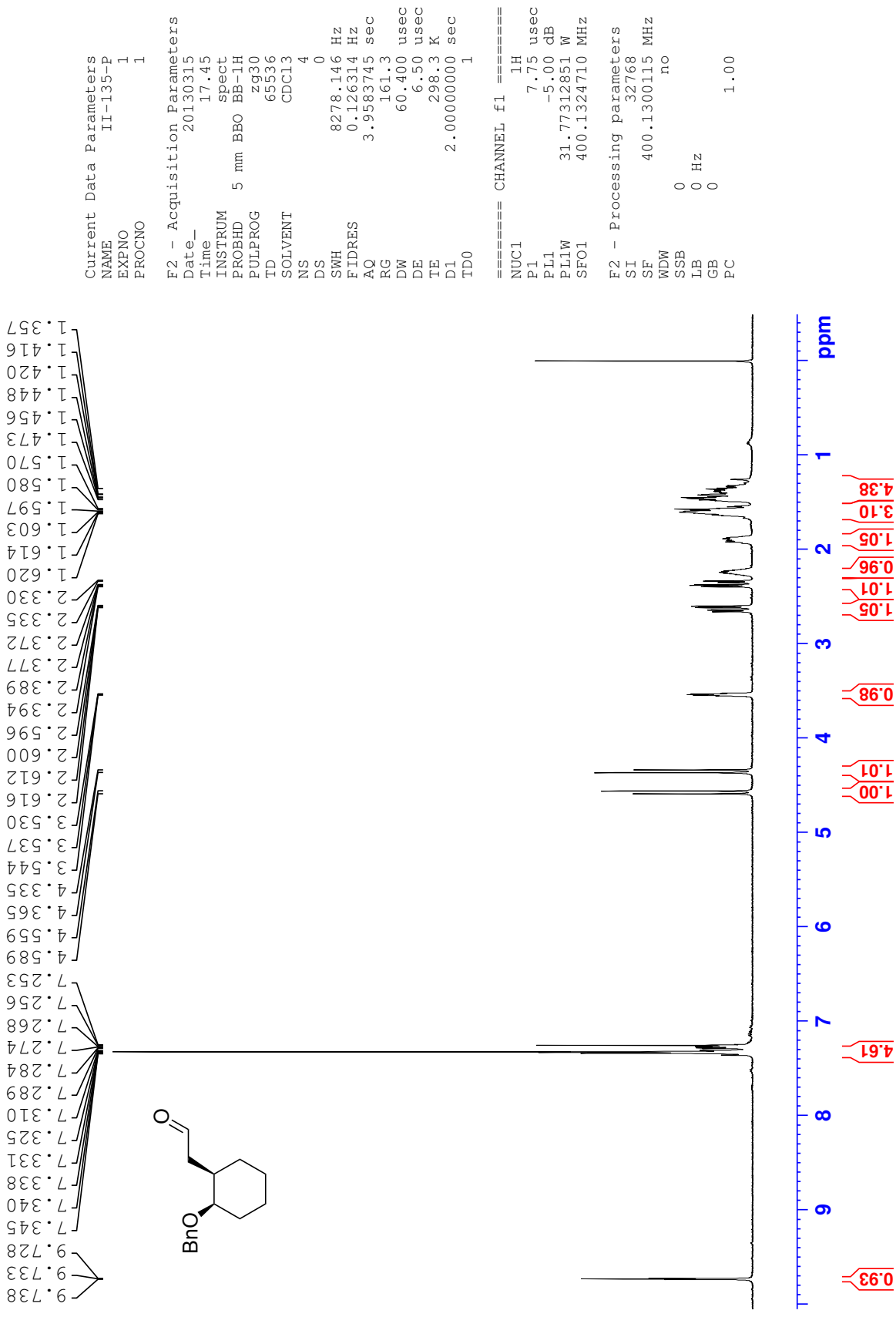

Current Data Parameters
NAME II-101-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130218
Time 12.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532032 sec
RG 23170.5
DW 23.700 usec
DE 6.00 usec
TE 298.3 K
D1 2.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -4.00 dB
PL1W 25.23829460 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -5.00 dB
PL12 13.84 dB
PL13 13.84 dB
PL2W 31.77312851 W
PL12W 0.41501135 W
PL13W 0.41501135 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 131072
SF 100.6127554 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40
166.04
136.77
136.25
132.99
132.88
131.14
129.68
129.66
128.50
116.34
72.73
69.30
40.60
38.02
37.09
30.36
27.60
25.34
21.16
16.83
0.14
PhOCO
cis-20
ppm
200
180
160
140
120
100
80
60
40
20

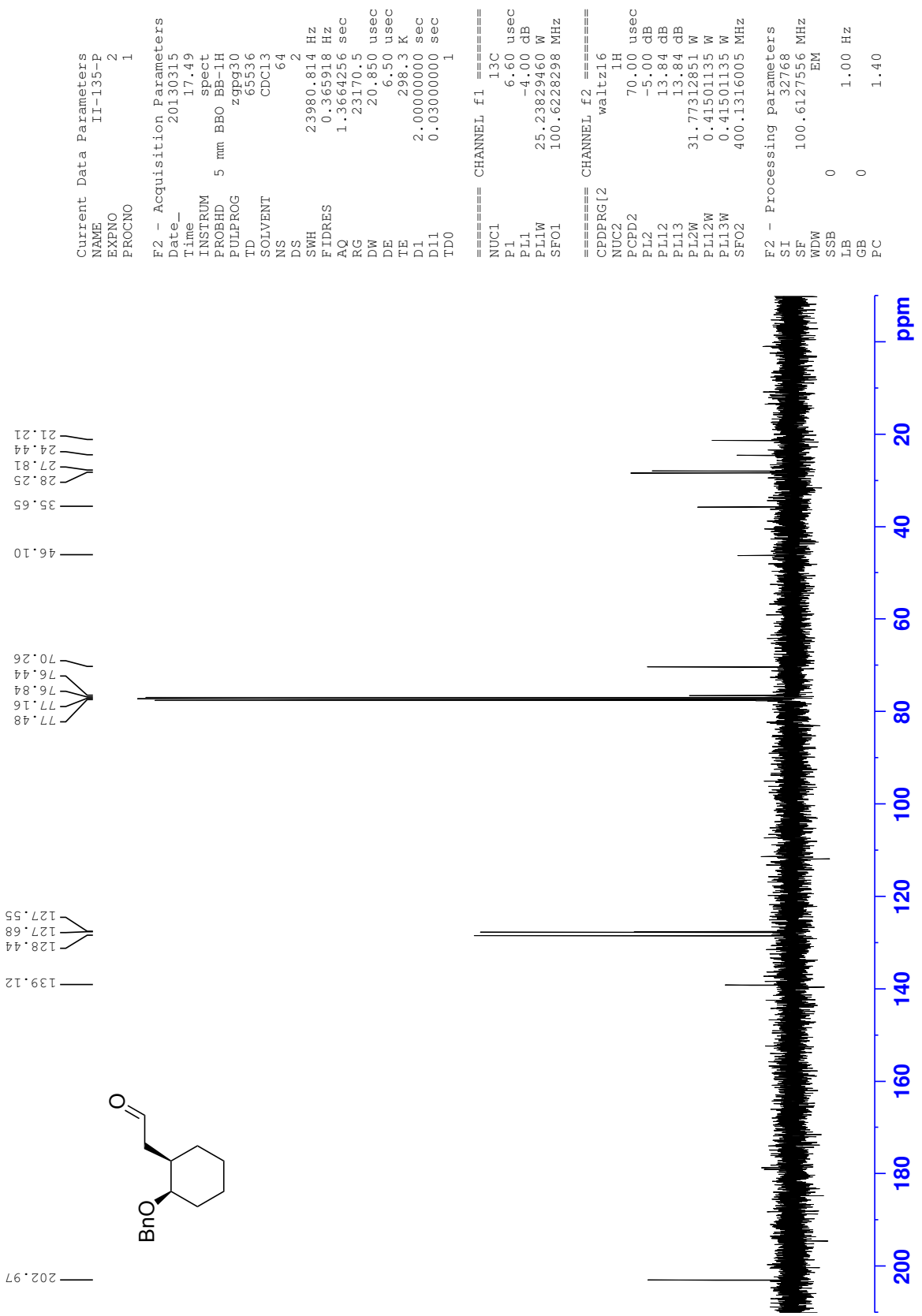

Current Data Parameters
NAME II-102-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130219
Time 15.36
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 85.84
DW 40.533 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.79 usec
PLW1 9.30000019 W
SFO1 600.1937064 MHz
F2 - Processing parameters
SI 65536
SF 600.1900111 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
-0.000
1.258
1.259
1.321
1.432
1.435
1.436
1.441
1.451
1.457
1.461
1.477
1.479
1.482
1.497
1.502
1.503
1.508
1.568
2.037
2.044
2.155
3.892
4.995
4.997
4.999
5.012
5.014
5.015
5.017
5.038
5.039
5.040
5.041
5.066
5.067
5.068
5.070
5.791
5.808
5.820
5.837
7.265
HO
cis-18
ppm
1
2
3
4
5
6
7
8
9
10.22
1.10
1.18
1.06
1.04
2.07
1.00

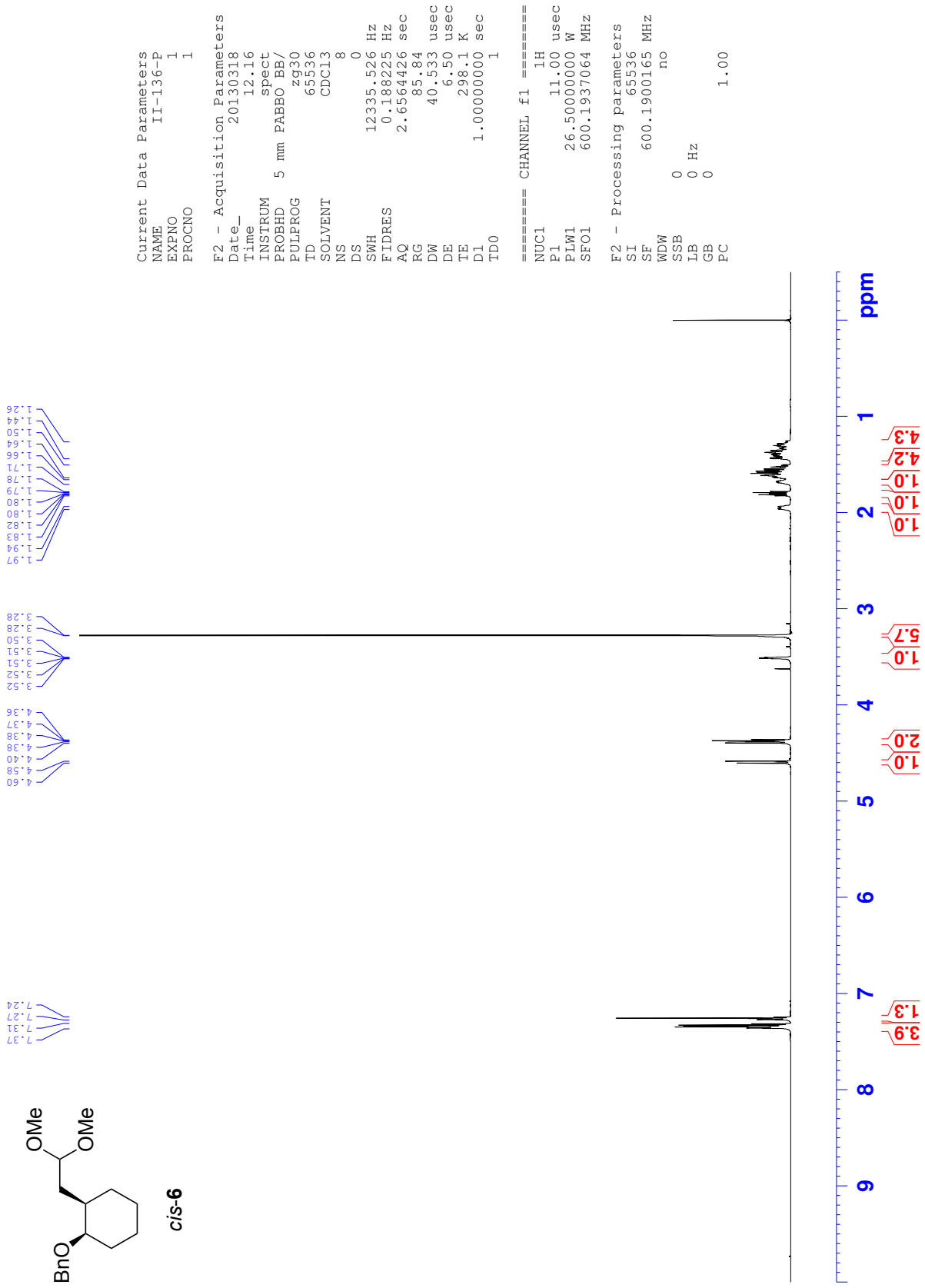

Current Data Parameters
NAME II-102-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130219
Time 15.38
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 184.65
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.00 usec
PLW1 106.00000000 W
SFO1 150.9329866 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 9.30000019 W
PLW12 0.18190999 W
PLW13 0.08913500 W
SFO2 600.1924008 MHz
F2 - Processing parameters
SI 32768
SF 150.9178749 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
20.60
25.25
26.52
33.17
36.83
41.40
69.24
76.95
77.16
77.37
115.89
137.64
HO
cis-18
ppm
200
180
160
140
120
100
80
60
40
20

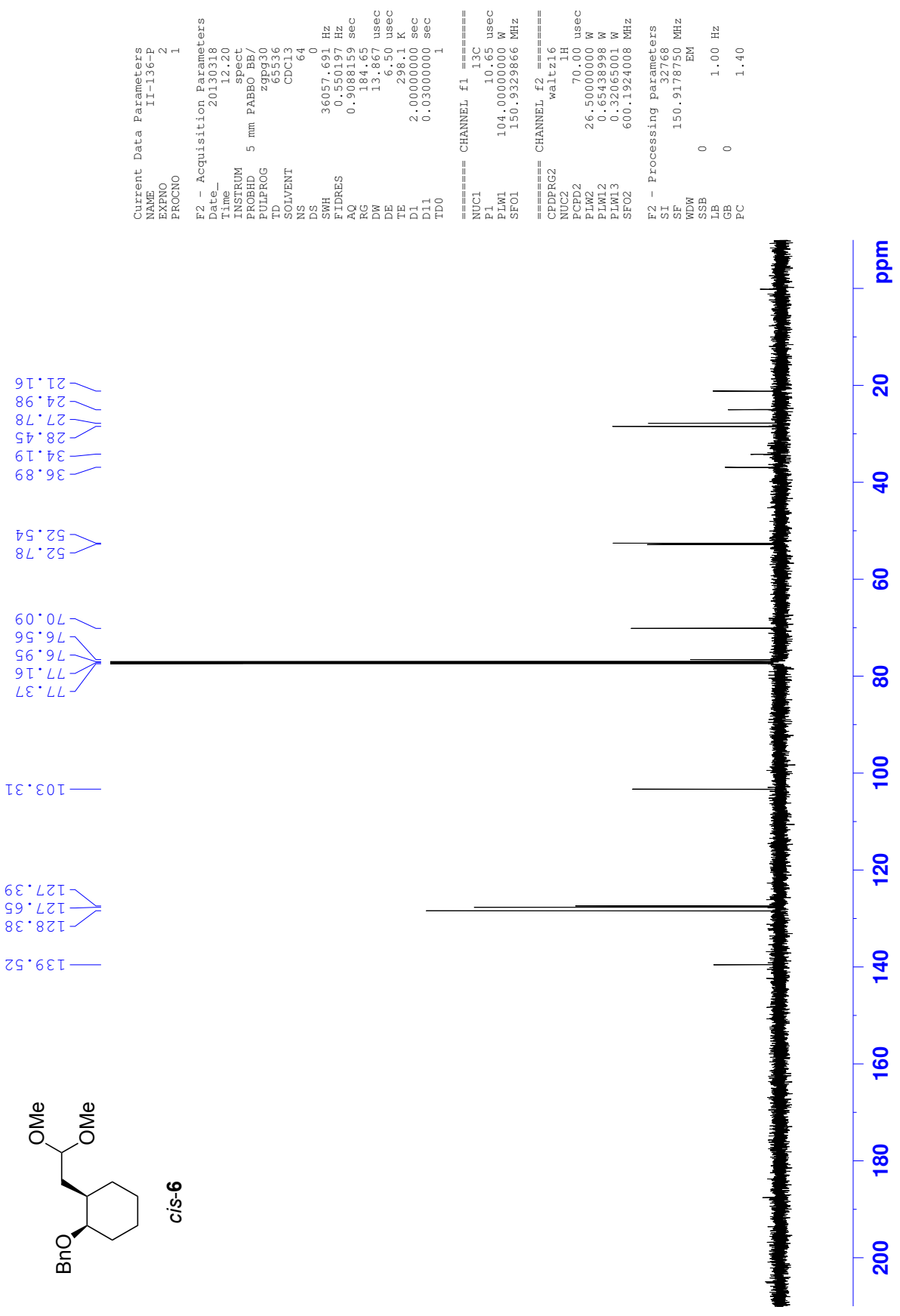

Current Data Parameters
NAME II-105-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130224
Time 15.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300148 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.38
7.36
7.34
7.32
7.29
7.27
7.26
7.26
7.78
5.77
5.02
5.02
4.98
4.98
4.96
4.61
4.58
4.41
4.38
3.56
3.56
3.55
2.26
2.24
2.07
2.05
1.67
1.64
1.63
1.60
1.58
1.57
1.56
1.53
1.51
1.44
1.43
1.42
1.41
1.37
1.33
1.32
1.29
1.29
BnO
cis-21
ppm
1
2
3
4
5
6
7
8
9
4.20
4.21
1.06
0.93
1.03
1.01
1.02
1.02
2.01
1.00
3.96
1.25

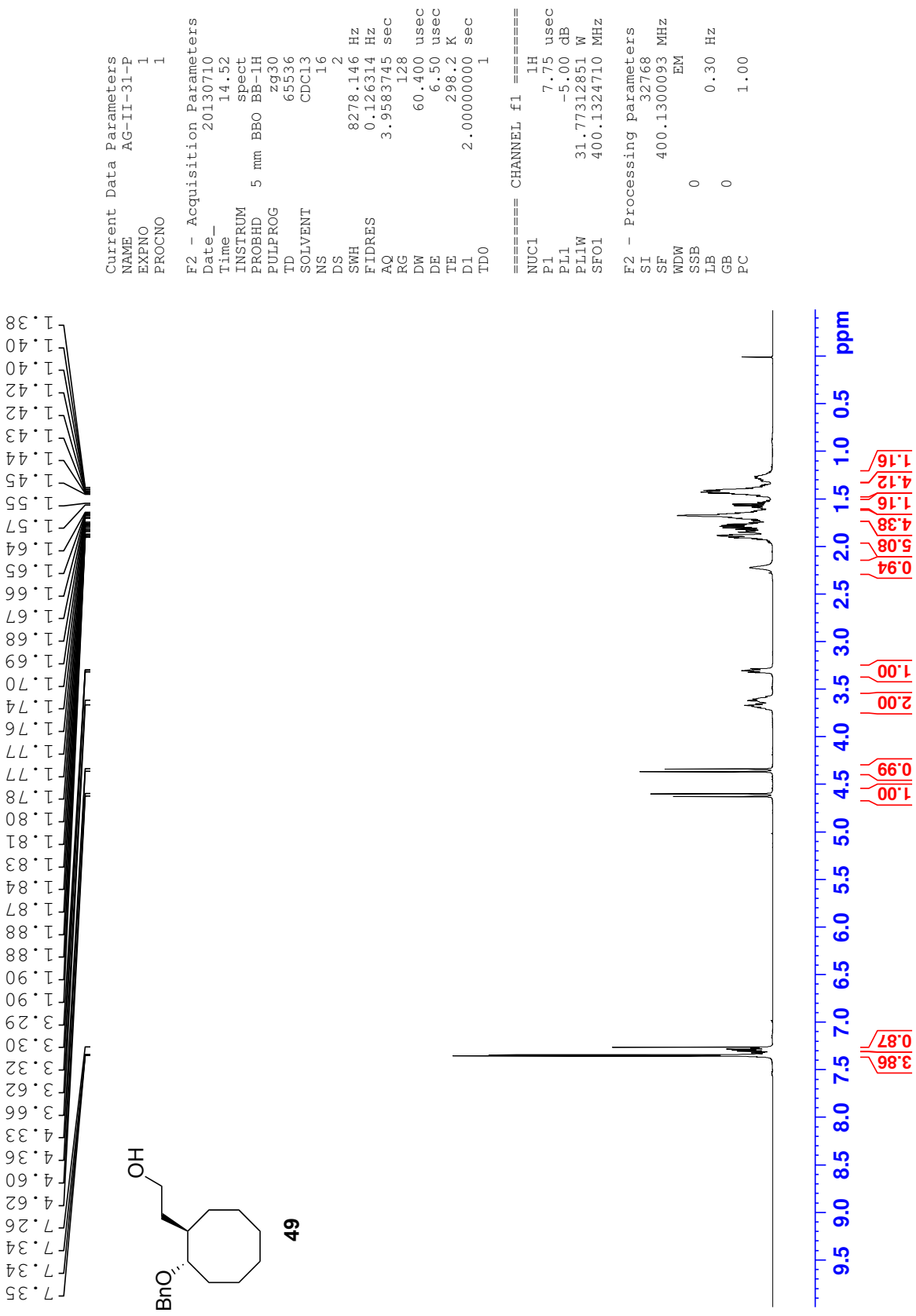

Current Data Parameters
NAME II-105-P
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130224
Time 15.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 65
DS 0
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532032 sec
RG 23170.5
DW 23.700 usec
DE 6.00 usec
TE 298.2 K
D1 2.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -4.00 dB
PL1W 25.23829460 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -5.00 dB
PL12 13.84 dB
PL13 13.84 dB
PL2W 31.77312851 W
PL12W 0.41501135 W
PL13W 0.41501135 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 131072
SF 100.6127556 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40
139.70
138.19
128.35
127.54
127.33
115.54
76.38
70.26
41.26
36.23
28.70
27.26
25.09
21.22
BnO
cis-21
ppm
200
180
160
140
120
100
80
60
40
20

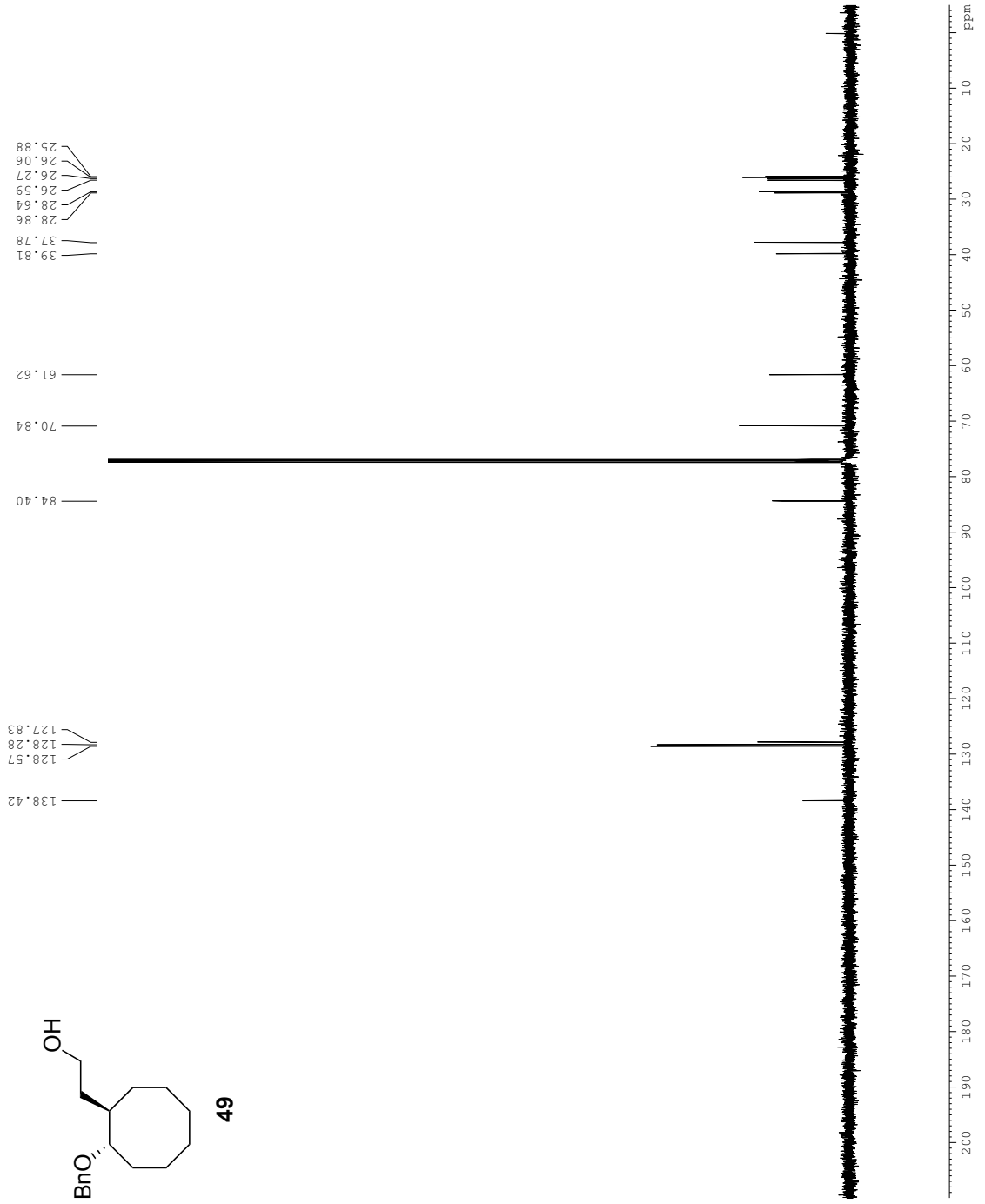

Current Data Parameters
NAME II-135-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time 17.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 161.3
DW 60.400 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300115 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9.738
9.733
9.728
7.345
7.340
7.338
7.331
7.325
7.310
7.289
7.284
7.274
7.268
7.256
7.253
4.589
4.559
4.365
4.335
3.544
3.537
3.530
2.616
2.612
2.600
2.596
2.394
2.389
2.377
2.372
2.335
2.330
1.620
1.614
1.603
1.597
1.580
1.570
1.473
1.456
1.448
1.420
1.416
1.357
BnO
O
ppm
1
2
3
4
5
6
7
8
9
0.93
4.61
1.00
1.01
0.98
1.05
1.01
0.96
1.05
3.10
4.38

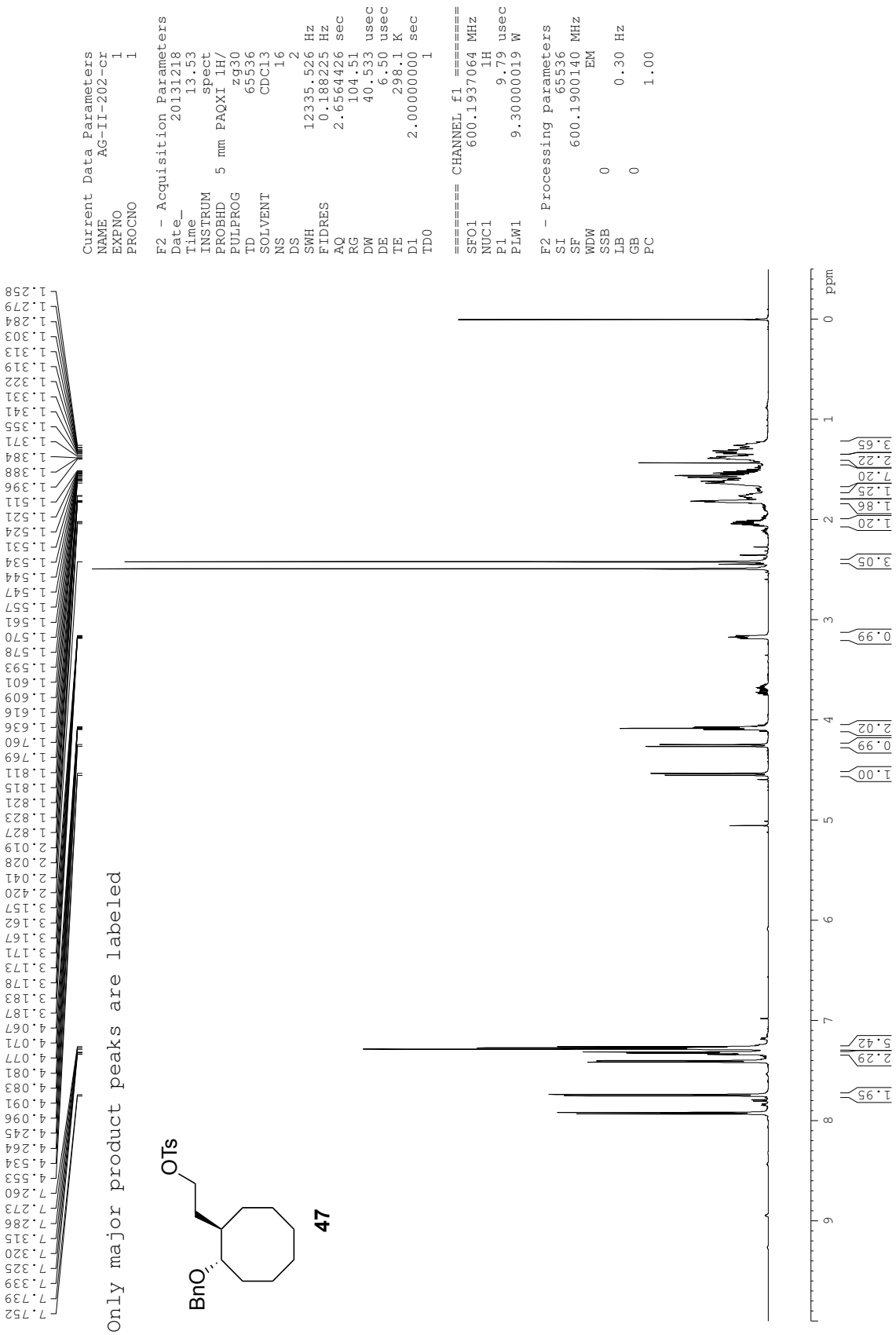

Current Data Parameters
NAME II-135-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time_ 17.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 23170.5
DW 20.850 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.60 usec
PL1 -4.00 dB
PL1W 25.23829460 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 -5.00 dB
PL12 13.84 dB
PL13 13.84 dB
PL2W 31.77312851 W
PL12W 0.41501135 W
PL13W 0.41501135 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127556 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
202.97
139.12
128.44
127.68
127.55
77.48
77.16
76.84
76.44
70.26
46.10
35.65
28.25
27.81
24.44
21.21
BnO
O
ppm
200
180
160
140
120
100
80
60
40
20

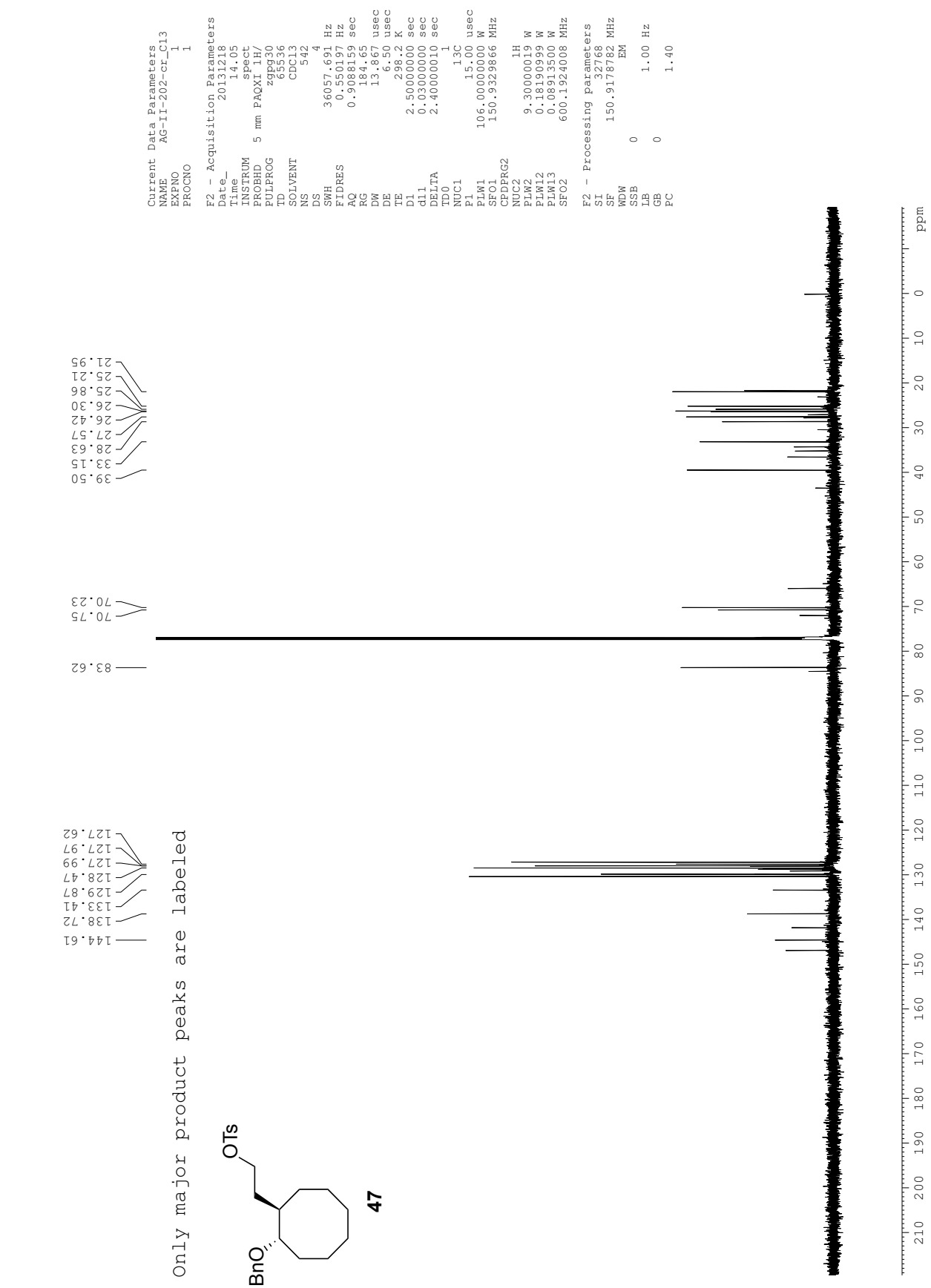

Current Data Parameters
NAME II-136-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130318
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 85.84
DW 40.533 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PLW1 26.50000000 W
SFO1 600.1937064 MHz
F2 - Processing parameters
SI 65536
SF 600.1900165 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
OMe
OMe
BnO
cis-6


Current Data Parameters
NAME 11-136-P
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130318
Time 12.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.90881591 sec
RG 184.65
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.65 usec
PLW1 104.00000000 W
SFO1 150.9329866 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PLW2 26.50000000 W
PLW12 0.65438998 W
PLW13 0.32065001 W
SFO2 600.1924008 MHz
F2 - Processing parameters
SI 32768
SF 150.9178750 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.16
24.98
27.78
28.45
34.19
36.89
52.54
52.78
70.09
76.56
76.95
77.16
77.37
103.31
127.39
127.65
128.38
139.52
ppm
20
40
60
80
100
120
140
160
180
200
OMe
OMe
BnO
cis-6


Current Data Parameters
NAME AG-II-31-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130710
Time 14.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 usec
PL1 -5.00 dB
PL1W 31.77312851 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OH
BnO
49
7.35
7.34
7.34
7.26
4.62
4.60
4.36
4.33
3.66
3.62
3.32
3.30
3.29
1.90
1.90
1.88
1.88
1.87
1.84
1.83
1.81
1.80
1.78
1.77
1.77
1.76
1.74
1.70
1.69
1.68
1.67
1.66
1.65
1.64
1.57
1.55
1.45
1.44
1.43
1.42
1.42
1.40
1.40
1.38
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
3.86
0.87
1.00
0.99
2.00
1.00
5.08
0.94
4.38
1.16
4.12
1.16

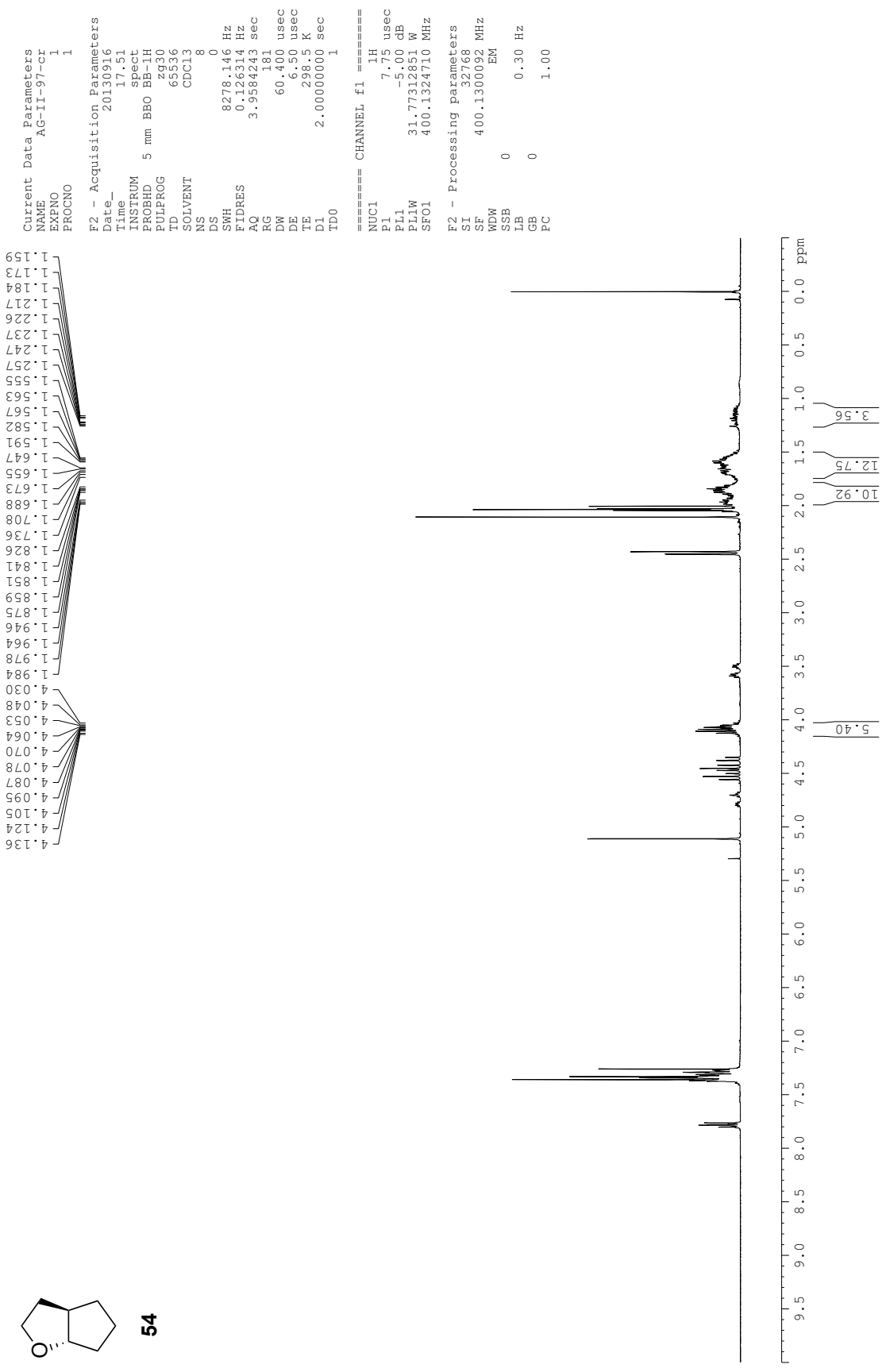

Current Data Parameters
NAME AG-II-31-P2_C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130924
Time_ 15.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 210
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 9195.2
DW 16.650 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.41 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 15.31 dB
PL13 18.31 dB
PL2W 37.58904266 W
PL12W 0.55470389 W
PL13W 0.27801058 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751222 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
25.88
26.06
26.27
26.59
28.64
28.86
37.78
39.81
61.62
70.84
84.40
127.83
128.28
128.57
138.42
ppm
OH
BnO
49

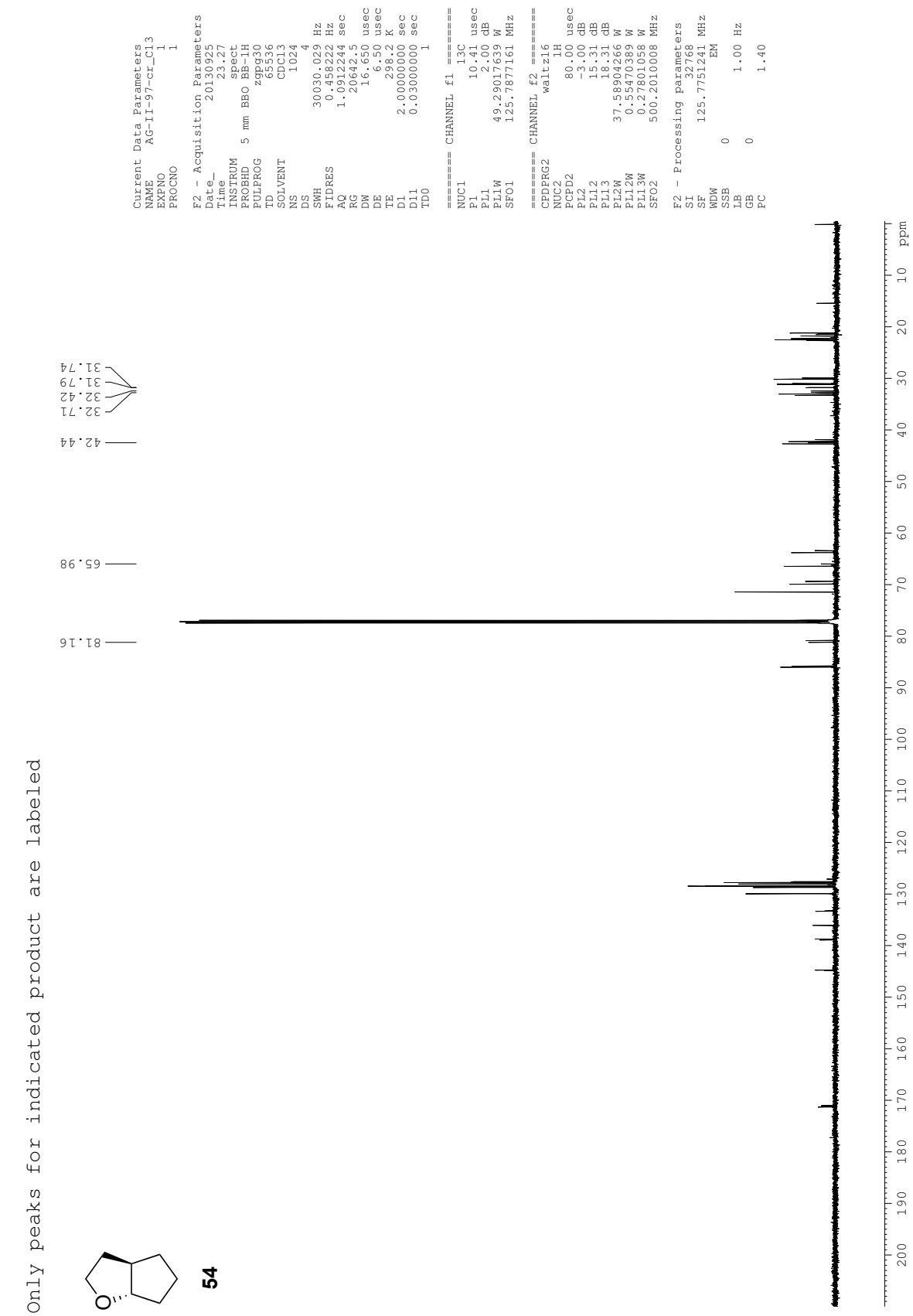

Current Data Parameters
NAME AG-II-202-cr
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131218
Time 13.53
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 104.51
DW 40.533 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 9.79 usec
PLW1 9.30000019 W
F2 - Processing parameters
SI 65536
SF 600.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Only major product peaks are labeled
OTs
BnO
47
ppm

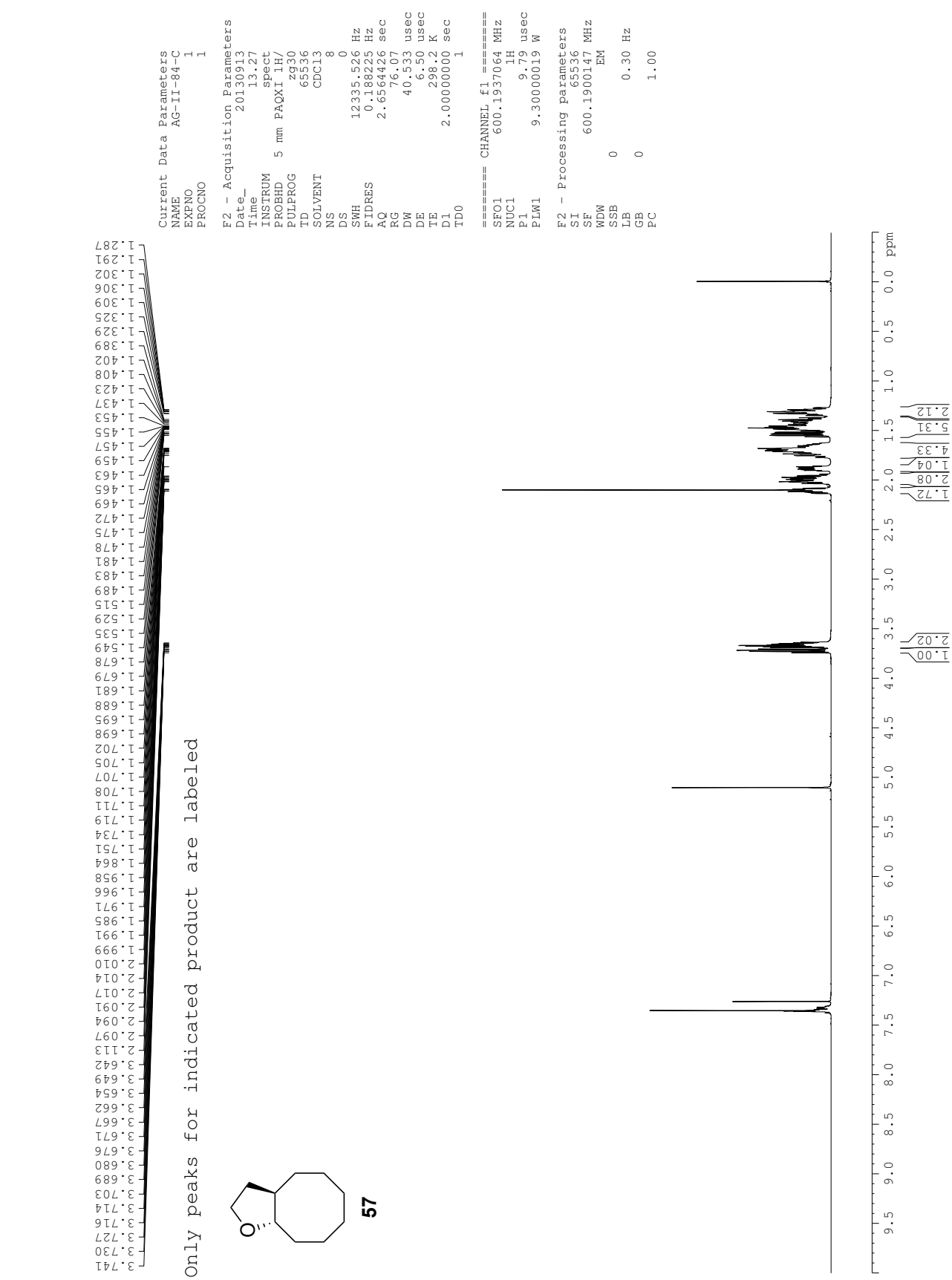

Current Data Parameters
NAME AG-II-202-cr_C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131218
Time_ 14.05
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 542
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.90881159 sec
RG 184.65
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.50000000 sec
d11 0.03000000 sec
DELTA 2.40000010 sec
TD0 1
NUC1 13C
P1 15.00 usec
PLW1 106.00000000 W
SFO1 150.9329866 MHz
CPDPRG2
NUC2 1H
PLW2 9.30000019 W
PLW12 0.18190999 W
PLW13 0.08913500 W
SFO2 600.1924008 MHz
F2 - Processing parameters
SI 32768
SF 150.9178782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.95
25.21
25.86
26.30
26.42
27.57
28.63
33.15
39.50
70.23
70.75
83.62
127.62
127.97
127.99
128.47
129.87
133.41
138.72
144.61
Only major product peaks are labeled
OTs
BnO
47
ppm

Only peaks for indicated product are labeled

54

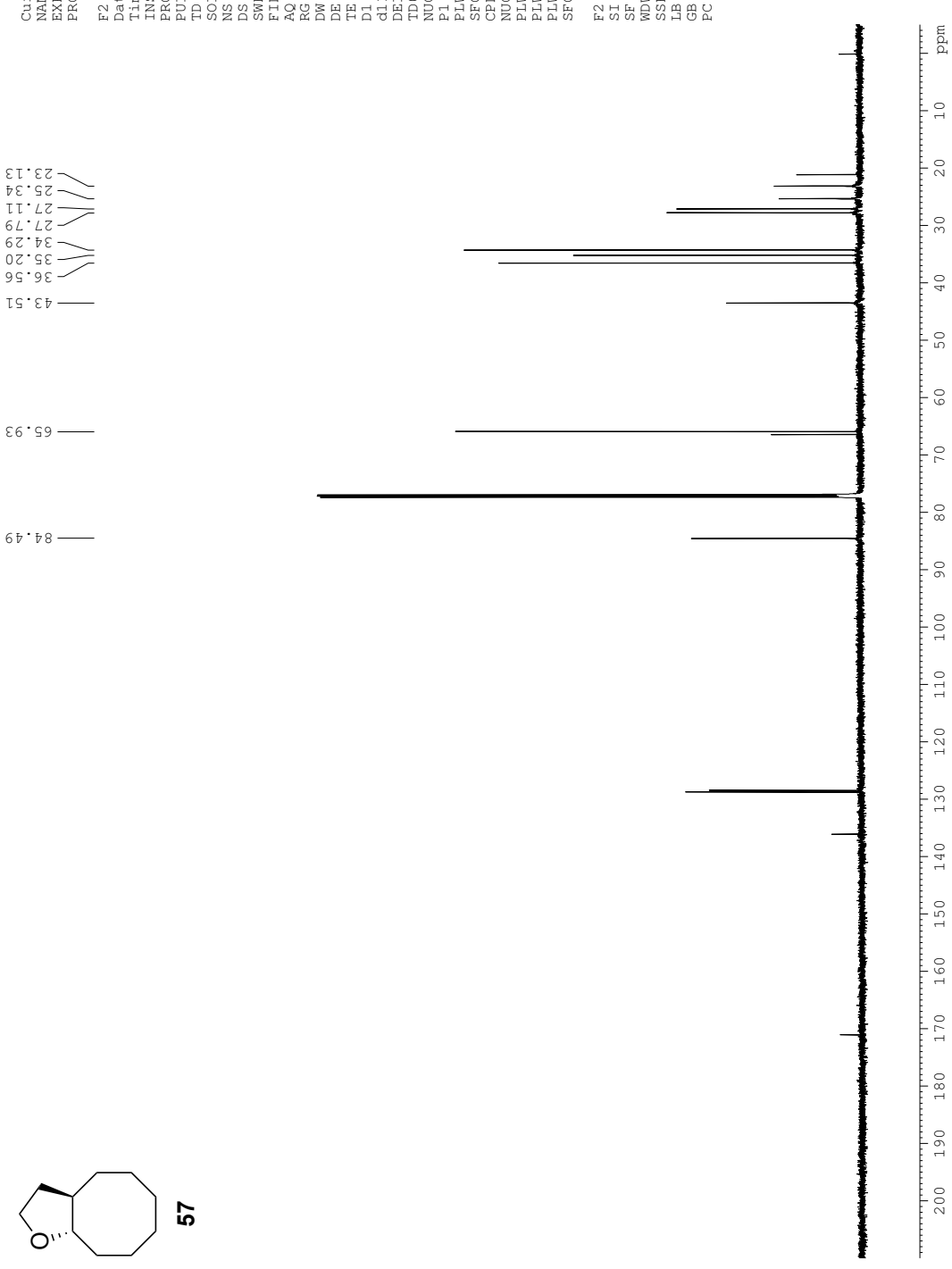



Only peaks for indicated product are labeled
54
Current Data Parameters
NAME AG-II-97-cr_C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130925
Time_ 23.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 20642.5
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.41 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 15.31 dB
PL13 18.31 dB
PL2W 37.58904266 W
PL12W 0.55470389 W
PL13W 0.27801058 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751241 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
81.16
65.98
42.44
32.71
32.42
31.79
31.74
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Current Data Parameters
NAME AG-II-84-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130913
Time 13.27
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 76.07
DW 40.533 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 600.1937064 MHz
NUC1 1H
P1 9.79 usec
PLW1 9.30000019 W
F2 - Processing parameters
SI 65536
SF 600.1900147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Only peaks for indicated product are labeled
57
1.00
2.02
1.72
2.08
1.04
4.33
5.31
2.12
ppm

Only peaks for indicated product are labeled

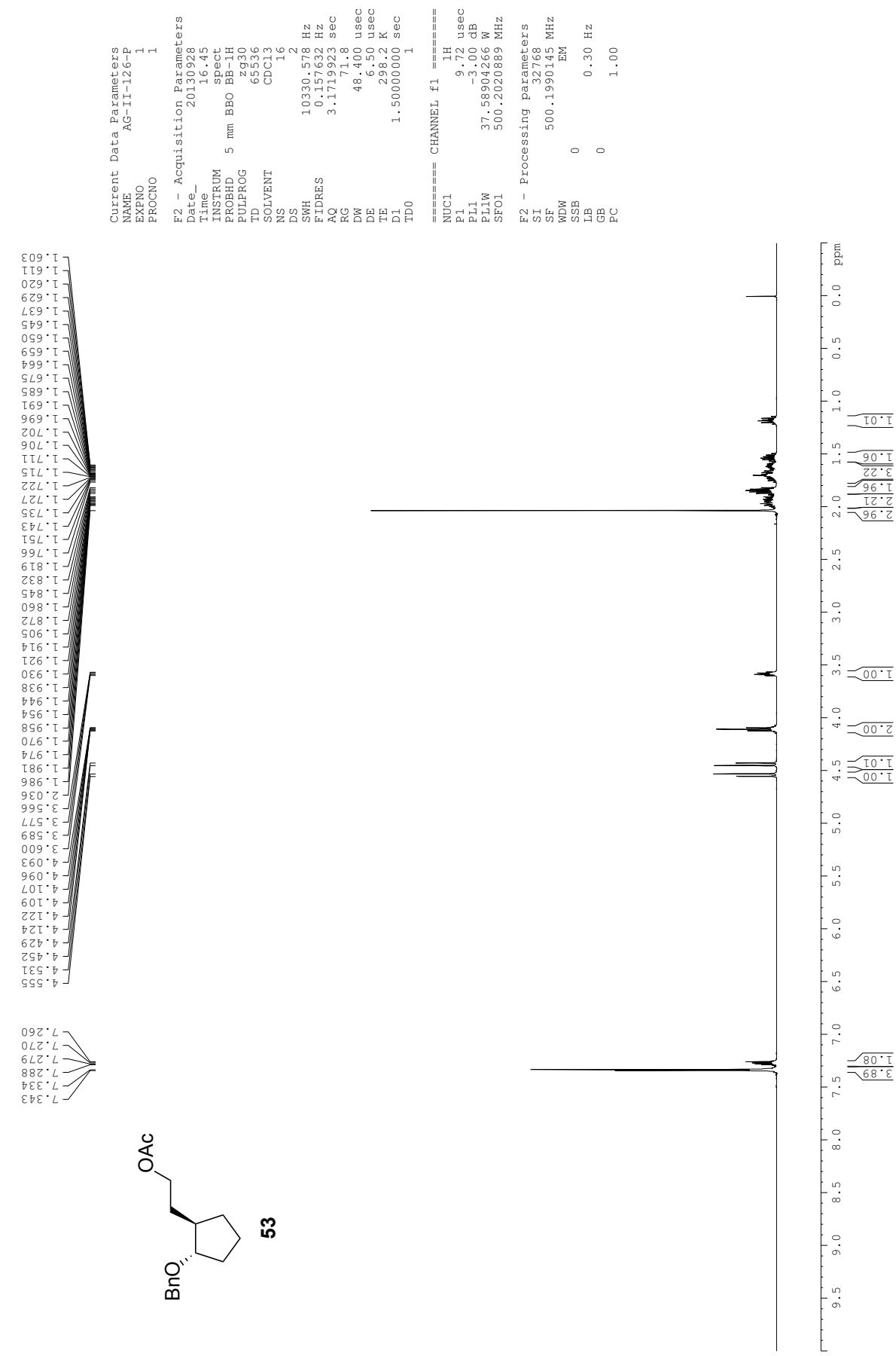
57




```
Current Data Parameters
NAME      AG-II-84-C_C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130913
Time               13.33
INSTRUM             spect
PROBHD   5 mm PAQXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  841
DS                    4
SWH           36057.691 Hz
FIDRES            0.550197 Hz
AQ                0.9088159 sec
RG                  184.65
DW                 13.867 usec
DE                  6.50 usec
TE                 298.1 K
D1              2.50000000 sec
d11             0.03000000 sec
DELTA           2.40000010 sec
TD0                    1
NUC1                 13C
P1                 15.00 usec
PLW1          106.00000000 W
SFO1          150.9329866 MHz
CPDPRG2
NUC2                  1H
PLW2           9.30000019 W
PLW12          0.18190999 W
PLW13          0.08913500 W
SFO2          600.1924008 MHz

F2 - Processing parameters
SI                 32768
SF          150.9178761 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```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Time_ 16.45
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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.72 usec
PL1 -3.00 dB
PL1W 37.58904266 W
SFO1 500.2020889 MHz
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OAc
BnO
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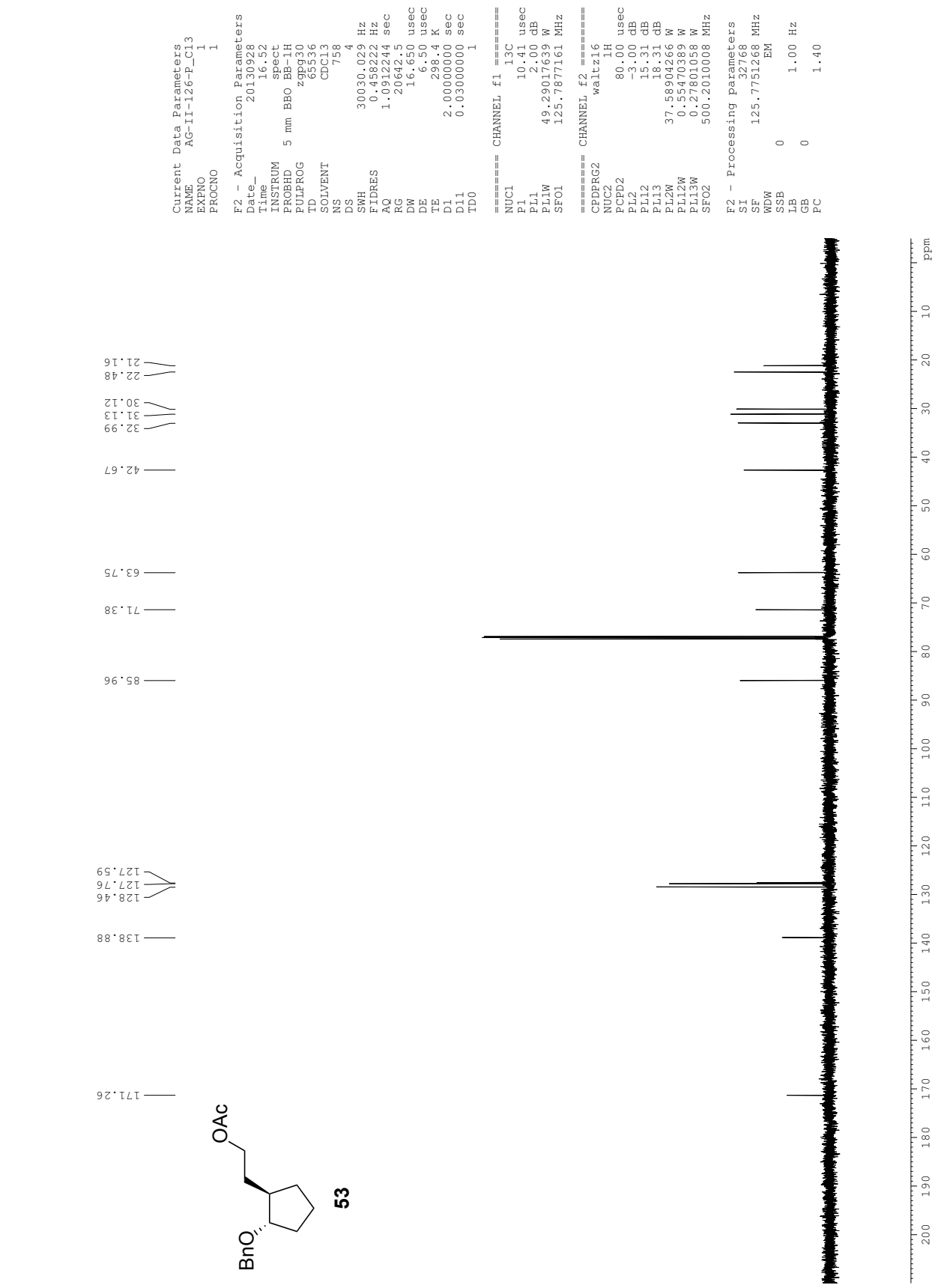
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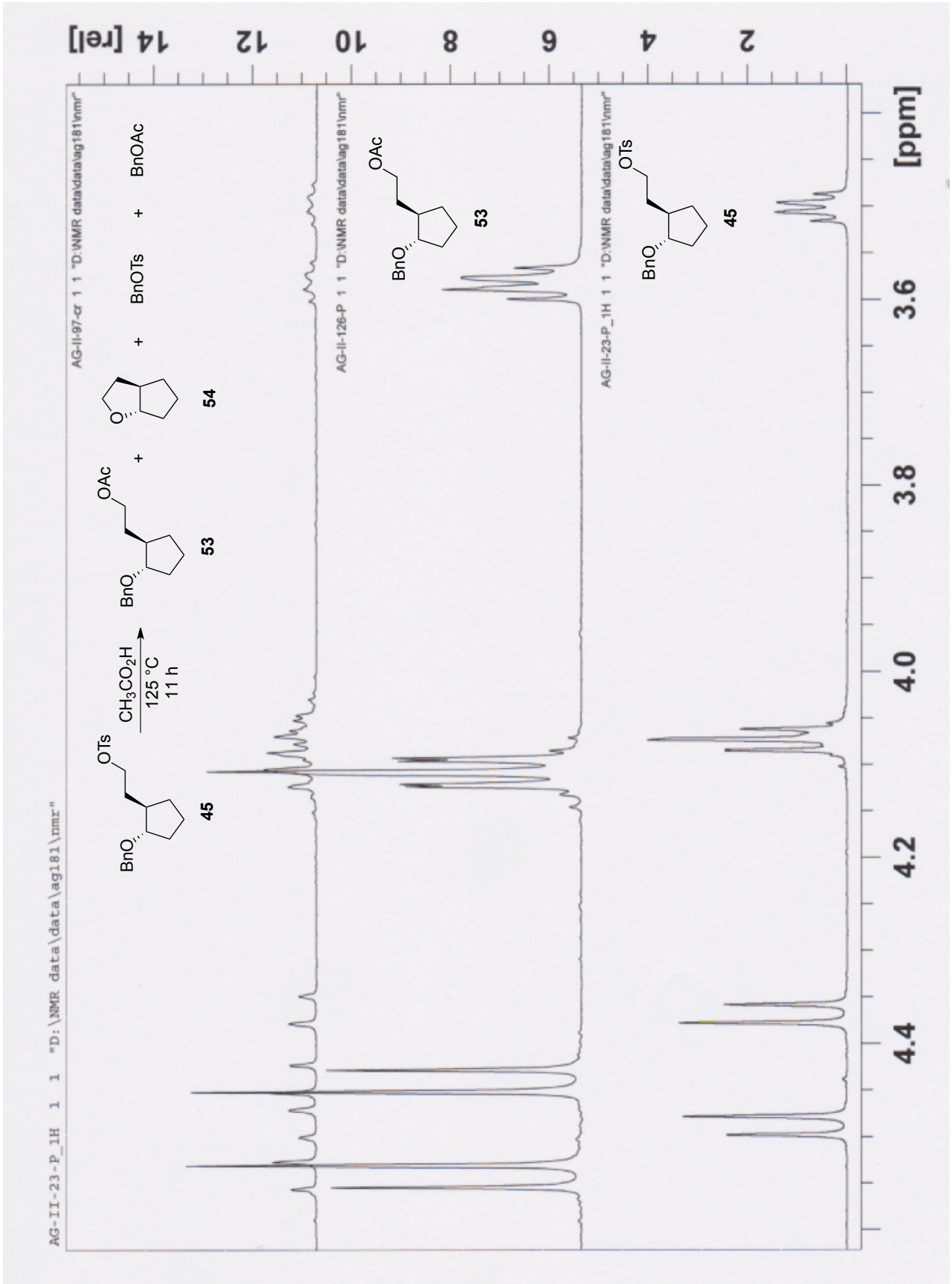
TD 65536
SOLVENT CDCl3
NS 758
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 20642.5
DW 16.650 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.41 usec
PL1 2.00 dB
PL1W 49.29017639 W
SFO1 125.7877161 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 15.31 dB
PL13 18.31 dB
PL2W 37.58904266 W
PL12W 0.55470389 W
PL13W 0.27801058 W
SFO2 500.2010008 MHz
F2 - Processing parameters
SI 32768
SF 125.7751268 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
21.16
22.48
30.12
31.13
32.99
42.67
63.75
71.38
85.96
127.59
127.76
128.46
138.88
171.26
OAc
BnO
53
ppm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OTs
BnO
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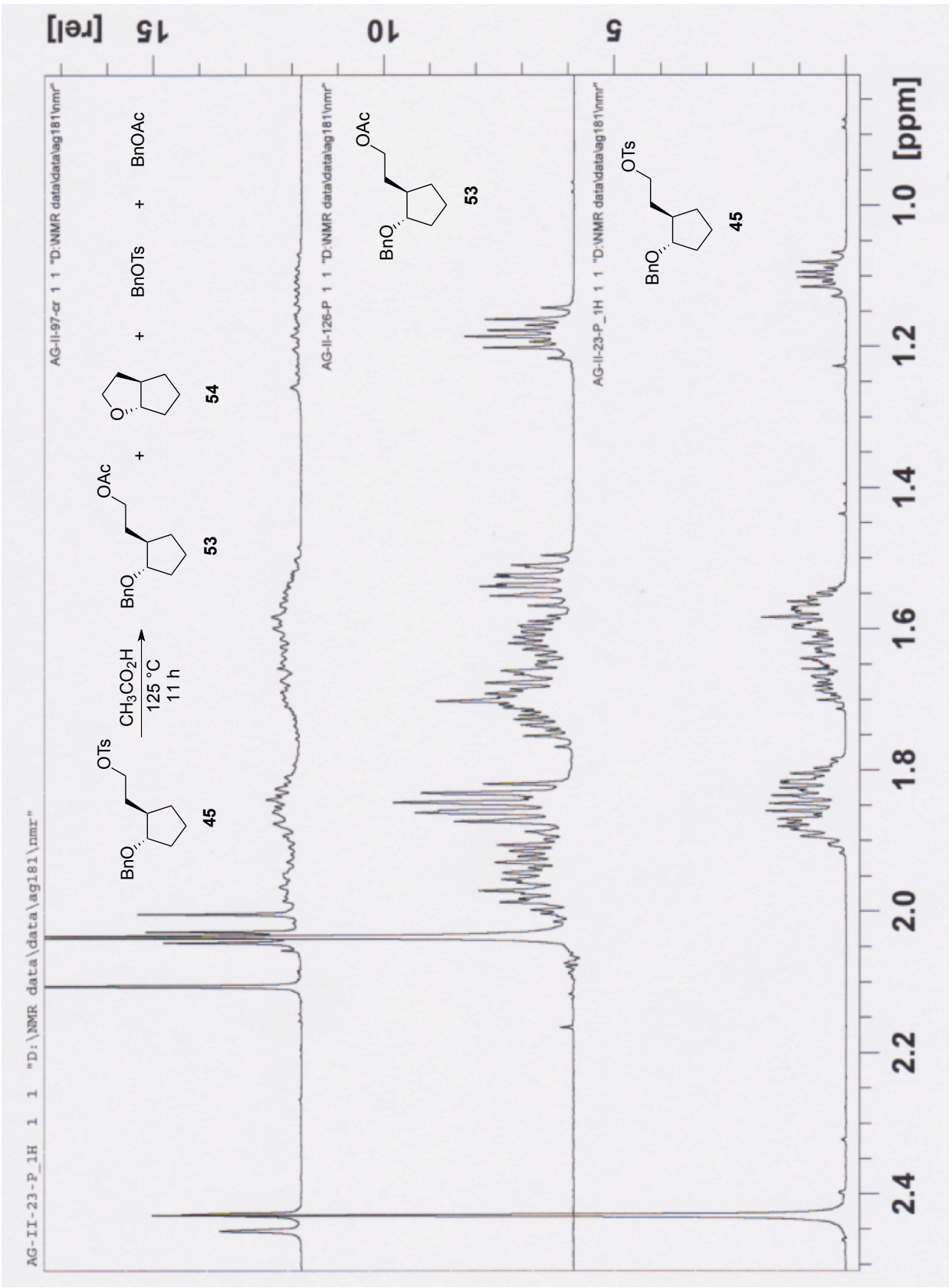
CH_3CO_2H
125 °C
11 h
OAc
BnO
53
54
BnOTs
BnOAc
[rel]
[ppm]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[rel]
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10
5
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0 [ppm]
OTs
BnO
45
CH3CO2H
125 °C
11 h
OAc
BnO
53
+
54
+ BnOTs + BnOAc
OAc
BnO
53
OTs
BnO
45