

## **Electronic Supporting Informations**

### **Self-assembly of novel benzimidazole *N*-glycosylamines to nanofibers and nanospheres**

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## **S.I. 1 Description of experimental techniques.**

### **S.I. 1.1: General procedure for gelation**

The gelation studies were carried as per reported procedures<sup>1</sup>. A definite amount of benzimidazole *N*-glycosylamine gelator **8-19** was added to 1 ml of a required solvent in a glass vial and warmed gently until clear solution was obtained. After allowing it to cool at ambient temperature, the vessel was turned upside down to verify the gel formation. The reversibility of the gelation was confirmed by repeated heating and cooling. The critical gelator concentration (CGC) of benzimidazole *N*-glycosylamine **8-19** was determined from the minimum amount of gelator required for the formation of gel formation at room temperature.

### **S.I. 1.2: Scanning electron microscopy (SEM)**

Scanning electron microscopic studies were performed by using Hitachi Scanning Electron Microscope SU3500. The samples were prepared by drop casting of gel of benzimidazole *N*-glycosylamines **18** and **19** on aluminum studs at their respective CGC at ambient conditions. SEM images were obtained after drying the sample at ambient temperature.

### **S.I. 1.3: Transmission electron microscopy (TEM)**

Transmission electron microscopic studies were performed by using Hitachi Transmission electron microscope H-9500. The samples were prepared by drop casting of solution, dispersed with gel of benzimidazole *N*-glycosylamines **18** on to carbon coated copper grids (400 mesh) at the concentration of  $1 \times 10^{-5}$  M at ambient conditions. TEM images were obtained after drying the sample and without staining in vacuum.

### **S.I. 1.4: Dropping ball method**

Gel to solution transition temperature ( $T_{\text{gel}}$ ) was determined by a 'dropping-ball method'. A small tin ball of approximate weight 100 mg was placed on top of the gel in a capped vial of diameter 1.0 cm, which was slowly warmed in a silicon oil bath. The temperature in which the tin ball reaches the bottom of the vial is assigned as  $T_{\text{gel}}$ . The experiment is duplicated one to obtain the reproducibility within  $\pm 2^\circ\text{C}$ . The same condition was repeated on increasing the concentration.

### **S.I. 1.5: Differential scanning calorimetry (DSC)**

DSC analysis of gels were performed on a NETZSCH phoenix DSC 204. The measurements were carried out under nitrogen atmosphere using 50 L sealed aluminium sample pans. Sample was heated from approx. 25 to 250 °C with a heating range of 10 °C min<sup>-1</sup> and sample weights of 10–21 mg were used in measurements.

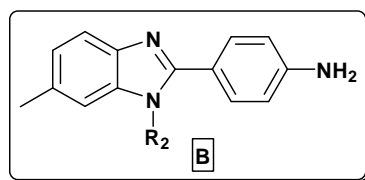
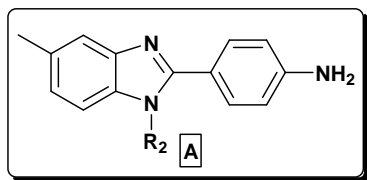
### S.I. 1.6: Response of gel towards $\text{Cu}^{2+}$

About 10  $\mu\text{l}$  of  $\text{Cu}_2(\text{OAc})\cdot\text{H}_2\text{O}$  solution (1%, ethanol) was added to gel of glycosylamines **8-19** in different solvent. The concentration of copper acetate monohydrate was increased gradually until gel turns to solution. Thus amount of copper acetate monohydrate required for the conversion of gel to solution was recorded.

#### Reference

- 1) G. S. Lim, B. M. Jung, S. J. Lee, H. H. Song, C. Kim, and J. Y. Chang *Chem. Mater.*, 2007, **19**, 460.

### S.I. 2.1 Chemical structure of regioisomers of compound **4-7**.







Current Data Parameters  
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PROCNO 1

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SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
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RG 161.3  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

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SFO1 300.1318534 MHz

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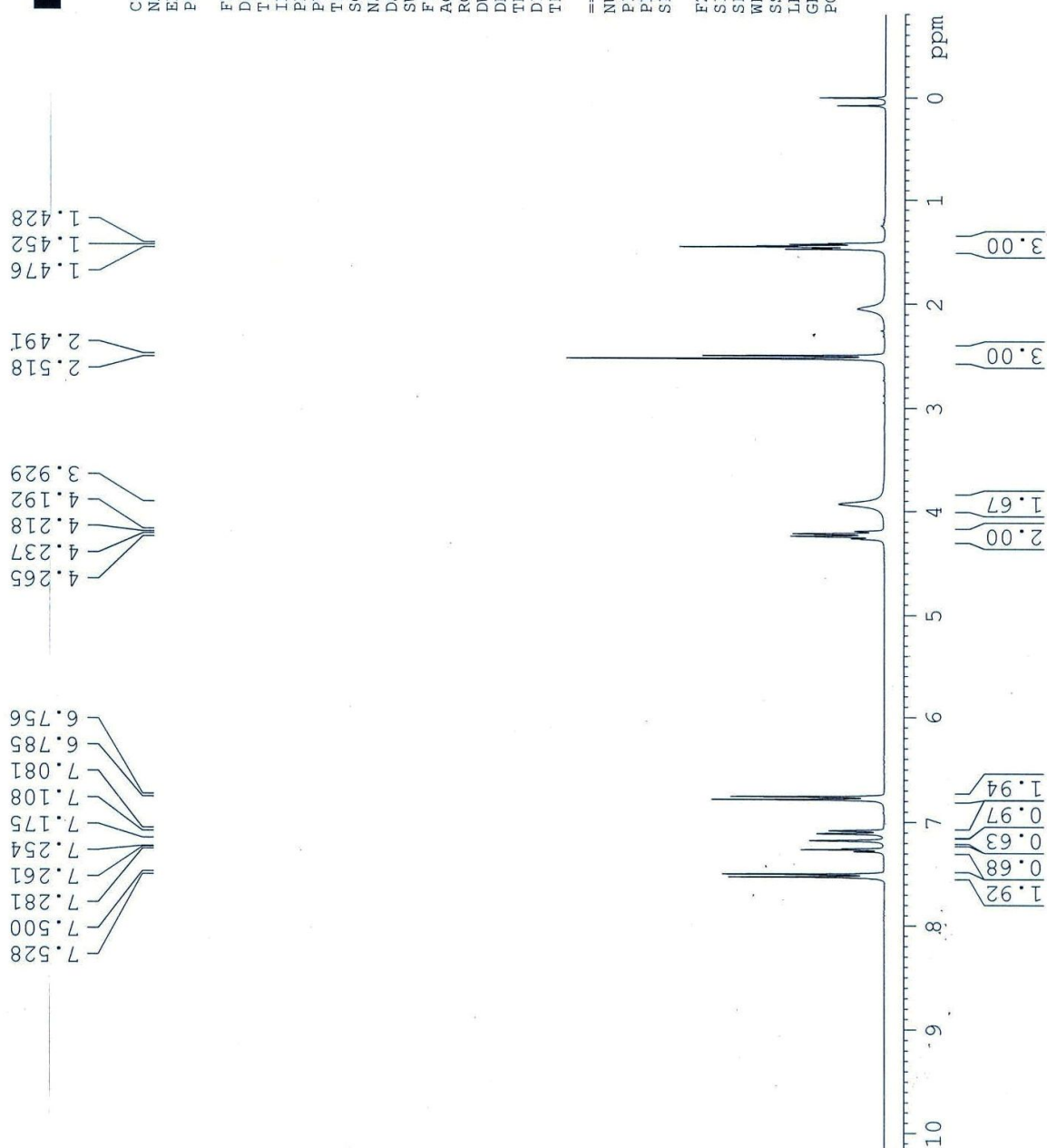


Figure S.I. 1:  $^1\text{H}$  NMR Spectrum of Compound **4**.



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PROCNO 1

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PULPROG zg30  
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SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 64  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

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PL1 0.00 dB  
SFO1 300.1318534 MHz

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SF 300.1300277 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

0.771  
0.803  
0.807  
1.146  
1.153  
1.176  
1.198  
1.722  
2.409  
2.439

4.048  
4.060  
4.081  
4.099

6.677  
6.705  
7.001  
7.029  
7.076  
7.165  
7.391  
7.419

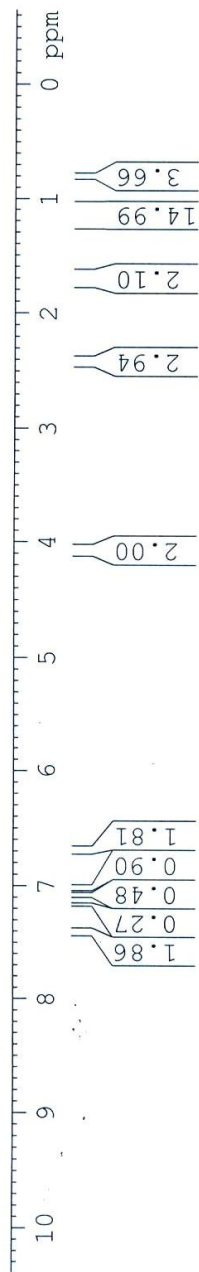
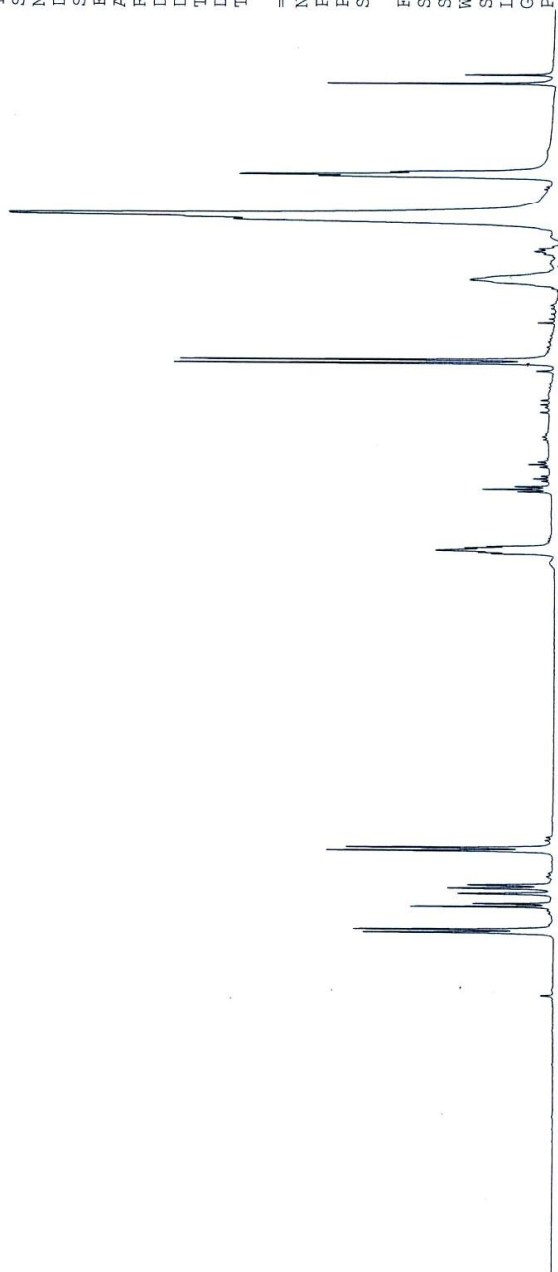


Figure S.I. 2:  $^1\text{H}$  NMR Spectrum of Compound 5.



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 PROCNO 1

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 Time 20.28  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 143.7  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 SFO1 300.1318534 MHz

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 GB 0  
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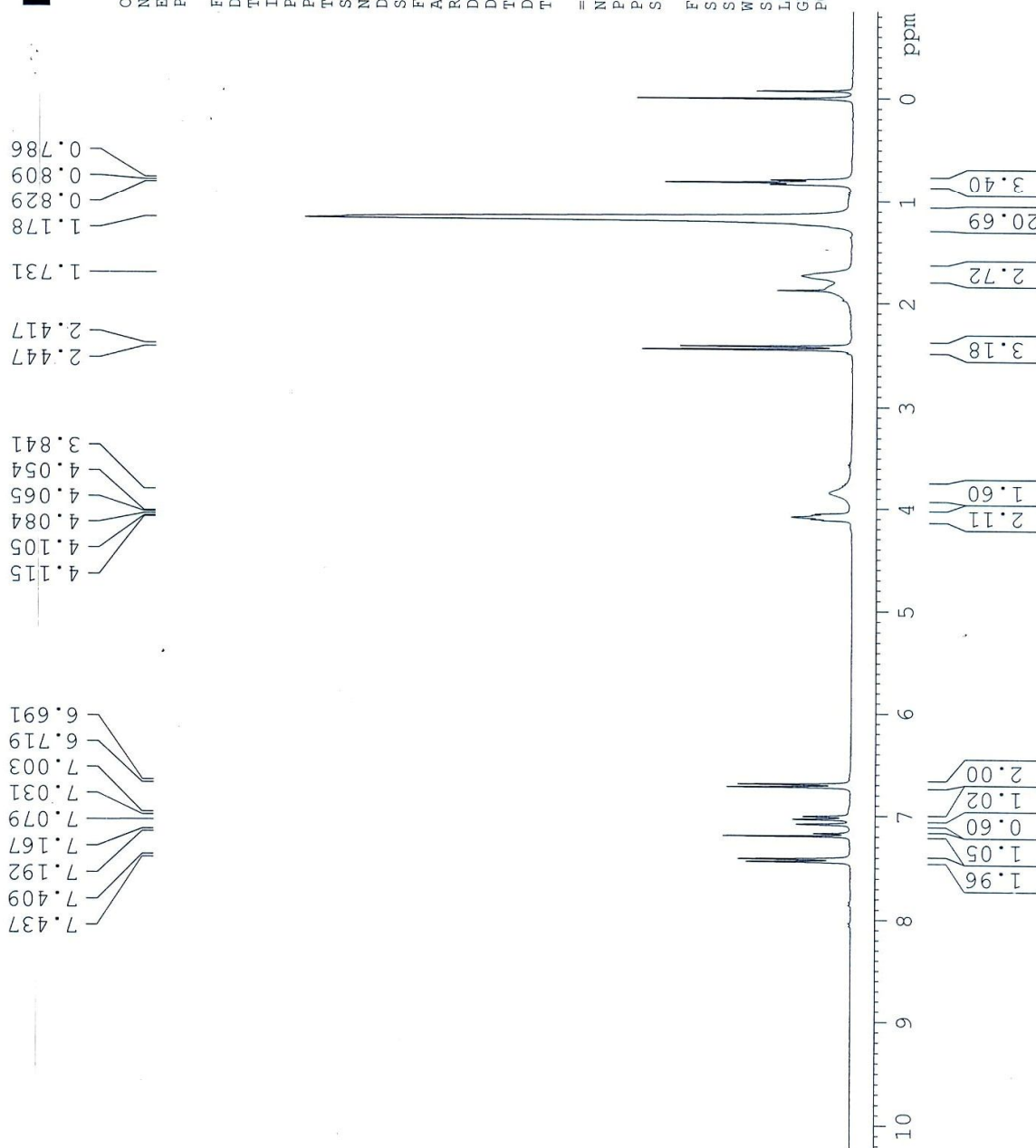


Figure S.I. 3:  $^1\text{H}$  NMR Spectrum of Compound 6.

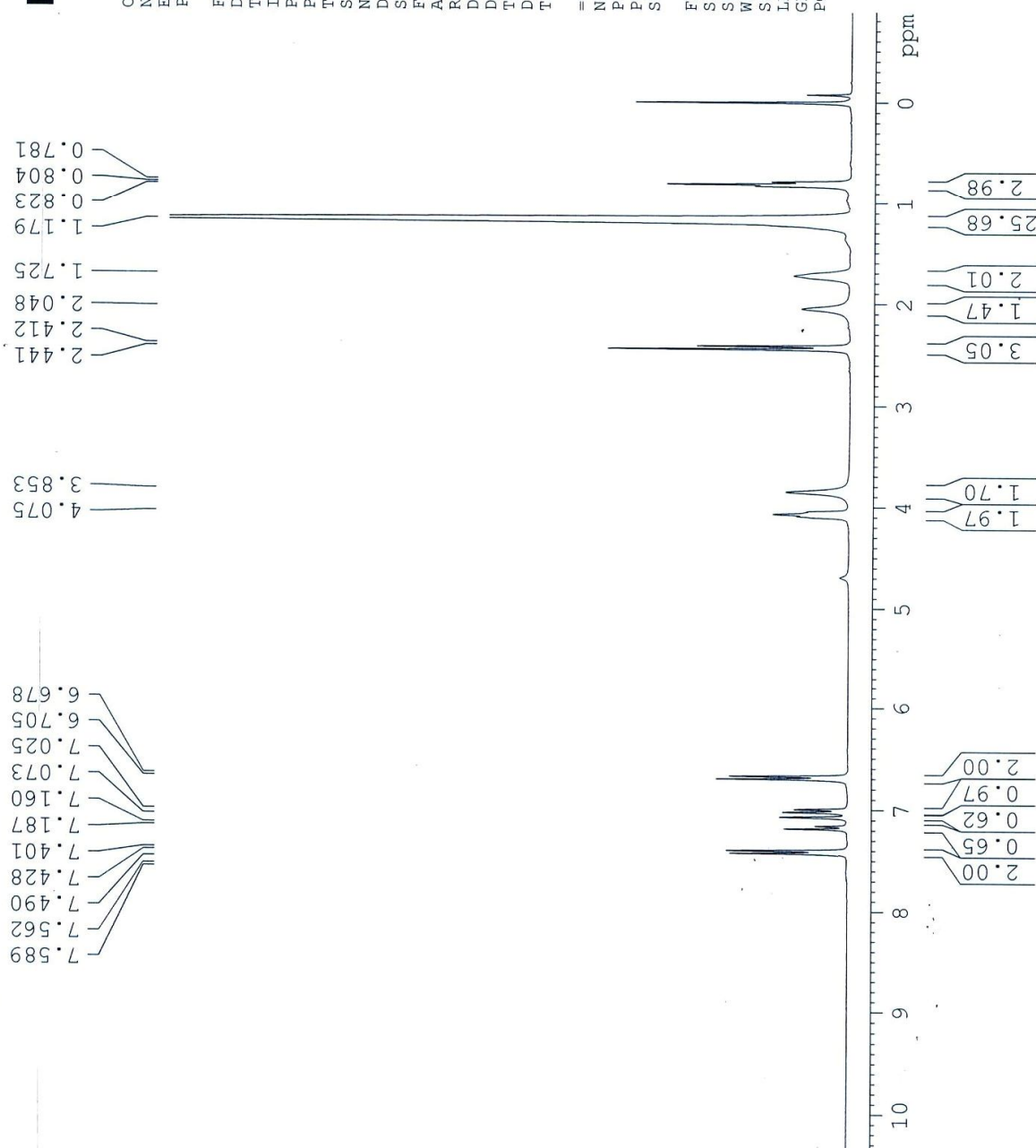


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 PULPROG zg30  
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 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 57  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 PL1 0.00 dB  
 SF01 300.1318534 MHz

F2 - Processing parameters  
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 SF 300.1300288 MHz  
 WDW EM  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00

Figure S.I. 4:  $^1\text{H}$  NMR Spectrum of Compound 7.



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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20121203  
Time\_ 19.49  
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PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 80.6  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.15 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
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SF 300.1314059 MHz  
WDW EM  
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LB 0.30 Hz  
GB 0  
PC 1.00

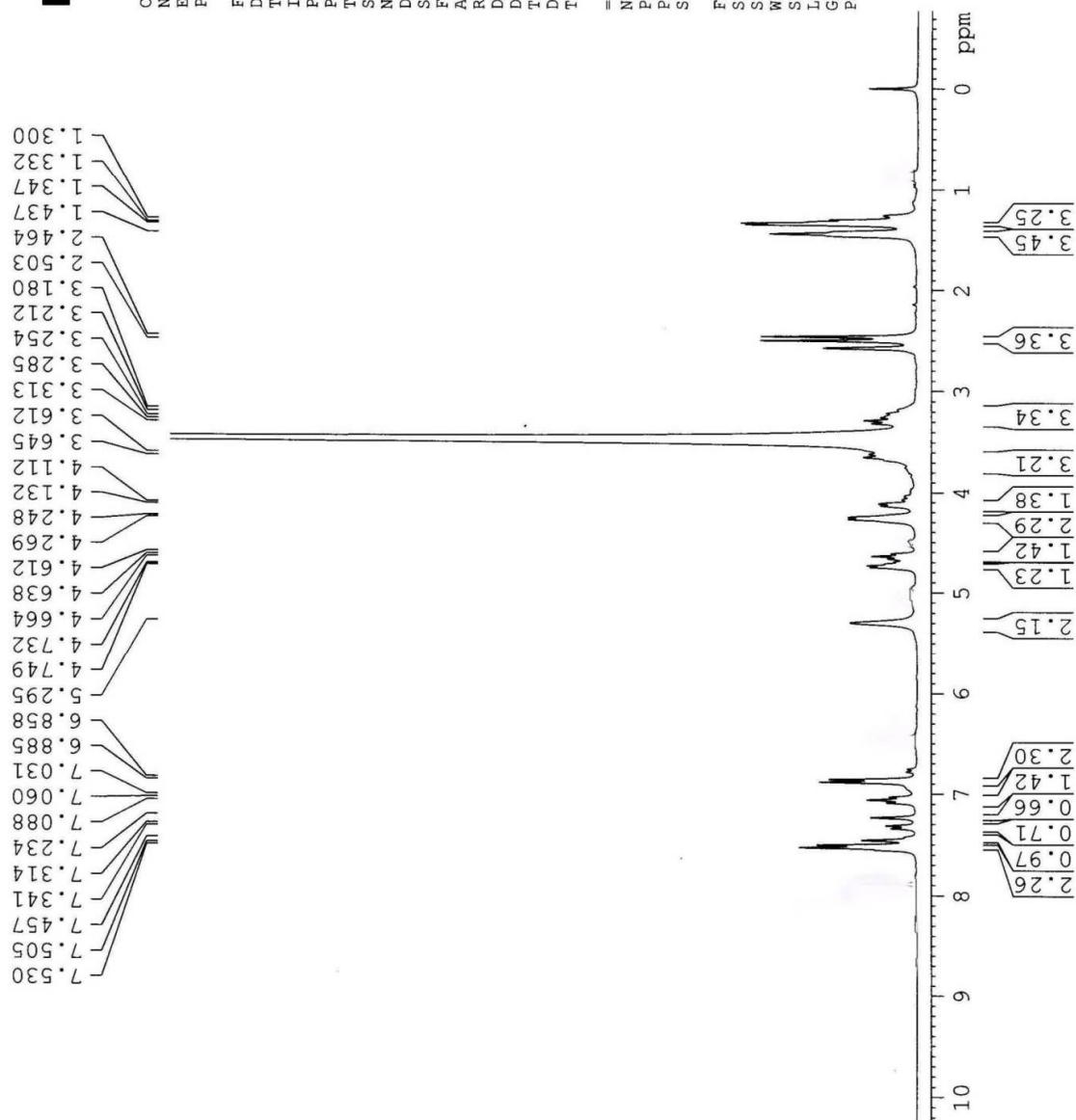


Figure S.I. 5:  $^1\text{H}$  NMR Spectrum of Compound **8**.



Current Data Parameters  
 NAME TMD-533  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20121204  
 Time 16.09  
 INSTRUM spect  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 354  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 812.7  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

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 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
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 PL2 0.00 dB  
 PL12 15.68 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

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 GB 0  
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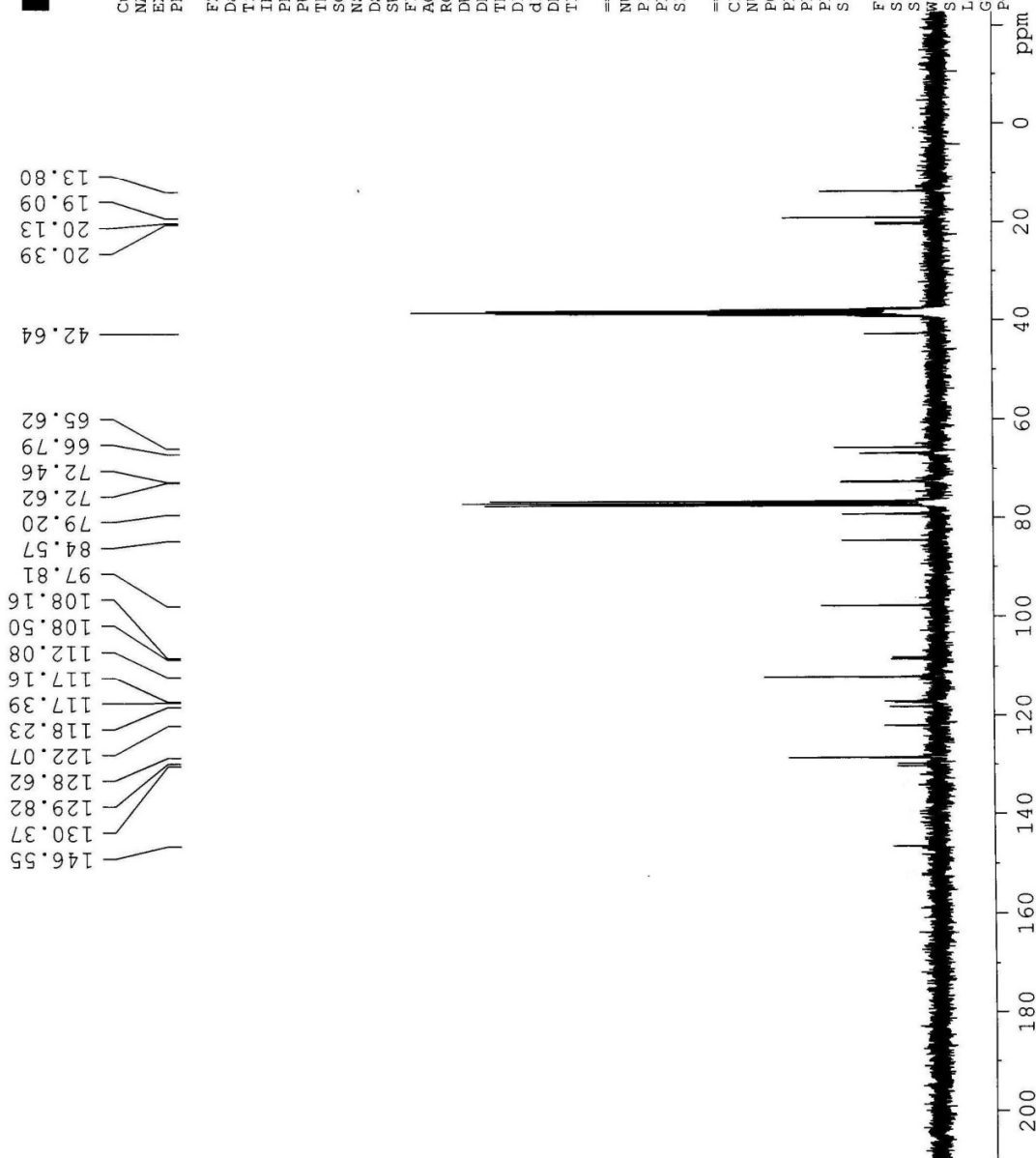


Figure S.I. 6:  $^{13}\text{C}$  NMR Spectrum of Compound 8.



Current Data Parameters  
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130308  
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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 143.7  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.15 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
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LB 0.30 Hz  
GB 0  
PC 1.00

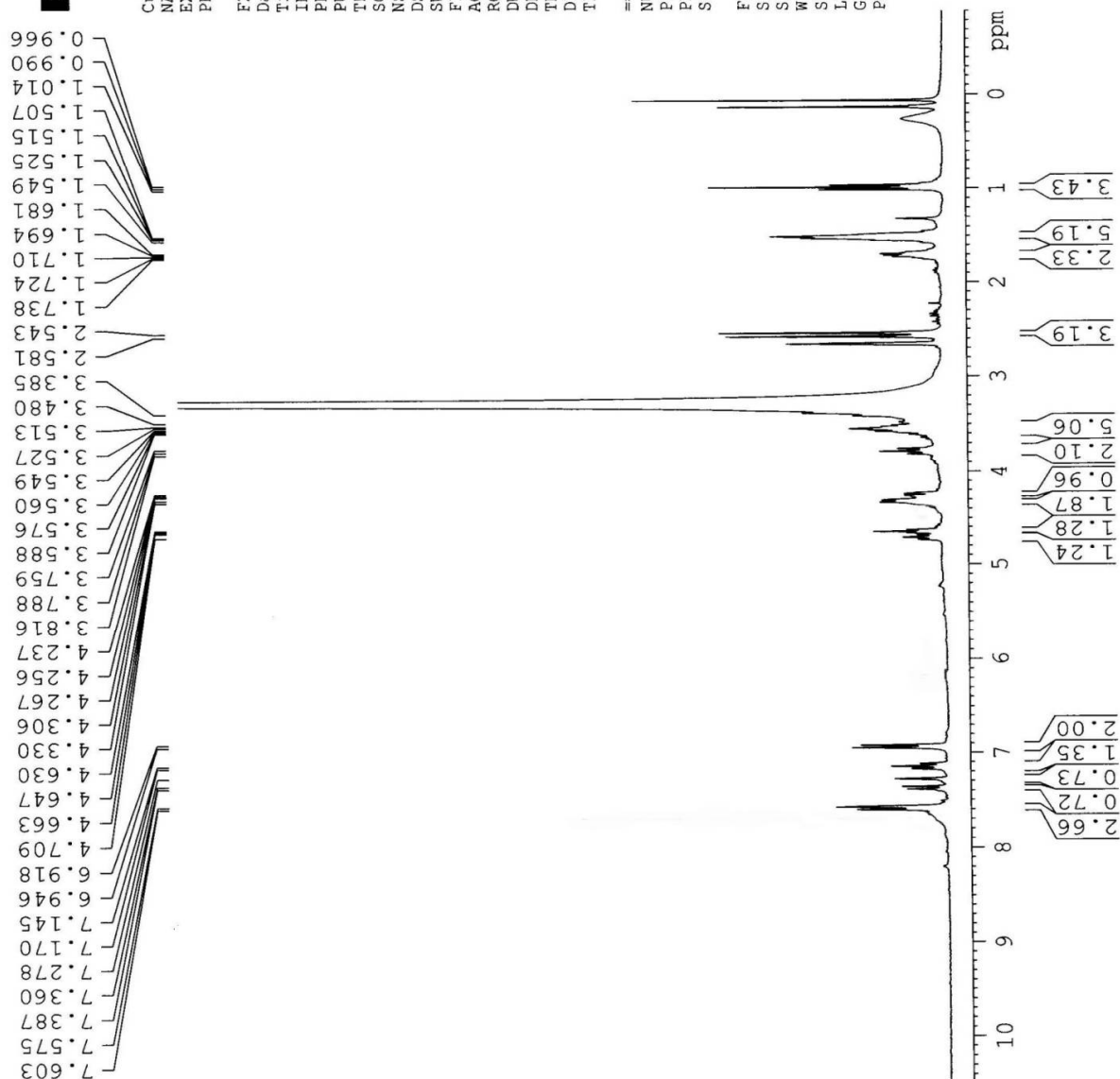


Figure S.I. 7:  $^1\text{H}$  NMR Spectrum of Compound **9**.

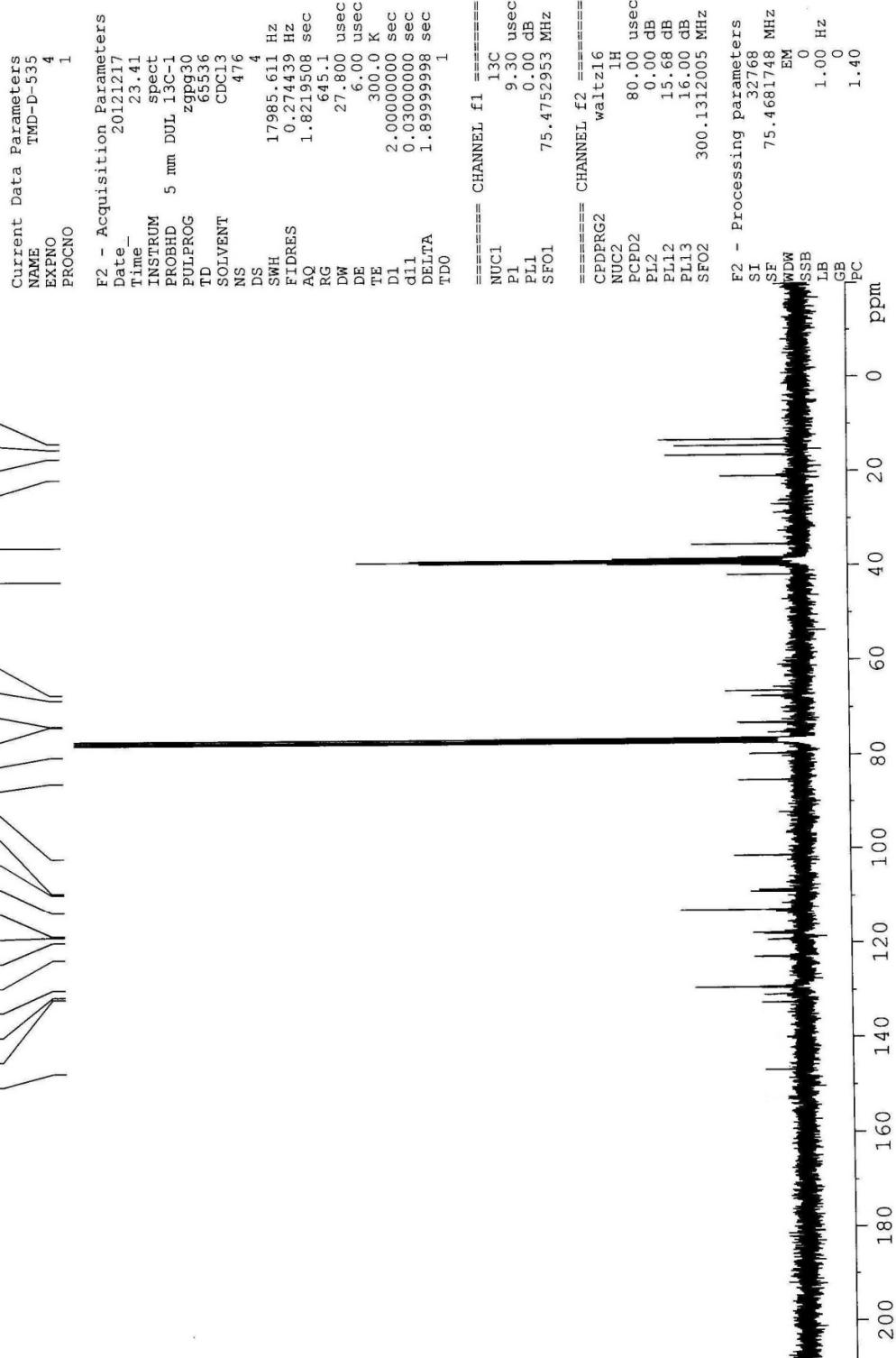


Figure S.I. 8:  $^{13}\text{C}$  NMR Spectrum of Compound **9**.



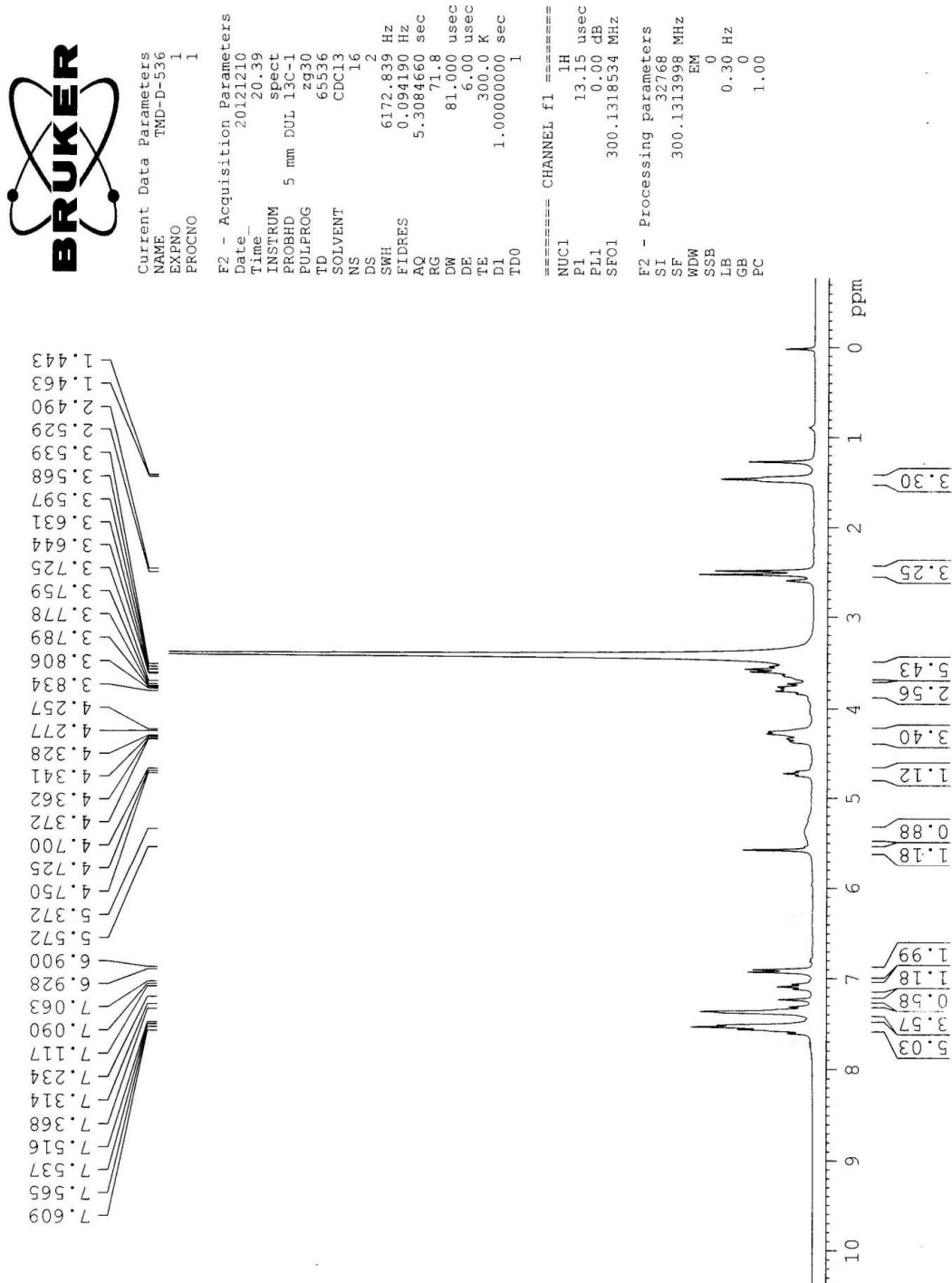


Figure S.I. 9:  $^1\text{H}$  NMR Spectrum of Compound **10**.

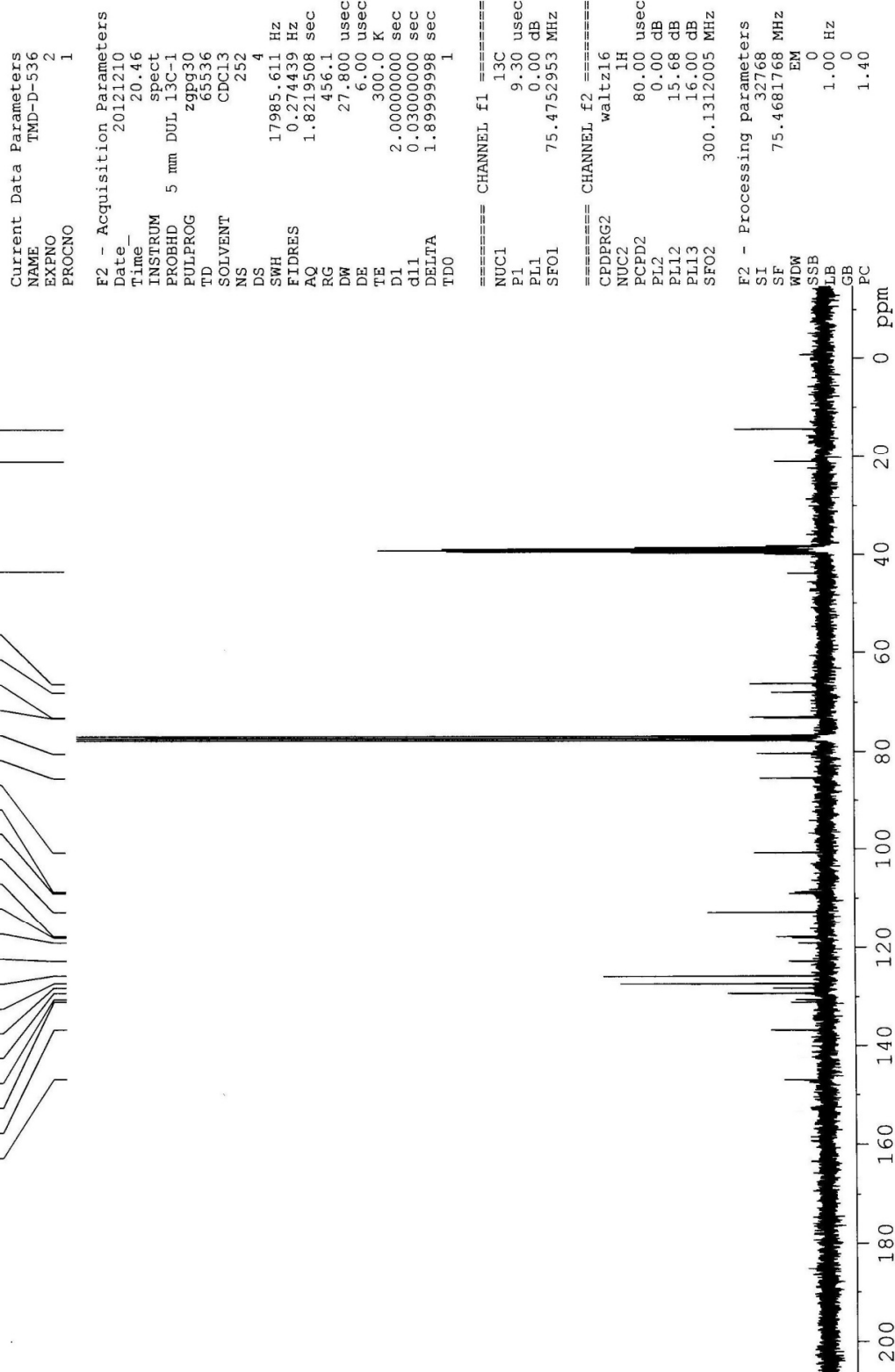


Figure S.I. 10:  $^{13}\text{C}$  NMR Spectrum of Compound 10.



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 PROCNO 1

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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 41  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
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 P1 13.15 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
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 GB 0  
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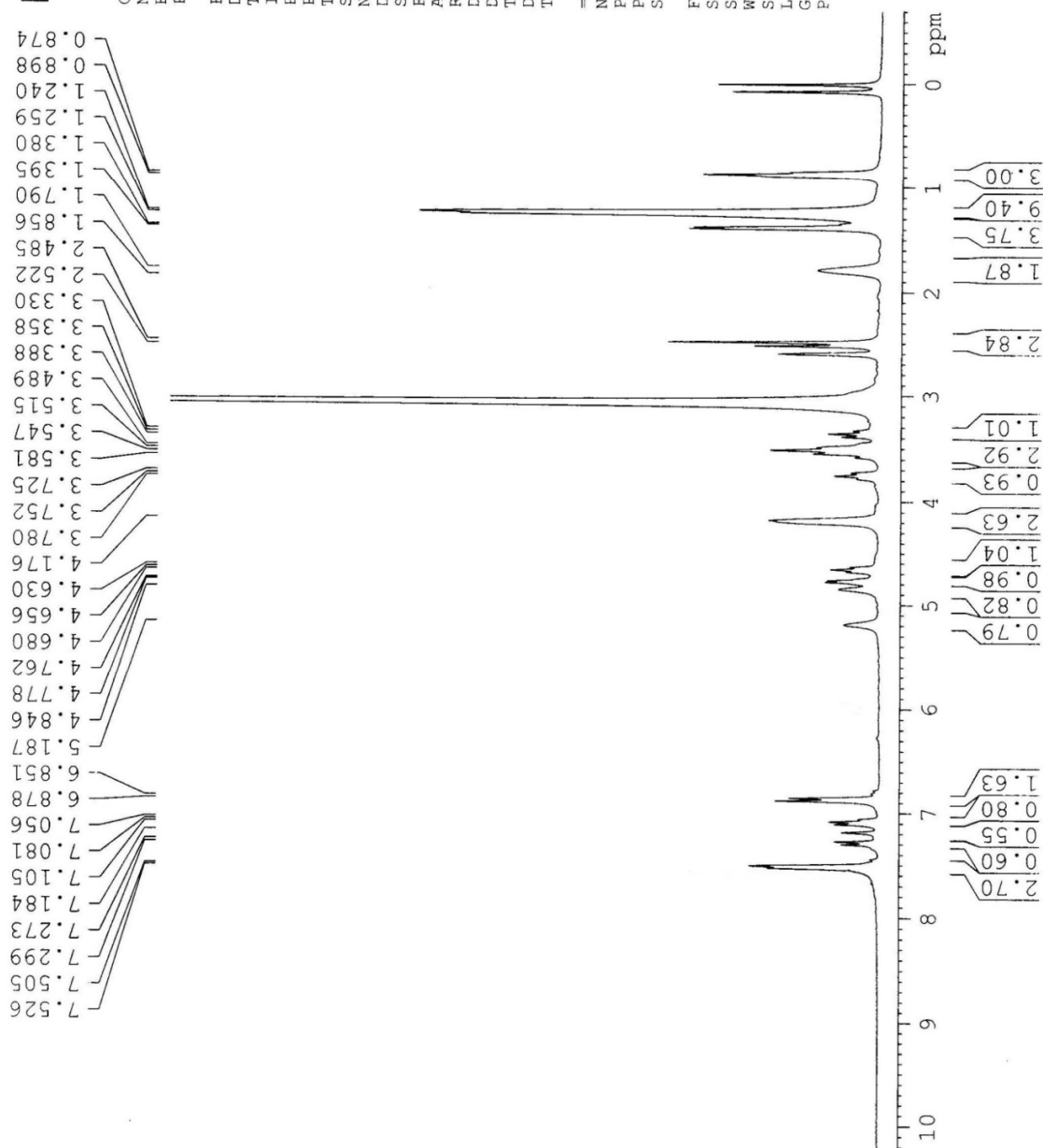
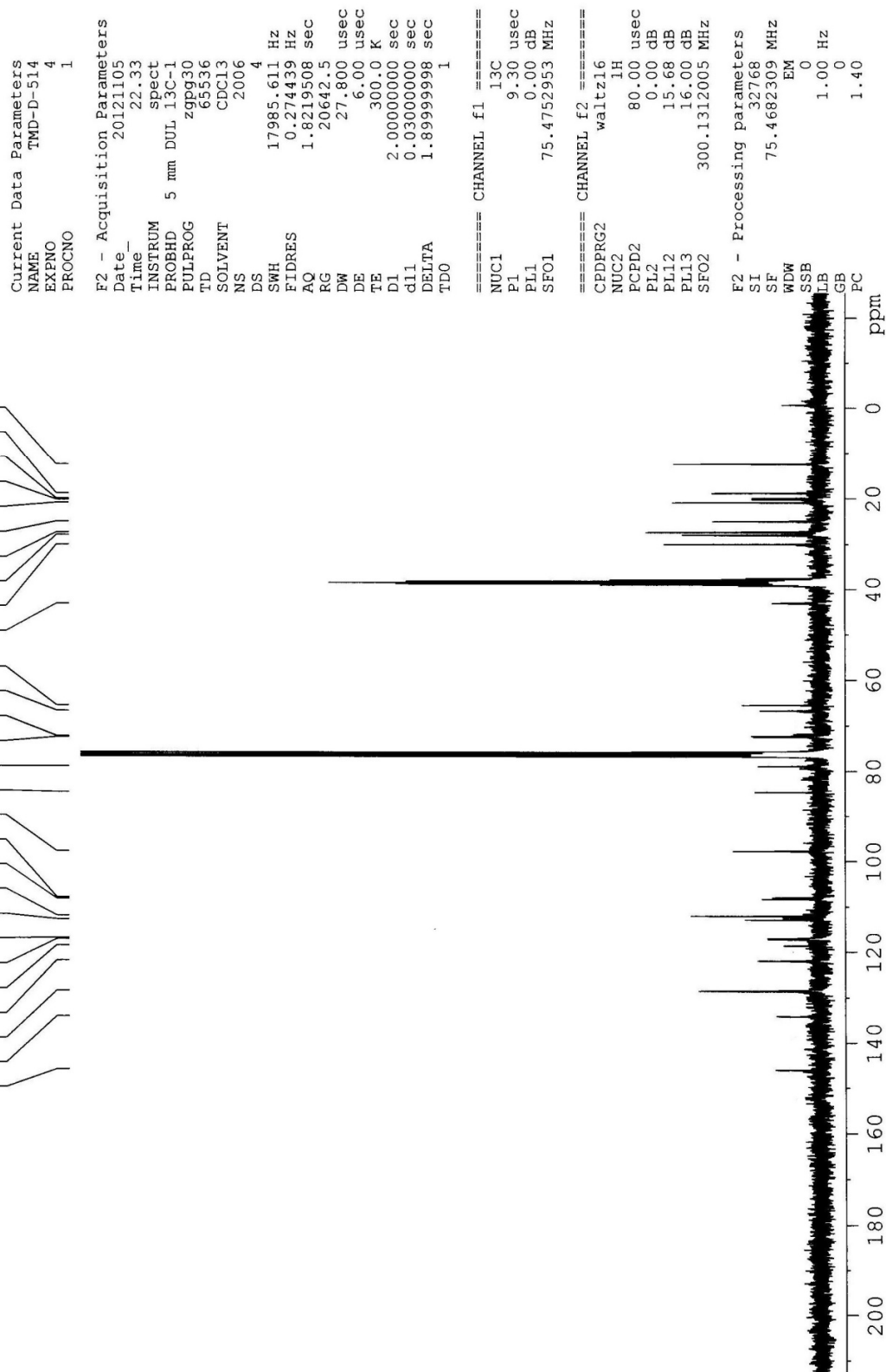


Figure S.I. 11:  $^1\text{H}$  NMR Spectrum of Compound 11.

Figure S.I. 12:  $^{13}\text{C}$  NMR Spectrum of Compound 11.



Current Data Parameters  
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 EXNO 2  
 PROCNO 1

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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 114  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 SFO1 300.1318534 MHz

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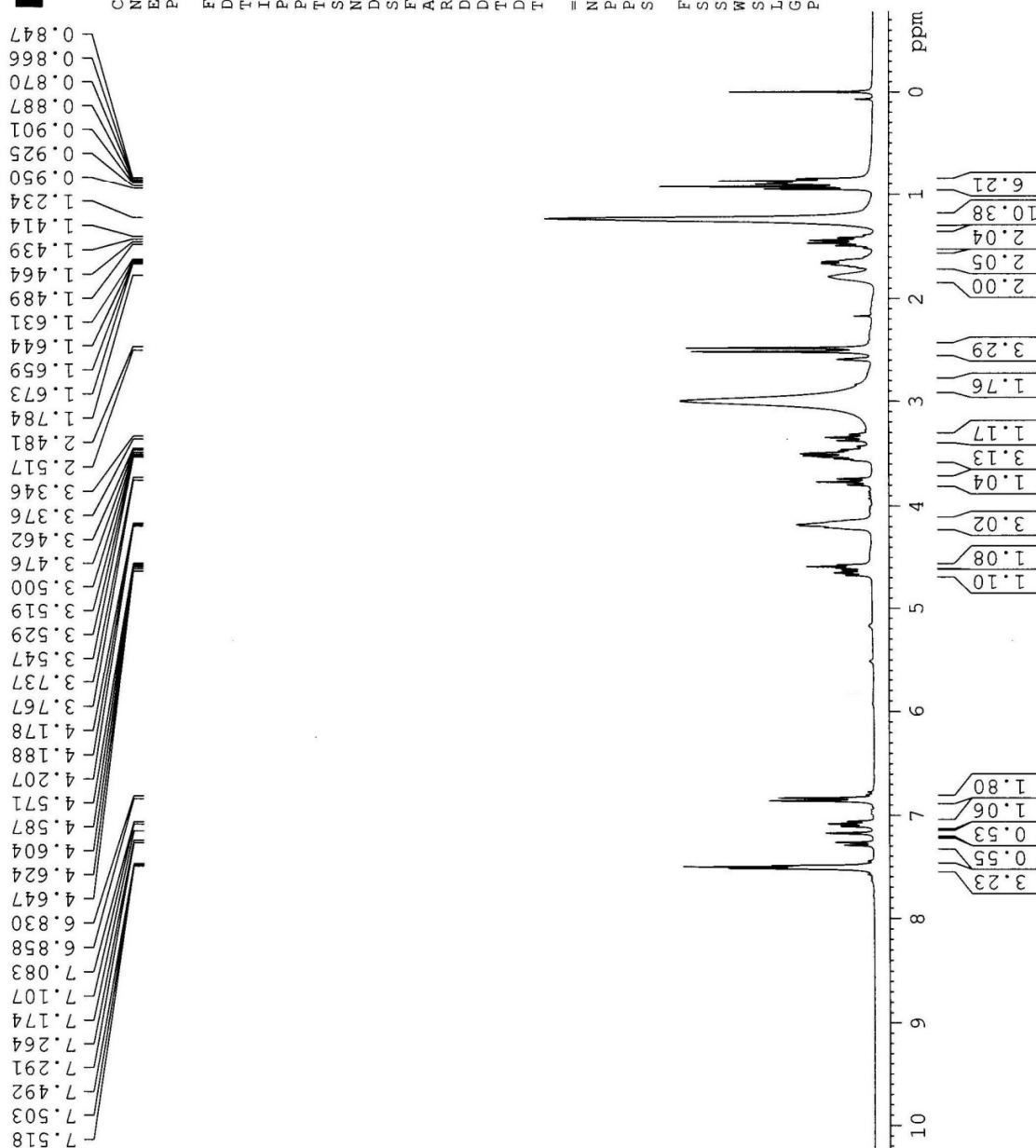


Figure S.I. 13:  $^1\text{H}$  NMR Spectrum of Compound 12.

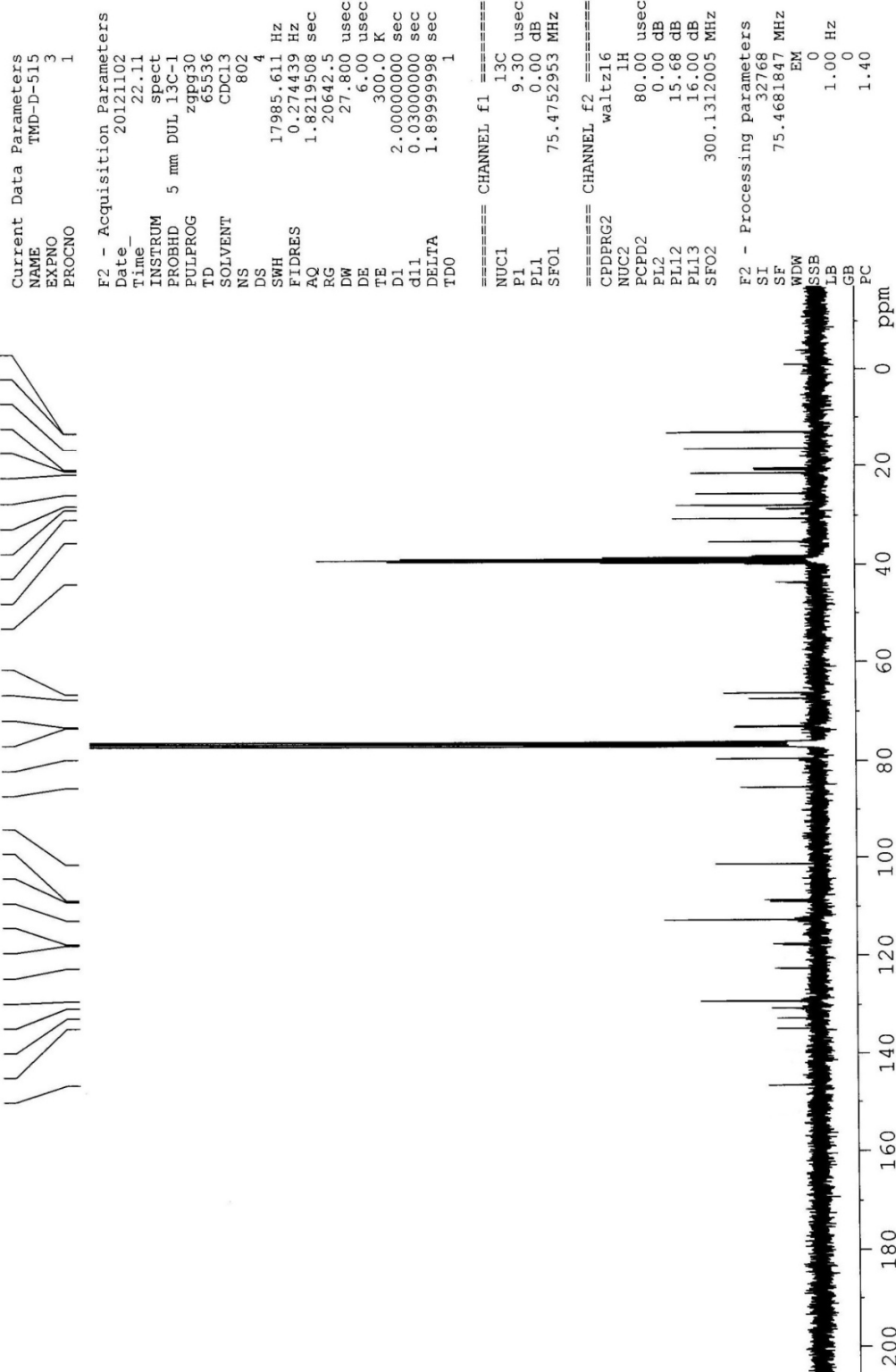


Figure S.I. 14:  $^{13}\text{C}$  NMR Spectrum of Compound 12.

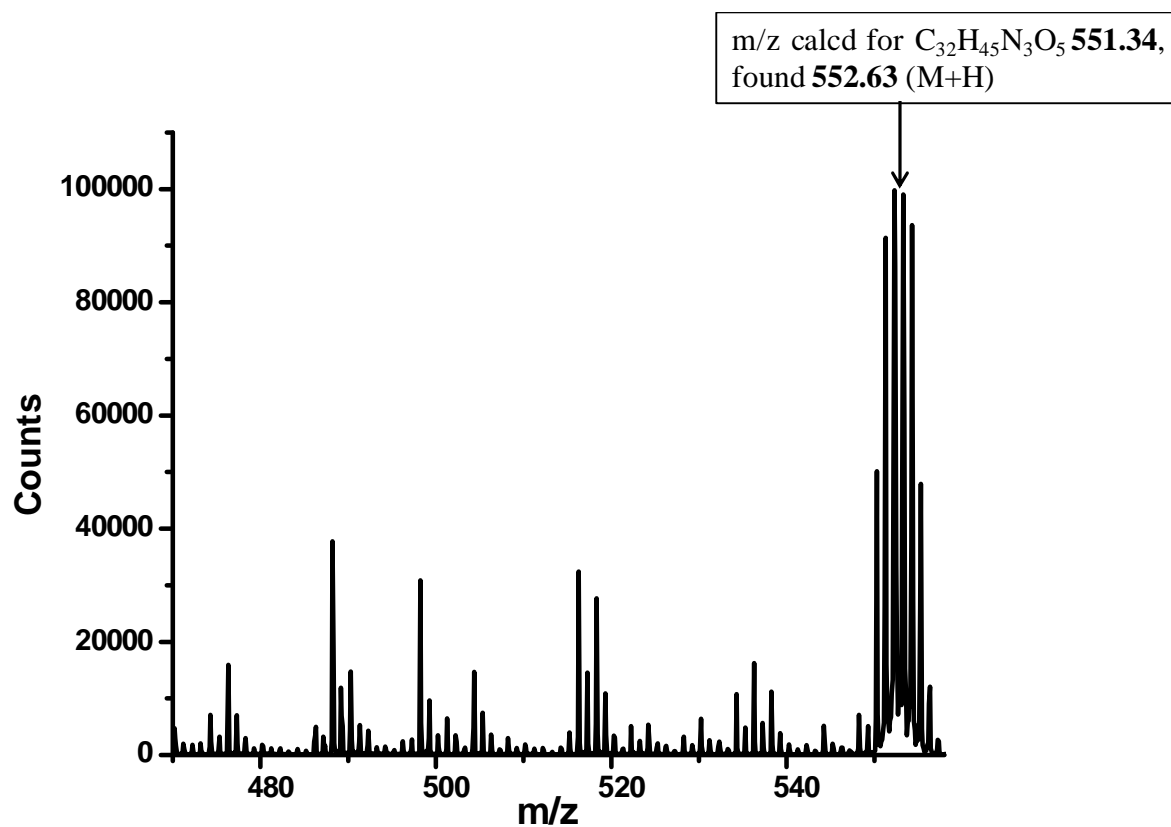


Figure S.I. 15: MALDI-TOF mass spectrum of Compound 12.

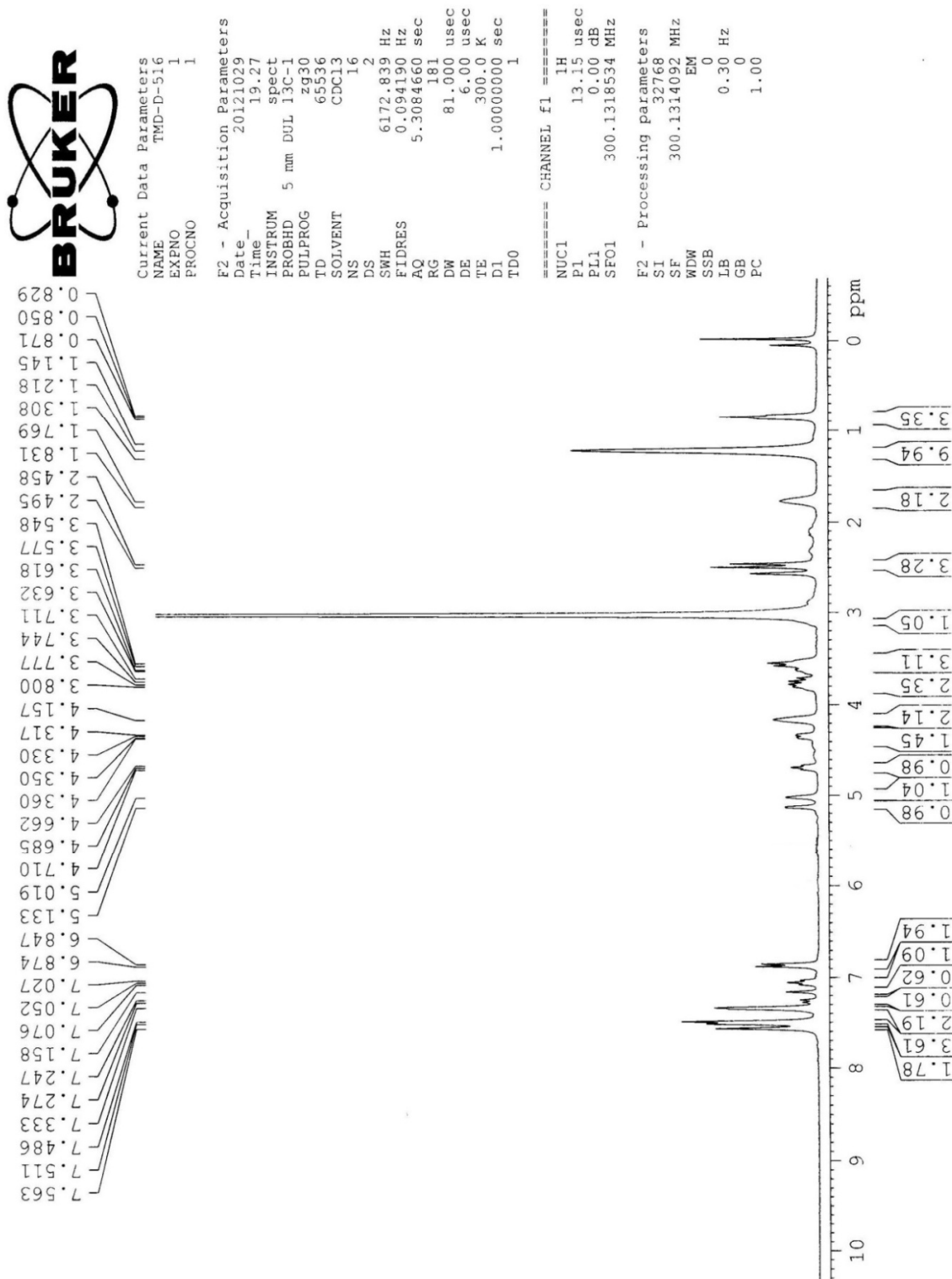


Figure S.I. 16:  $^1\text{H}$  NMR Spectrum of Compound **13**.



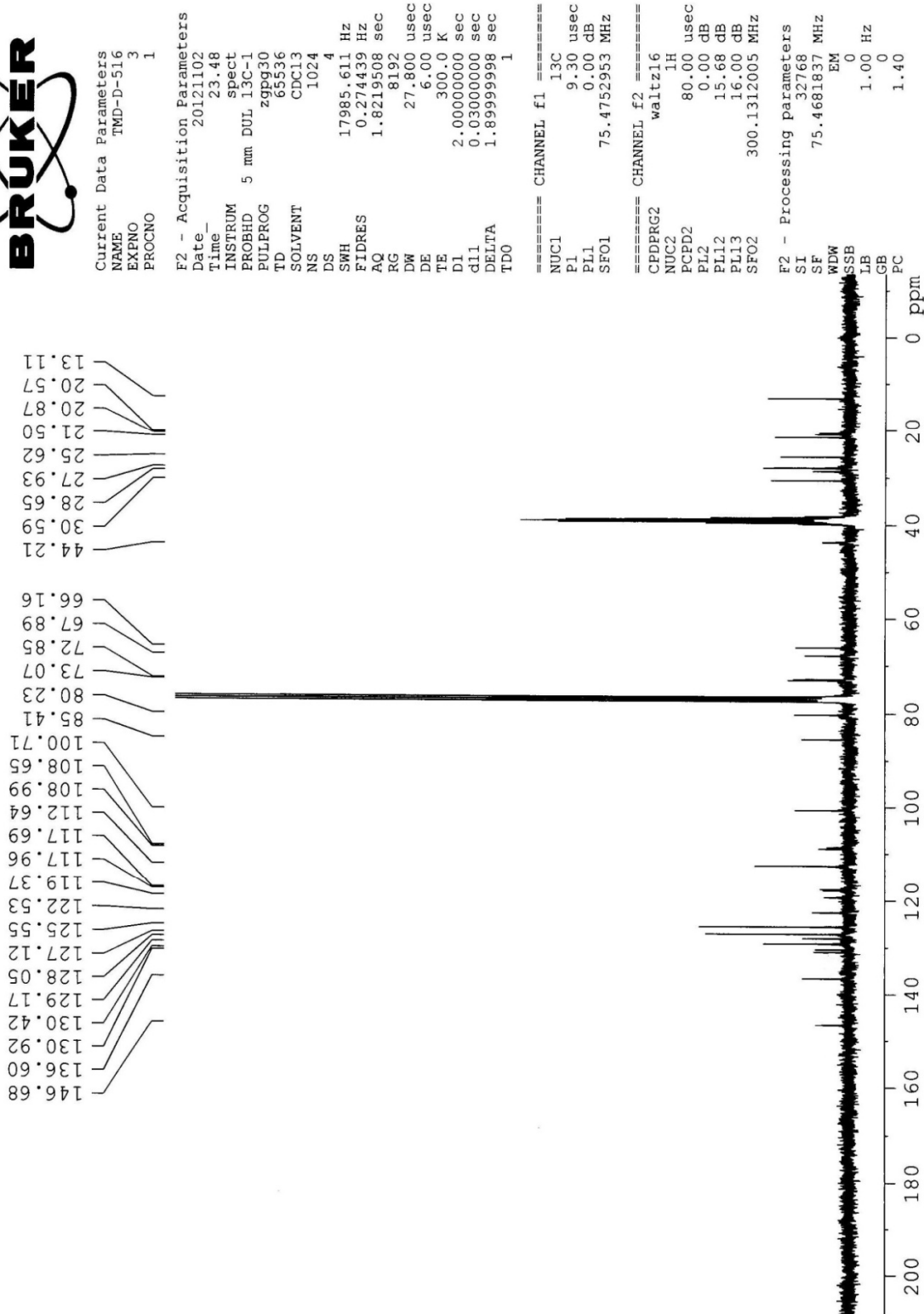


Figure S.I. 17:  $^{13}\text{C}$  NMR Spectrum of Compound 13.



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 PROCNO 1

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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 PL1 0.00 dB  
 SFO1 300.1318534 MHz

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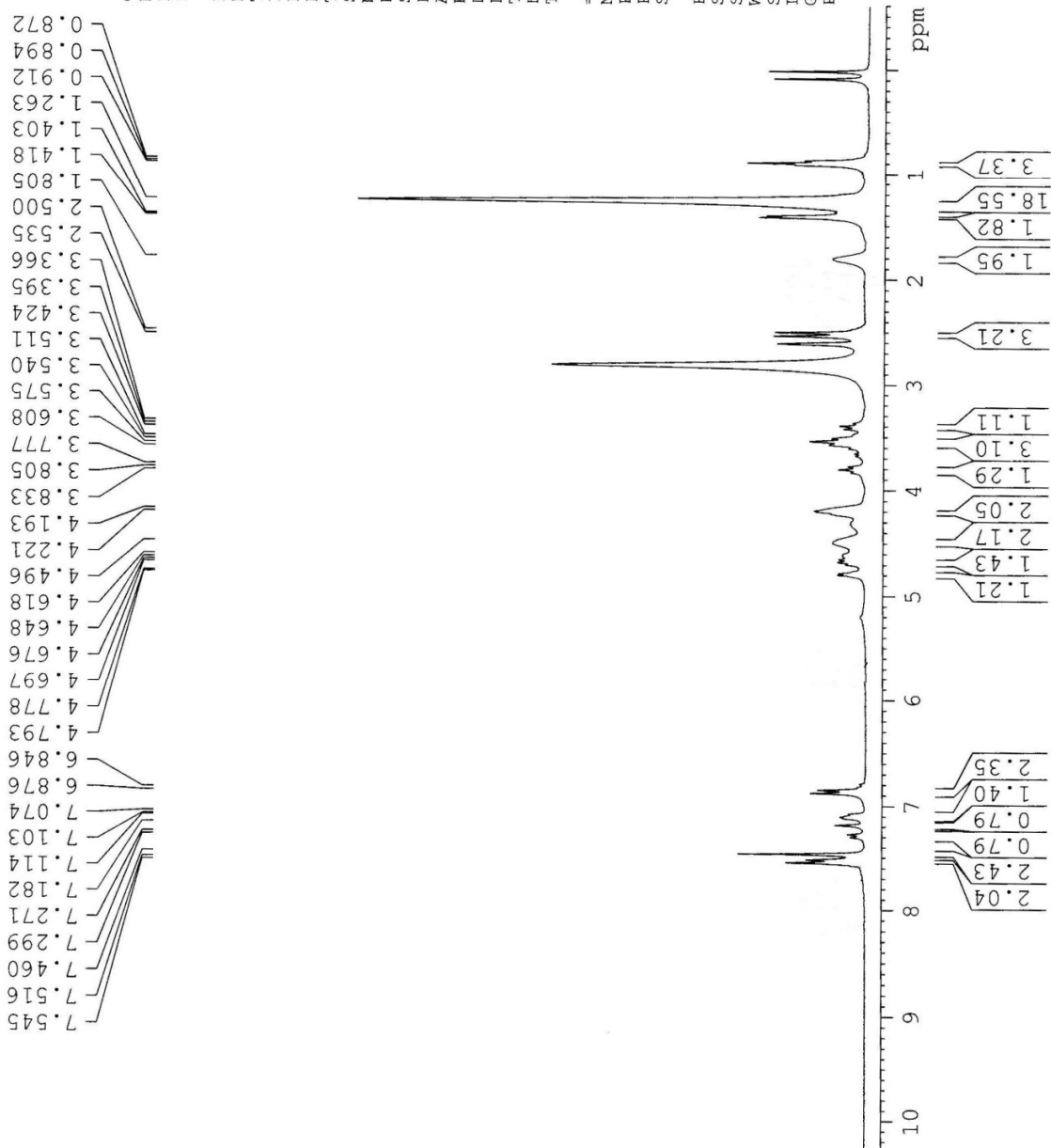


Figure S.I. 18:  $^1\text{H}$  NMR Spectrum of Compound **14**.

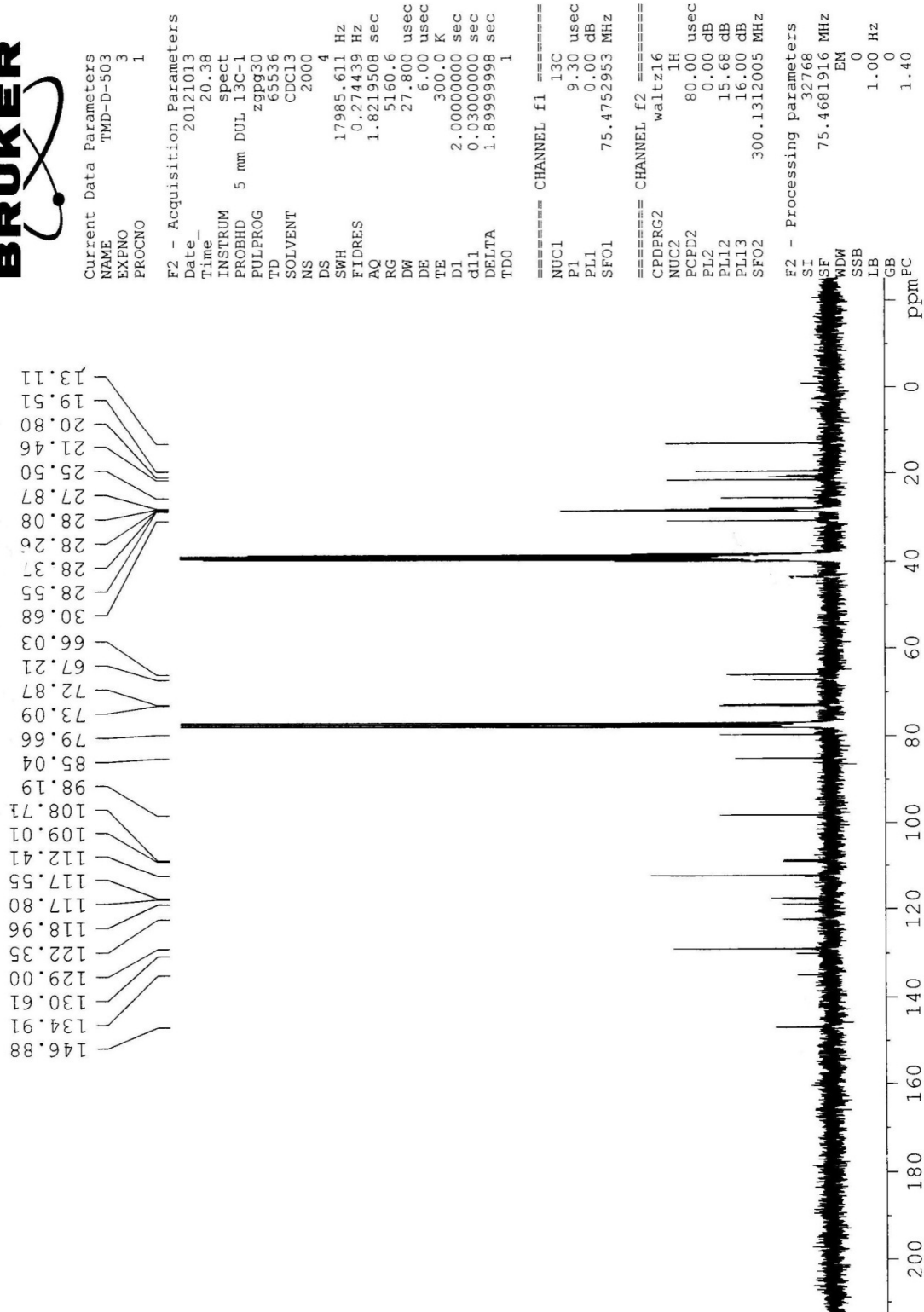


Figure S.I. 19:  $^{13}\text{C}$  NMR Spectrum of Compound 14.



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PROCNO 1

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PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
RW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
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PL1 0.00 dB  
SF01 300.1318534 MHz

F2 - Processing parameters  
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WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

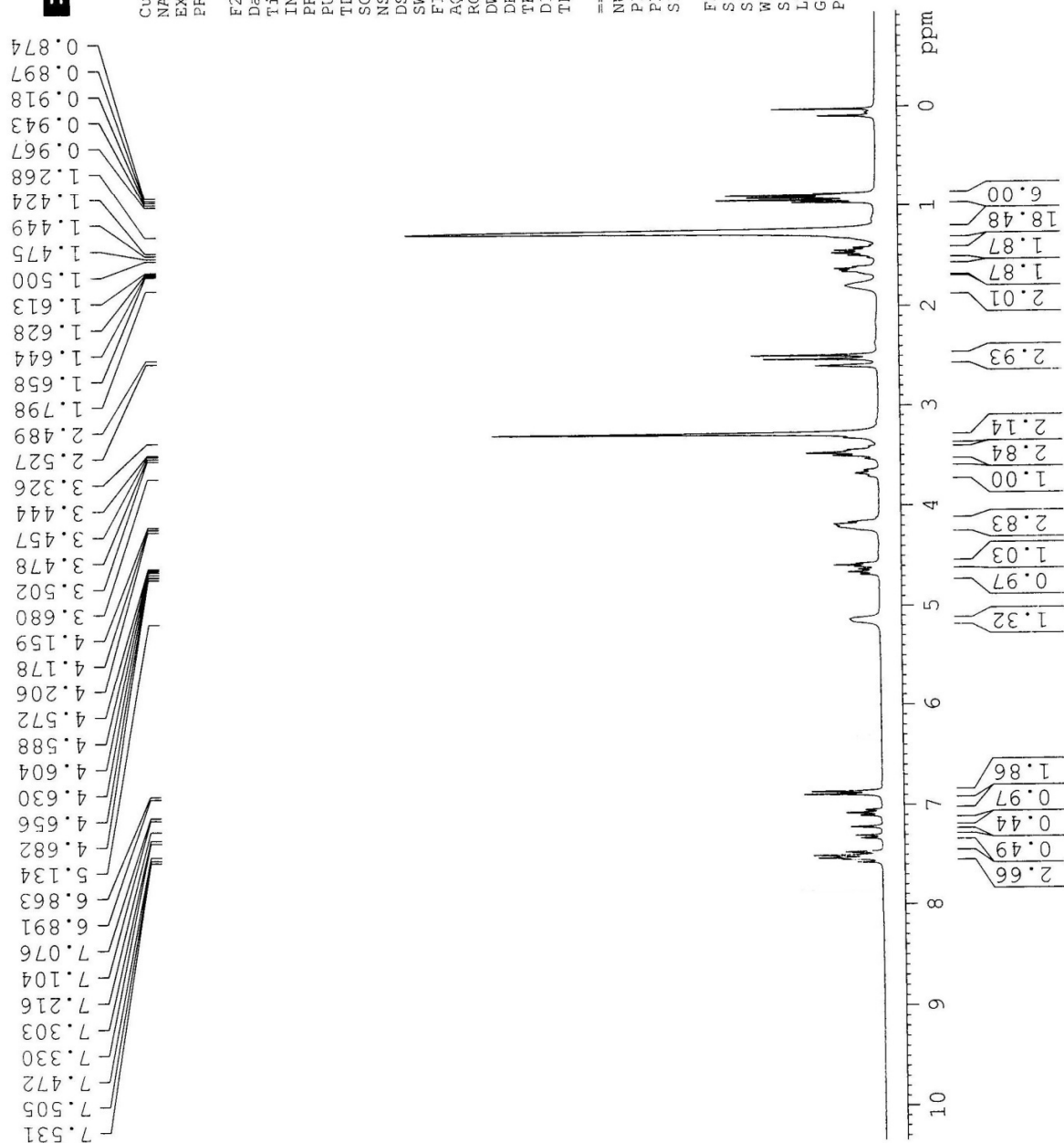


Figure S.I. 20:  $^1\text{H}$  NMR Spectrum of Compound **15**.

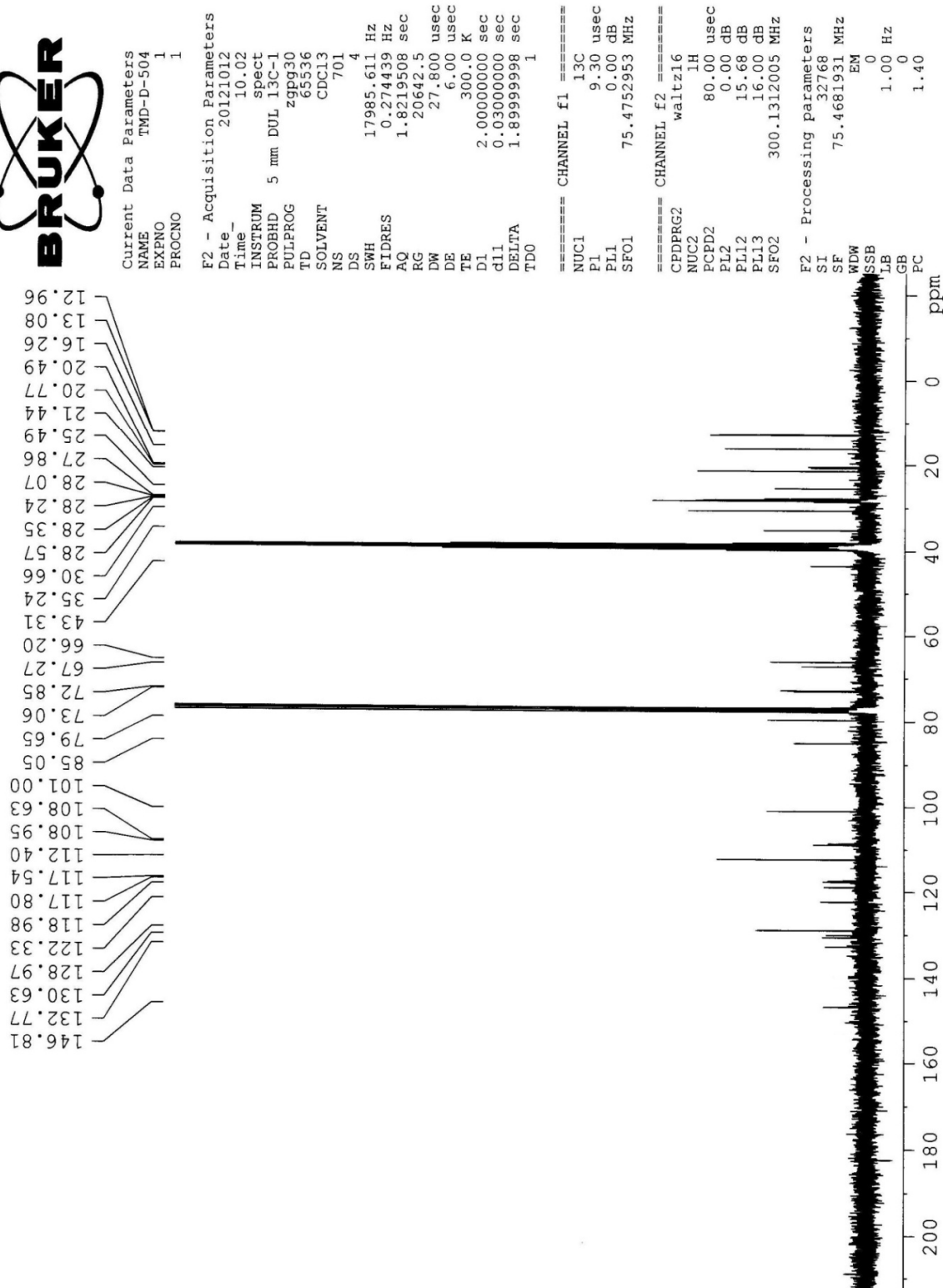


Figure S.I. 21:  $^{13}\text{C}$  NMR Spectrum of Compound **15**.



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PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120926  
Time 22.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 7  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 143.7  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.15 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1314026 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

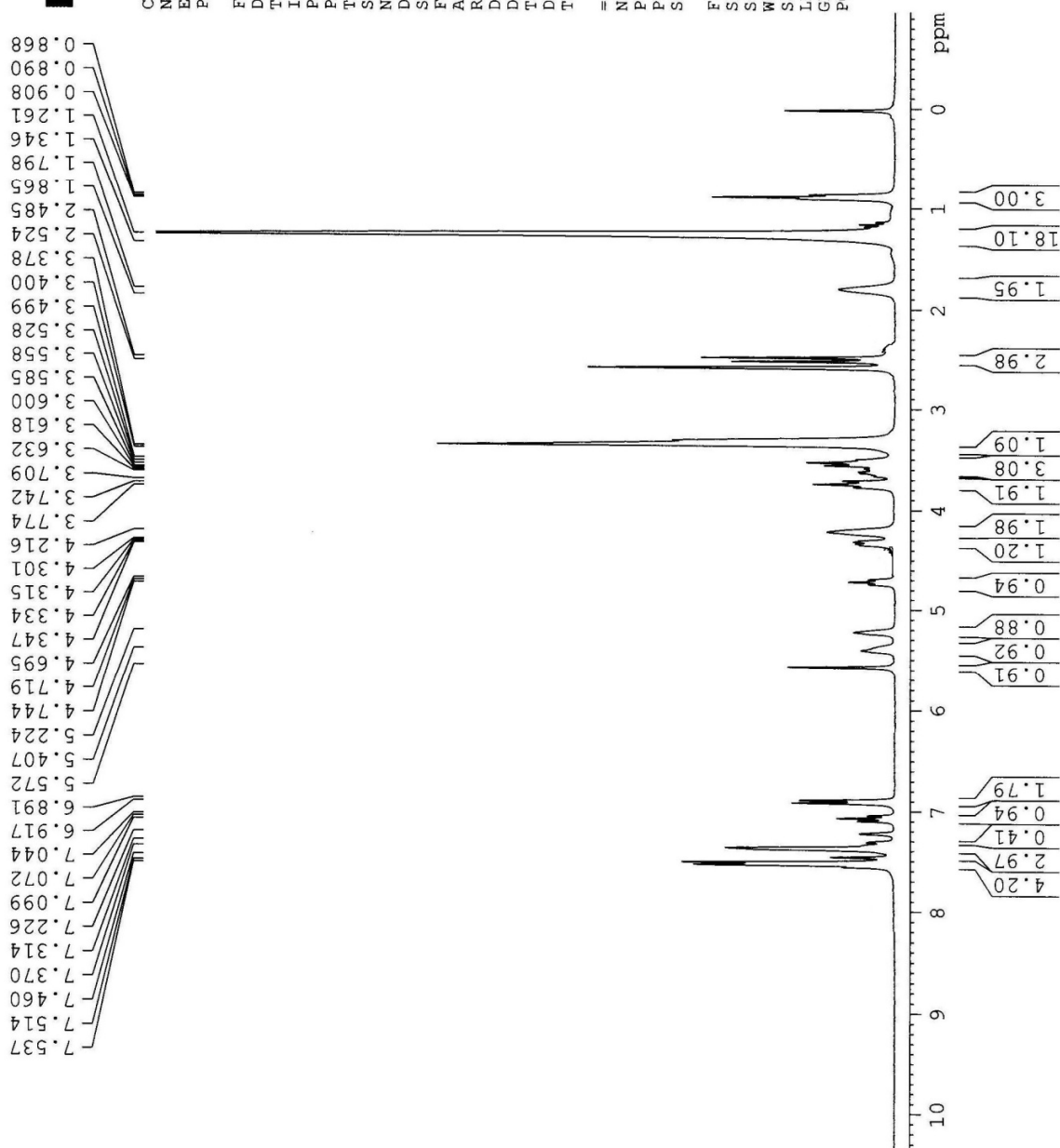


Figure S.I. 22:  $^1\text{H}$  NMR Spectrum of Compound 16.



Current Data Parameters  
 NAME TMD-D-506  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121013  
 Time 23.34  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5792.6  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.30 usec  
 PL1 0.00 dB  
 SF01 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.68 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4681873 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

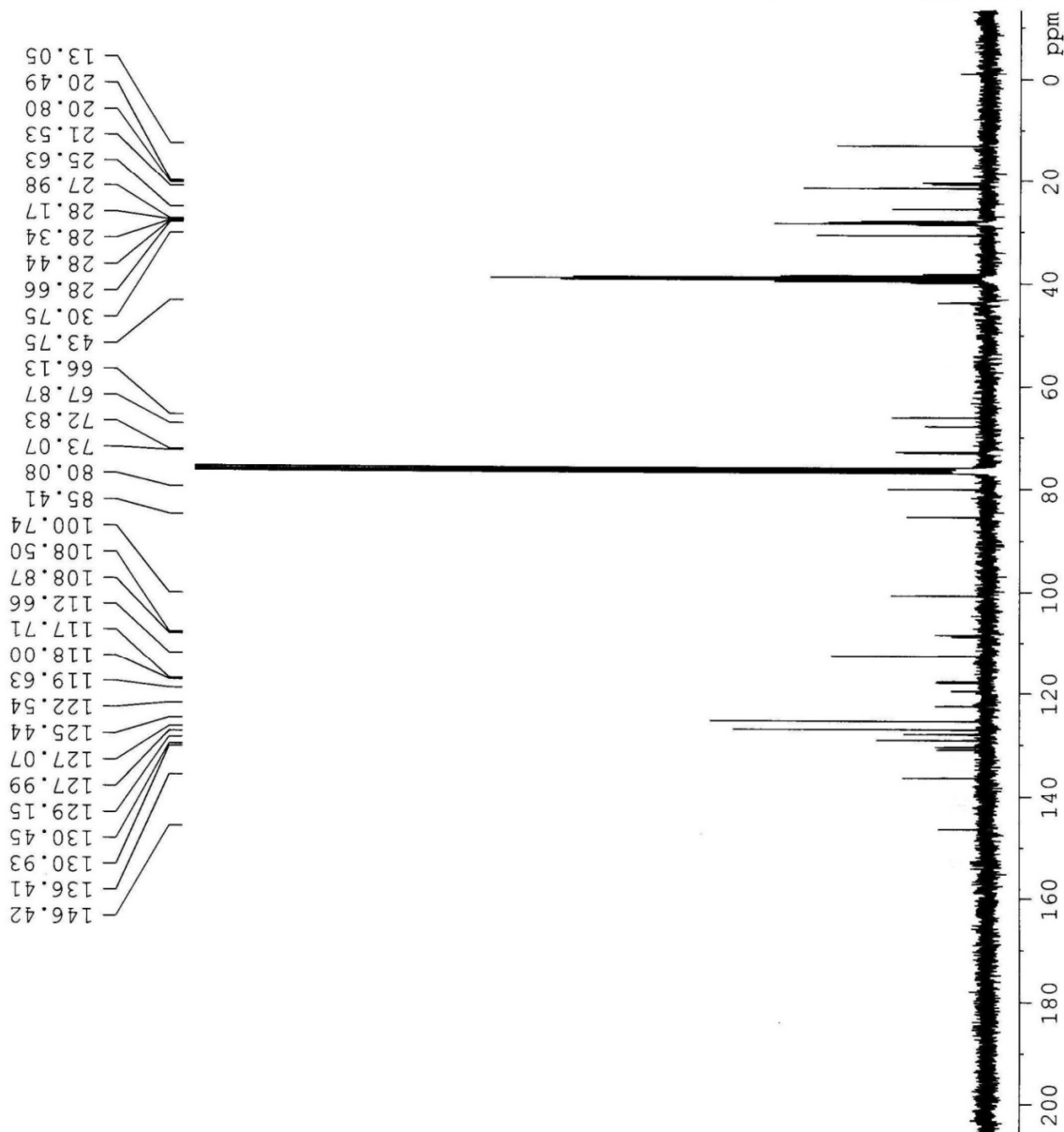


Figure S.I. 23:  $^{13}\text{C}$  NMR Spectrum of Compound 16.

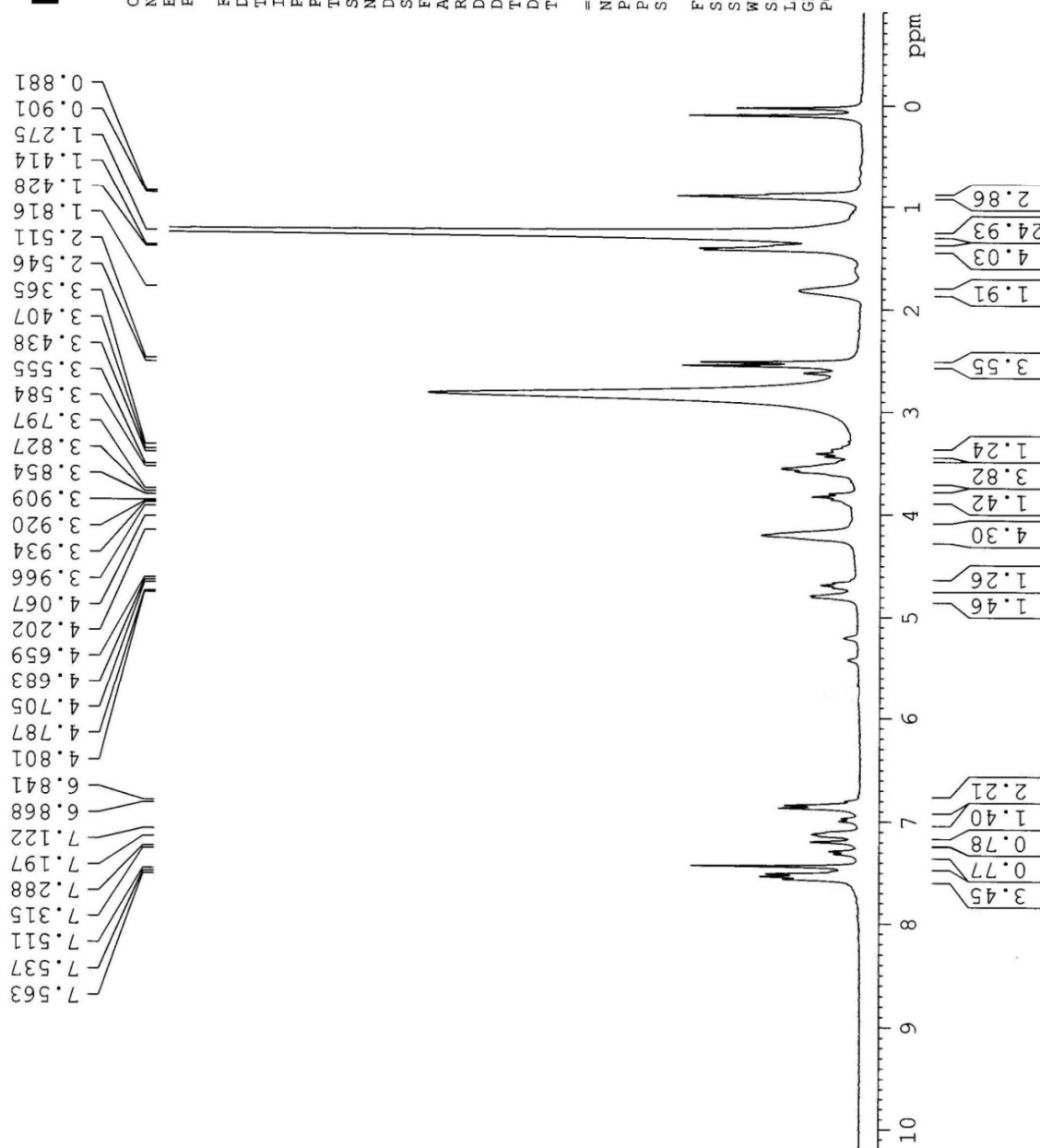


Current Data Parameters  
 NAME TMD-507  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121028  
 Time\_ 9.52  
 INSTRUM spect  
 PROBD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 128  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.15 usec  
 PL1 0.00 dB  
 SF01 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1313941 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Figure S.I. 24:  $^1\text{H}$  NMR Spectrum of Compound 17.





Current Data Parameters  
 NAME TMD-D-507  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121021  
 Time\_ 12.57  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4000  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 7298.2  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.30 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.68 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4681892 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

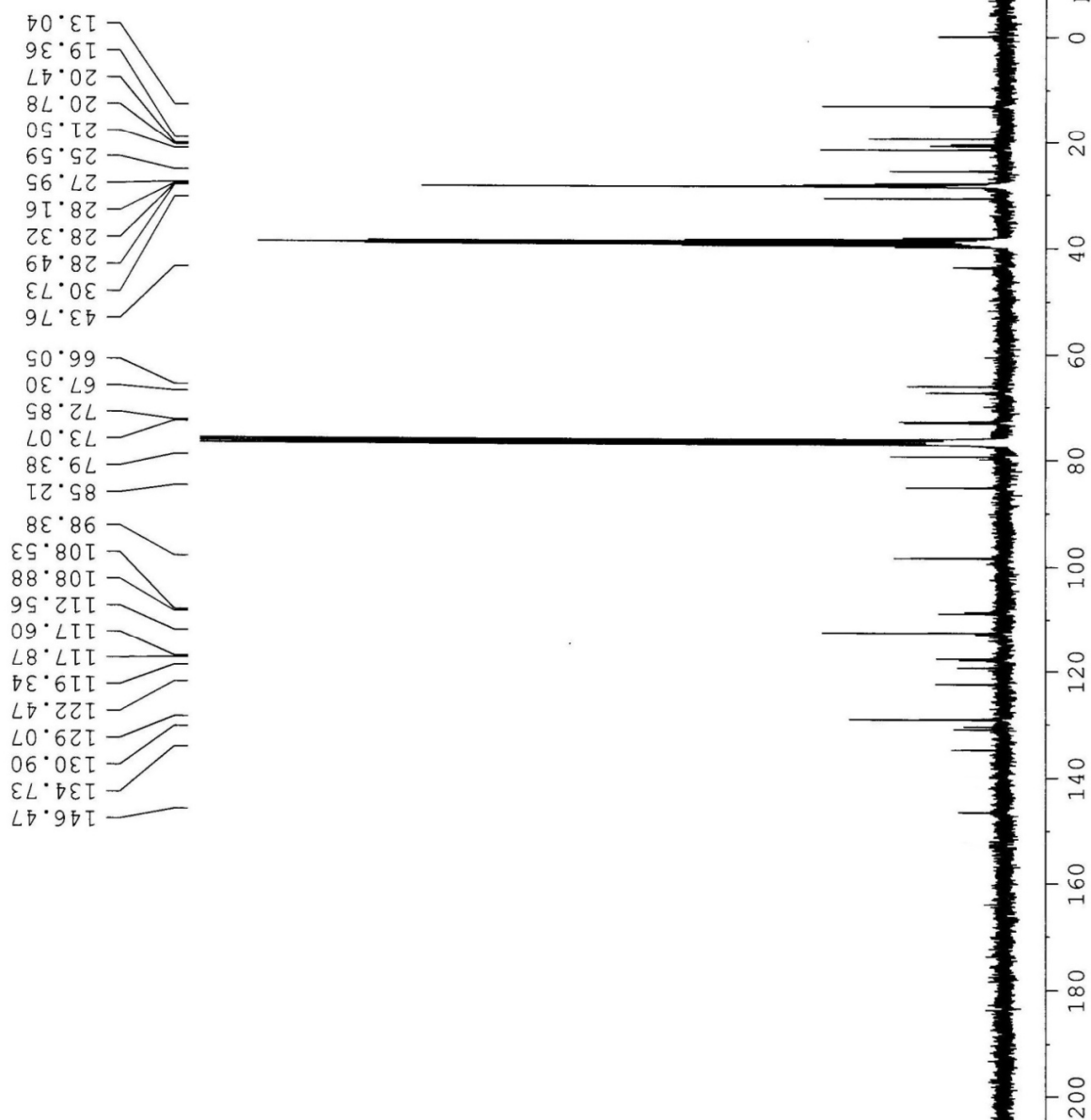


figure S.I. 25:  $^{13}\text{C}$  NMR Spectrum of Compound 17.



Current Data Parameters  
 NAME TMD-D-508  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20121015  
 Time 21.15  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.15 usec  
 PL1 0.00 dB  
 SF01 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1314059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

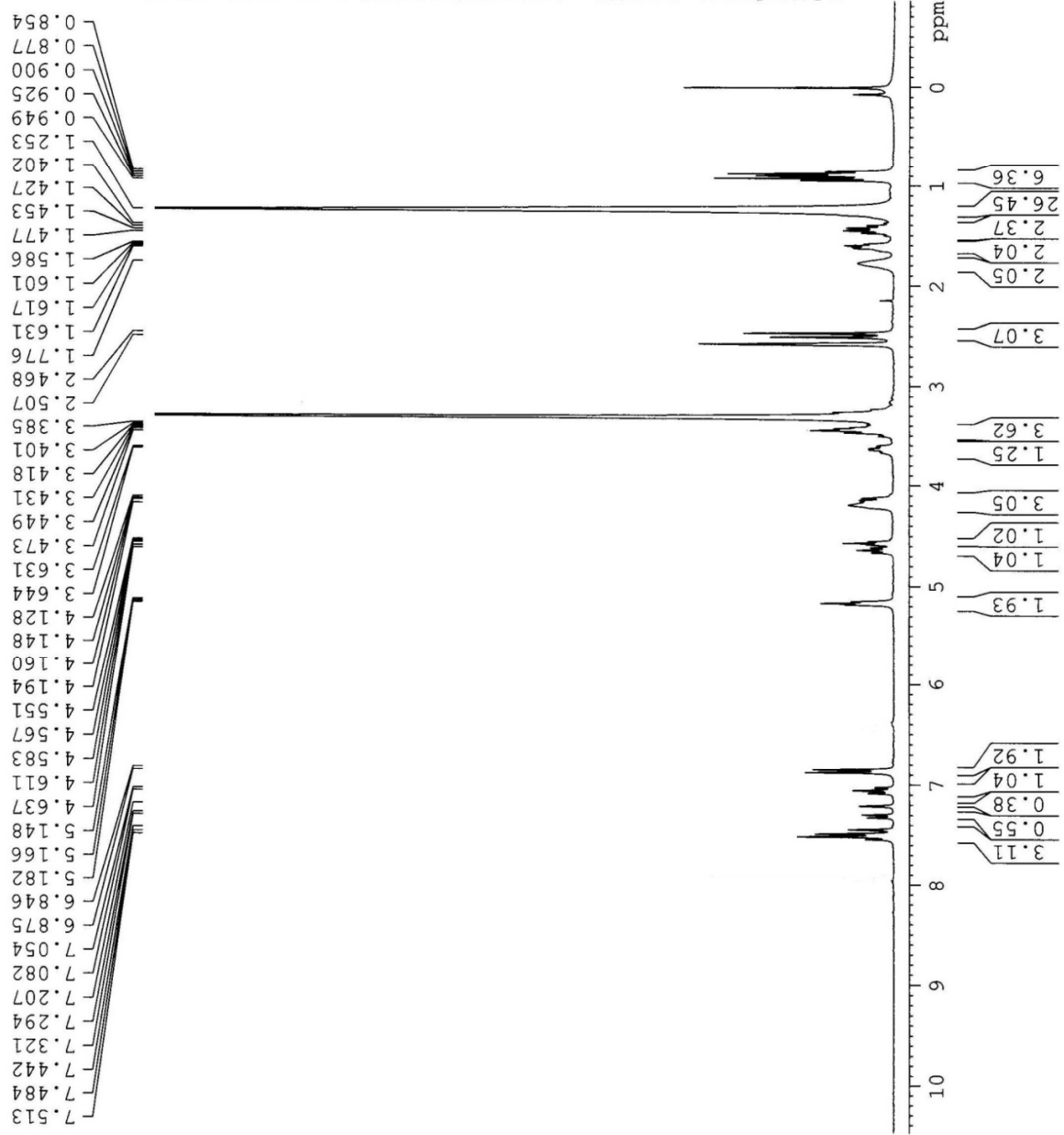


Figure S.I. 26:  $^1\text{H}$  NMR Spectrum of Compound **18**.

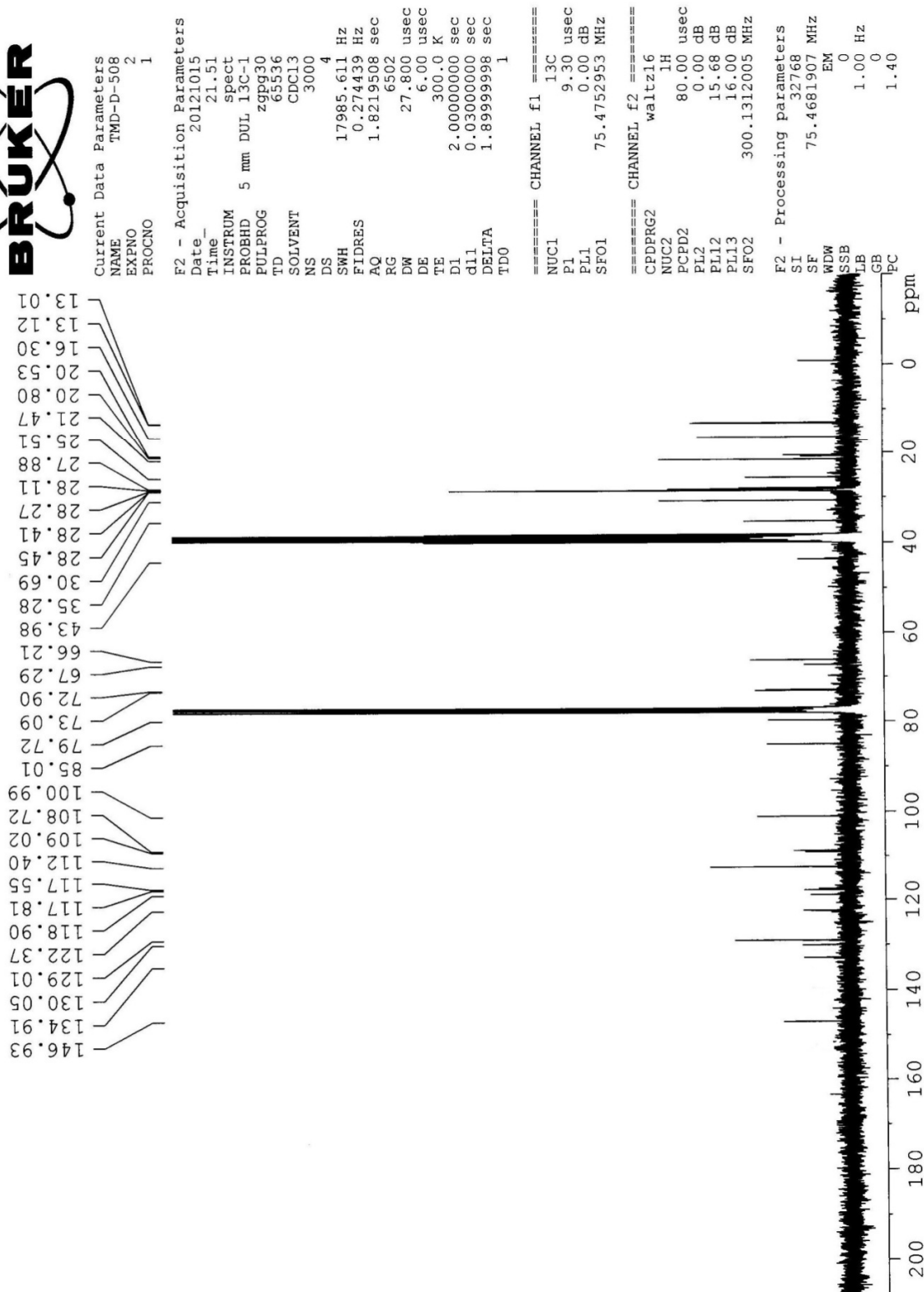


Figure S.I. 27:  $^{13}\text{C}$  NMR Spectrum of Compound 18.

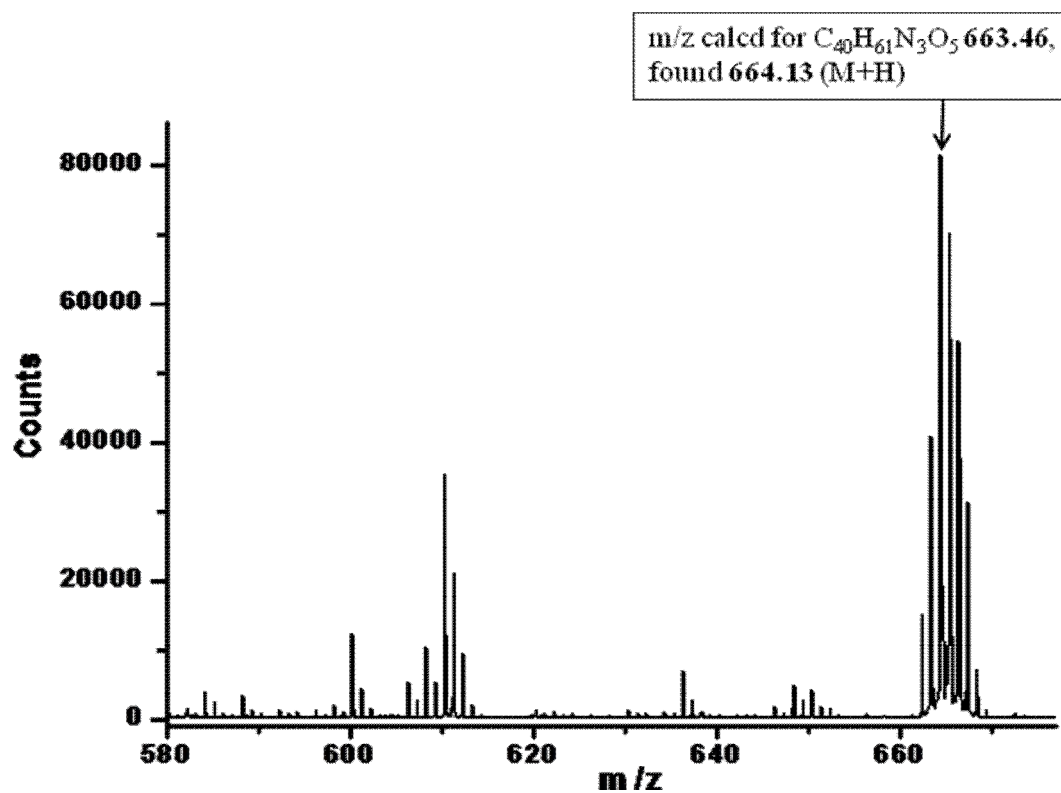


Figure S.I. 28: MALDI-TOF mass spectrum of Compound 18.

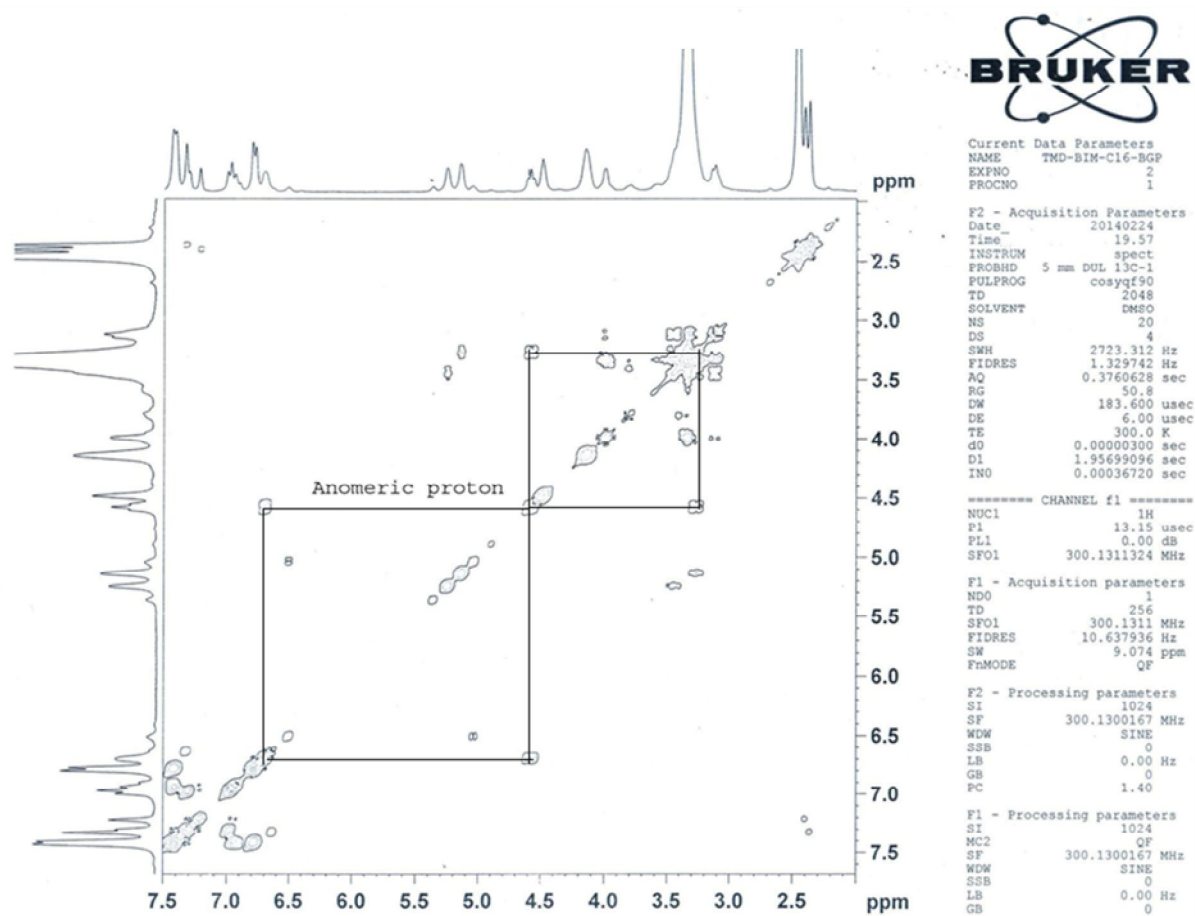


Figure S.I. 29: HH-COSY NMR Spectrum of Compound **18**.

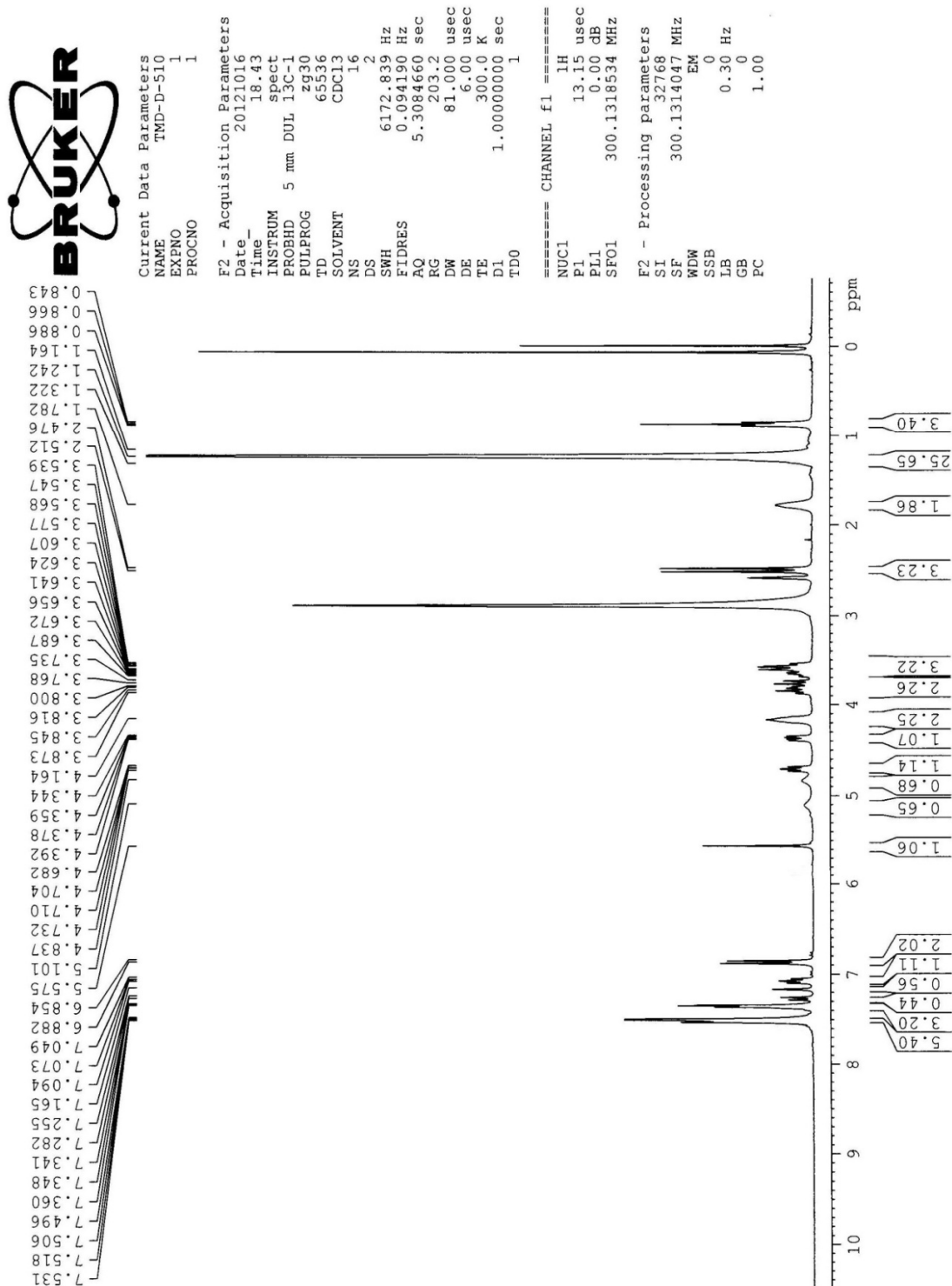


Figure S.I. 30:  $^1\text{H}$  NMR Spectrum of Compound **19**.

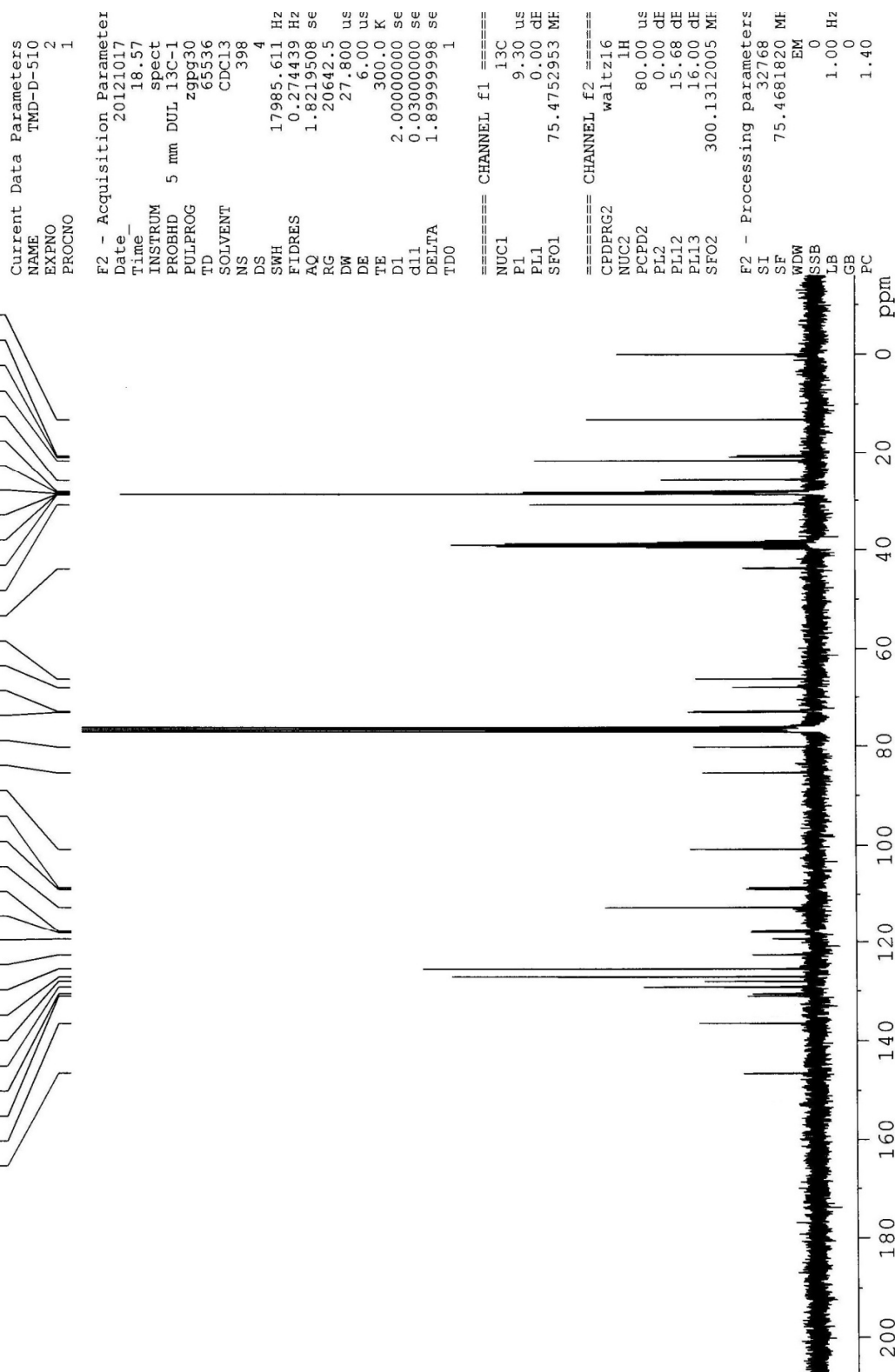


Figure S.I. 31:  $^{13}\text{C}$  NMR Spectrum of Compound 19.

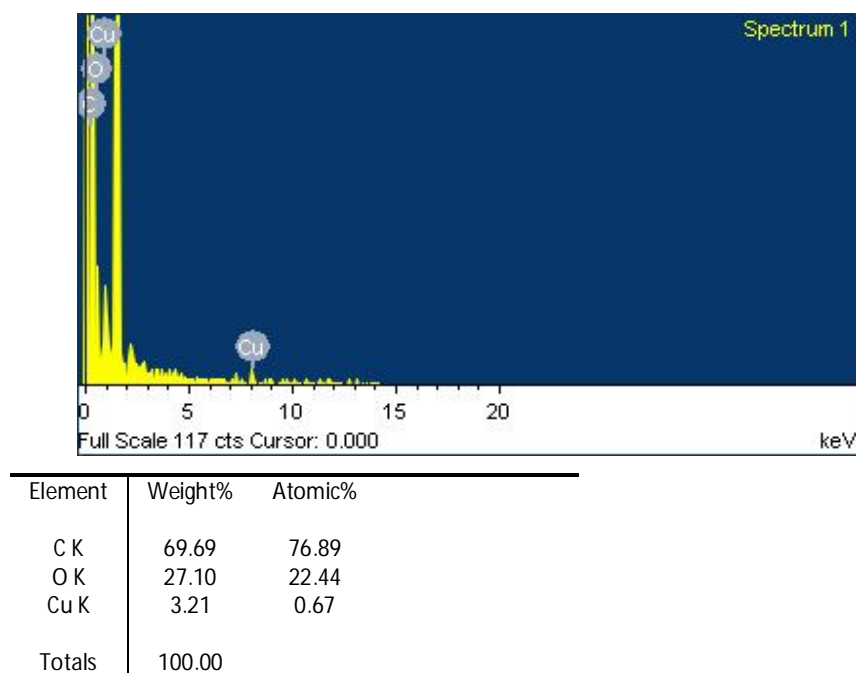


Figure S.I. 32: EDAX spectrum of solution derived from gel **18** in ethanol with  $\text{Cu}^{2+}$  ion (20  $\mu\text{L}$  of 0.1 % in ethanol).