Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

Polymers from biomass: One pot two steps synthesis of furilydenepropanenitrile derivatives with MIL-100 (Fe) catalyst

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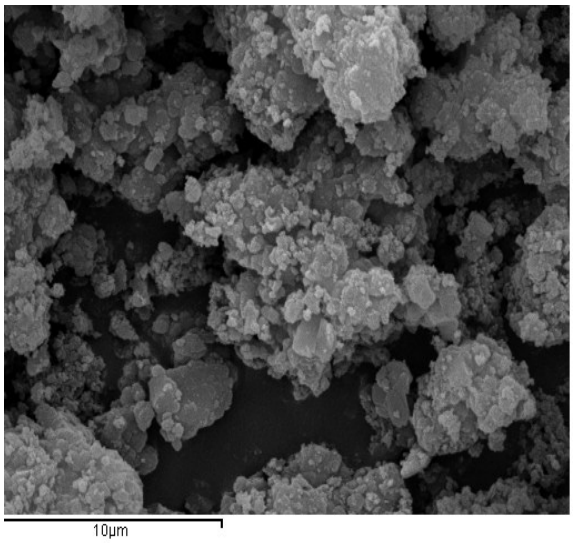
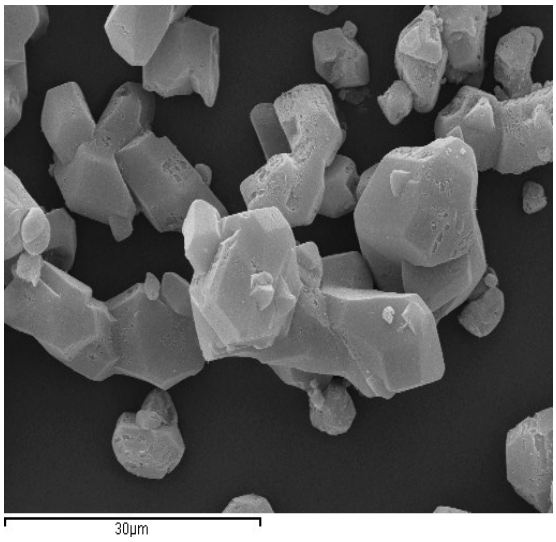
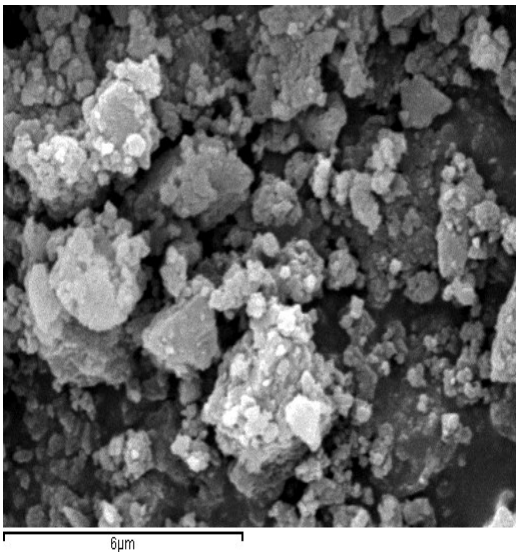


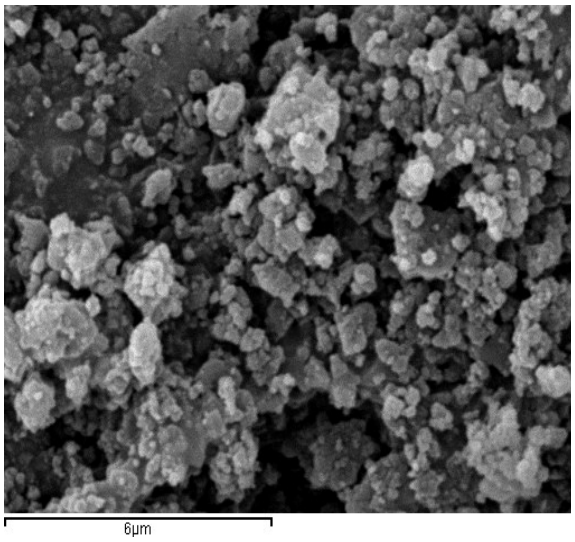
Fe(BTC)



$Cu_3(BTC)_2$



MIL100 (Fe)



MIL100 (Fe)-NH_4F

Figure S1. SEM image analysis of different MOFs

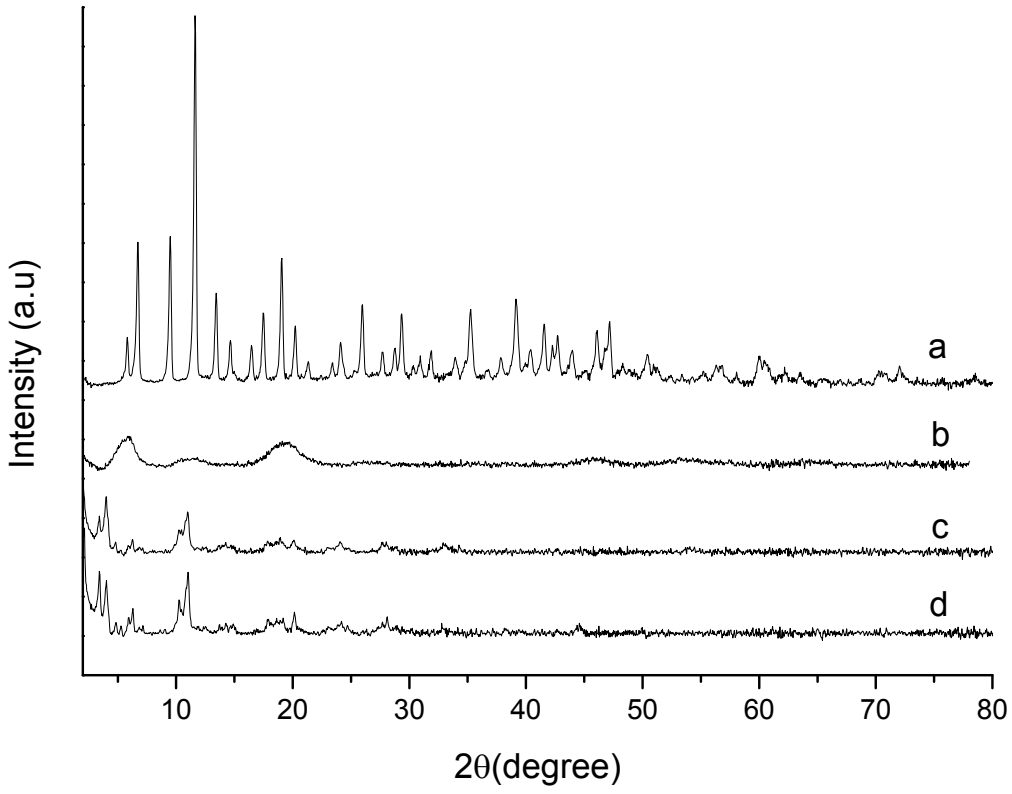


Figure S2. XRD patterns of (a) $Cu_3(BTC)_2$, (b) Fe(BTC), (c) MIL-100(Fe) and (d) MIL-100 (Fe)-NH_4F.

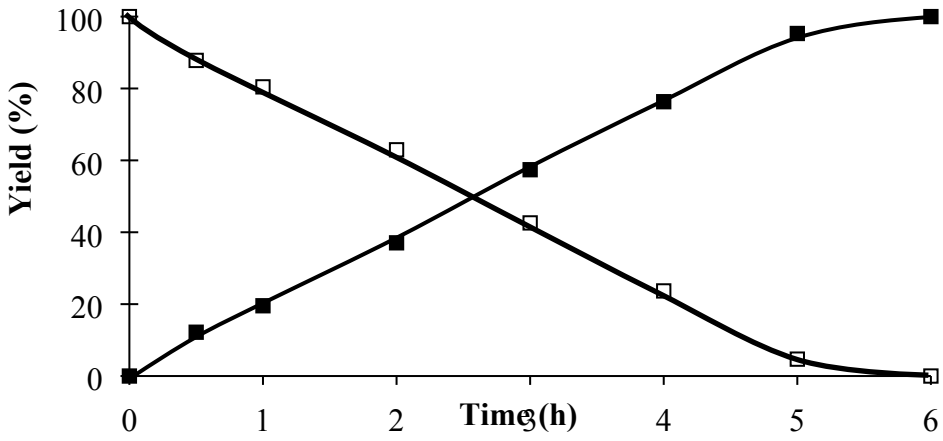


Figure S3. DFF yield versus time plot for the aerobic oxidation of HMF to DFF catalyzed by MIL-100 (Fe)-NH_4F. Reaction Conditions: HMF (1 mmol, 126 mg), catalyst (45 mg, 0.17 mmol of Fe); TEMPO (0.076 mmol, 12 mg); $NaNO_2$ (0.14 mmol; 10 mg); CH_3CN (5 mL) at 75 °C under atmospheric pressure of oxygen.(□) HMF; (■) DFF.

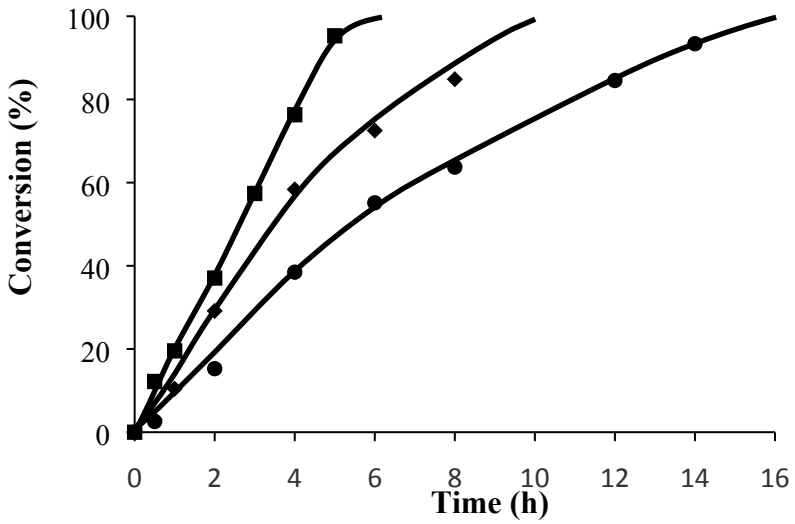


Figure S4. Conversion of 5-HMF versus time plot for oxidation of 5-HMF during reuses of MIL-100 (Fe)-NH_4F. Reaction conditions: 5-HMF (1 mmol, 126 mg); MIL-100 (Fe)-NH_4F (45 mg); TEMPO (0.076 mmol; 12 mg); $NaNO_2$ (0.14 mmol, 10 mg); at 75 °C, in CH_3CN -5ml under atmospheric pressure of oxygen. 1st cycle (■), 2nd cycle (♦), 3th cycle(●).

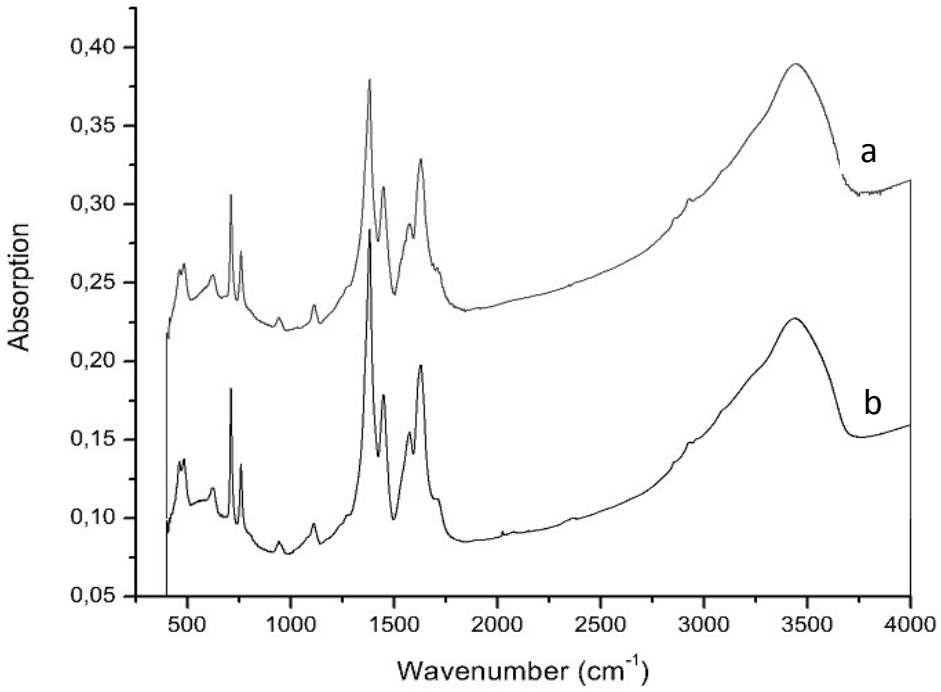


Figure S5. IR spectra of MIL-100(Fe)-NH_4F a) fresh and b) reused catalyst

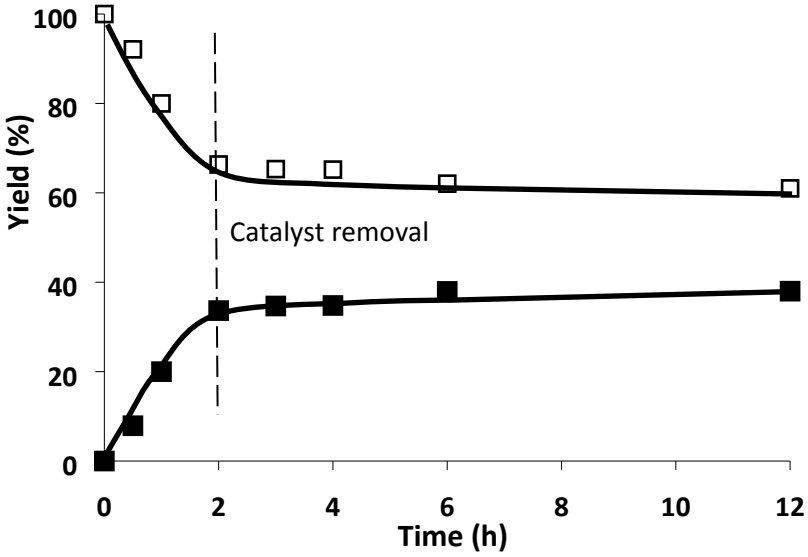
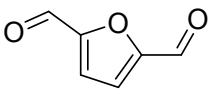
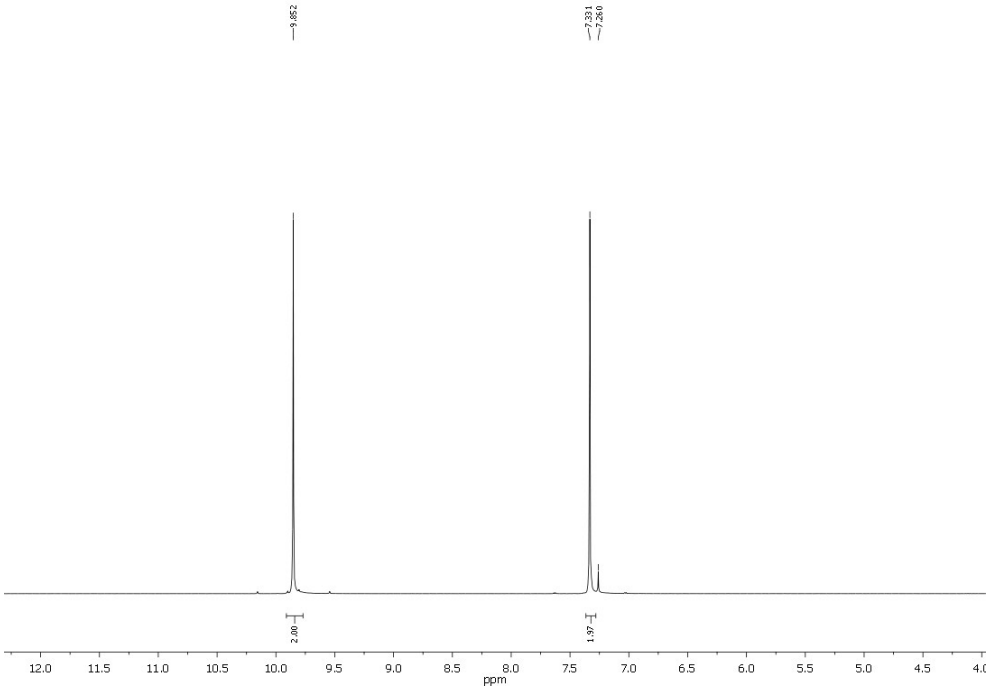


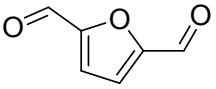
Figure S6. Leaching test of MIL-100 (Fe)-NH_4F catalysts.

Table S1. Physical and chemical properties of different studied catalysts

Catalyst	Metal content (wt %)	S_{BET} (m^2/g)	Total pore volume V_{total} (cm^3/g)	Crystal size (μm)
Fe(BTC)	21	613	0.36	0.48
MIL-100 (Fe)-NH_4F	21	1370	0.84	0.57
MIL-100 (Fe)	20	993	0.69	0.47
$Cu_3(BTC)_2$	25	1341	0.75	8.70
HY-Fe	5.3	544	0.46	-


O
O
O


9.852
7.331
7.260
2.00
1.97
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5
ppm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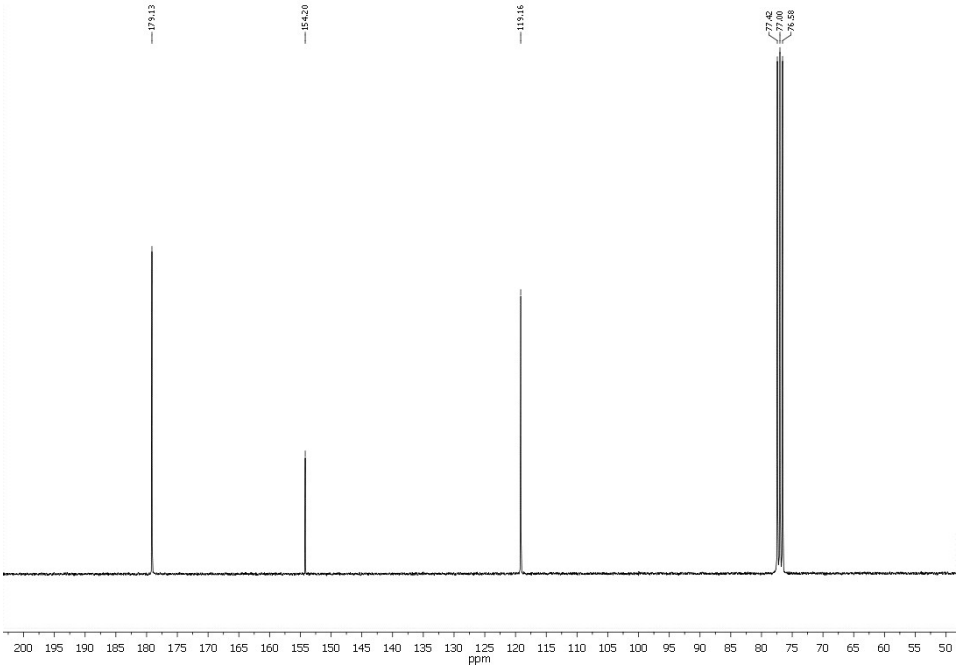
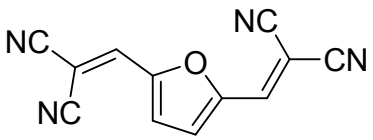
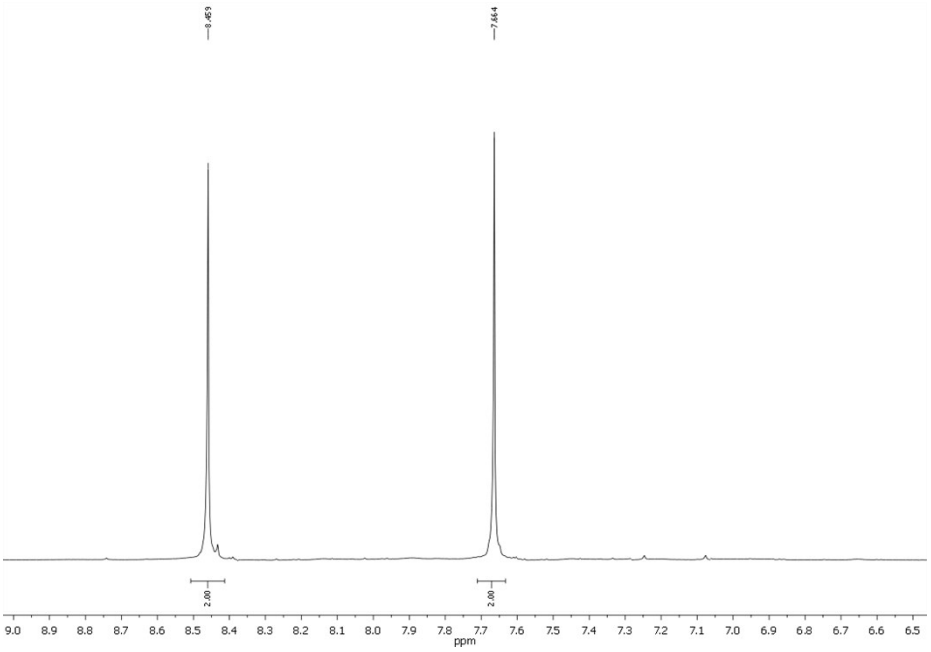
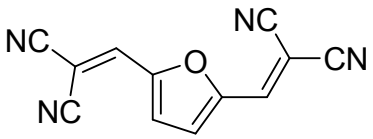
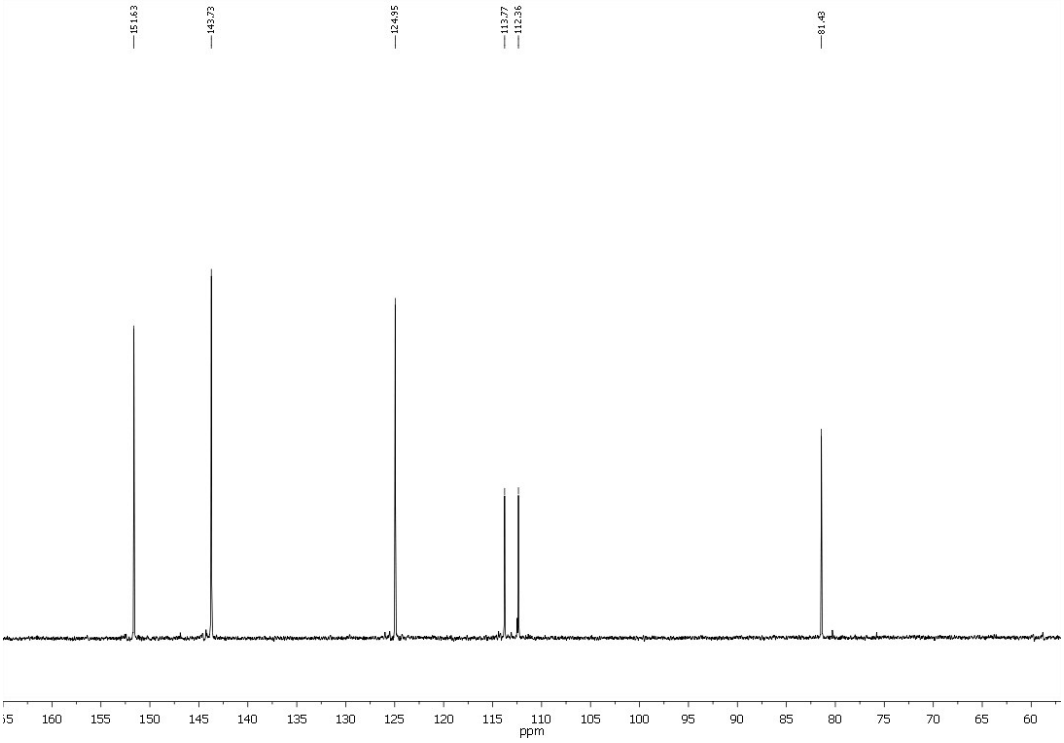
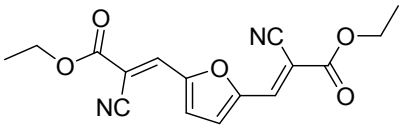

179.13
154.20
119.16
77.42
77.00
76.58
200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
ppm

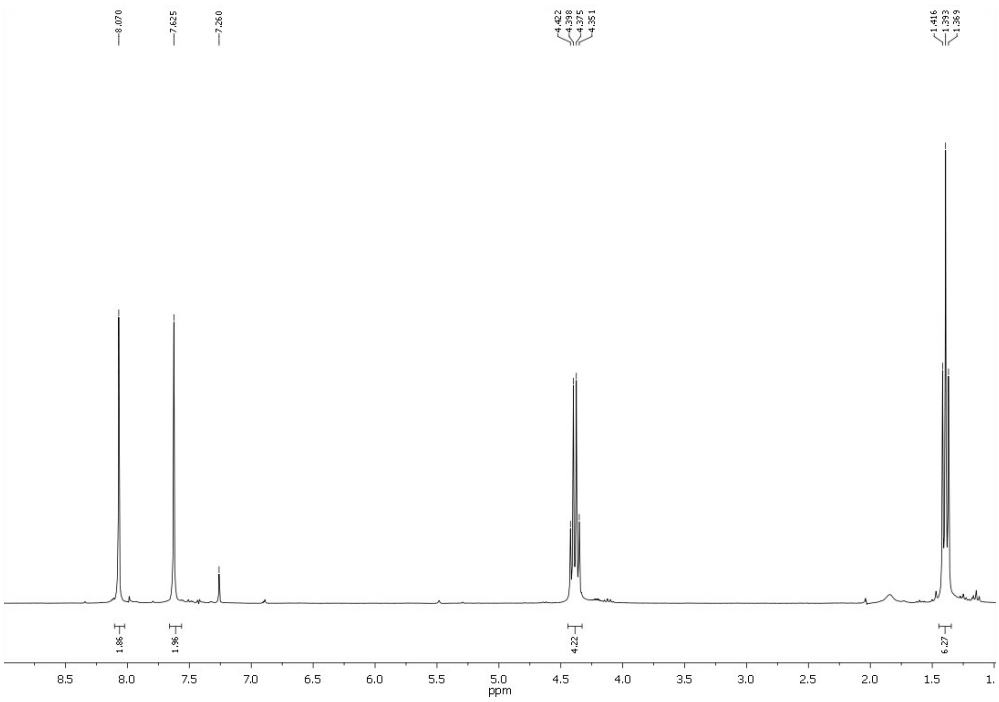

NC
NC
O
NC
CN

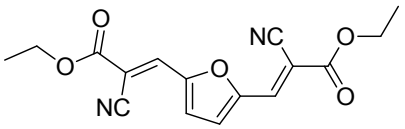

8.469
7.664
2.00
2.00
9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5
ppm


NC
NC
O
NC
CN


151.63
143.73
124.95
113.77
112.36
81.48
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60
ppm


O
O
NC
NC
O
O
O


8.070
7.625
7.260
4.402
4.398
4.375
4.351
1.416
1.393
1.369
1.88
1.96
4.22
6.27
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
ppm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NC
NC
O
O
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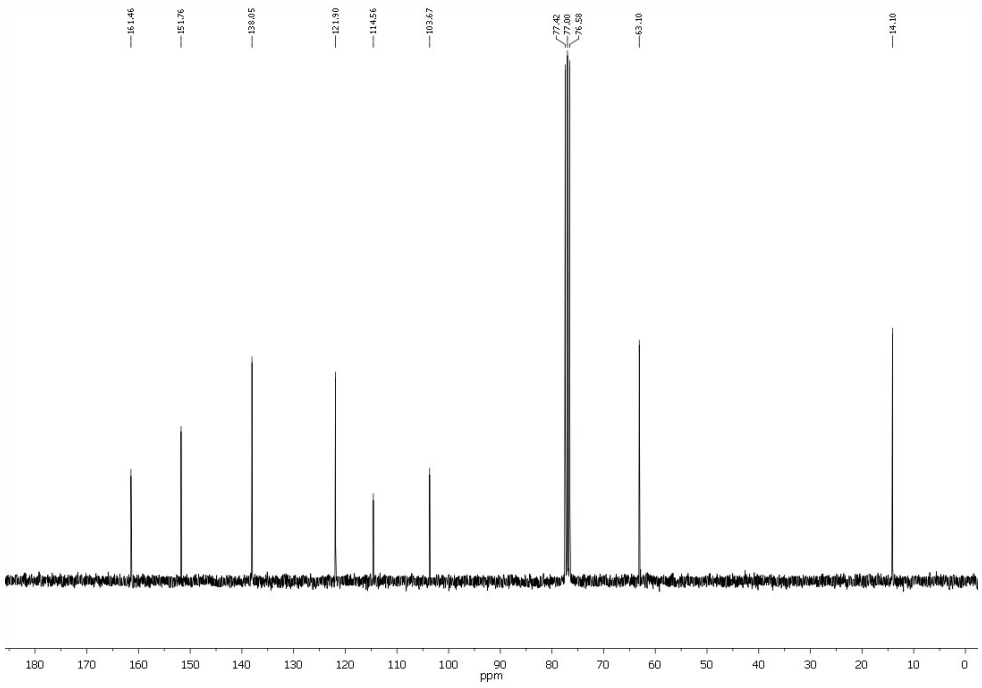
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138.05
121.30
114.56
103.67
77.42
77.00
76.58
63.10
14.10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm