10.1071/CH14400_AC

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SUPPLEMENTARY MATERIAL

Synthesis and thermal stability of new polynitrostilbenes

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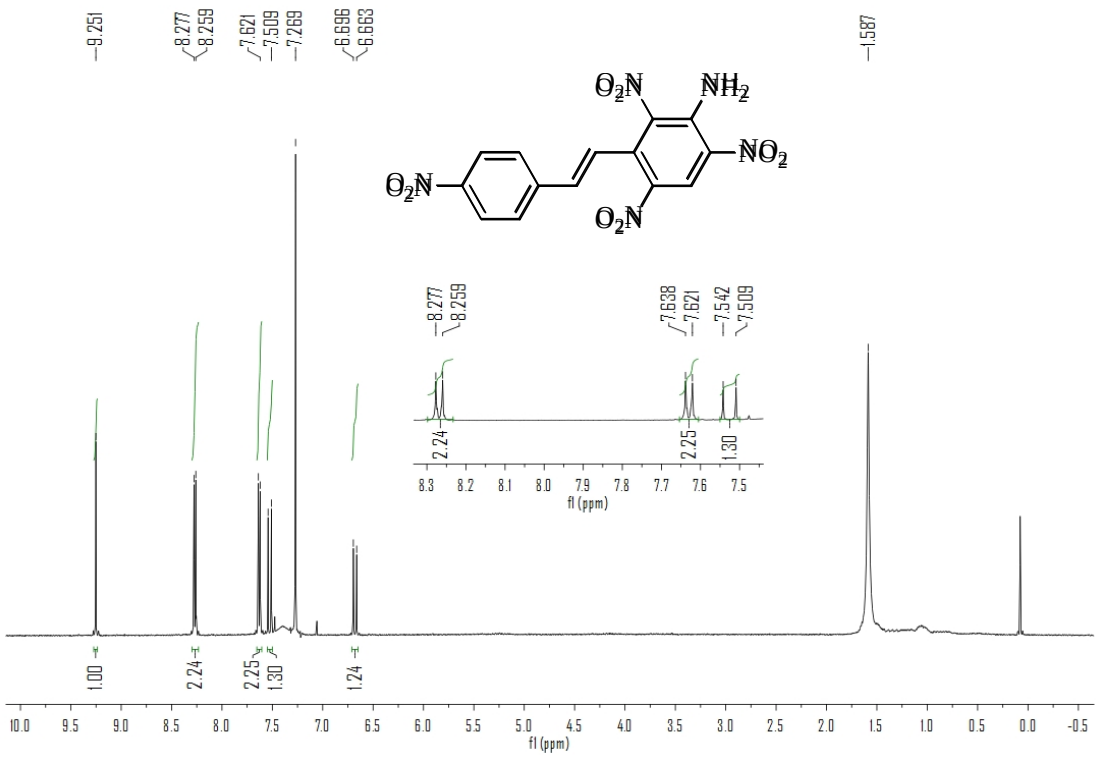
[B] Corresponding author. Email: xhpeng@mail.njust.edu.cn

NMR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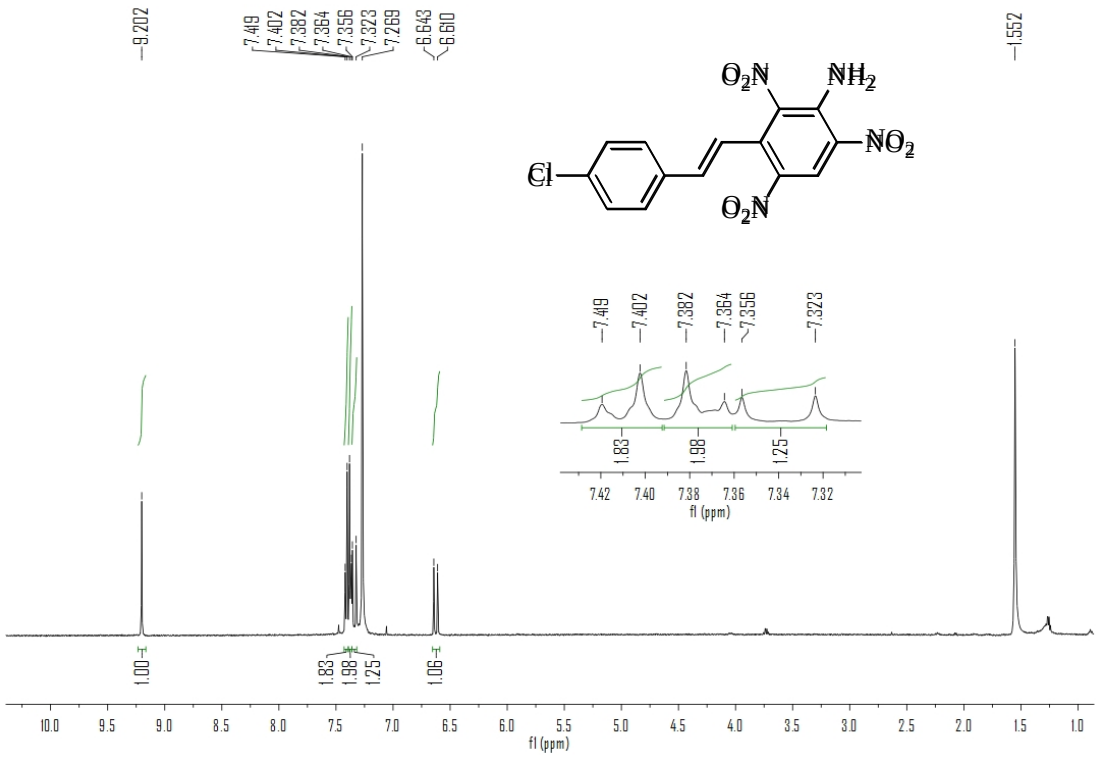
7.621
7.509
7.269
6.696
6.663
1.587
O2N
NH2
NO2
O2N
O2N
8.277
8.259
7.638
7.621
7.542
7.509
2.24
2.25
1.30
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)
1.00
2.24
2.25
1.30
1.24
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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7.356
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7.269
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6.610
1.552
O2N
NH2
NO2
Cl
O2N
7.419
7.402
7.382
7.364
7.356
7.323
1.83
1.98
1.25
7.42 7.40 7.38 7.36 7.34 7.32
f1 (ppm)
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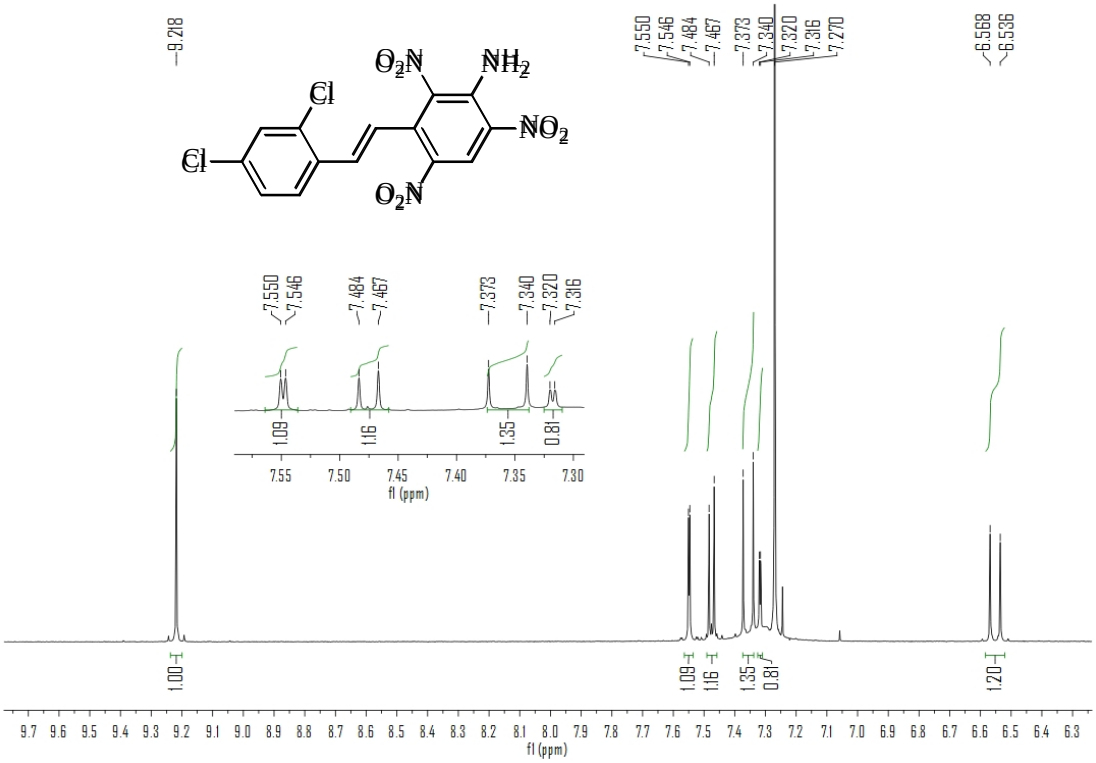
1.83
1.98
1.25
1.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)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1.09
1.16
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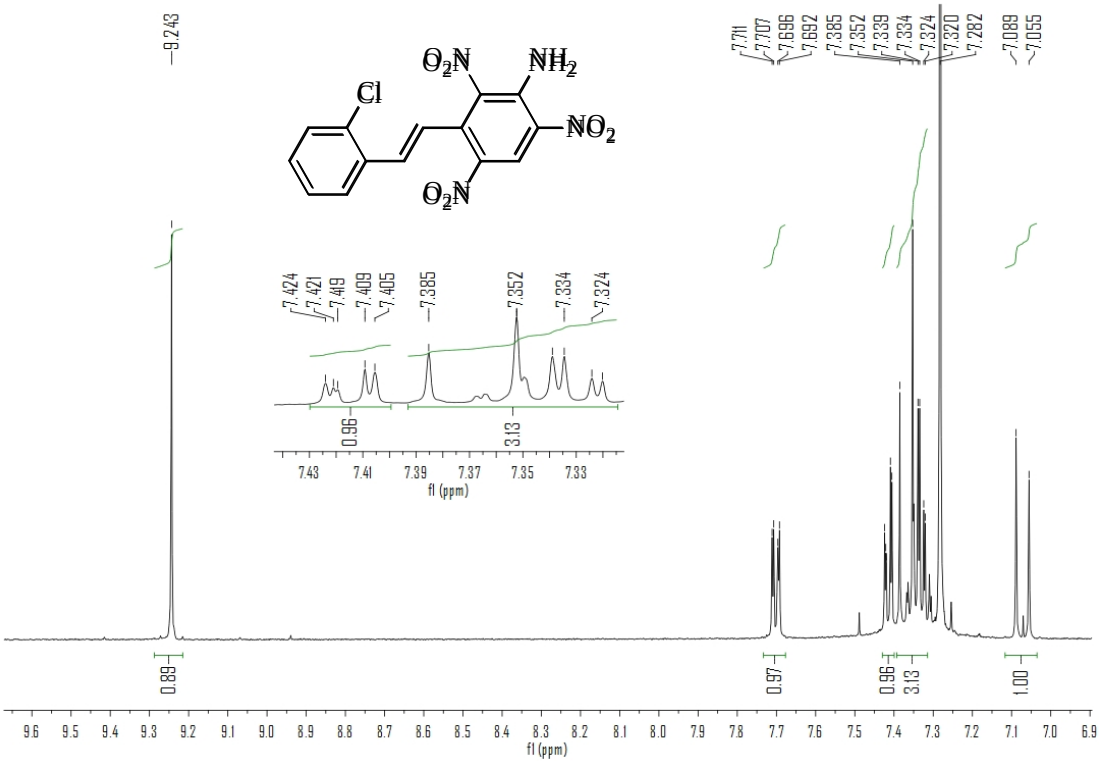
f1 (ppm)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7.339
7.334
7.324
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7.282
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7.055
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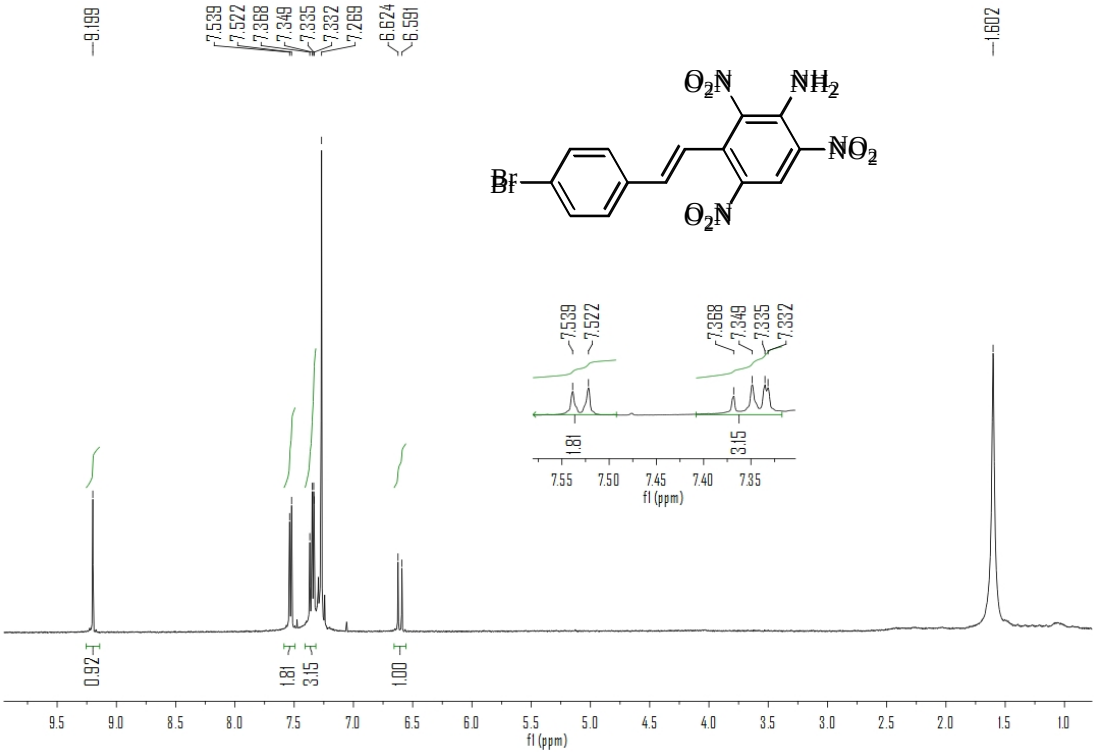
0.96
3.13
1.00
f1 (ppm)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6.591
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NO2
O2N
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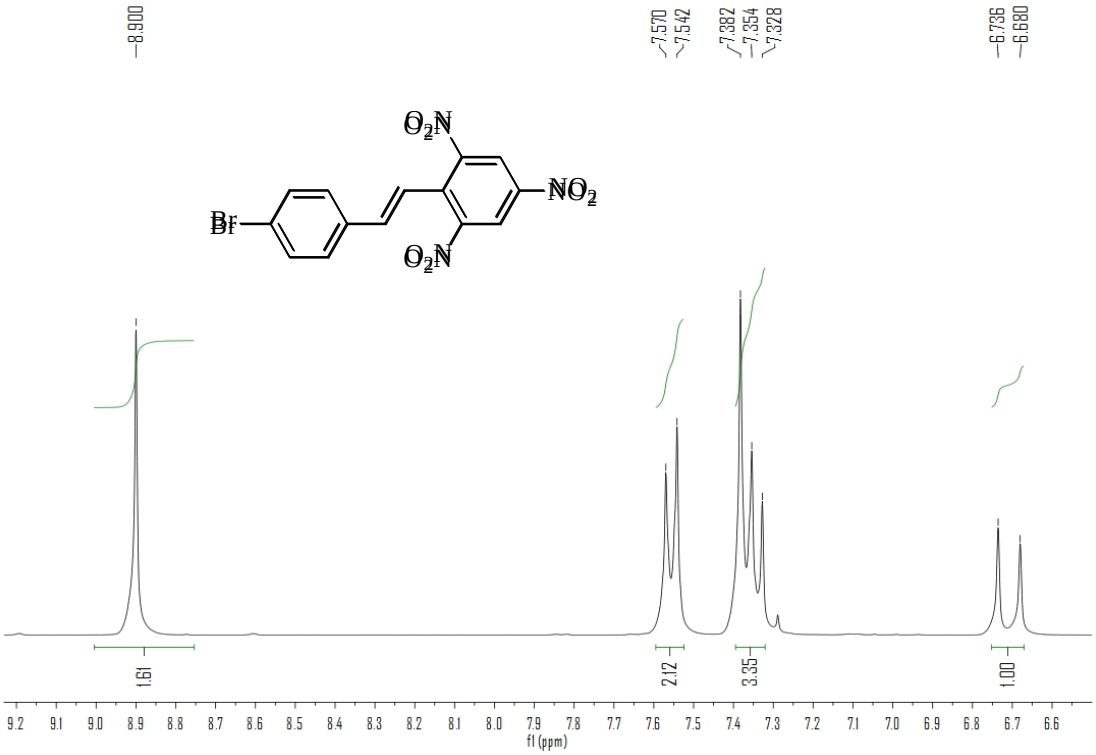
1.00
1.81
3.15
f1 (ppm)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O2N
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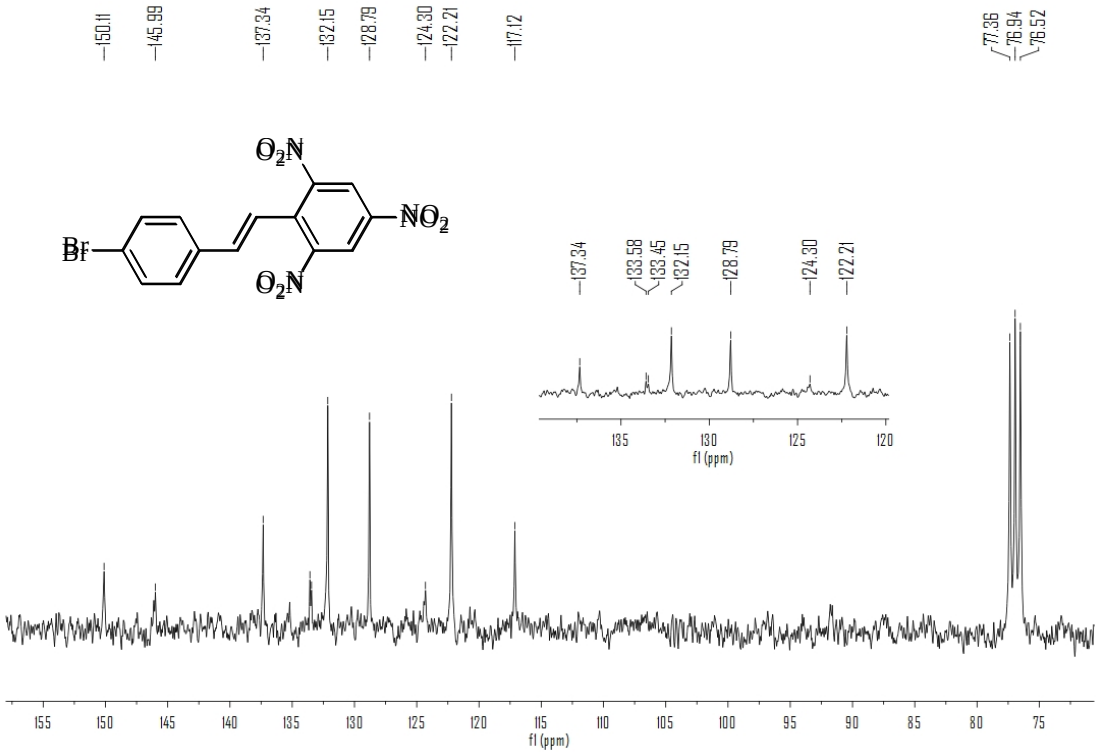
1.00
f1 (ppm)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132.15
128.79
124.30
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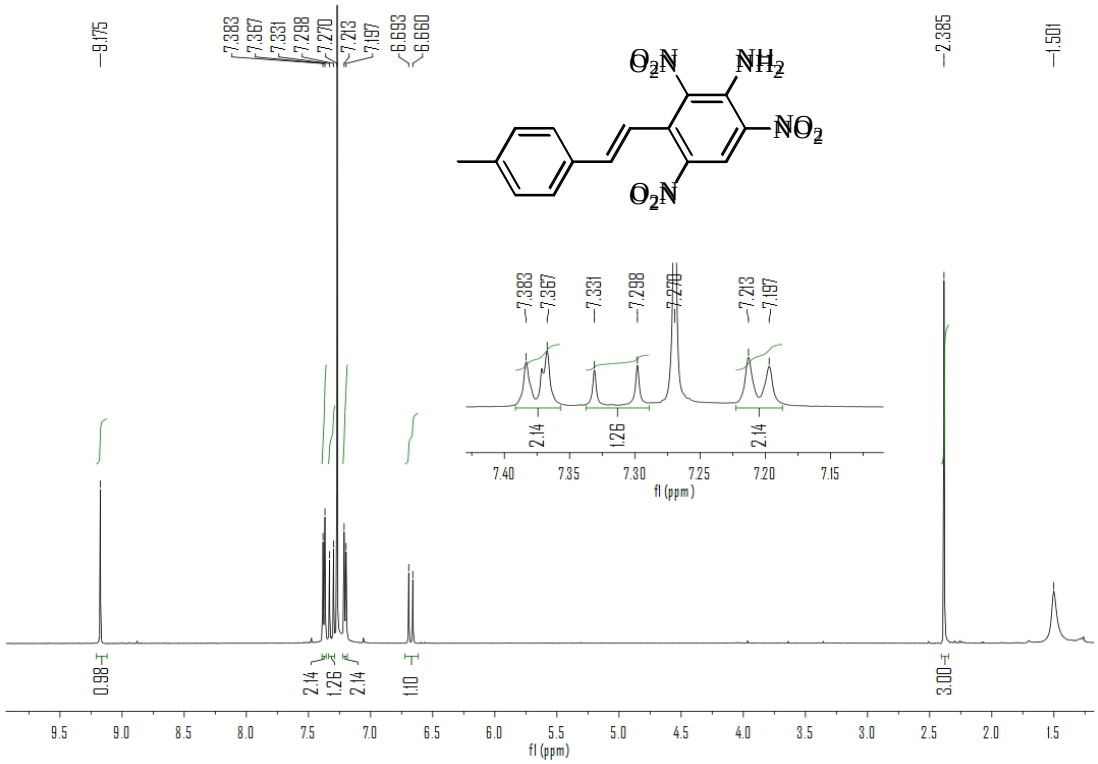
NO2
O2N
133.58
133.45
f1 (ppm)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6.660
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NO2
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1.26
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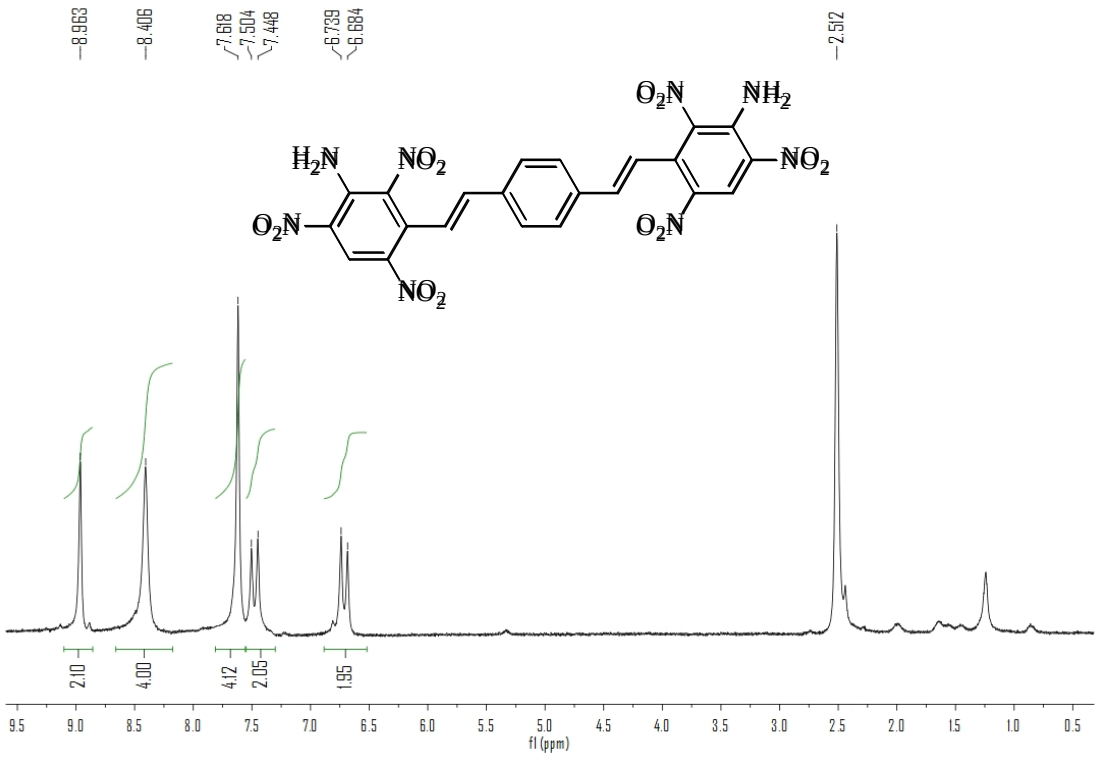
3.00
f1 (ppm)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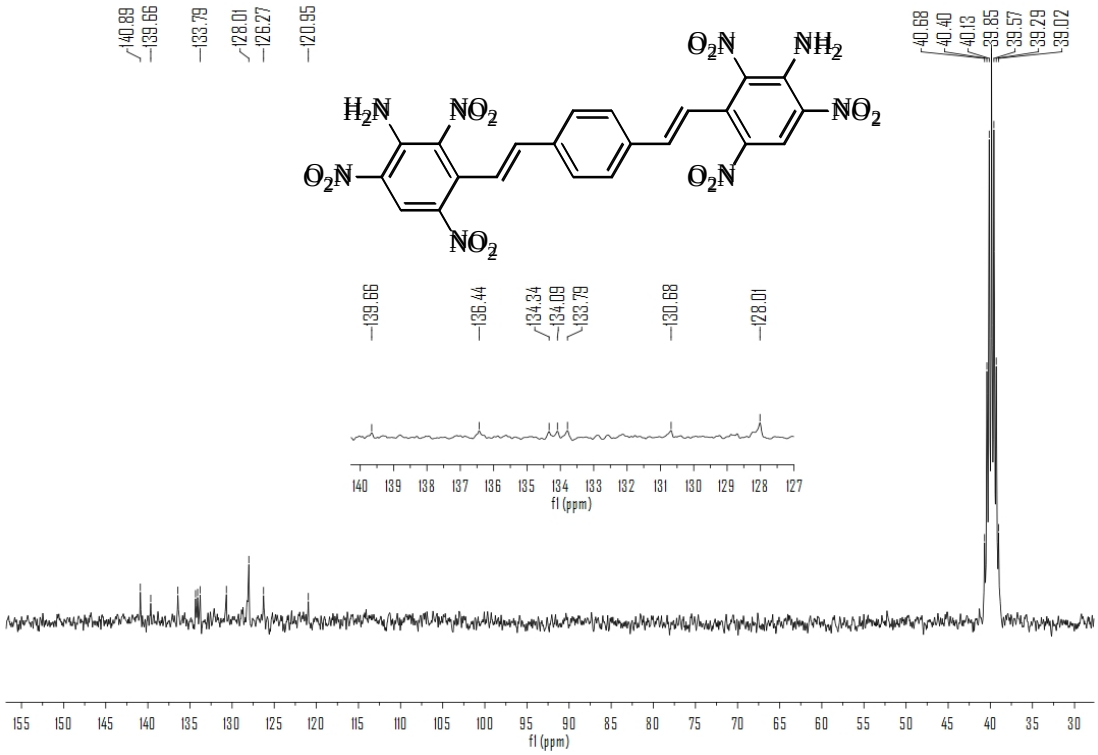
f1 (ppm)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133.79
128.01
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120.95
40.68
40.40
40.13
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39.02
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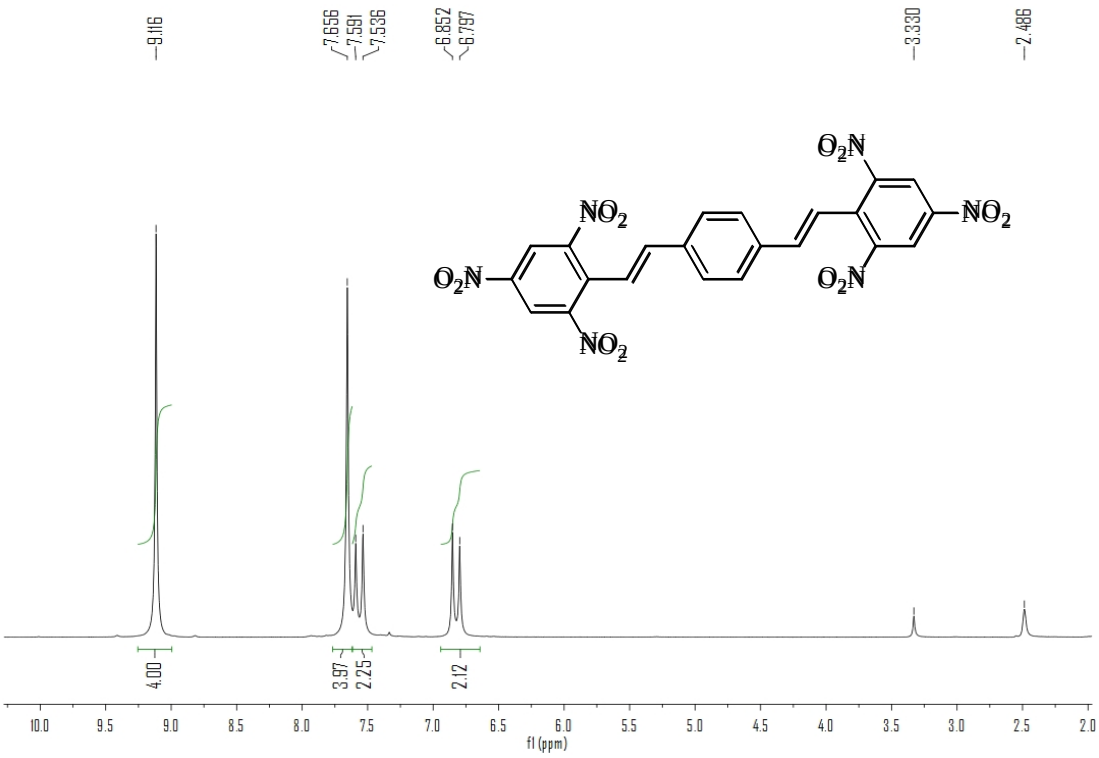
134.34
134.09
133.79
130.68
128.01
f1 (ppm)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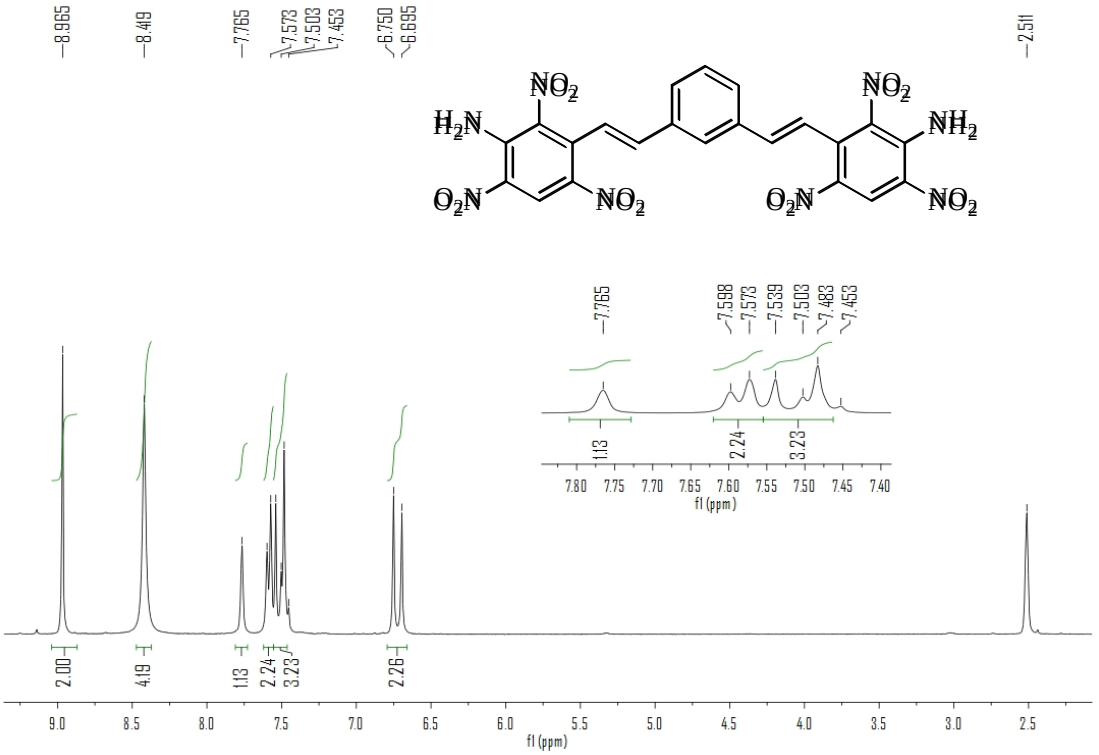
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6.695
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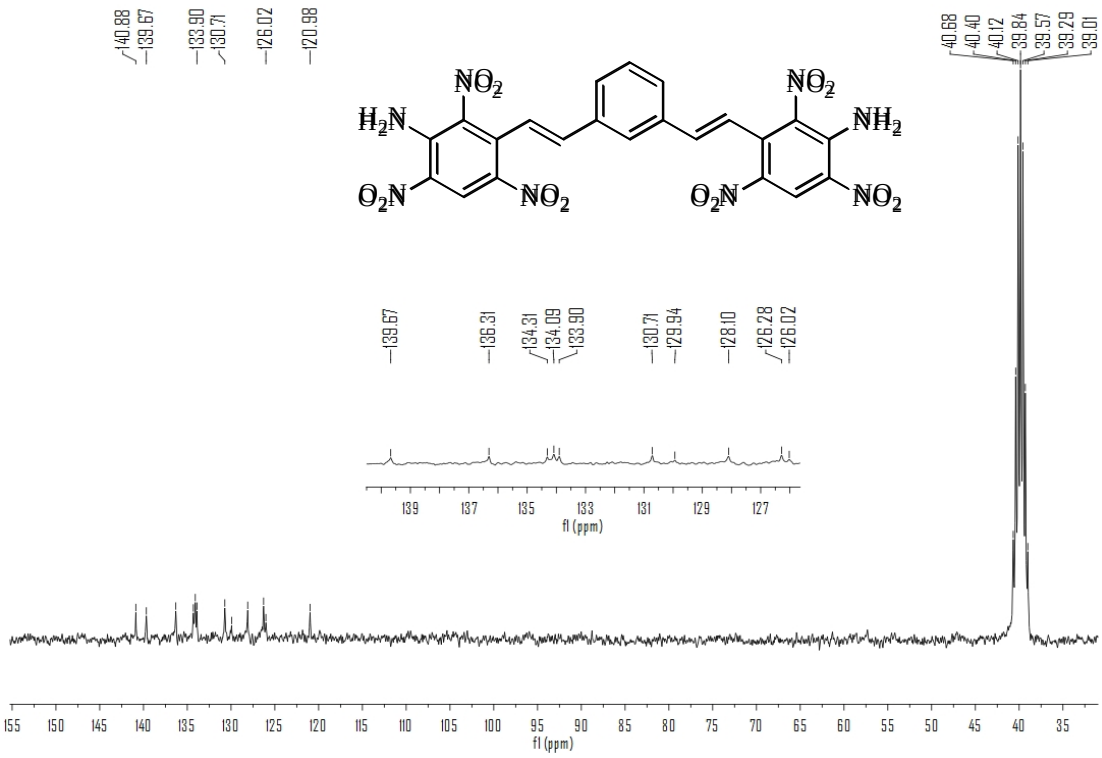
2.00
4.19
1.13
2.24
3.23
2.26
f1 (ppm)


140.88
139.67
133.90
130.71
126.02
120.98
40.68
40.40
40.12
39.84
39.57
39.29
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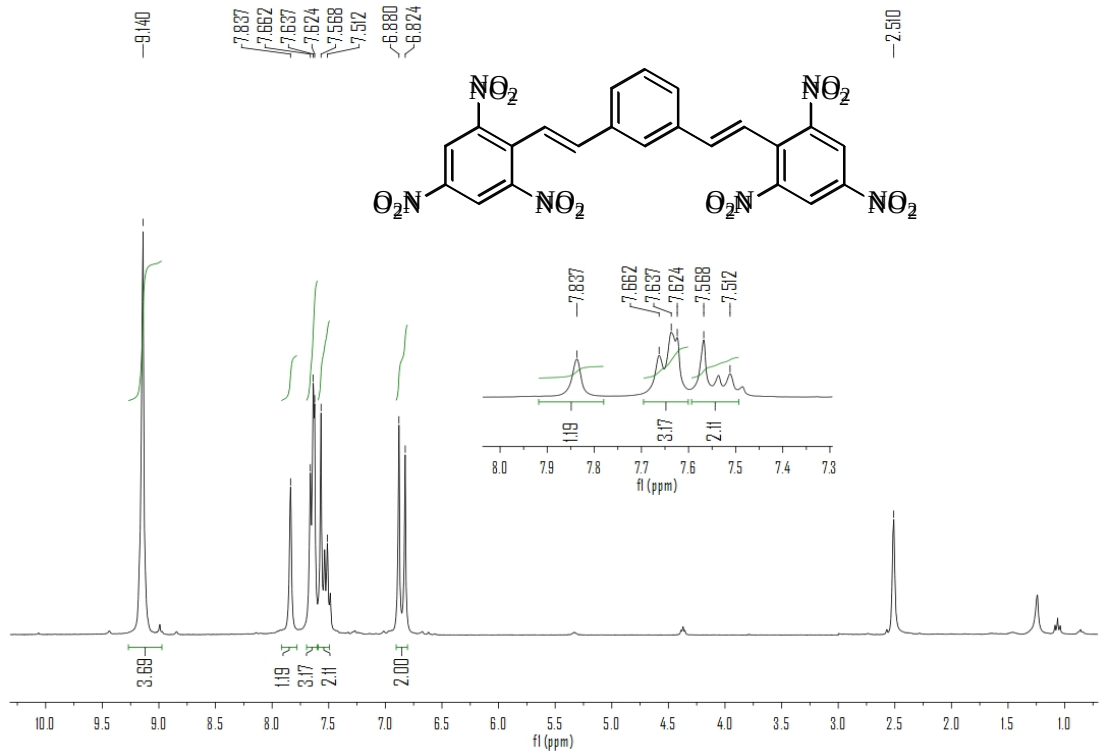
126.02
f1 (ppm)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7.662
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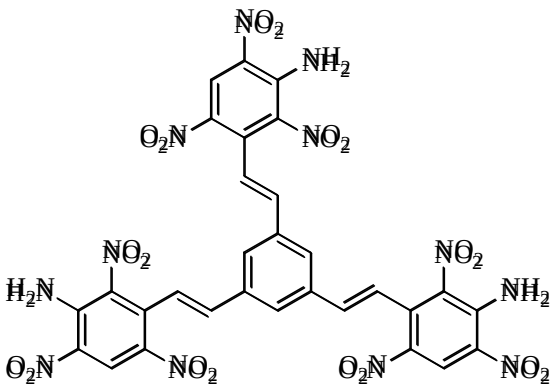
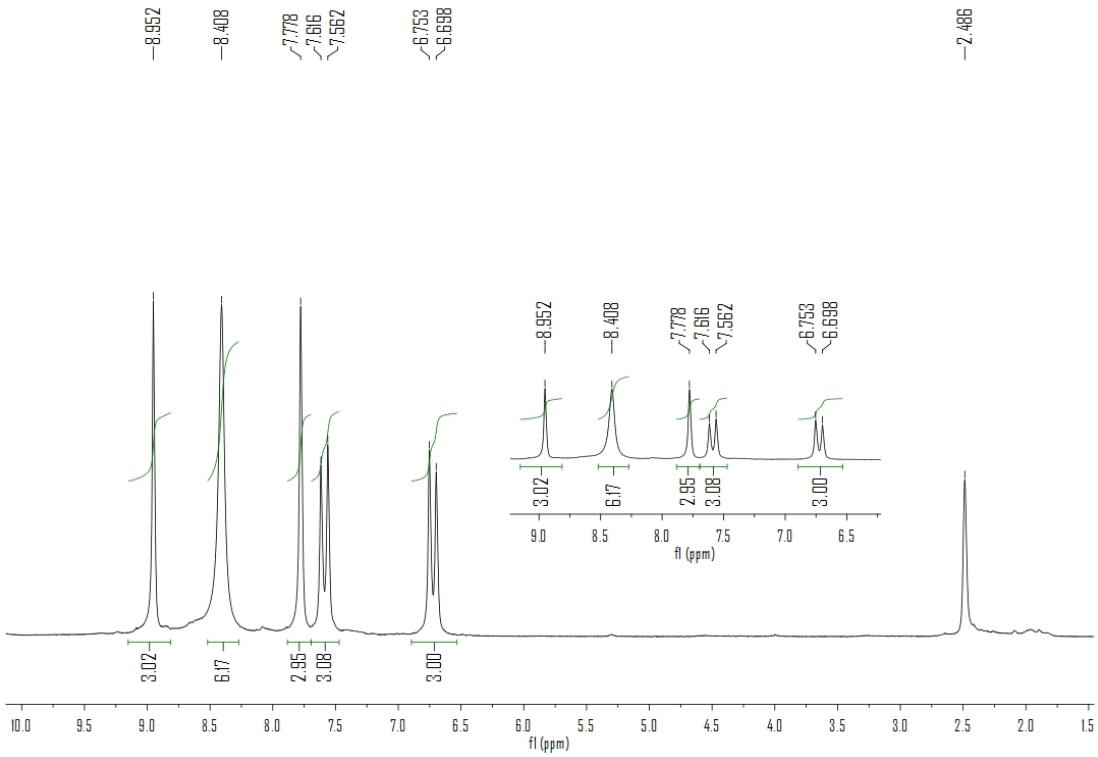
f1 (ppm)

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6.17
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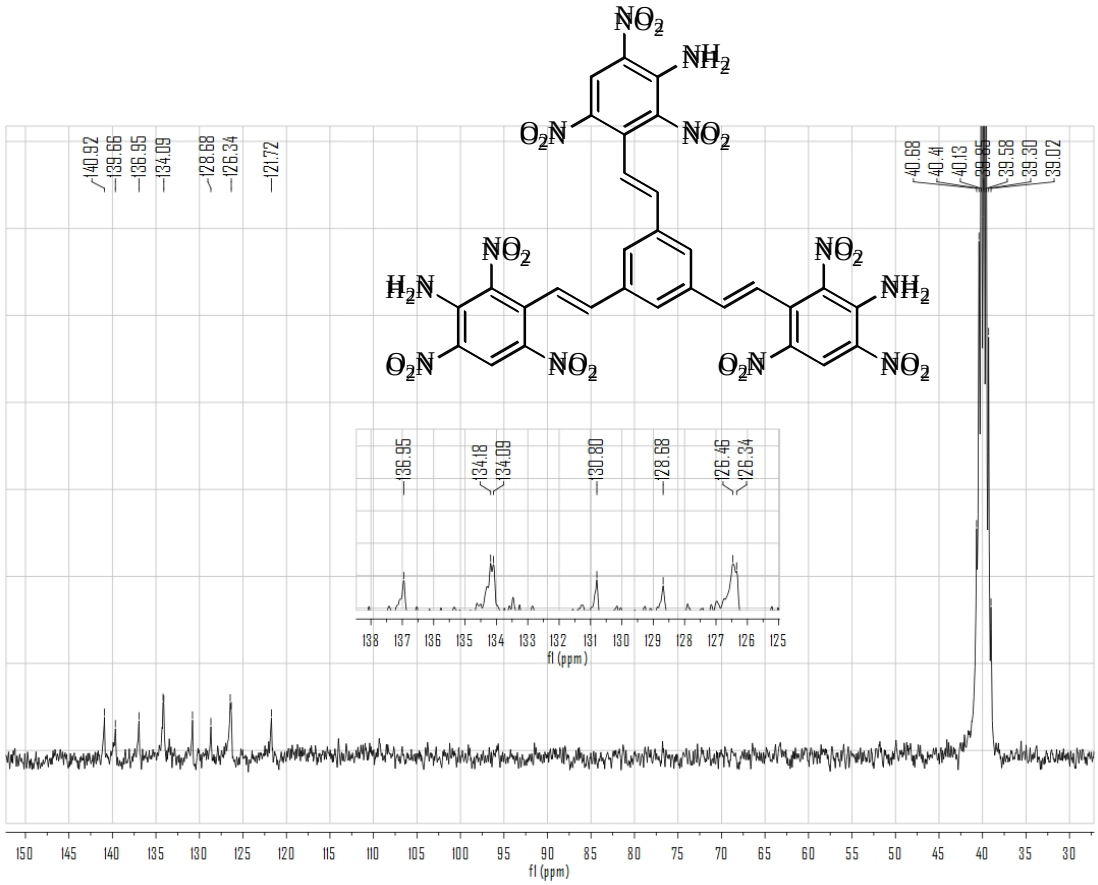
f1 (ppm)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134.09
128.68
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40.13
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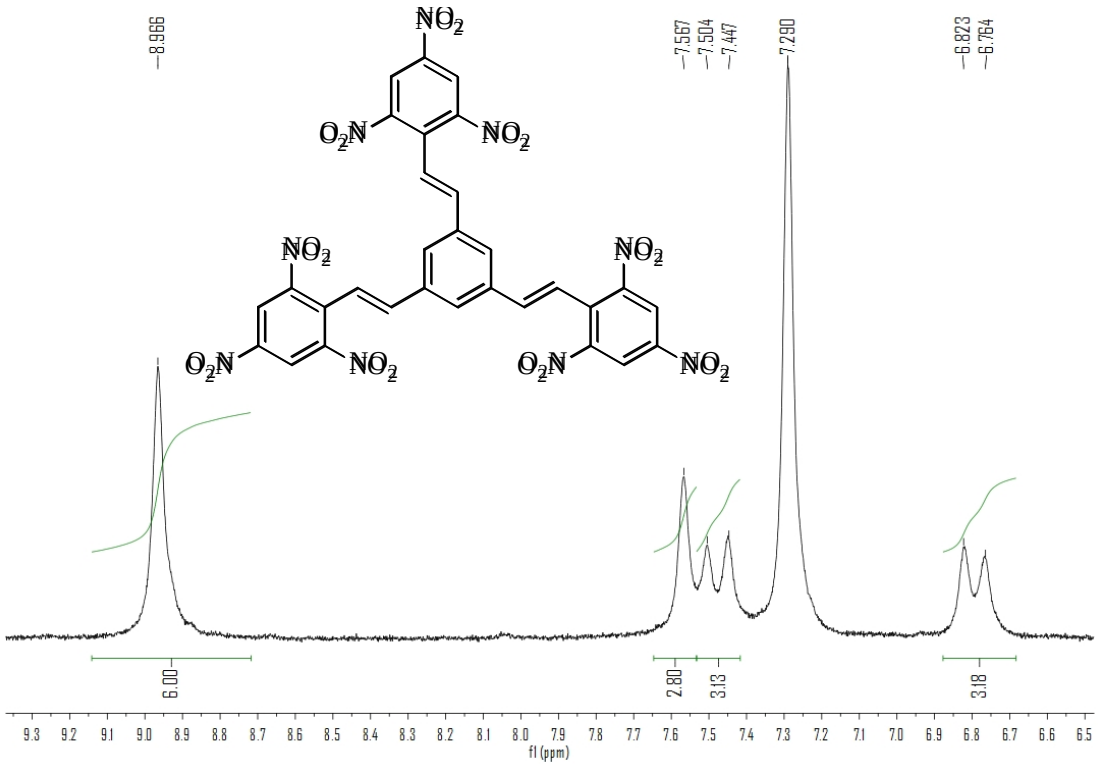
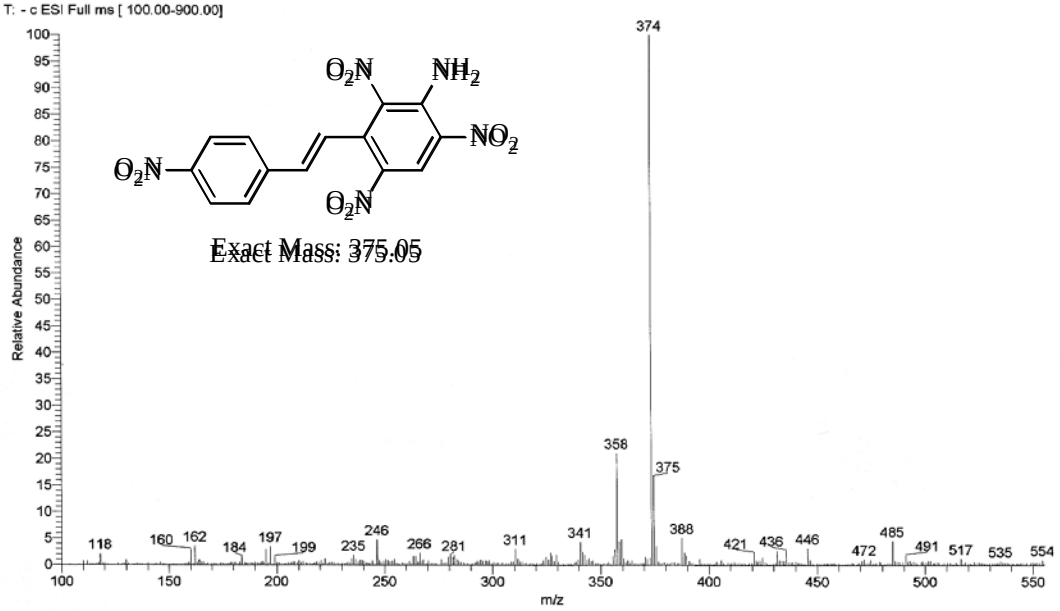
f1 (ppm)



MS

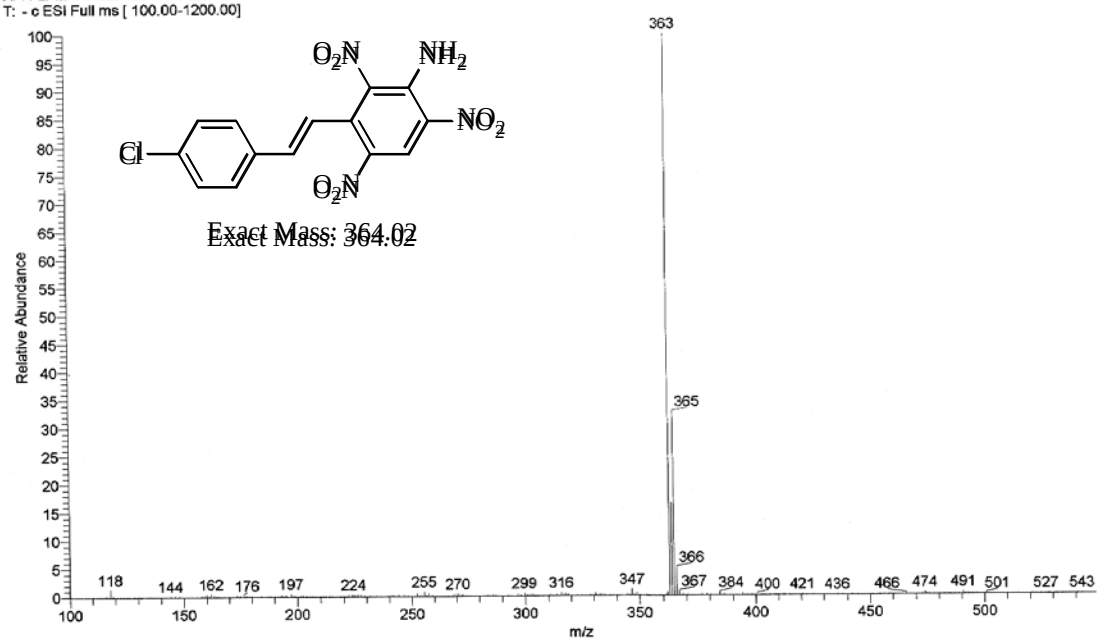
F:\data\XFN-LFM-4 2013-06-21 13:41:39

XFN-LFM-4 #43-65 RT: 0.93-1.26 AV: 23 NL: 6.78E6
T: - c ESI Full ms [100.00-900.00]



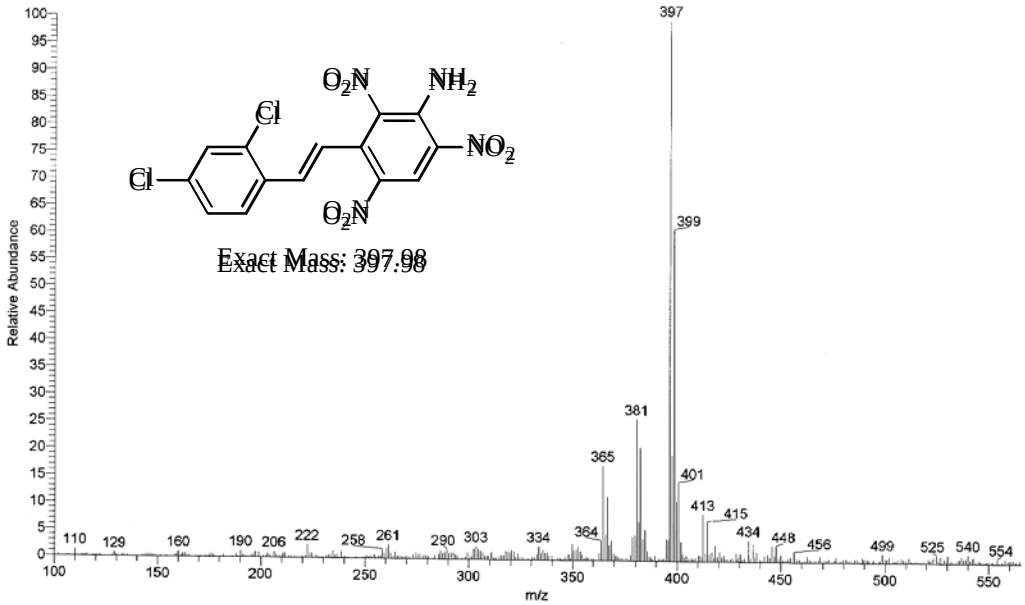
F:\data\XFN-LFM-1 2013-06-21 11:34:07

XFN-LFM-1 #122-138 RT: 2.59-2.85 AV: 17 NL: 3.79E7
T: - c ESI Full ms [100.00-1200.00]



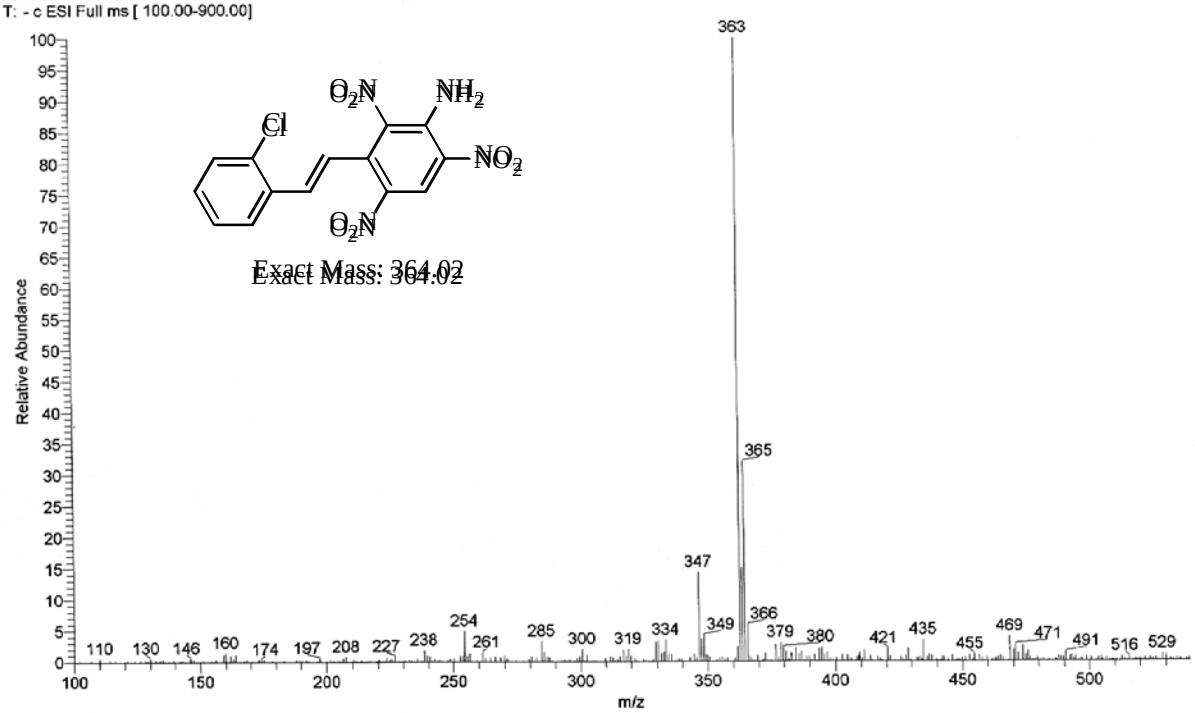
F:\DATA\XFN-LFM-6 2013-06-21 13:55:42

XFN-LFM-6 #32-44 RT: 0.78-0.94 AV: 13 SB: 2 0.50, 1.61 NL: 1.63E7
T: - c ESI Full ms [100.00-900.00]



F:\data\XFN-LFM--2 2013-06-21 13:26:26

XFN-LFM--2 #22-26 RT: 0.64-0.70 AV: 5 SB: 2 0.57, 0.85 NL: 2.36E7
T: - c ESI Full ms [100.00-900.00]



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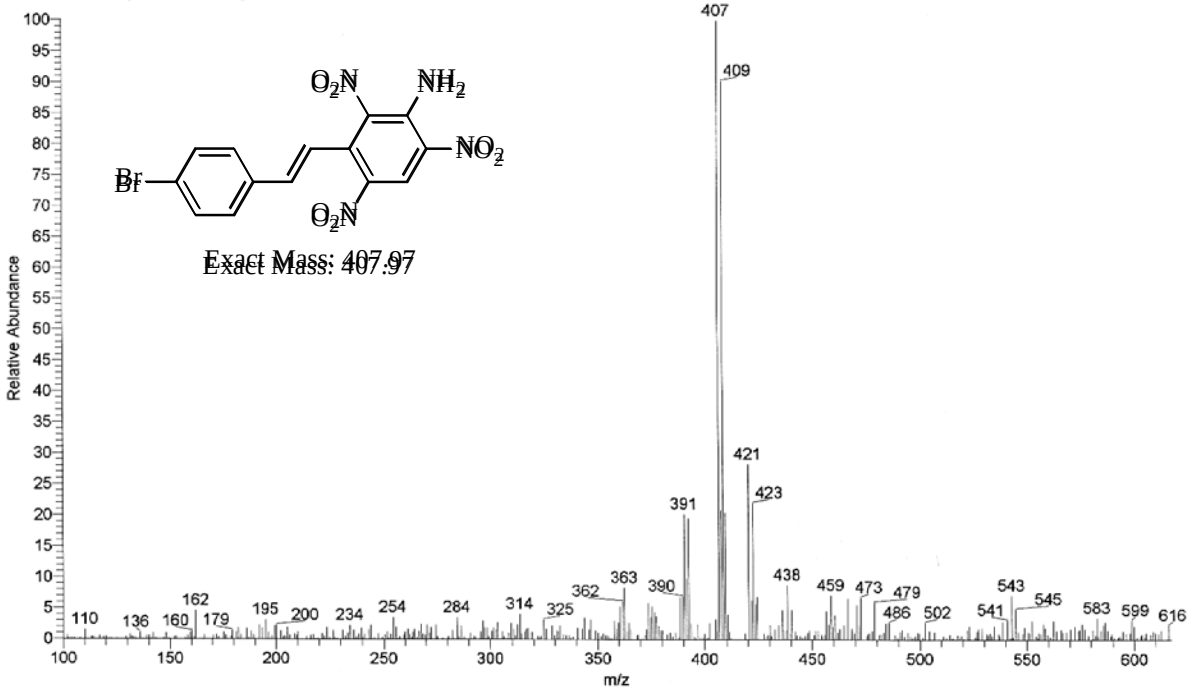
XFN-LFM-5 #48-54 RT: 1.00-1.09 AV: 7 SB: 2 0.51, 1.18 NL: 1.64E6
T: - c ESI Full ms [100.00-900.00]



F:\data\XFN-LFM-3 2013-06-21 13:33:38

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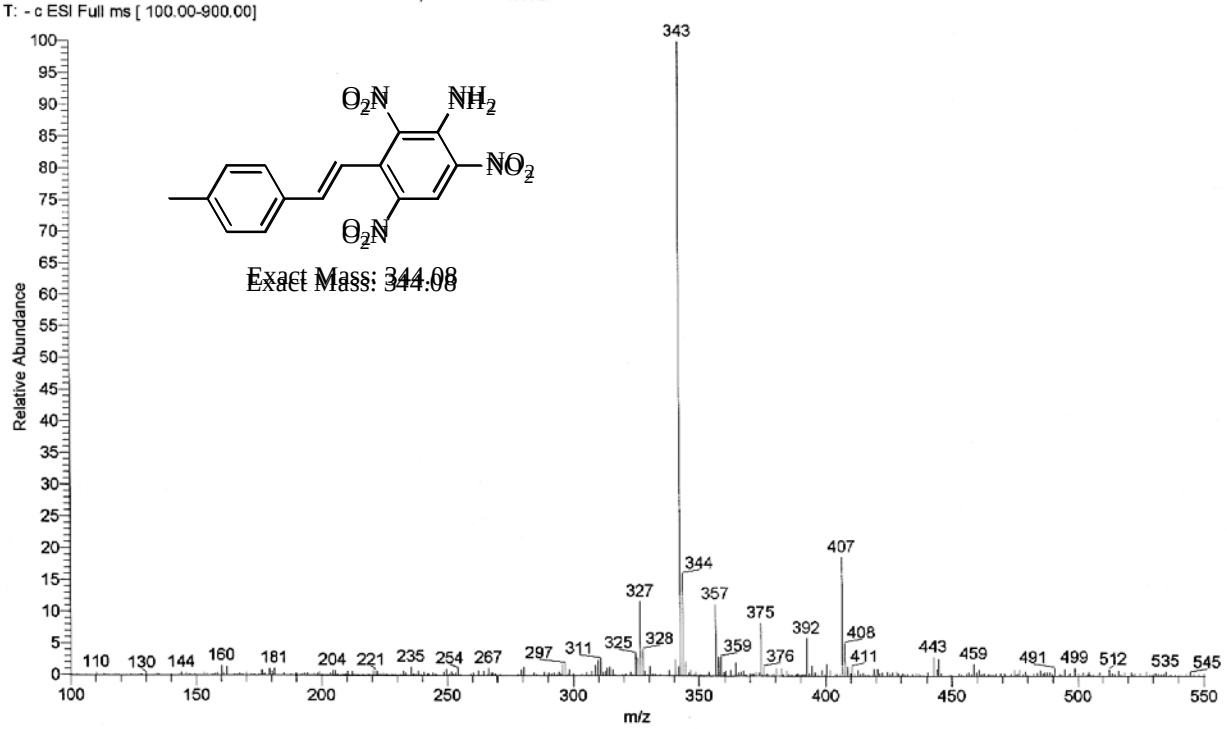

20140411-SMN-2 #134 RT: 1.56 AV: 1 NL: 6.67E5
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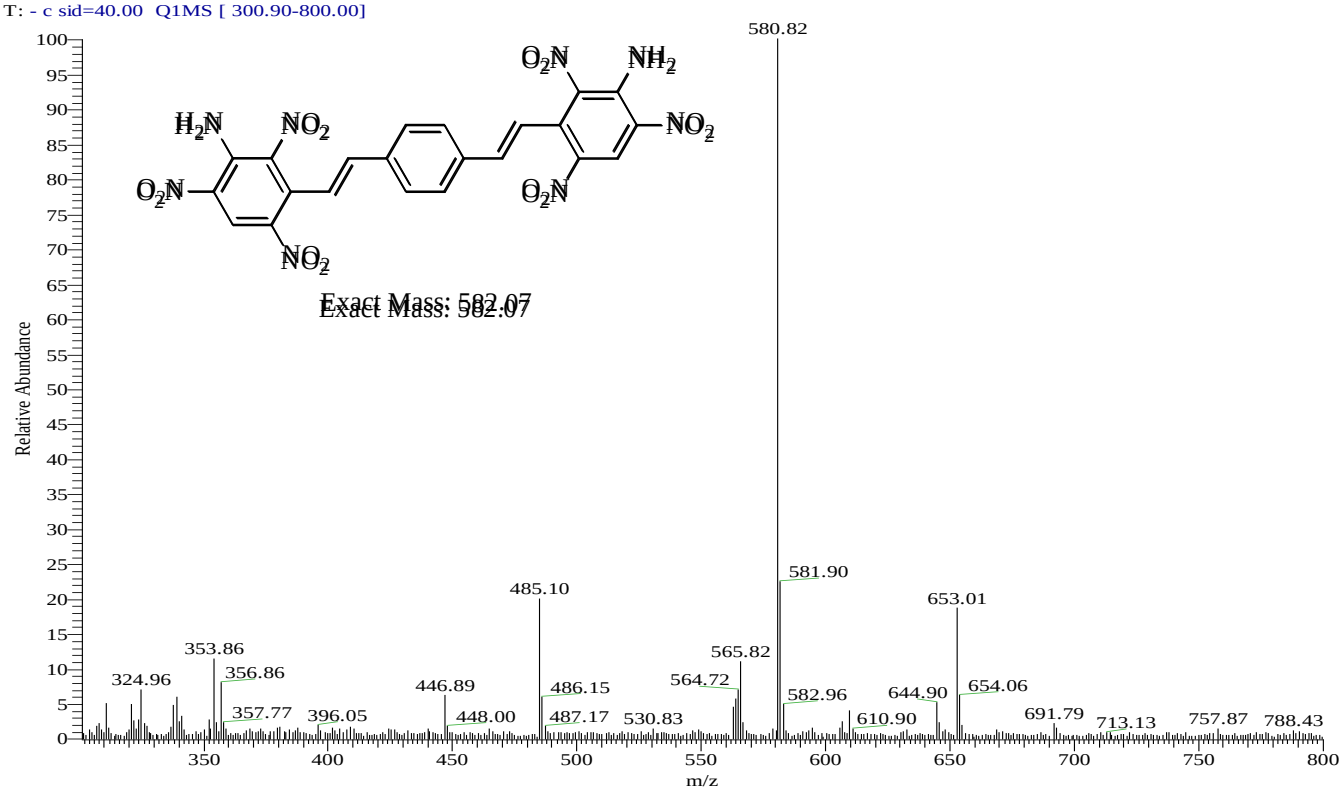
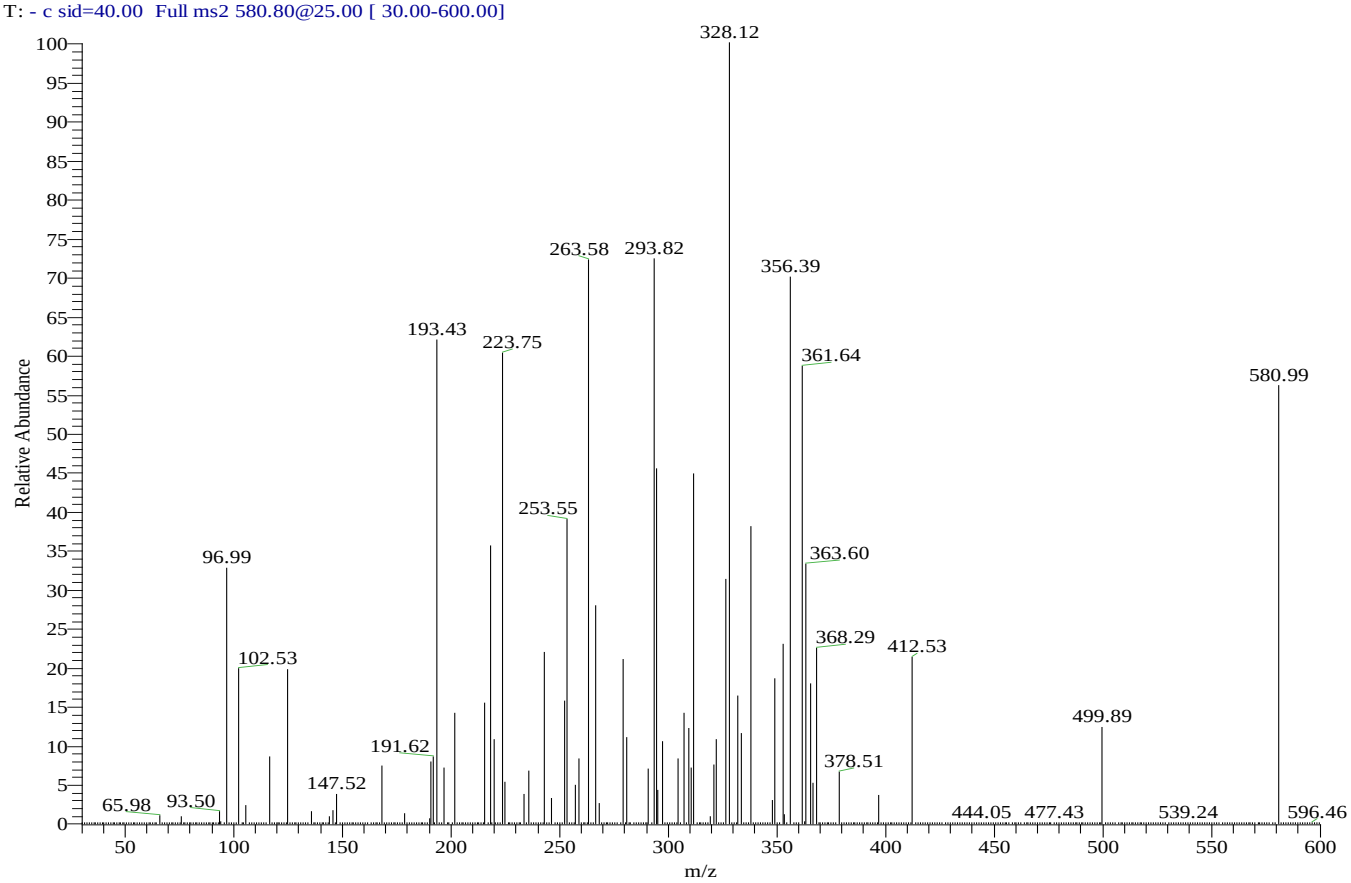


20140411-SMN-2 #157 RT: 1.83 AV: 1 NL: 6.17E3
T: - c sid=40.00 Full ms2 580.80@25.00 [30.00-600.00]



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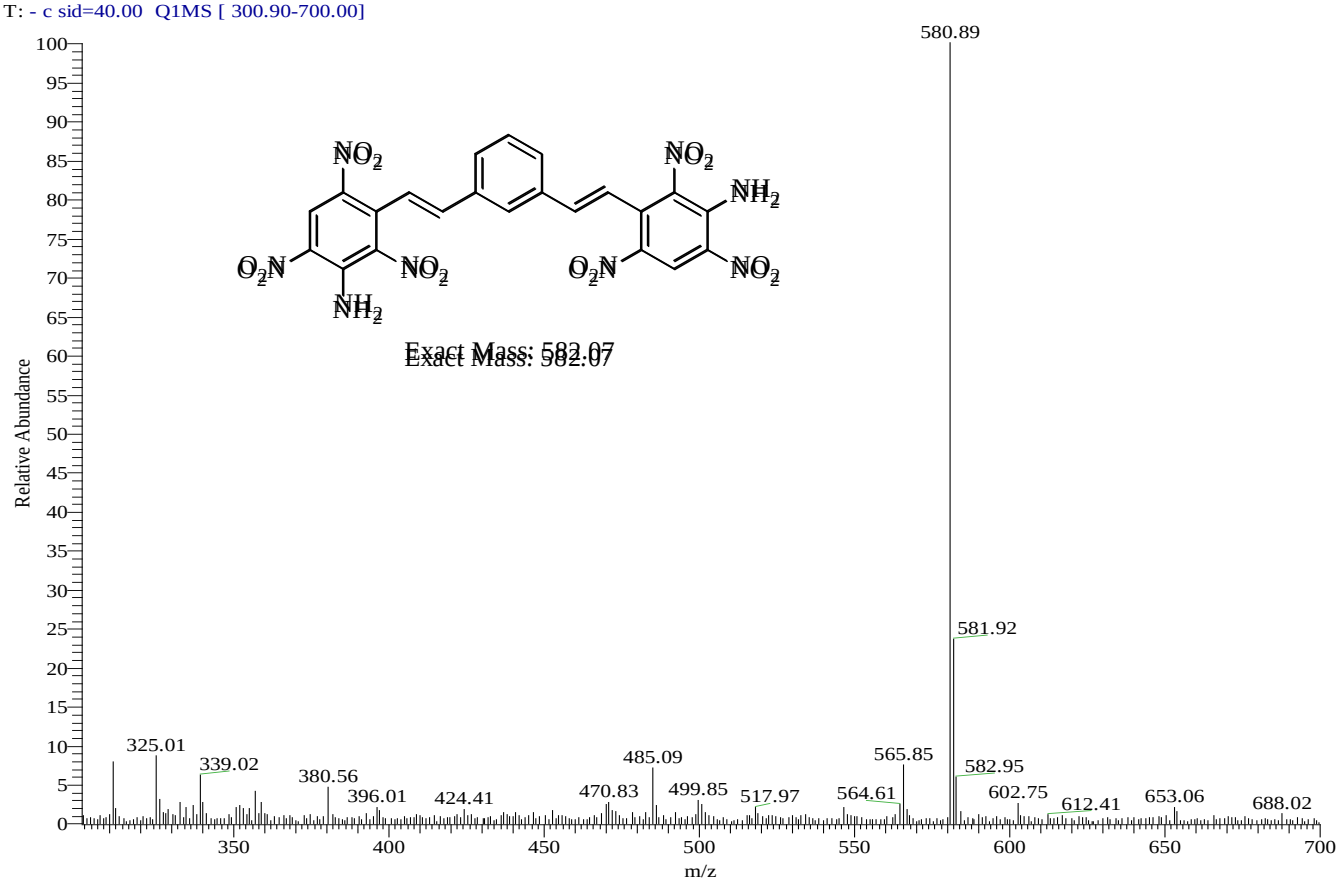
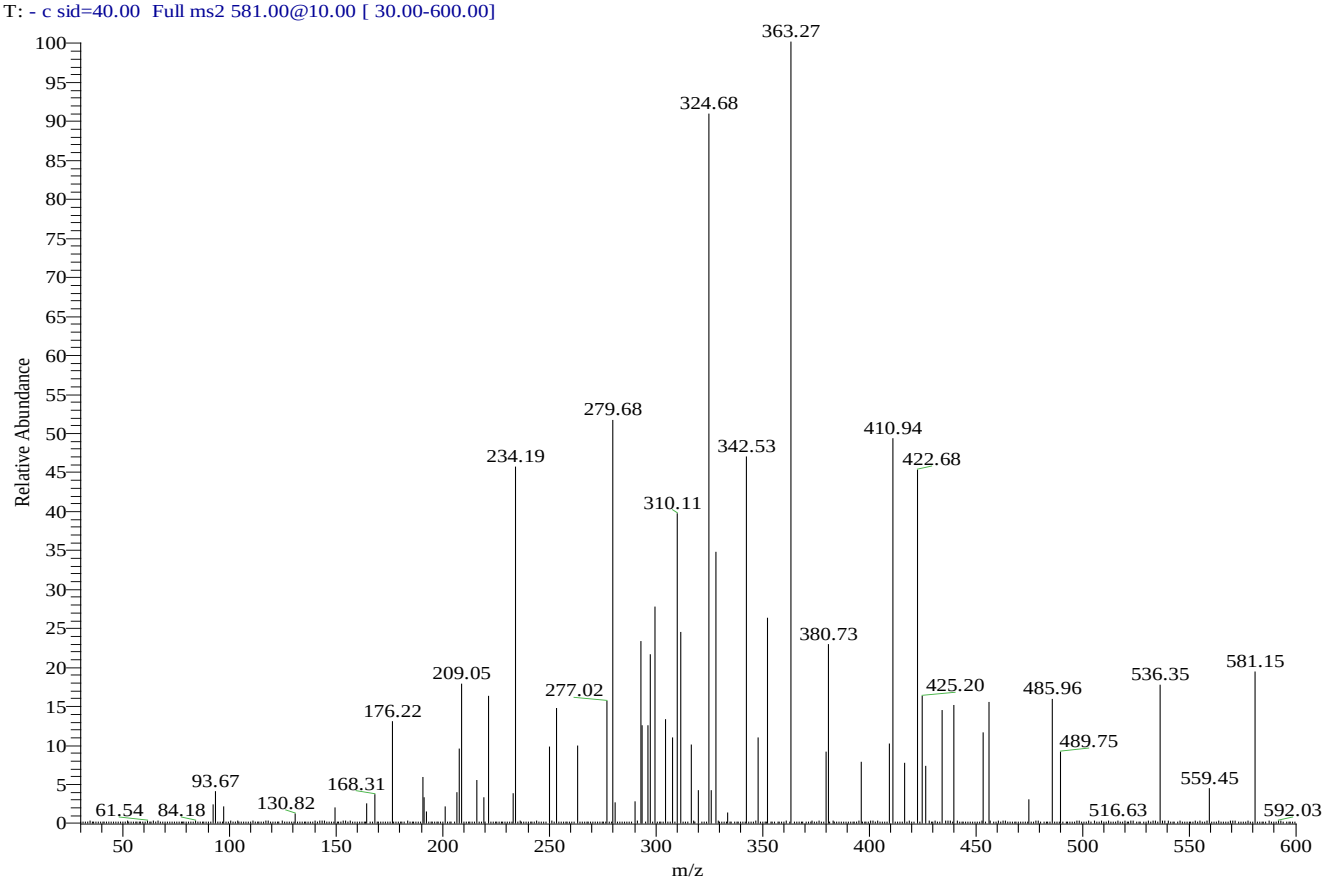


20140411-SMN-4 #106 RT: 1.36 AV: 1 NL: 3.86E3
T: - c sid=40.00 Full ms2 581.00@10.00 [30.00-600.00]



20140411-SMN-1 #73 RT: 0.95 AV: 1 NL: 2.16E5
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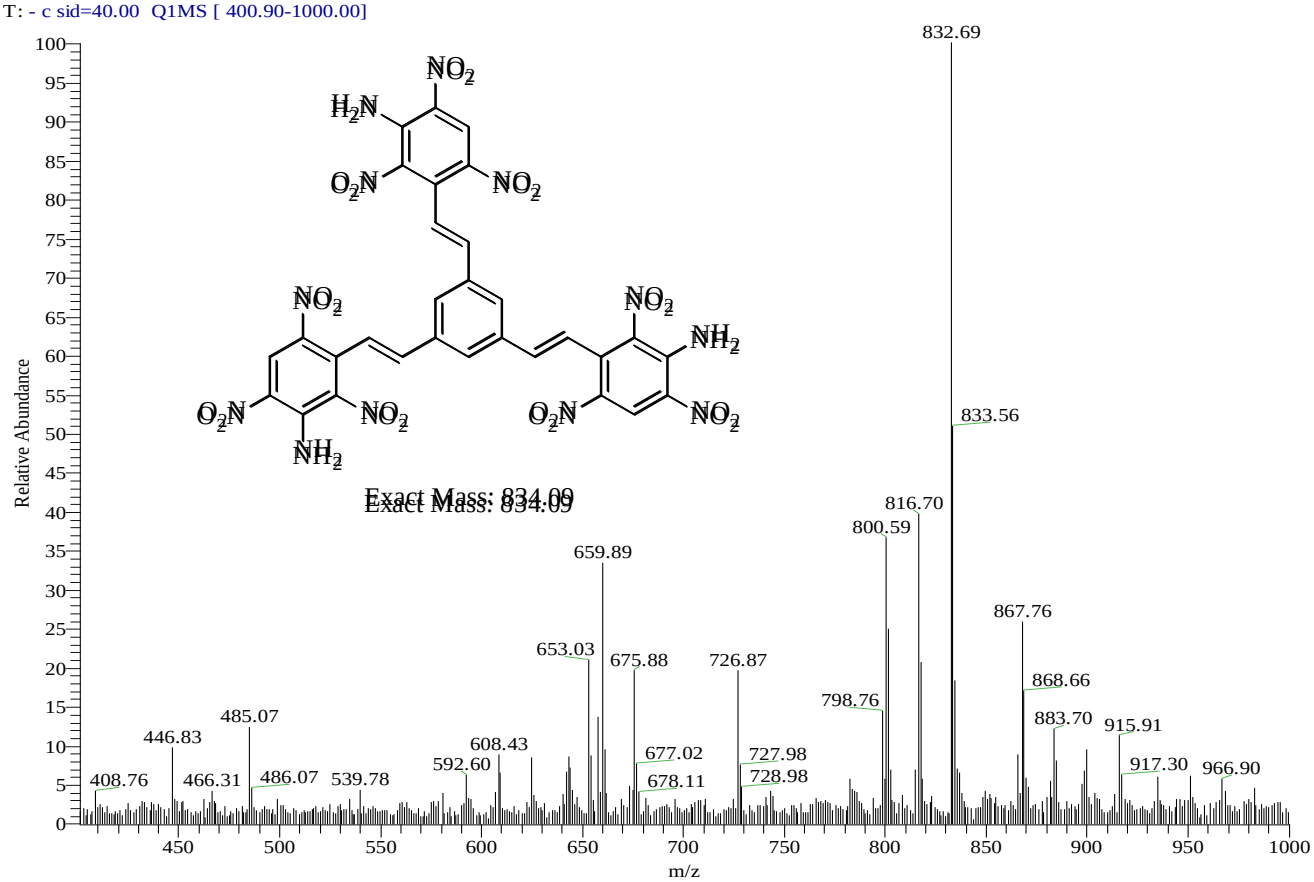
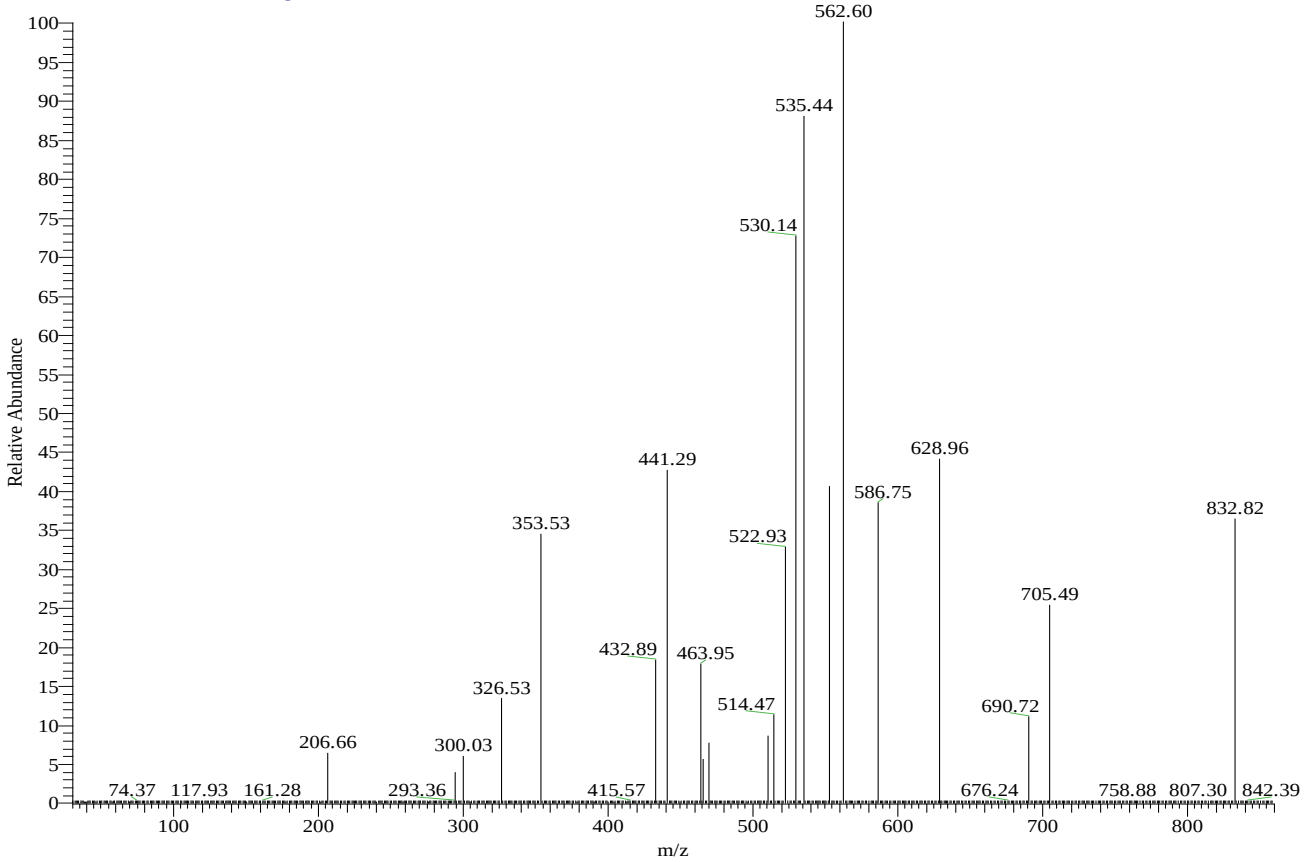
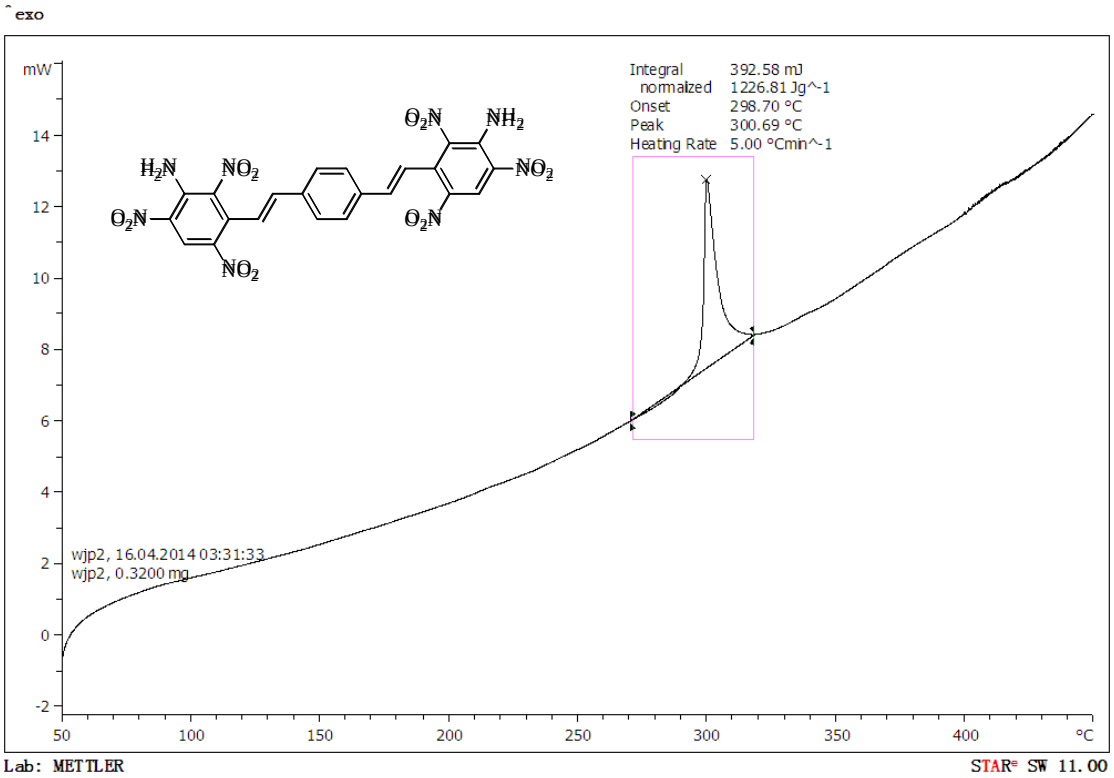
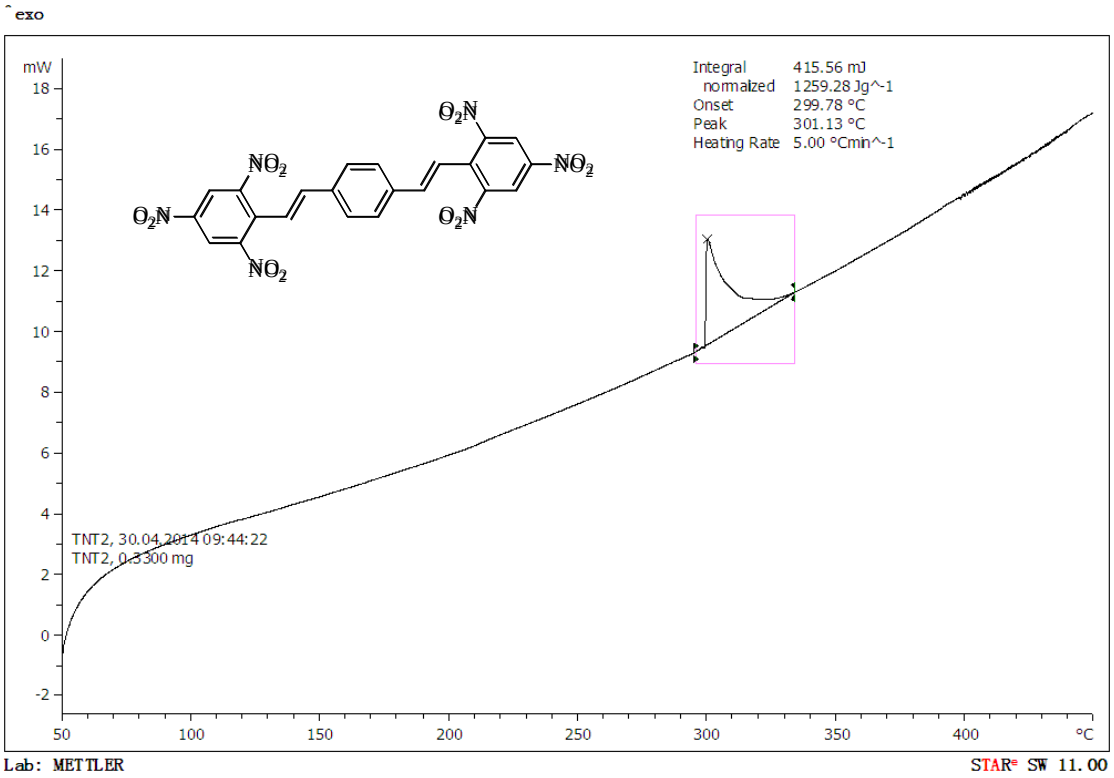


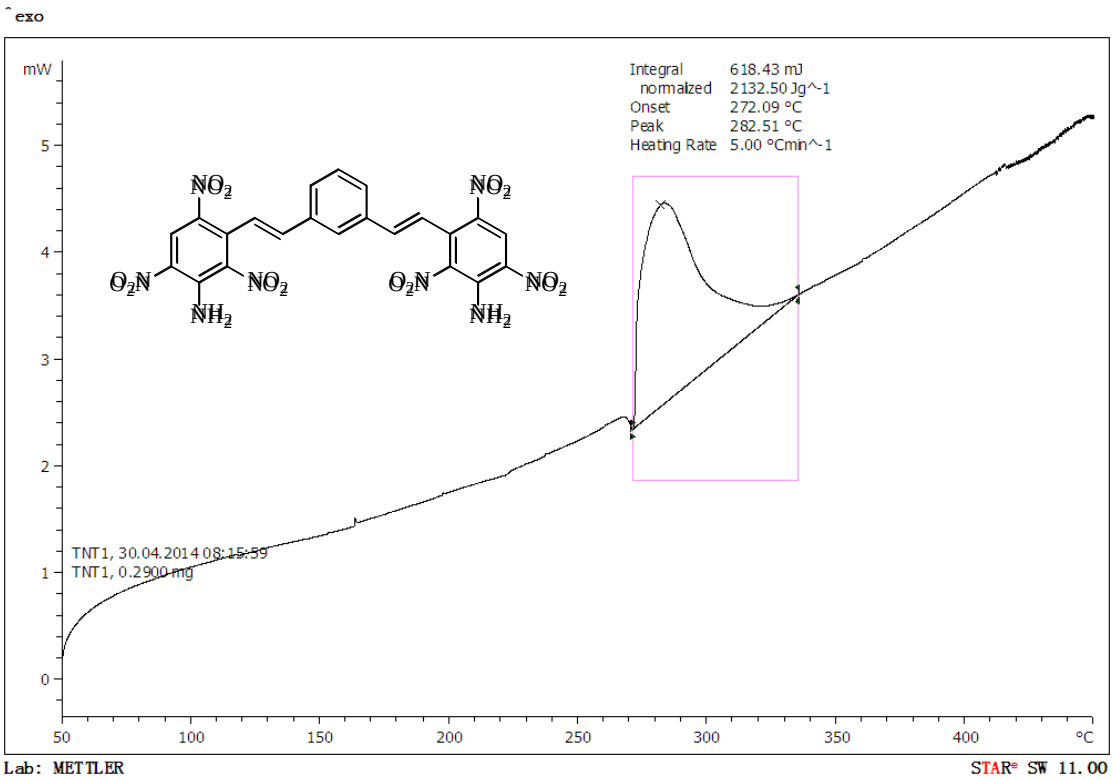
20140411-SMN-1 #124 RT: 1.49 AV: 1 NL: 2.59E3
T: - c sid=40.00 Full ms2 832.70@15.00 [30.00-860.00]

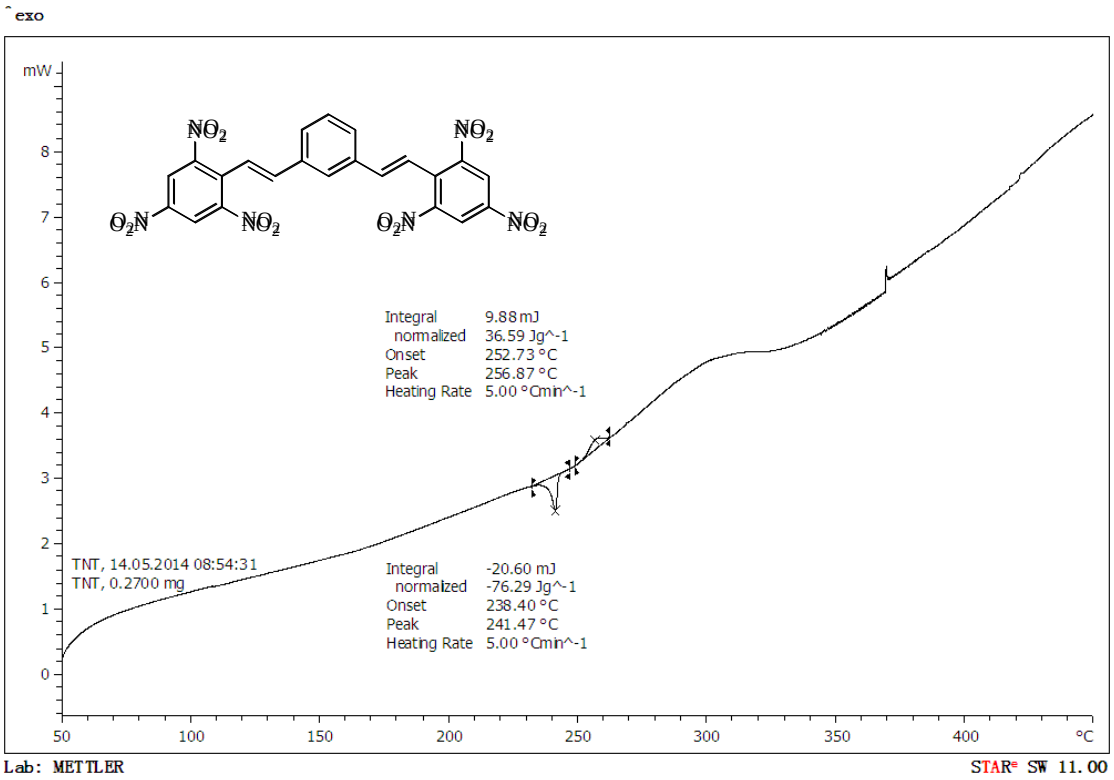


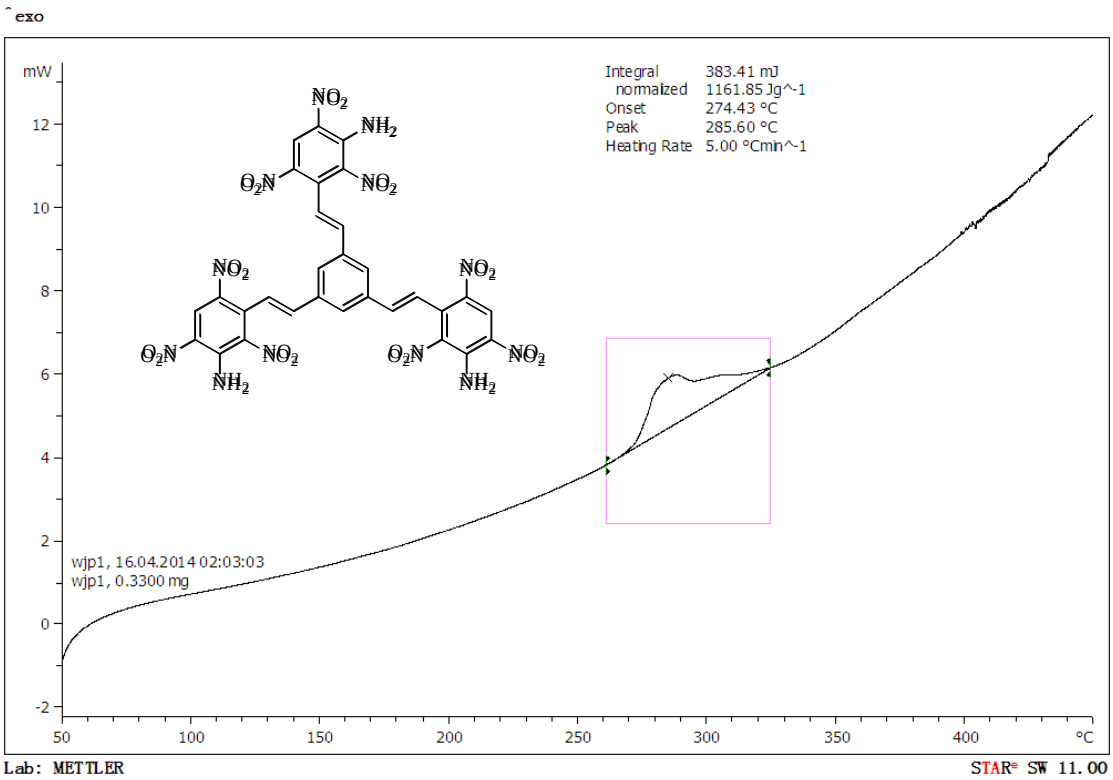
DSC

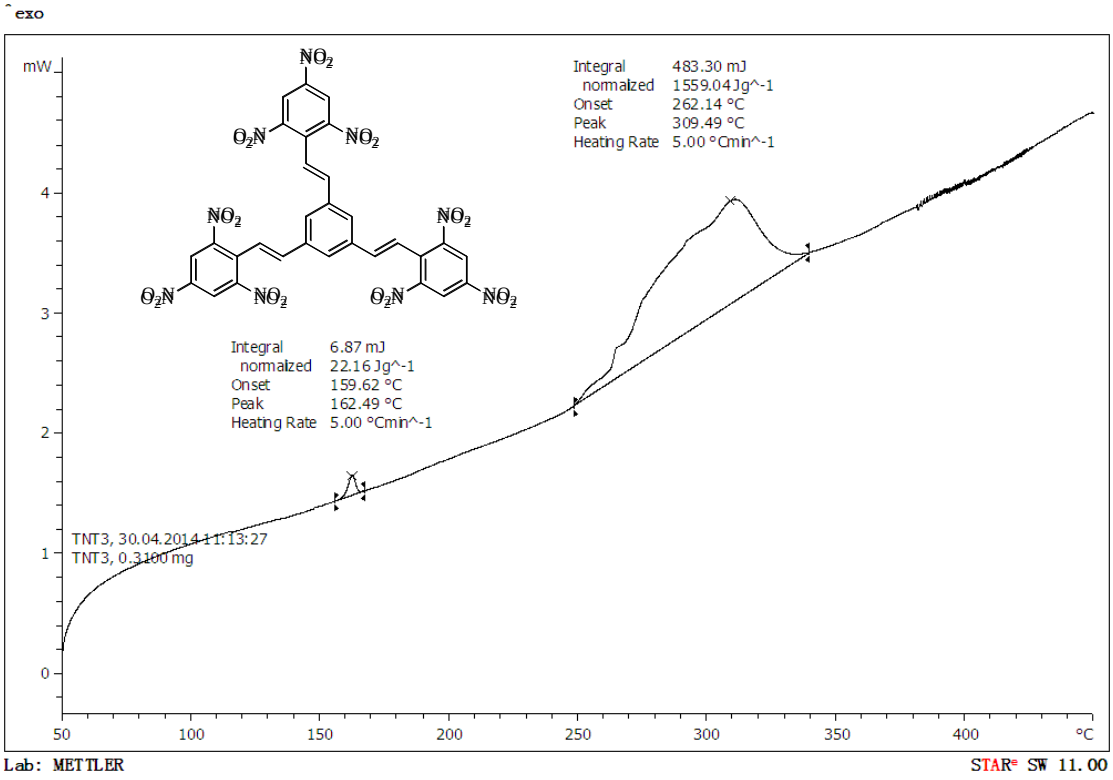

^exo
mW
Integral 392.58 mJ
normalized 1226.81 Jg^-1
Onset 298.70 °C
Peak 300.69 °C
Heating Rate 5.00 °Cmin^-1
wjp2, 16.04.2014 03:31:33
wjp2, 0.3200 mg
°C
Lab: METTLER
STAR® SW 11.00


^exo
mW
Integral 415.56 mJ
normalized 1259.28 Jg^-1
Onset 299.78 °C
Peak 301.13 °C
Heating Rate 5.00 °Cmin^-1
TNT2, 30.04.2014 09:44:22
TNT2, 0.3300 mg
°C
Lab: METTLER
STAR® SW 11.00


^exo
mW
Integral 618.43 mJ
normalized 2132.50 Jg^-1
Onset 272.09 °C
Peak 282.51 °C
Heating Rate 5.00 °Cmin^-1
TNT1, 30.04.2014 08:15:59
TNT1, 0.2900 mg
°C
Lab: METTLER
STAR® SW 11.00


^exo
mW
Integral 9.88 mJ
normalized 36.59 Jg^-1
Onset 252.73 °C
Peak 256.87 °C
Heating Rate 5.00 °Cmin^-1
TNT, 14.05.2014 08:54:31
TNT, 0.2700 mg
Integral -20.60 mJ
normalized -76.29 Jg^-1
Onset 238.40 °C
Peak 241.47 °C
Heating Rate 5.00 °Cmin^-1
°C
Lab: METTLER
STAR® SW 11.00


^exo
mW
Integral 383.41 mJ
normalized 1161.85 Jg^-1
Onset 274.43 °C
Peak 285.60 °C
Heating Rate 5.00 °Cmin^-1
wjp1, 16.04.2014 02:03:03
wjp1, 0.3300 mg
°C
Lab: METTLER
STAR® SW 11.00


^exo
mW
Integral 483.30 mJ
normalized 1559.04 Jg^-1
Onset 262.14 °C
Peak 309.49 °C
Heating Rate 5.00 °Cmin^-1
Integral 6.87 mJ
normalized 22.16 Jg^-1
Onset 159.62 °C
Peak 162.49 °C
Heating Rate 5.00 °Cmin^-1
TNT3, 30.04.2014 11:13:27
TNT3, 0.3100 mg
°C
Lab: METTLER
STAR® SW 11.00