

## SUPPLEMENTARY INFORMATION

### **Synthesis, photophysical, electrochemical and DSSC application of novel donor-acceptor triazole bridged dendrimers with triphenylamine core and benzoheterazole as surface unit**

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## S-1 Abbreviations

TPA	:	Triphenylamine
$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$	:	Copper sulphate pentahydrate
NaAsc	:	Sodium ascorbate
$\text{CDCl}_3$	:	Chloroform-d
DMSO- $d_6$	:	Dimethyl sulfoxide- $d_6$
UV	:	Ultraviolet
CV	:	Cyclic Voltammetry
DFT	:	Density functional theory
ESI-Mass	:	Electrospray ionization
NMR	:	Nuclear Magnetic Resonance

## S-2

### General procedure for dendritic chloride

A mixture of 2-(4-(azidomethyl)phenyl)benzoheterazole **13** and **14** (2.2 equiv.) and 3,5-bis(propargloxy) benzyl chloride **16** (1.0 equiv.) was dissolved in a mixture of t-BuOH and water (1:1; 20 mL) and sodium ascorbate (10 mol%) was added followed by the addition of CuSO<sub>4</sub>·5H<sub>2</sub>O (5 mol%). The reaction mixture was stirred for 12 h at room temperature and then the solvent was evaporated, the crude product was dissolved with CHCl<sub>3</sub> (3 x100 mL), washed with water (200 mL) and brine (50 mL), dried over Na<sub>2</sub>SO<sub>4</sub> and concentrated to give the crude triazole, which was purified by column chromatography (SiO<sub>2</sub>) with CHCl<sub>3</sub> or CHCl<sub>3</sub>-MeOH as eluent to give the corresponding dendritic chlorides.

### Dendritic chloride 17 (G1-Cl)

Yield: 90%; mp: 154-156 °C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 4.47 (s, 2H); 5.16 (s, 4H); 5.55 (s, 4H); 6.56 (s, 4H); 6.61 (s, 2H); 7.07 (d, *J* = 16.2 Hz, 2H); 7.30 (t, *J* = 8.7 Hz, 8H); 7.53 (t, *J* = 5.1 Hz, 2H); 7.59 (d, *J* = 7.2 Hz, 6H); 7.71 (t, *J* = 4.8 Hz, 3H); 7.75 (d, *J* = 16.5 Hz, 1H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>C</sub> 46.9, 53.8, 62.1, 101.9, 108.0, 110.3, 115.0, 119.9, 123.0, 124.6, 125.4, 128.2, 128.6, 135.7, 135.8, 138.2, 140.0, 142.1, 144.3, 150.4, 159.4, 162.4. ESI-MS *m/z* 825 [M + H]<sup>+</sup>. Anal. Calcd. for C<sub>45</sub>H<sub>35</sub>ClN<sub>8</sub>O<sub>4</sub>: C, 68.65; H, 4.48; N, 14.23. Found: C, 68.74; H, 4.55; N, 14.18.

### Dendritic chloride 18 (G1-Cl)

Yield: 87%; mp: 184-188 °C; <sup>1</sup>H NMR (300 MHz, DMSO-d<sub>6</sub>): δ<sub>H</sub> 4.66 (s, 2H); 5.15 (s, 4H); 5.66(s, 4H); 6.72 (s, 2H); 7.37 (d, *J* = 7.5 Hz, 4H); 7.45 (d, *J* = 7.5 Hz, 2H); 7.52 (t, *J* = 7.8 Hz, 2H); 7.64 (s, 4H); 7.79 (d, *J* = 7.5 Hz, 4H); 7.98 (d, *J* = 7.8 Hz, 2H); 8.09 (d, *J* = 7.5 Hz, 2H); 8.33 (s, 2H). <sup>13</sup>C NMR (75 MHz, DMSO-d<sub>6</sub>): δ<sub>C</sub> 45.9, 52.5, 61.2, 101.4, 107.9,

122.2, 122.5, 124.7, 125.4, 126.5, 128.0, 128.4, 134.0, 135.0, 136.6, 137.1, 139.7, 142.8, 153.4, 159.1, 166.2. ESI-MS  $m/z$  818  $[M + H]^+$ . Anal.Calcl.for  $C_{45}H_{35}ClN_8O_2S_2$ : C, 65.96; H, 4.31; N, 13.68. Found: C, 66.05; H, 4.38; N, 13.60.

### General procedure for dendritic azide

To the corresponding dendritic chloride **17** and **18** (1.0 equiv.) in dry DMF (10 mL), sodium azide (1.5 equiv.) was added and stirred at room temperature for 24 h. The reaction mixture was poured into the water (50 mL) and extracted with  $CHCl_3$  (3 x100 mL). The organic layer was washed with water (100 mL) and brine (50 mL), dried over  $Na_2SO_4$ . The solvent was evaporated under reduced pressure to afford the crude product, which was purified by column chromatography ( $SiO_2$ ), using  $CHCl_3$  or  $CHCl_3$ -MeOH as eluent to give the corresponding first generation dendritic azides.

### Dendritic azide 19 (G1-N<sub>3</sub>)

Yield: 87%; mp: 168-172 °C;  $^1H$  NMR (300 MHz, DMSO- $d_6$ ):  $\delta$  4.34 (s, 2H); 5.14 (s, 4H); 5.65 (s, 4H); 6.64 (s, 2H); 6.72 (s, 1H); 7.36 (t,  $J = 7.2$  Hz, 9 H); 7.70-7.80 (m, 10 H); 8.23 (s, 2 H).  $^{13}C$  NMR (75 MHz, DMSO- $d_6$ ):  $\delta_c$  40.1, 52.5, 61.1, 101.1, 107.4, 110.5, 114.1, 119.5, 124.7, 124.8, 125.5, 128.2, 128.4, 134.7, 137.4, 137.8, 138.7, 141.5, 142.8, 149.7, 159.2, 162.2. ESI-MS  $m/z$  793  $[M + H]^+$ . Anal.Calcl.for  $C_{45}H_{35}N_{11}O_4$ : C, 68.09; H, 4.44; N, 19.41. Found: C, 68.09; H, 4.54; N, 19.34.

### Dendritic azide 20 (G1-N<sub>3</sub>)

Yield: 86%; mp: 164-168 °C;  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta$  4.22 (s, 2H); 5.15 (s, 4H); 5.52 (s, 4H); 6.53 (s, 2H); 6.57 (s, 1H); 7.27 (d,  $J = 7.8$  Hz, 4H); 7.35 (d,  $J = 5.7$  Hz, 2H); 7.40 (s, 2H); 7.44 (d,  $J = 5.9$  Hz, 3H); 7.50 (d,  $J = 5.7$  Hz, 1H); 7.56 (t,  $J = 8.1$  Hz, 6H); 7.84 (d,  $J = 7.8$  Hz, 2H), 7.98 (d,  $J = 8.1$ Hz, 2H).  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ):  $\delta_c$  53.8, 54.6, 62.1, 101.7, 107.5, 121.5, 122.8, 123.0, 125.5, 126.4, 128.0, 128.6, 134.4, 135.4, 136.0,

136.3, 137.8, 144.3, 153.8, 159.6, 166.5. ESI-MS  $m/z$  825  $[M + H]^+$ . Anal.Calcl.for  $C_{45}H_{35}N_{11}O_2S_2$ : C, 65.44; H, 4.27; N, 18.65. Found: C, 65.44; H, 4.37; N, 18.58.

### **General procedure for bis and tris[4-(trimethylsilylethynyl)phenyl]phenylamine or amine**

A flame-dried Schlenk tube was charged with di and tribromo triphenylamine (1 equiv.),  $PdCl_2(PPh_3)_2$  (0.06 equiv. / 0.08 equiv.), CuI (0.03 equiv. / 0.04 equiv.), and  $PPh_3$  (0.02 equiv. / 0.06 equiv.) in dry THF and  $Et_3N$  (3:1 / 1:3 ratio) were added and the mixture was degassed by three successive nitrogen cycles. Trimethylsilylacetylene (3.0 equiv. / 4.5 equiv.) was added, the Schlenk tube was sealed, once addition is over the reaction mixture turned black. The reaction mixture was heated at 80 °C for 3 h and then cooled to room temperature. After the completion of the reaction, the reaction mixture was diluted with DCM (150 mL), filtered over Celite, and concentrated under reduced pressure, which was purified silica gel column chromatography with gradient elution of hexane-ethyl acetate (95:5) to give trimethylsilylated ethynyl compounds.

### **N, N'-bis-[4-(trimethylsilylethynyl)phenyl]phenylamine 23**

Yield: 70%; mp: 148-152°C;  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta_H$  0.23 (s, 18H); 6.95 (d,  $J = 8.4$  Hz, 4H); 7.06 (d,  $J = 8.4$  Hz, 2H); 7.26 (d,  $J = 3.6$  Hz, 2H); 7.32 (d,  $J = 8.4$  Hz, 6H).  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ):  $\delta_C$  0.01, 93.5, 105.1, 117.0, 123.2, 124.1, 125.4, 129.5, 133.1, 146.4, 147.3.

### **N, N', N''-tris-[4-(trimethylsilylethynyl)phenyl]phenylamine 24**

Yield: 82%; mp: 148-152°C;  $^1H$  NMR (300 MHz,  $CDCl_3$ ):  $\delta_H$  0.26 (s, 27H); 6.98 (d,  $J = 8.4$  Hz, 6H); 7.36 (d,  $J = 8.4$  Hz, 6H).  $^{13}C$  NMR (75 MHz,  $CDCl_3$ ):  $\delta_C$  0.38, 94.3, 105.2, 118.2, 124.1, 133.5, 147.1.

### **Bis and tris(4-ethynylphenyl)phenylamine or amine**

Anhydrous potassium carbonate (5 equiv. / 7.5 equiv.) was added to a mixture of bis and tris [4-(trimethylsilylethynyl)phenyl]phenylamine or amine (1 equiv.) in dry methanol (50 mL), and the mixture was stirred for 24 h at room temperature. The mixture was concentrated at reduced pressure, and the residue was taken in DCM (150 mL) and filtered over celite. The filtrate was evaporated and the solid was dried under vacuum. The title of the compounds was obtained as yellow solid.

### **N, N'-Bis-(4-ethynylphenyl)phenylamine 25**

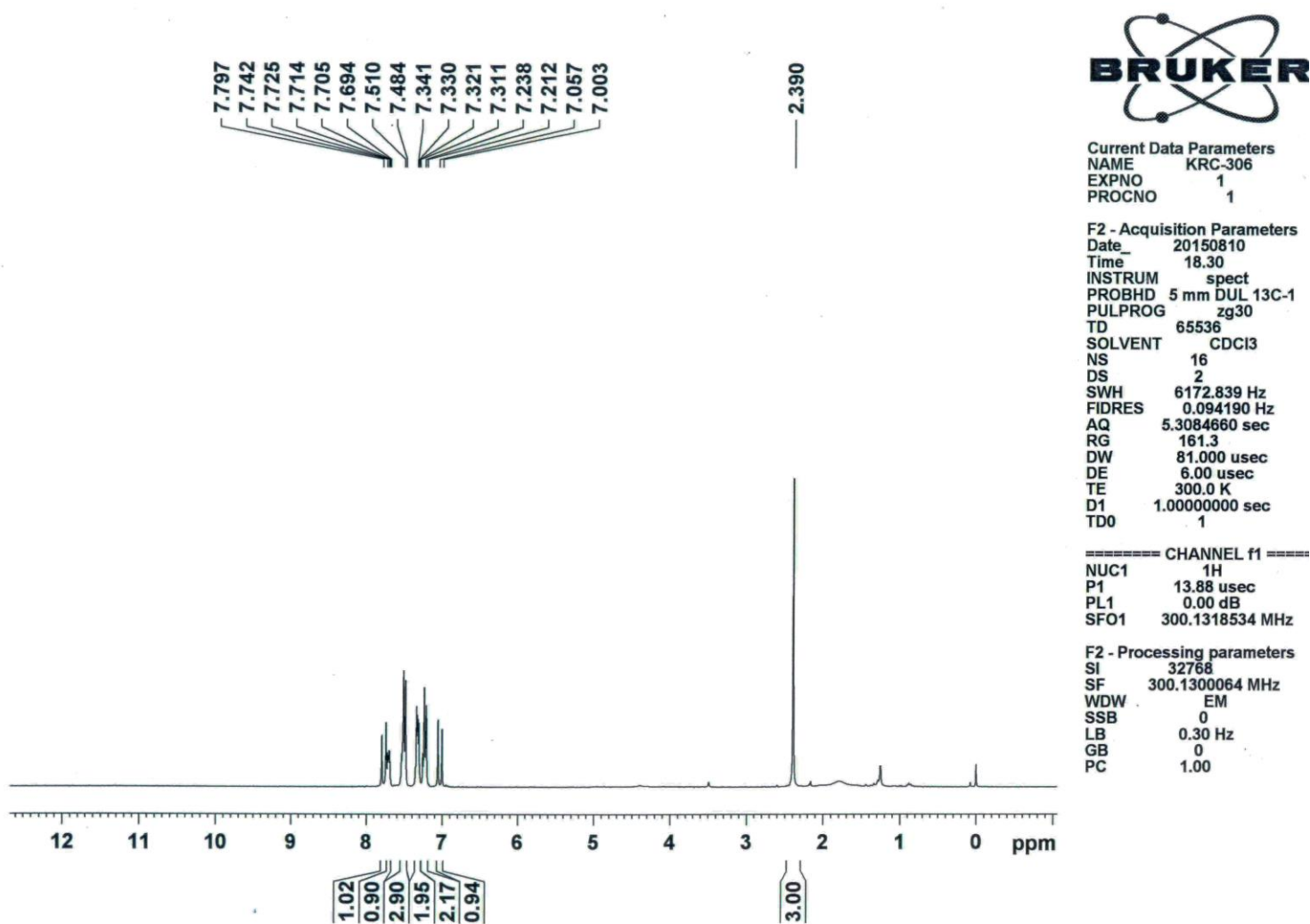
Yield: 90%; mp: 94-96°C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 3.04 (s, 2H); 6.99 (d, *J* = 8.7 Hz, 4H); 7.09 (d, *J* = 8.1 Hz, 2H); 7.29 (t, *J* = 7.8 Hz, 1H); 7.35 (d, *J* = 8.4 Hz, 6H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>c</sub> 76.6, 83.6, 115.9, 123.1, 124.3, 125.5, 129.6, 133.2, 146.5, 147.6.

### **N, N', N''-Tris-(4-ethynylphenyl)phenylamine 26**

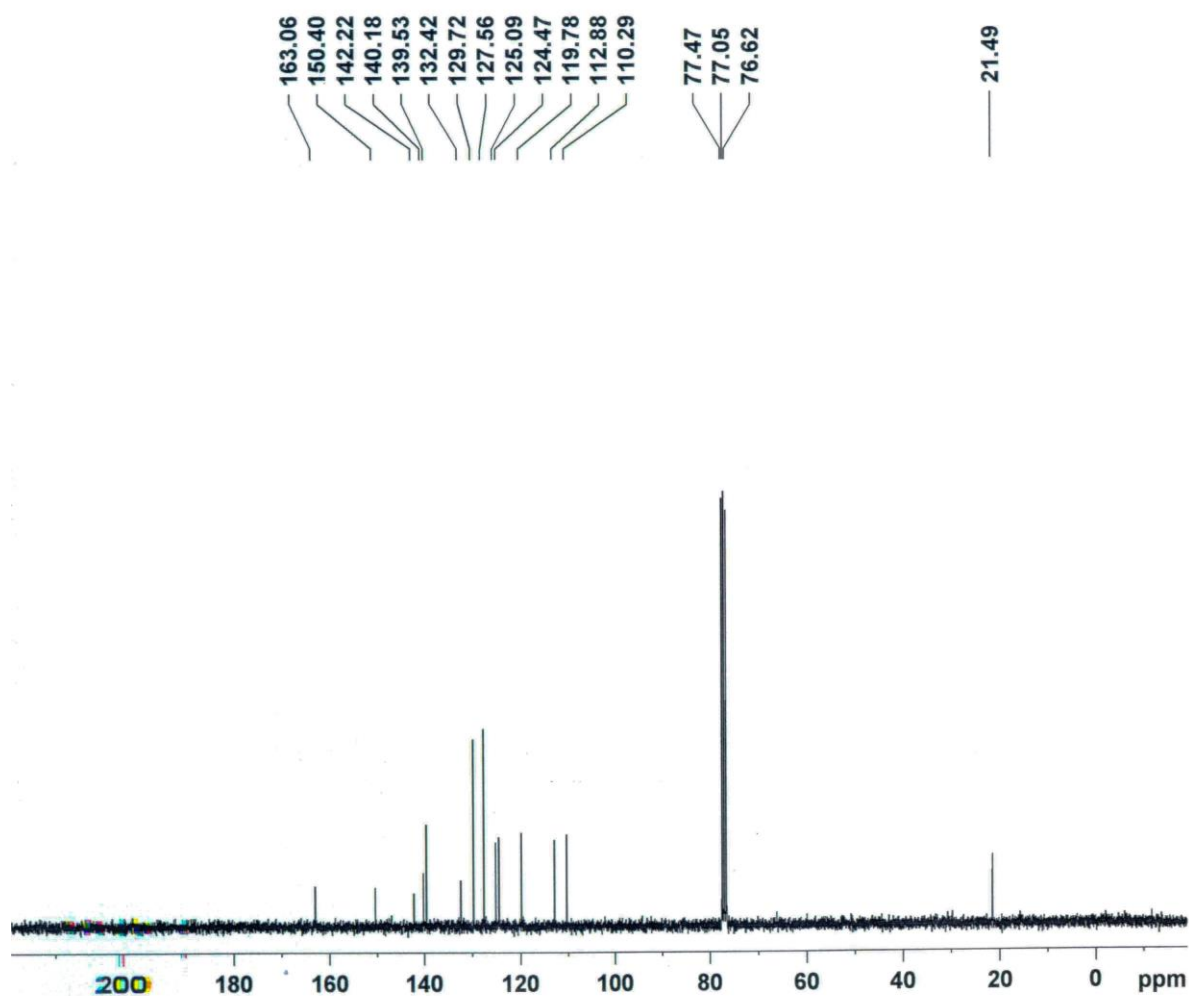
Yield: 80%; mp: 96-98°C; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 3.05 (s, 3H); 7.00 (d, *J* = 8.4 Hz, 6H); 7.38 (d, *J* = 8.4 Hz, 6H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>c</sub> 77.0, 83.4, 116.8, 124.0, 133.3, 147.0.

S-3

### Spectroscopic data



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the compound 9



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$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **9**



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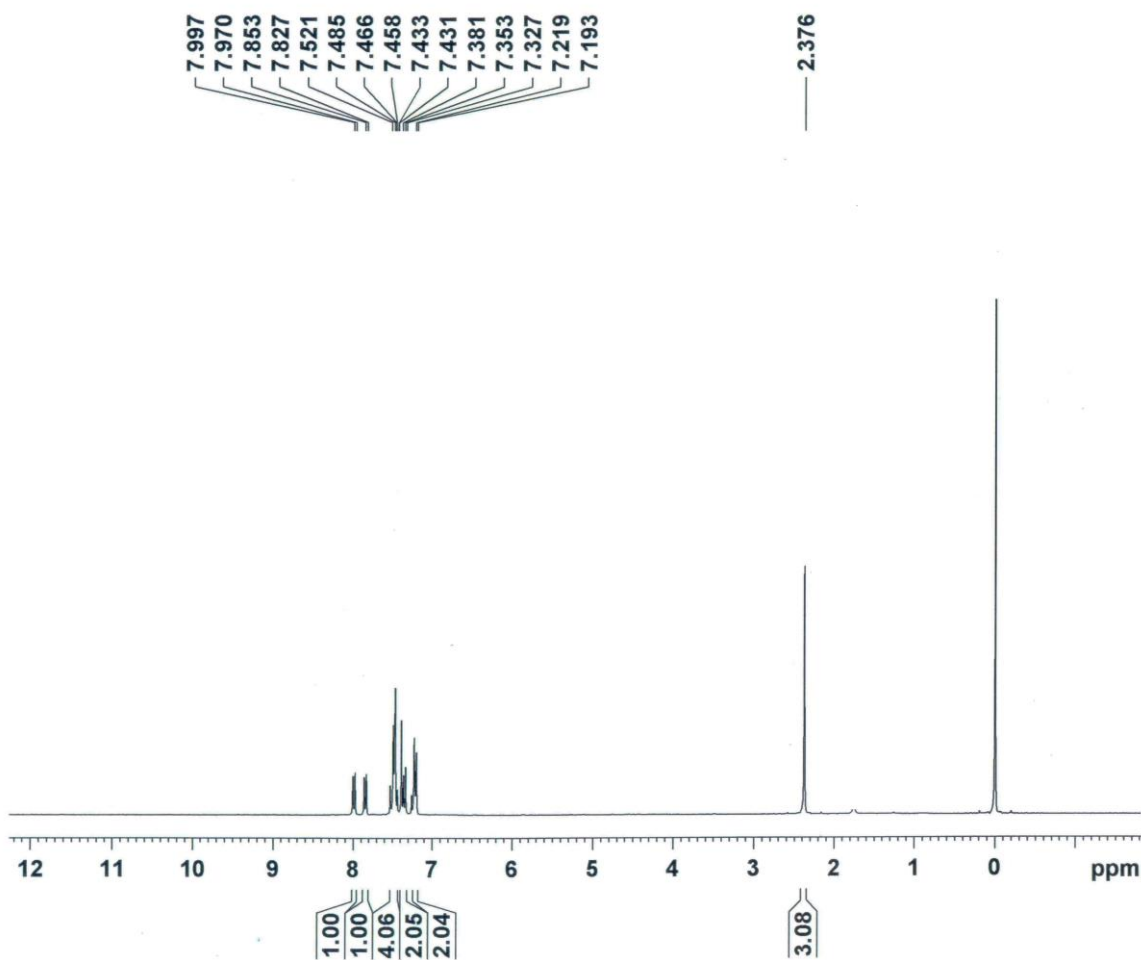


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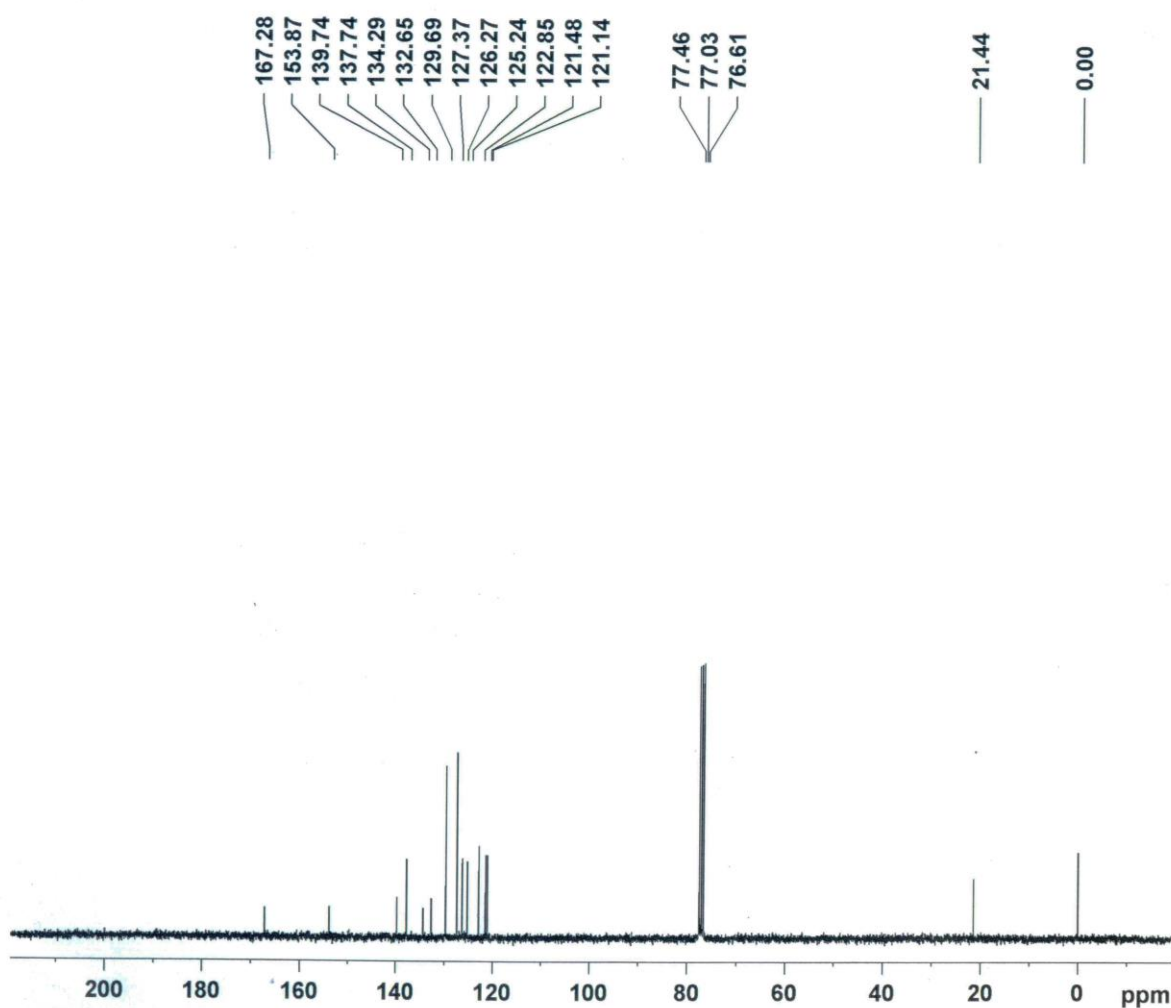
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$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **10**

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$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **10**



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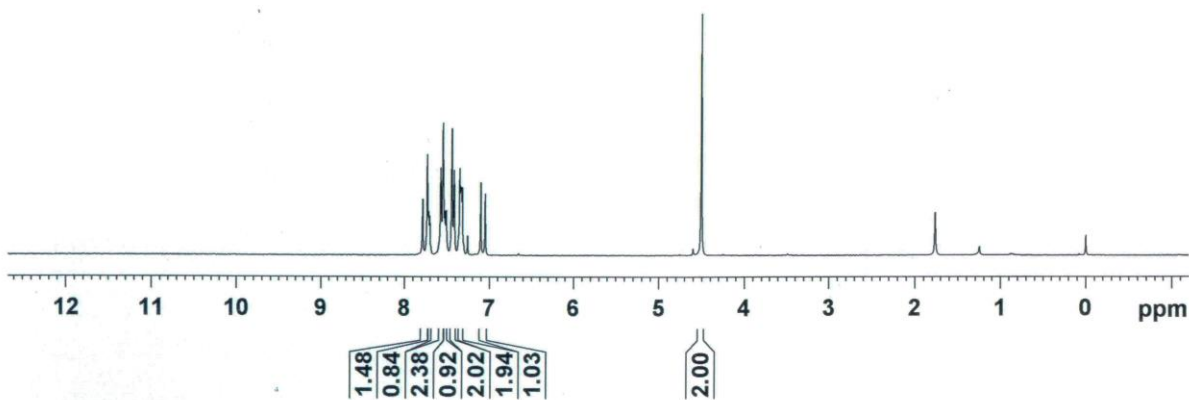
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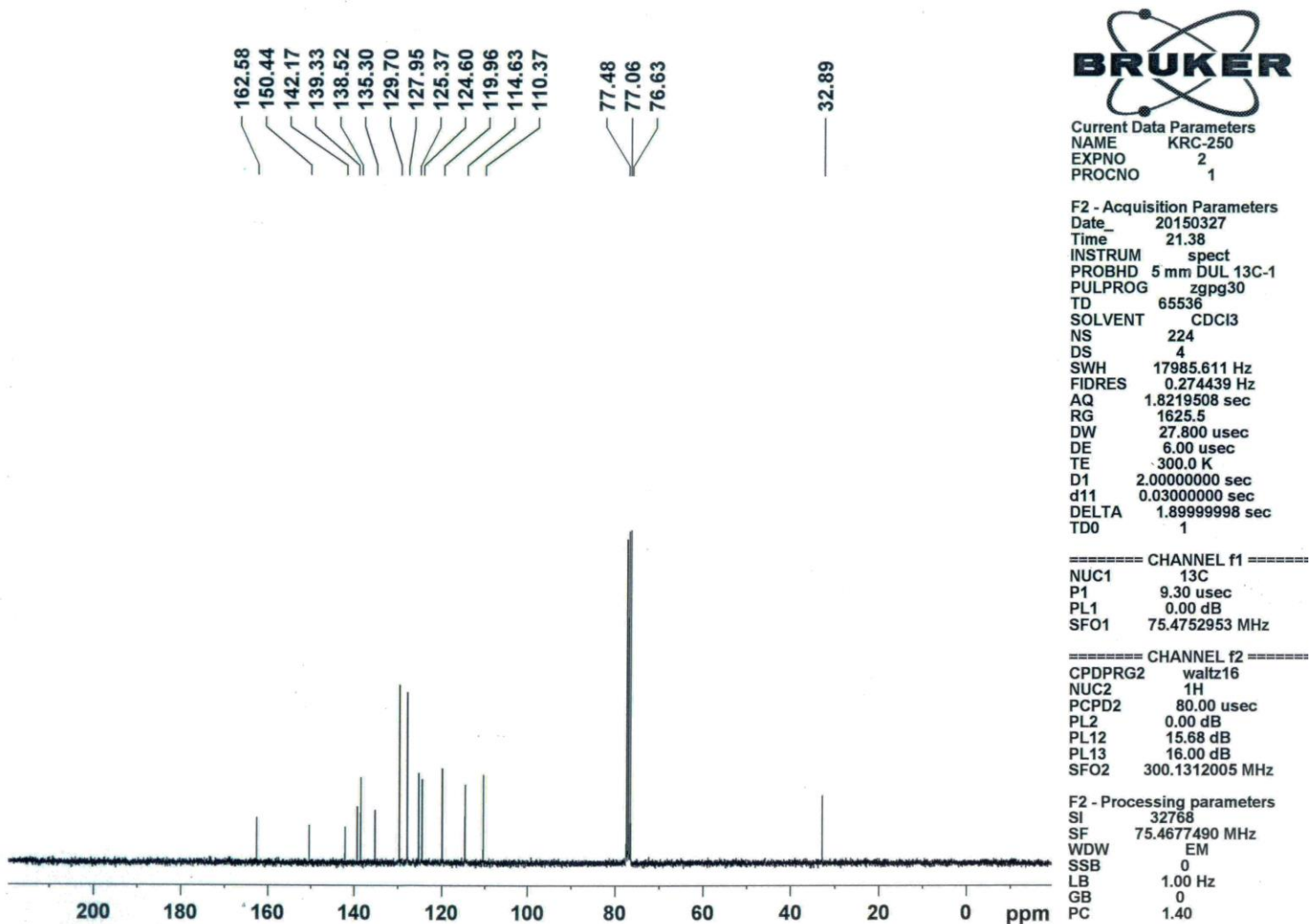
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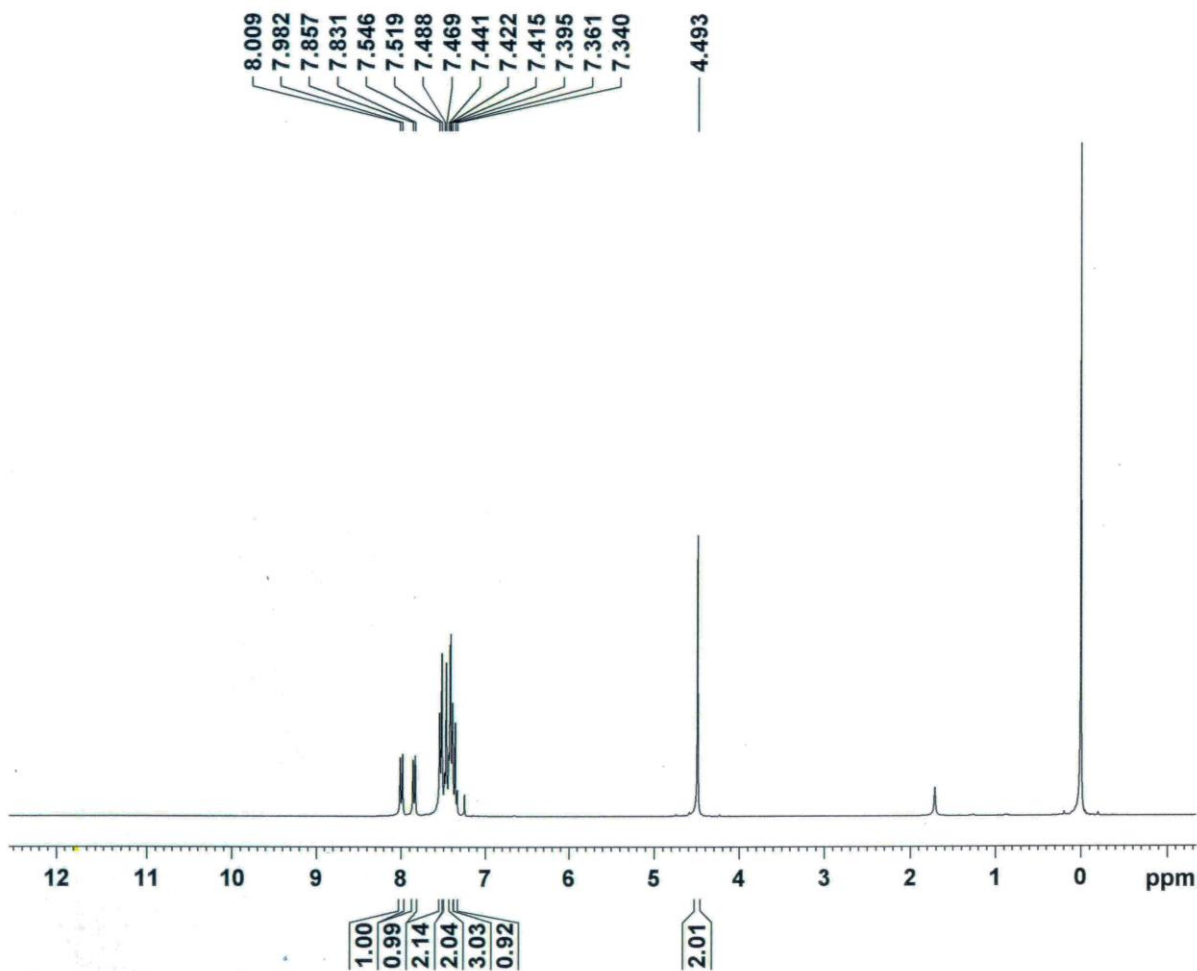
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4.505



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **11**



<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) spectrum of the compound **11**



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$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **12**



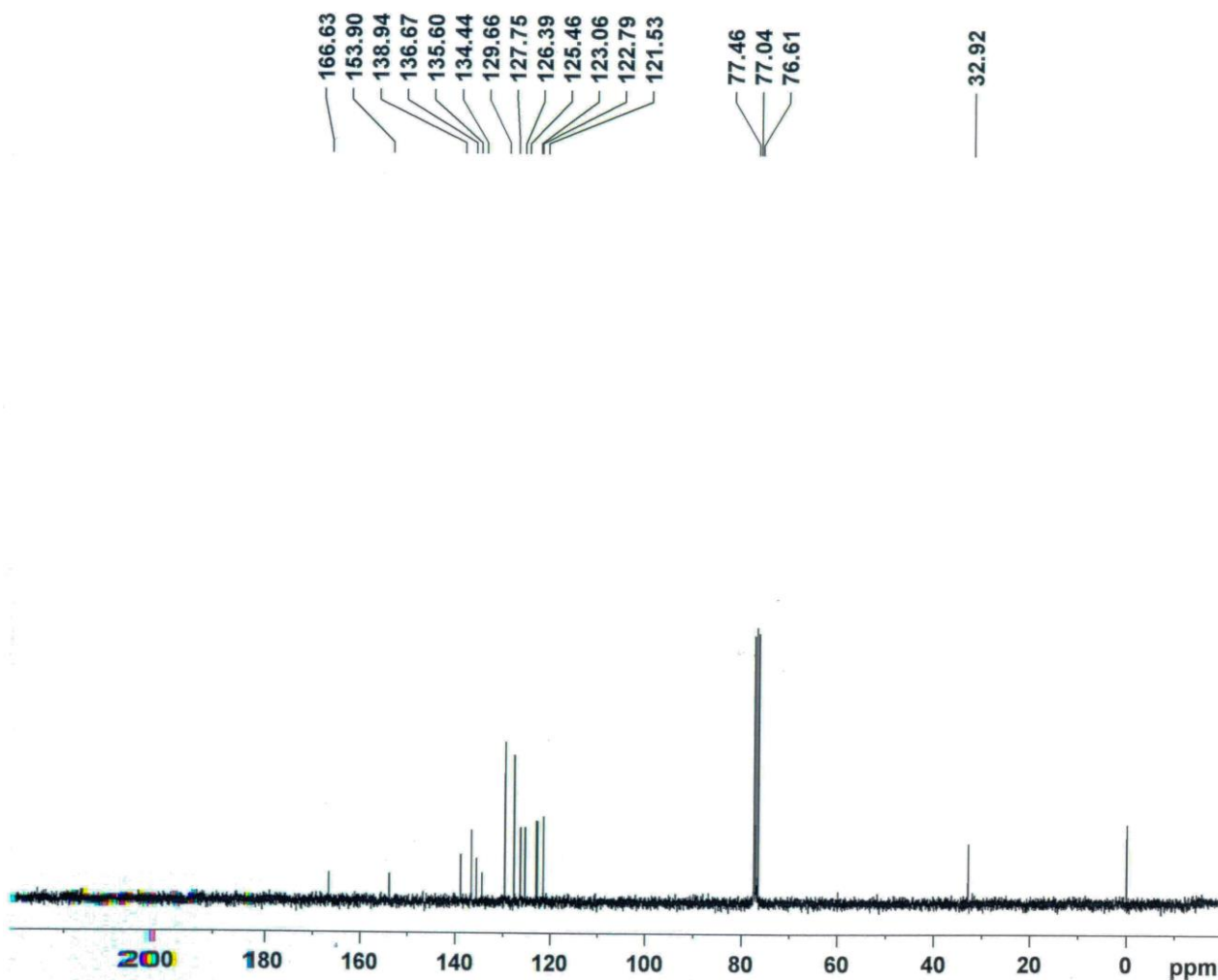
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$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **12**

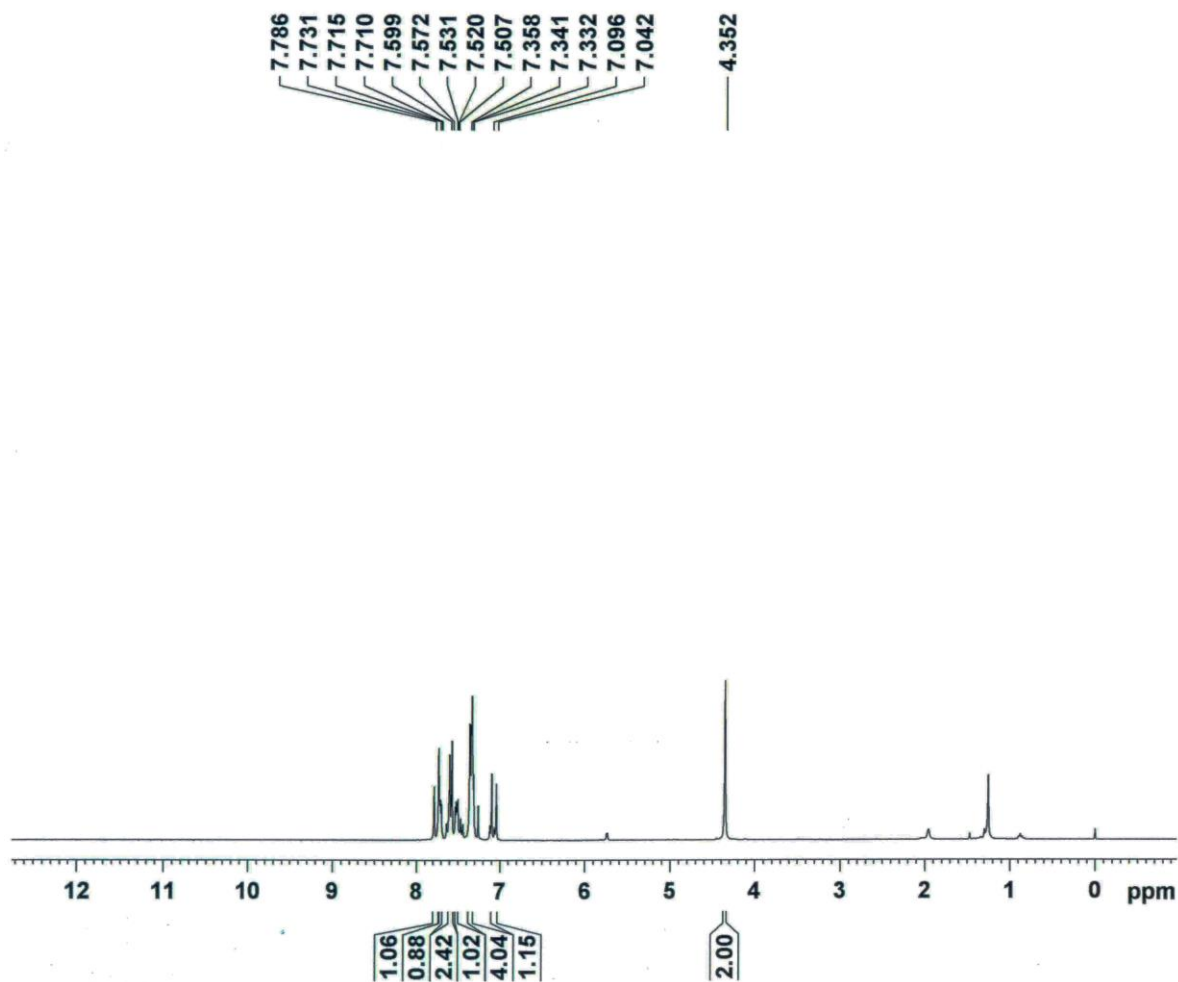


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$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **13**

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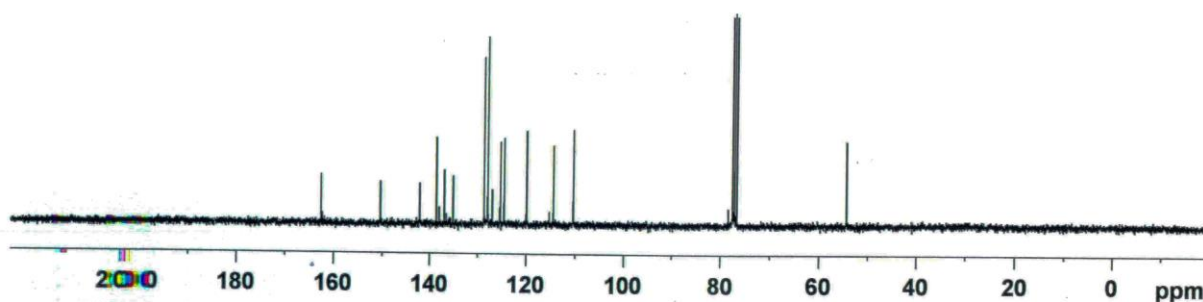
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DE 6.00 usec  
TE 300.0 K  
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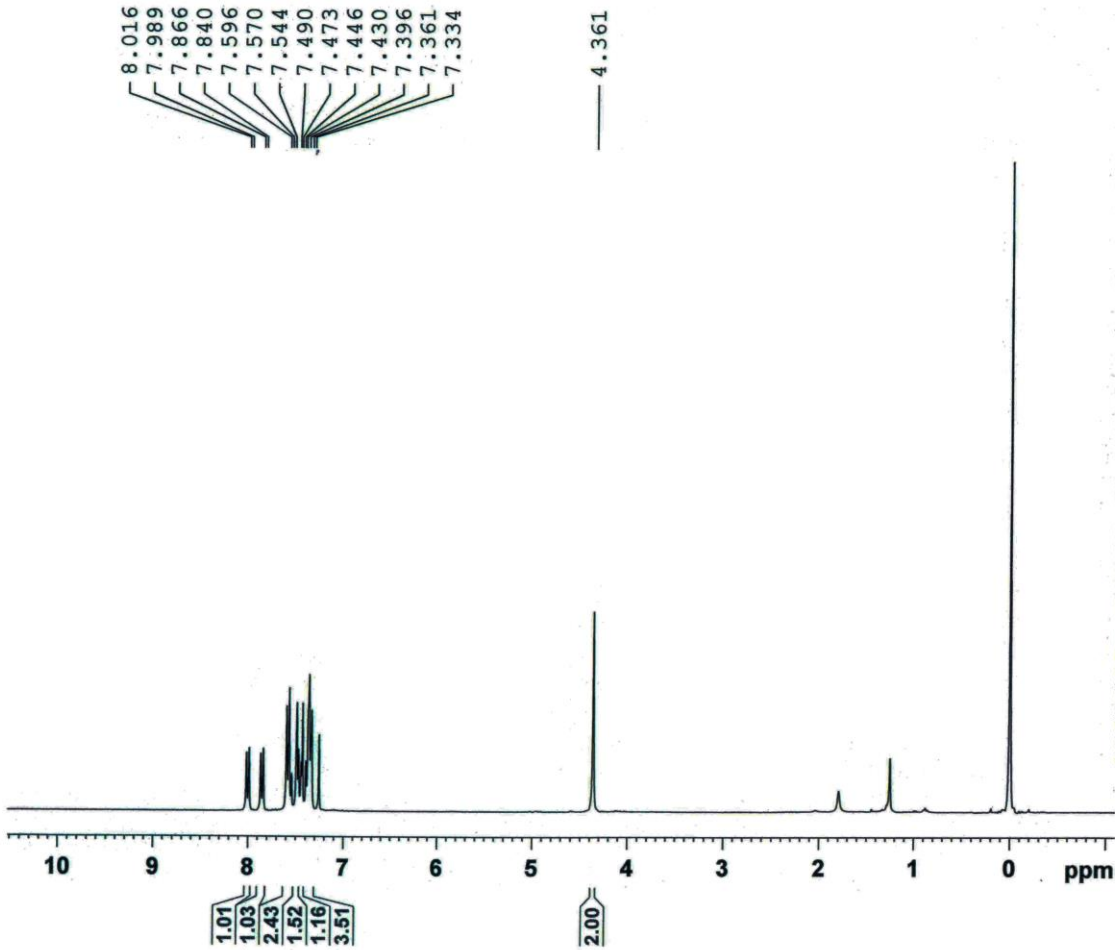
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$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **13**



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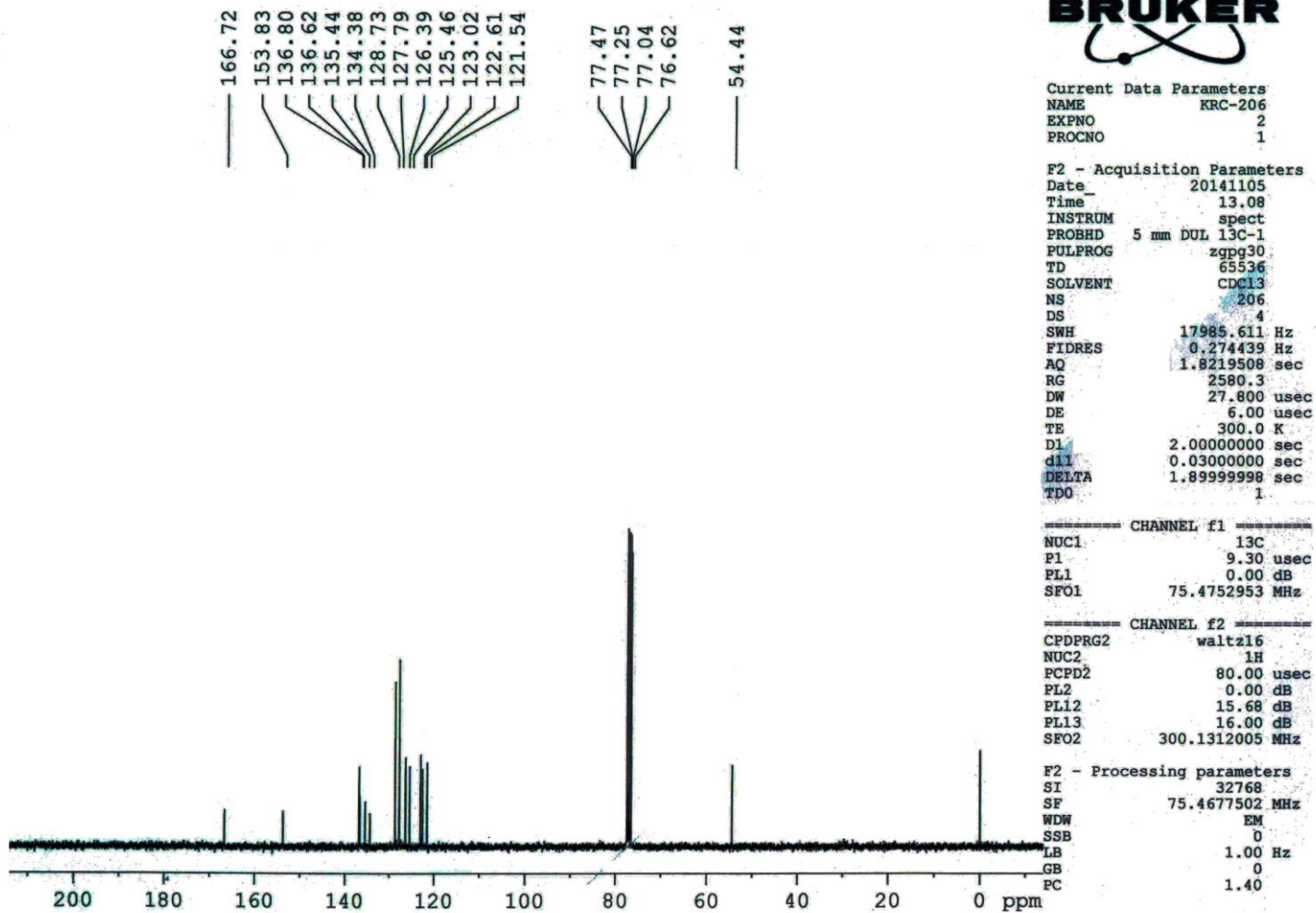
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DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

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

F2 - Processing parameters  
SI 32768  
SF 300.1300085 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

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



$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **14**

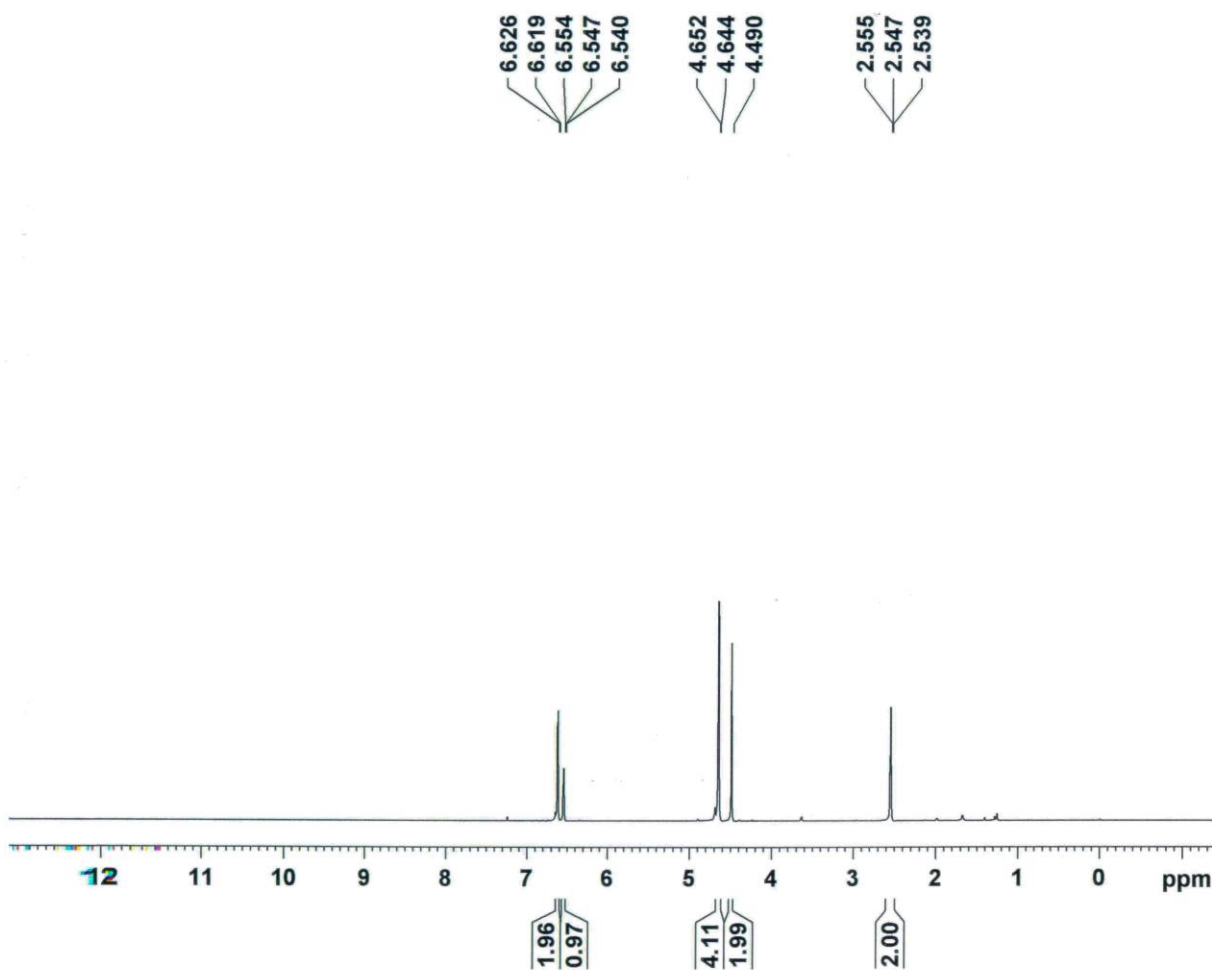


Current Data Parameters  
NAME KR-14  
EXPNO 1  
PROCNO 1

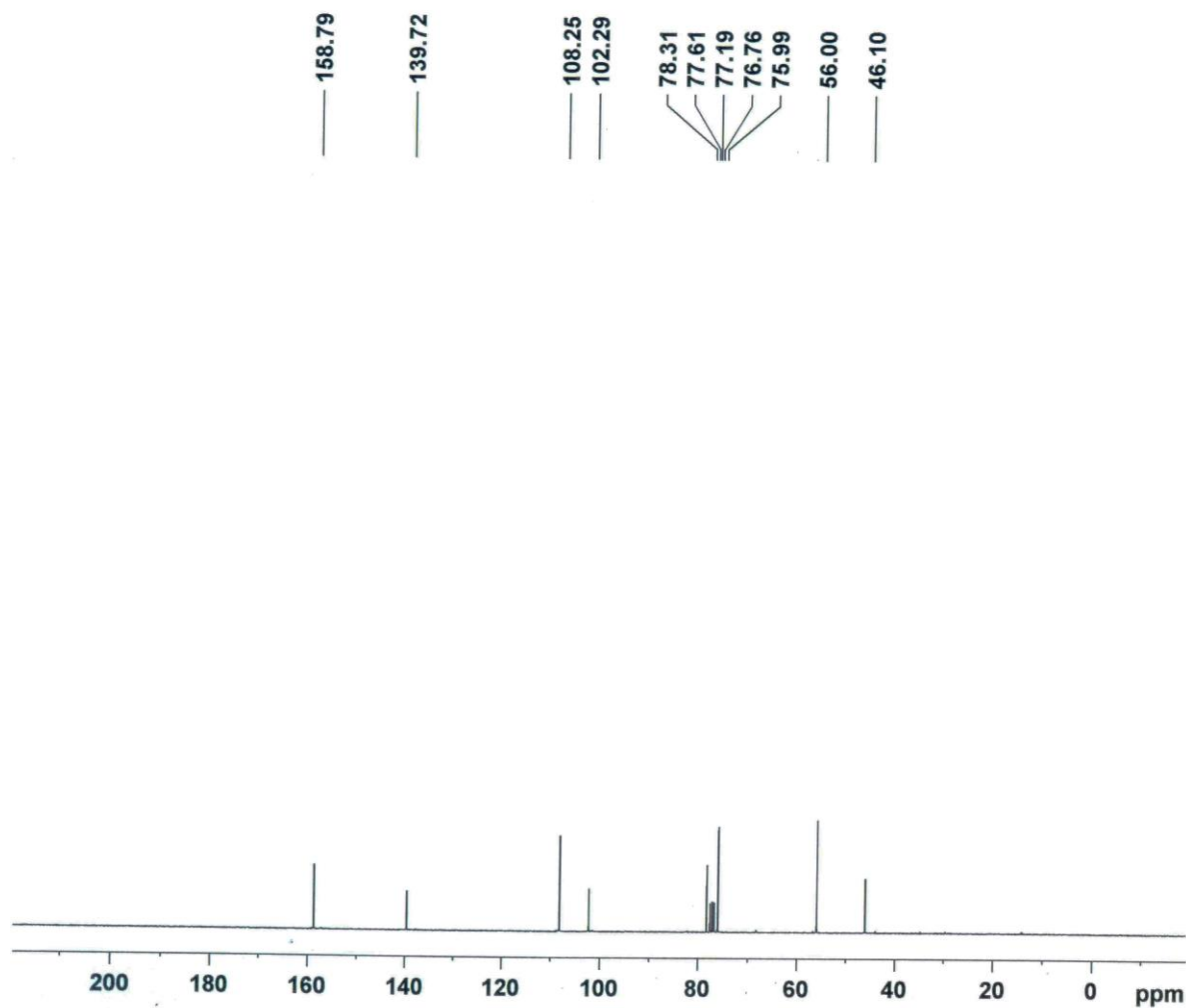
F2 - Acquisition Parameters  
Date\_ 20130404  
Time 20.10  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 11  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 28.5  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

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

F2 - Processing parameters  
SI 32768  
SF 300.1300113 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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



Current Data Parameters  
 NAME KR-14  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20130404  
 Time 20.17  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 126  
 DS 4  
 SV 1 17985.611 Hz  
 FI RES 0.274439 Hz  
 AC 1.8219508 sec  
 RC 2580.3  
 DV 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d1 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 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 75.4677490 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>) spectrum of the compound **16**



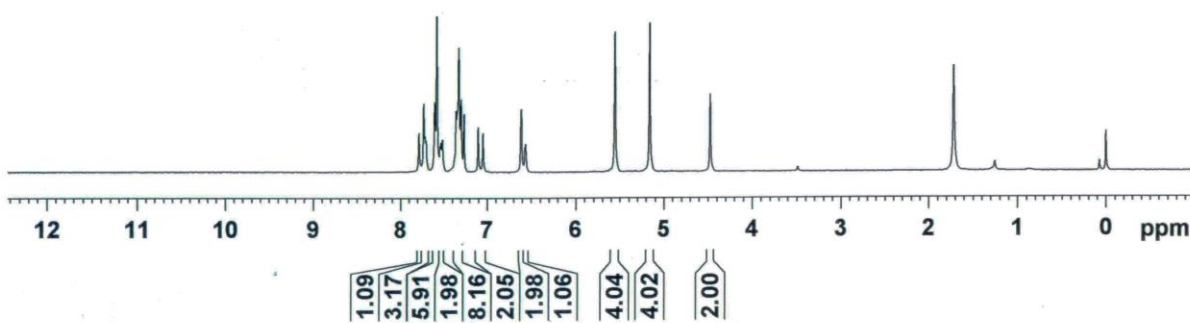
Current Data Parameters  
 NAME KRC-261  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150411  
 Time 13.19  
 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 256  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

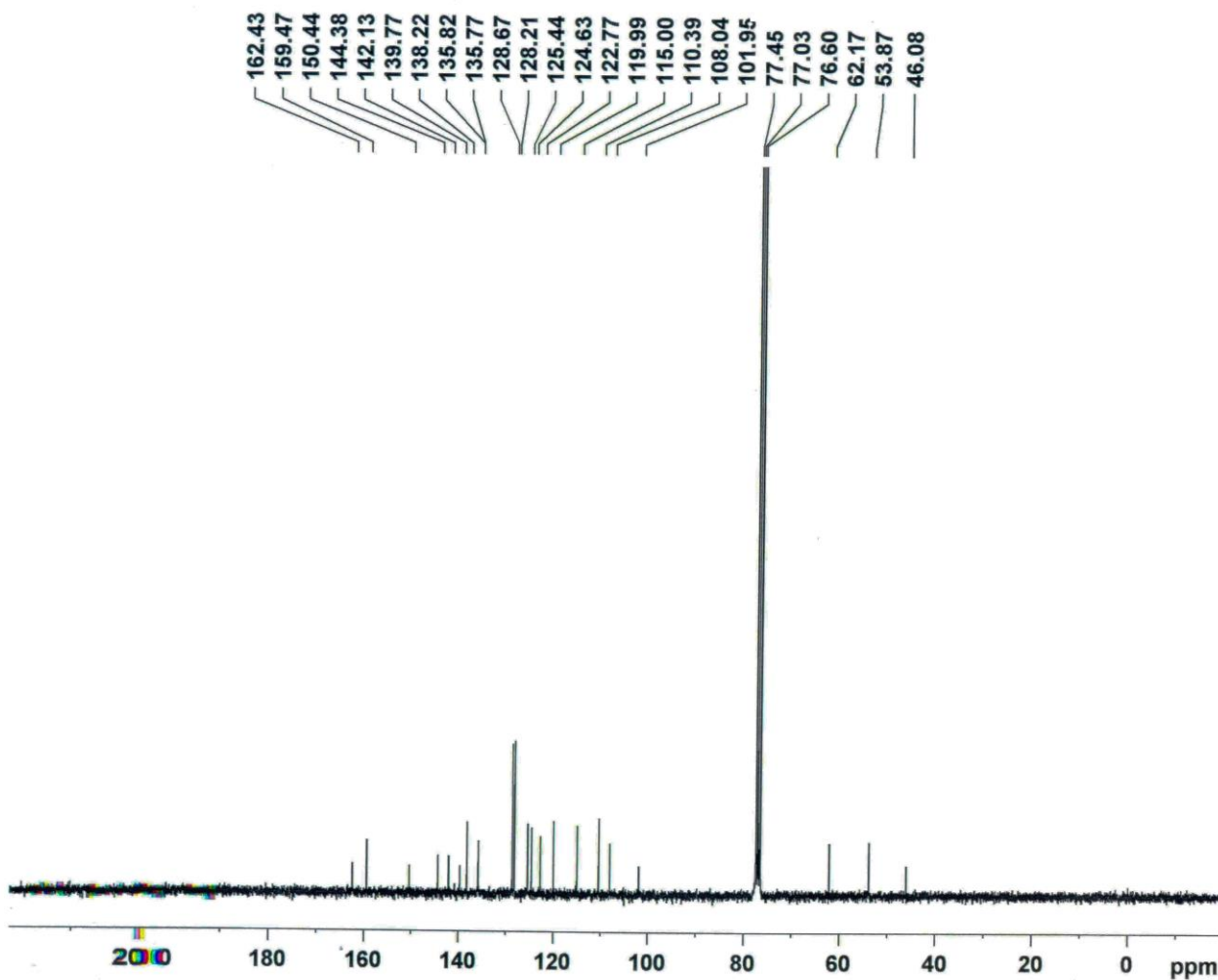
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.15 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300060 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

7.787  
 7.732  
 7.716  
 7.705  
 7.605  
 7.581  
 7.545  
 7.533  
 7.516  
 7.356  
 7.327  
 7.300  
 7.265  
 7.104  
 7.050  
 6.613  
 6.566  
 5.558  
 5.163  
 4.474



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of the dendritic chloride **17**



Current Data Parameters  
 NAME KRC-261  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150411  
 Time 13.45  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 853  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2896.3  
 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

===== 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 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the dendritic chloride **17**

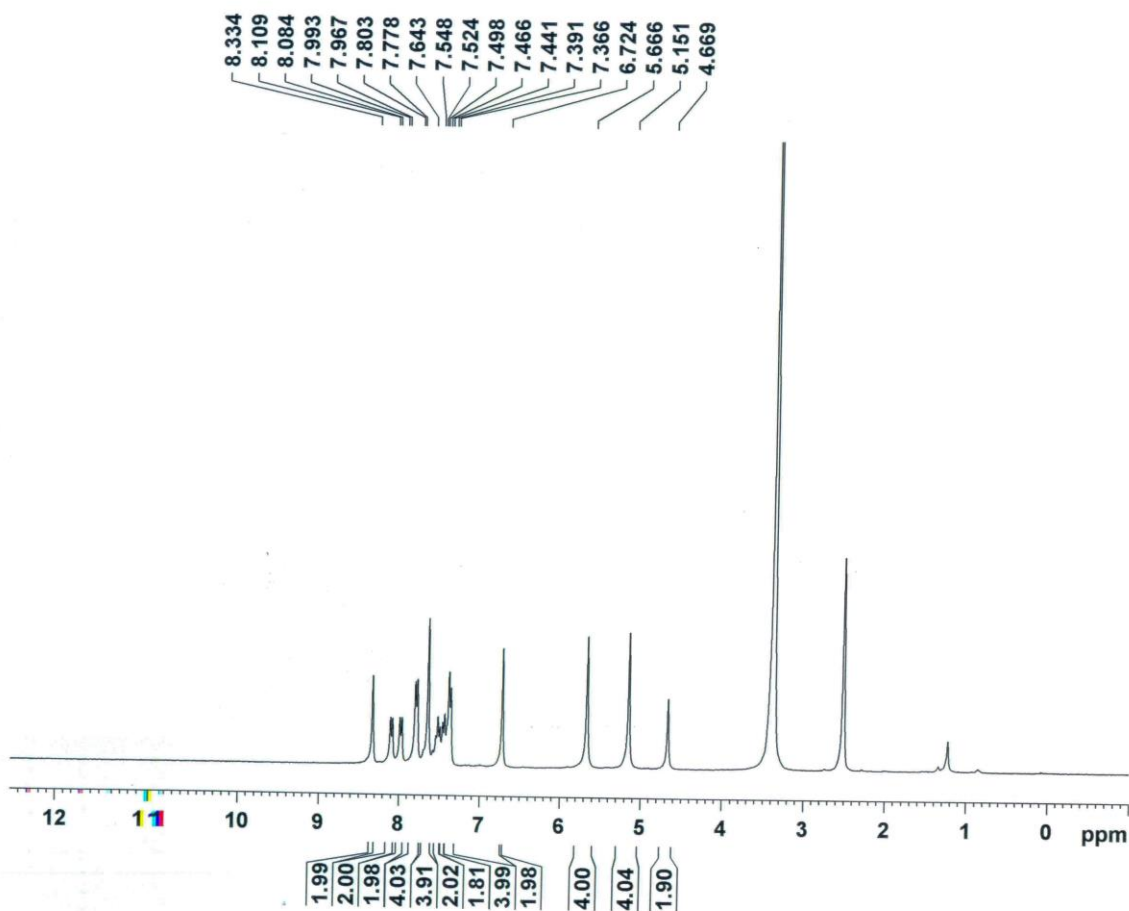


Current Data Parameters  
NAME KRC-210  
EXPNO 3  
PROCNO 1

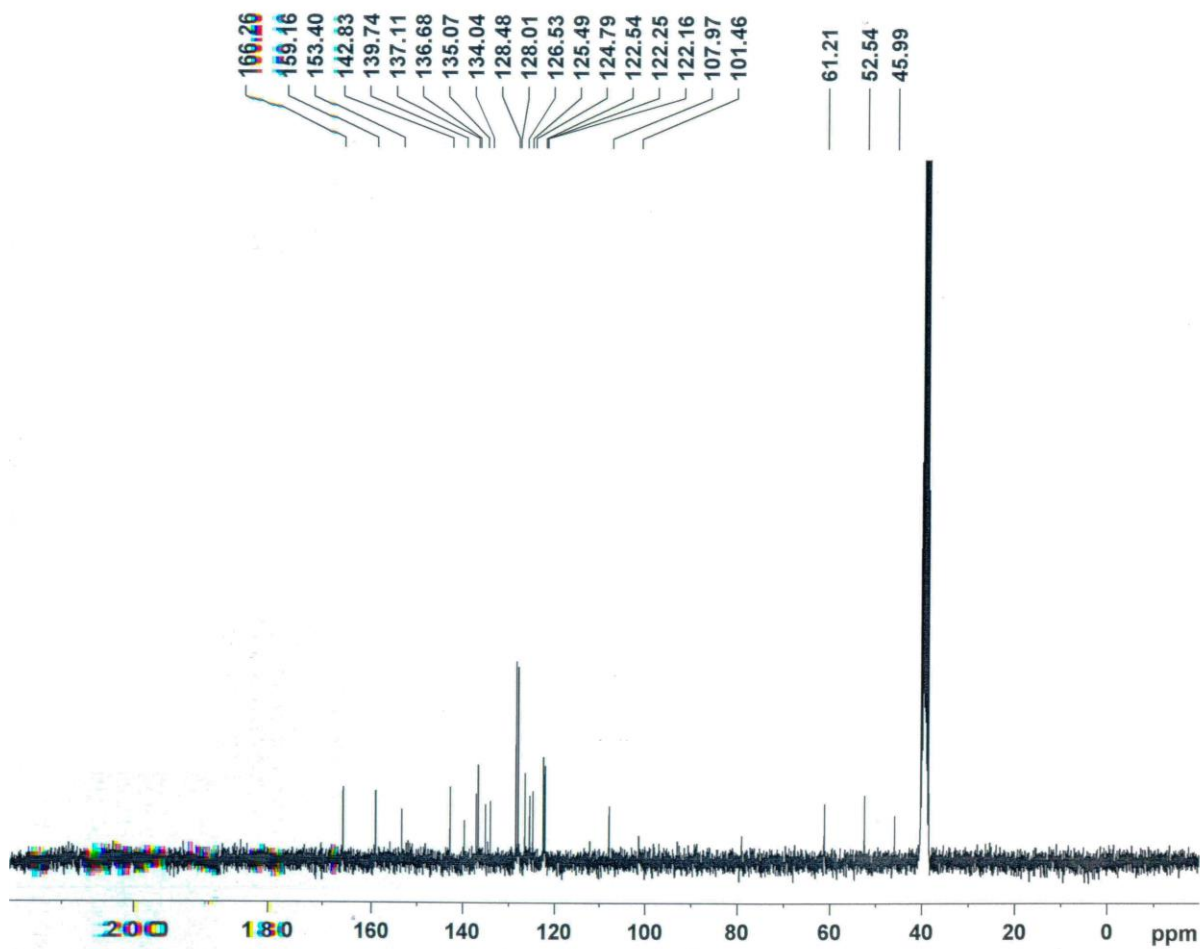
F2 - Acquisition Parameters  
Date\_ 20141113  
Time 18.31  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 143.7  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

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

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



$^1\text{H}$  NMR (300 MHz,  $\text{DMSO-d}_6$ ) spectrum of the dendritic chloride **18**



Current Data Parameters  
 NAME KRC-210  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20141114  
 Time 22.58  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 663  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 1024  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.89999998 sec  
 TD0 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 75.4677867 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) spectrum of the dendritic chloride **18**



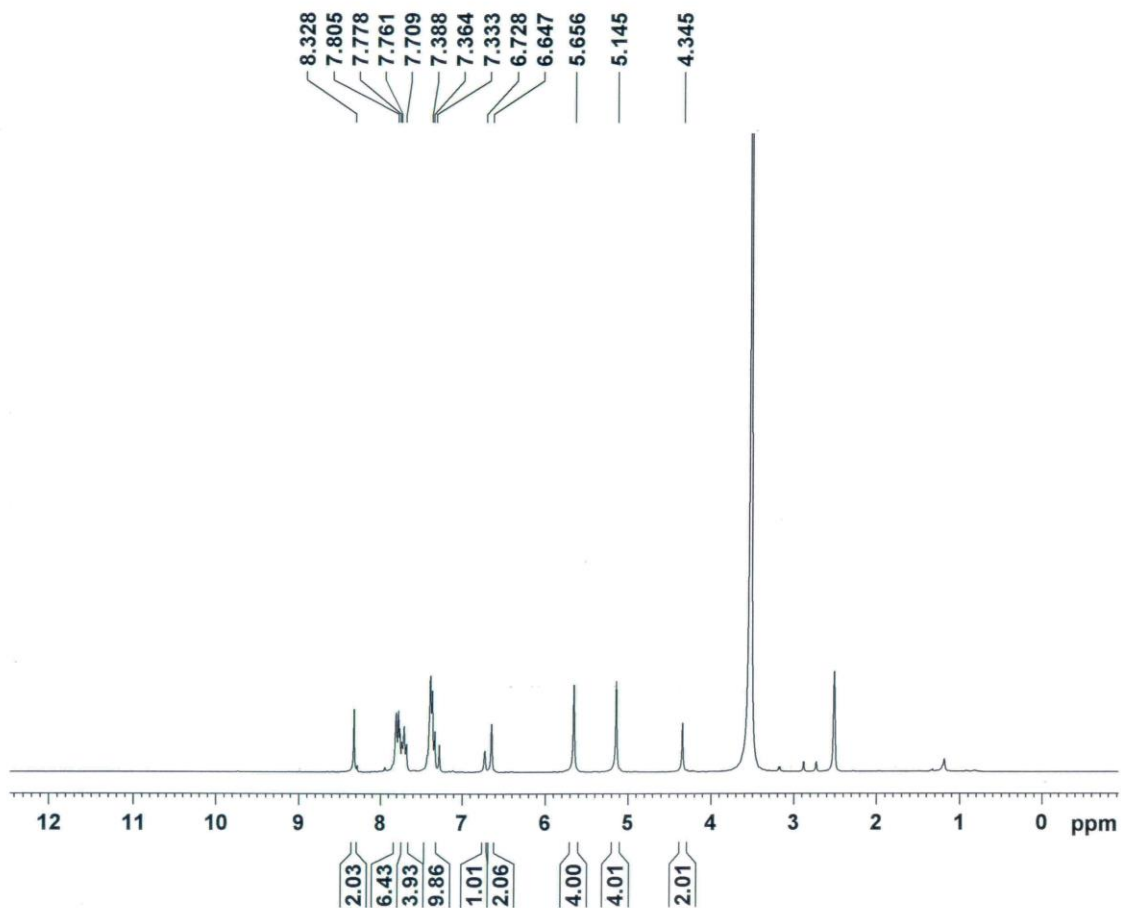


Current Data Parameters  
 NAME KRC-264  
 EXPNO 1  
 PROCNO 1

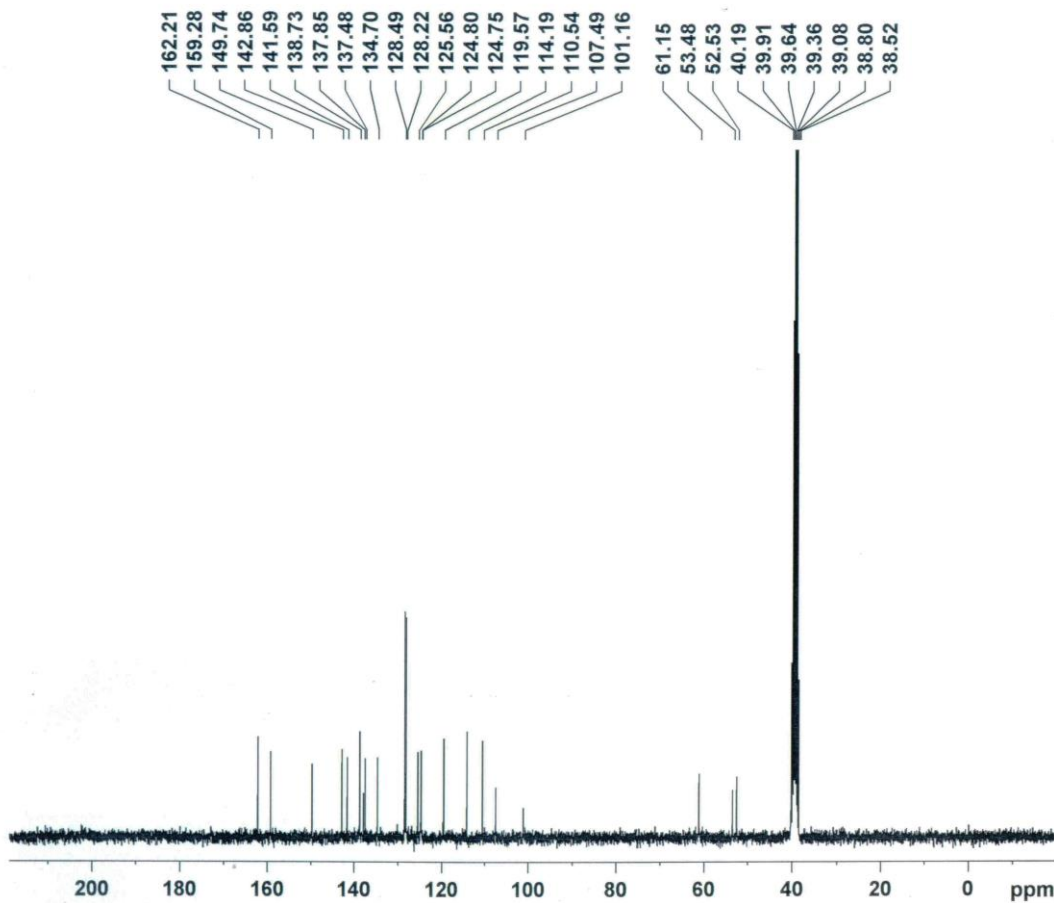
F2 - Acquisition Parameters  
 Date\_ 20150416  
 Time 12.56  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 45.3  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.15 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



$^1\text{H}$  NMR (300 MHz,  $\text{DMSO-d}_6$ ) spectrum of the dendritic azide **19**



Current Data Parameters  
 NAME KRC-264  
 EXPNO 2  
 PROCNO 1

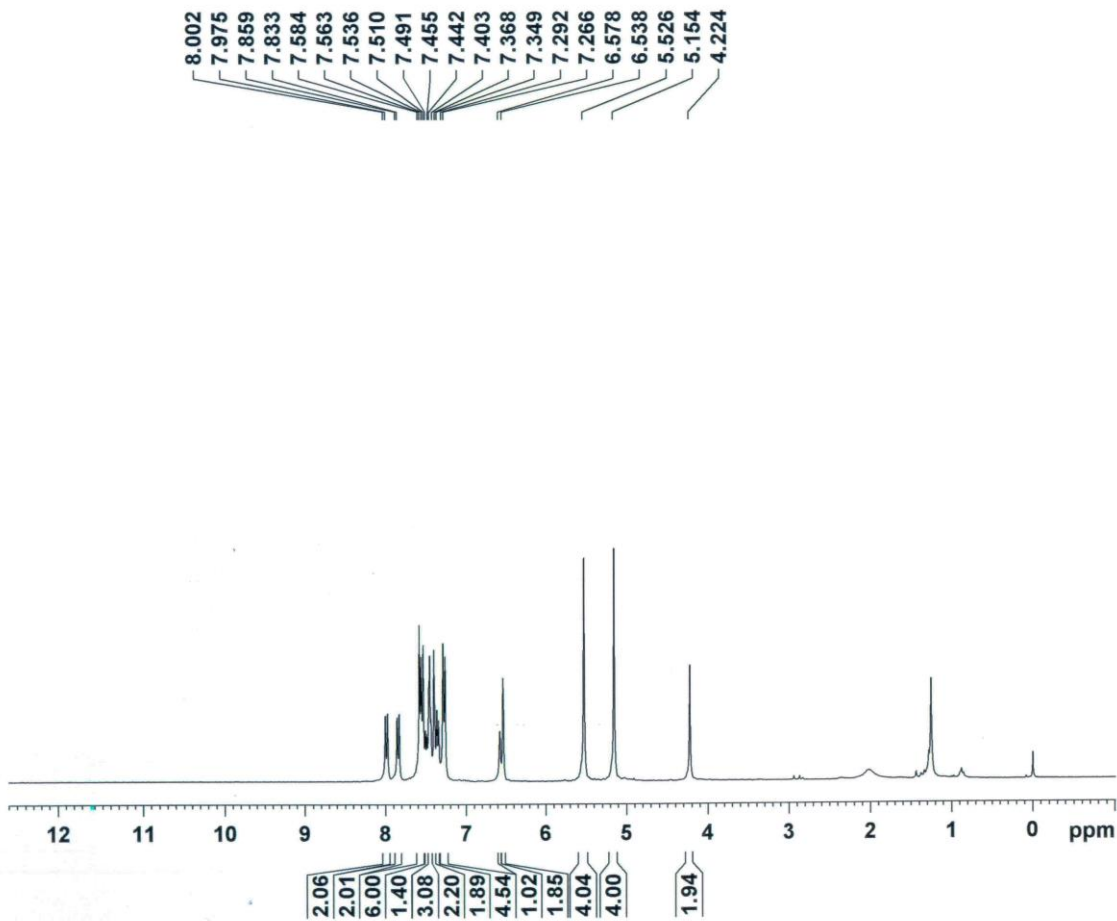
F2 - Acquisition Parameters  
 Date\_ 20150416  
 Time 13.14  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 400  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 912.3  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1

===== 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 75.4677867 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR (75 MHz, DMSO-d<sub>6</sub>) spectrum of the dendritic azide **19**



Current Data Parameters  
 NAME KRC-218  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150307  
 Time 14.00  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3  
 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 13.15 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300048 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the dendritic azide **20**



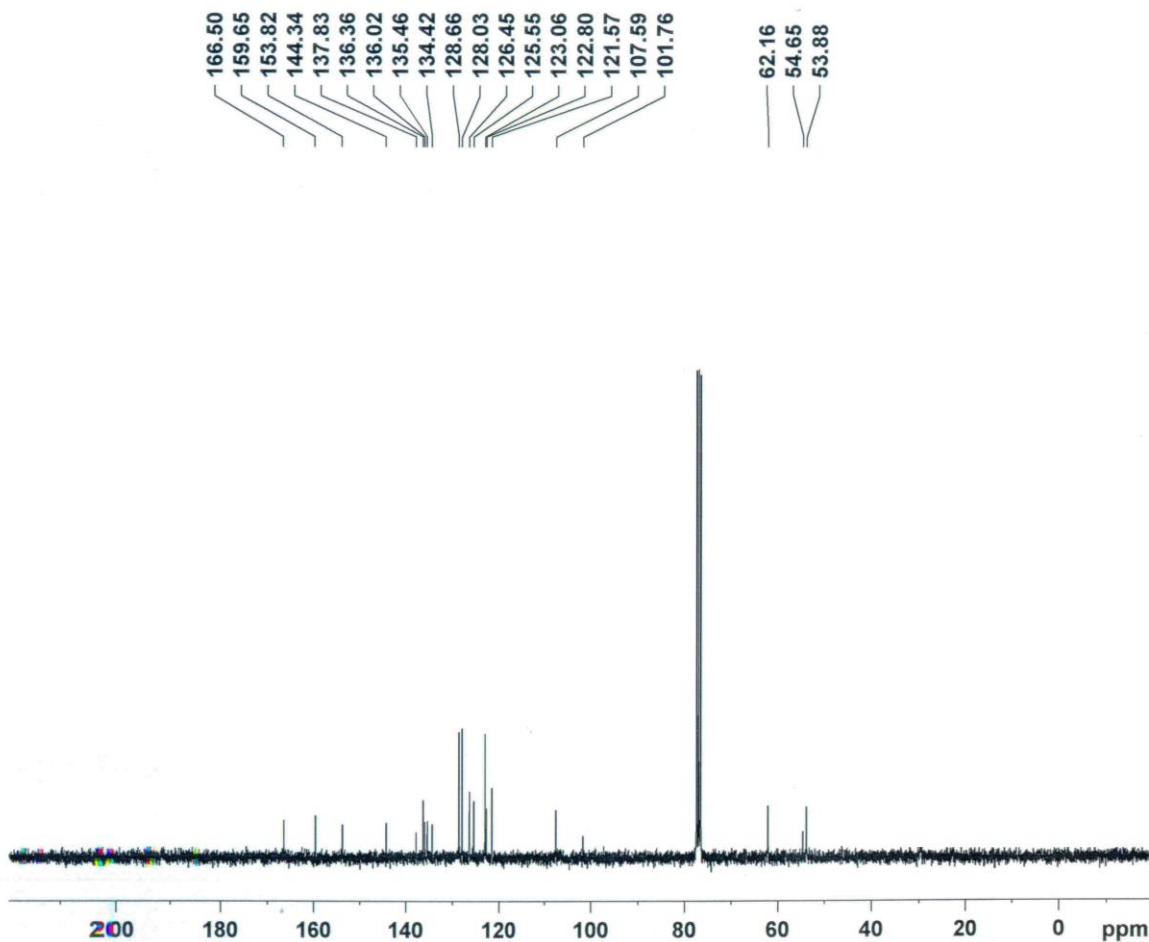
Current Data Parameters  
NAME KRC-218  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141203  
Time 13.35  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 231  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3649.1  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TD0 1

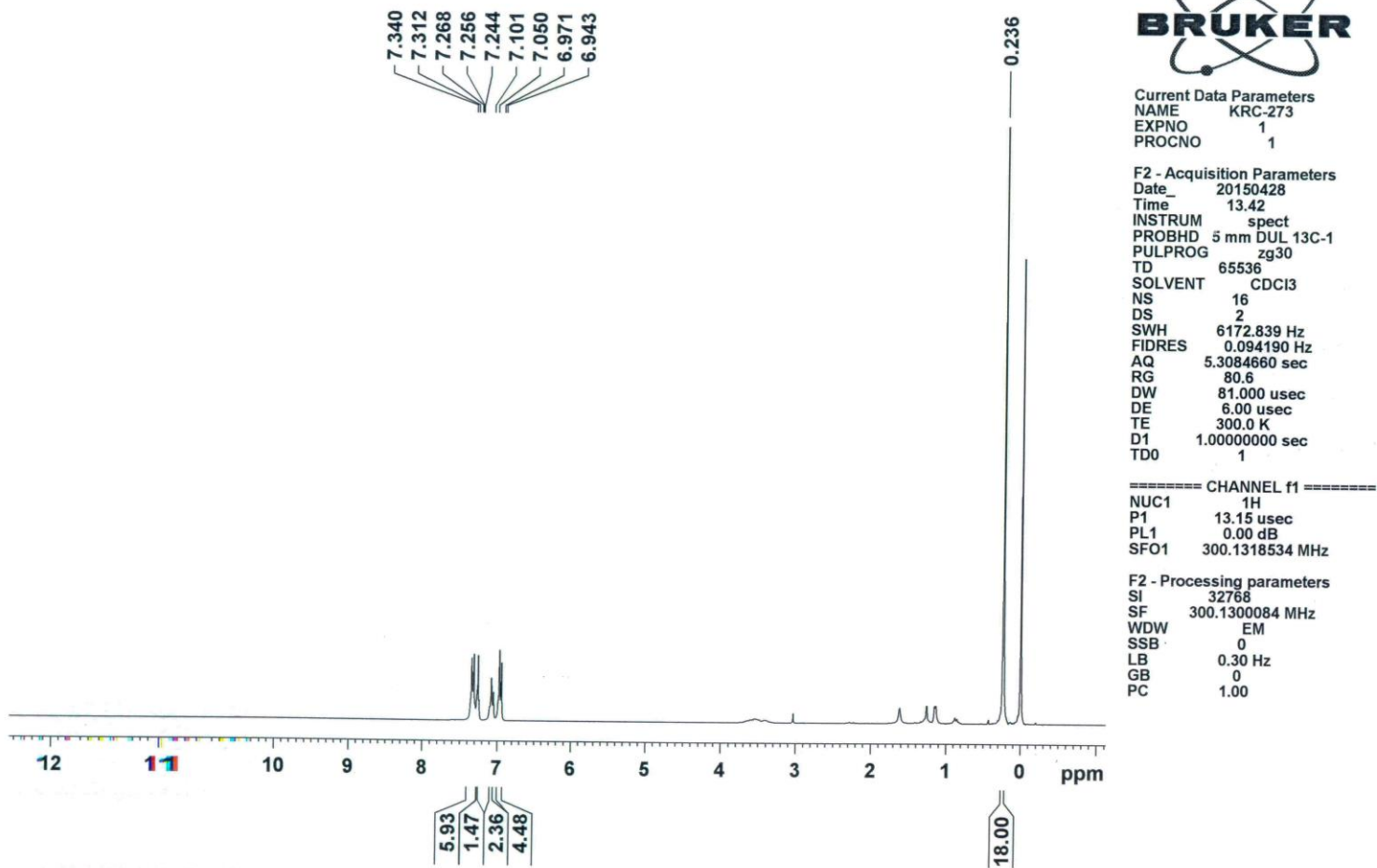
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.30 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

===== 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 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the dendritic azide **20**



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **23**



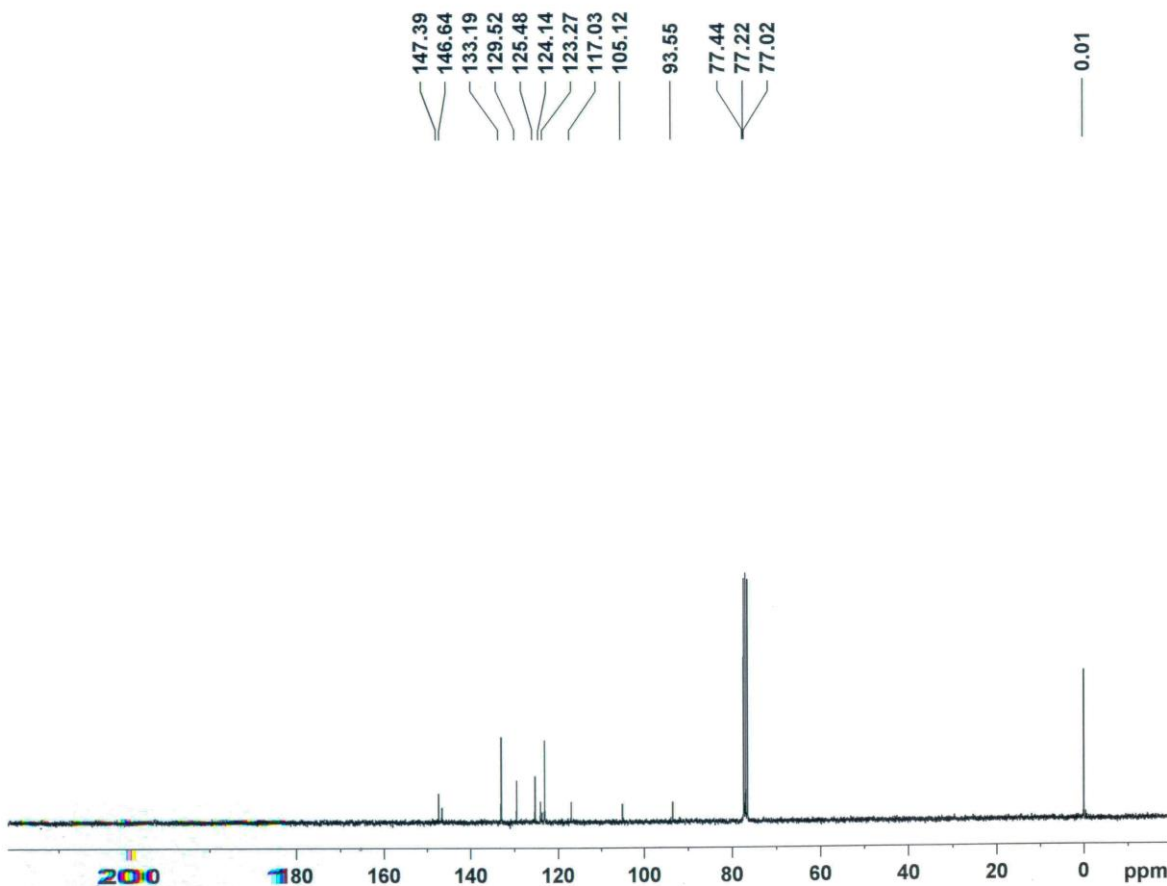
Current Data Parameters  
 NAME KRC-273  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150428  
 Time 13.48  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 201  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 1824.6  
 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 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 75.4677490 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>) spectrum of the compound **23**

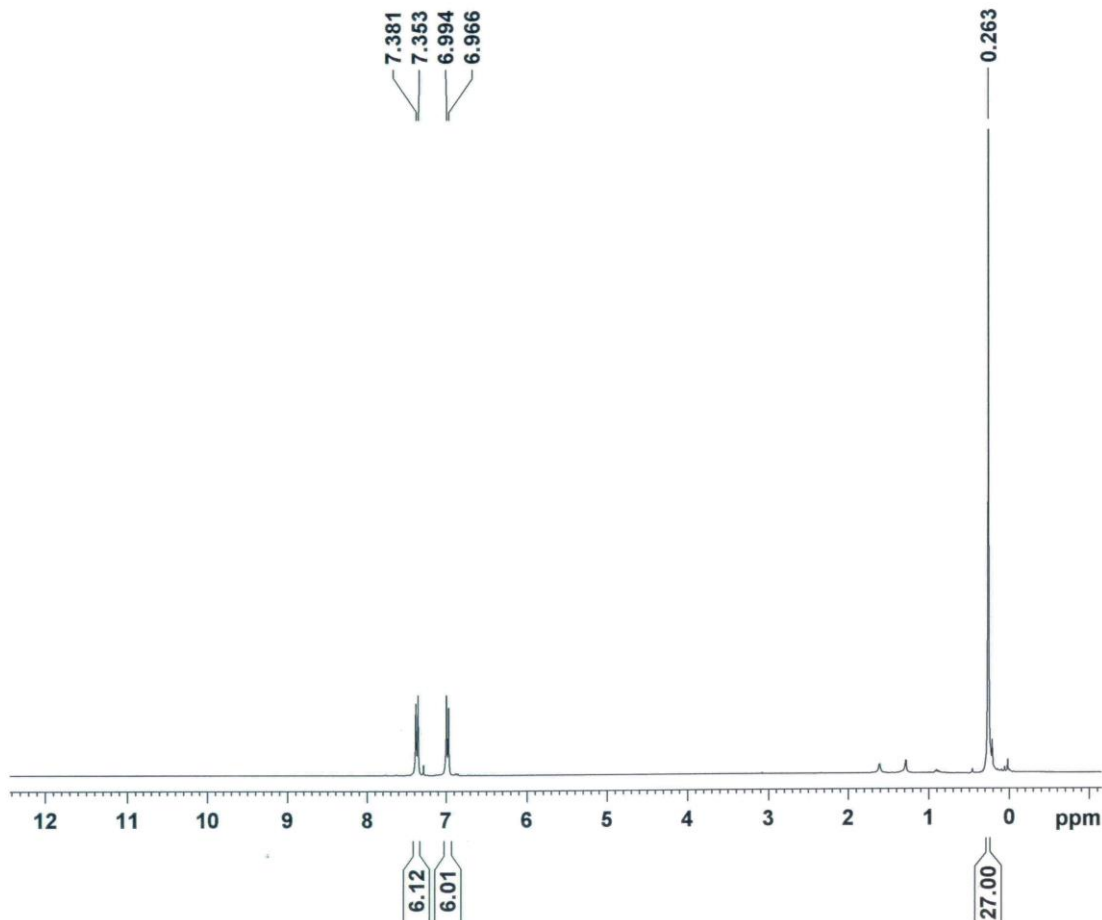


Current Data Parameters  
 NAME KRC-242-Re  
 EXPNO 1  
 PROCNO 1

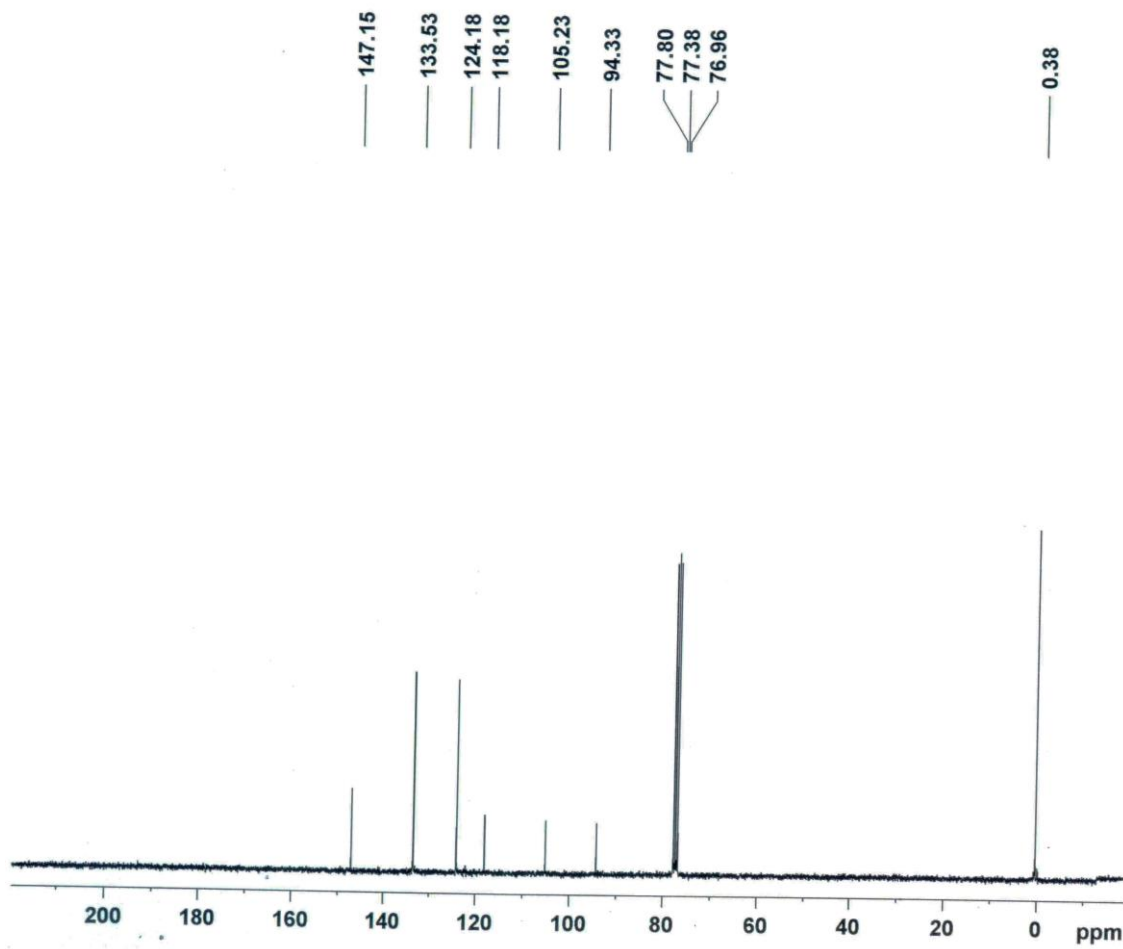
F2 - Acquisition Parameters  
 Date\_ 20150305  
 Time 13.02  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 80.6  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

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

F2 - Processing parameters  
 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>) spectrum of the compound **24**



Current Data Parameters  
 NAME KRC-242-Re  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150305  
 Time 13.08  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 350  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 1625.5  
 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

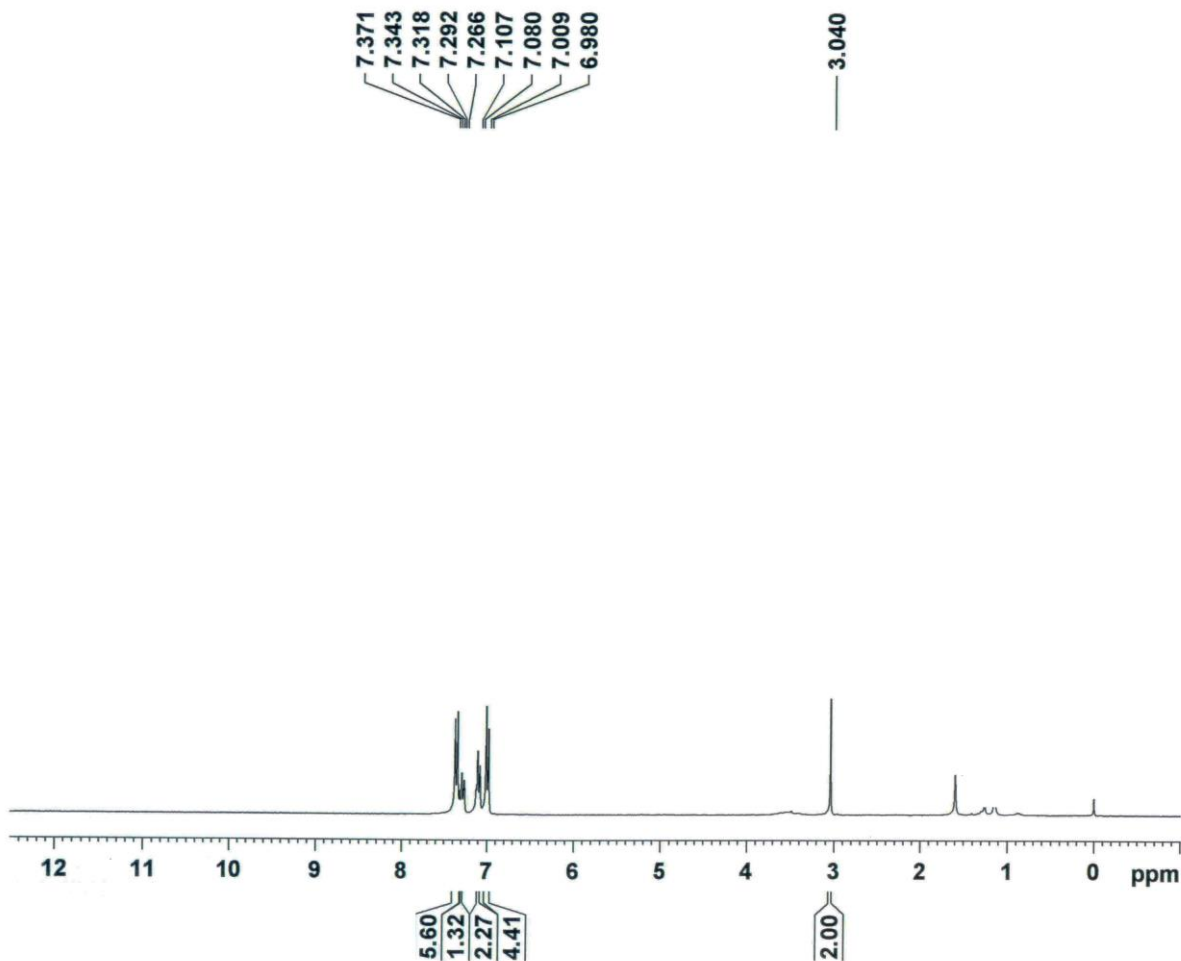
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.30 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== 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 75.4677218 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>) spectrum of the compound **24**





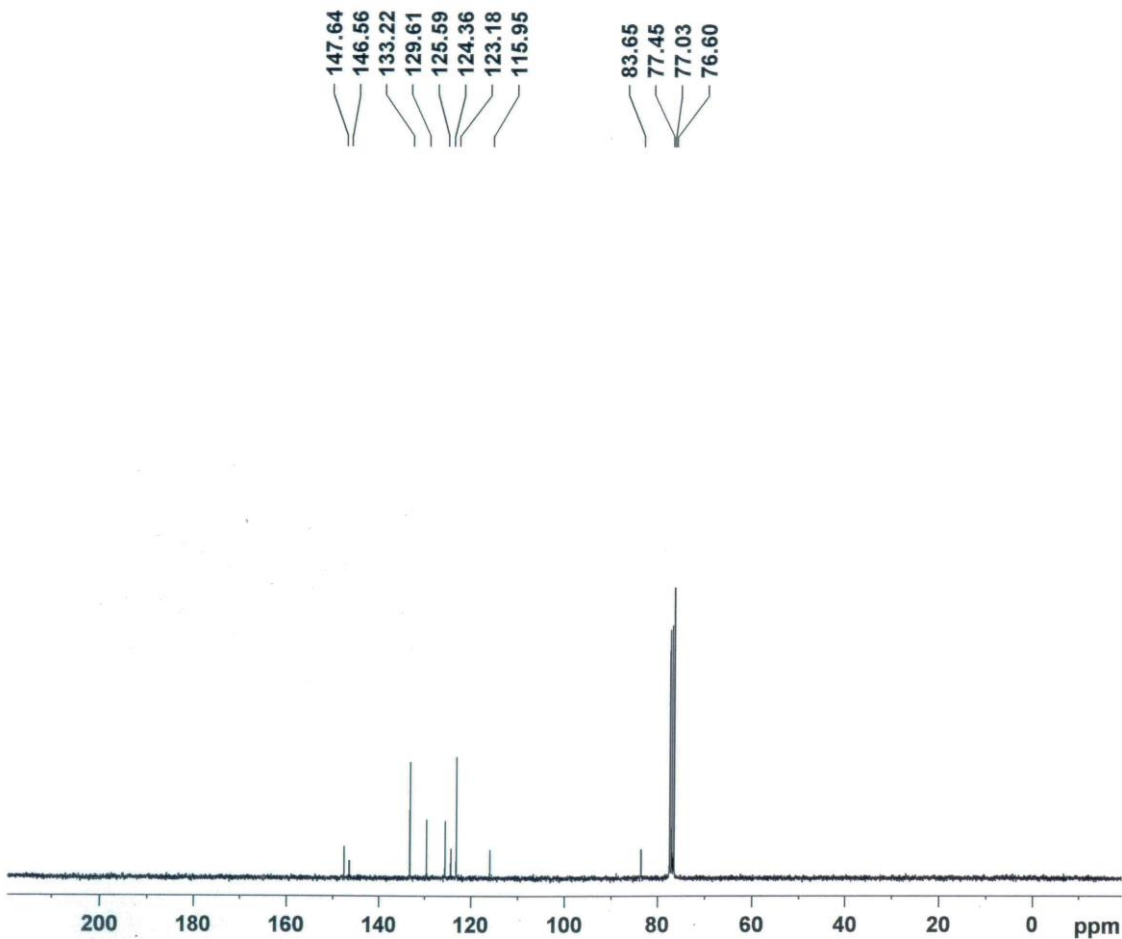
Current Data Parameters  
 NAME KRC-277  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150506  
 Time 18.03  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 203.2  
 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 300.1300076 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **25**



Current Data Parameters  
 NAME KRC-277  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150506  
 Time 18.06  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 314  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 1625.5  
 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 9.30 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 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **25**

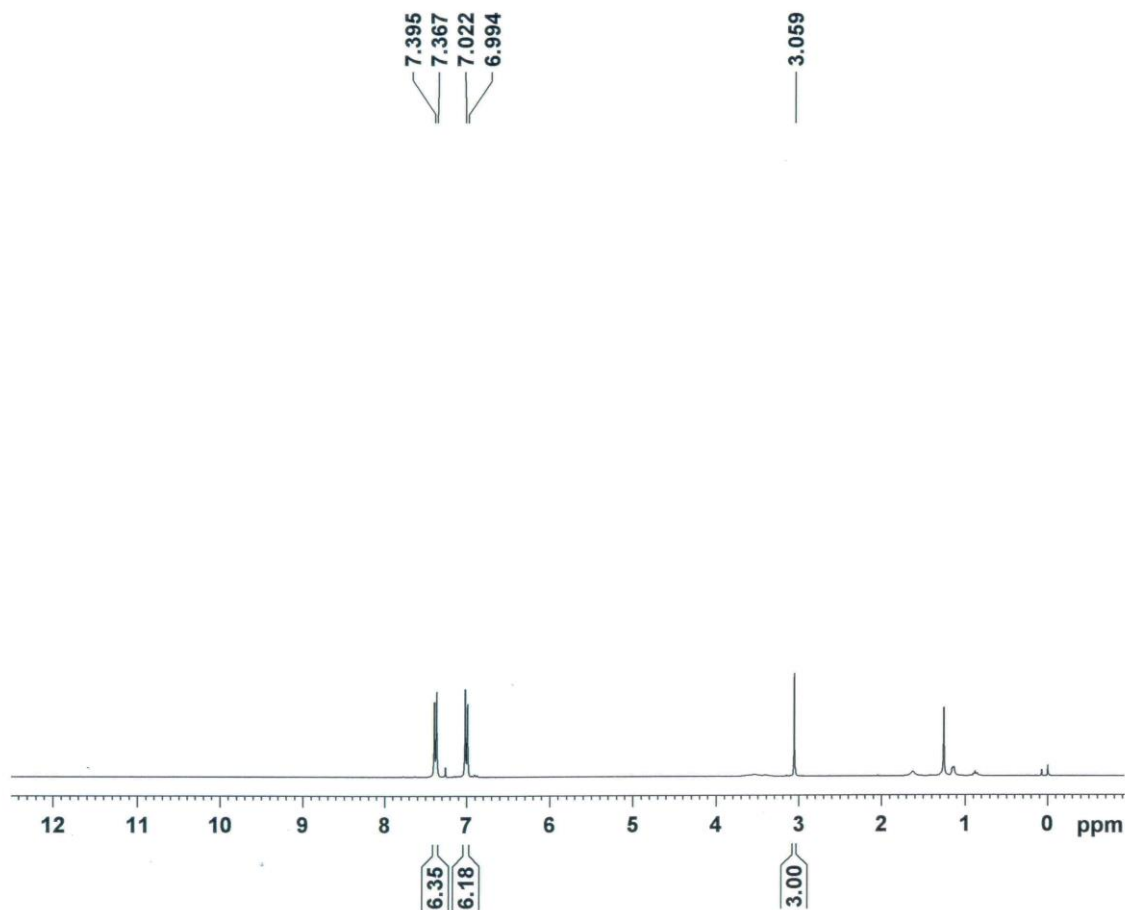


Current Data Parameters  
NAME KRC-251  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150316  
Time 17.50  
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 128  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 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 300.1300070 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **26**



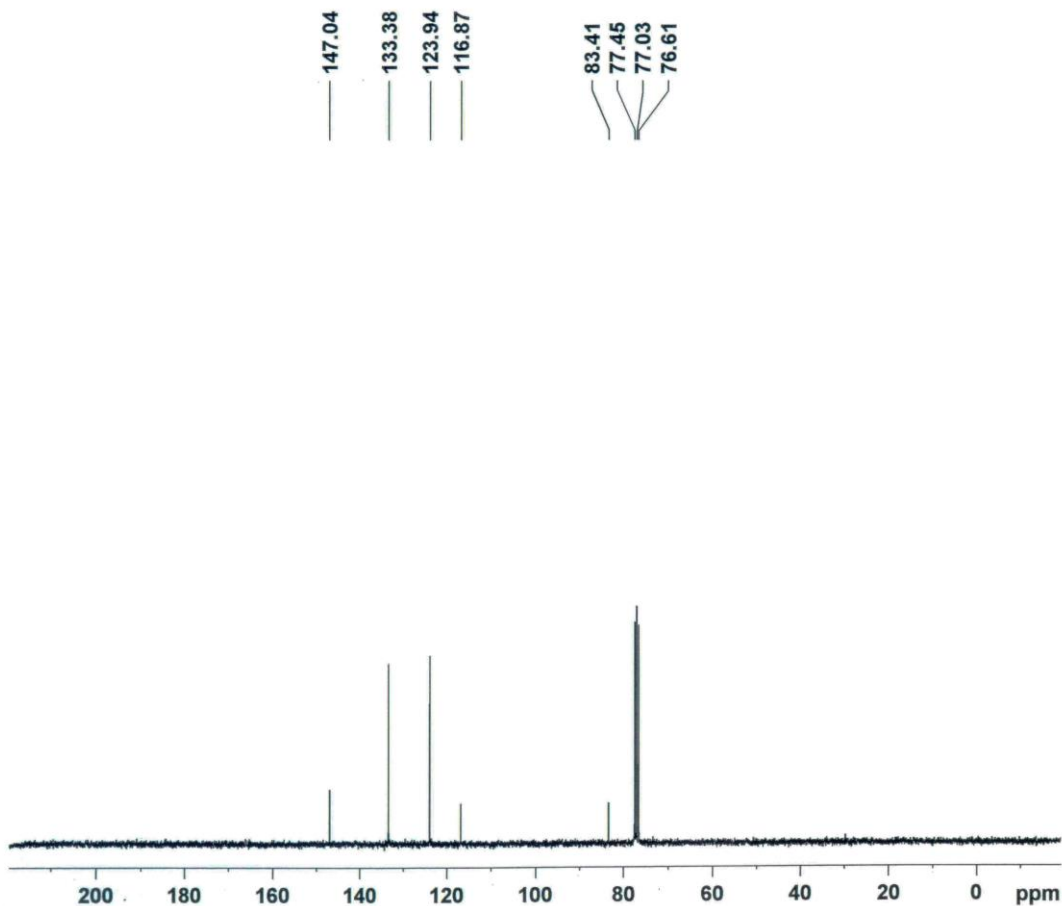
Current Data Parameters  
 NAME KRC-251  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150316  
 Time 17.55  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 103  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2896.3  
 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

===== 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 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the compound **26**

7.798  
7.743  
7.717  
7.703  
7.694  
7.665  
7.639  
7.617  
7.590  
7.545  
7.532  
7.515  
7.352  
7.327  
7.288  
7.263  
7.236  
7.130  
7.110  
7.102  
7.070  
7.056  
5.602

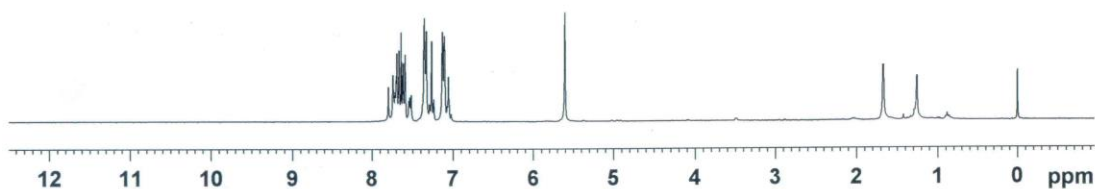


Current Data Parameters  
NAME KRC-290  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150627  
Time 0.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 203.2  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

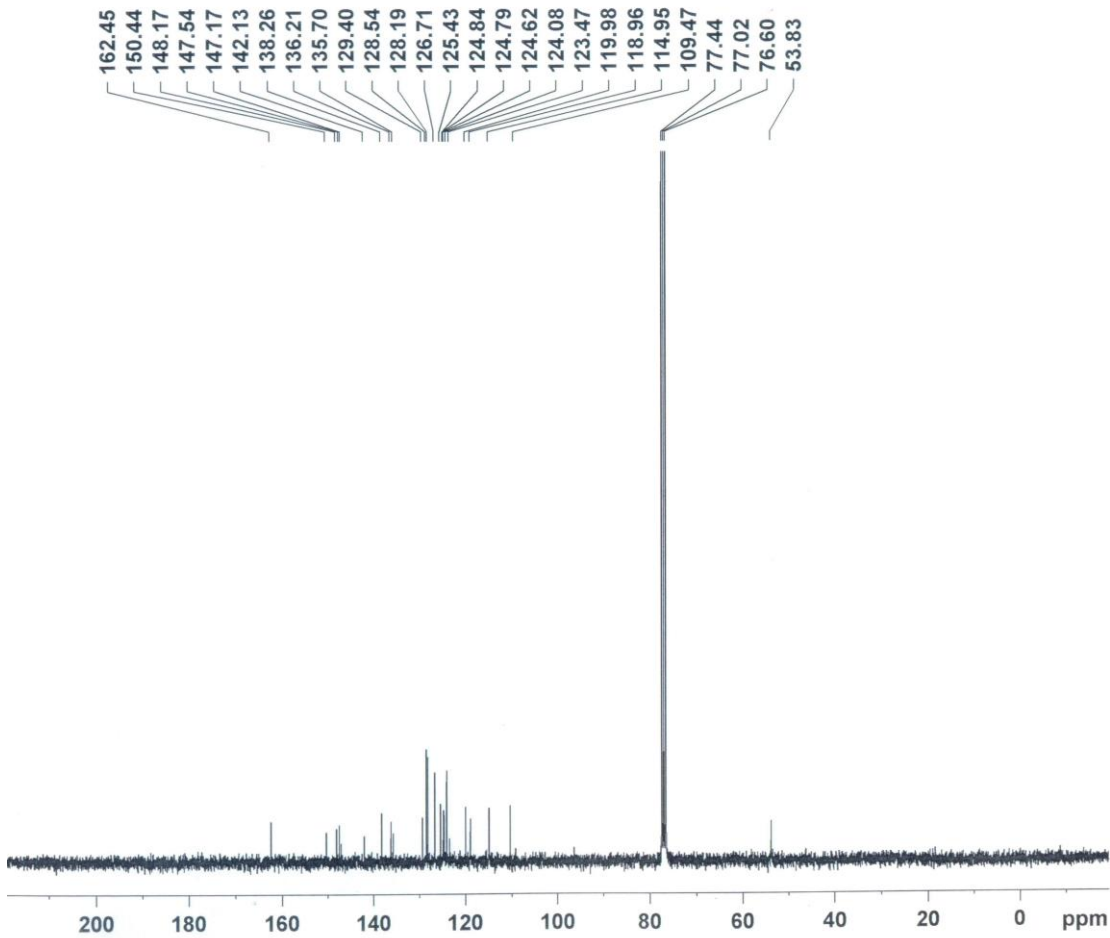
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.88 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300052 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.00  
1.89  
3.39  
2.30  
1.95  
4.11  
1.95  
8.24  
3.32  
3.24  
3.73  
1.85  
4.02

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **1**



Current Data Parameters  
NAME KRC-290  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150627  
Time 0.17  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 322  
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 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 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

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **1**

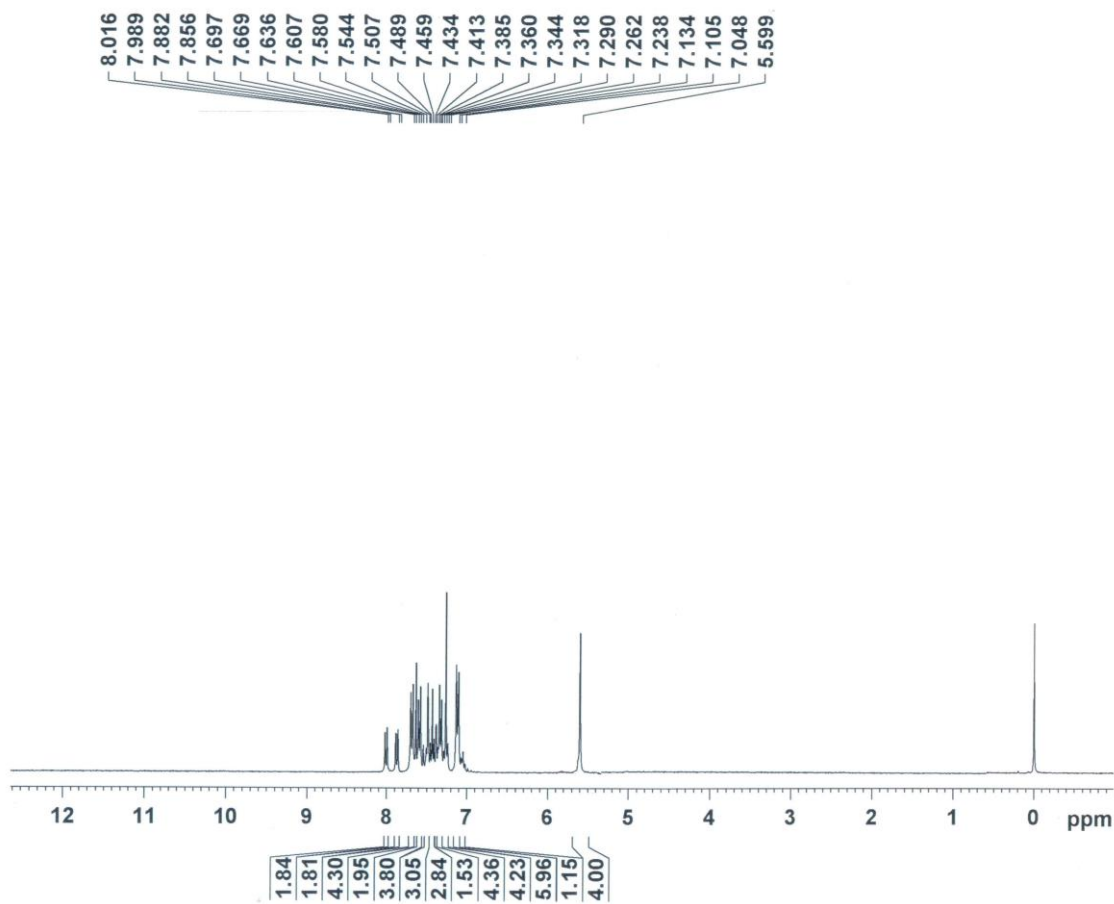


Current Data Parameters  
NAME KRC-289  
EXPNO 1  
PROCNO 1

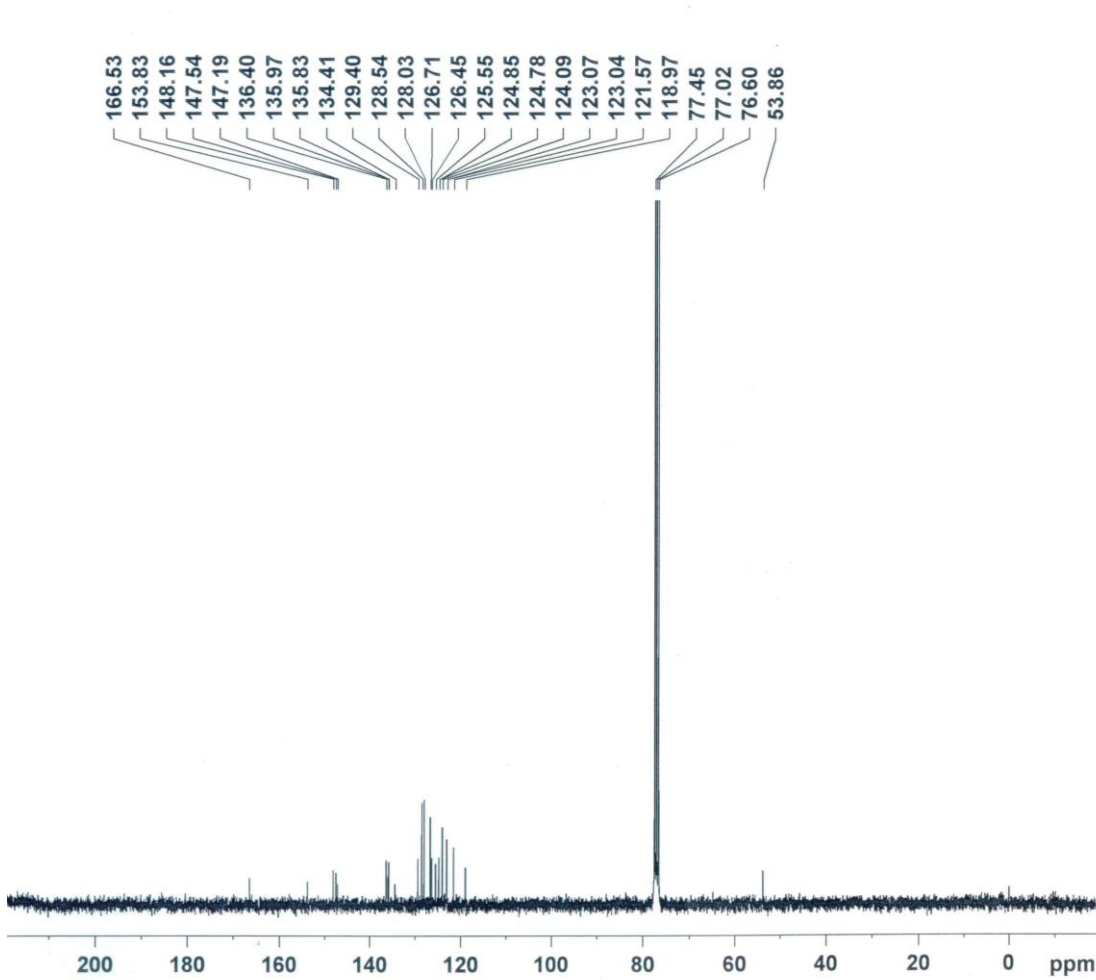
F2 - Acquisition Parameters  
Date\_ 20150627  
Time 0.35  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 11  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

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

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



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer 2



Current Data Parameters  
NAME KRC-289  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150628  
Time 20.59  
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 2896.3  
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 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 75.4677487 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **2**



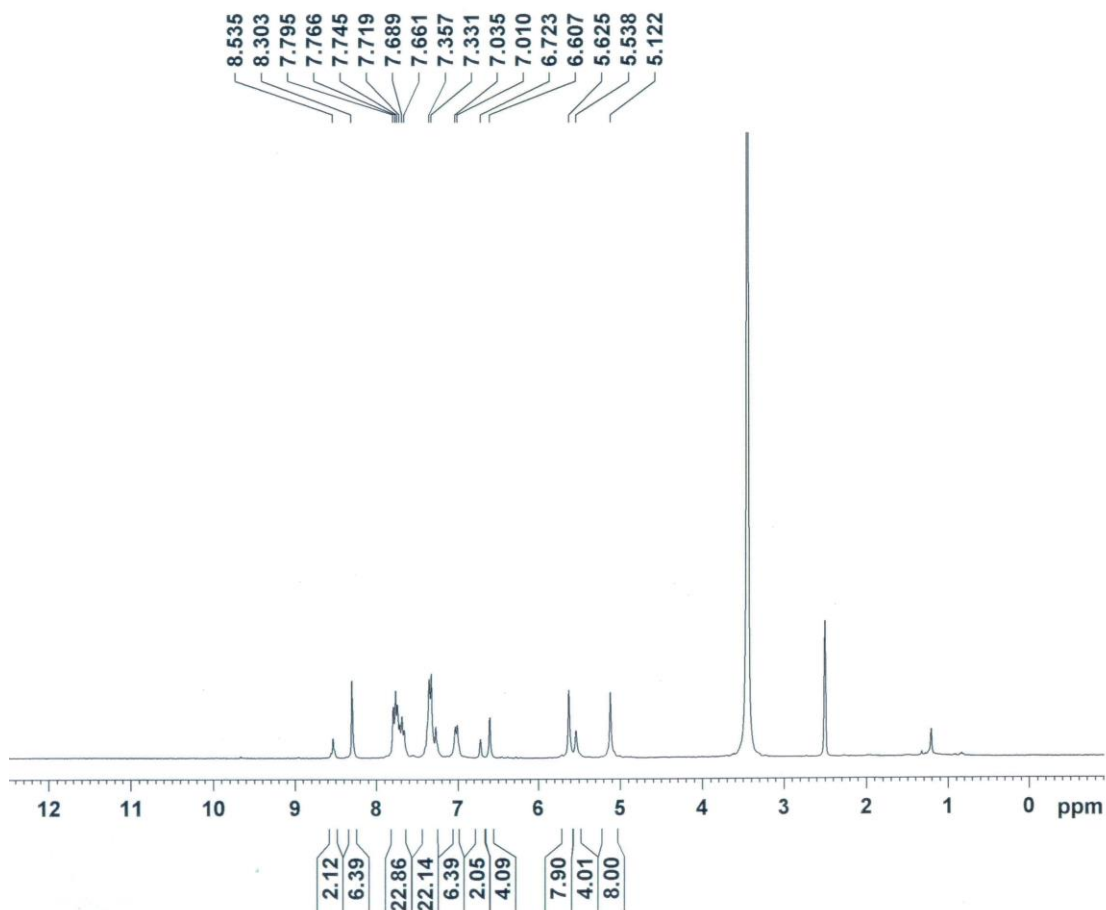


Current Data Parameters  
NAME KRC-292  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150707  
Time 7.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
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 1.0000000 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 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



$^1\text{H}$  NMR (300 MHz, DMSO- $d_6$ ) spectrum of the dendrimer **3**



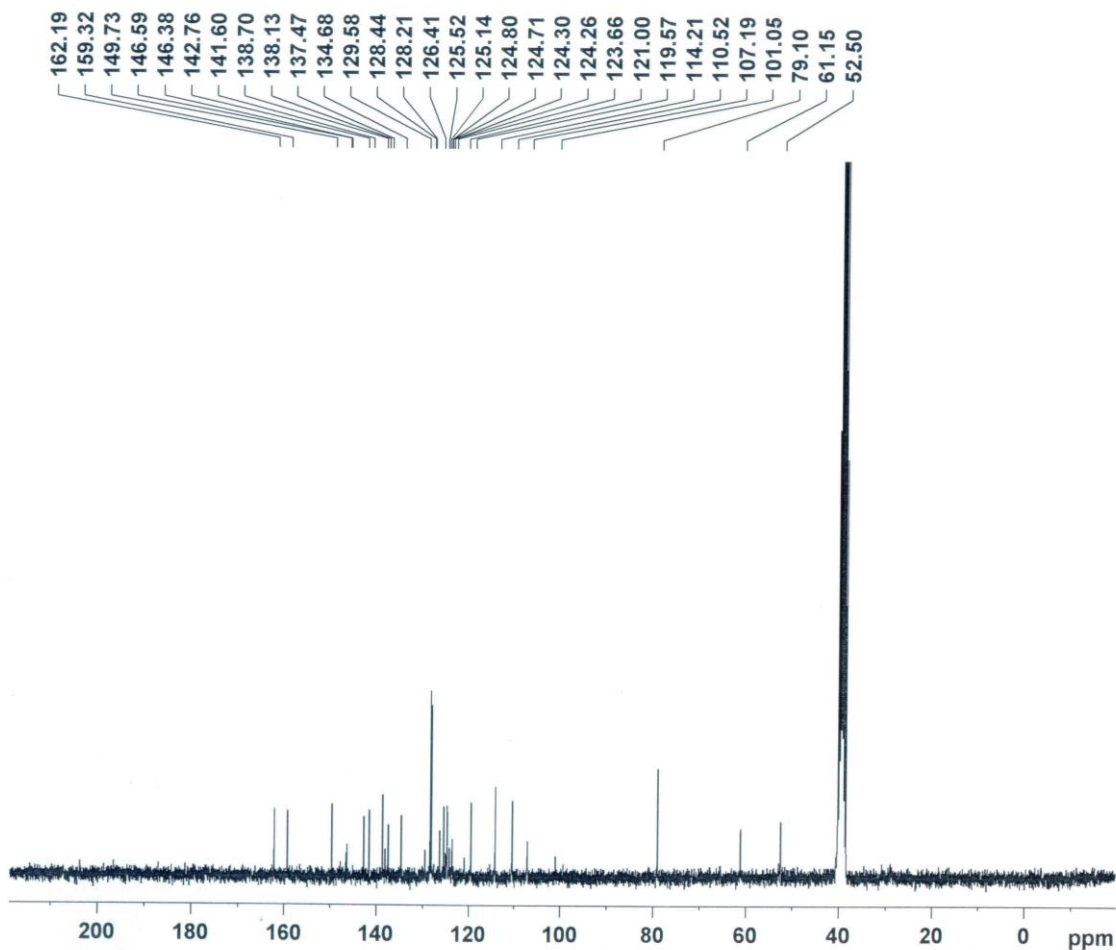
Current Data Parameters  
NAME KRC-292  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150708  
Time 0.46  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2343  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2896.3  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

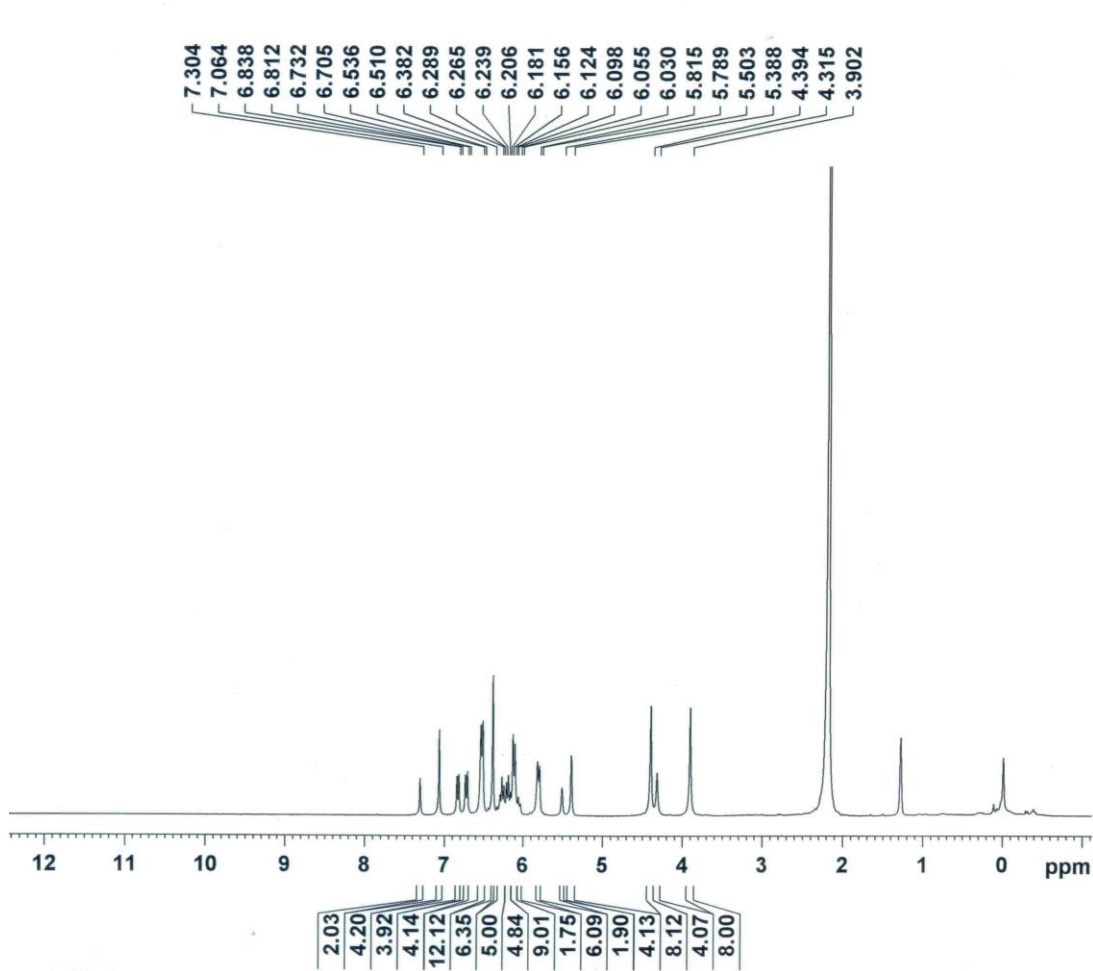
===== CHANNEL f1 =====  
NUC1 13C  
P1 10.38 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

===== 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 75.4677867 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) spectrum of the dendrimer **3**



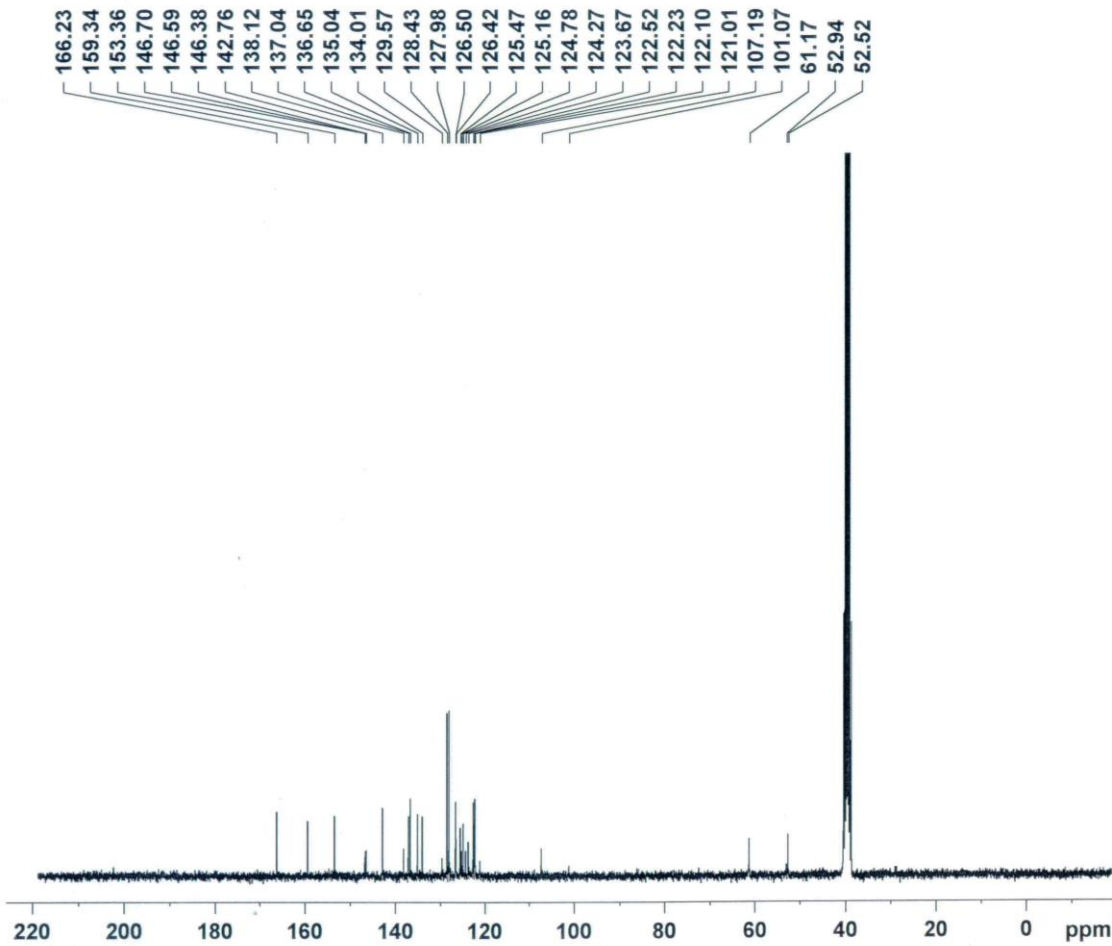
Current Data Parameters  
 NAME KRC-291  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150626  
 Time 23.21  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 12  
 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 13.88 usec  
 PL1 0.00 dB  
 SFO1 300.1318534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1303685 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR (300 MHz, DMSO-d<sub>6</sub>) spectrum of the dendrimer 4



Current Data Parameters  
 NAME KRC-291  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150629  
 Time 22.21  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1716  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2896.3  
 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

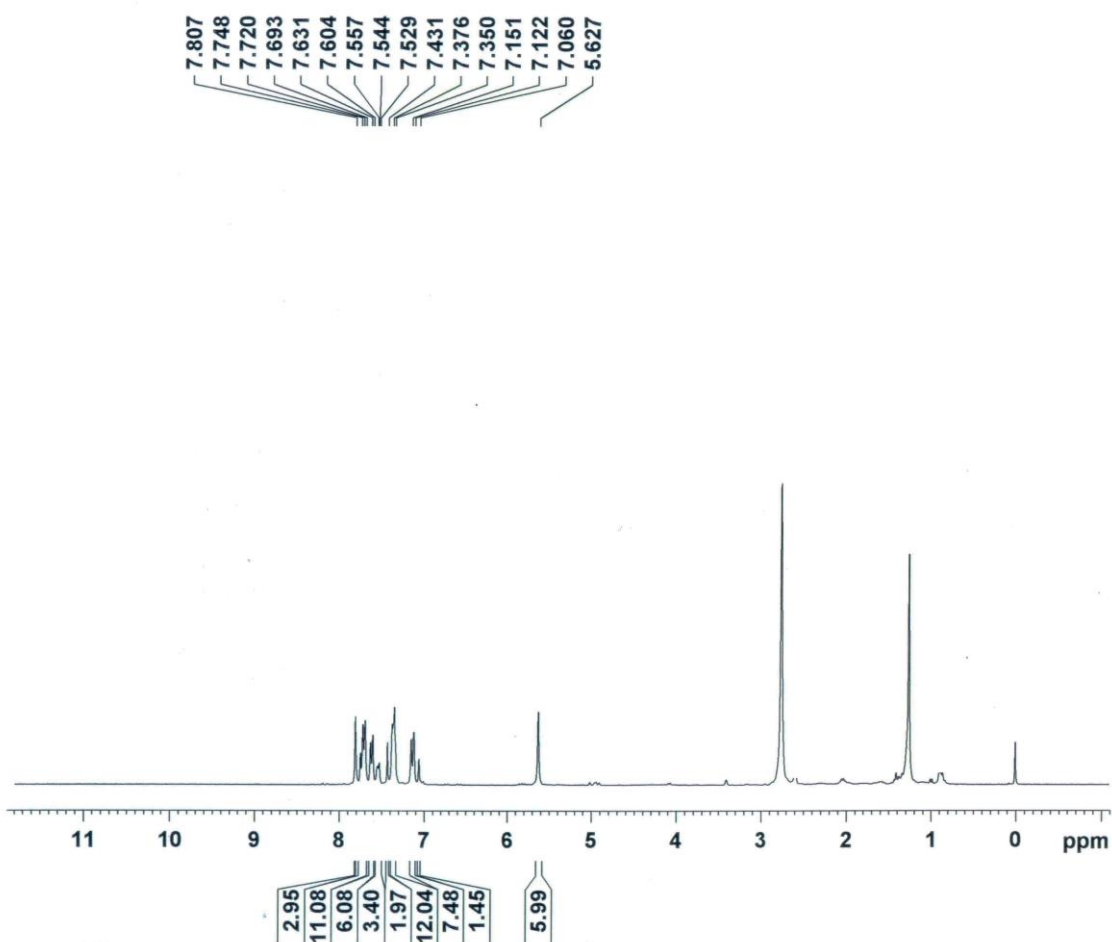
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.38 usec  
 PL1 0.00 dB  
 SFO1 75.4752953 MHz

===== 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 75.4677867 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) spectrum of the dendrimer **4**

UNI. OF MADRAS



Current Data Parameters  
NAME KRC-259  
EXPNO 1  
PROCNO 1

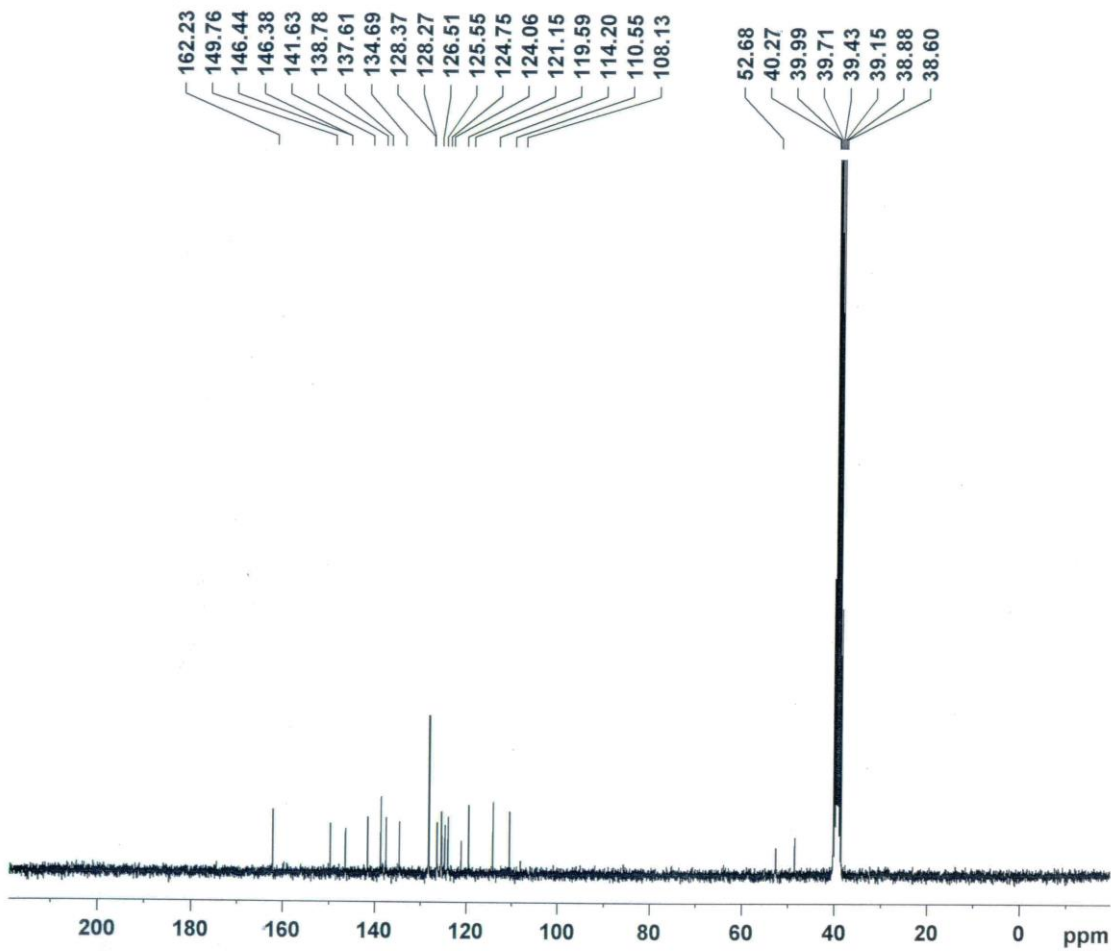
F2 - Acquisition Parameters  
Date\_ 20150401  
Time 13.07  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 228.1  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

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

F2 - Processing parameters  
SI 32768  
SF 300.1314015 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **5**

UNI. OF MADRAS



Current Data Parameters  
NAME KRC-259A  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150401  
Time 14.36  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 1824.6  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1

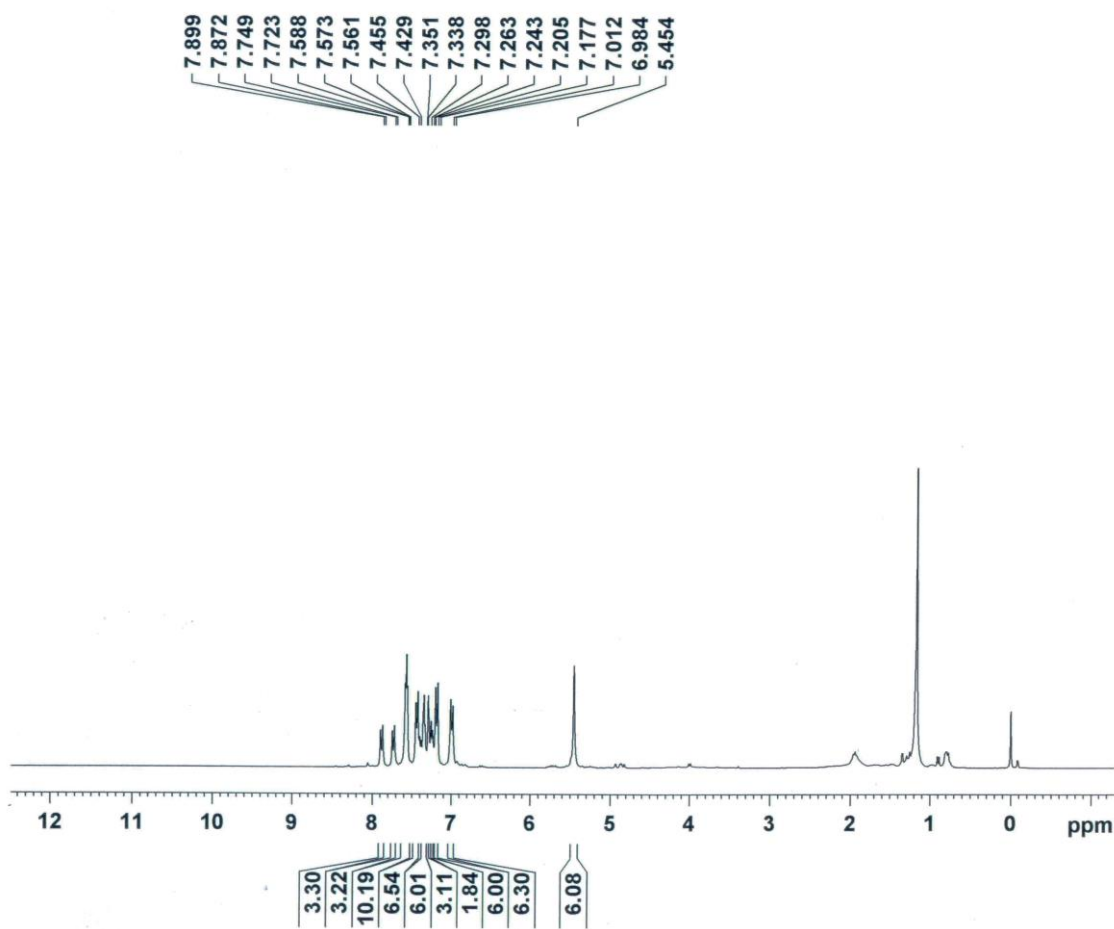
=====  
CHANNEL f1  
=====  
NUC1 13C  
P1 9.30 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

=====  
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 75.4677867 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{DMSO-d}_6$ ) spectrum of the dendrimer **5**

UNIV. OF MADRAS



$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **6**



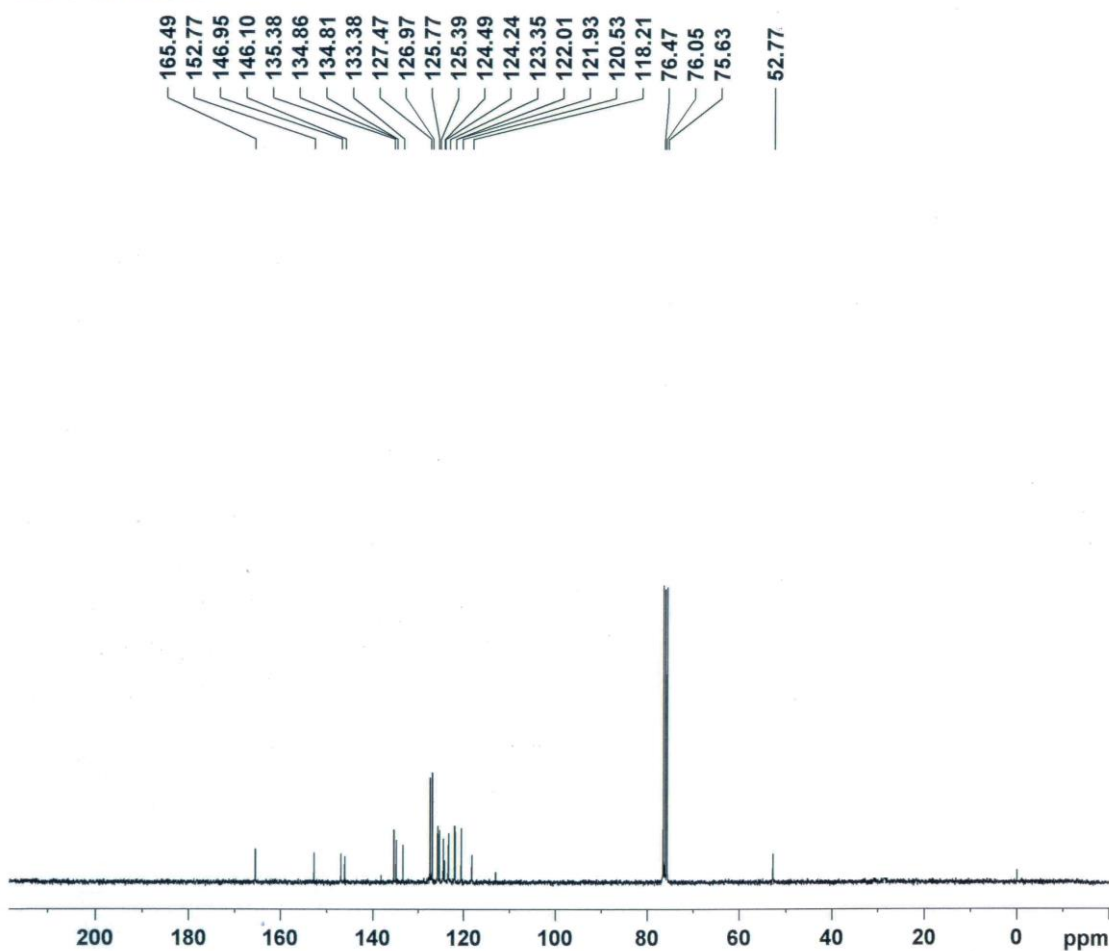
Current Data Parameters  
NAME KRC-254  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150324  
Time 14.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT  $\text{CDCl}_3$   
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

===== CHANNEL f1 =====  
NUC1  $^1\text{H}$   
P1 13.15 usec  
PL1 0.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300328 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

UNIV. OF MADRAS



Current Data Parameters  
NAME KRC-254  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150324  
Time 14.31  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 431  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2580.3  
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

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

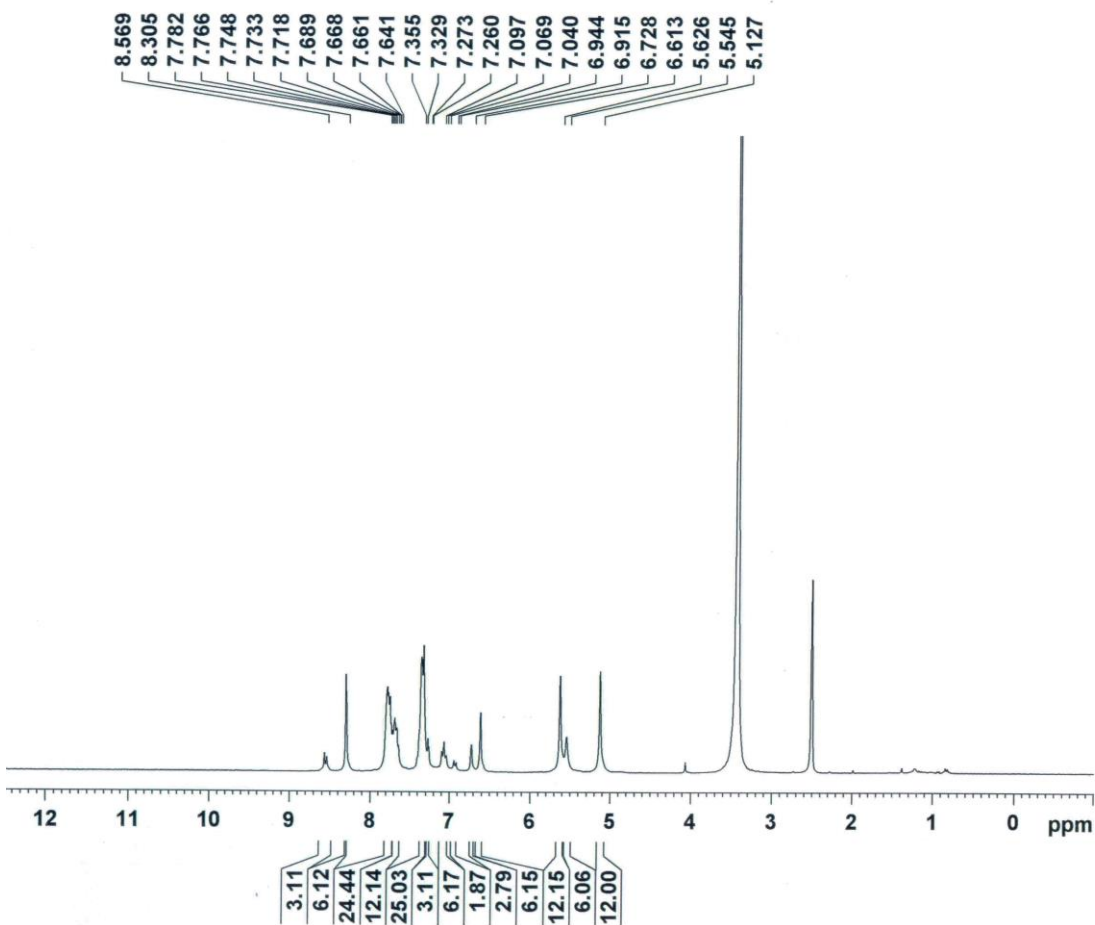
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 0.00 dB  
PL12 15.68 dB  
PL13 16.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4678267 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) spectrum of the dendrimer **6**



UNIV. OF MADRAS



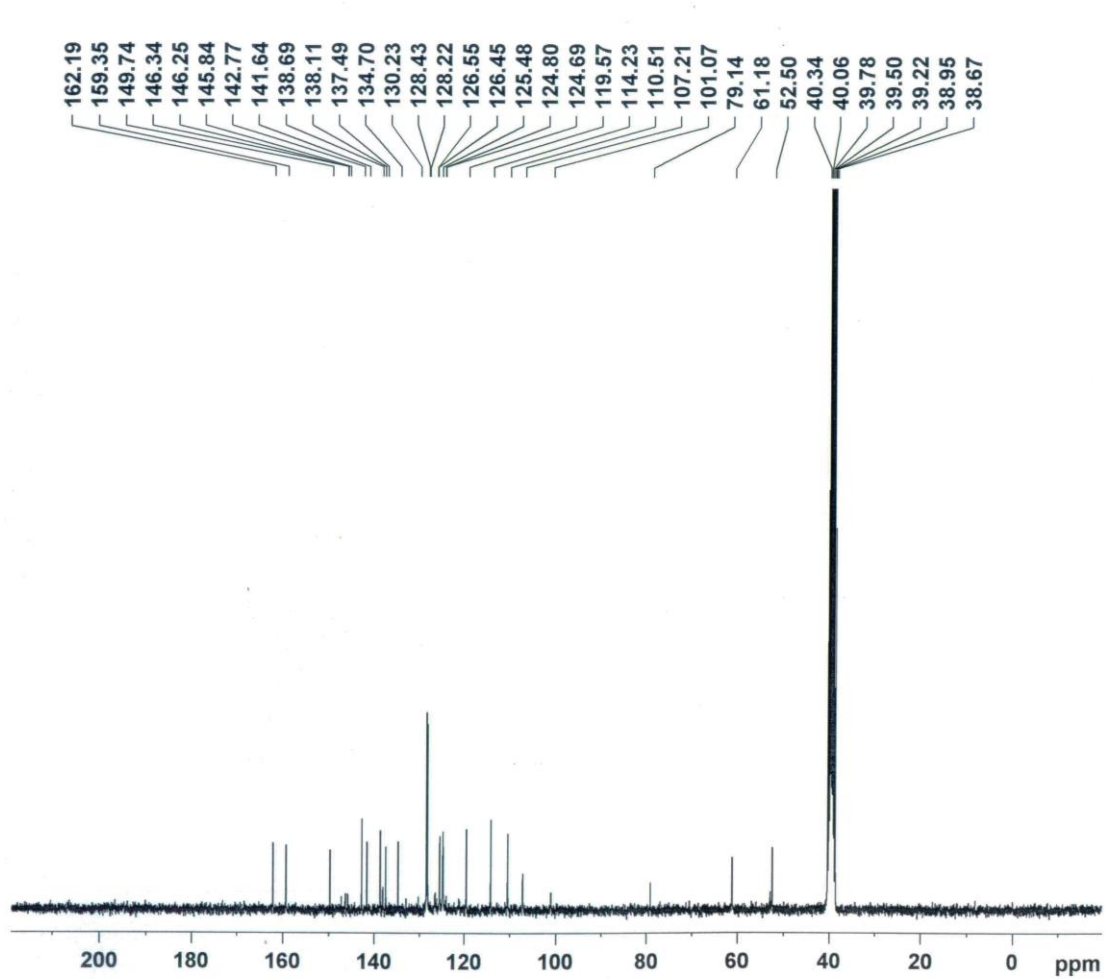
Current Data Parameters  
NAME KRC-286  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150611  
Time 17.54  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
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 1.0000000 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 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

$^1\text{H}$  NMR (300 MHz, DMSO- $\text{d}_6$ ) spectrum of the dendrimer **7**



Current Data Parameters  
NAME KRC-286  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150704  
Time 14.57  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 2000  
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 2.0000000 sec  
d11 0.0300000 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 75.4677867 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) spectrum of the dendrimer **7**

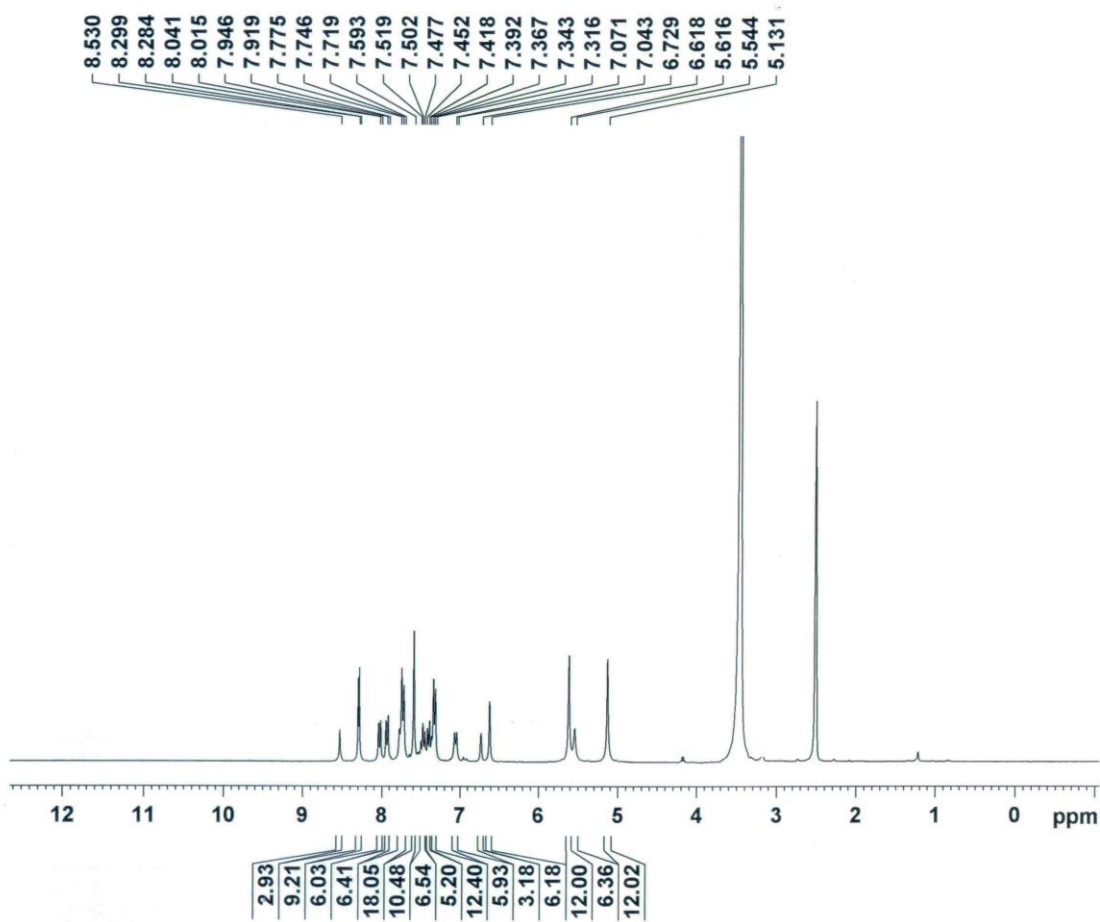


Current Data Parameters  
 NAME KRC-262  
 EXPNO 1  
 PROCNO 1

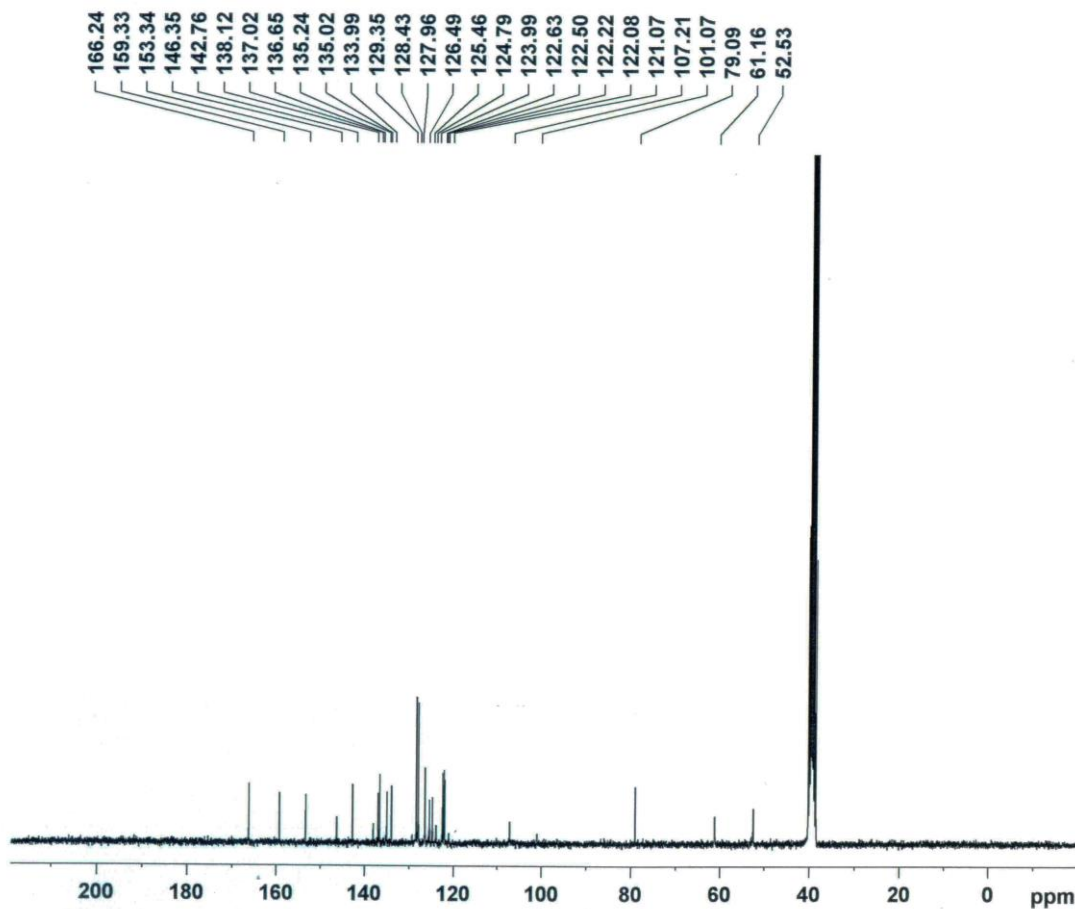
F2 - Acquisition Parameters  
 Date\_ 20150415  
 Time 15.16  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 64  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.15 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, DMSO-d<sub>6</sub>) spectrum of the dendrimer **8**



Current Data Parameters  
NAME KRC-262  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150417  
Time 21.54  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 3735  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 9195.2  
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 9.30 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 75.4677867 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^{13}\text{C}$  NMR (75 MHz, DMSO- $d_6$ ) spectrum of the dendrimer **8**

## BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

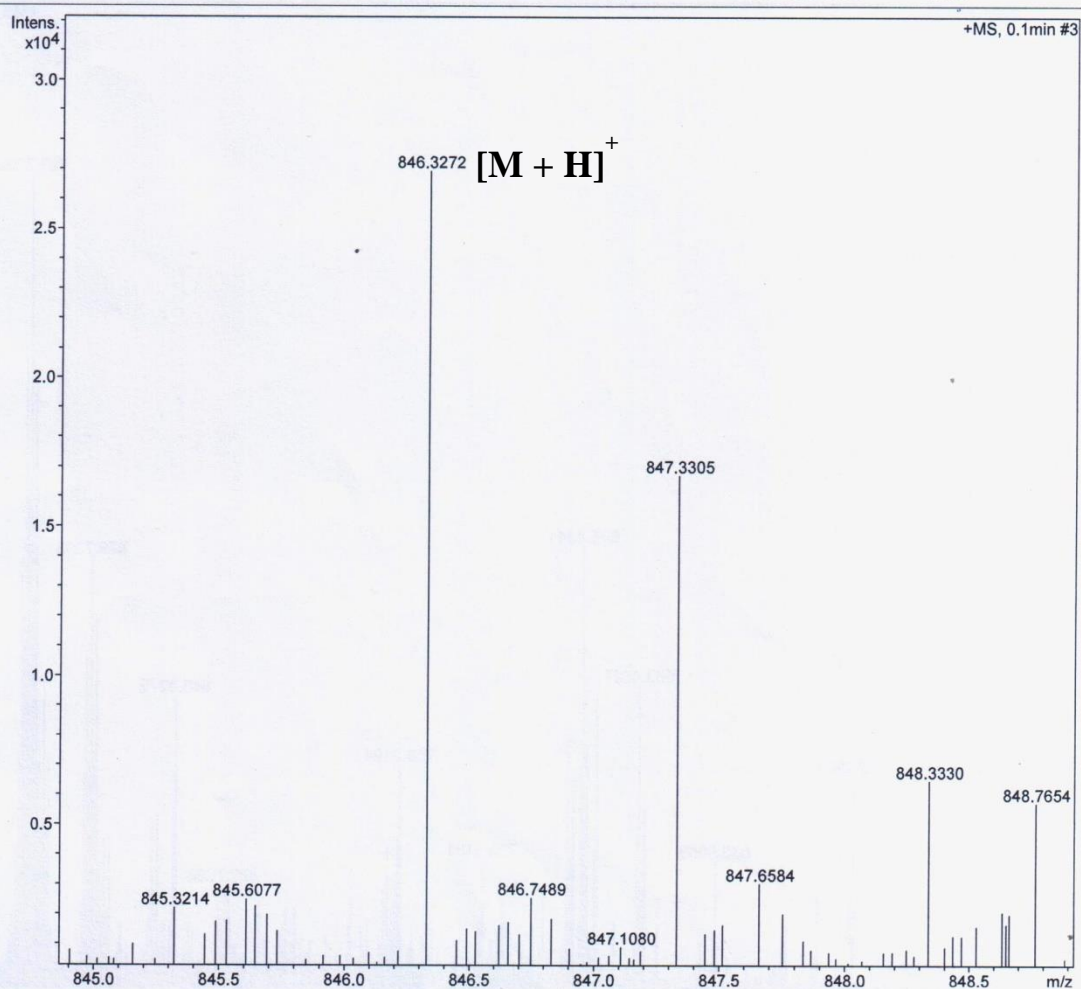
Analysis Name D:\Data\2015\DrNagarajan\NOV\BSN-V1-R.d  
Method tune\_low\_Pos.m  
Sample Name BSN-V1-CHCL3-MEOH  
Comment

Acquisition Date 11/24/2015 12:54:25 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



ESI mass spectrum of dendrimer 1

# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

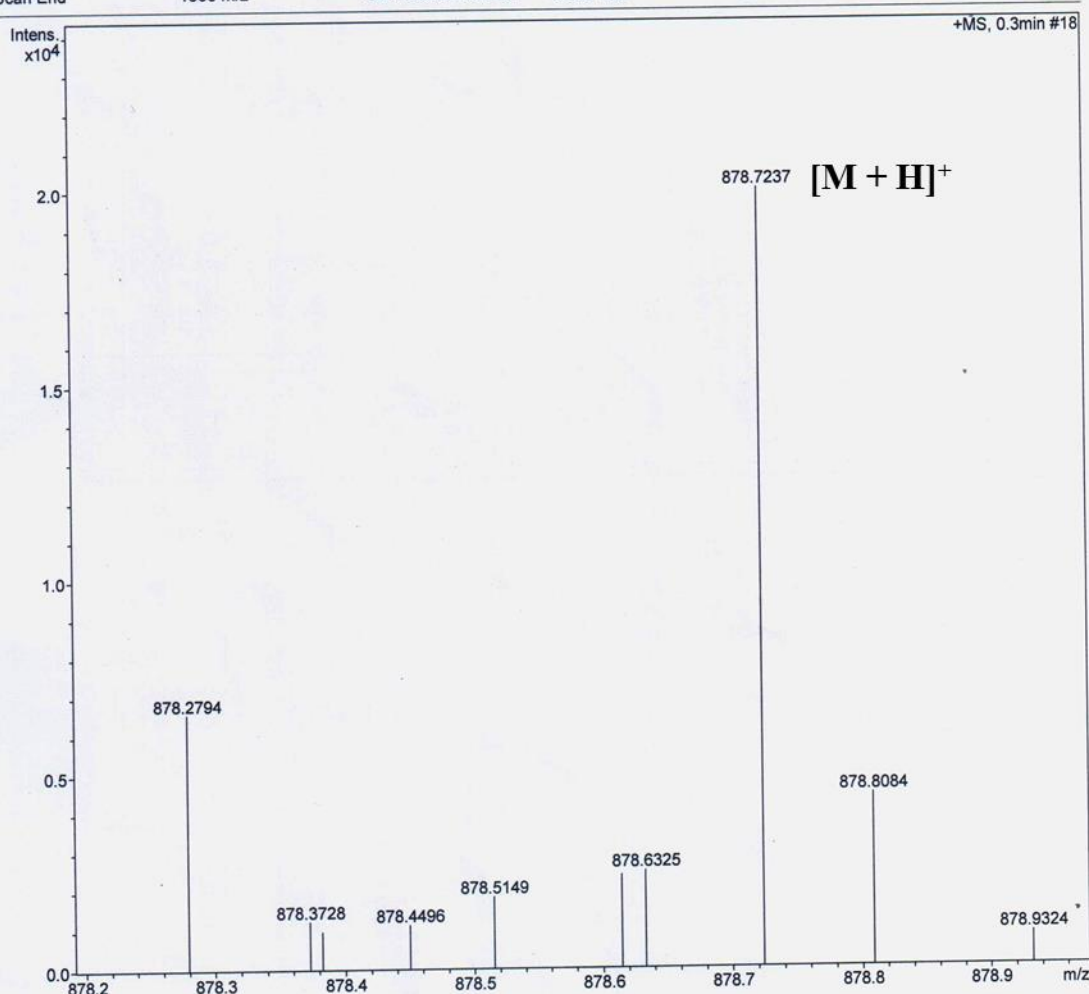
Analysis Name D:\Data\2015\DrNagarajan\NOV\BSN-V2.d  
Method tune\_low\_Pos.m  
Sample Name BSN-V2-CHCL3-MEOH  
Comment

Acquisition Date 11/24/2015 1:05:47 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



ESI mass spectrum of dendrimer 2

# BRUKER MAXIS HRMS REPORT

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## Analysis Info

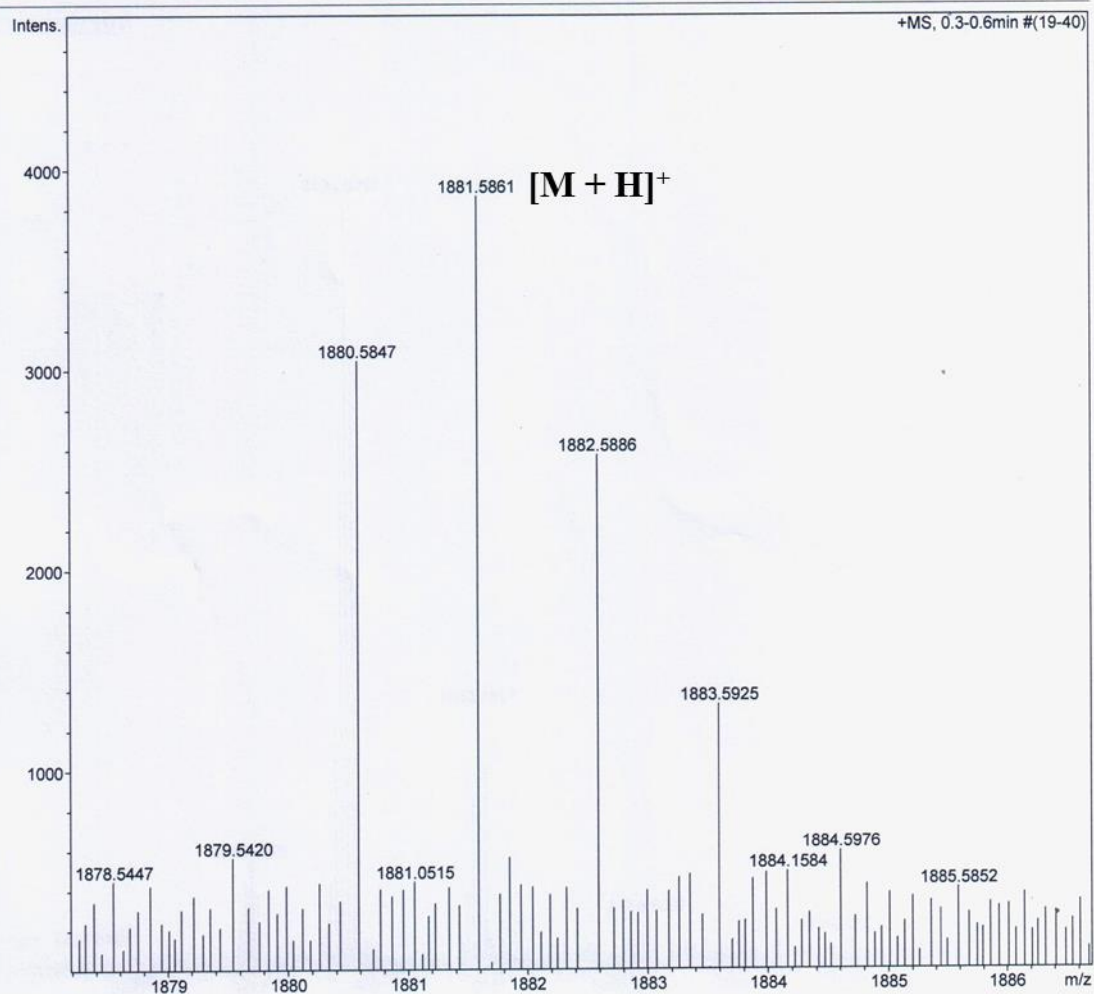
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Method tune\_wide\_PosR.m  
Sample Name BSN-V5-CHCL3-MEOH  
Comment

Acquisition Date 11/27/2015 12:02:50 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
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Scan End	2200 m/z	Set Collision Cell RF	2500.0 Vpp	Set Divert Valve	Source



ESI mass spectrum of dendrimer 3

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## Analysis Info

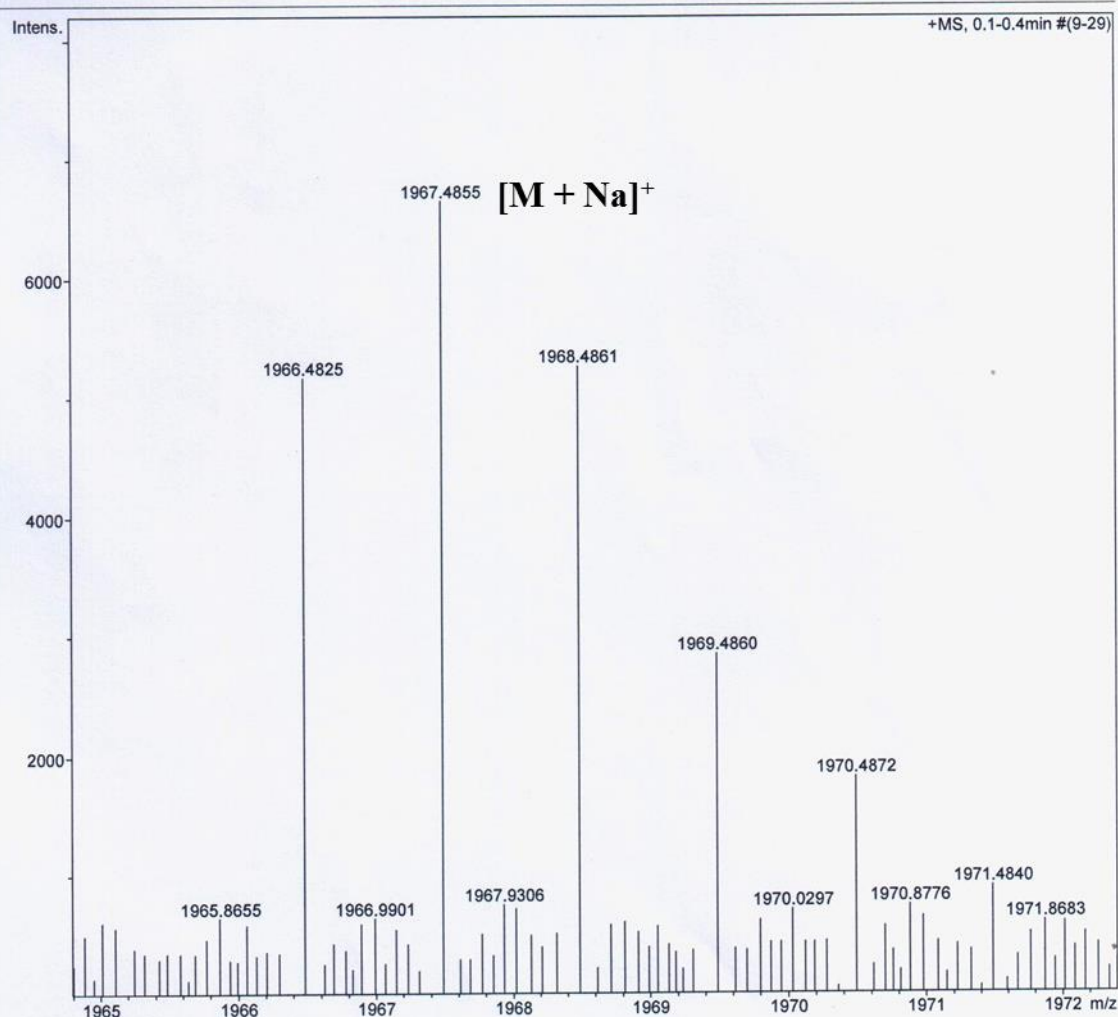
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Acquisition Date 11/17/2015 1:08:22 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2400 m/z	Set Collision Cell RF	2500.0 Vpp	Set Divert Valve	Source



ESI mass spectrum of dendrimer 4



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Analysis Info

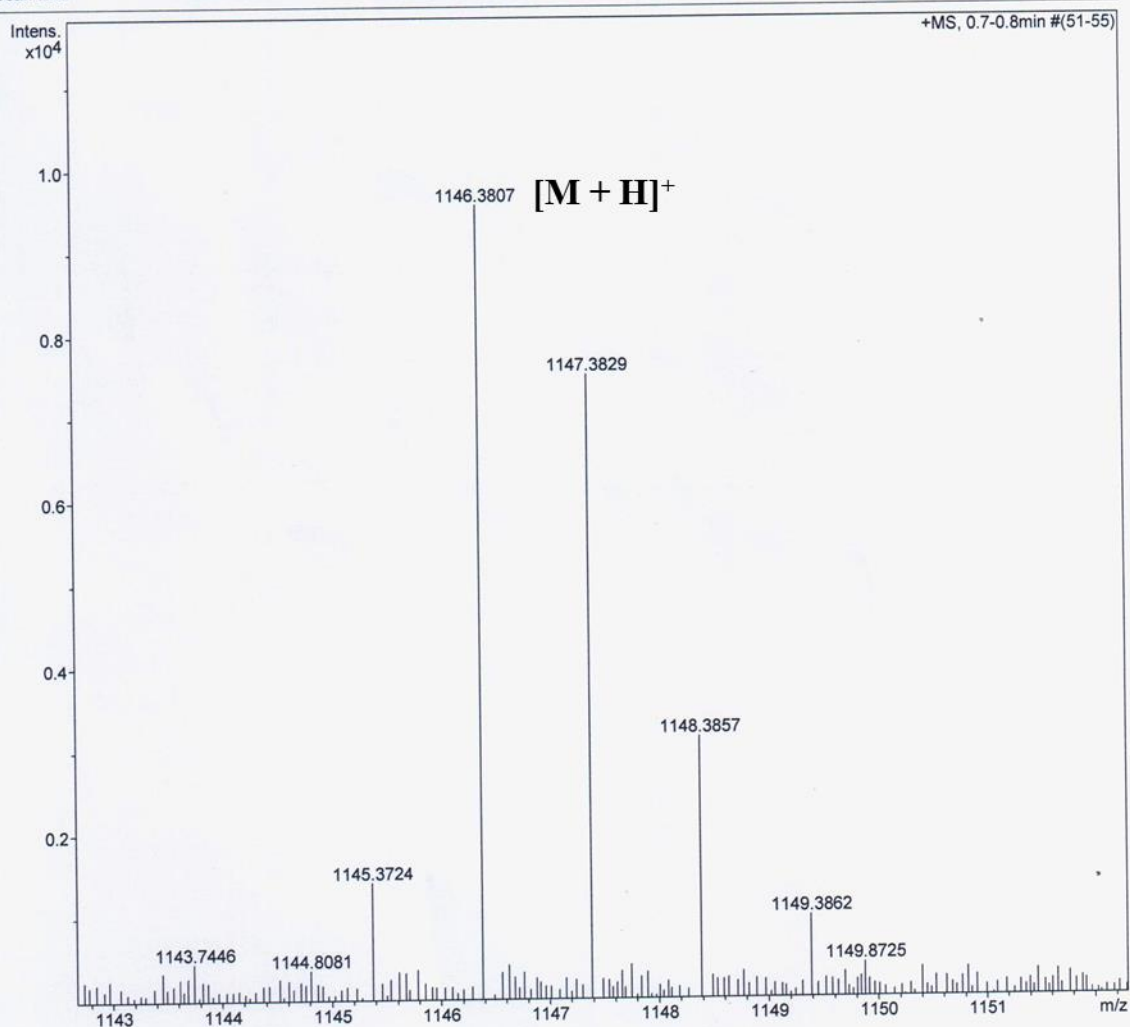
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Sample Name BSN-V3-CHCL3-MEOH  
Comment

Acquisition Date 12/1/2015 12:52:33 PM

Operator Ramu Sridhar  
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2500.0 Vpp	Set Divert Valve	Source



ESI mass spectrum of dendrimer 5

# BRUKER MAXIS HRMS REPORT

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## Analysis Info

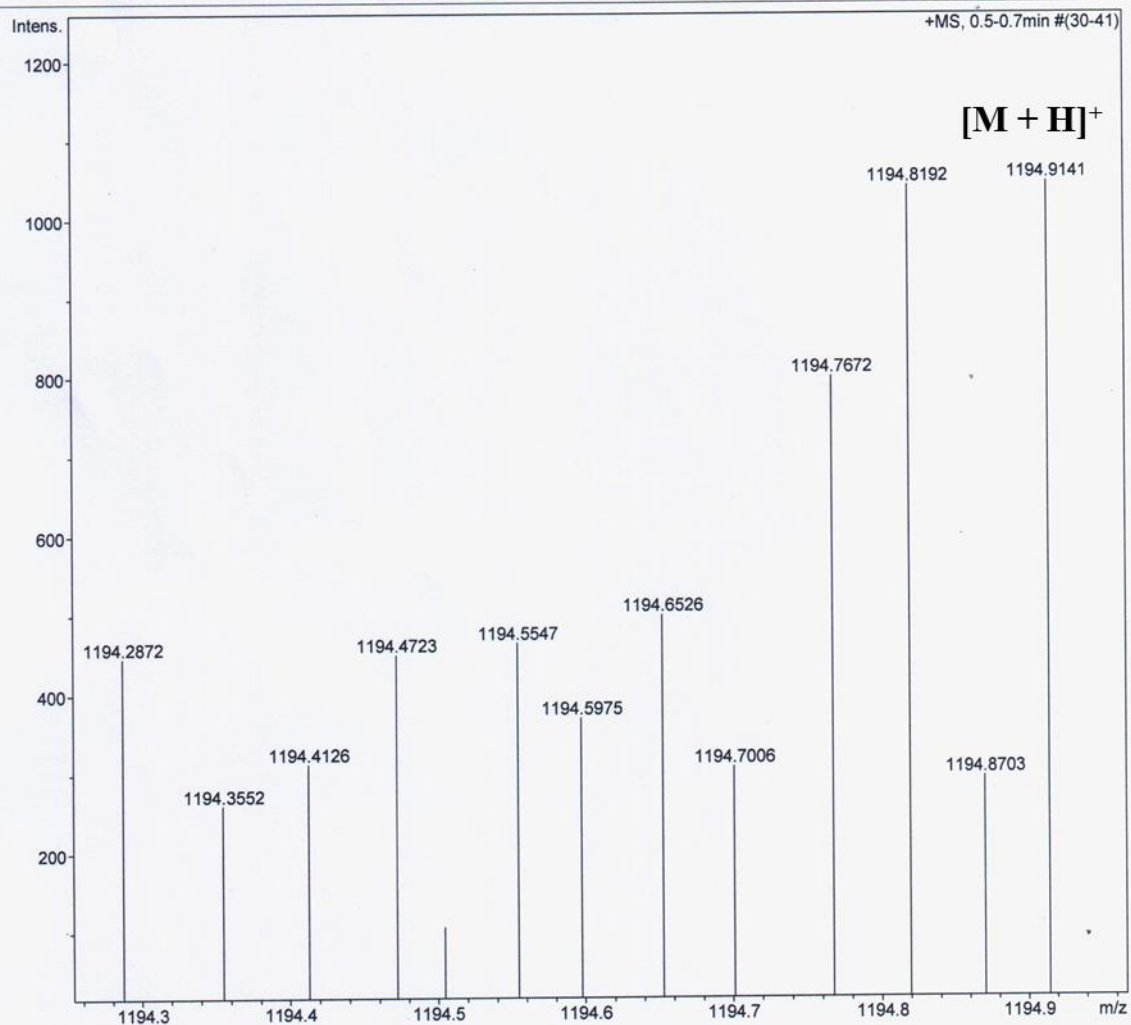
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Comment

Acquisition Date 11/27/2015 11:52:26 AM

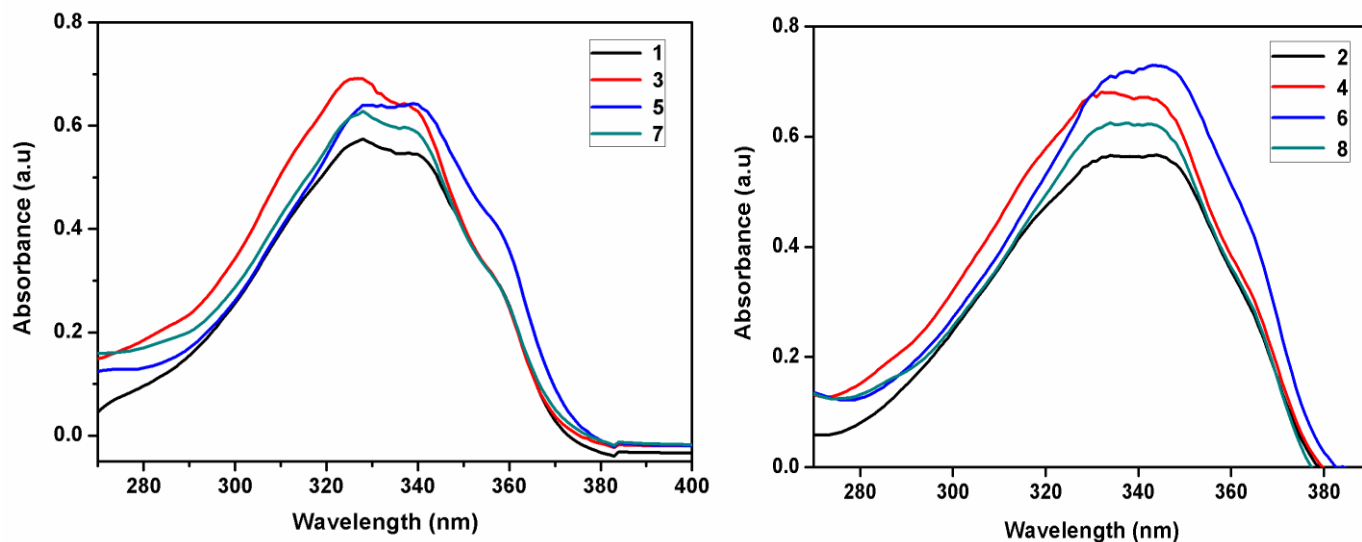
Operator Ramu Sridhar  
Instrument maXis 10138

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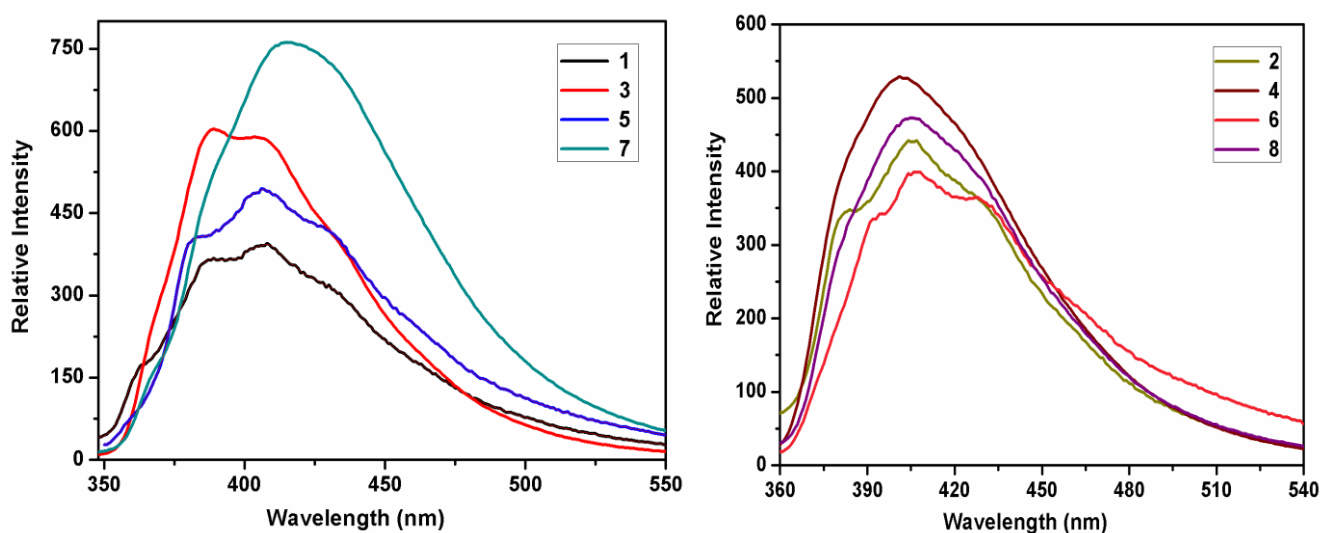
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Scan End	3500 m/z	Set Collision Cell RF	2500.0 Vpp	Set Divert Valve	Source



ESI mass spectrum of dendrimer **6**

**Absorption spectra of benzoheterazole dendrimer 1-8**

**Fig. 1** UV- vis absorption spectra of benzoxazole dendrimer **1, 3, 5, 7** and benzothiazole dendrimer **2, 4, 6, 8** in DMF ( $1 \times 10^{-3} \text{ mol L}^{-1}$ ).

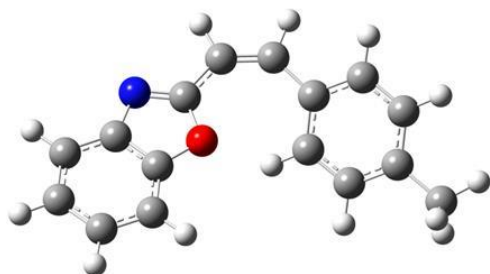
**Emission studies**

**Fig. 2** Emission spectra of benzoxazole dendrimer **1, 3, 5, 7** and benzothiazole dendrimer **2, 4, 6, 8** in DMF ( $1 \times 10^{-3} \text{ mol L}^{-1}$ )

### Energy minimization studies

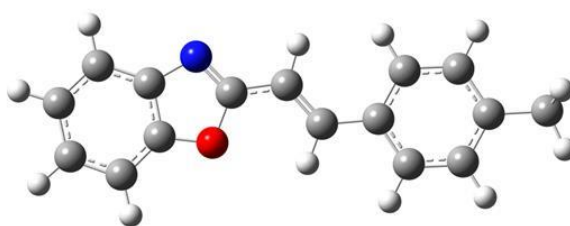
#### Benzoxazole 9

Cis



Total energy = -469081.4272 kcal/mol

Trans

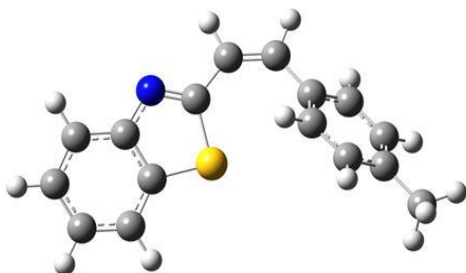


= -469087.4913 kcal/mol

**Trans energy is -6.0641276 kcal/mol less than Cis**

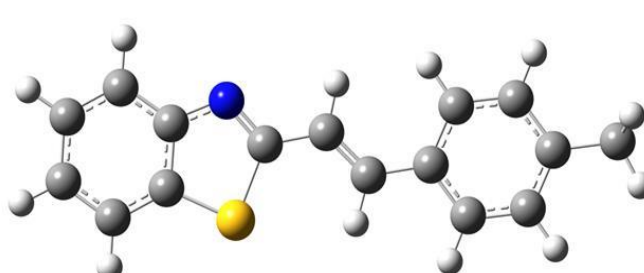
#### Benzothiazole 10

Cis



Total energy = -671748.6600kcal/mol

Trans

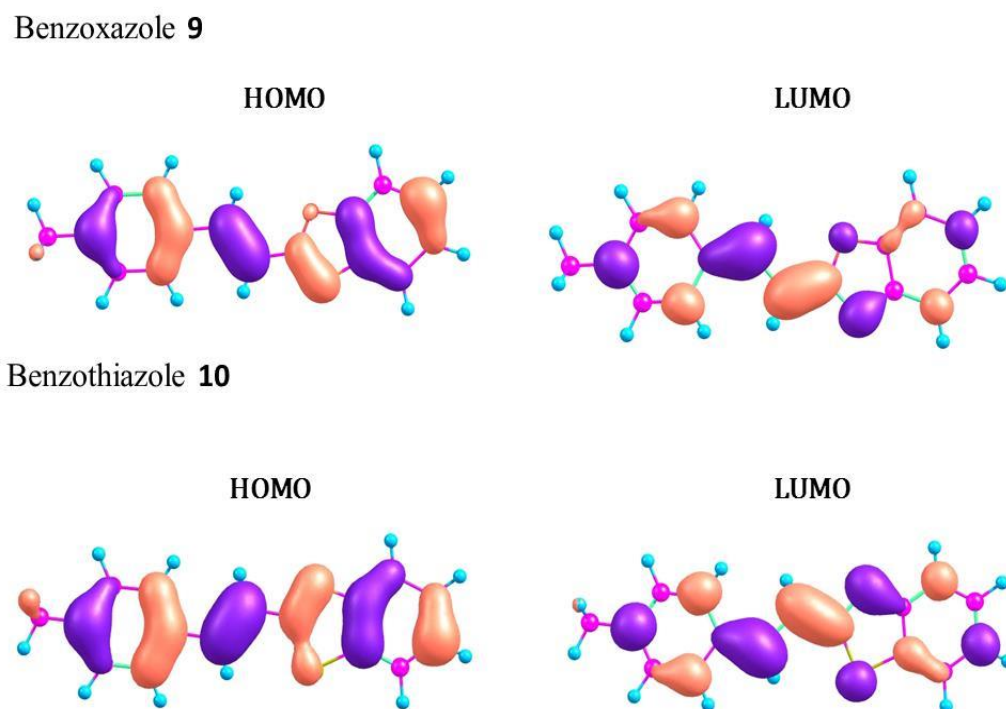


= -671755.0593kcal/mol

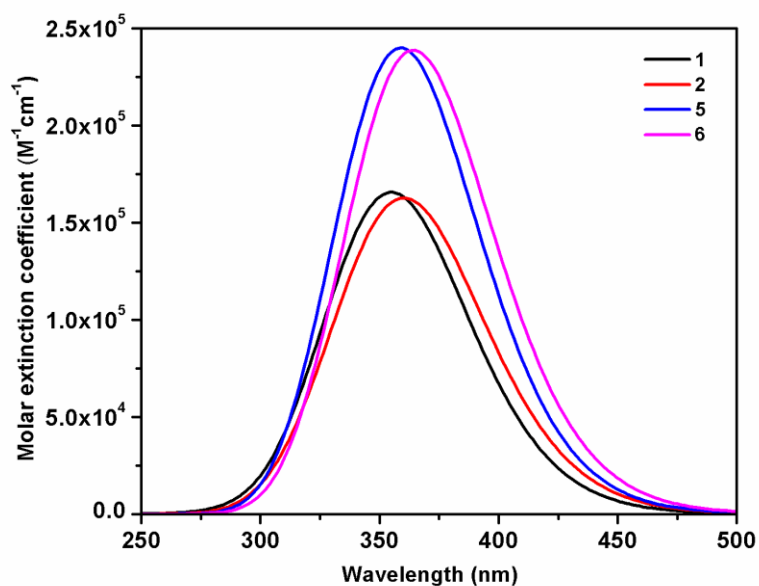
**Trans energy is -6.39921 kcal/mol less than Cis**

**Fig. 3** Energy minimized studies of benzoxazole 9 and benzothiazole 10

## Theoretical calculations



**Fig. 4** Density functional theory calculations of benzoxazole **9** and benzothiazole **10**



**Fig. 5** Density functional theory calculations of zeroth generation benzoheterazole dendrimer **1**, **2**, **5** and **6**

**Table 1** Oscillator strength and excitation energy of zeroth generation benzoheterazole dendrimer **1**, **2**, **5** and **6**

<b>Dendrimer</b>	<b>Oscillator strength (f)</b>	<b>Excitation energy (eV)</b>
1	1.6005	3.42 eV (362 nm)
	1.0640	3.48 eV (356 nm)
	1.3065	3.54 eV (349 nm)
2	1.7555	3.38 eV (367 nm)
	1.5554	3.42 eV (363 nm)
	1.0039	3.52 eV (352 nm)
5	1.6300	3.40 eV (365 nm)
	1.6647	3.41 eV (363 nm)
	1.3487	3.52 eV (352 nm)
6	1.3910	3.36 eV (369 nm)
	2.4833	3.37 eV (368 nm)
	1.0405	3.49 eV (355 nm)