

**Synthesis, photophysical, electrochemical properties and DSSC application of triphenylamine chalcone dendrimers via click chemistry**

Devaraj Anandkumar,<sup>a</sup> Perumal Rajakumar,<sup>a\*</sup> Shanmugam Ganesan<sup>b</sup> and  
Pichai Maruthamuthu<sup>c</sup>

<sup>a</sup>Department of Organic Chemistry, University of Madras, Guindy Campus Chennai 600 025, TamilNadu, India

<sup>b</sup>Department of Chemistry, SRM University, SRM Nagar, Kattankulathur, Chennai-603 203, India

<sup>c</sup>Department of Energy, University of Madras, Guindy Campus, Chennai 600 025, India

E-mail: perumalrajakumar@gmail.com; Tel: +91 044 2220 2814

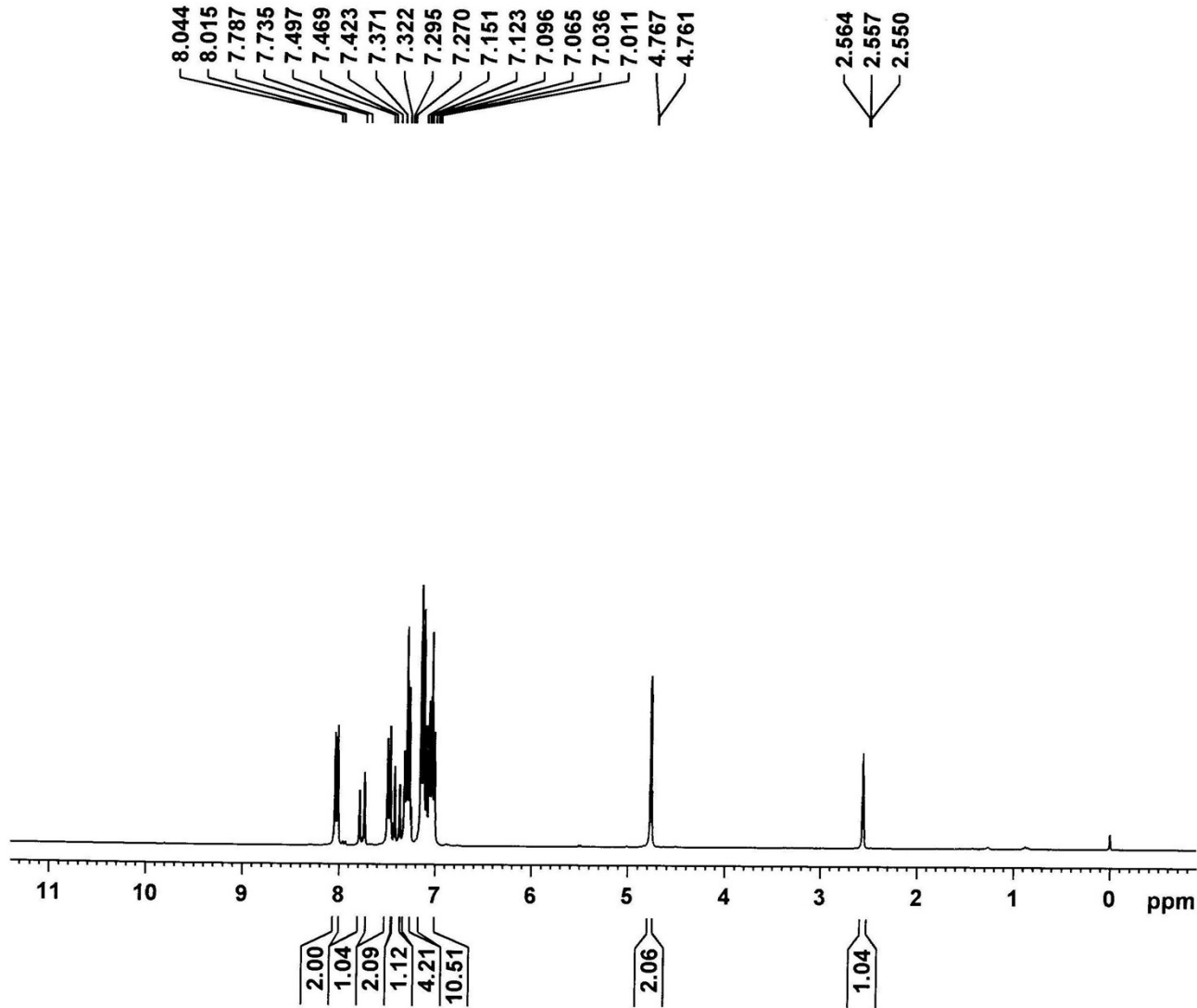


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PROCNO 1

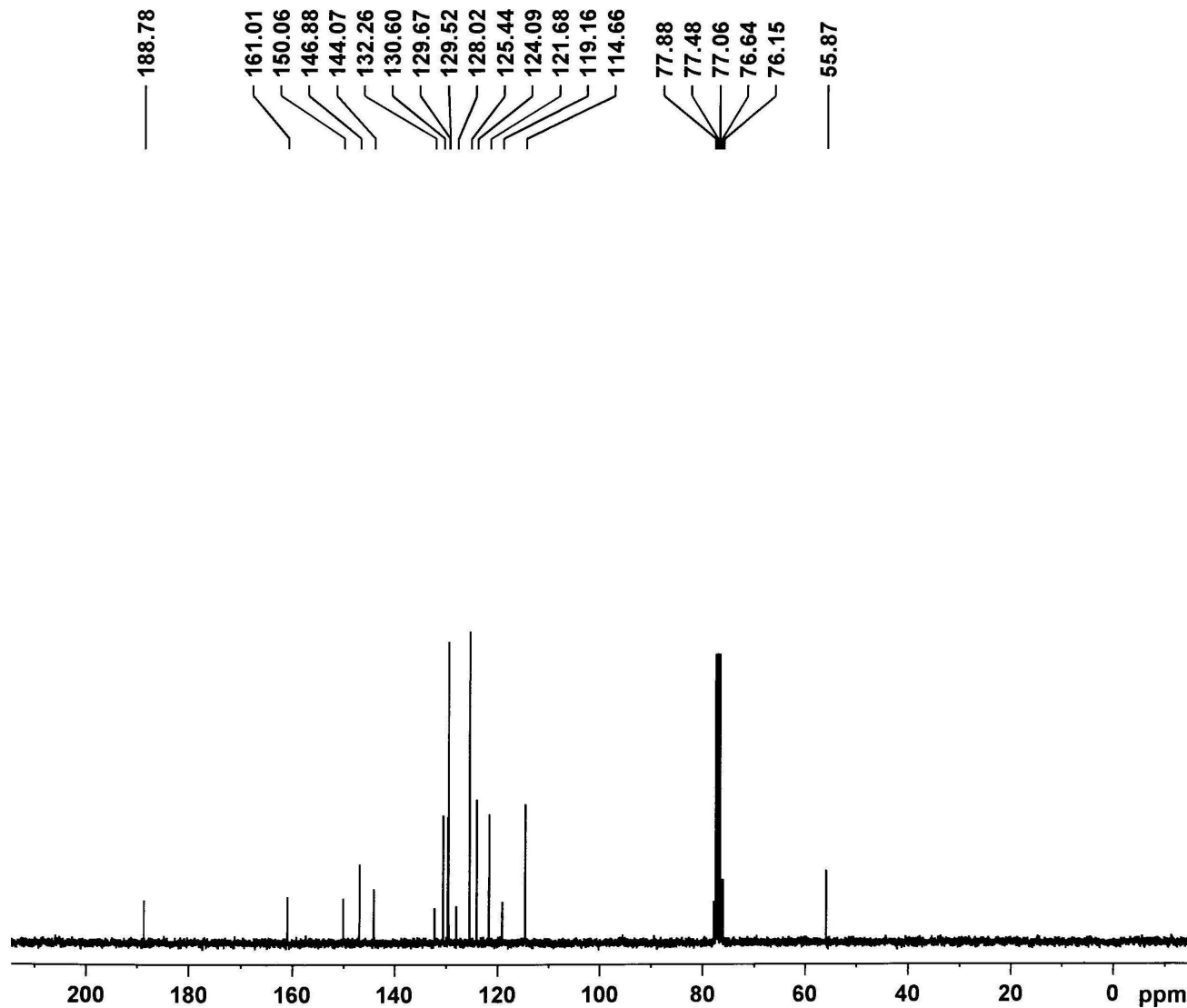
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TD 65536  
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NS 16  
DS 2  
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FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 80.6  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.88 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300084 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound **10**



Current Data Parameters  
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 EXPNO 2  
 PROCNO 1

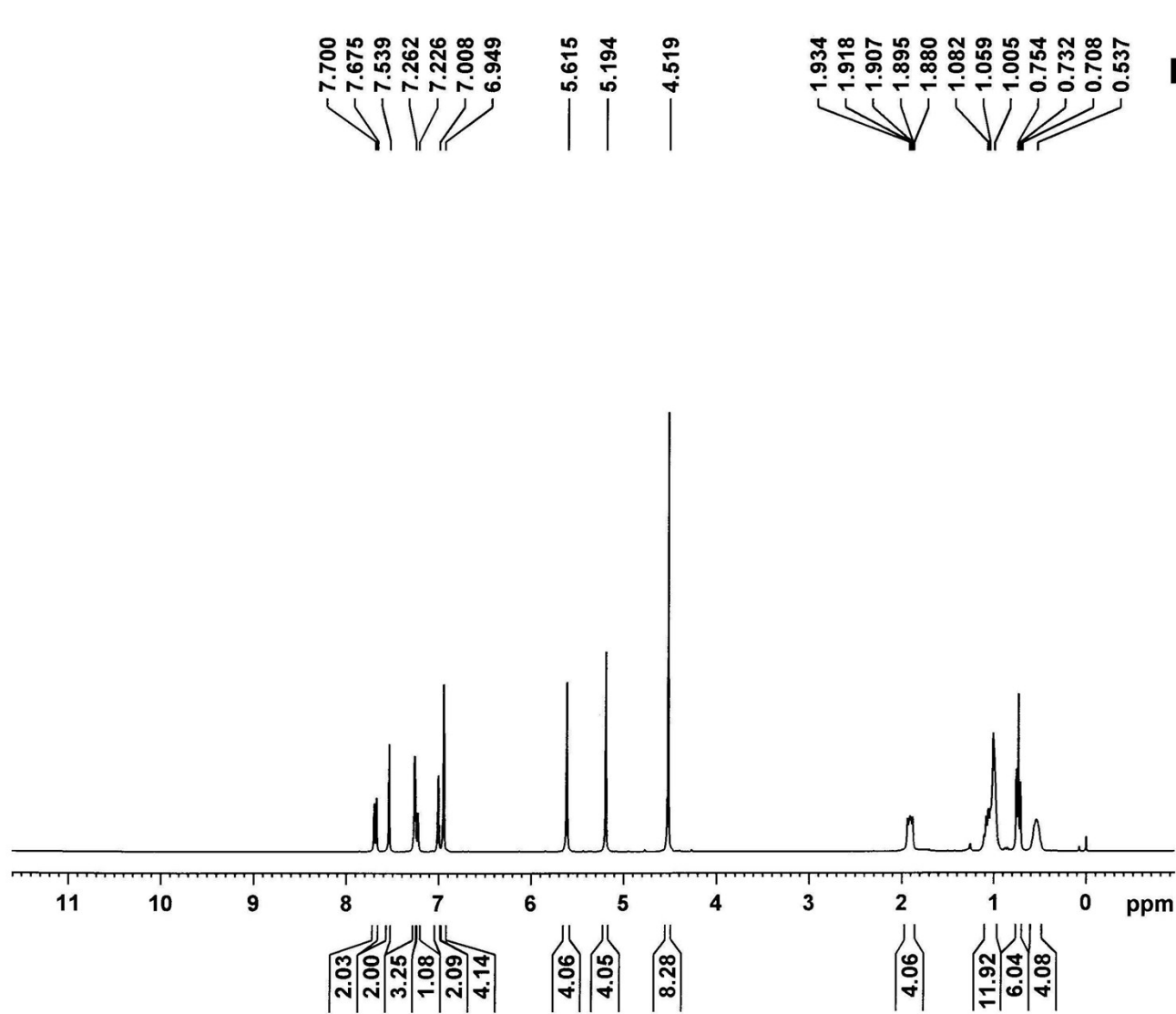
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 SOLVENT CDCl3  
 NS 100  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 18390.4  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.38 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.21 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
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 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 10



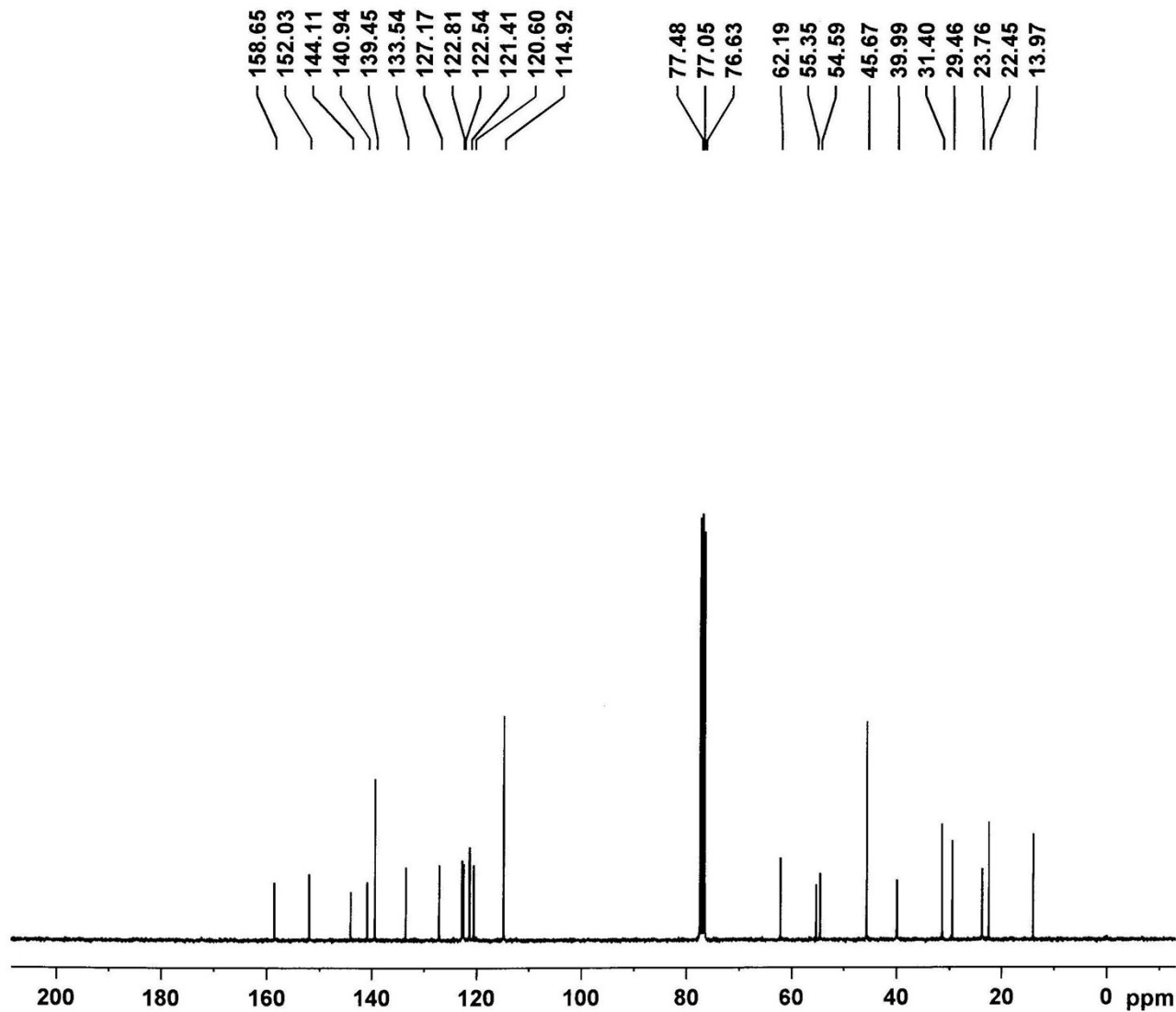
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F2 - Acquisition Parameters  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 71.8  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.88 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300042 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound 14



<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 14



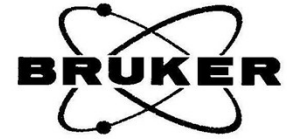
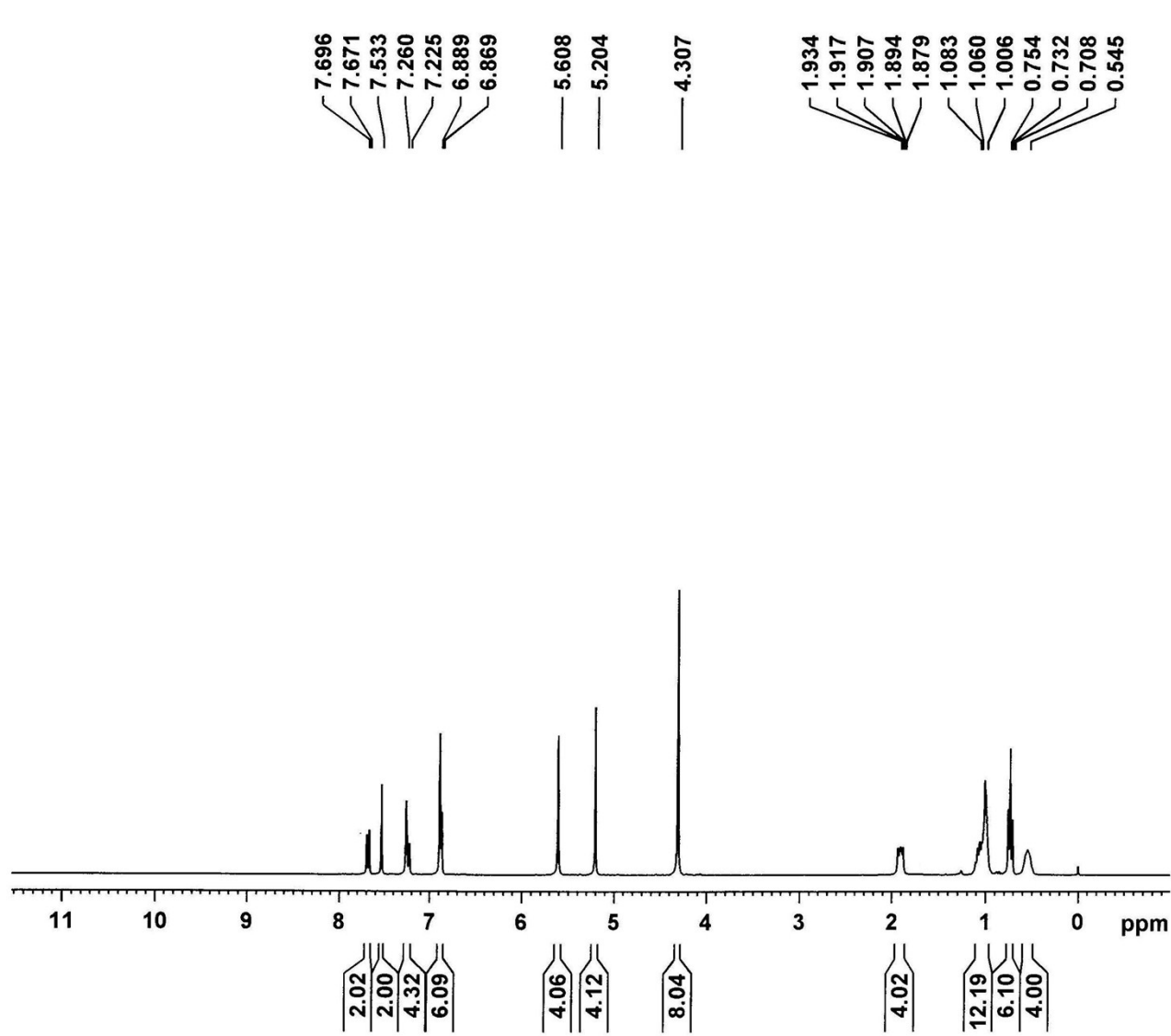
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 PROCNO 1

F2 - Acquisition Parameters  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 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  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.38 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.21 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



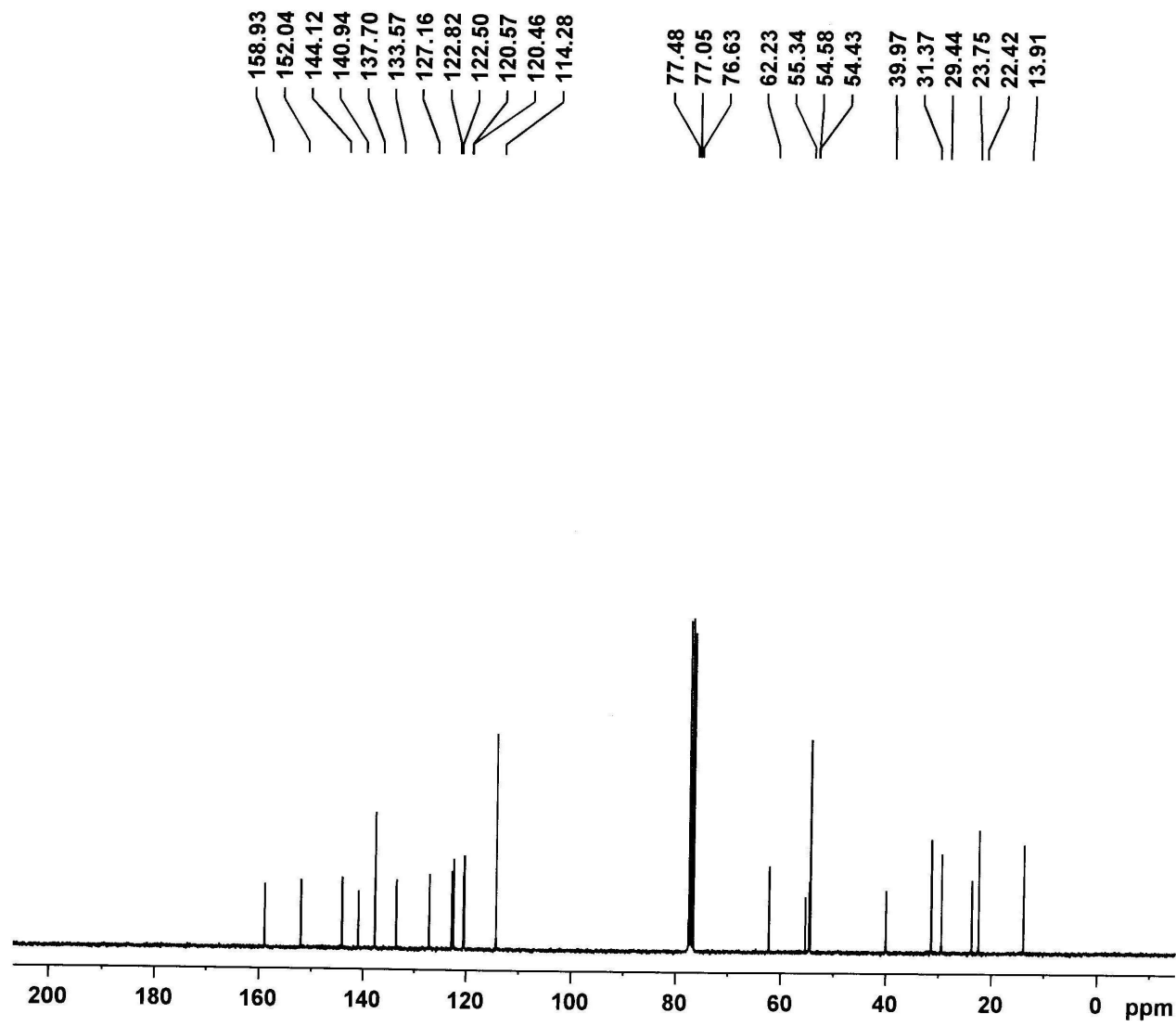
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 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 90.5  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.88 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300043 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 15



Current Data Parameters  
 NAME DA-534  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151004  
 Time 19.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1500  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 3251  
 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 10.38 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.21 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 15



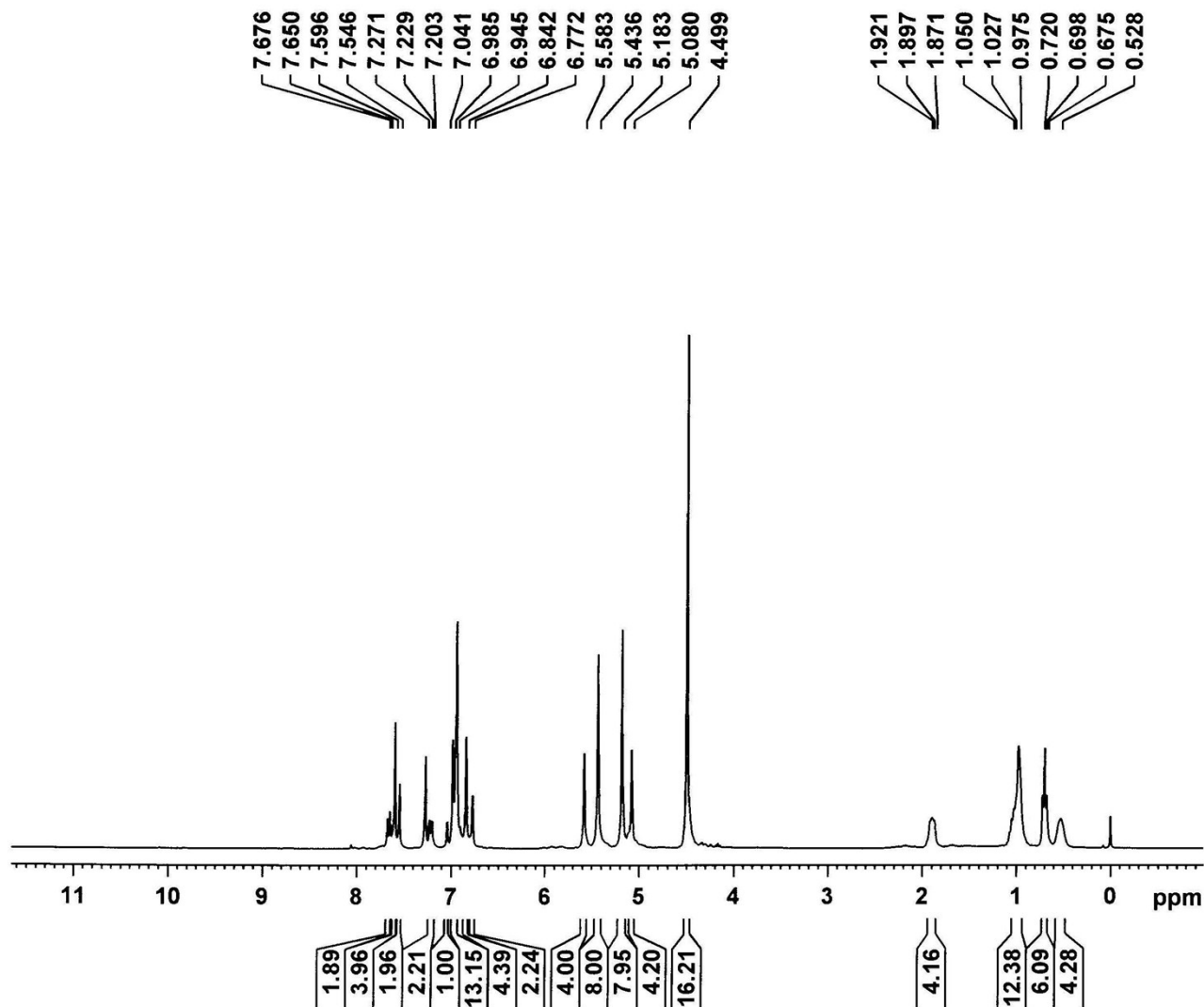


Current Data Parameters  
 NAME DA-587  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160323  
 Time 15.51  
 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 64  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

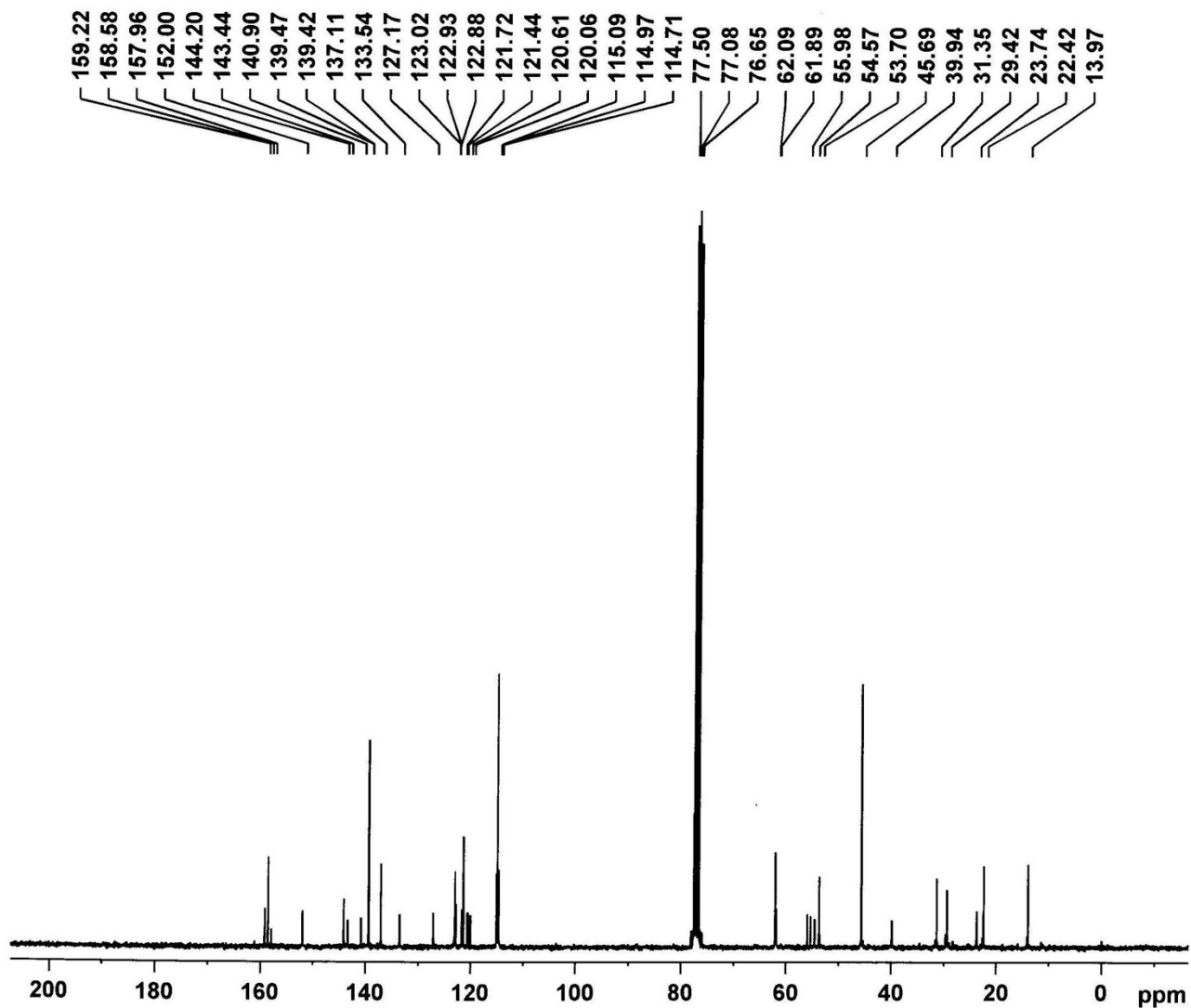
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 NUC1 1H  
 P1 12.45 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300030 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound 16

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Current Data Parameters  
NAME DA-587  
EXPNO 2  
PROCNO 1

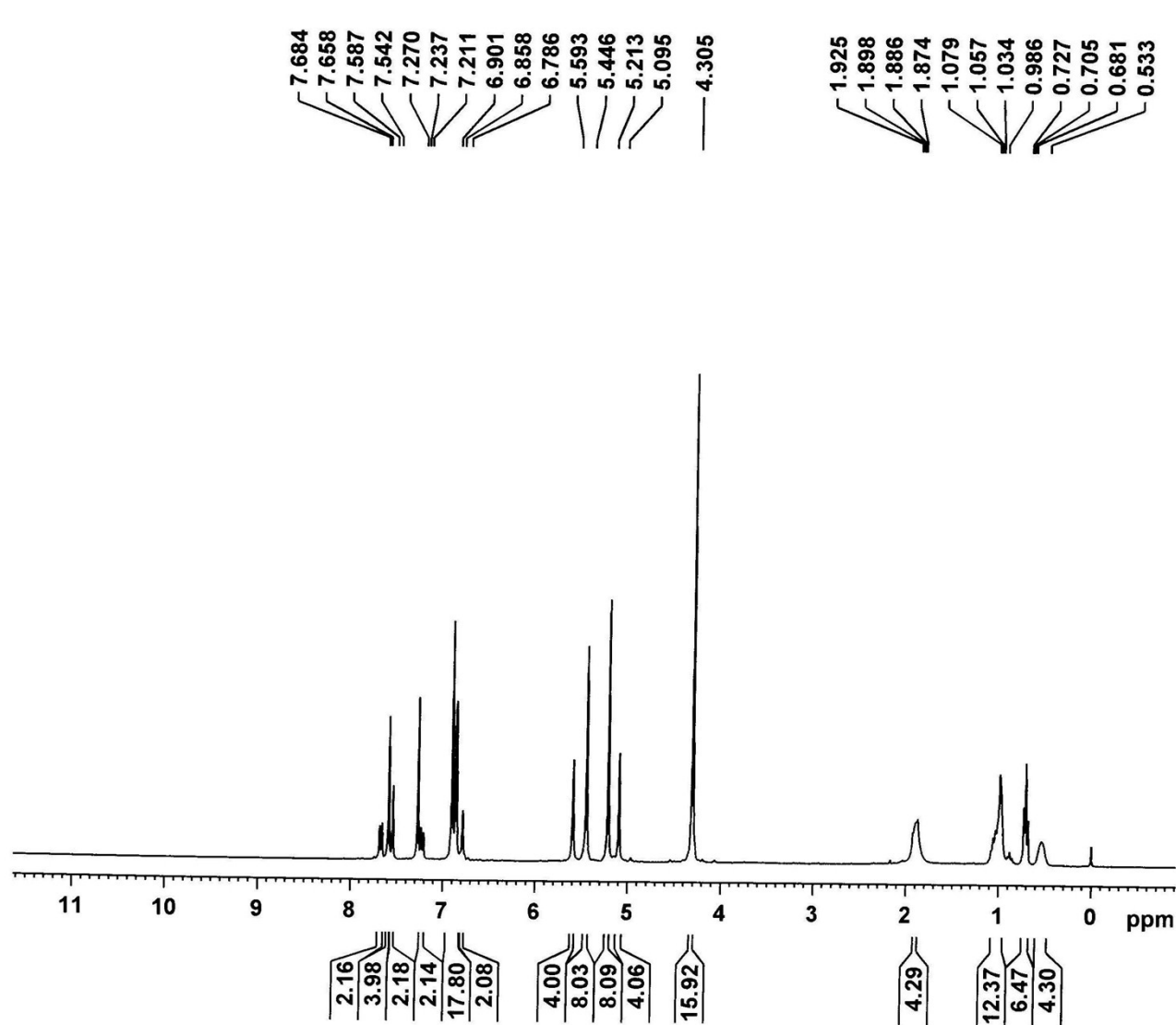
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2000  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 11585.2  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.63 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 0.00 dB  
PL12 16.16 dB  
PL13 16.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 16



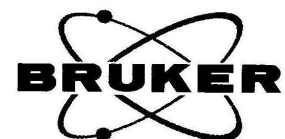
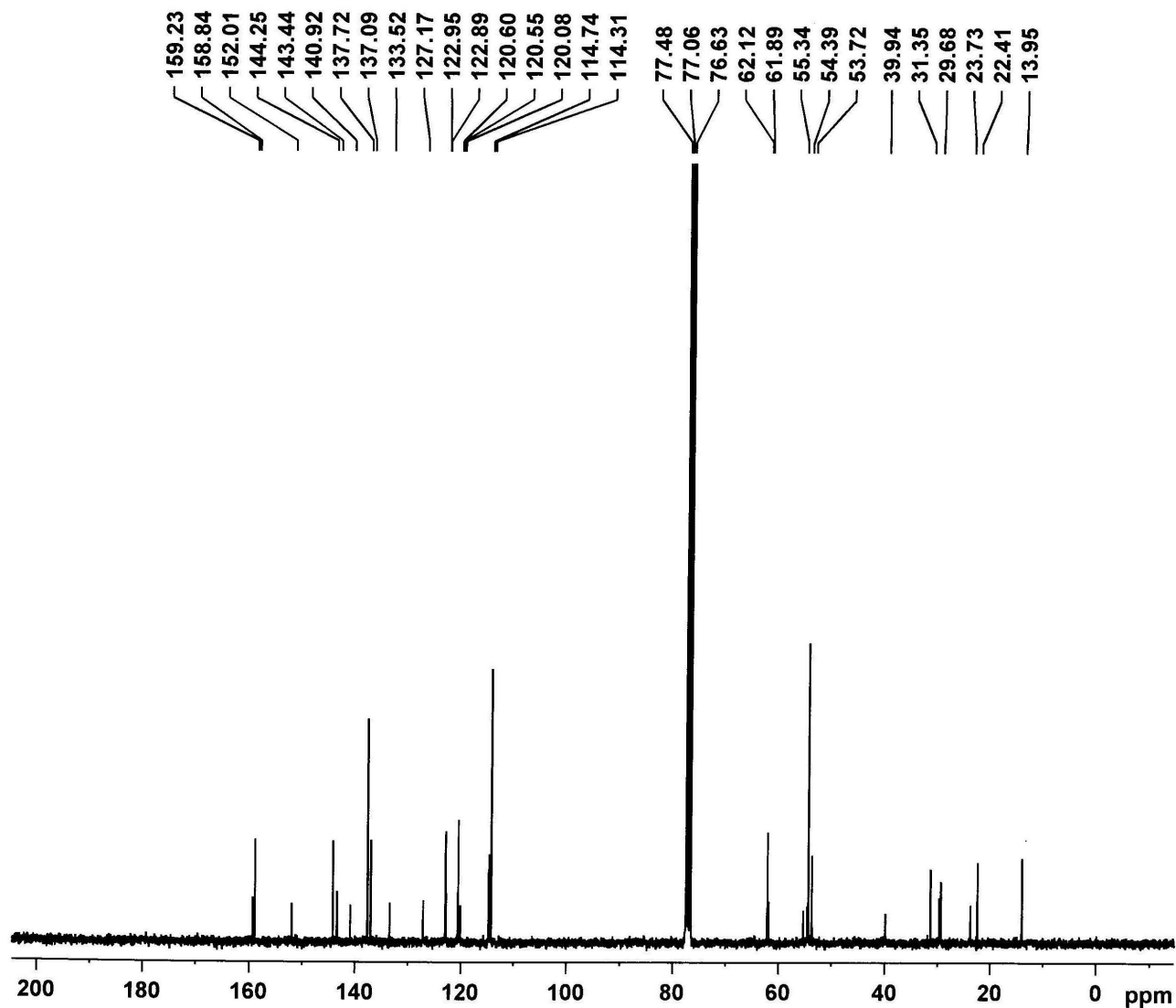
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 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
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 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 101.6  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.45 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300033 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 17



Current Data Parameters  
 NAME DA-595  
 EXPNO 2  
 PROCNO 1

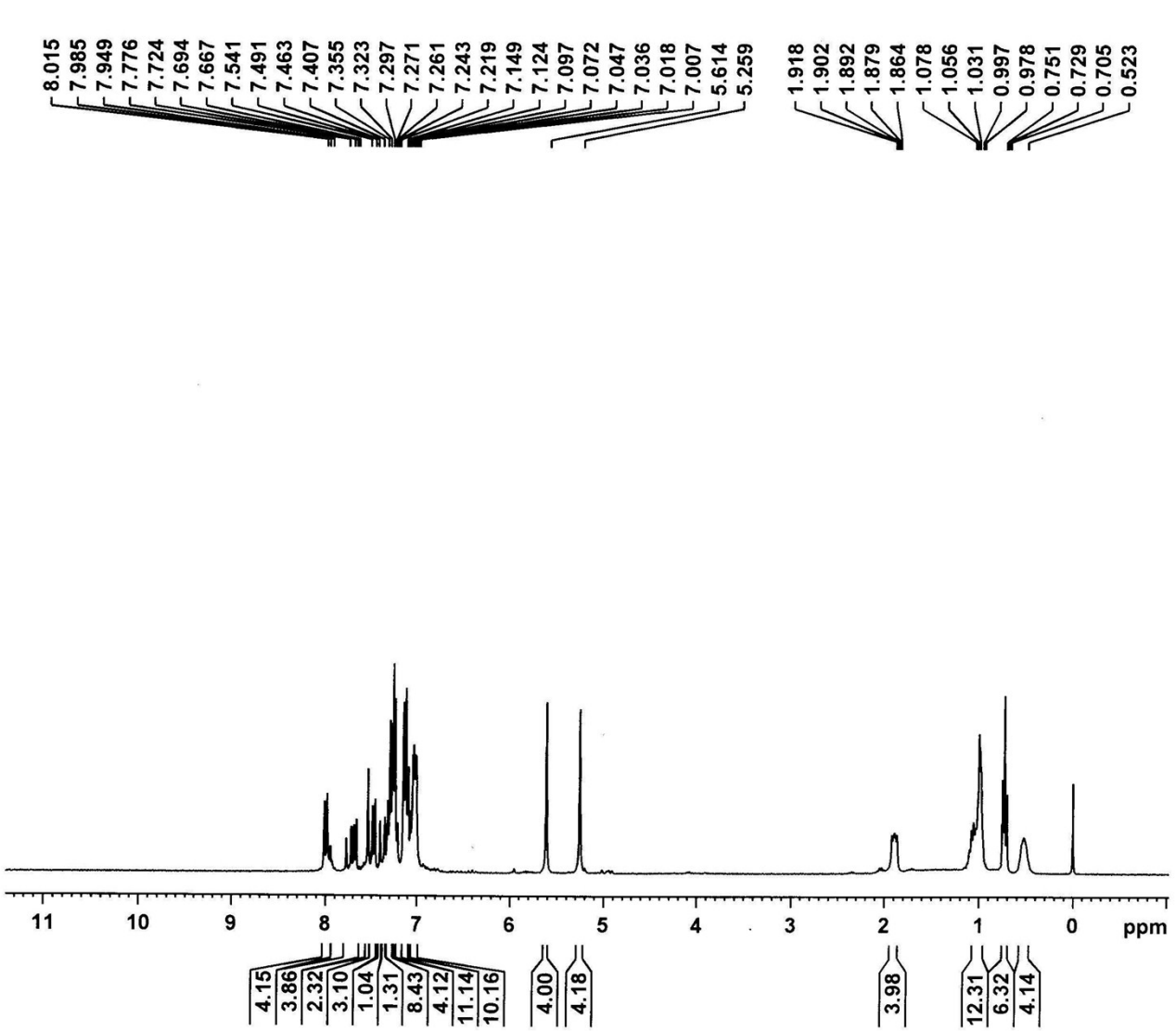
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 6502  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.63 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 16.16 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 17



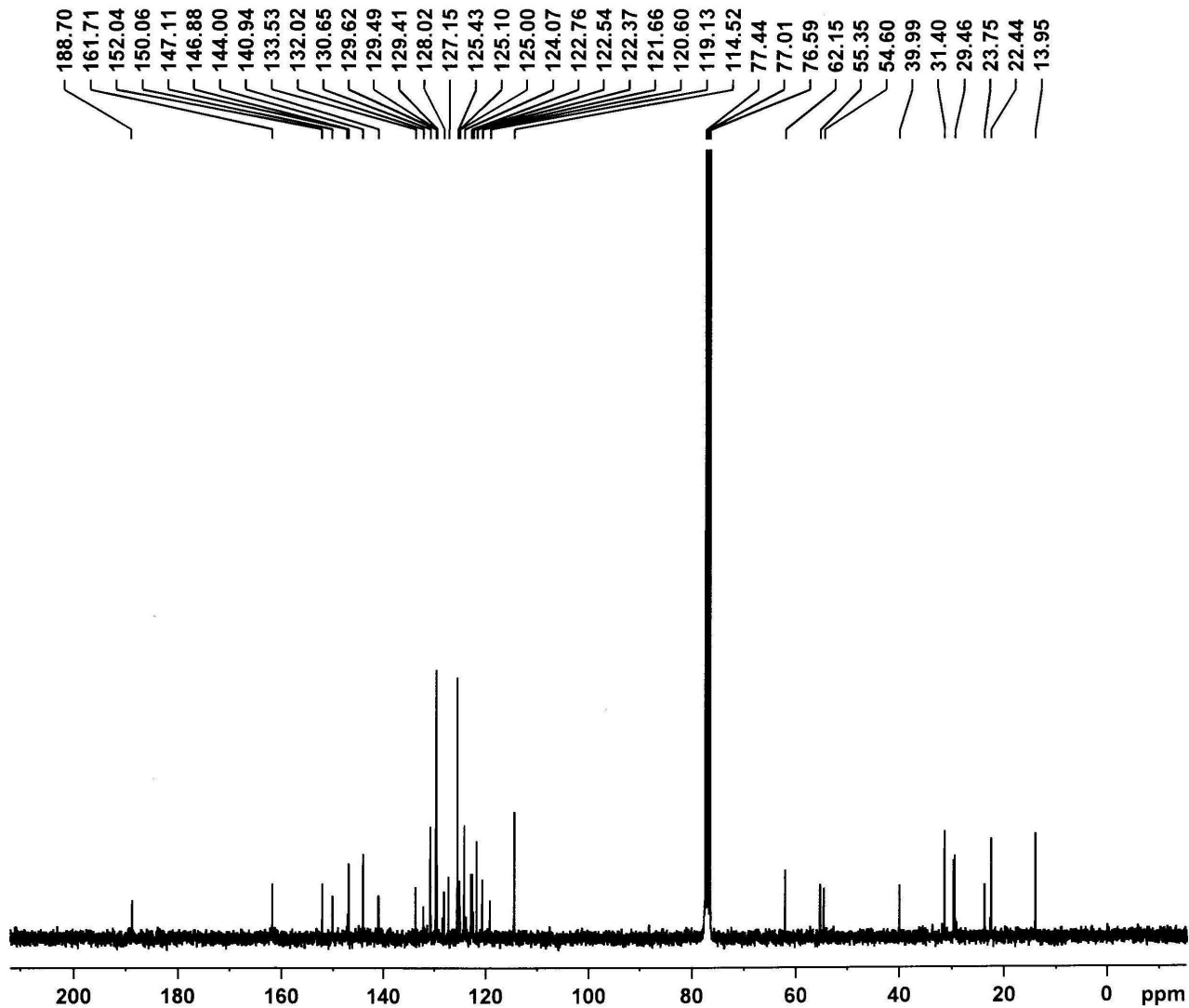
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 EXPNO 1  
 PROCNO 1

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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 161.3  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.88 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 1



Current Data Parameters  
 NAME DA-520  
 EXPNO 2  
 PROCNO 1

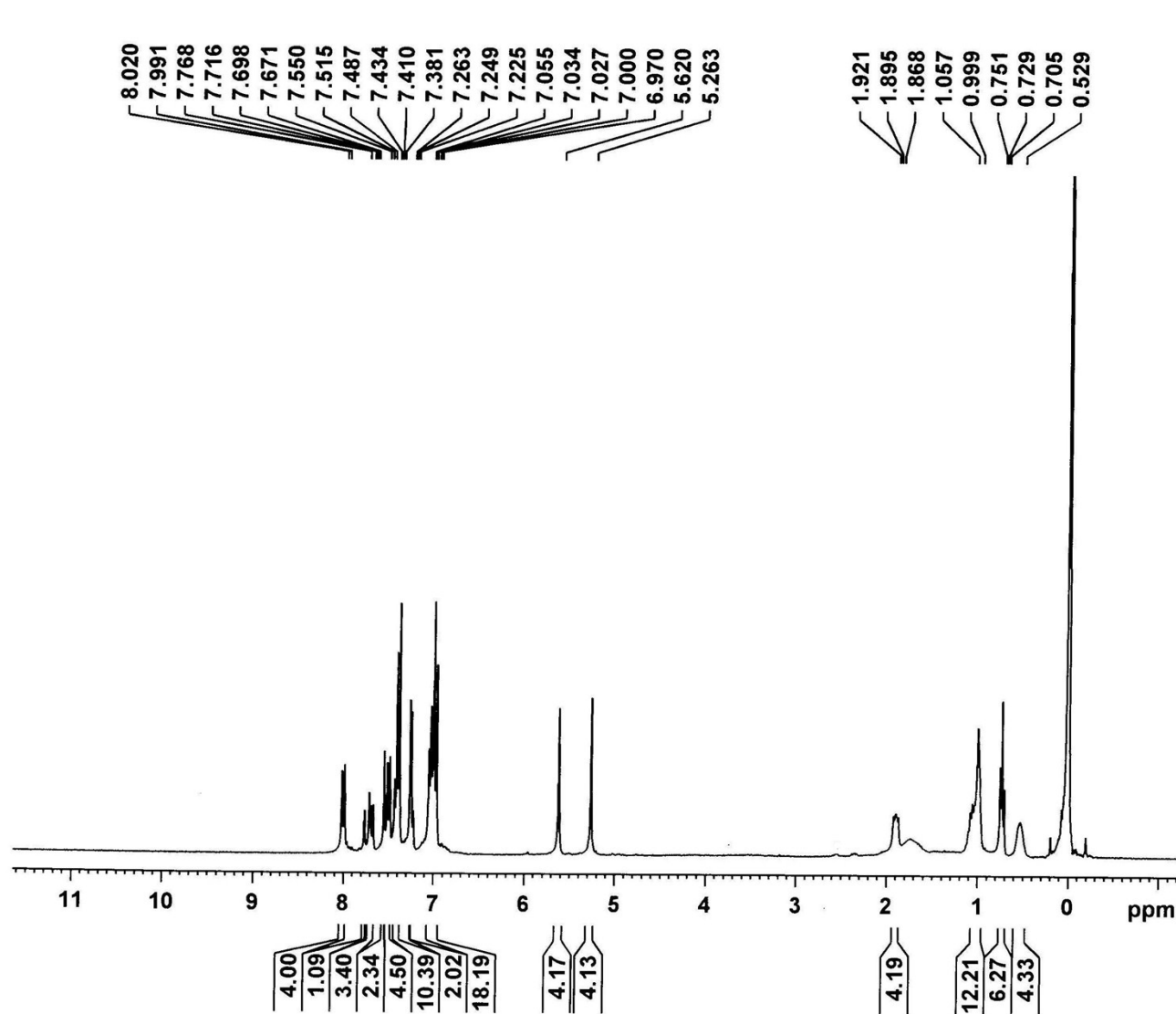
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 PULPROG zgpg30  
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 SOLVENT CDCl3  
 NS 1500  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 4597.6  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.38 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 15.21 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 1



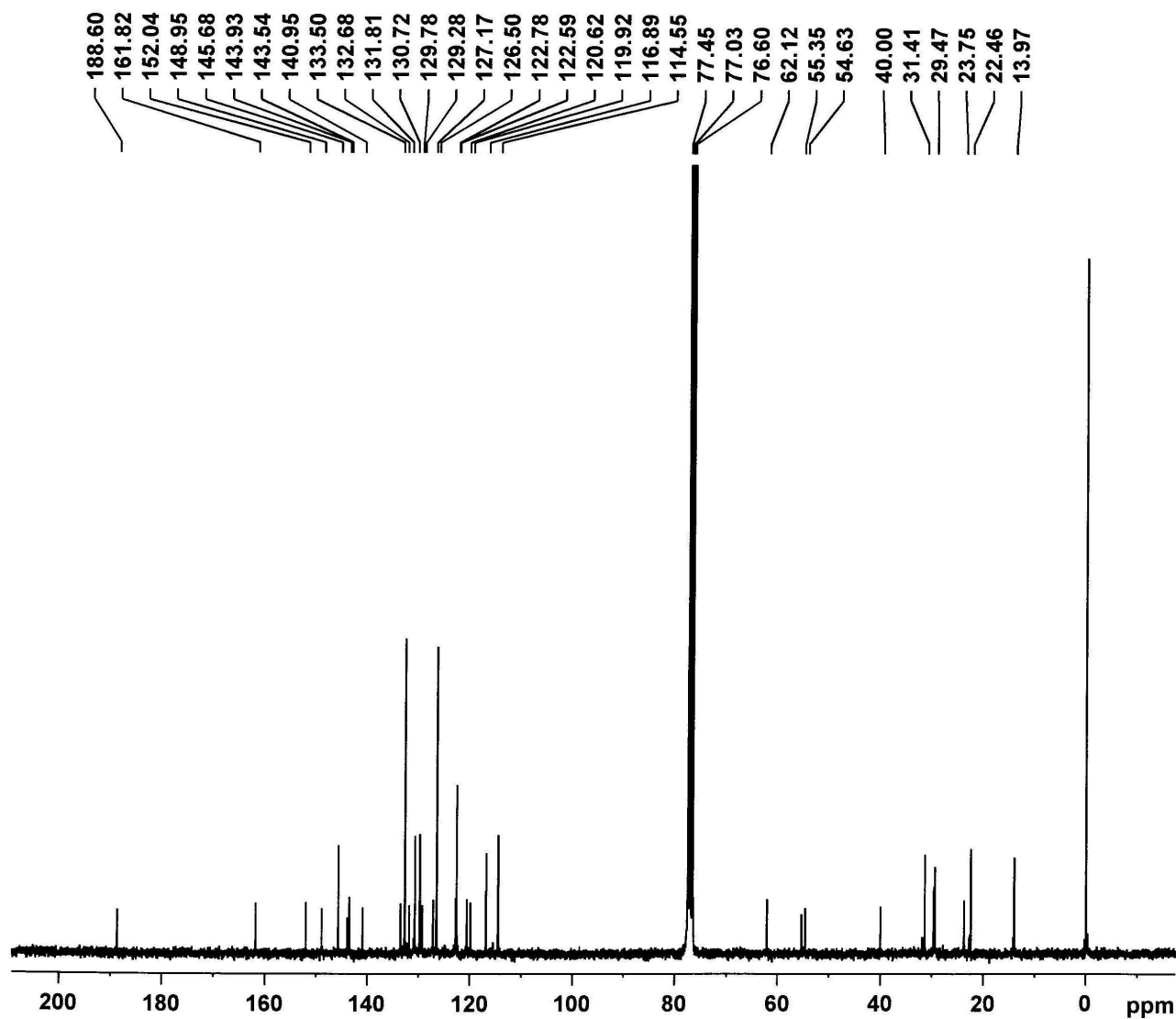
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 143.7  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.45 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300054 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 2



Current Data Parameters  
 NAME DA-578  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160220  
 Time 8.03  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7000  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 912.3  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

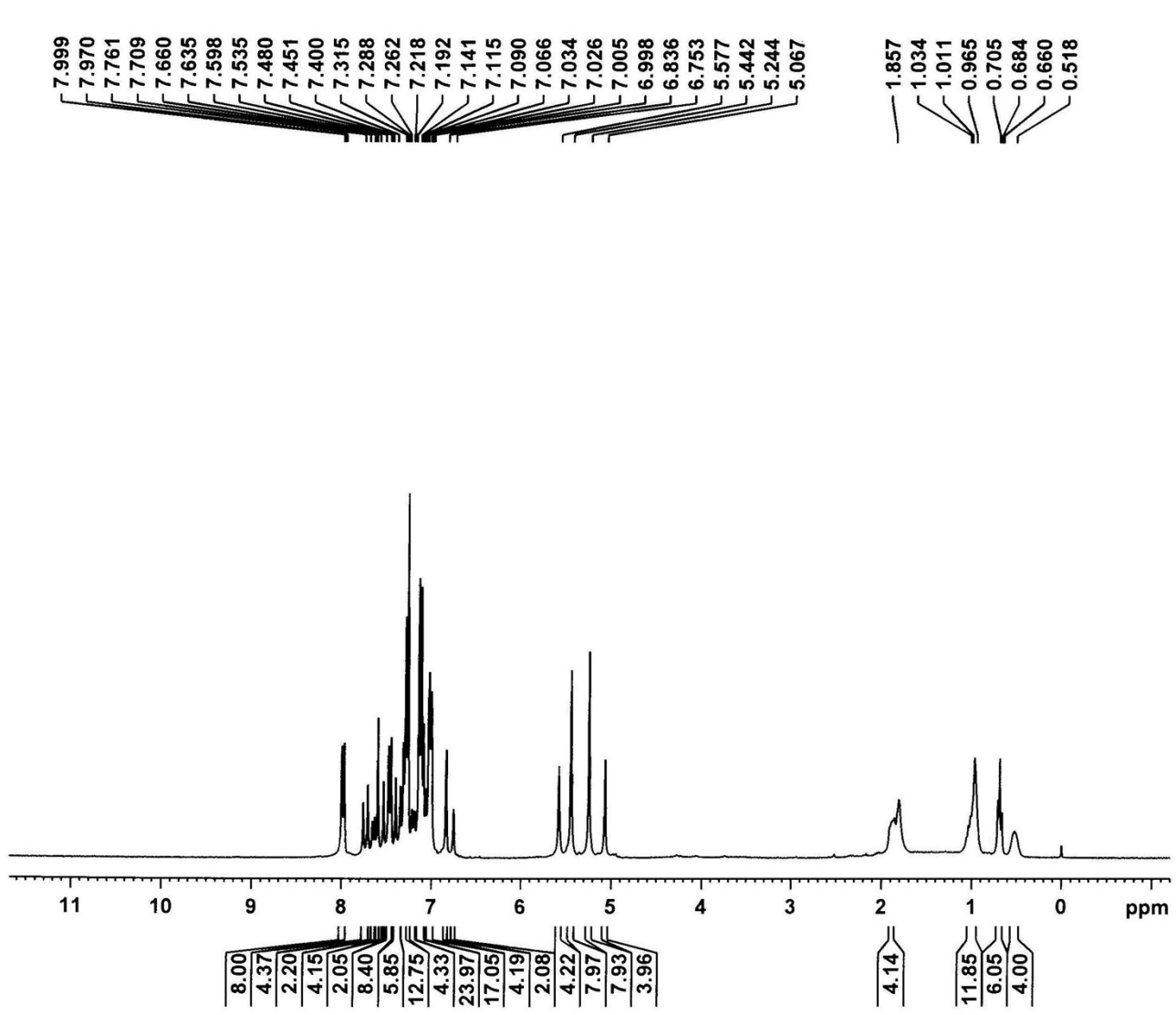
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 NUC1 13C  
 P1 9.63 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 16.16 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 2





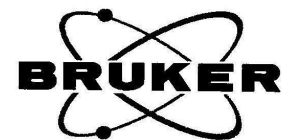
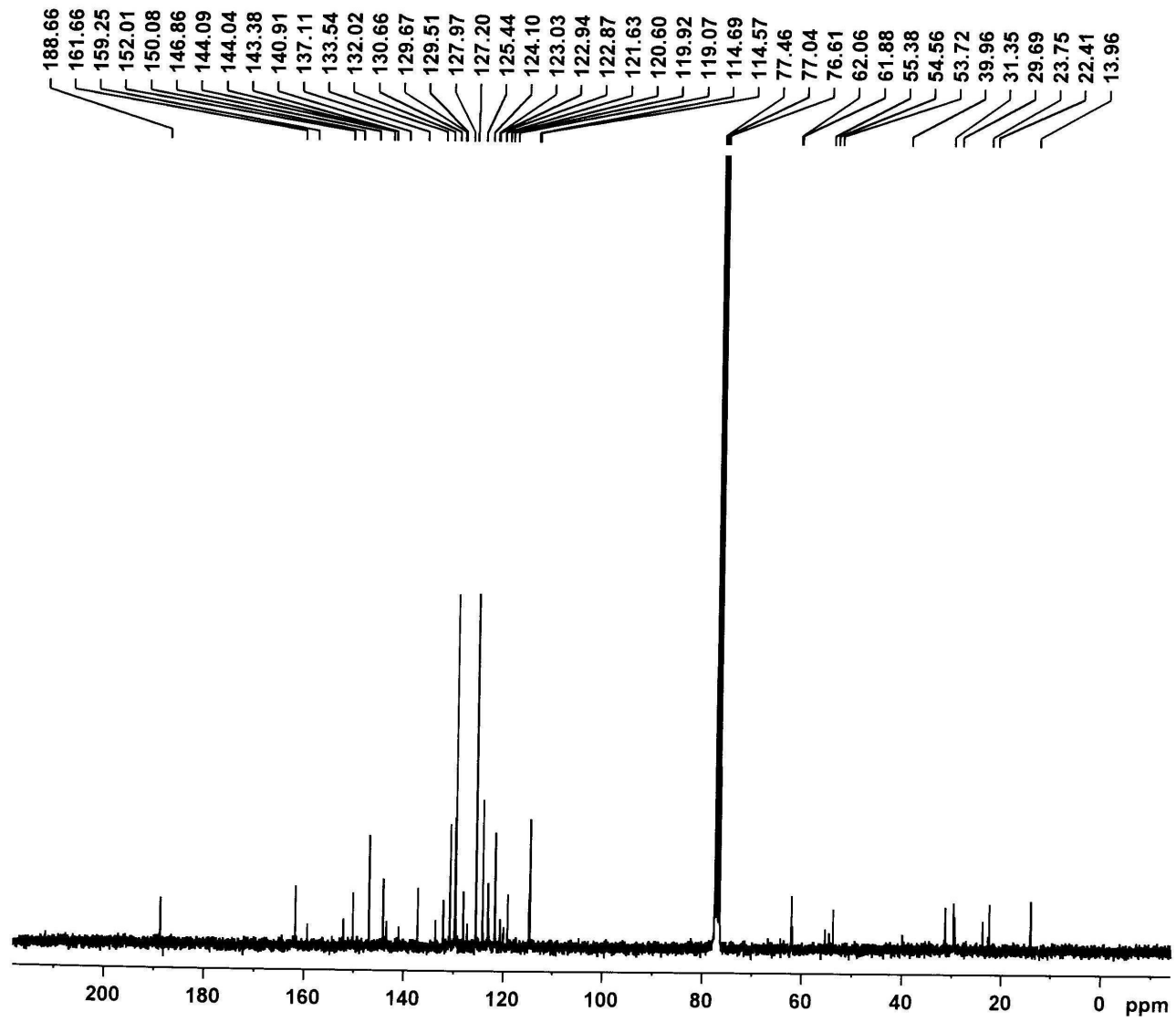
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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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 101.6  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.45 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300058 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 3



Current Data Parameters  
 NAME DA-568  
 EXPNO 2  
 PROCNO 1

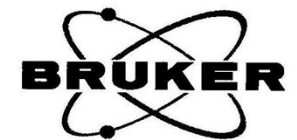
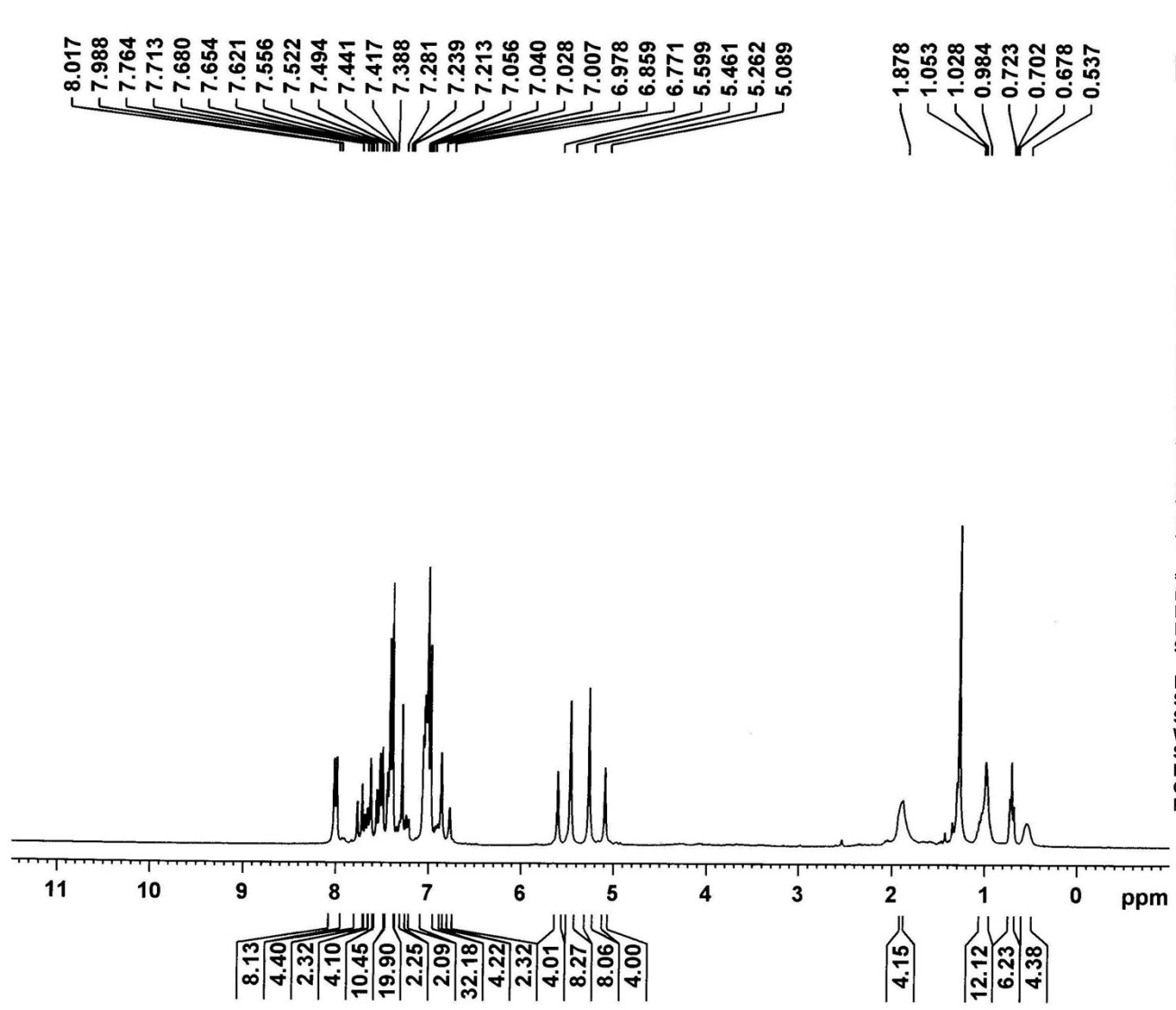
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 Time 0.10  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2000  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 1448.2  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.63 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 16.16 dB  
 PL13 16.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **3**



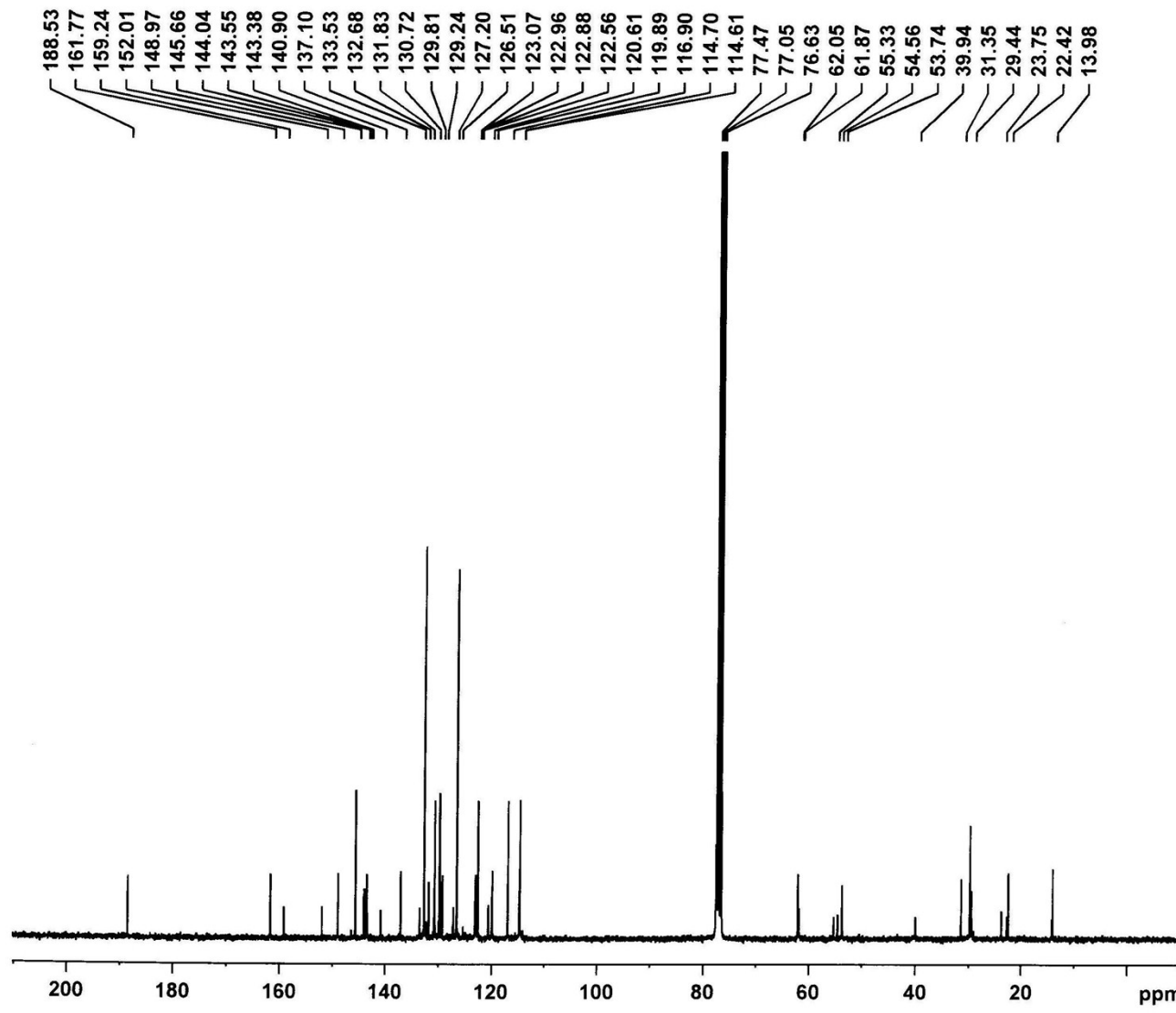
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 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160314  
 Time 7.49  
 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 101.6  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.45 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 4



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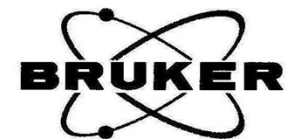
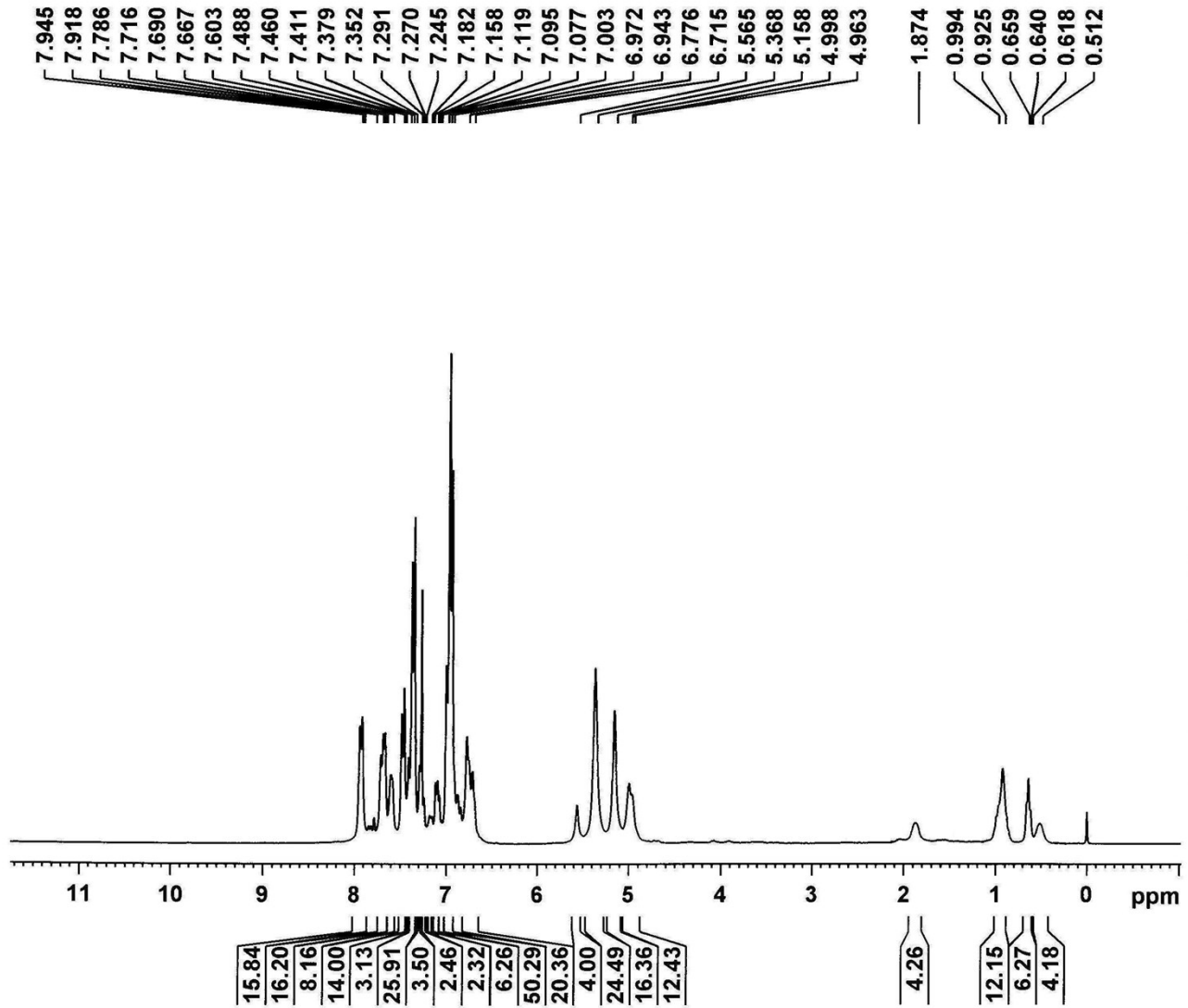
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 PL1 0.00 dB  
 SFO1 75.4752953 MHz

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F2 - Processing parameters  
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<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 4



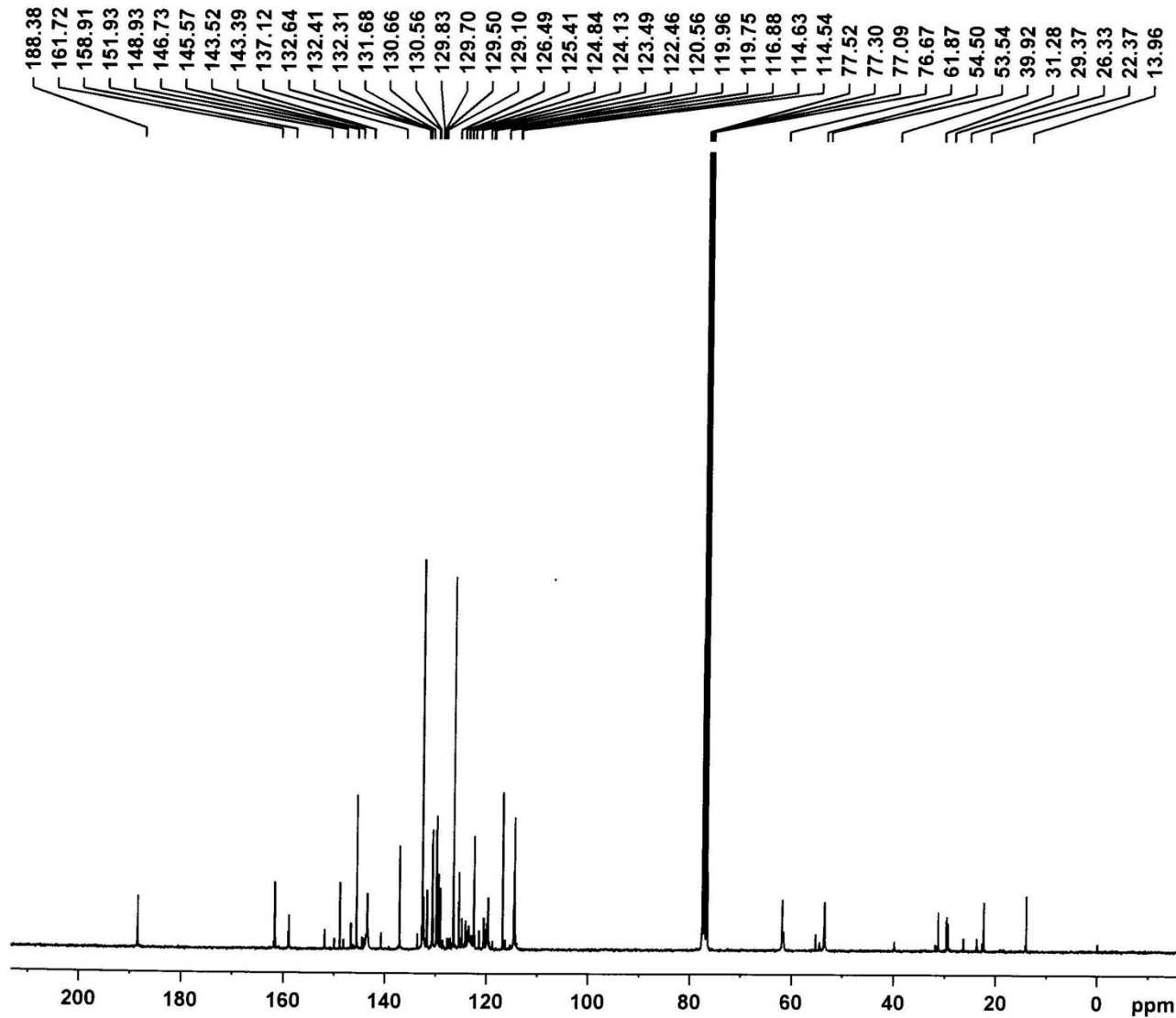
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<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 6



Current Data Parameters  
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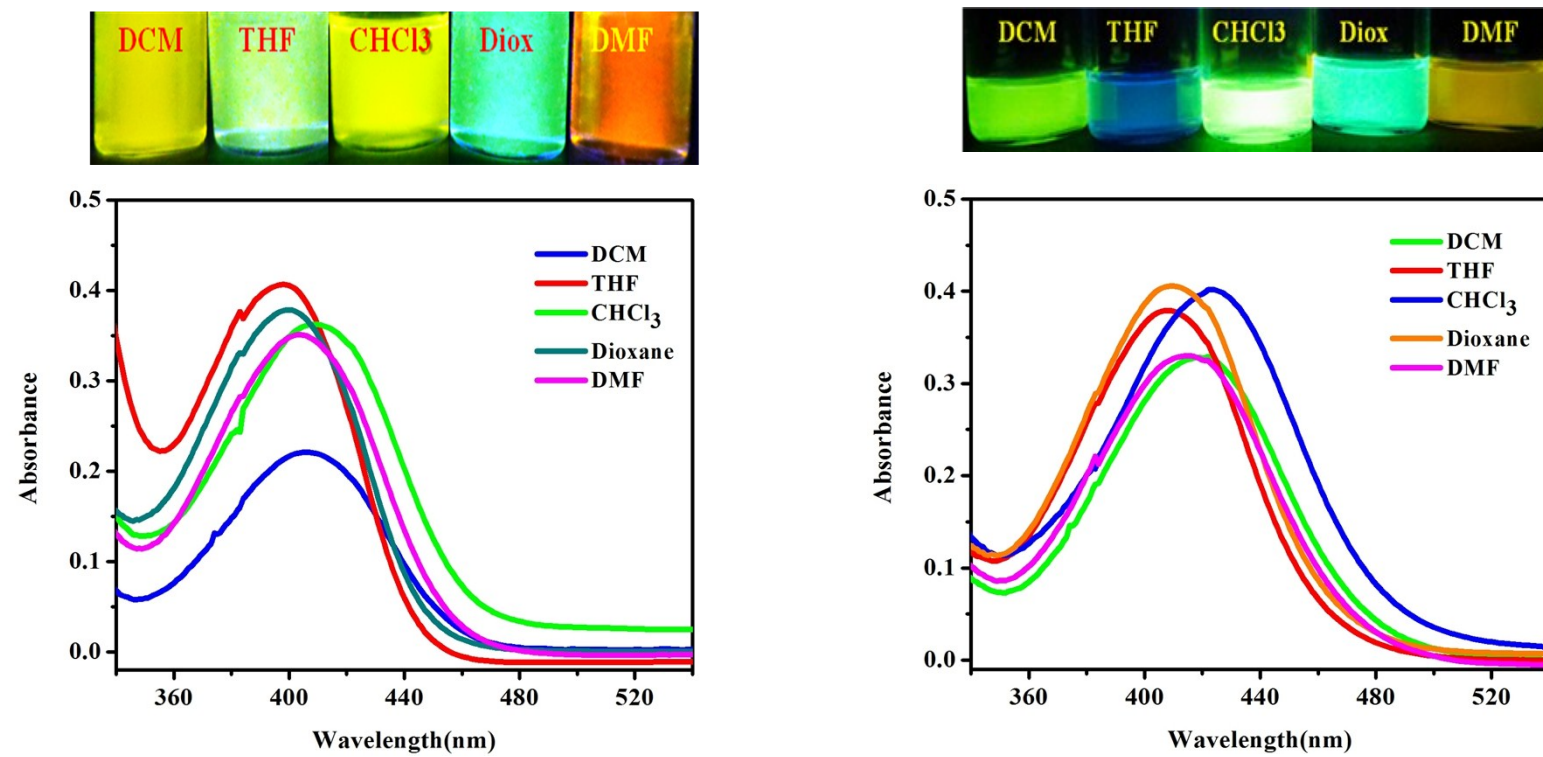
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===== CHANNEL f1 =====  
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 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
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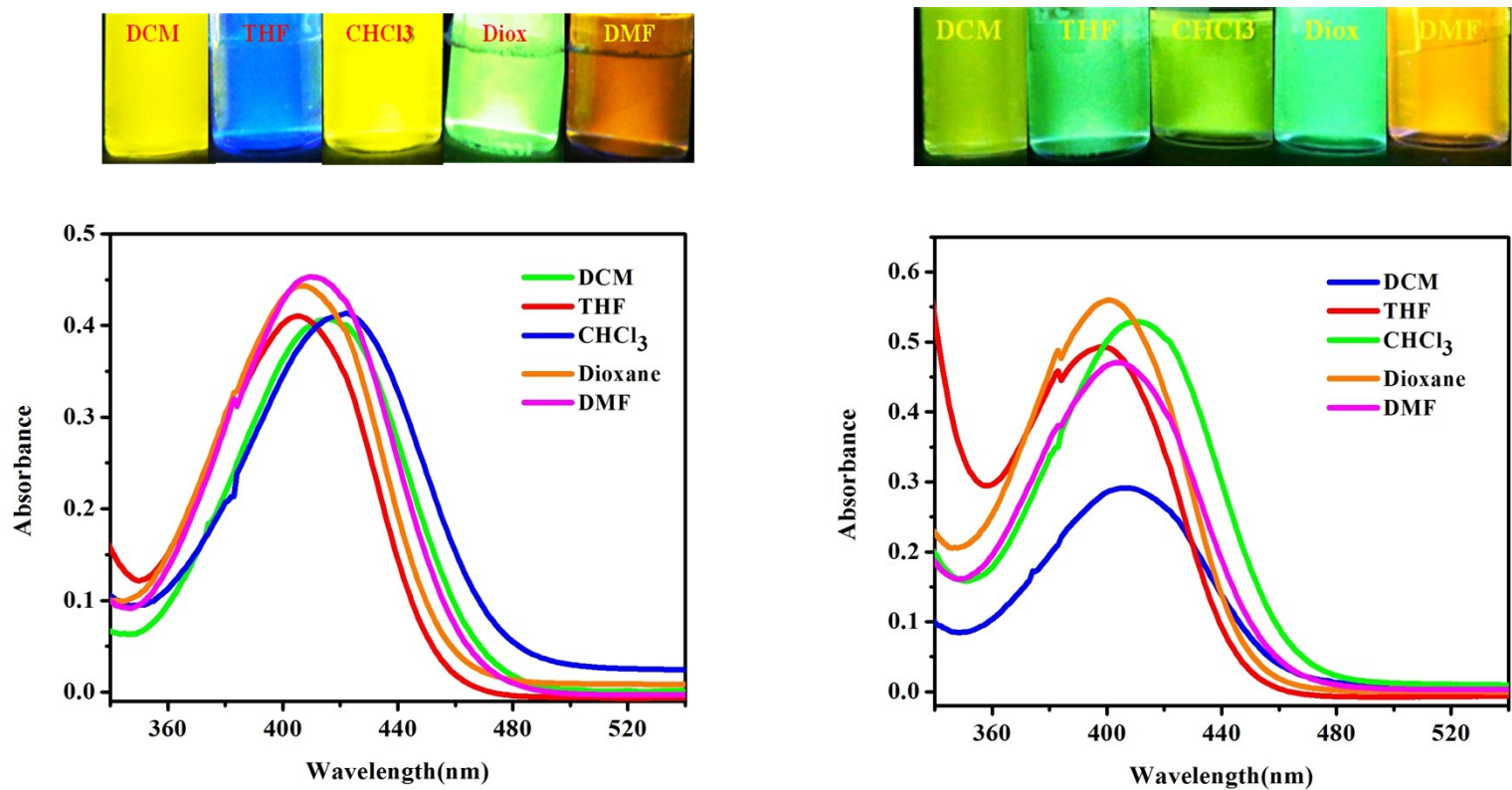
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<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 6



**Figure 1** Absorption spectra of 1 and 2 recorded in selected solvents of different polarity.

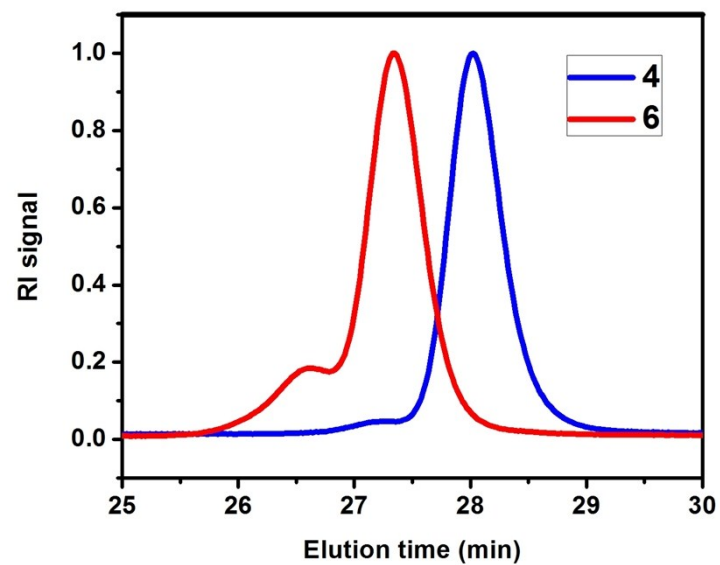




**Figure 2** Absorption spectra of 3 and 4 recorded in selected solvents of different polarity.

**Table 1** Absorption data for compounds **1-4** recorded in different solvents.

<b>Compound</b>	<b>Solvent</b>	$\lambda_{ab}^{max}$ (nm)	$\epsilon_{max}$ (L M <sup>-1</sup> cm <sup>-1</sup> × 10 <sup>6</sup> )
<b>1</b>	DCM	421	0.3275
	THF	408	0.3788
	CHCl <sub>3</sub>	424	0.4022
	Dioxane	410	0.4060
	DMF	415	0.3304
<b>2</b>	DCM	406	0.2208
	THF	398	0.4054
	CHCl <sub>3</sub>	410	0.3636
	Dioxane	400	0.3787
	DMF	404	0.5463
<b>3</b>	DCM	416	0.4060
	THF	406	0.4103
	CHCl <sub>3</sub>	423	0.4132
	Dioxane	407	0.4419
	DMF	410	0.4538
<b>4</b>	DCM	406	0.2919
	THF	399	0.4919
	CHCl <sub>3</sub>	411	0.5282
	Dioxane	401	0.5599
	DMF	405	0.4706



**Fig. 3** GPC diagrams of dendrimers **4** and **6** using THF eluent

**Table 2** Molecular weight data of dendrimers **4** and **6**

S.No	Dendrimers	$M_n$ (g mol <sup>-1</sup> )	$M_w$ (g mol <sup>-1</sup> )	PDI
1	<b>4</b>	3540	3700	1.04
2	<b>6</b>	6380	6960	1.09

### **Fabrication of dye-sensitized solar cells (DSSC)**

The dye-sensitized solar cell (DSSC) was fabricated on a conducting glass covered with fluorinated tin oxide (F: SnO<sub>2</sub>) (FTO) and nanocrystalline TiO<sub>2</sub> coated by reported procedure by Srimanne et al. [P. M. Sirimanne, T. Shirata, T. Soga, J. Solid. State Chem. 166 (2002) 142]. The prepared TiO<sub>2</sub> electrodes were immersed in a  $5 \times 10^{-5}$  M solution of the photosensitizer such as, cis-dithiocyanato bis (2, 2'-bipyridyl- 4,4'-dicarboxylate)- ruthenium (II) (N3 dye) in ethanol for 24 h at room temperature and dried in air and it act as working electrode. The Pt coated conducting plate act as counter electrode. The synthesized triphenylamine chalcone dendrimer derivatives based electrolyte solution was injected into the space between two electrodes. The electrolyte solution was composed of KI is 0.15g ; I<sub>2</sub> is 0.06g, synthesized organic dendrimers is 0.03g additives in 10ml DMF solvent. The active area of newly synthesized dendrimer doped electrolyte based dye-sensitized solar cells is 1 cm<sup>2</sup>. The solar cells activity carried out under illumination of 70 mW cm<sup>-2</sup> at AM 1.5.