Science Advances
AAAS

Supplementary Materials for

An enzyme-mimic single Fe-N_3 atom catalyst for the oxidative synthesis of nitriles via C─C bond cleavage strategy

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Sci. Adv. **8**, eadd1267 (2022)
DOI: 10.1126/sciadv.add1267

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Supplementary NMR data
Supplementary mass spectrometry and NMR spectrometry

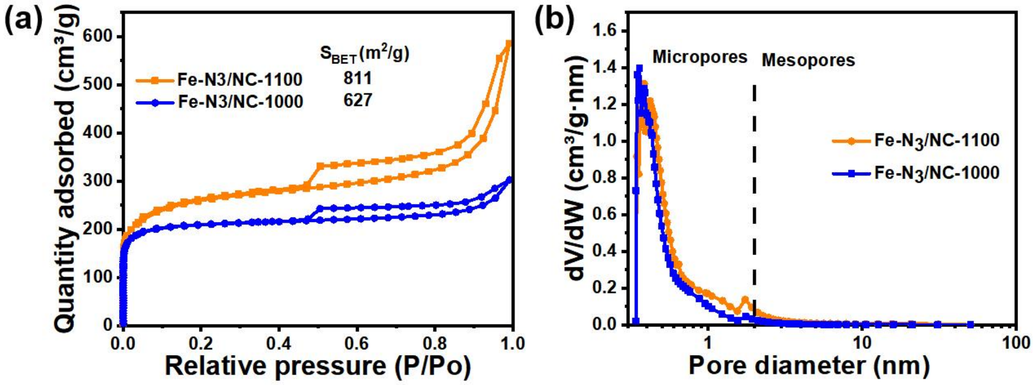


Fig. S1. Characterization of the surface area of the catalyst by nitrogen physisorption measurements. Nitrogen adsorption-desorption isotherms (**a**) and pore size distribution (**b**) of the Fe catalysts.

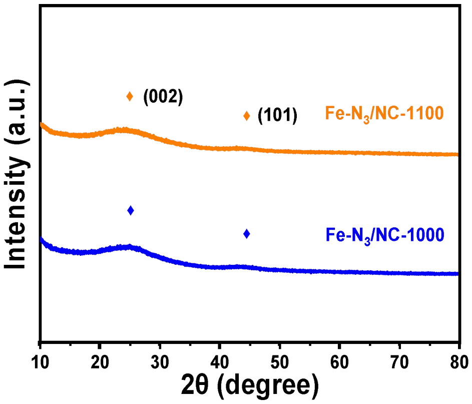


Fig. S2. XRD patterns of the as-prepared Fe catalysts. XRD patterns of Fe-N_3/NC-1100 also gave no diffraction peaks of Fe species, but showed two weak peaks at 24.4° and 44.6°, assigning to the (002) and (101) planes of graphitic carbon.

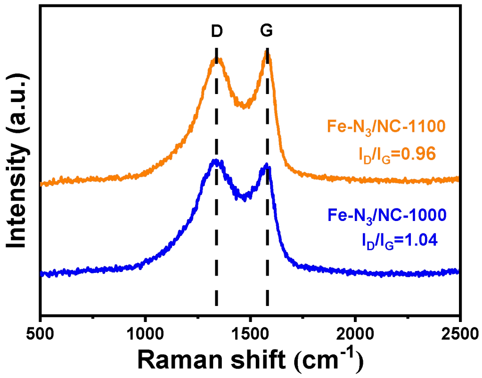


Fig. S3. Raman spectra of the as-prepared Fe catalysts. Two peaks with the Raman shifts around 1350 (called D bond) and 1570 cm^{-1} (called G bond) were observed.

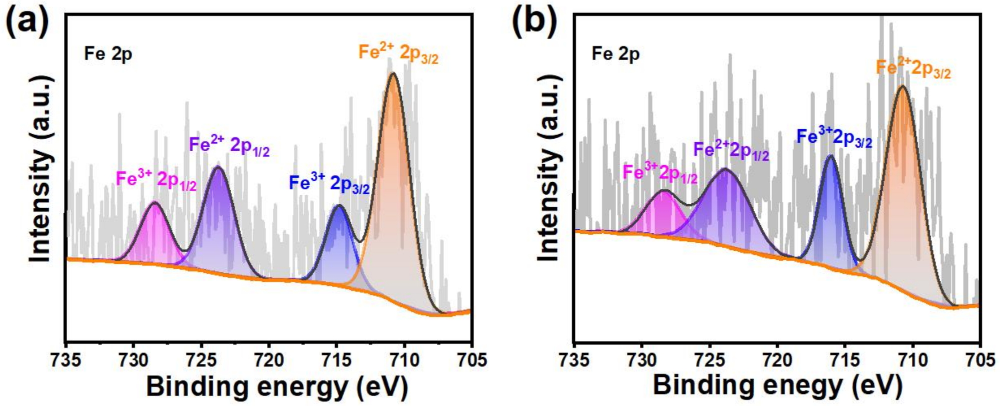
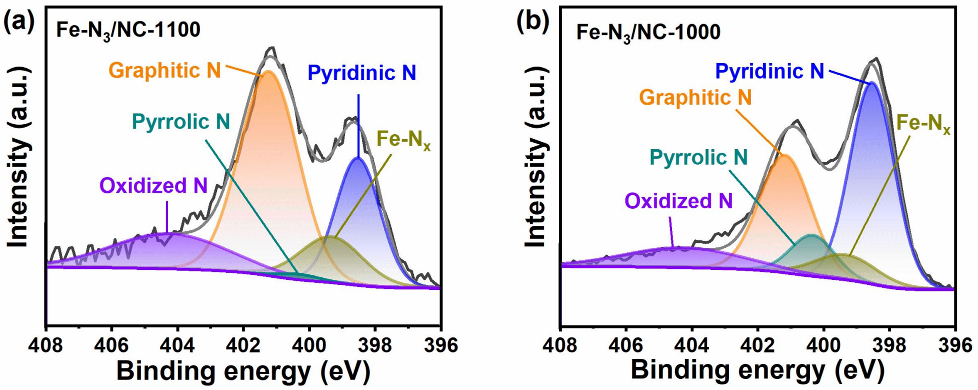


Fig. S4. Fe 2p XPS spectra of the as-prepared Fe catalysts. (**a**) Fe-N_3/NC-1100; (**b**) Fe-N_3/NC-1000.



(c)

Types of N atoms	Pyridinic N	Fe-N$_x$	Pyrrolic N	Graphitic N	Oxidized N
Binding energy (eV) Content (%) Sample	398.5	399.3	400.3	401.2	404.3
Fe-N$_3$/NC-1100	22.6	11.4	1.0	48.9	16.1
Fe-N$_3$/NC-1000	43.7	7.4	8.6	29.3	11.0

Fig. S5. N 1s XPS spectra and content of the as-prepared Fe catalysts. (**a**) Fe-N$_3$/NC-1100; (**b**) Fe-N$_3$/NC-1000; (**c**) Content of types of N atoms.

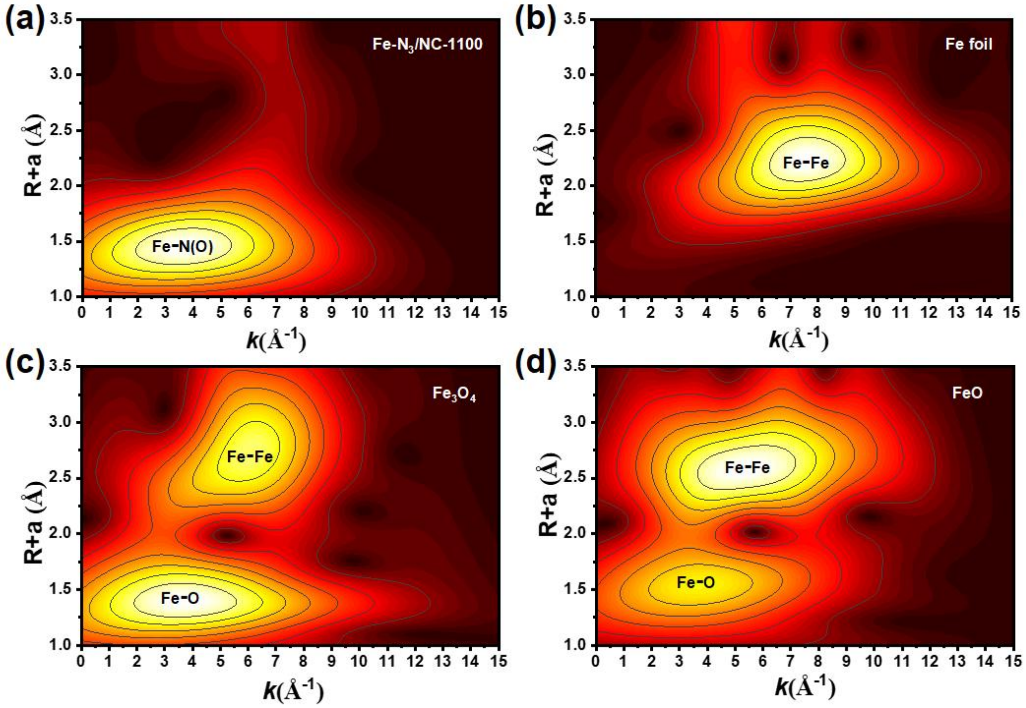


Fig. S6. Wavelet-transformed k^3 -weighted EXAFS spectra. (**a**) Fe-N$_3$/NC-1100; (**b**) Fe foil; (**c**) Fe$_3$O$_4$; (**d**) FeO.

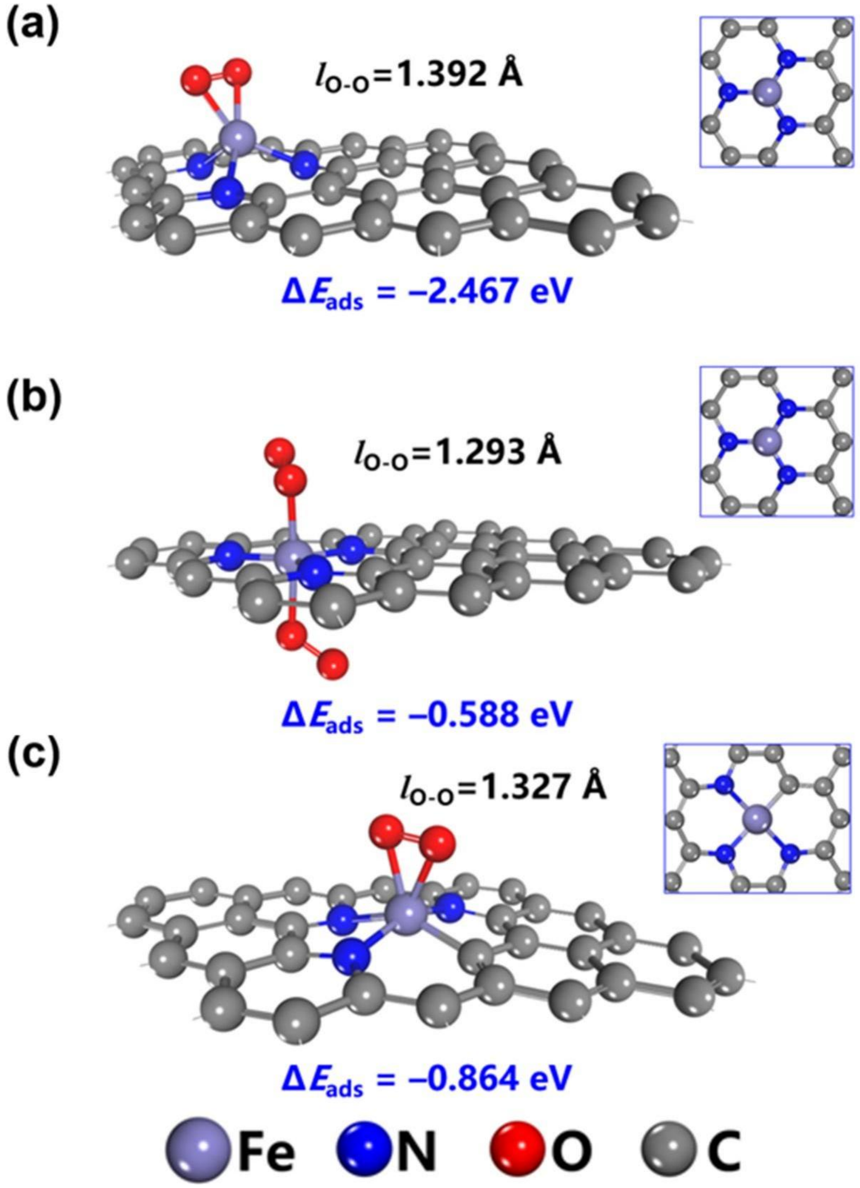


Fig. S7. The possible structures of Fe-N_3/NC-1100 were further studied by DFT calculation.

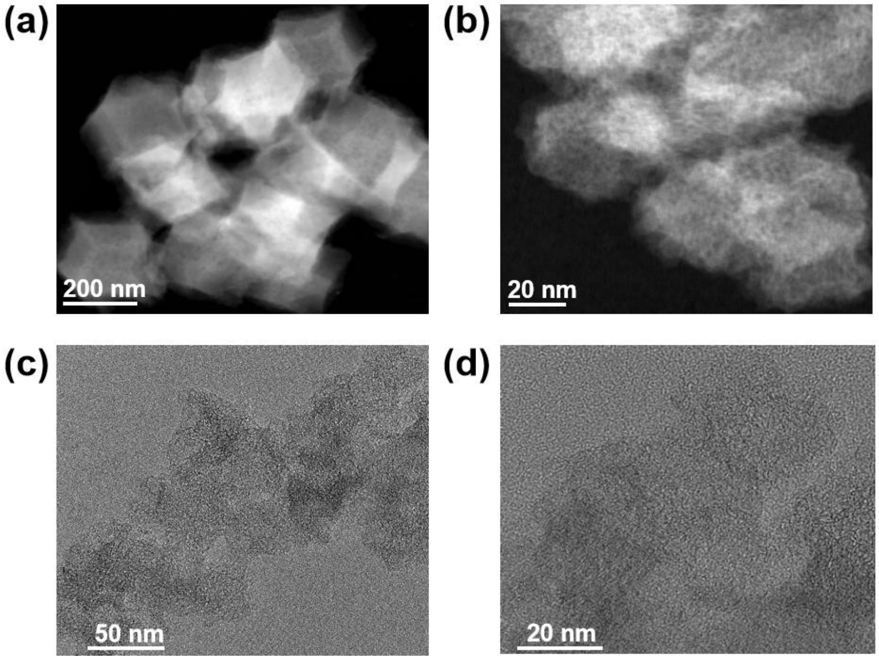


Fig. S8. STEM images of the Fe-N$_3$/NC-1000 catalyst. (**a~b**) SEM; (**c~d**) TEM.

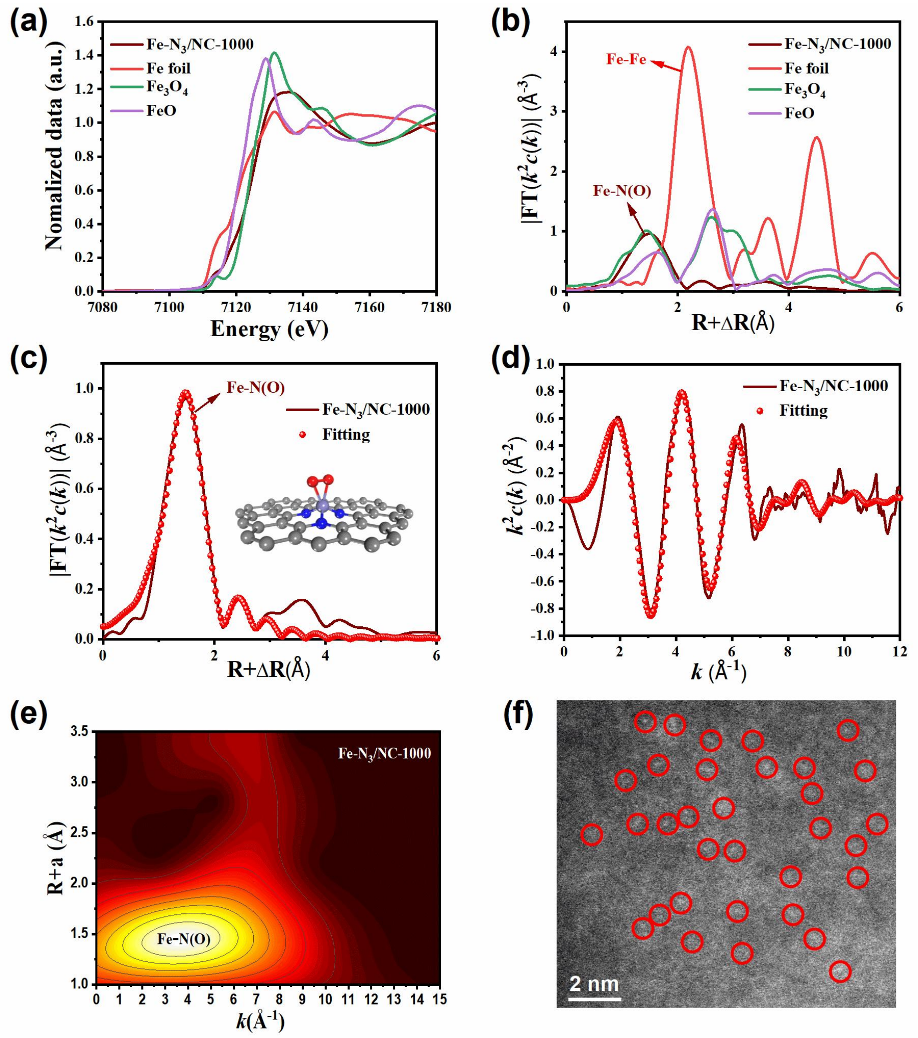


Fig. S9. Characterization of the Fe-N_3/NC-1000 catalyst. (**a**) XANES spectra at the Fe K-edge; (**b**) FT-EXAFS spectra of the Fe foil, Fe_3O_4, FeO and Fe-N_3/NC-1000; (**c**) R space and (**d**) k space of Fe-N_3/NC-1000; (**e**) Wavelet-transformed k^3 -weighted EXAFS spectra of Fe-N_3/NC-1000; (**f**) HAADF-STEM image of Fe-N_3/NC-1000 (single-atom Fe is highlighted with red circles).

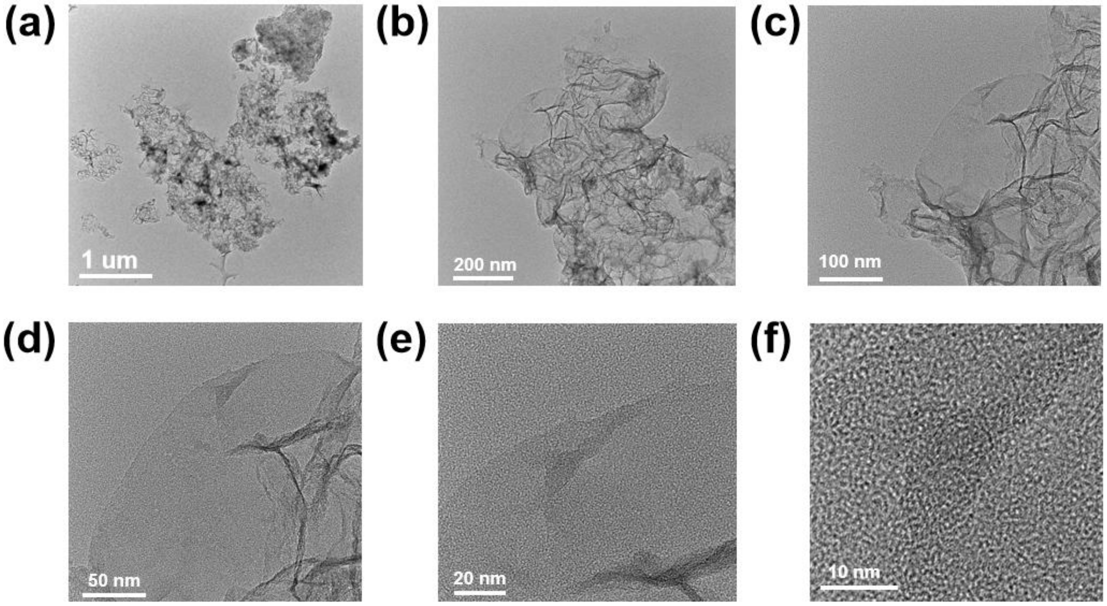


Fig. S10. STEM images of the Fe-N_4/NC-800 catalyst. (**a~d**) STEM images of Fe-N_4/NC-800; (**e~f**) HRTEM images of Fe-N_4/NC-800.

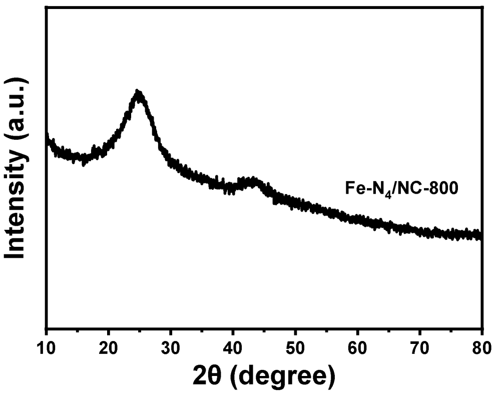


Fig. S11. XRD patterns of the Fe-N_4/NC-800 catalyst. XRD patterns of Fe-N_4/NC-800 also gave no diffraction peaks of Fe species, but showed two weak peaks at 25.4° and 43.6°.

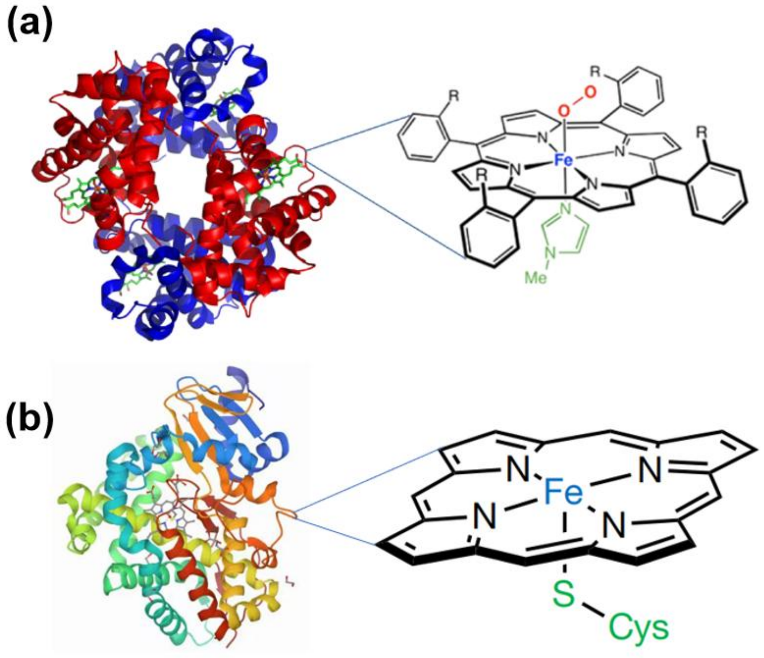


Fig. S12. The structure of the hemoglobin molecule and cytochrome P450 in organism. (**a**) hemoglobin molecule; (**b**) cytochrome P450.

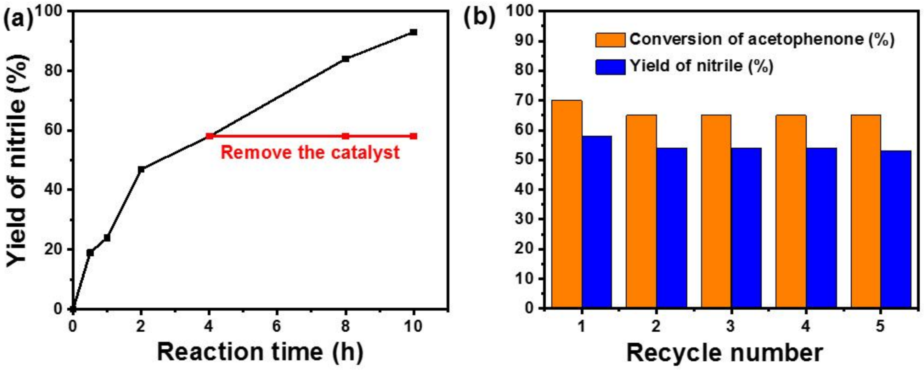


Fig. S13. The recycling test of the Fe-N_3/NC-1100 catalyst. (**a**) Time-yield plots over Fe-N_3/NC-1100 (black line) or removing Fe-N_3/NC-1100 after 4 h (red line); (**b**) Recycling experiment of the oxidative transformation of acetophenone into benzonitrile. Reaction conditions: Acetophenone (0.20 mmol), toluene (1.5 mL), Fe-N_3/NC-1100 (20 mg, 0.93 mmol %), $NH_3 \cdot H_2O$ (26.5 wt.% 400 μL), 150 °C, O_2 (10 bar) and 4 h.

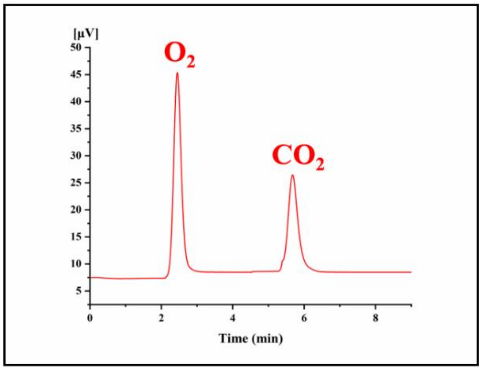


Fig. S14. CO_2 was detected by mass spectrometry.

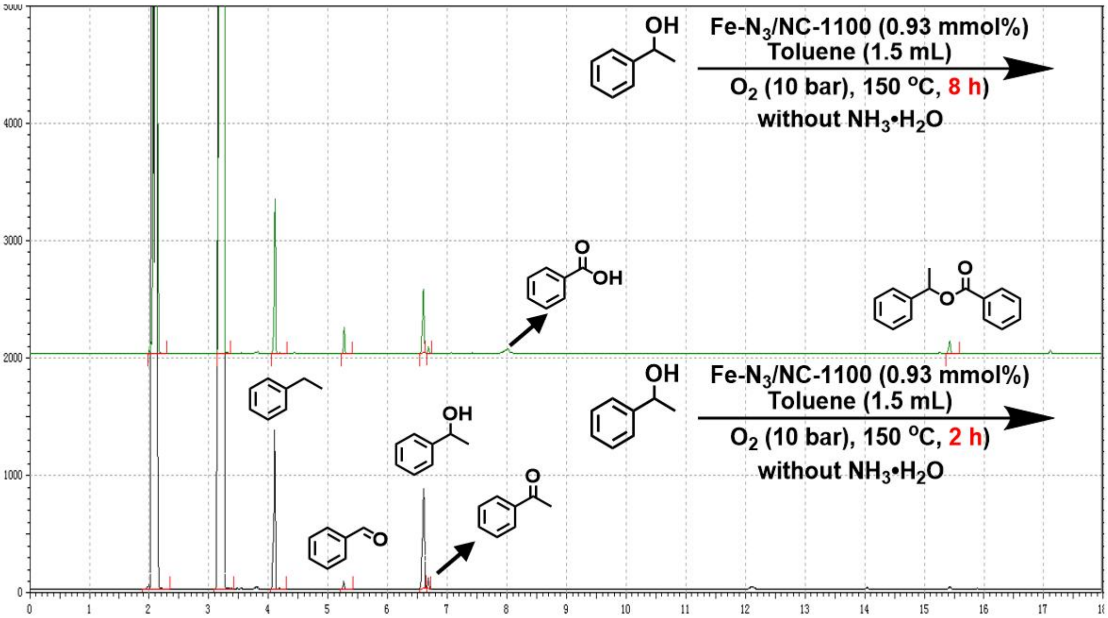
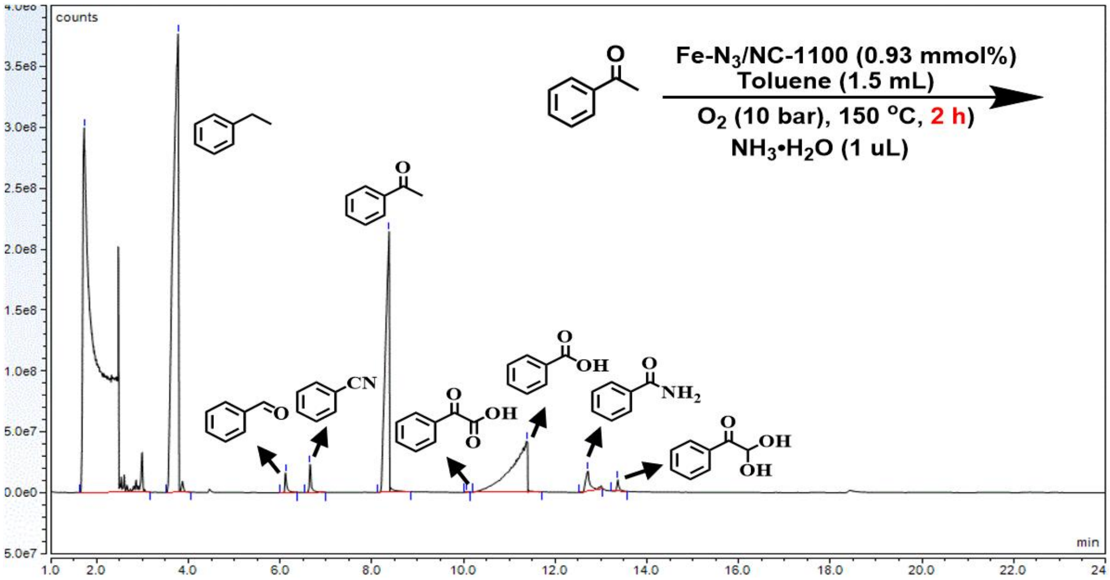
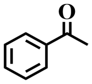
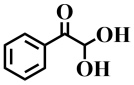
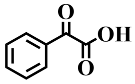
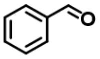
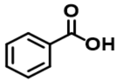
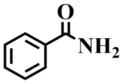


Fig. S15. GC spectrum of the intermediate generated from the aerobic oxidation cleavage and functionalization of DL-1-phenethylalcohol in toluene.



(acetophenone); (2,2-dihydroxy-acetophenon); (phenylglyoxylic acid); (benzaldehyde); (benzoic acid); (benzamide);

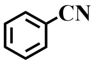
(benzonitrile)

Fig. S16. GC-MS spectrum of the intermediate generated from the aerobic oxidation cleavage and functionalization of acetophenone in toluene.

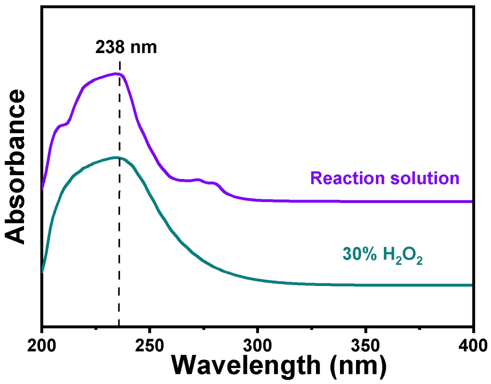


Fig. S17. Detection of H_2O_2. UV/visible spectrophotometer of 30% H_2O_2 solution and solution after reaction in methanol.

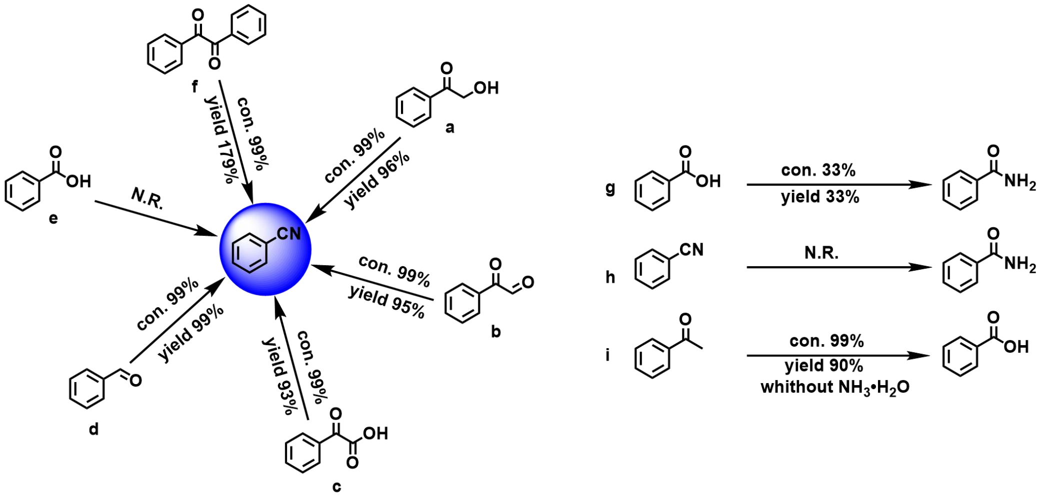


Fig. S18. Some important intermediates for the synthesis of benzonitrile. Reaction conditions: Substrate (0.20 mmol), Fe-N_3/NC-1100 (20 mg 0.98 mmol%), NH_3•H_2O (26.5 wt.% 400 μL), toluene (1.5 mL), O_2 (10 bar), 150 °C and 10 h.

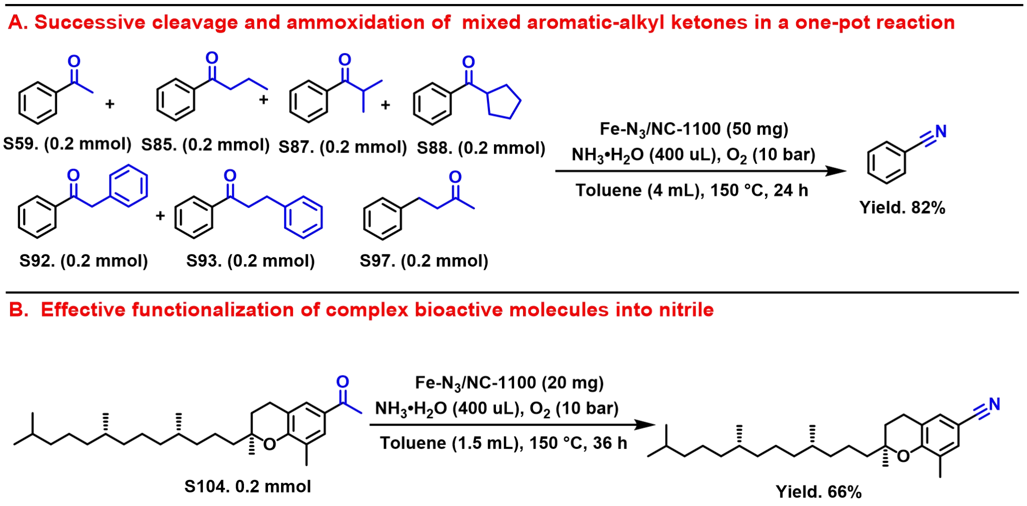


Fig. S19. Practical applications of developed catalytic methods.

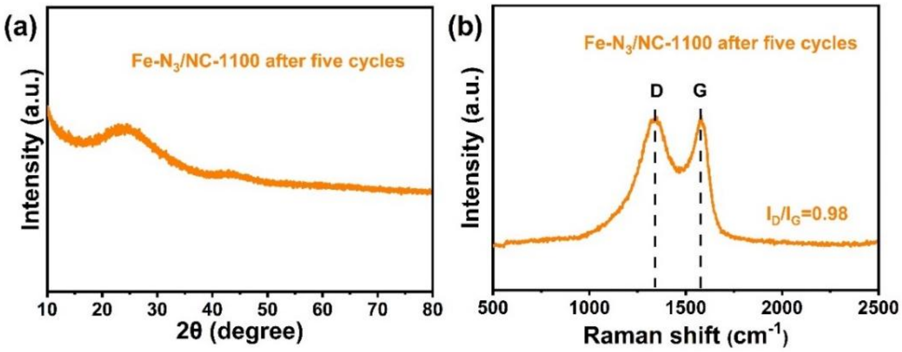


Fig. S20. XRD and Raman patterns of Fe-N$_3$/NC-1100 after five large-scale cycles. (**a**) XRD; (**b**) Raman.

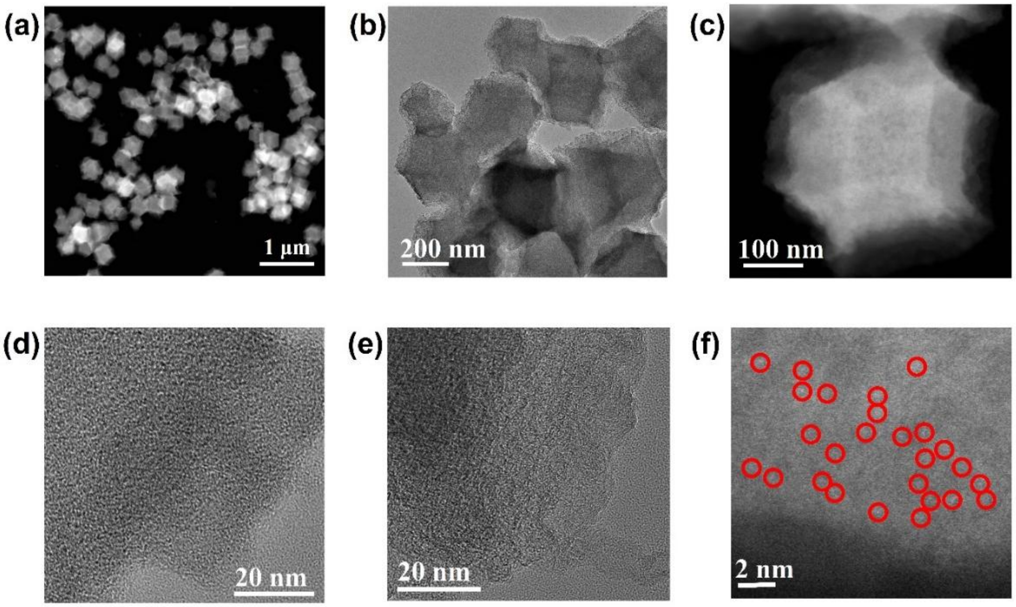
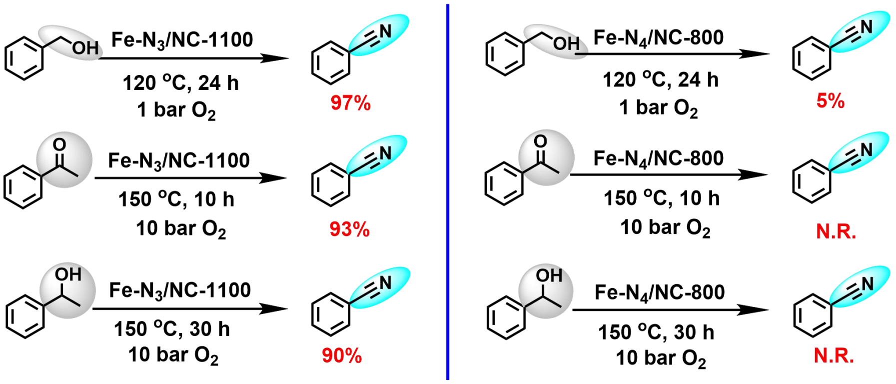


Fig. S21. STEM images of the Fe-N$_3$/NC-1100 after five large-scale cycles. (a~e) STEM images; (**f**) HAADF-STEM image (single-atom Fe is highlighted with red circles).



Reaction conditions: substrates (0.20 mmol), catalyst (20 mg), NH_3•H_2O (26.5 wt.%, 400 μL), toluene (1.5 mL).

Fig. S22. Comparison of catalytic activity of Fe-N$_3$/NC-1100 and Fe-N$_4$/NC-800.

Table S1. Texture properties and elements content in the Fe catalysts.

Sample	S_{BET} (m^2/g)	Pore Volume (cm^3/g)	Pore Size (nm)	Content	
				Fe (wt.%)[a]	Zn (wt.%)[a]
Fe-N_3/NC-1100	811	0.67	3.3	0.52	0.05
Fe-N_3/NC-1000	627	0.40	2.6	0.76	0.54

[a] Measured by ICP-AES.

Table S2. Elements content in the Fe catalysts. [a]

Sample	C (at.%)	N (at.%)	O (at.%)	Fe (at.%)	Zn (at.%)
Fe-N_3/NC-1100	89.67	1.71	8.42	0.2	0
Fe-N_3/NC-1000	87.45	5.46	6.08	0	1.01

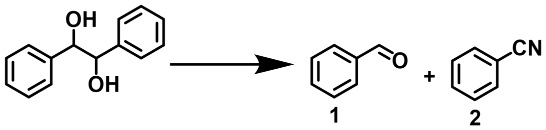
[a] Measured by XPS.

Table S3. EXAFS fitting parameters at the Fe K-edge for various samples (S_0^2=0.811).

Sample	Shell	CN^a	R(Å)^b	σ^2(Å^2)^c	ΔE_0(eV)^d	R factor
Fe K-edge						
Fe foil	Fe-Fe	8*	2.46±0.01	0.0048	5.8	0.0055
	Fe-Fe	6*	2.85±0.01	0.0055		
FeO	Fe-O	6.0	2.12±0.01	0.0147	-2.2	0.0074
	Fe-Fe	12.0	3.07±0.01	0.0119		
Fe_3O_4	Fe-O	6.0	2.00±0.01	0.0135	-0.9	0.0092
	Fe-Fe	8.0	3.00±0.02	0.0145		
	Fe-Fe	8.0	3.50±0.01	0.0092		
Fe-N_3/NC-1000	Fe-N	2.9±0.6	1.97±0.01	0.0111	-7.9	0.0048
	Fe-O	2.3±0.5	1.70±0.03	0.0111		
Fe-N_3/NC-1100	Fe-N	2.7±0.4	1.98±0.01	0.0101	-6.6	0.0035
	Fe-O	2.1±0.3	1.72±0.02	0.0101		

^{a}*CN*, coordination number; ^{b}*R*, distance between absorber and backscatter atoms; $^c\sigma^2$, Debye-Waller factor to account for both thermal and structural disorders; $^d\Delta E_0$, inner potential correction; *R* factor indicates the goodness of the fit. $S0^2$ was fixed to 0.811, according to the experimental EXAFS fit of Fe foil by fixing CN as the known crystallographic value. Fitting range: $3.0 \leq k$ (/Å) ≤ 12.5 and $1.0 \leq R$ (Å) ≤ 3.0 (Fe foil, FeO and Fe3O4); $2.0 \leq k$ (/Å) $\leq \sim9.5$ and $1.0 \leq R$ (Å) $\leq \sim3.0$ (Fe-1000 and Fe-1100). A reasonable range of EXAFS fitting parameters: $0.700 < S_0^2 < 1.000$; $CN > 0$; $\sigma^2 > 0$ Å^2; $\Delta E_0 < 10$ eV; *R* factor < 0.02.

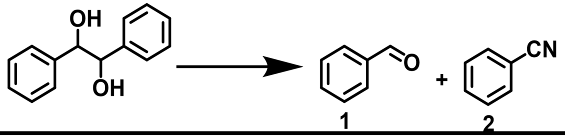
Table S4. Oxidative transformation of *R,R*-hydrobenzoin in different solvents. [a]



Entry	Solvent	Con. (%)	Sel. of 1 (%)	Sel.of 2 (%)
1	Toluene	> 99	40	60
2	Methanol	> 99	14	58
3	THF	> 99	43	46
4	Hexane	> 99	10	31
5	1,4-Dioxane	43	93	7
6	Acetonitrile	> 99	45	26

[a] Reaction conditions: *R,R*-hydrobenzoin (0.20 mmol), Fe-N_3/NC-1100 (20 mg, 0.93 mmol%), $NH_3 \cdot H_2O$ (26.5 wt.%, 200 μL), solvent (1.5 mL), O_2 (1 bar), 25 °C and 8 h.

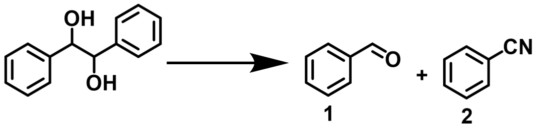
Table S5. The effect of $NH_3{\bullet}H_2O$ loading on the oxidative transformation of *R,R*-hydrobenzoin. [a]



Entry	$NH_3{\bullet}H_2O$ (μL)	Con. (%)	Sel. of 1 (%)	Sel. of 2 (%)
1	50	> 99	55	45
2	100	> 99	50	50
3	200	> 99	40	60
4	300	> 99	29	71
5	400	> 99	21	79

[a] Reaction conditions: *R,R*-hydrobenzoin (0.20 mmol), Fe-N_3/NC-1100 (20 mg, 0.93 mmol%), $NH_3{\bullet}H_2O$ (26.5 wt.%, 50~400 μL), toluene (1.5 mL), O_2 (1 bar), 25 °C and 8 h.

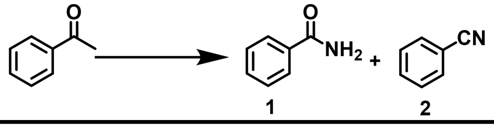
Table S6. Time course of the products distribution during the oxidative transformation of *R,R*-hydrobenzoin. [a]



Entry	Time (h)	Con. (%)	Sel. of 1 (%)	Sel. of 2 (%)
1	0.5	62	96	4
2	1	87	81	19
3	2	> 99	67	33
4	4	> 99	37	63
5	8	> 99	29	71
6	16	> 99	5	95
7	24	> 99	0	> 99

[a] Reaction conditions: *R,R*-hydrobenzoin (0.20 mmol), Fe-N$_3$/NC-1100 (20 mg, 0.93 mmol%), NH$_3$•H$_2$O (26.5 wt.%, 400 μL), toluene (1.5 mL), O$_2$ (1 bar) and 25 ^{o}C.

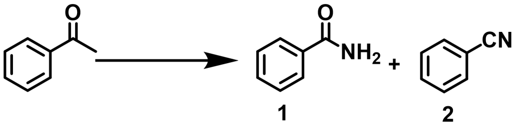
Table S7. The effect of the reaction temperature and oxygen pressure on the oxidative transformation of acetophenone. [a]



Entry	T (°C)	O_2 pressure (bar)	Con. (%)	Sel. of 1 (%)	Sel. of 2 (%)
1	120	1	0	-	-
2	140	1	0	-	-
3	150	1	4	0	100
4	150	2.5	15	27	73
5	150	5	36	14	86
6	150	7.5	70	19	81
7	150	10	70	9	91

[a] Reaction conditions: Acetophenone (0.20 mmol), toluene (1.5 mL), Fe-N_3/NC-1100 (20 mg, 0.93 mmol%), NH_3•H_2O (26.5 wt.%, 400 μL) and 4 h.

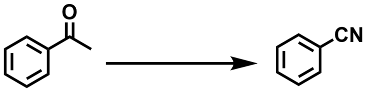
Table S8. Time course of the products distribution during the oxidative transformation of acetophenone. [a]



Entry	Time (h)	Con. (%)	Yield of 1 (%)	Yield of 2 (%)
1	0.5	21	1	20
2	1	31	2	29
3	2	50	3	47
4	4	70	5	65
5	8	90	6	84
6	10	100	7	93

[a] Reaction conditions: Acetophenone (0.20 mmol), toluene (1.5 mL), Fe-N_3/NC-1100 (20 mg, 0.93 mmol%), NH_3•H_2O (26.5 wt.%, 400 μL), 150 °C and O_2 (10 bar).

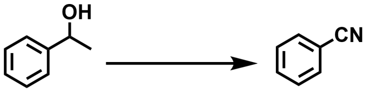
Table S9. Control experiments for the oxidative transformation of ketones into nitriles. [a]



Entry	Catalyst	T (ºC)	Time (h)	Con. (%)	Yield (%)
1	Fe-N_3/NC-1100	150	4	70	65
2	NC-1100	150	4	0	-
3	Fe-N_3/NC-1100-H^+	150	4	76	74
4	Fe-N_3/NC-1100-H^+ + KSCN (2 equiv.)	150	4	13	12

[a] Reaction conditions: Acetophenone (0.20 mmol), toluene (1.5 mL), catalyst (20 mg, 0.93 mmol%), NH_3•H_2O (26.5 wt.%, 400 μL), 150 ºC and O_2 (10 bar) and 4 h.

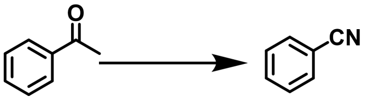
Table S10. Control experiments for the oxidative transformation of secondary alcohols into nitriles. [a]



Entry	Catalyst	T (°C)	Time (h)	Con. (%)	Yield (%)
1	Fe-N_3/NC-1100	150	30	99	90
2	NC-1100	150	30	0	-
3	Fe-N_3/NC-1100-H^+	150	30	99	94
4	Fe-N_3/NC-1100-H^+ + KSCN (2 equiv.)	150	30	28	27

[a] Reaction conditions: DL-1-phenethylalcohol (0.20 mmol), toluene (1.5 mL), catalyst (20 mg, 0.93 mmol%), NH_3•H_2O (26.5 wt.%, 400 μL), 150 °C and O_2 (10 bar) and 30 h.

Table S11. The radical inhibition experiments of the oxidative transformation of acetophenone into benzonitrile. [a]



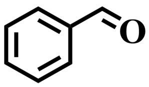
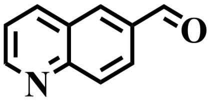
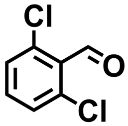
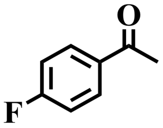
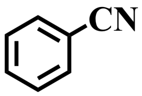
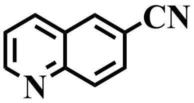
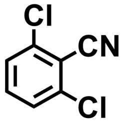
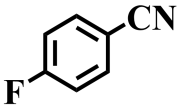
Entry	Additive	Conversion (%)	Yield (%)
1	-	70	58
2	BHT	18	18
3	1,4-Benzoquinone	16	13
4	Furfuryl alcohol	65	54
5	Isopropyl alcohol	72	62

[a] Reaction conditions: Acetophenone (0.20 mmol), Fe-N_3/NC-1100 catalyst (20 mg, 0.93 mmol%), additive (2 equiv.), $NH_3•H_2O$ (26.5 wt.%, 400 μL), toluene (1.5 mL), O_2 (10 bar), 150 °C and 4 h.

Table S12. Methods for the preparation of Fe-N_3/NC-1100 with 1～5 gram scale.

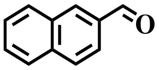
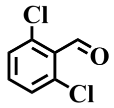
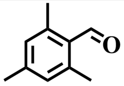
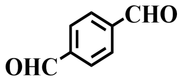
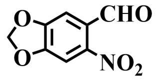
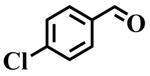
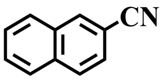
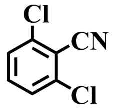
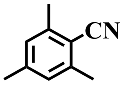
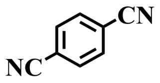
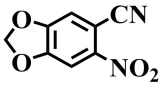
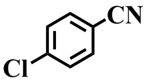
Entry	Ferrocene	ZIF-8	Pyrolysis (at ramp. 5 °C/min)	Catalyst mass (g)
1	56 mg	4 g	1100 ^{o}C, 2 h	1.46
2	112 mg	8 g	1100 ^{o}C, 2 h	3.28
3	168 mg	12 g	1100 ^{o}C, 2 h	5.12

Table S13. Activity test of the prepared catalyst in difference scale. [a]

Substrates				
Products				
Catalyst from 1.46 g of scale	97% yield	92% yield	99% yield	85% yield[b]
Catalyst from 3.28 g of scale	99% yield	89% yield	99% yield	88% yield[b]
Catalyst from 5.12 g of scale	95% yield	90% yield	99% yield	86% yield[b]

[a] Reaction conditions: Substrate (0.20 mmol), catalyst (20 mg), $NH_3 \cdot H_2O$ (26.5 wt.%, 400 μL) toluene (1.5 mL), O_2 (1 bar), 25 °C and 24 h; [b]O_2 (10 bar). 150 °C and 10 h.

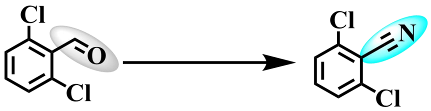
Table S14. Large-scale applications in the synthesis of nitriles. [a]

Substrates						
Products						
Yield	86%	93%	83%	88%	93%	95%

[a] Reaction conditions: Substrates (2 g), catalyst (500 mg), $NH_3 \cdot H_2O$ (26.5 wt.%, 1 mL) acetonitrile (10 mL), O_2 (10 bar), 80 °C and 24 h.

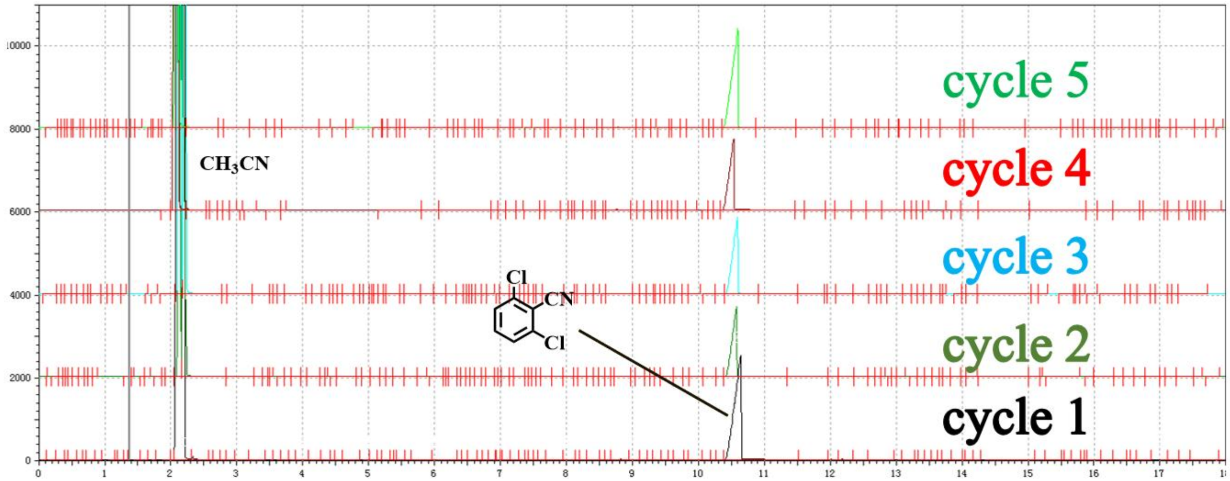
The figure of products

Table S15. Large-scale cycle experiment in the synthesis of nitriles. [a]



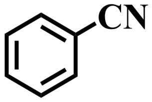
Entry	Catalyst	T (°C)	Time (h)	Yield. (%)
1	Fe-N$_3$/NC-1100	80	24	99
2		80	24	99
3		80	24	99
4		80	24	99
5		80	24	99

[a] Reaction conditions: 2,6-dichlorobenzaldehyde (1 g), Fe-N$_3$/NC-1100 (500 mg), NH$_3$•H$_2$O (26.5 wt.%, 1 mL), acetonitrile (10 mL), O$_2$ (10 bar), 80 °C and 24 h.



GC spectrum of cycle

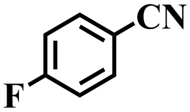
Benzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63-7.51 (m, 3H), 7.43 (t, *J*=7.7 Hz, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 132.71, 131.97, 129.03, 118.73, 112.19.

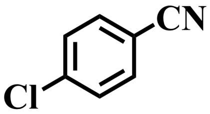
4-Fluorobenzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.70-7.57 (m, 2H), 7.19-7.06 (m, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 166.20, 163.65, 134.68, 134.59, 117.97, 116.88, 116.66, 108.46, 108.42.

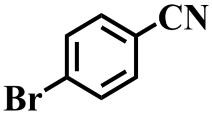
4-Chlorobenzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.56 (d, *J*=8.5 Hz, 2H), 7.42 (d, *J*=8.4 Hz, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 139.39, 133.32, 129.59, 117.89, 110.66.

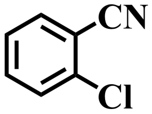
4-Bromobenzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.61-7.55 (m, 2H), 7.52-7.46 (m, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 133.36, 132.54, 127.91, 117.99, 111.11.

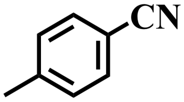
2-Chlorobenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J*=7.7, 1.5 Hz, 1H), 7.57-7.43 (m, 2H), 7.40-7.32 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.64, 133.95, 129.98, 127.21, 115.93, 113.17.

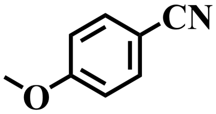
4-Methylbenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J*=8.0 Hz, 2H), 7.22 (d, *J*=8.0 Hz, 2H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.60, 131.82, 129.71, 119.00, 109.05, 21.64.

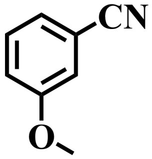
4-Methoxybenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J*=8.9 Hz, 2H), 6.89 (d, *J*=8.9 Hz, 2H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.74, 133.81, 119.13, 114.66, 103.67, 55.44.

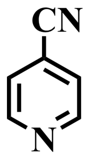
3-Methoxybenzonitrile



^{1}H NMR (400 MHz, CD_3OD) δ 7.46-7.33 (m, 1H), 7.27-7.10 (m, 3H), 3.84-3.72 (m, 3H).

^{13}C NMR (101 MHz, CD_3OD) δ 161.17, 131.59, 125.32, 120.40, 119.60, 117.85, 114.03, 56.07.

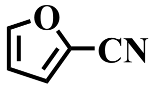
Isonicotinonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 8.76-8.65 (m, 2H), 7.46 (dd, *J*=4.5, 1.5 Hz, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 150.60, 125.12, 120.18, 116.26.

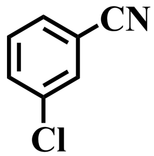
Furan-2-carbonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.85-7.70 (m, 1H), 7.28 (d, *J*=3.6 Hz, 1H), 6.63 (dd, *J*=3.6, 1.8 Hz, 1H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 149.43, 127.11, 123.48, 112.65, 112.32.

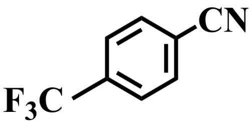
3-Chlorobenzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.62-7.50 (m, 3H), 7.45-7.37 (m, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 135.15, 133.22, 131.84, 130.52, 130.29, 117.41, 113.89.

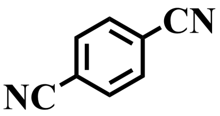
4-(Trifluoromethyl)benzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.79 (d, *J*=8.3 Hz, 2H), 7.73 (d, *J*=8.4 Hz, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 132.73, 126.23, 126.20, 126.16, 126.12, 124.46, 121.75, 117.48, 116.07.

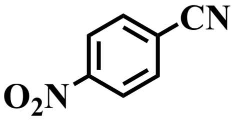
1,4-Dicyanobenzene



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 132.85, 117.07, 116.75.

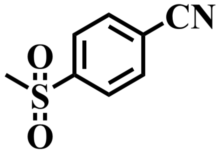
4-Nitrobenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J*=8.7 Hz, 2H), 7.89 (d, *J*=8.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.04, 133.57, 124.33, 118.32, 116.90.

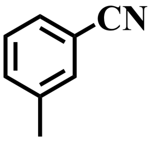
4-(Methylsulfonyl)benzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J*=8.5 Hz, 2H), 7.87 (d, *J*=8.5 Hz, 2H), 3.08 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.42, 133.26, 128.22, 117.53, 117.14, 44.21.

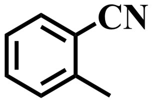
3-Methylbenzonitrile



^{1}H NMR (400 MHz, CD_3OD) δ 7.61-7.10 (m, 4H), 2.34 (s, 3H).

^{13}C NMR (101 MHz, CD_3OD) δ 140.74, 134.85, 133.34, 130.22, 130.21, 119.82, 113.05, 21.06.

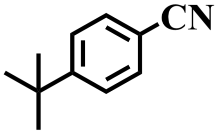
2-Methylbenzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.64-7.43 (m, 2H), 7.38-7.21 (m, 2H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 142.89, 133.94, 133.42, 131.31, 127.44, 118.83, 113.46, 20.39.

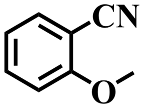
4-Tert-Butylbenzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.58 (dd, *J*=19.5, 8.5 Hz, 4H), 1.31 (s, 9H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 157.84, 132.80, 127.26, 119.69, 110.02, 35.87, 31.07.

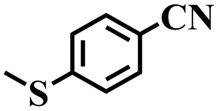
2-Methoxybenzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.34-7.27 (m, 2H), 7.26-7.20 (m, 1H), 2.89-2.78 (m, 1H), 2.60 (qd, *J*=7.2, 1.7 Hz, 3H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 162.52, 135.90, 134.65, 121.89, 117.32, 112.68, 102.14, 56.61.

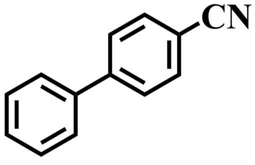
4-Cyanothioanisole



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 11.4 Hz, 2H), 2.47 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 146.03, 131.99, 125.30, 118.87, 107.37, 14.52.

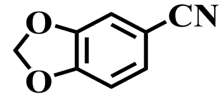
[1,1'-Biphenyl]-4-carbonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.68 (q, *J*=8.5 Hz, 4H), 7.63-7.54 (m, 2H), 7.54-7.40 (m, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 145.49, 139.00, 132.51, 129.07, 128.63, 127.62, 127.14, 118.91, 110.77.

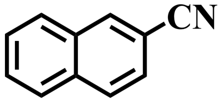
Benzo[d][1,3]dioxole-5-carbonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.16 (dd, *J*=8.1, 1.5 Hz, 1H), 6.98 (d, *J*=1.4 Hz, 1H), 6.83 (d, *J*=8.1 Hz, 1H), 6.04 (s, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 151.50, 147.98, 128.15, 118.87, 111.28, 109.08, 104.78, 102.25.

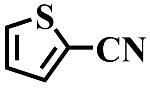
Naphthonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 8.14 (s, 1H), 7.88-7.78 (m, 3H), 7.65-7.50 (m, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 134.50, 134.01, 132.09, 129.09, 128.98, 128.31, 127.96, 127.59, 126.18, 119.21, 109.20.

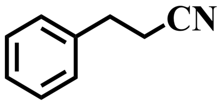
Thiophene-2-carbonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63-7.55 (m, 2H), 7.14-7.04 (m, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 147.38, 137.41, 132.68, 127.64, 122.04, 114.21, 109.61.

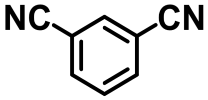
Phenylpropanenitrile



^{1}H NMR (400 MHz, CD_3OD) δ 7.34-7.27 (m, 2H), 7.26-7.20 (m, 3H), 2.89-2.78 (m, 2H), 2.60 (qd, *J*=7.2, 1.7 Hz, 2H).

^{13}C NMR (101 MHz, CD_3OD) δ 139.86, 129.62, 129.36, 127.92, 120.66, 32.16, 19.49.

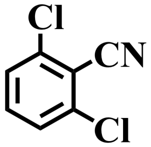
1,3-Dicyanobenzene



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.81 (m, 3H), 7.66 (t, *J*=7.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 136.02, 135.39, 130.34, 116.62, 114.02.

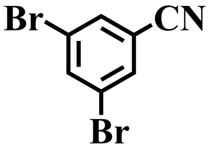
2,6-Dichlorobenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.35 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.49, 133.97, 128.21, 114.38, 113.40.

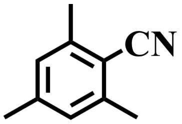
3,5-Dibromobenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.85 (m, 1H), 7.73 (d, *J*=1.3 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.85, 133.47, 123.61, 115.94, 115.45.

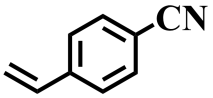
2,4,6-Trimethylbenzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.23-6.71 (m, 2H), 2.75-1.80 (m, 9H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 144.34, 142.80, 129.09, 118.05, 110.75, 21.39, 20.39.

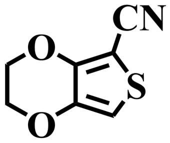
4-Vinylbenzonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 (d, *J*=8.2 Hz, 2H), 7.47 (t, *J*=10.7 Hz, 2H), 6.70 (dd, *J*=17.6, 10.9 Hz, 1H), 5.86 (d, *J*=17.6 Hz, 1H), 5.43 (d, *J*=10.9 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 141.82, 135.27, 132.31, 126.69, 118.87, 117.71, 110.99.

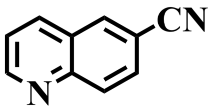
2,3-Dihydrothieno[3,4-b][1,4]dioxine-5-carbonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 6.83 (s, 1H), 4.43-4.30 (m, 2H), 4.25 (dd, *J*=5.3, 3.0 Hz, 2H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 151.14, 142.16, 113.41, 108.61, 85.23, 66.75, 65.37.

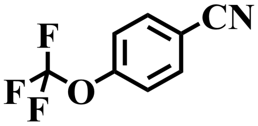
Quinoline-6-carbonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 8.90 (s, 1H), 8.26-7.87 (m, 3H), 7.66 (d, *J*=6.6 Hz, 1H), 7.39 (s, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 152.91, 148.65, 136.04, 133.83, 130.62, 129.69, 127.16, 122.47, 118.19, 109.88.

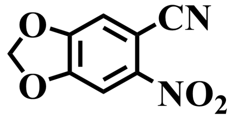
4-(Trifluoromethoxy)benzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.85 (d, *J*=8.6 Hz, 2H), 7.45 (d, *J*=8.2 Hz, 2H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 153.26, 135.50, 122.43, 118.41, 112.02.

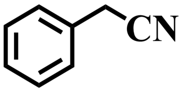
6-Nitrobenzo[d][1,3]dioxole-5-carbonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.82 (s, 1H), 7.40 (d, *J*=8.4 Hz, 1H), 6.31 (s, 2H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 113.78, 106.80, 106.30.

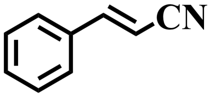
2-Phenylacetonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.58-6.89 (m, 5H), 4.07-3.52 (m, 2H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 131.89, 129.92, 128.88, 128.69, 119.59, 23.44.

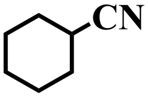
Cinnamonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 7.80-6.93 (m, 6H), 5.85 (d, *J*=16.6 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 150.36, 133.31, 131.06, 128.94, 127.23, 118.08, 96.13.

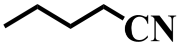
Cyclohexanecarbonitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 2.58 (dt, *J*=11.9, 4.0 Hz, 1H), 1.98-1.54 (m, 6H), 1.53-1.17 (m, 4H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 122.50, 29.33, 27.79, 25.08, 23.90.

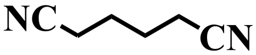
Pentanenitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 2.26 (t, *J*=7.1 Hz, 2H), 1.55 (dt, *J*=15.1, 7.1 Hz, 2H), 1.46-1.29 (m, 2H), 0.86 (t, *J*=7.3 Hz, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 119.61, 27.03, 21.51, 16.47, 12.90.

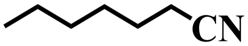
Adiponitrile



^{1}H NMR (400 MHz, CDCl$_3$) δ 2.59-1.95 (m, 4H), 1.90-1.39 (m, 4H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 118.73, 23.59, 15.83.

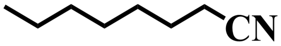
Heptanenitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 2.78-2.13 (m, 2H), 1.91-0.51 (m, 11H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 120.91, 31.87, 29.18, 26.23, 23.23, 17.11, 14.13.

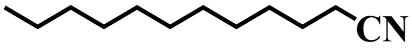
Octanenitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 2.52-2.25 (m, 2H), 1.81-1.17 (m, 10H), 1.00-0.76 (m, 3H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 120.90, 32.50, 29.48, 29.37, 26.28, 23.39, 17.11, 14.23.

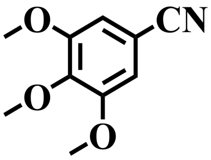
Dodecanenitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 2.67-2.12 (m, 2H), 1.80-1.09 (m, 16H), 1.06-0.68 (m, 3H).

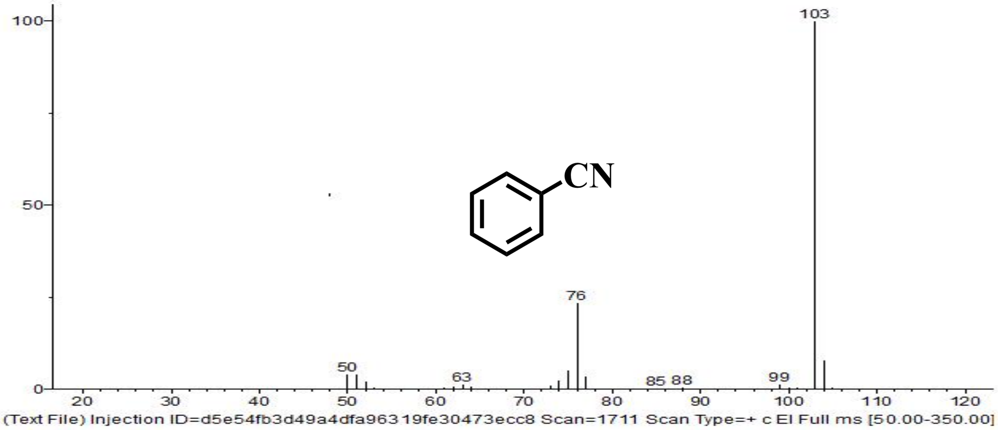
^{13}C NMR (101 MHz, CD$_3$OD) δ 120.86, 32.88, 30.54, 30.50, 30.33, 30.29, 29.75, 29.56, 26.31, 23.56, 17.13, 14.34.

3,4,5-Trimethoxybenzonitrile



^{1}H NMR (400 MHz, CD$_3$OD) δ 7.01 (s, 2H), 4.09-3.49 (m, 9H).

^{13}C NMR (101 MHz, CD$_3$OD) δ 154.77, 110.53, 61.01, 56.73.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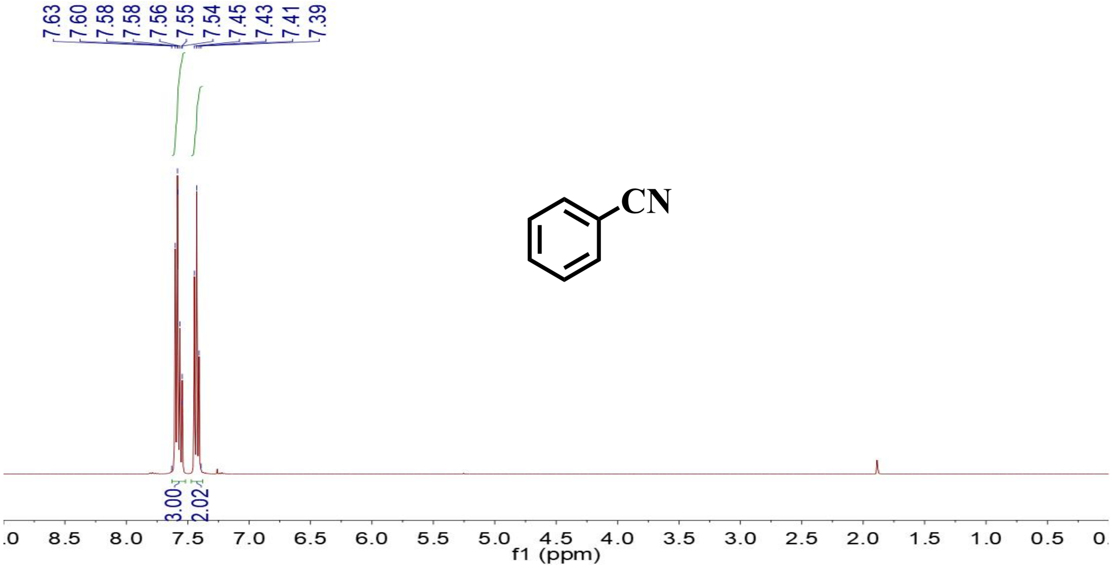
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7.41
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2.02
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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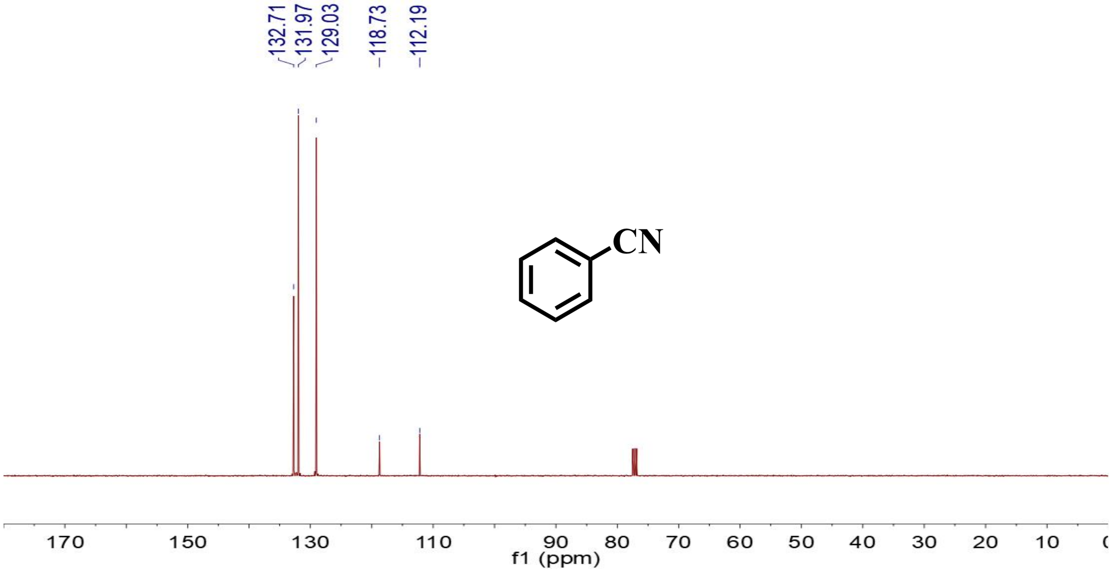
f1 (ppm)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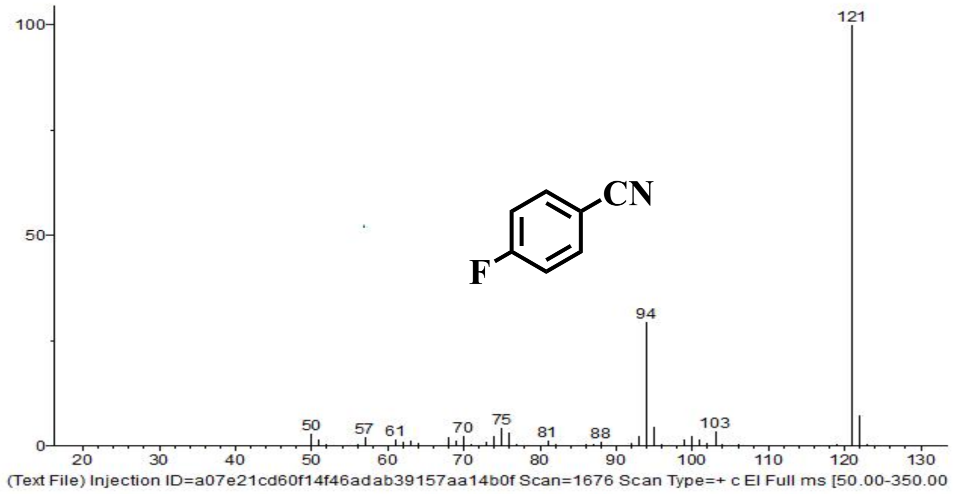
f1 (ppm)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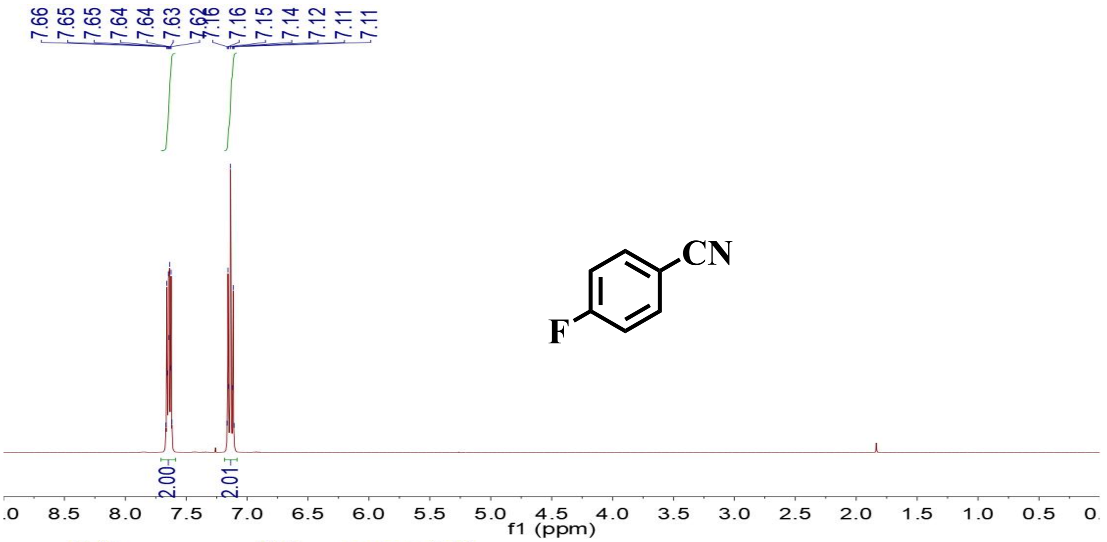
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7.11
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2.01
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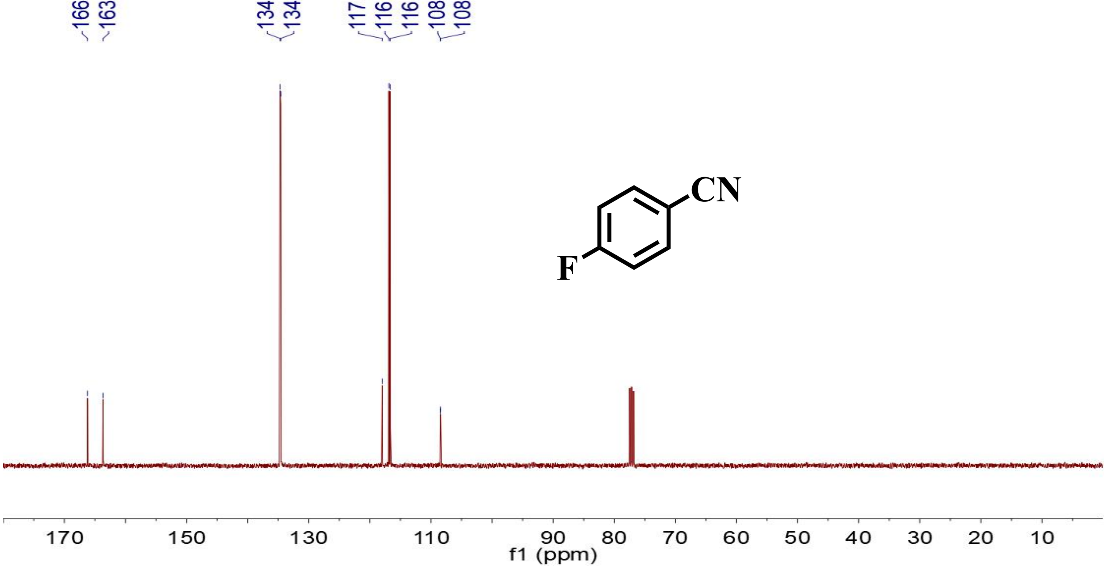
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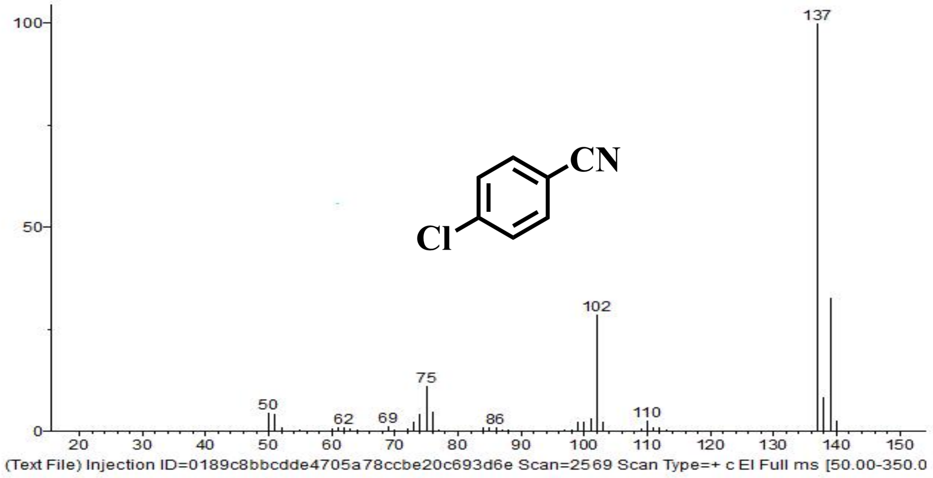
f1 (ppm)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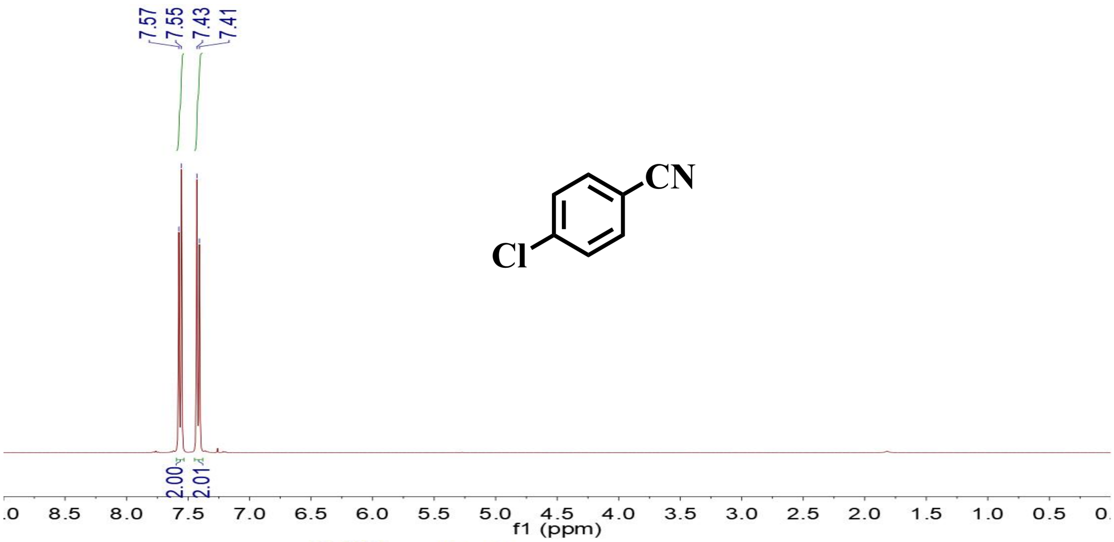
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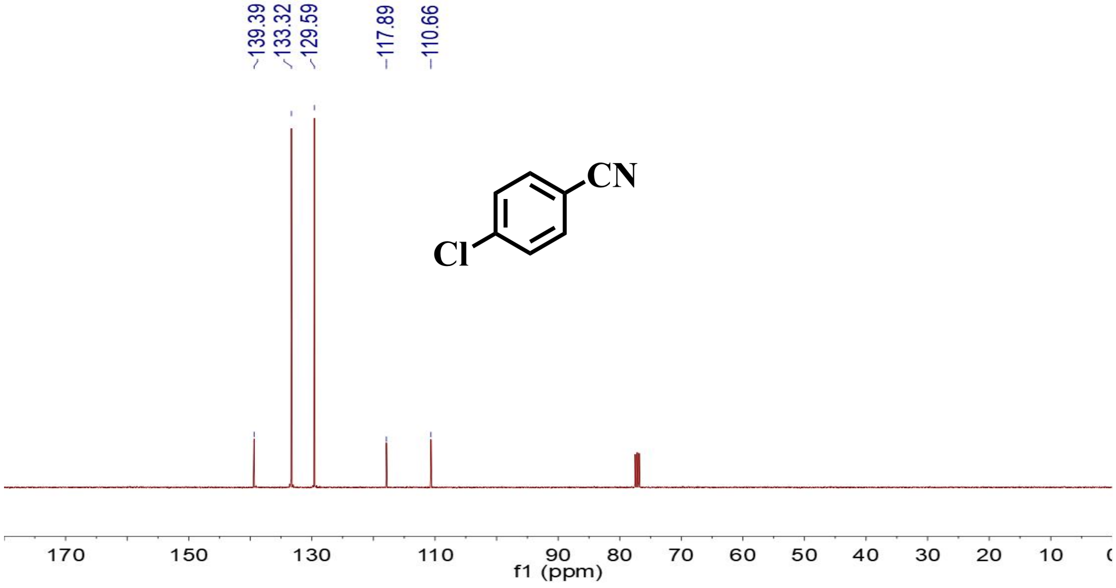
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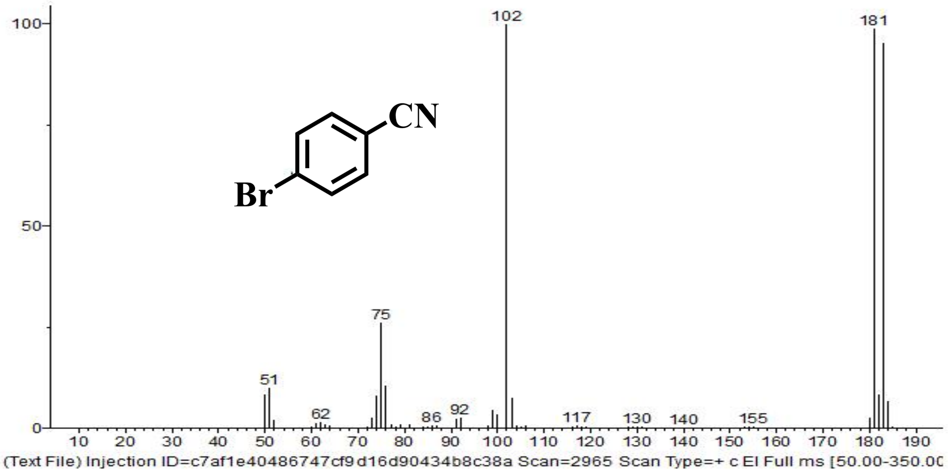

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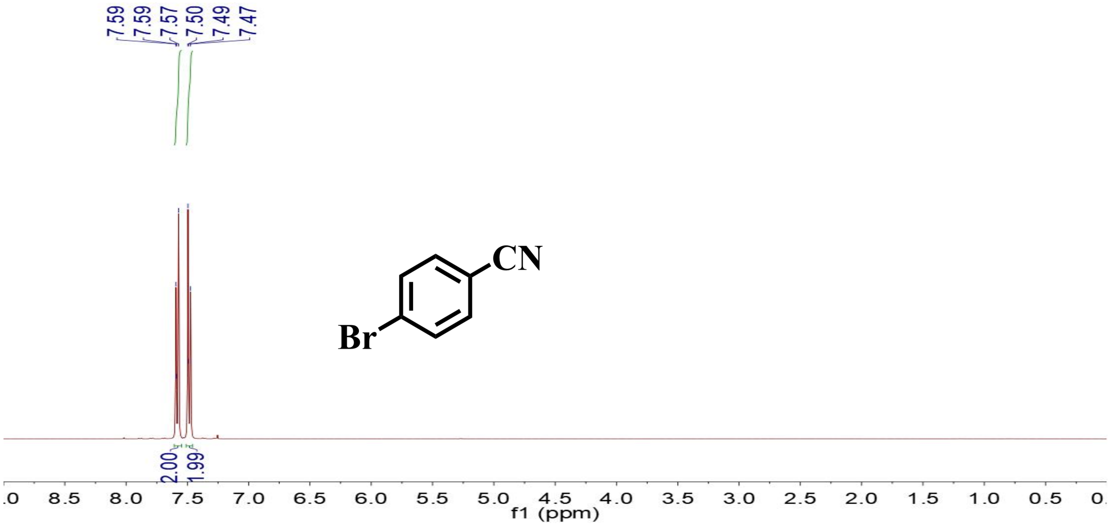
Br



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Br
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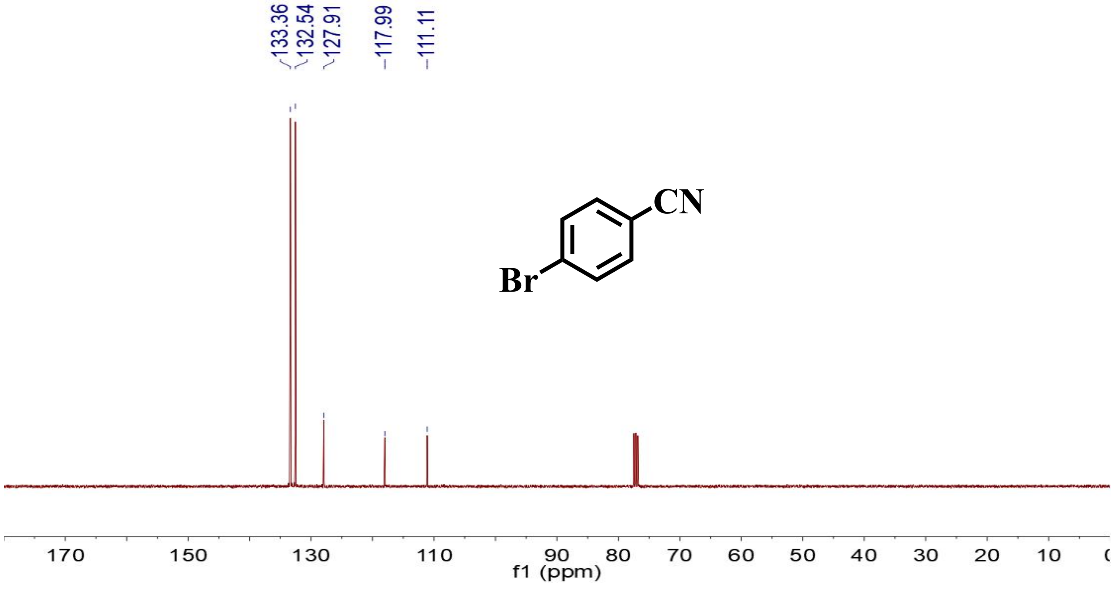

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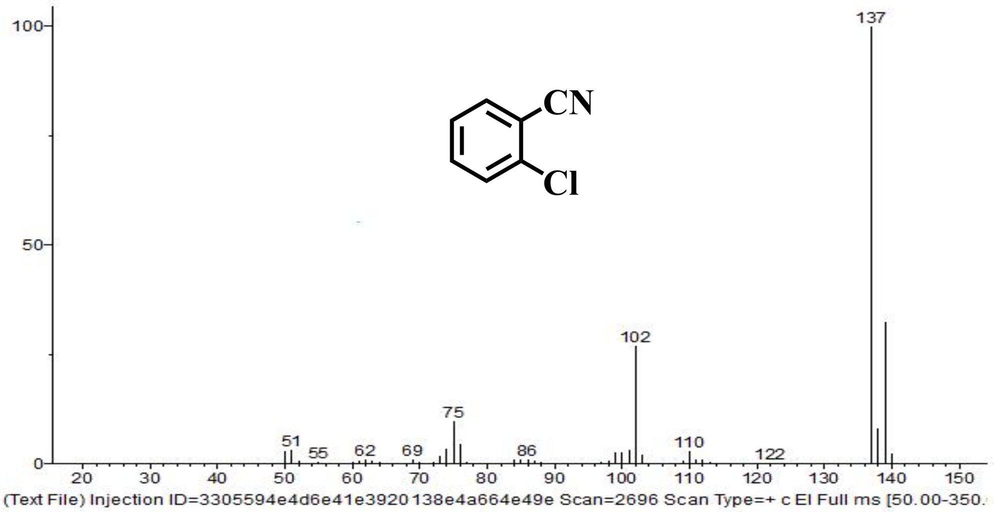
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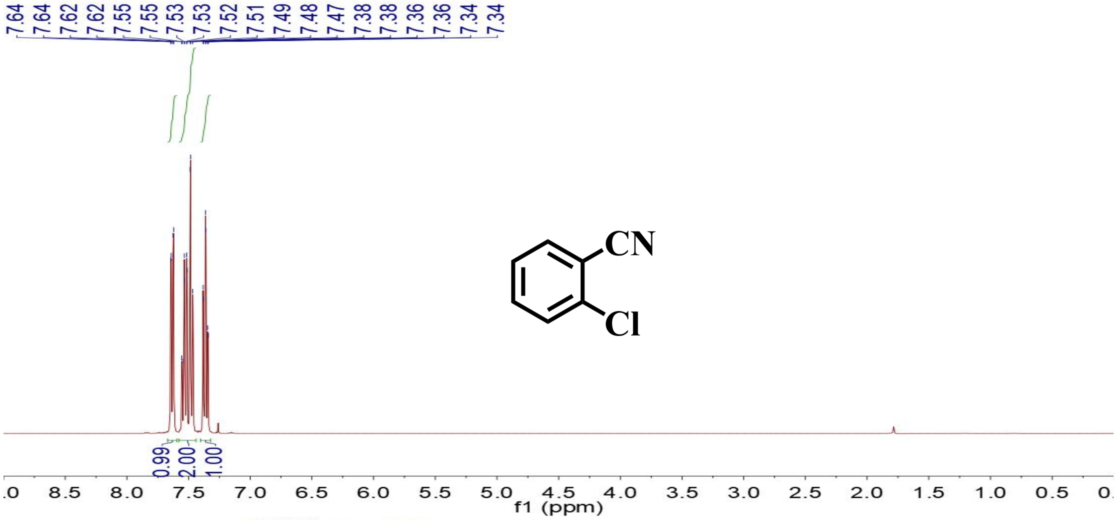
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7.34
CN
Cl
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1.00
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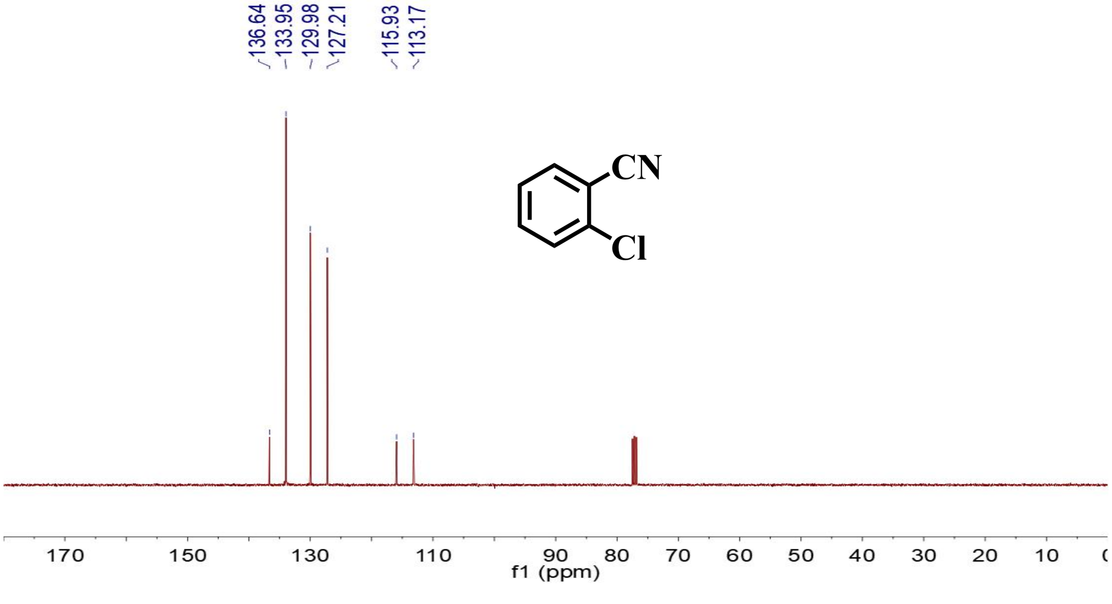
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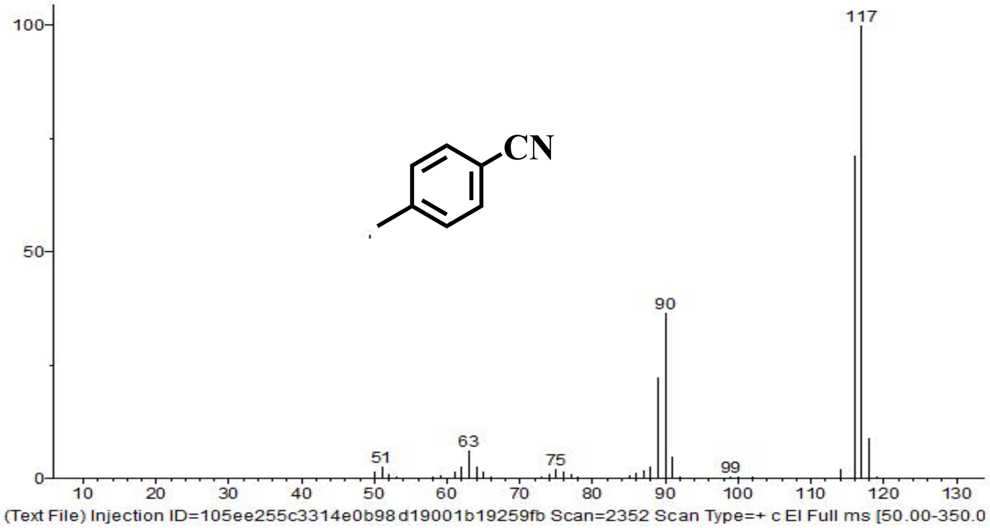
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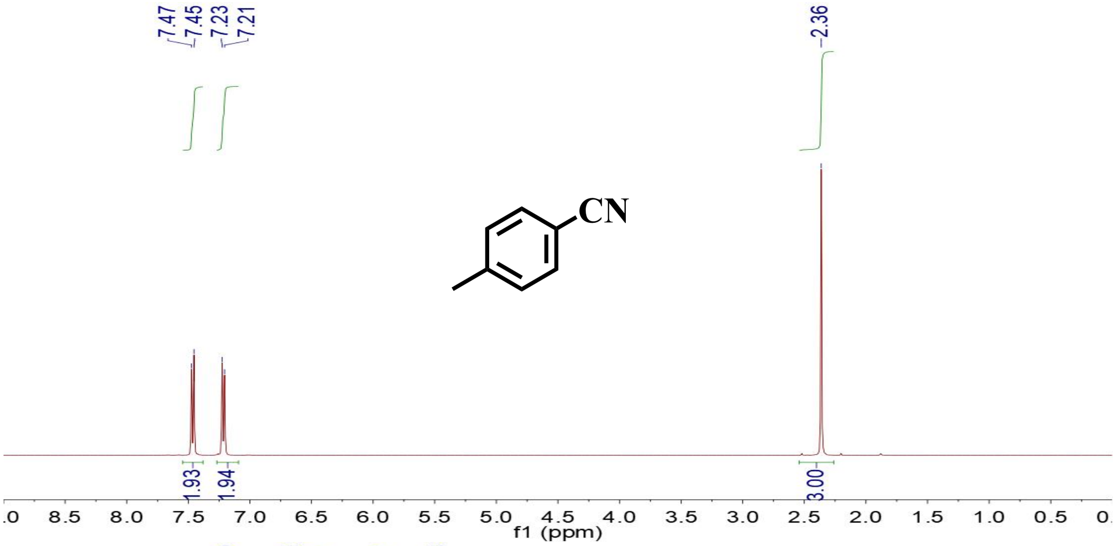
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3.00
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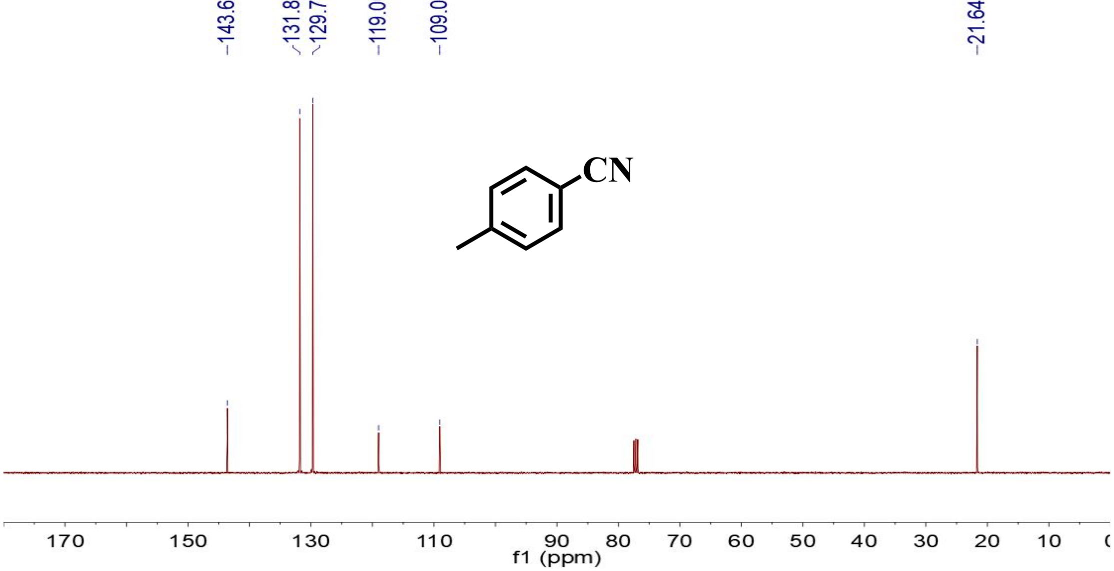
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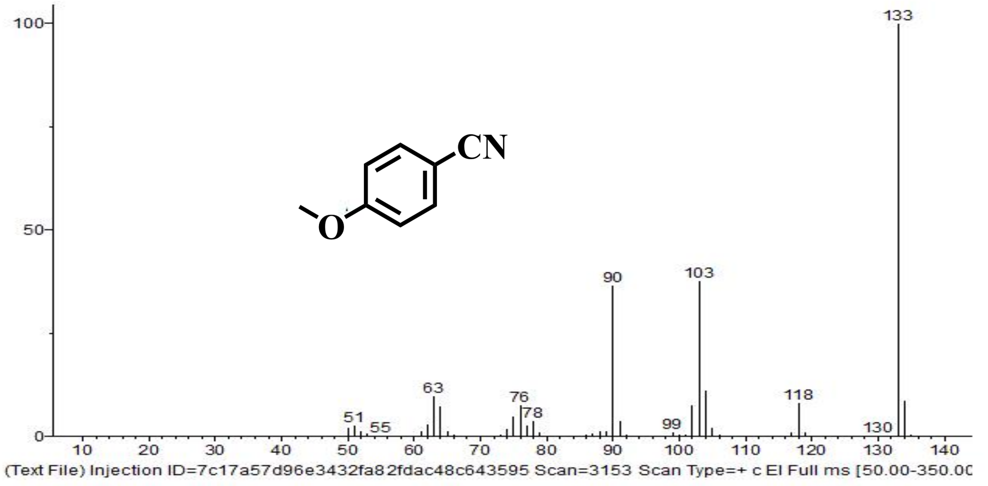
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10 20 30 40 50 60 70 80 90 100 110 120 130 140
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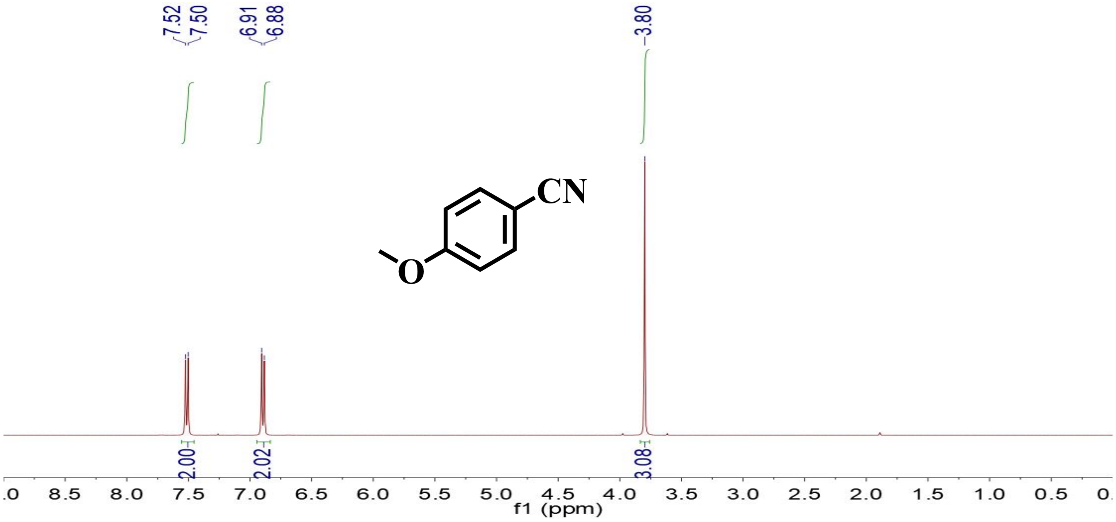
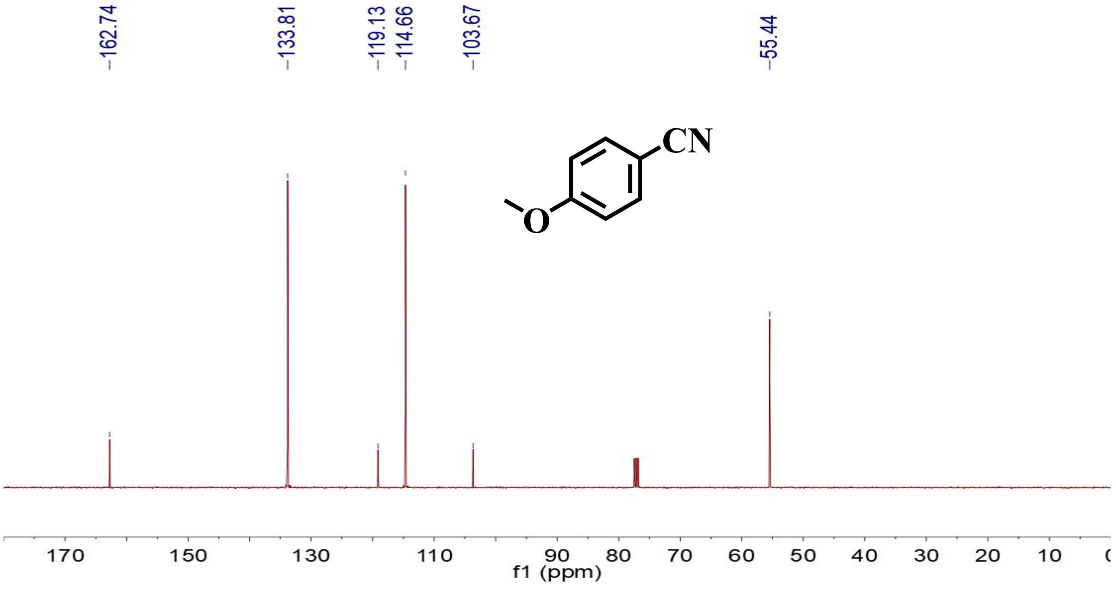
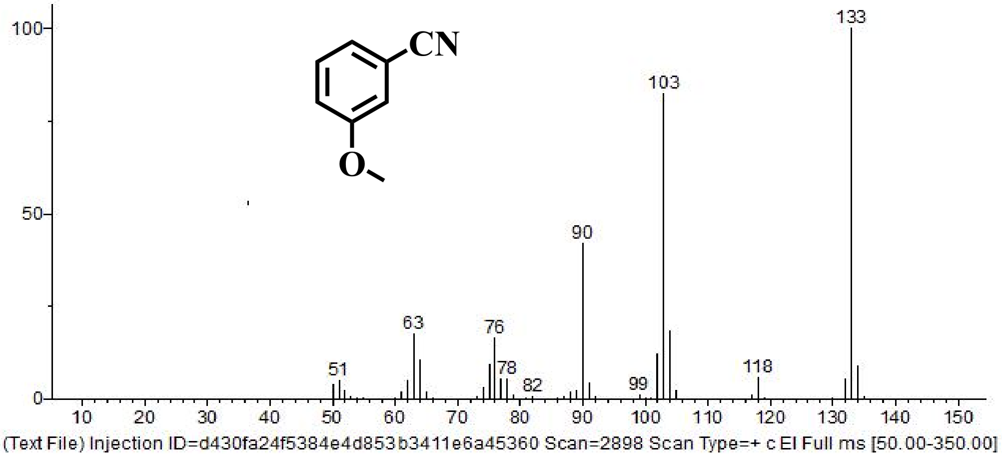
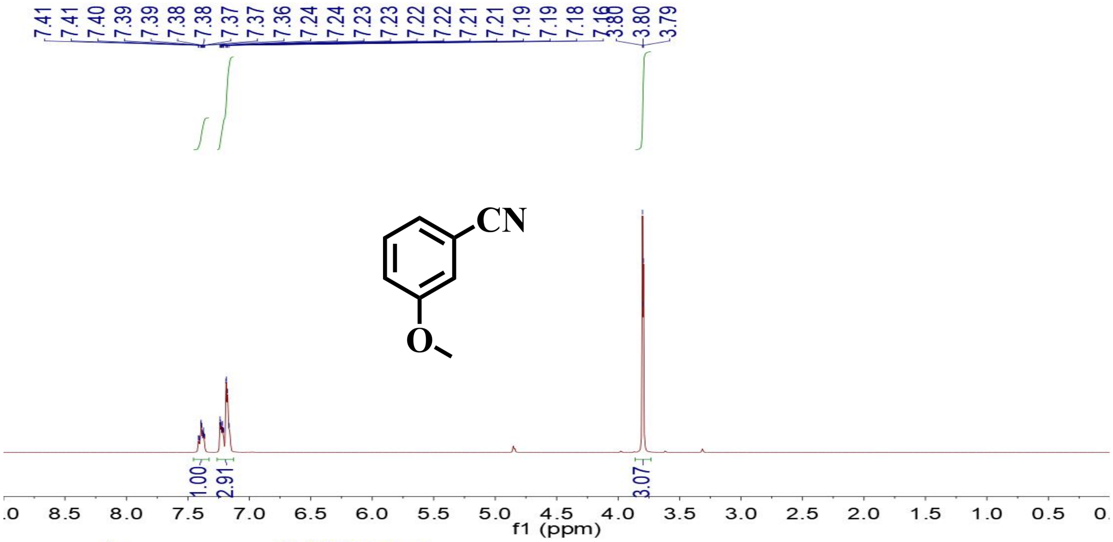
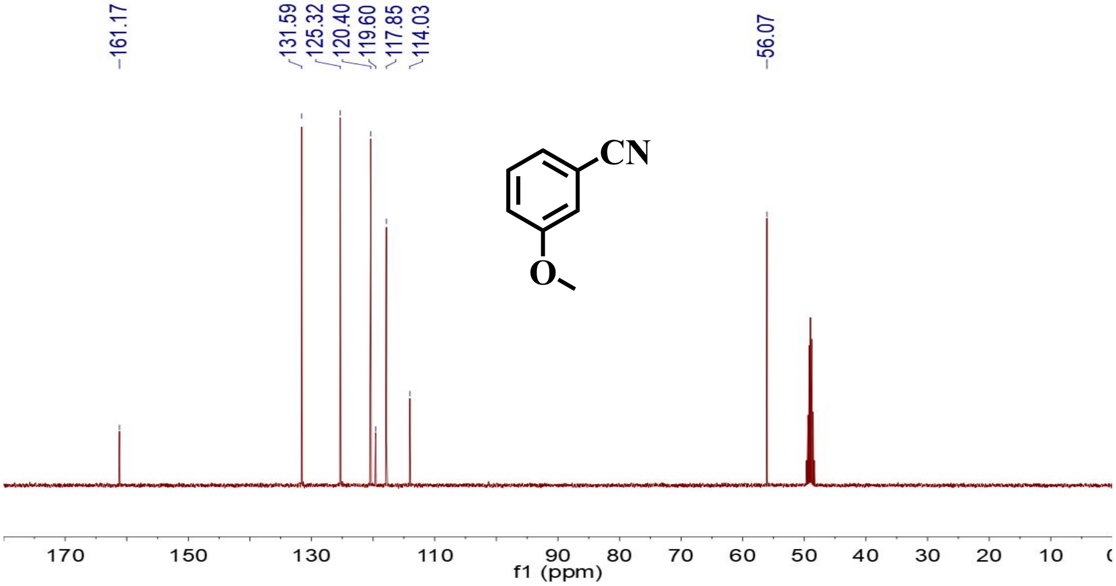
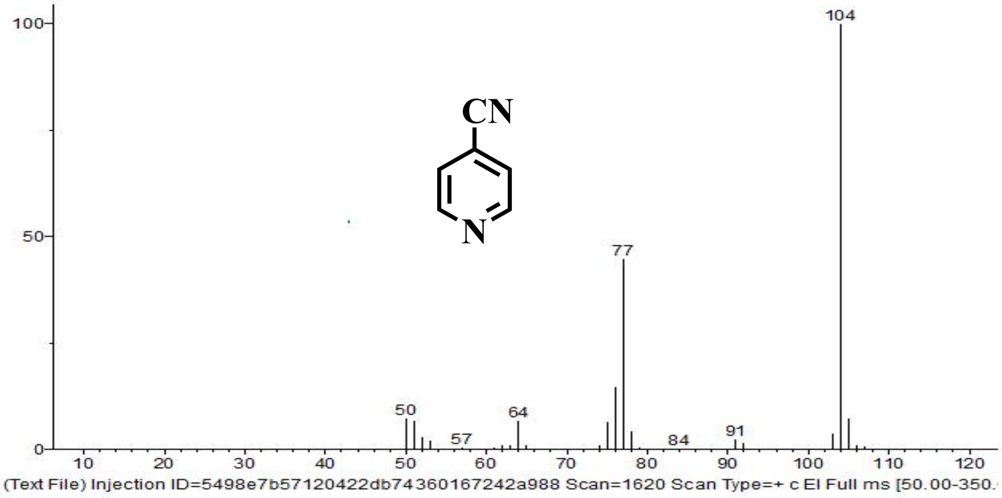

7.52
7.50
6.91
6.88
3.80
CN
O
2.00
2.02
3.08
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

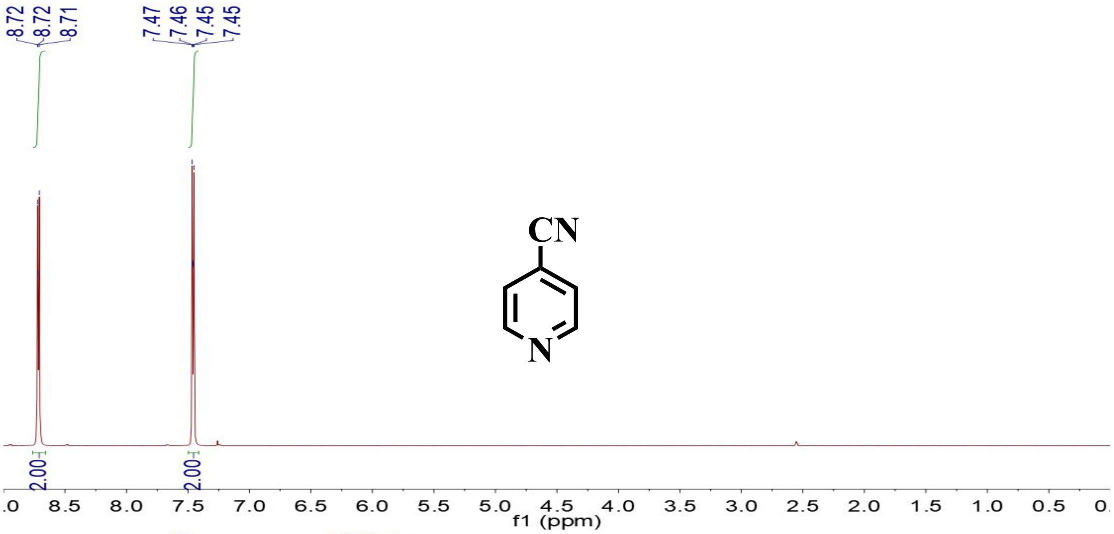

162.74
133.81
119.13
114.66
103.67
55.44
CN
O
170 150 130 110 90 80 70 60 50 40 30 20 10 (
f1 (ppm)

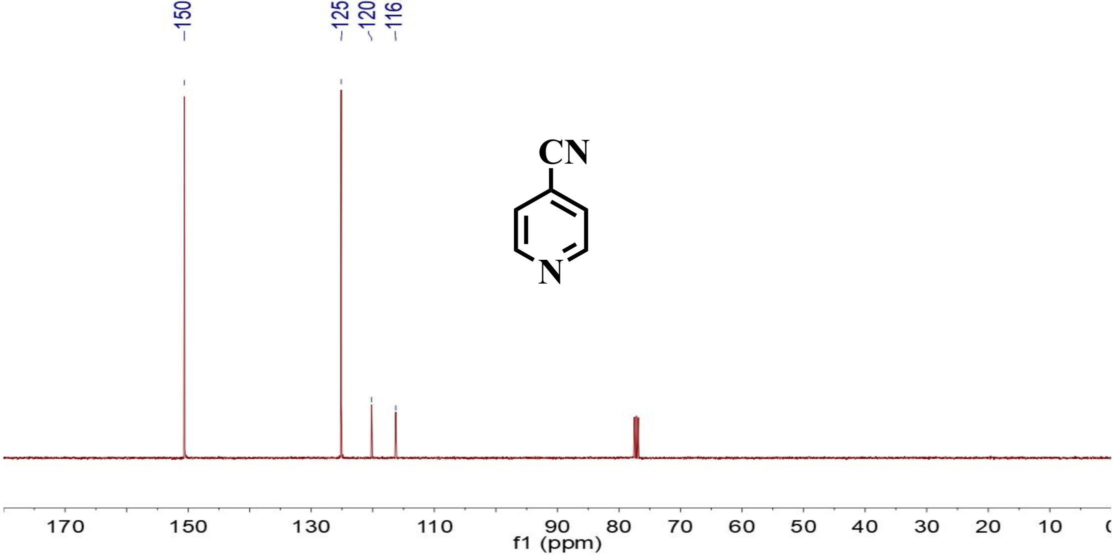

100
50
0
133
103
90
63
76
78
82
51
99
118
CN
O
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
(Text File) Injection ID=d430fa24f5384e4d853b3411e6a45360 Scan=2898 Scan Type=+ c EI Full ms [50.00-350.00]

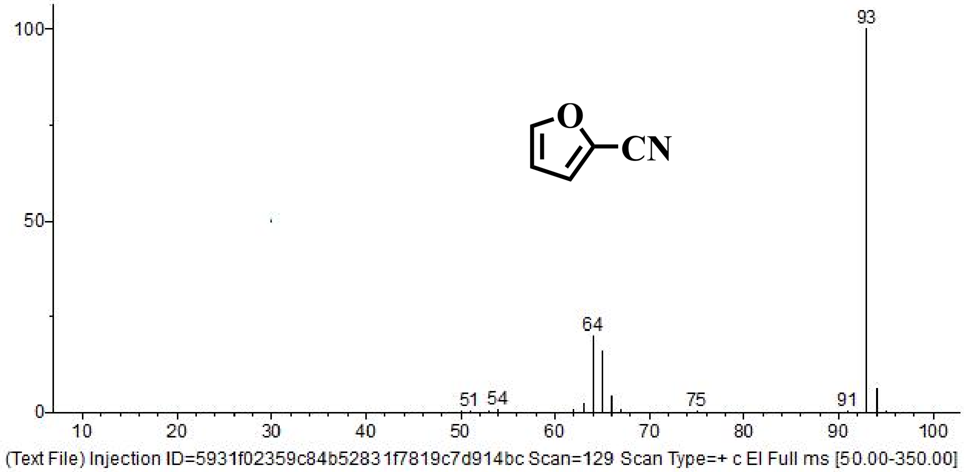

7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.24
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.19
7.19
7.18
7.16
3.80
3.80
3.79
CN
O
1.00
2.91
3.07
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

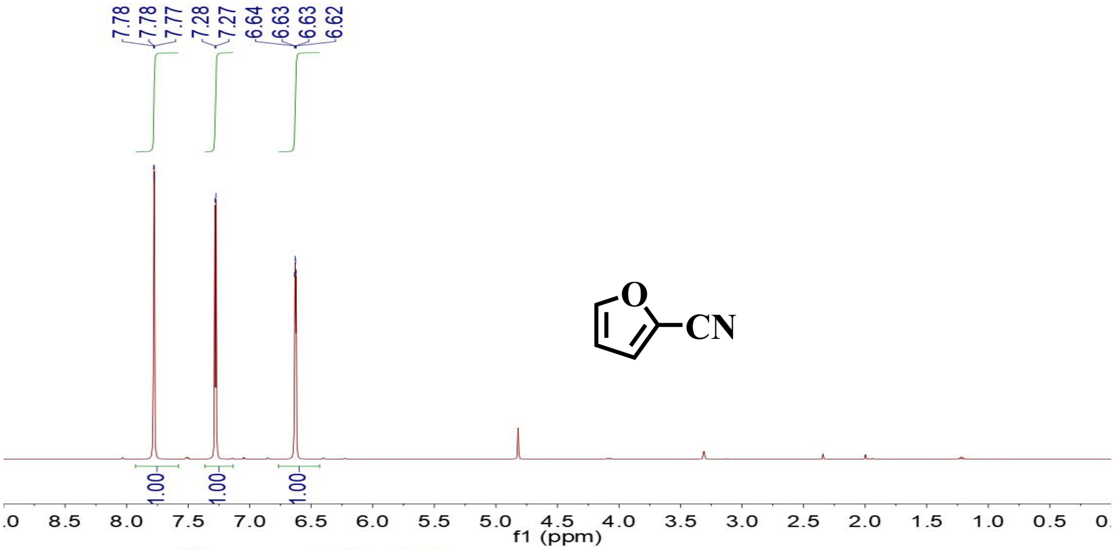

161.17
131.59
125.32
120.40
119.60
117.85
114.03
56.07
CN
O
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

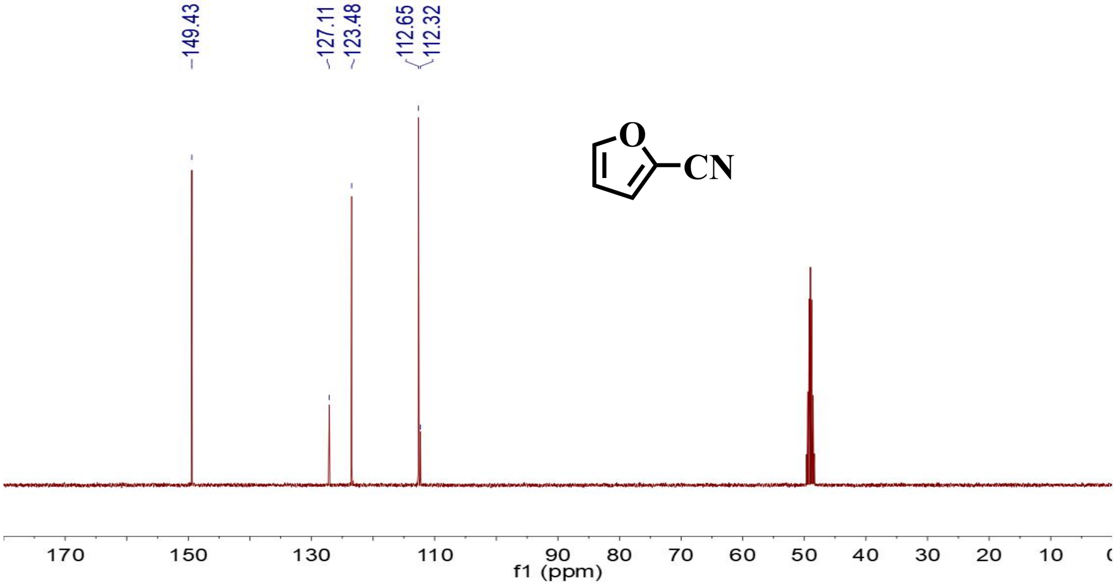

100
50
0
104
77
50
64
57
84
91
CN
N
10
20
30
40
50
60
70
80
90
100
110
120
(Text File) Injection ID=5498e7b57120422db74360167242a988 Scan=1620 Scan Type=+ c EI Full ms [50.00-350.

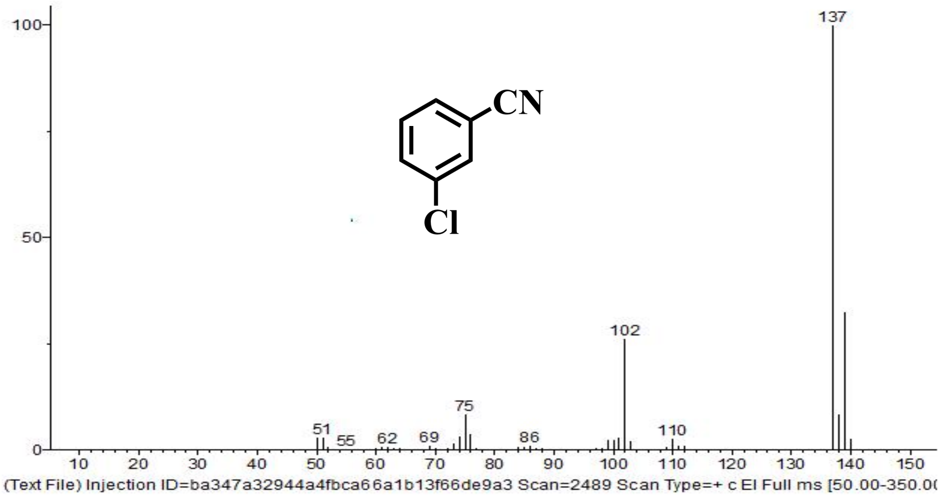

8.72
8.72
8.71
7.47
7.46
7.45
7.45
CN
N
2.00
2.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

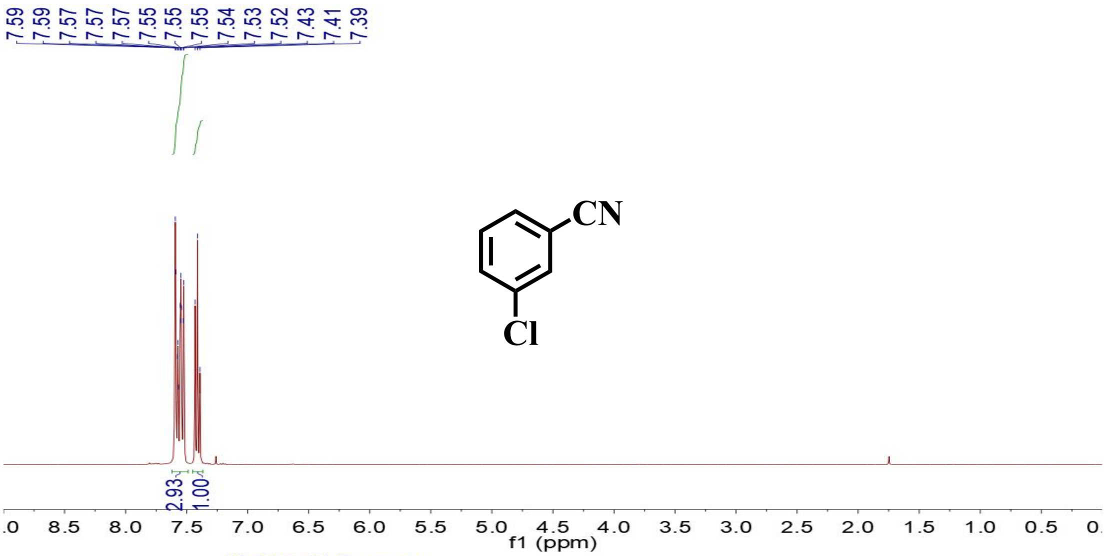

150.60
125.12
120.18
116.26
CN
N
170
150
130
110
90
80
70
60
50
40
30
20
10
(
f1 (ppm)

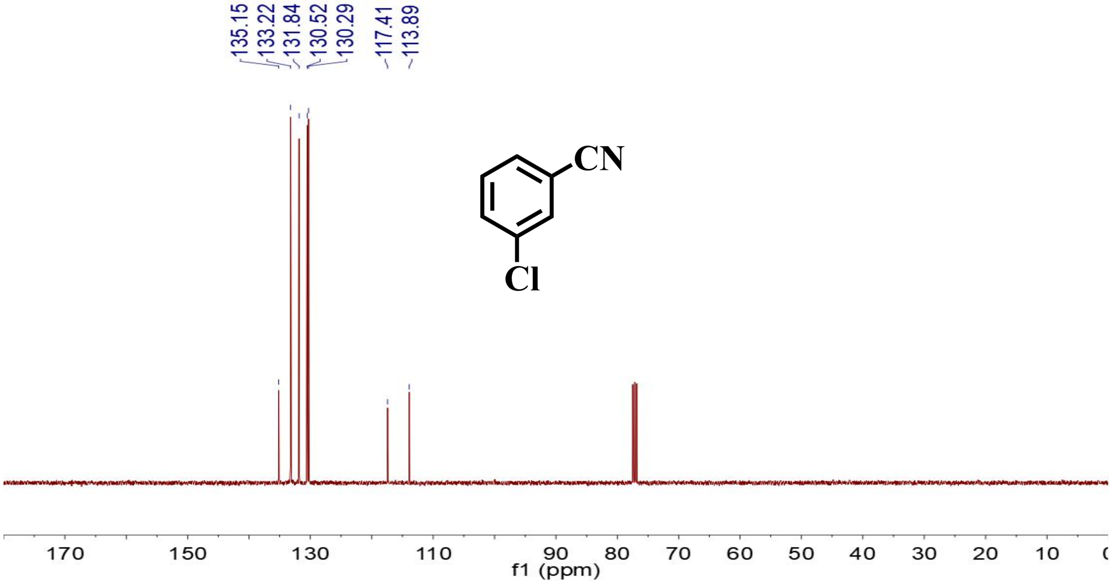

93
64
51
54
75
91
100
50
0
10
20
30
40
50
60
70
80
90
100
O
CN
(Text File) Injection ID=5931f02359c84b52831f7819c7d914bc Scan=129 Scan Type=+ c EI Full ms [50.00-350.00]

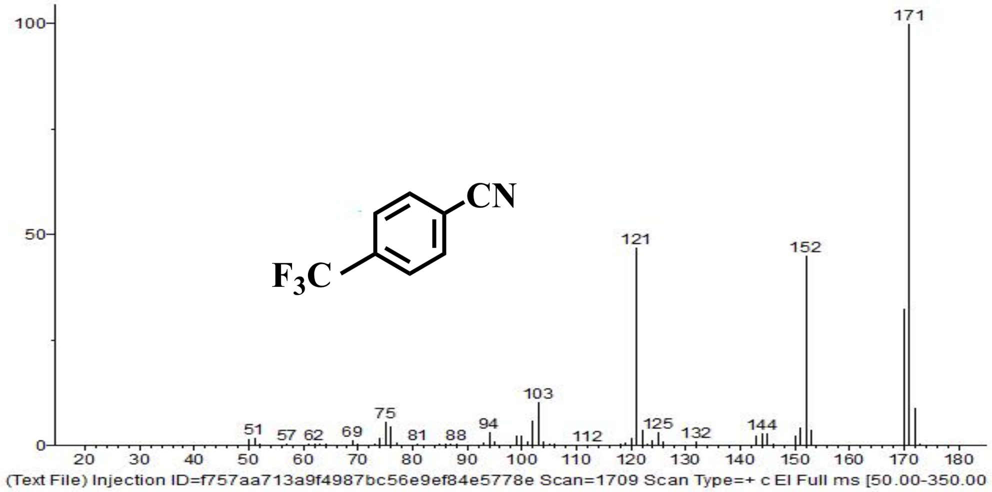

7.78
7.78
7.77
7.28
7.27
6.64
6.63
6.63
6.62
1.00
1.00
1.00
O
CN
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

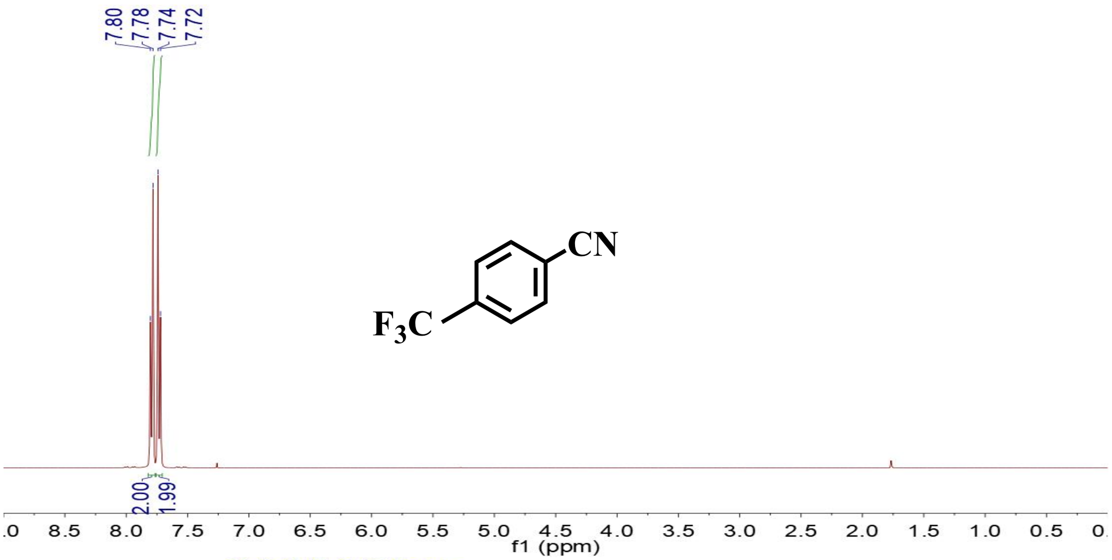

149.43
127.11
123.48
112.65
112.32
O
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

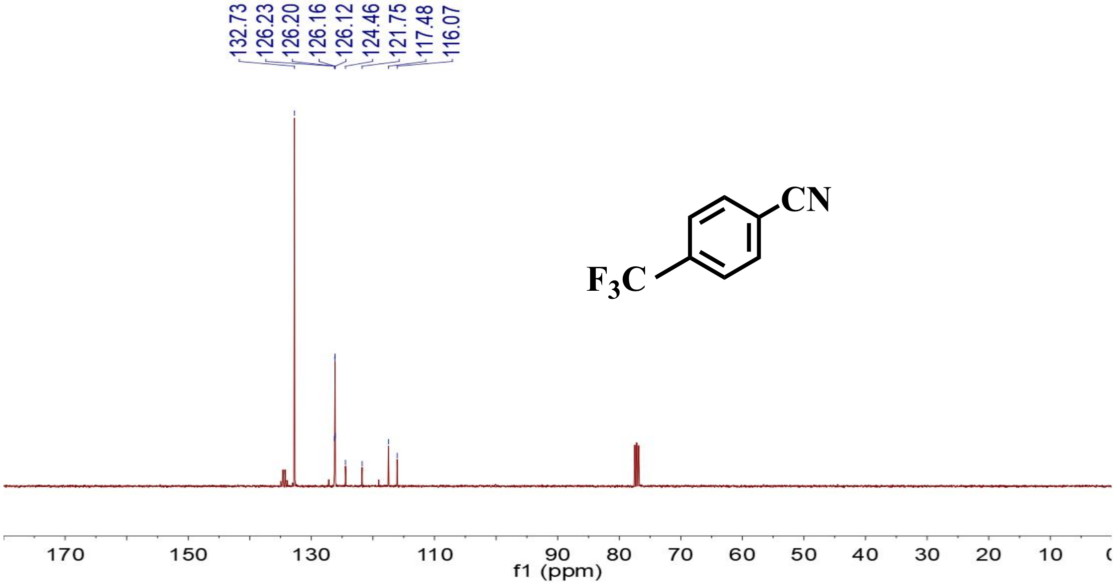

100
50
0
137
102
75
51
55
62
69
86
110
CN
Cl
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150
(Text File) Injection ID=ba347a32944a4fbca66a1b13f66de9a3 Scan=2489 Scan Type=+ c EI Full ms [50.00-350.0

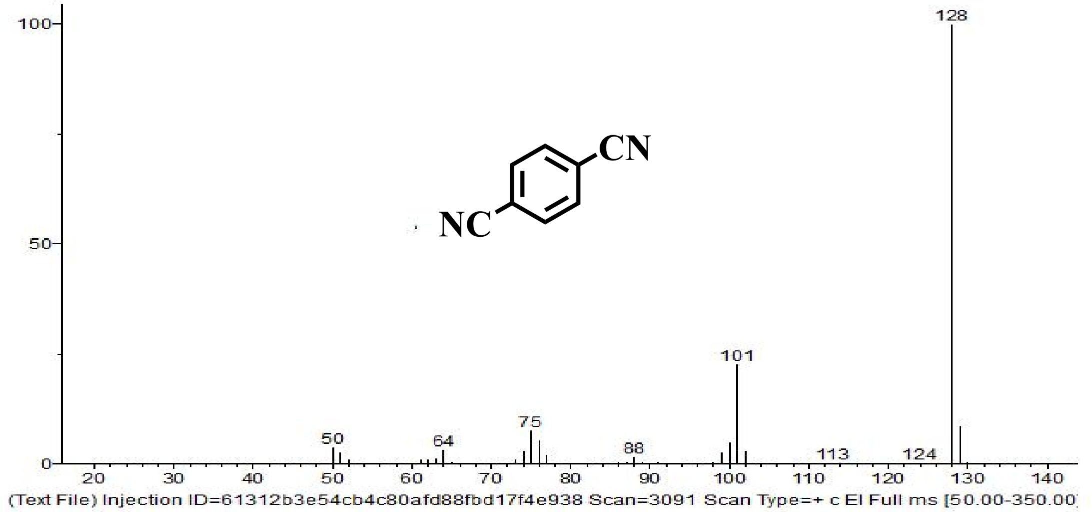

7.59
7.59
7.57
7.57
7.57
7.55
7.55
7.55
7.54
7.53
7.52
7.43
7.41
7.39
CN
Cl
2.93
1.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

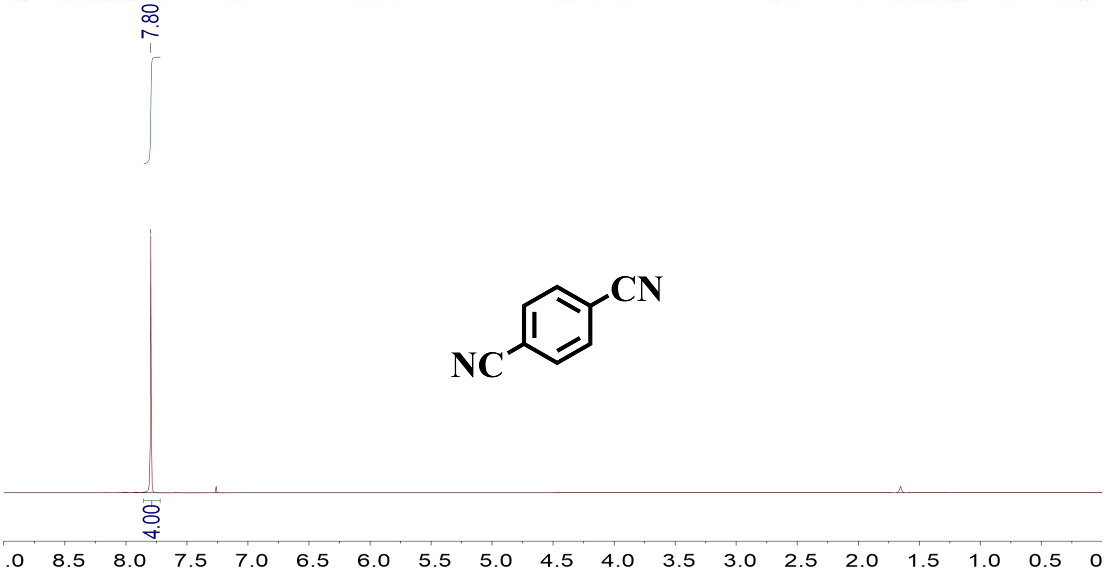

135.15
133.22
131.84
130.52
130.29
117.41
113.89
CN
Cl
170 150 130 110 90 80 70 60 50 40 30 20 10 (
f1 (ppm)

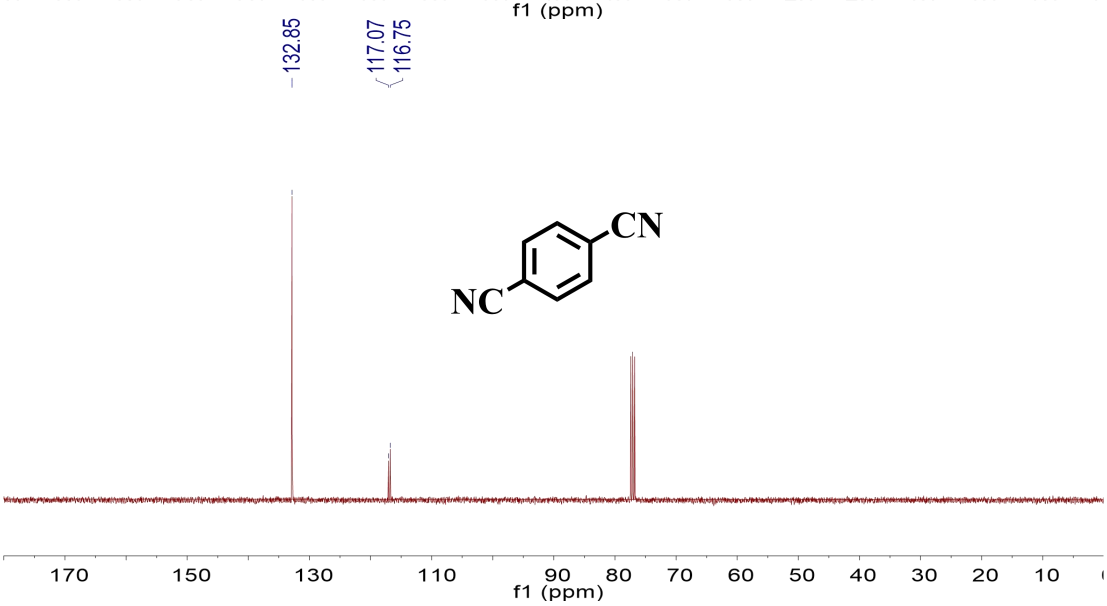

100
50
0
171
121
152
103
75
51
57
62
69
81
88
94
112
125
132
144
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180
CN
F3C
(Text File) Injection ID=f757aa713a9f4987bc56e9ef84e5778e Scan=1709 Scan Type=+ c EI Full ms [50.00-350.00

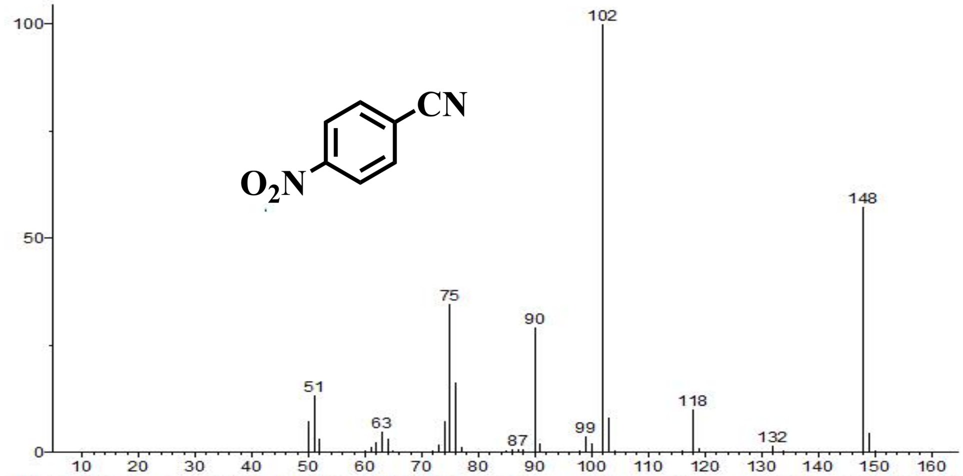

7.80
7.78
7.74
7.72
CN
F3C
2.00
1.99
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)


132.73
126.23
126.20
126.16
126.12
124.46
121.75
117.48
116.07
CN
F3C
170 150 130 110 90 80 70 60 50 40 30 20 10 (
f1 (ppm)

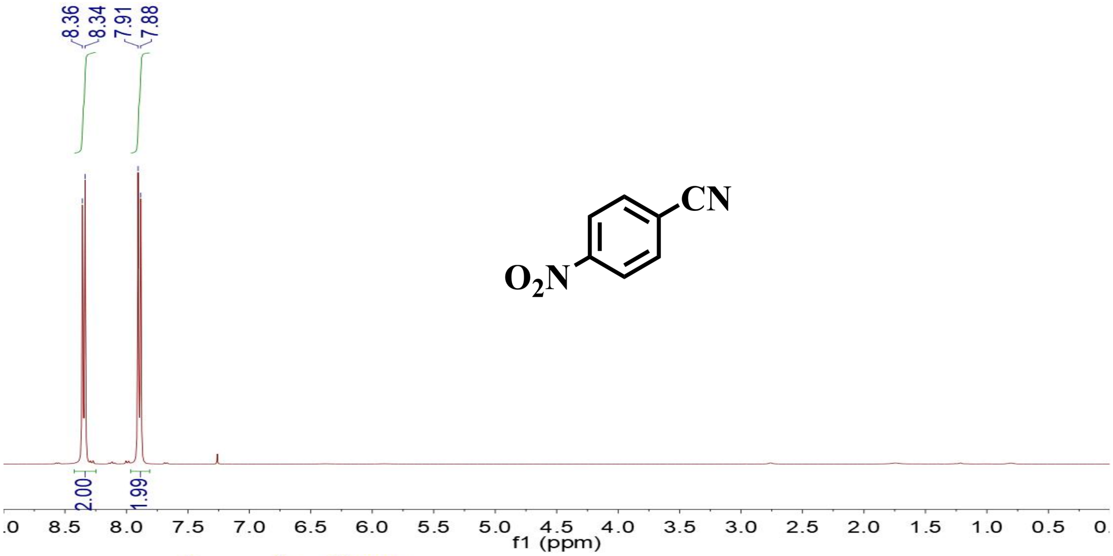

100
50
0
128
101
75
50
64
88
113
124
20
30
40
50
60
70
80
90
100
110
120
130
140
CN
NC
(Text File) Injection ID=61312b3e54cb4c80afd88fbd17f4e938 Scan=3091 Scan Type=+ c EI Full ms [50.00-350.00

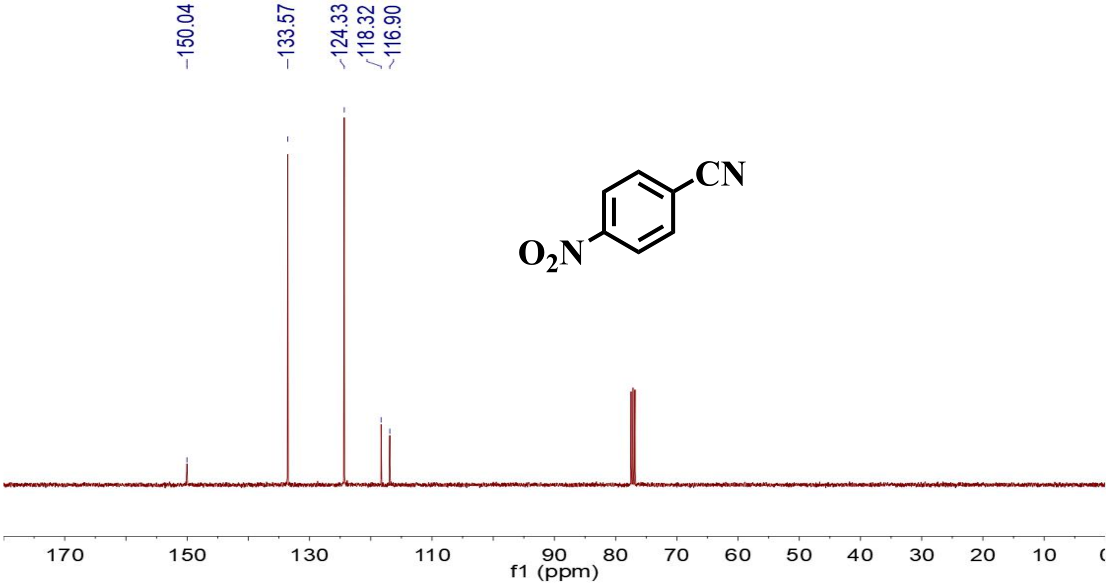

7.80
CN
NC
4.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

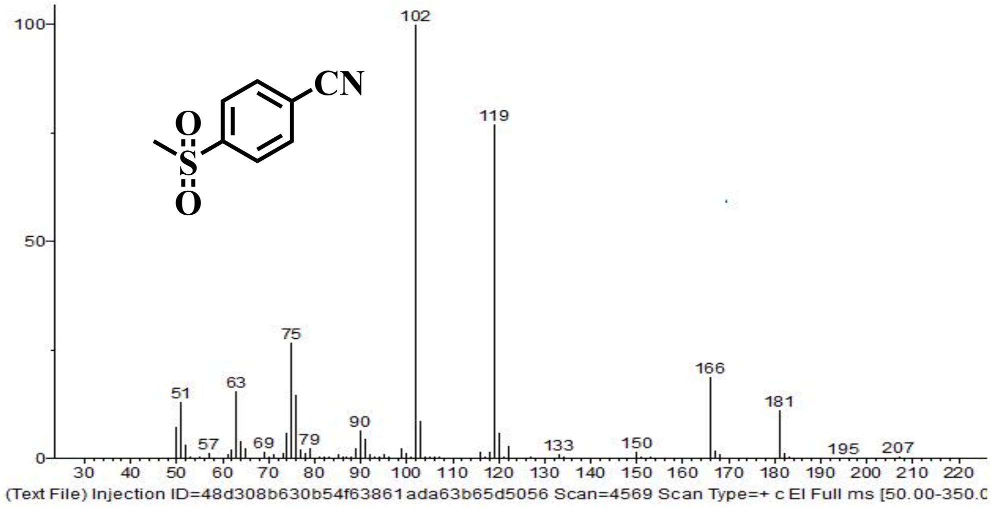

132.85
117.07
116.75
CN
NC
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

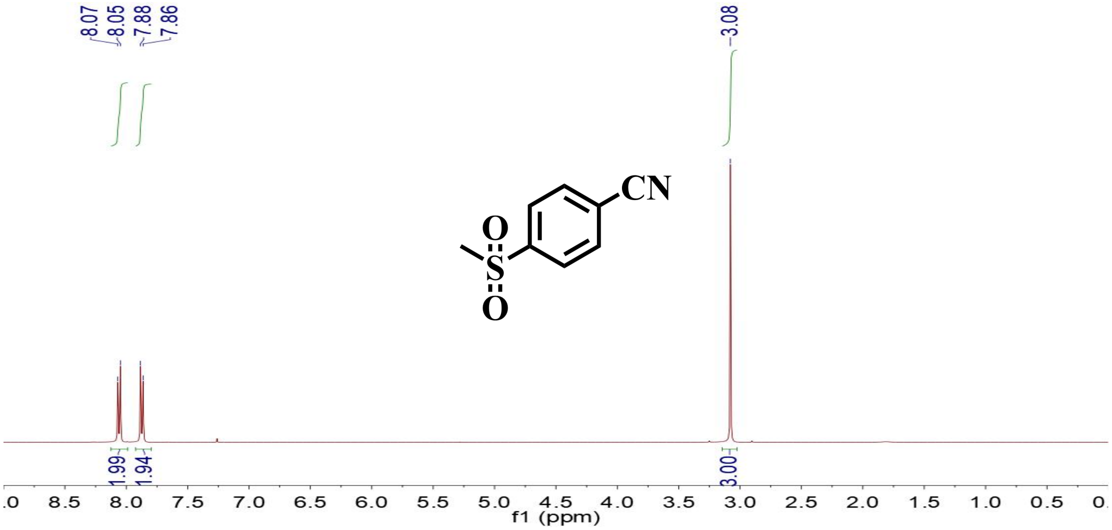


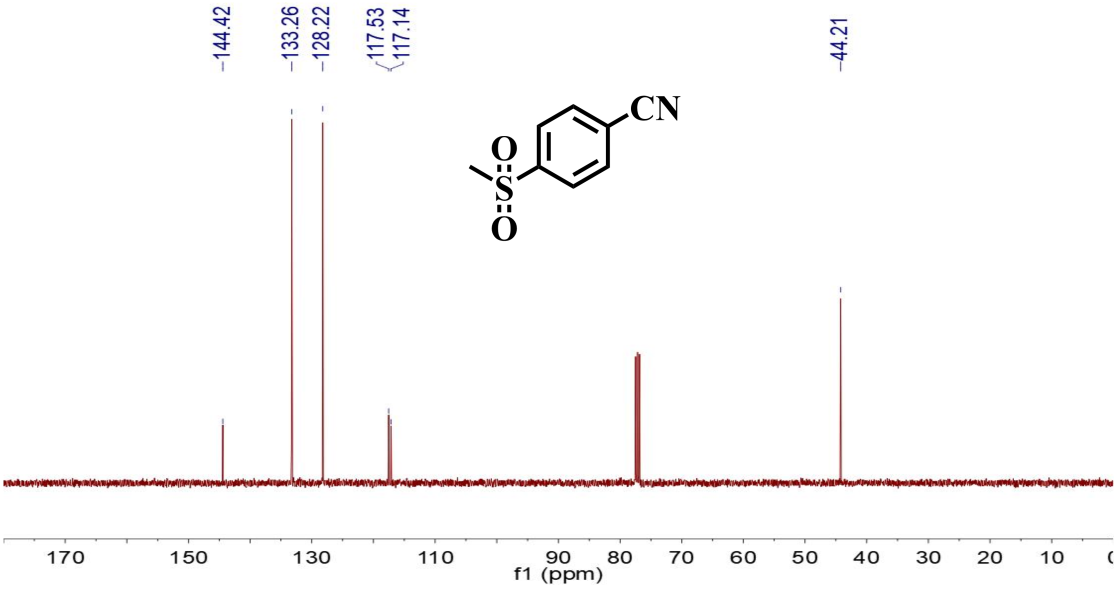
(Text File) Injection ID=39df1d5cf8674c8ba0913d206eec7593 Scan=3447 Scan Type=+ c EI Full ms [50.00-350.00

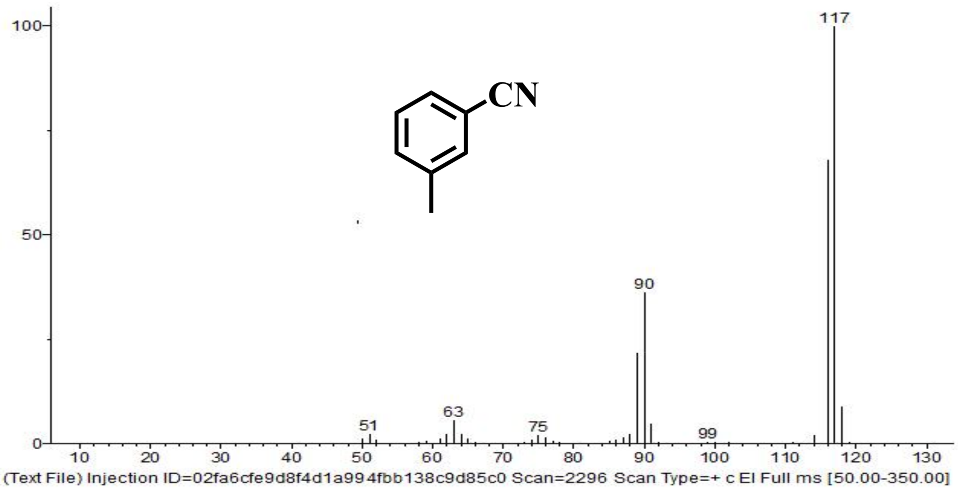


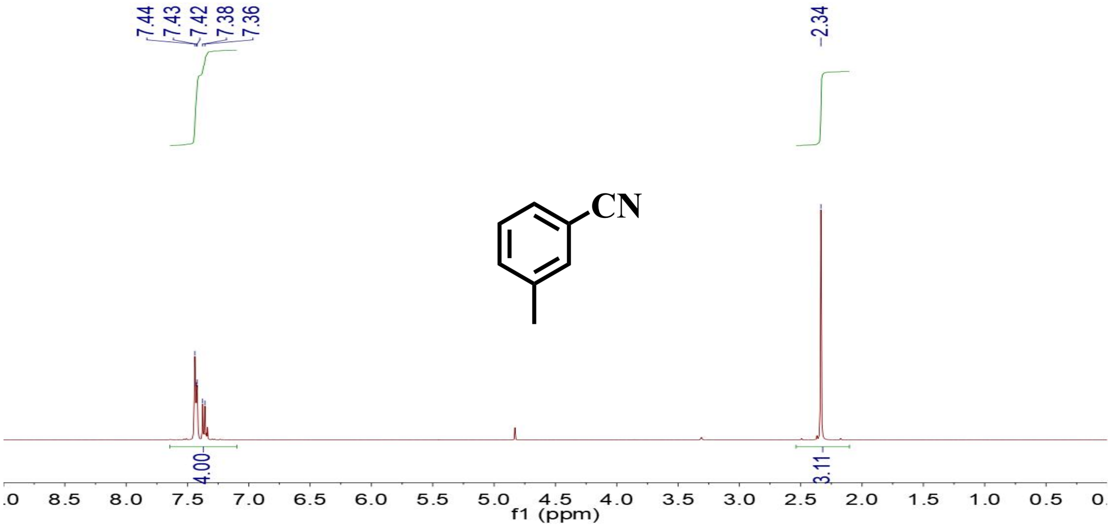


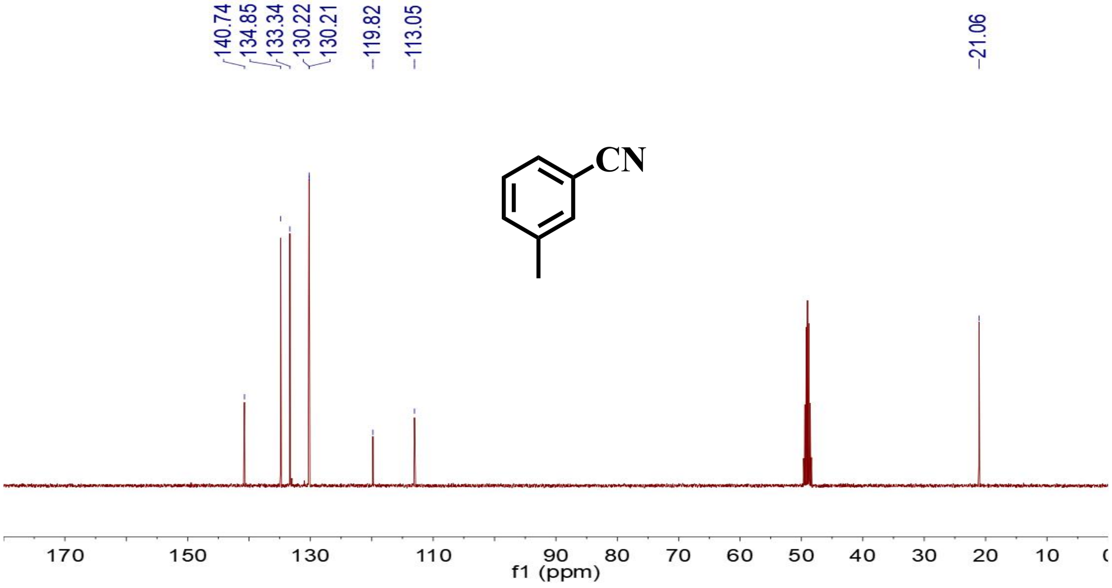

100
50
0
102
119
75
63
51
57
69
79
90
133
150
166
181
195
207
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220
CN
O
S
O
(Text File) Injection ID=48d308b630b54f63861ada63b65d5056 Scan=4569 Scan Type=+ c EI Full ms [50.00-350.C

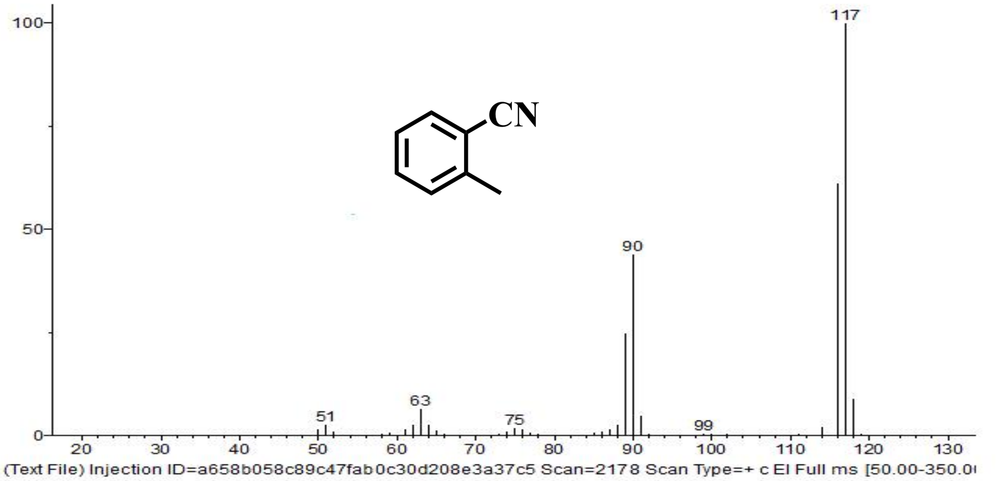

8.07
8.05
7.88
7.86
3.08
CN
O
S
O
1.99
1.94
3.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)


144.42
133.26
128.22
117.53
117.14
44.21
CN
O
S
O
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

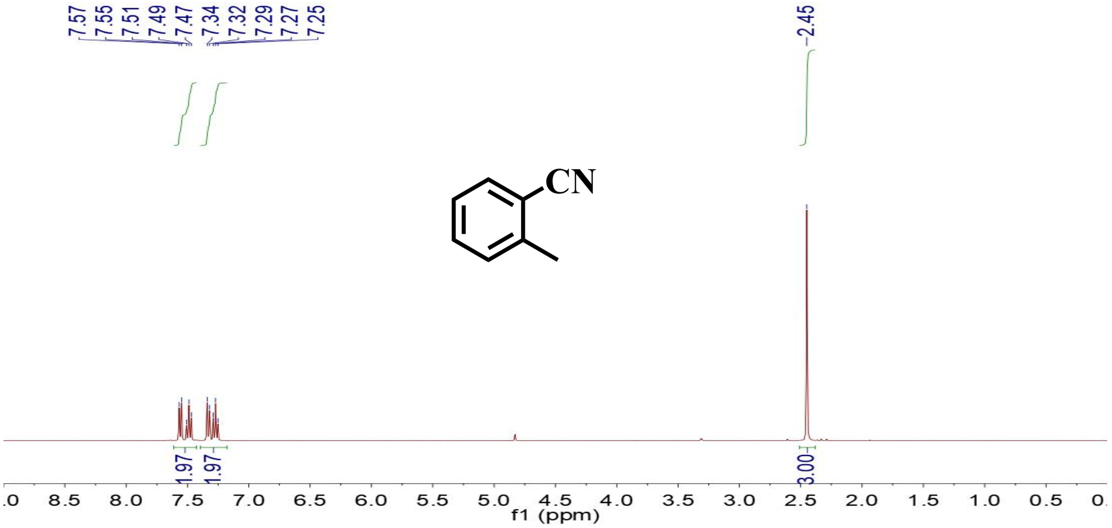

100
50
0
117
CN
90
51
63
75
99
10
20
30
40
50
60
70
80
90
100
110
120
130
(Text File) Injection ID=02fa6cfe9d8f4d1a994fbb138c9d85c0 Scan=2296 Scan Type=+ c EI Full ms [50.00-350.00]


7.44
7.43
7.42
7.38
7.36
-2.34
CN
4.00
3.11
.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.
f1 (ppm)

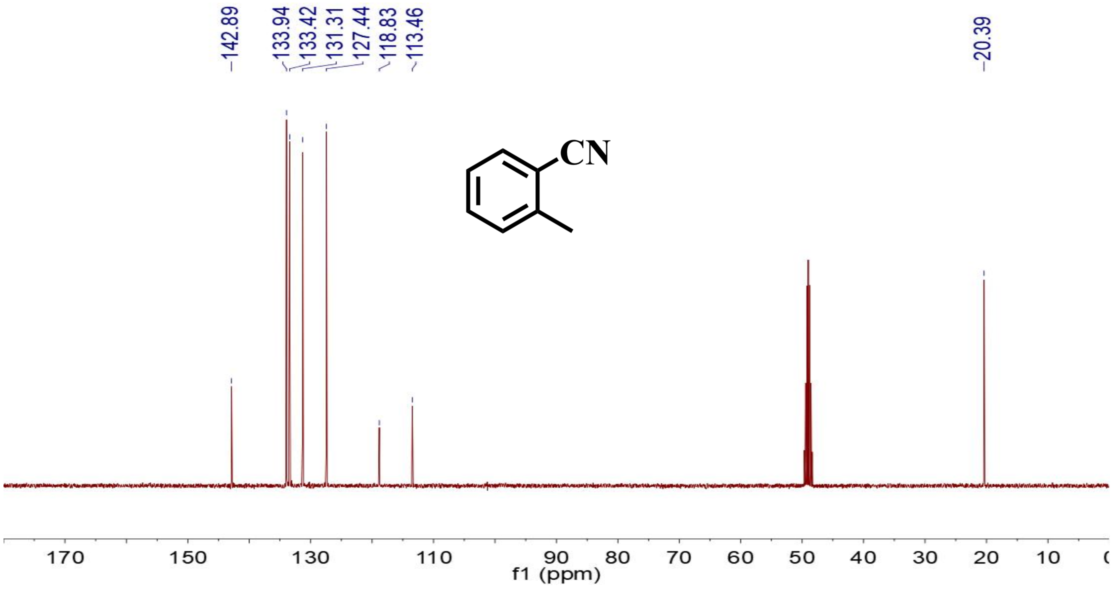

140.74
134.85
133.34
130.22
130.21
-119.82
-113.05
-21.06
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)



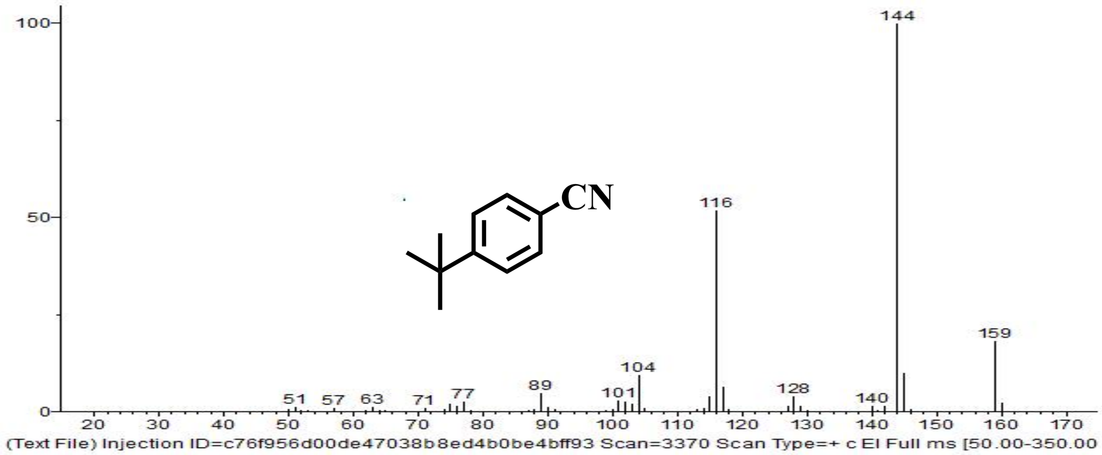
CN
117
90
63
51
75
99
100
50
0
20
30
40
50
60
70
80
90
100
110
120
130
(Text File) Injection ID=a658b058c89c47fab0c30d208e3a37c5 Scan=2178 Scan Type=+ c EI Full ms [50.00-350.0

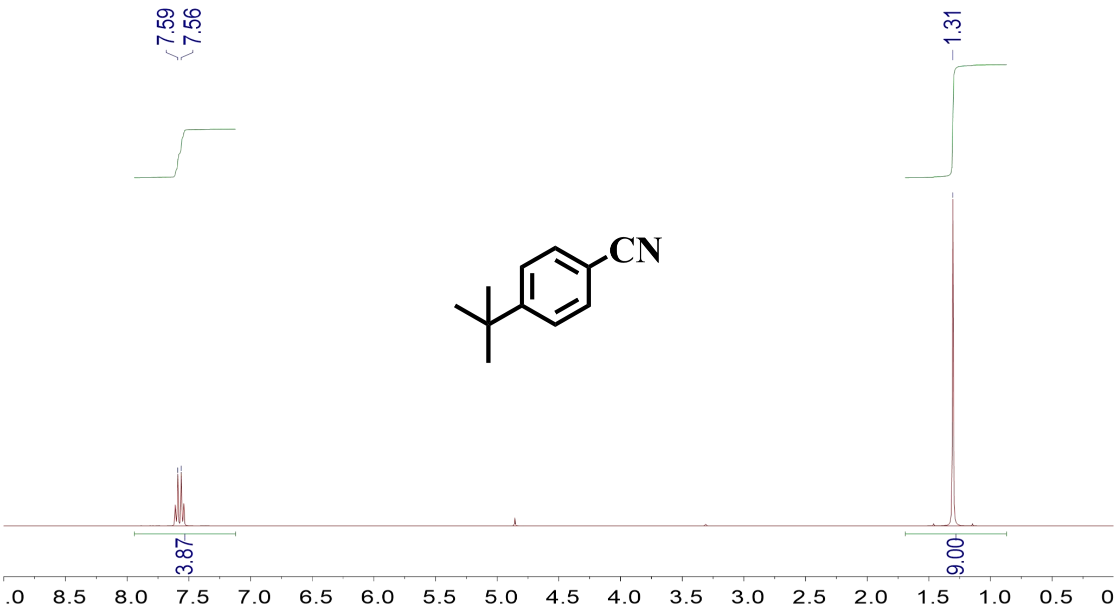


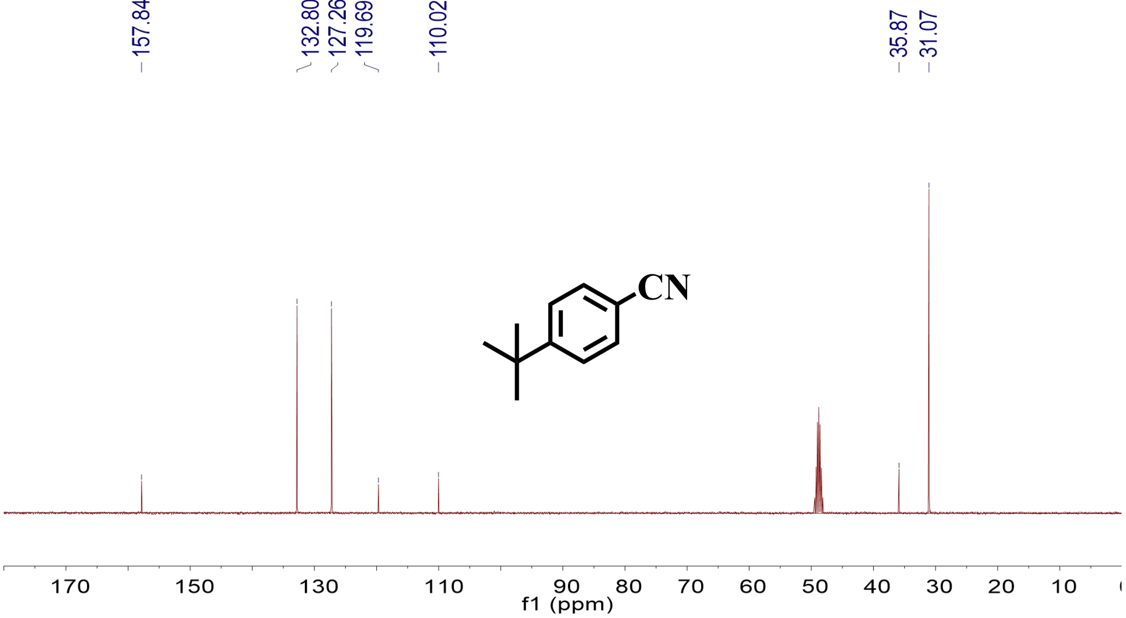
7.57
7.55
7.51
7.49
7.47
7.34
7.32
7.29
7.27
7.25
2.45
CN
1.97
1.97
3.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

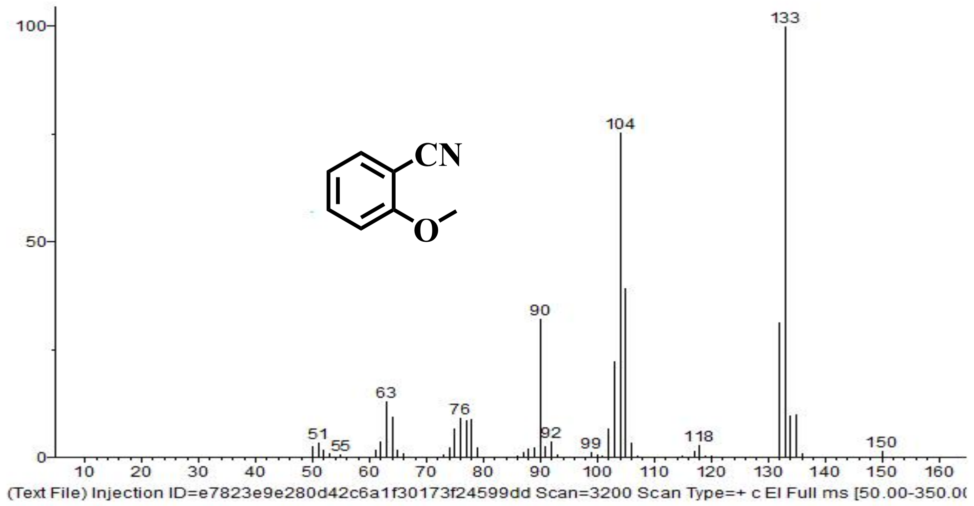


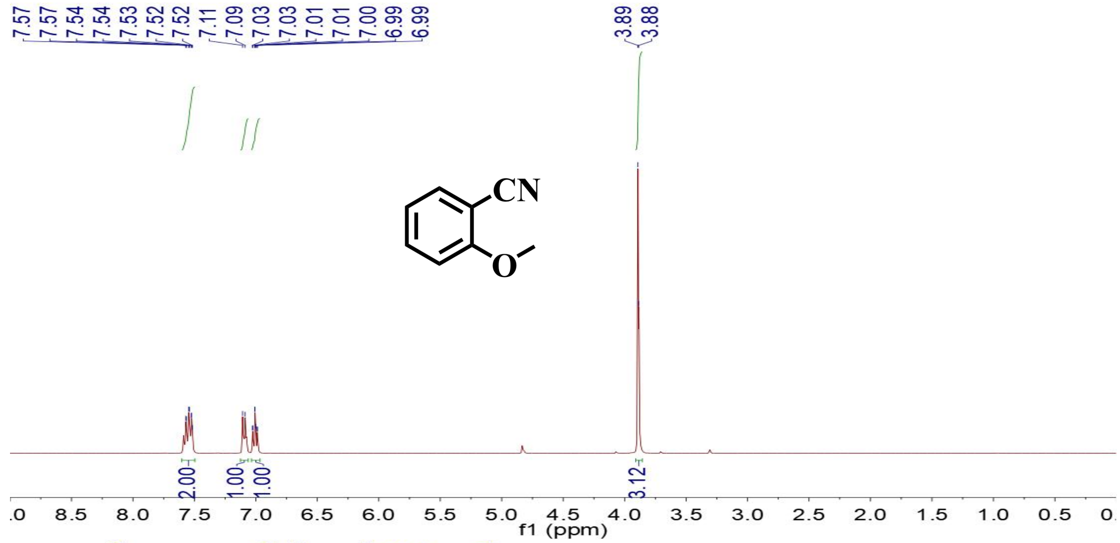
142.89
133.94
133.42
131.31
127.44
118.83
113.46
20.39
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

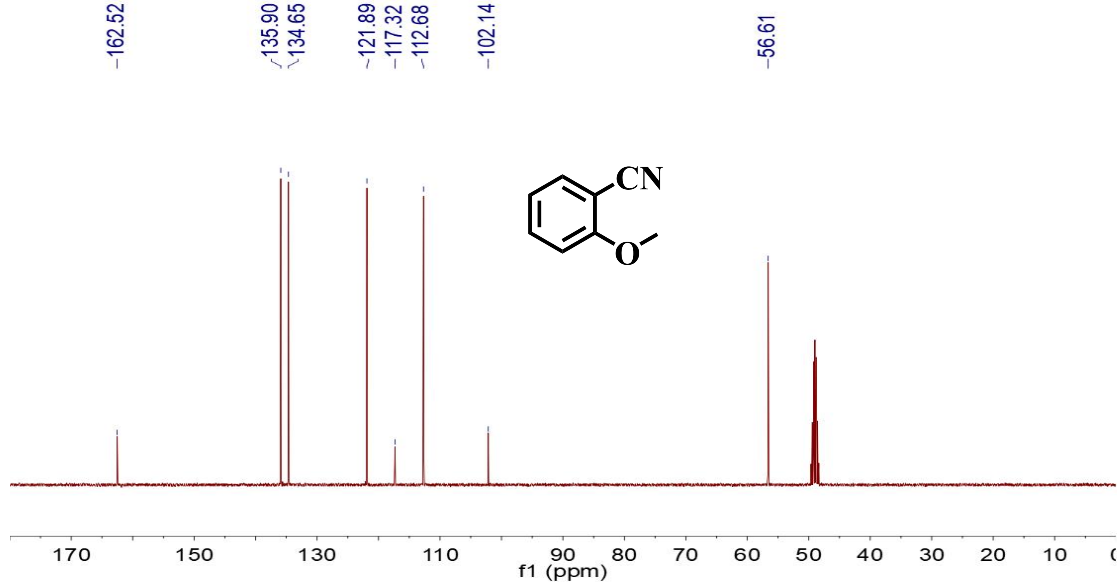

CN
100
50
0
144
116
159
104
128
140
101
89
77
71
63
57
51
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170
(Text File) Injection ID=c76f956d00de47038b8ed4b0be4bff93 Scan=3370 Scan Type=+ c EI Full ms [50.00-350.00

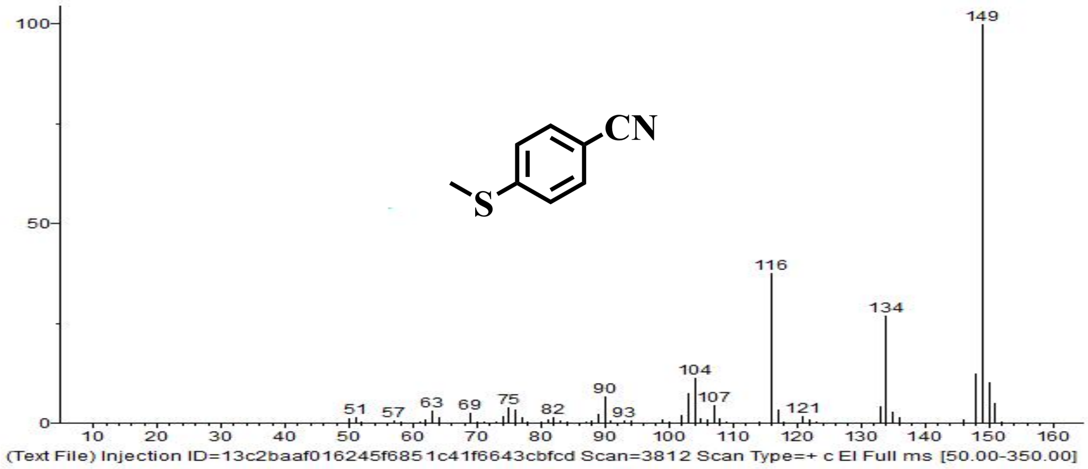

7.59
7.56
1.31
CN
3.87
9.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

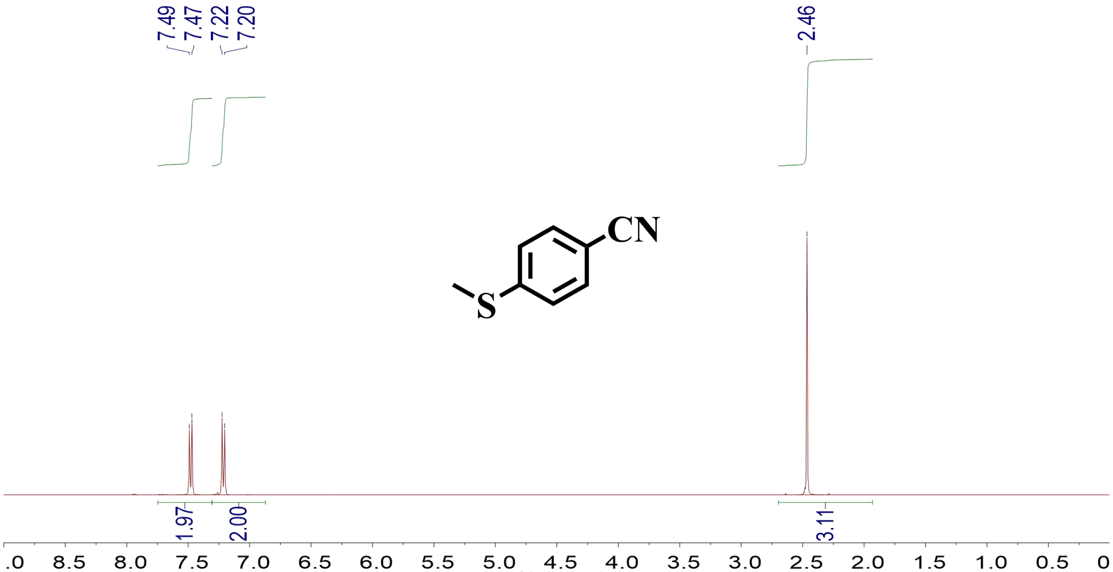

157.84
132.80
127.26
119.69
110.02
35.87
31.07
CN
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

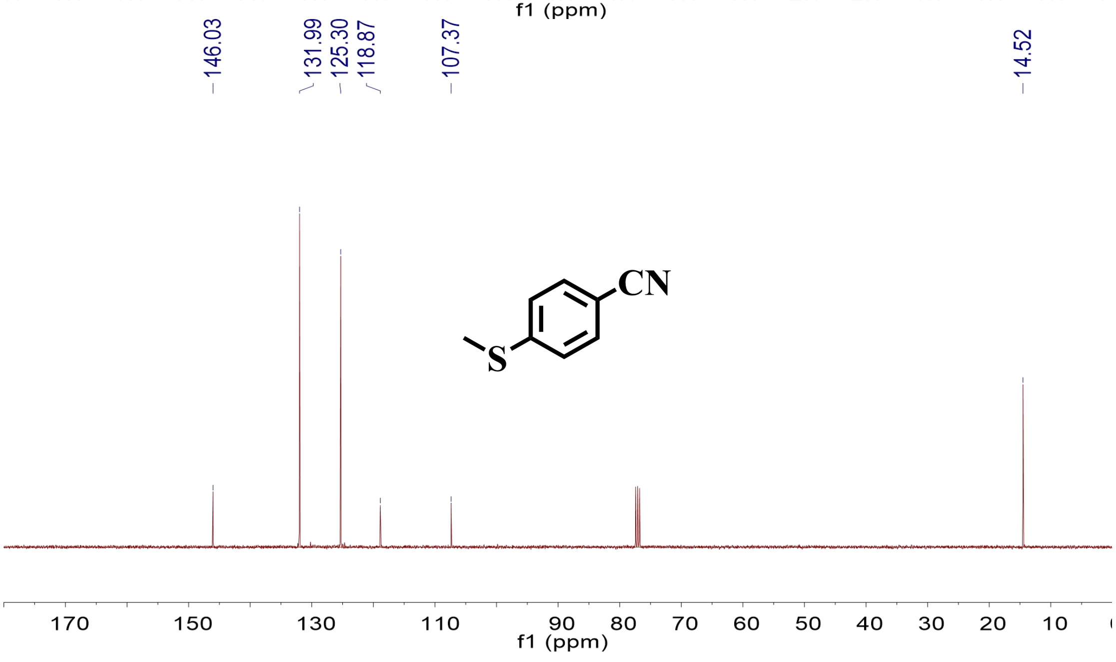

100
50
0
133
104
90
63
76
92
51
55
99
118
150
CN
O
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
(Text File) Injection ID=e7823e9e280d42c6a1f30173f24599dd Scan=3200 Scan Type=+ c EI Full ms [50.00-350.0

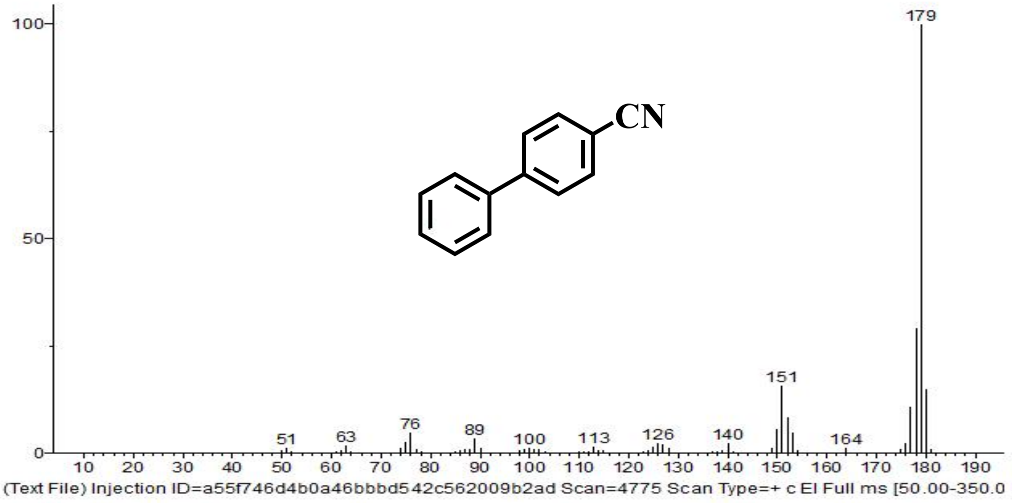

7.57
7.57
7.54
7.54
7.53
7.52
7.52
7.11
7.09
7.03
7.03
7.01
7.01
7.00
6.99
6.99
3.89
3.88
CN
O
2.00
1.00
1.00
3.12
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

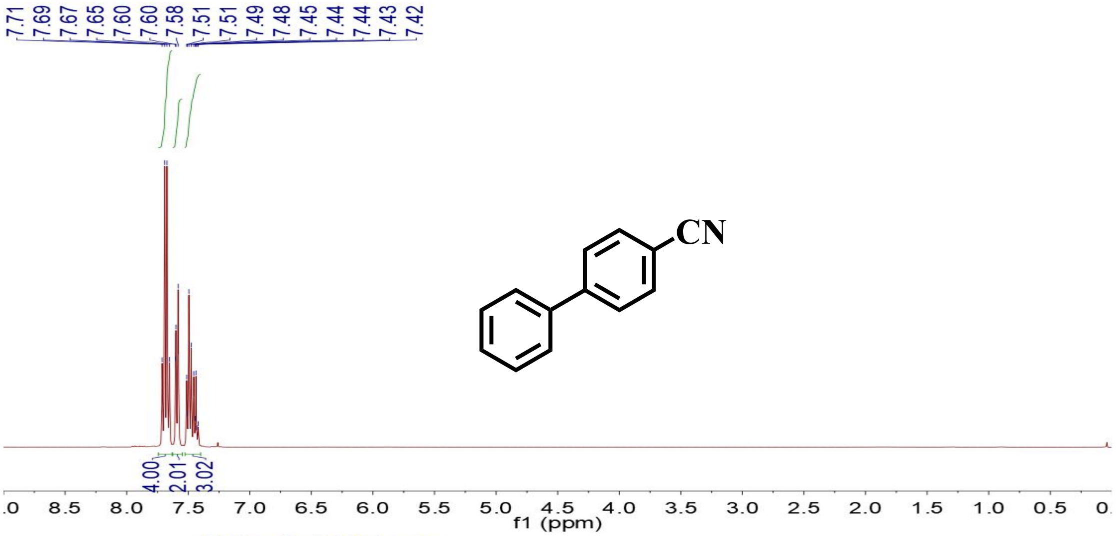

162.52
135.90
134.65
121.89
117.32
112.68
102.14
56.61
CN
O
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

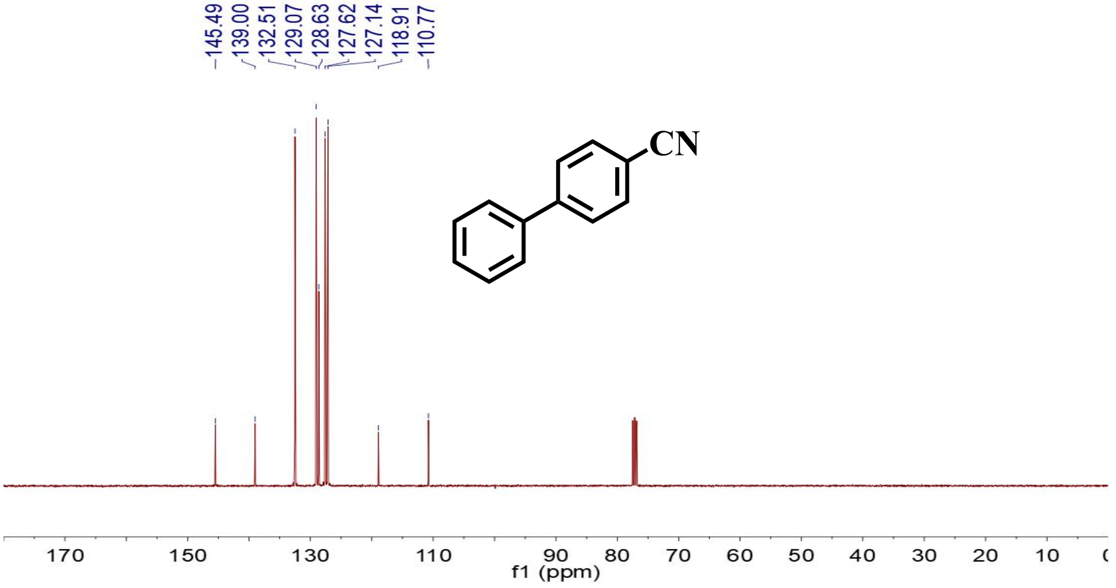

100
50
0
149
116
134
104
107
90
93
75
82
63
69
51
57
121
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
CN
S
(Text File) Injection ID=13c2baaf016245f6851c41f6643cbfcd Scan=3812 Scan Type=+ c EI Full ms [50.00-350.00]

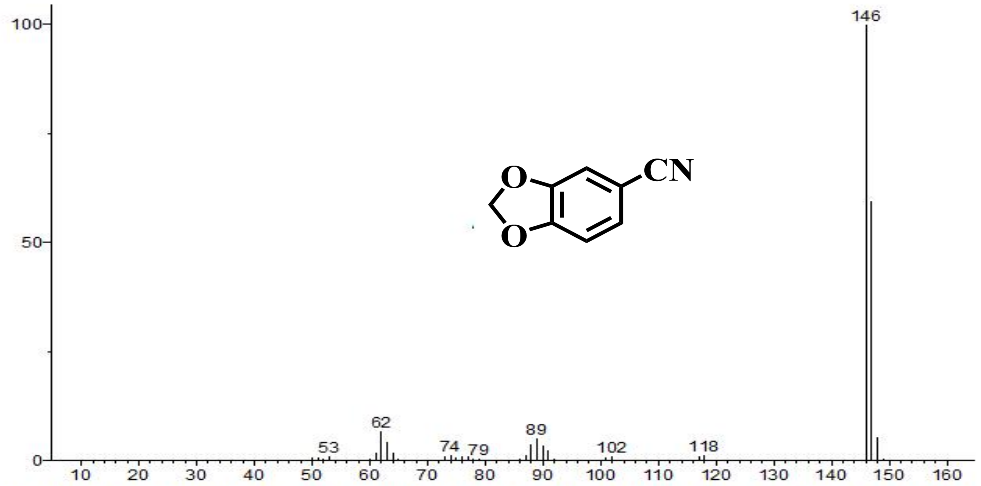

7.49
7.47
7.22
7.20
2.46
CN
S
1.97
2.00
3.11
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)


146.03
131.99
125.30
118.87
107.37
14.52
CN
S
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

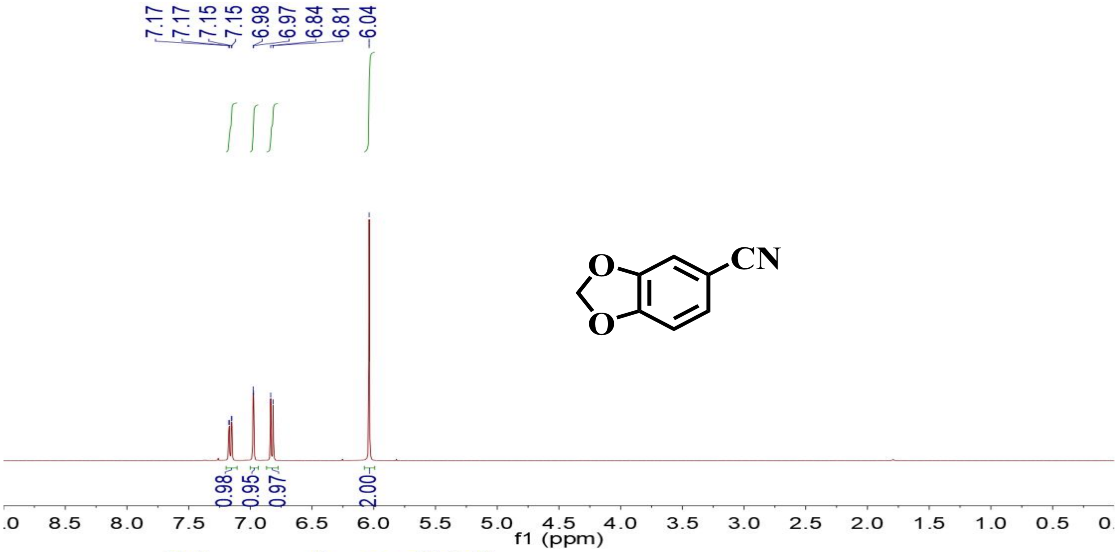

100
50
0
179
151
164
140
126
113
100
89
76
63
51
CN
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190
(Text File) Injection ID=a55f746d4b0a46bbbd542c562009b2ad Scan=4775 Scan Type=+ c EI Full ms [50.00-350.0

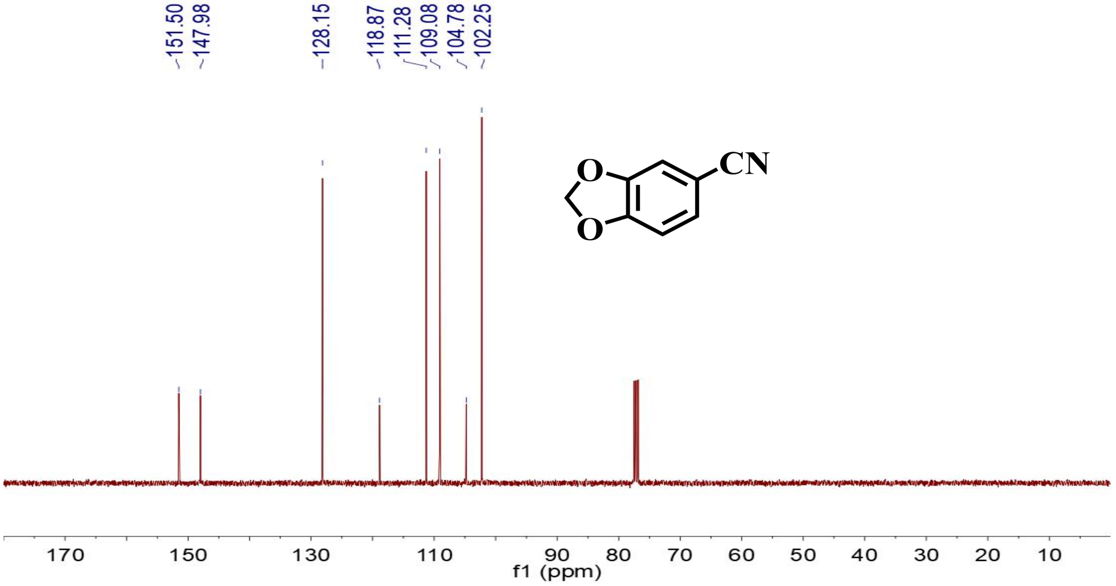

7.71
7.69
7.67
7.65
7.60
7.60
7.58
7.51
7.51
7.49
7.48
7.45
7.44
7.44
7.43
7.42
CN
4.00
2.01
3.02
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

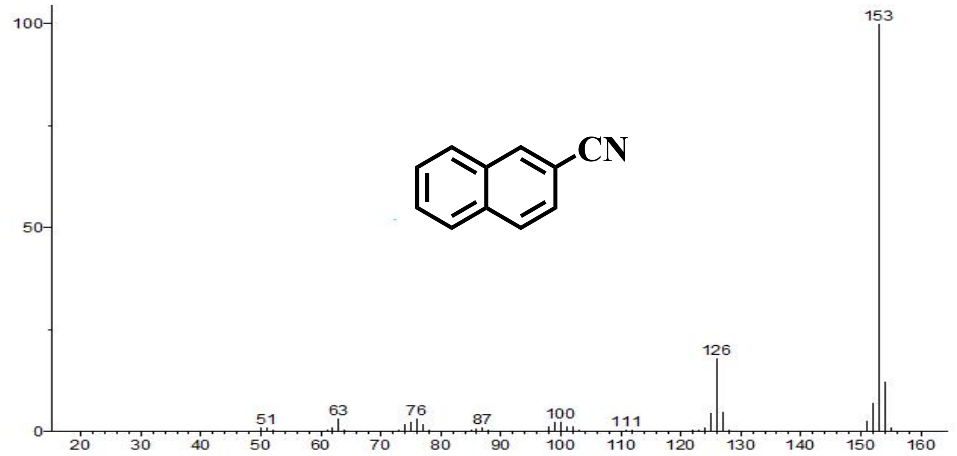

145.49
139.00
132.51
129.07
128.63
127.62
127.14
118.91
110.77
CN
170 150 130 110 90 80 70 60 50 40 30 20 10 (
f1 (ppm)



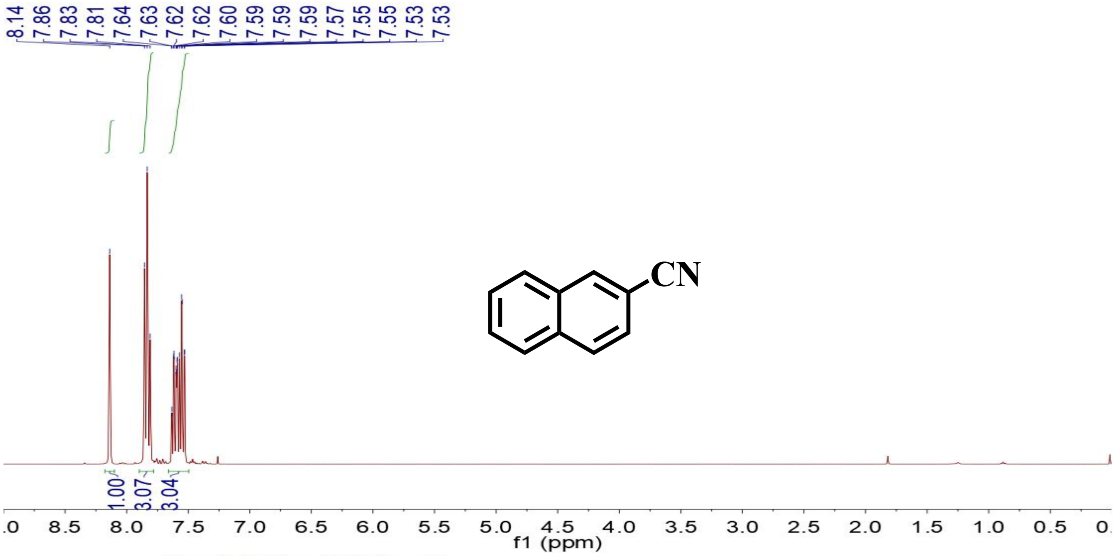
(Text File) Injection ID=e481a6eed7114847afe8da963e8e0c0b Scan=3447 Scan Type=+ c EI Full ms [50.00-350.0

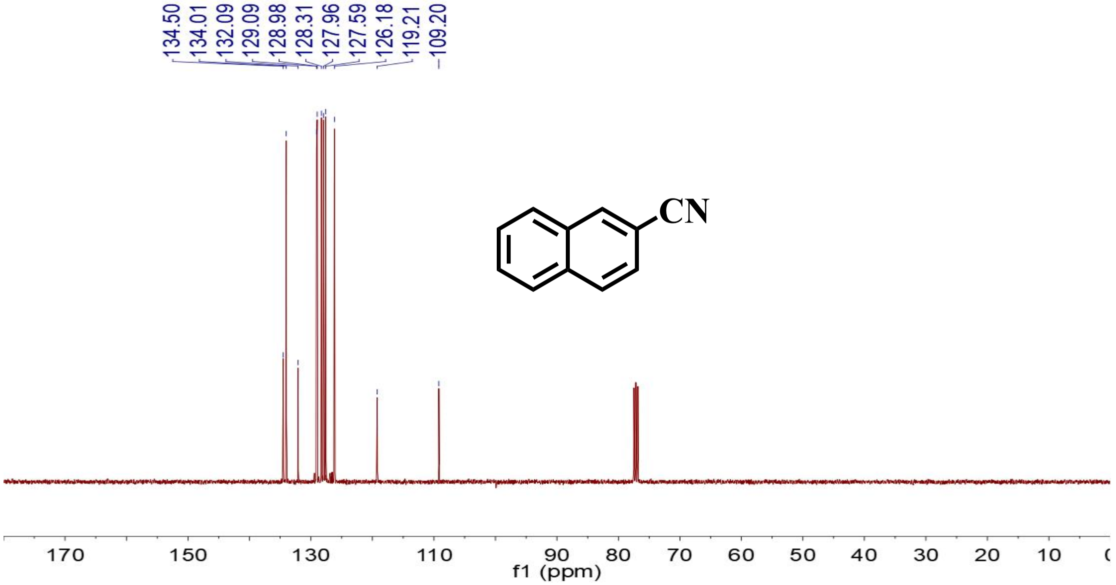


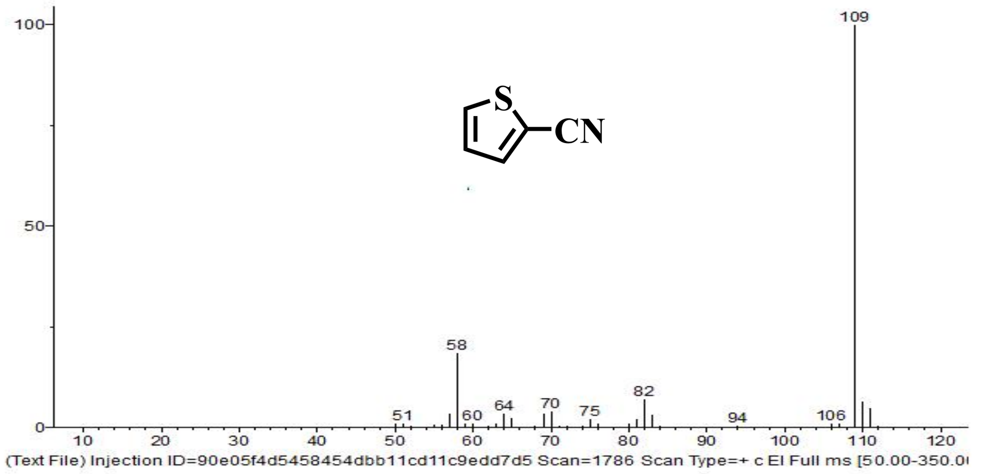


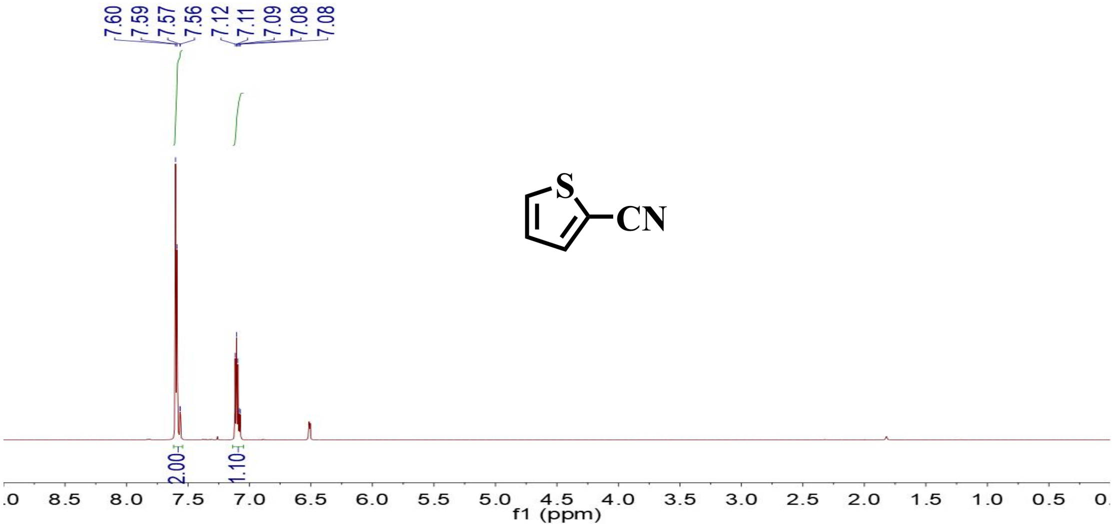


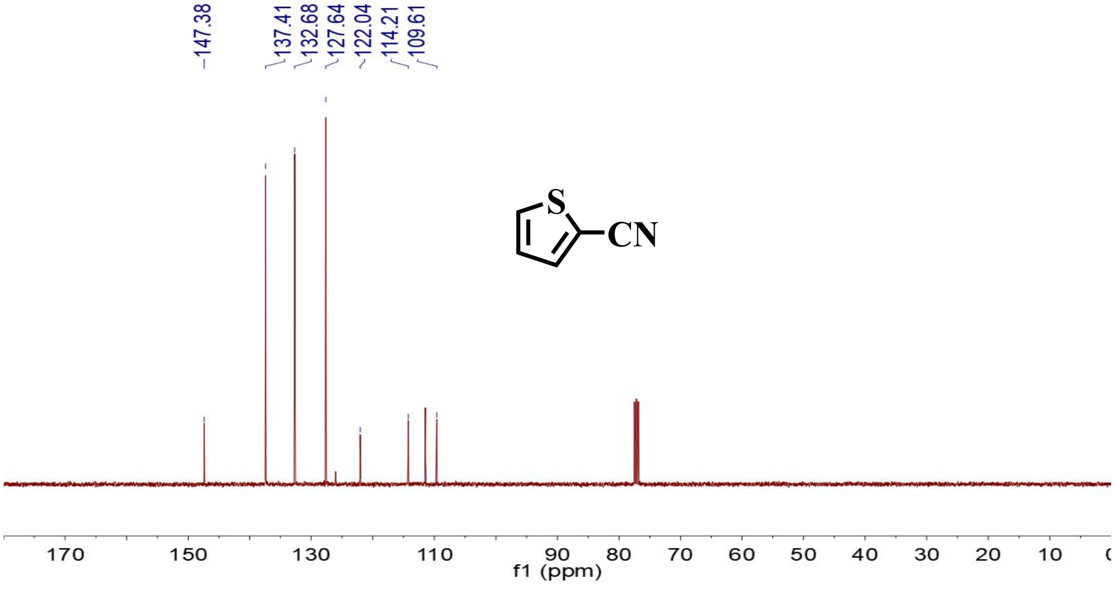
(Text File) Injection ID=337b0bdf976e476a87b58e88d4efcfaa Scan=4094 Scan Type=+ c EI Full ms [50.00-350.00

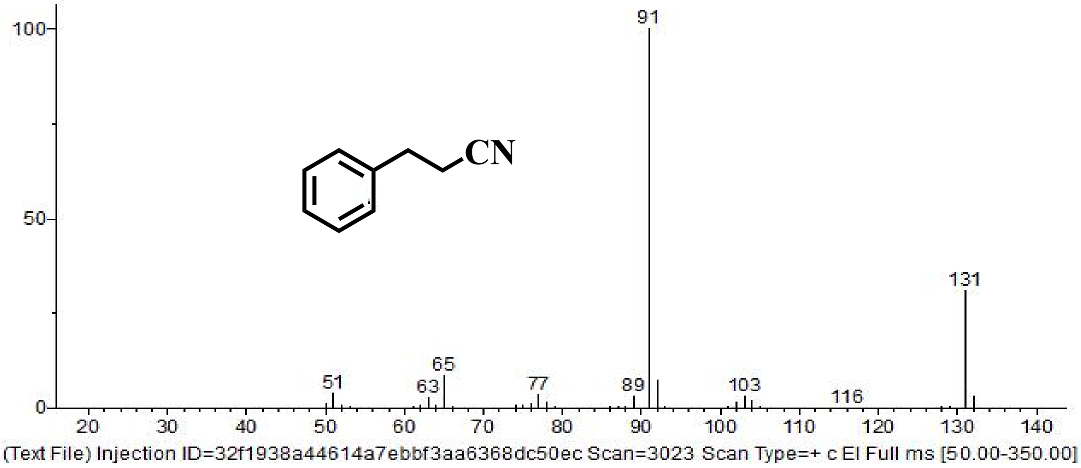


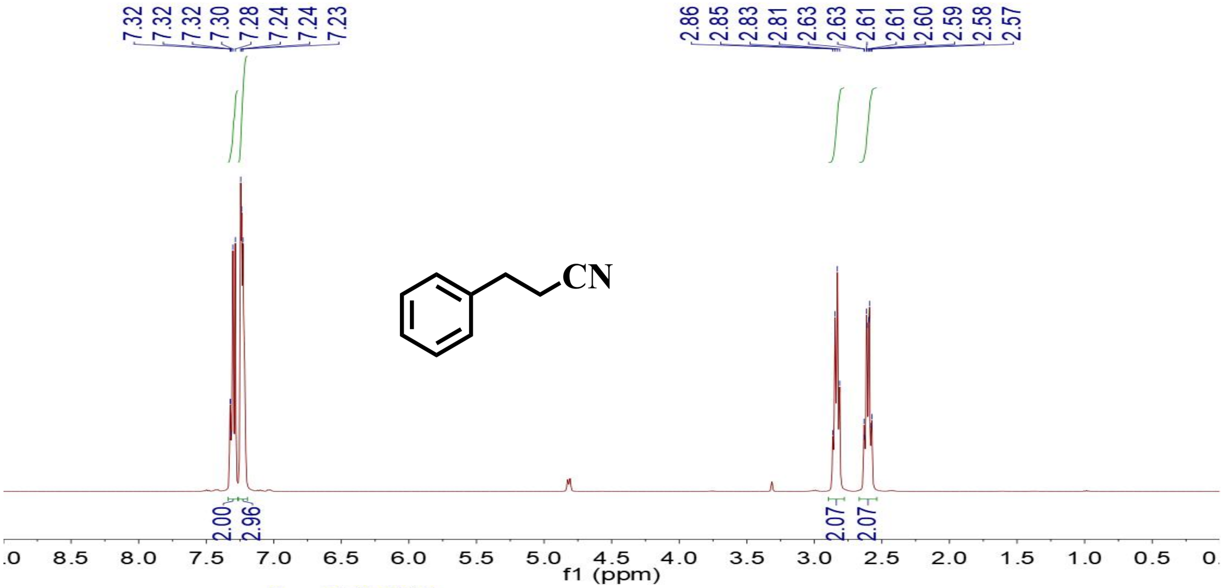


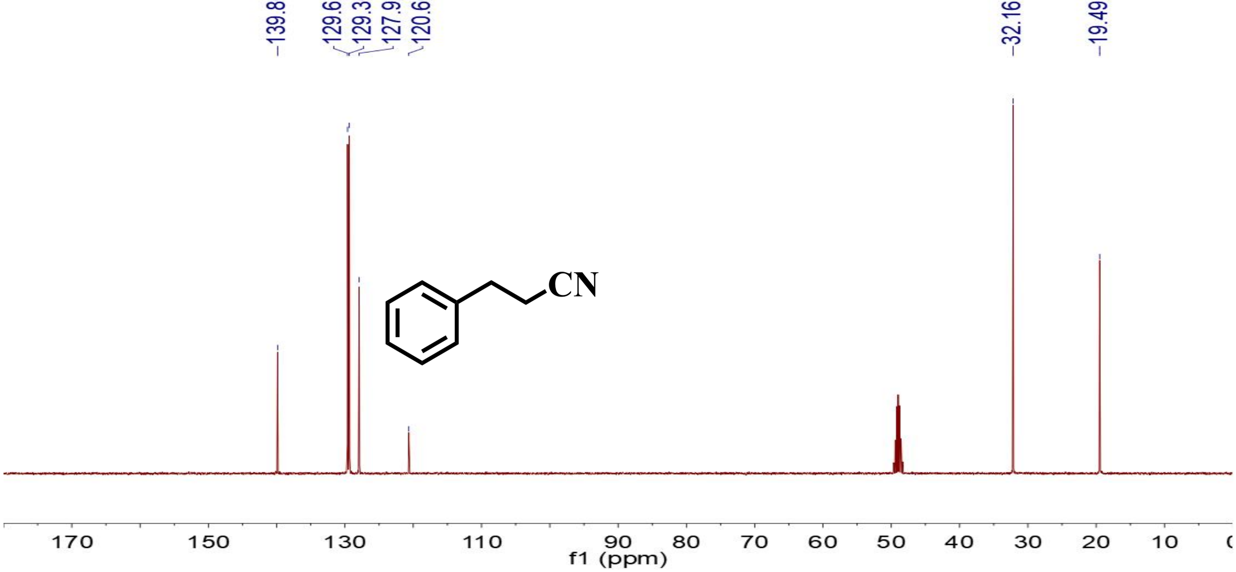

100
50
0
109
58
51
60
64
70
75
82
94
106
S
CN
10
20
30
40
50
60
70
80
90
100
110
120
(Text File) Injection ID=90e05f4d5458454dbb11cd11c9edd7d5 Scan=1786 Scan Type=+ c EI Full ms [50.00-350.0

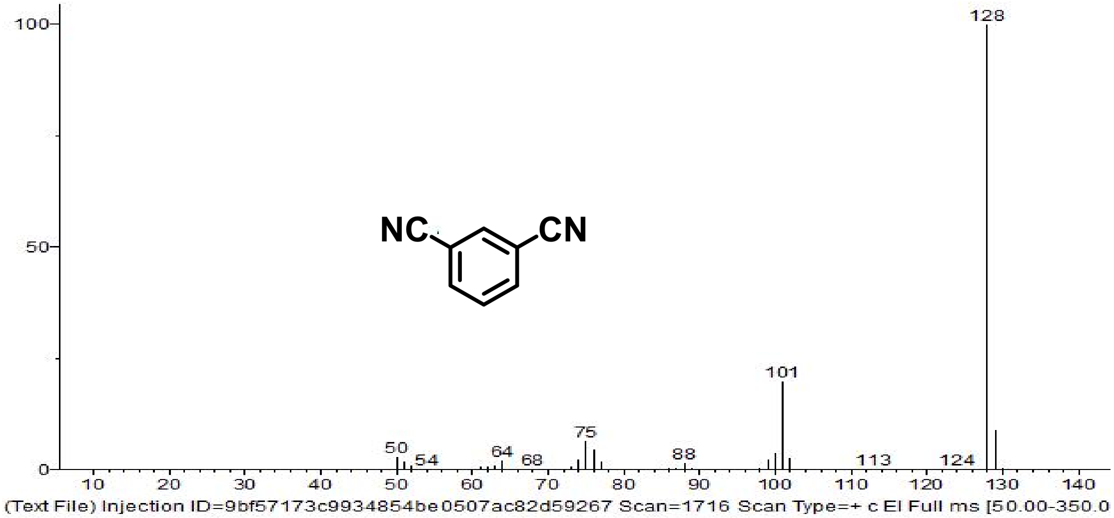

7.60
7.59
7.57
7.56
7.12
7.11
7.09
7.08
7.08
S
CN
2.00
1.10
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

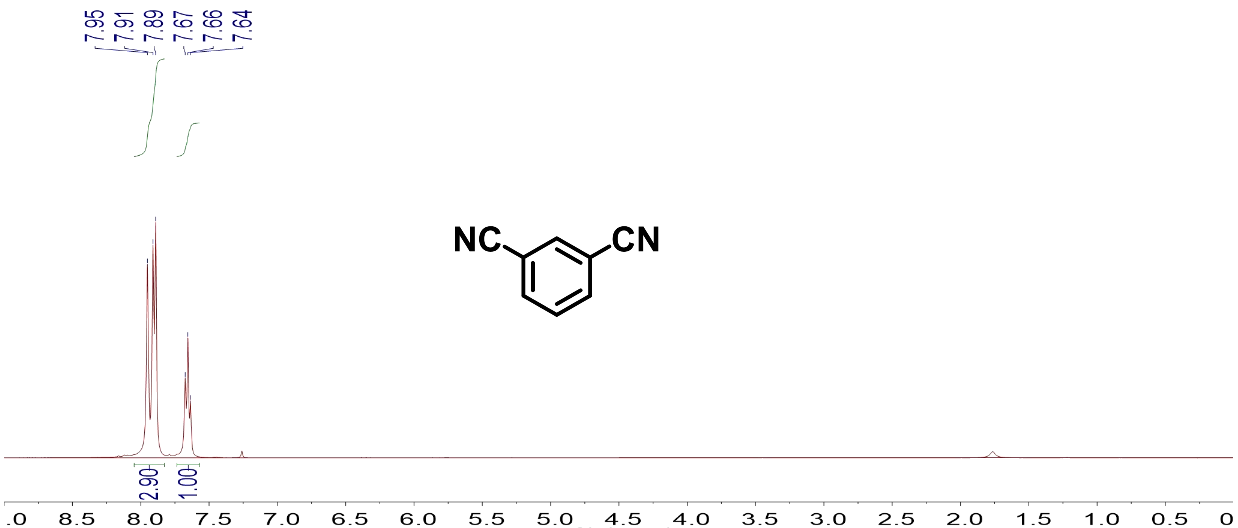

147.38
137.41
132.68
127.64
122.04
114.21
109.61
S
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
(
f1 (ppm)

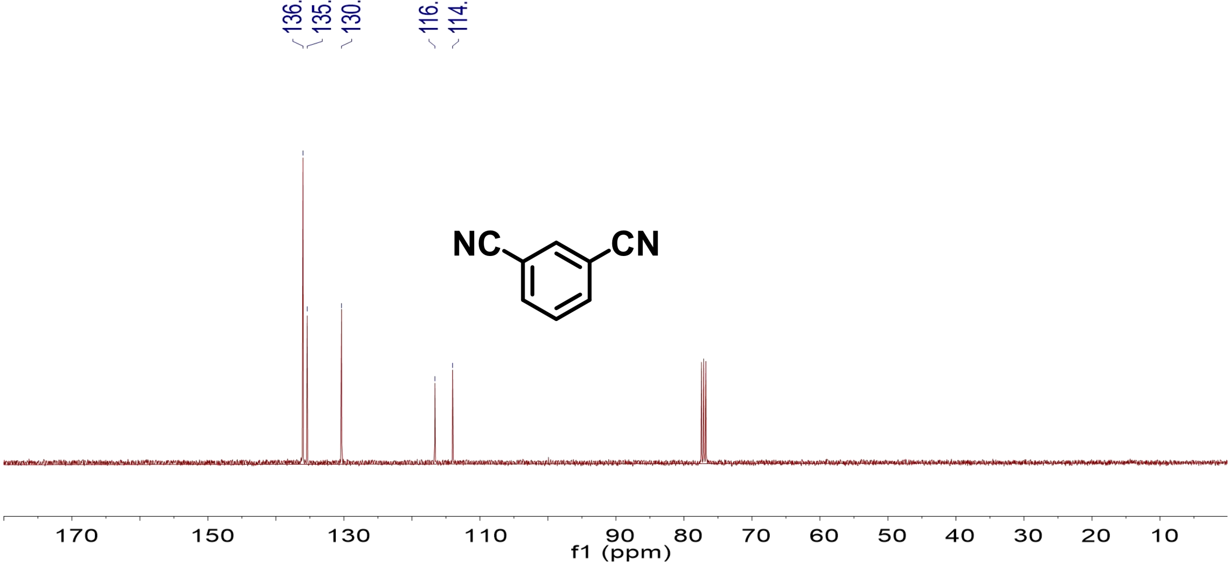

100
50
0
91
131
51
63
65
77
89
103
116
CN
20
30
40
50
60
70
80
90
100
110
120
130
140
(Text File) Injection ID=32f1938a44614a7ebbf3aa6368dc50ec Scan=3023 Scan Type=+ c EI Full ms [50.00-350.00]

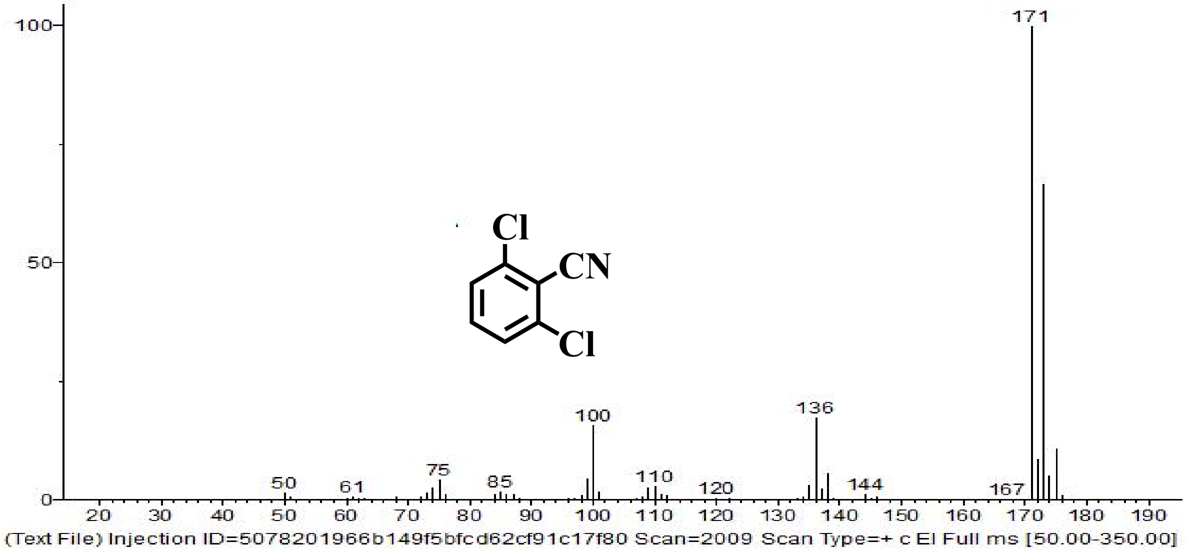

7.32
7.32
7.32
7.30
7.28
7.24
7.24
7.23
2.86
2.85
2.83
2.81
2.63
2.63
2.61
2.61
2.60
2.59
2.58
2.57
CN
2.00
2.96
2.07
2.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


139.86
129.62
129.36
127.92
120.66
32.16
19.49
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

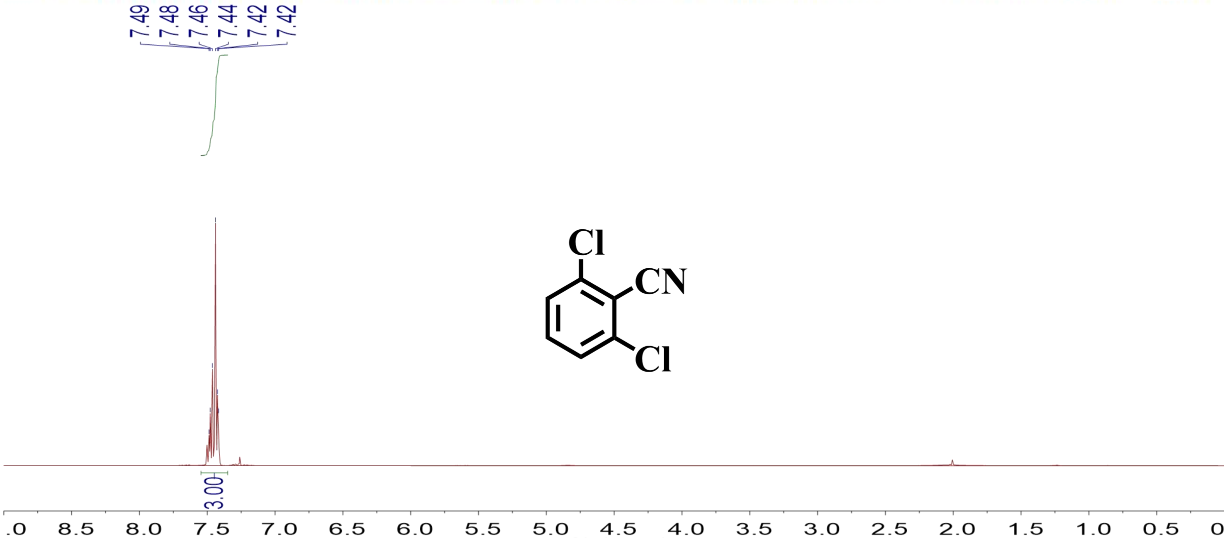

100
50
0
128
101
75
64
50
54
68
88
113
124
NC
CN
10
20
30
40
50
60
70
80
90
100
110
120
130
140
(Text File) Injection ID=9bf57173c9934854be0507ac82d59267 Scan=1716 Scan Type=+ c EI Full ms [50.00-350.0


7.95
7.91
7.89
7.67
7.66
7.64
NC
CN
2.90
1.00
.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
f1 (ppm)

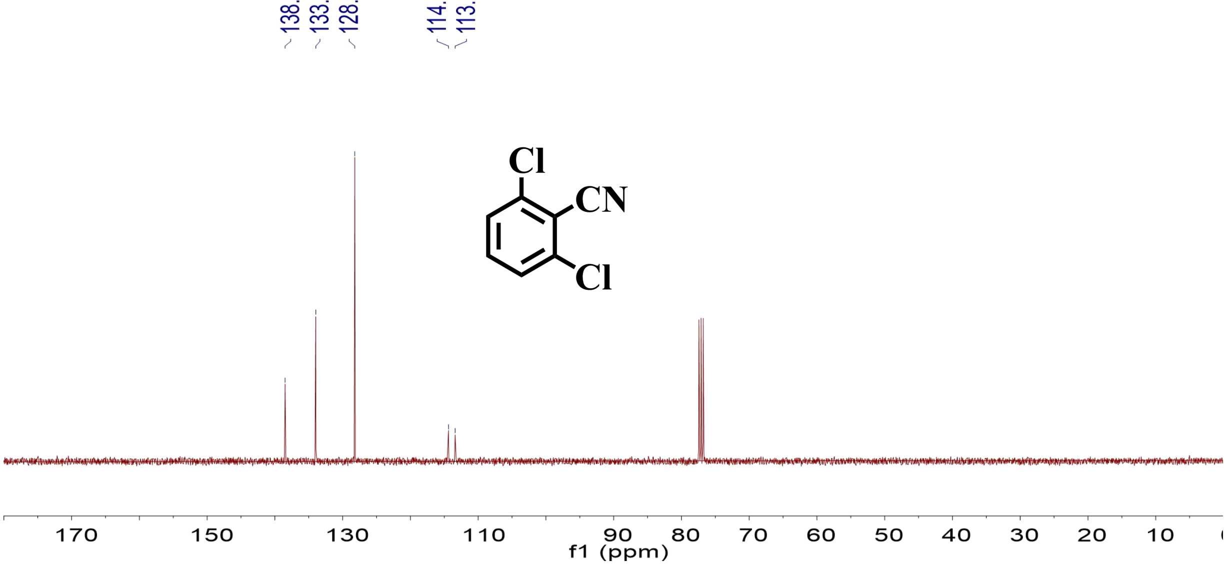

136.02
135.39
130.34
116.62
114.02
NC
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)



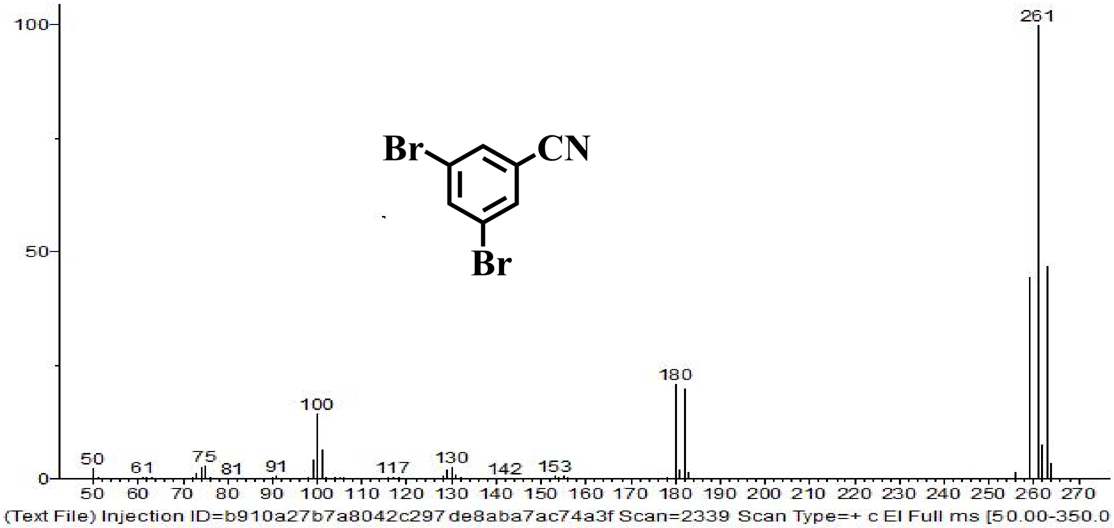
100
50
0
171
167
144
136
120
110
100
85
75
61
50
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190
(Text File) Injection ID=507820196 6b149f5bfcd62cf91c17f80 Scan=2009 Scan Type=+ c EI Full ms [50.00-350.00]
Cl
CN
Cl



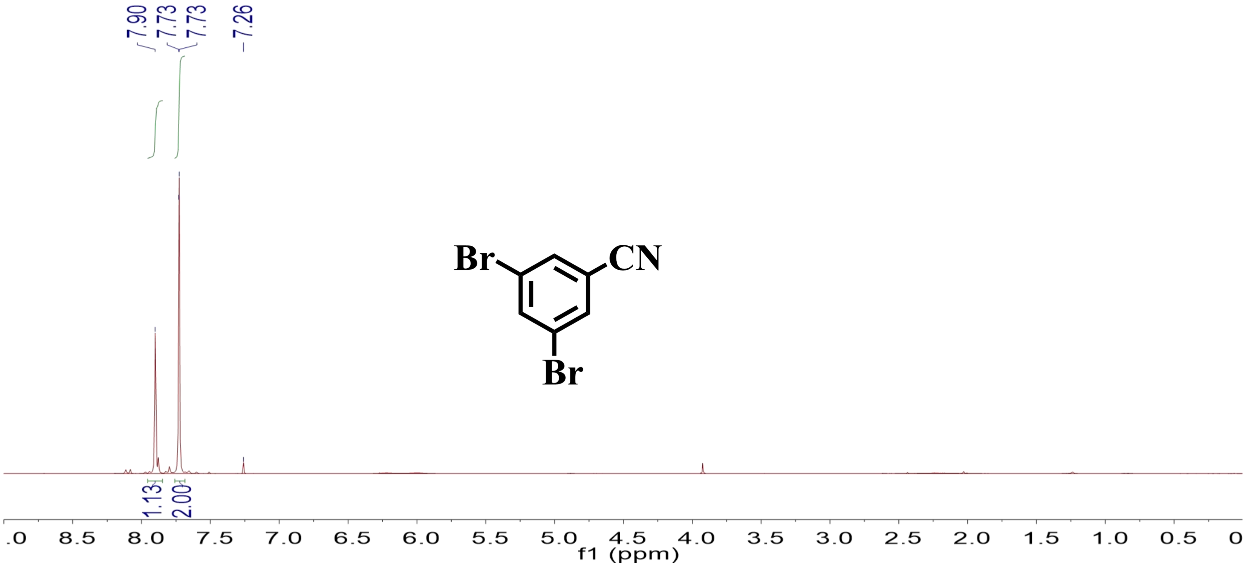
7.49
7.48
7.46
7.44
7.42
7.42
3.00
Cl
CN
Cl
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)



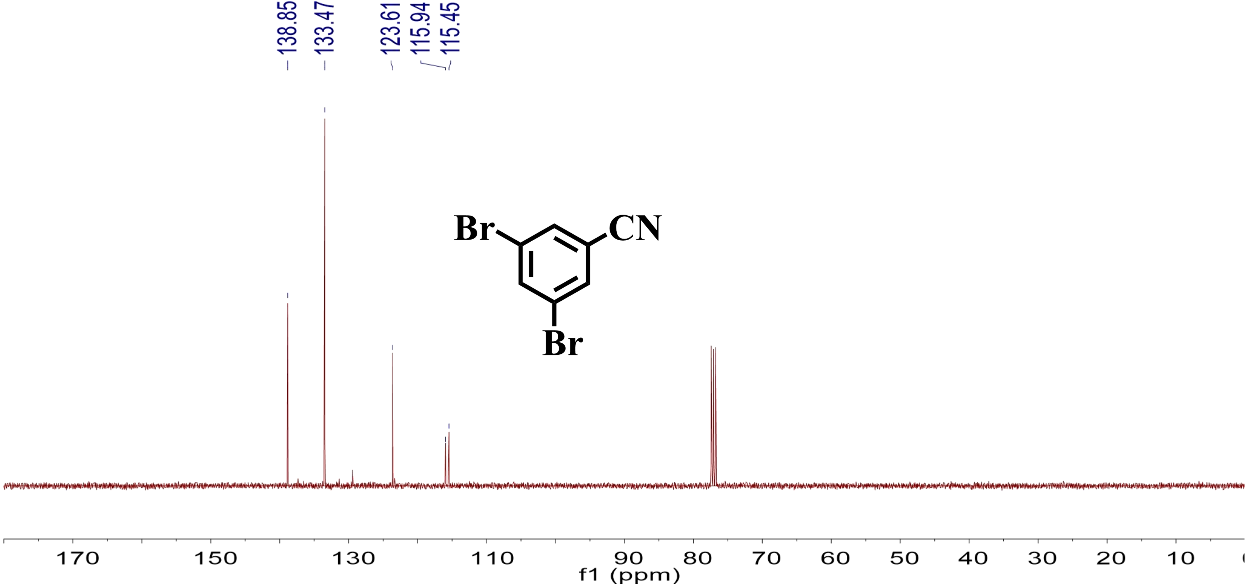
138.49
133.97
128.21
114.38
113.40
Cl
CN
Cl
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)



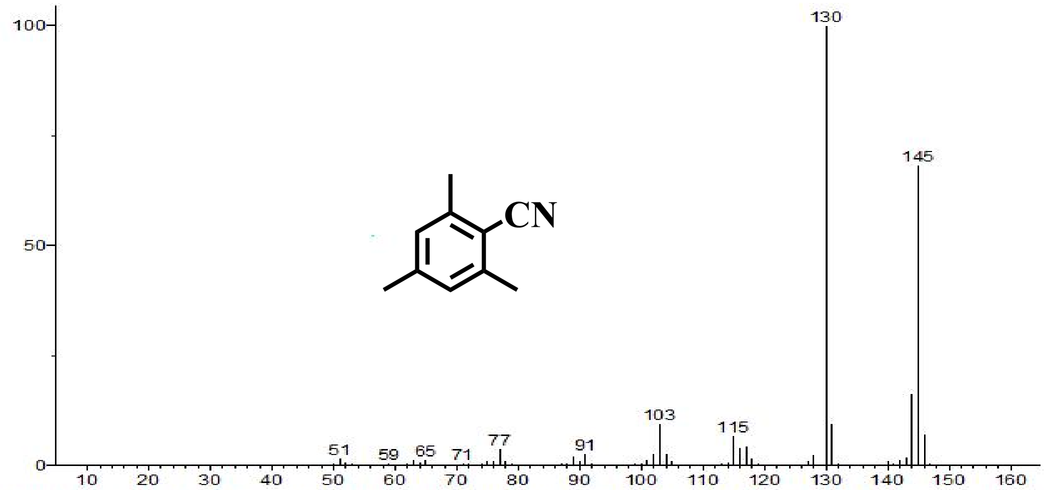
100
50
0
261
180
100
50
61
75
81
91
117
130
142
153
50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270
Br
CN
Br
(Text File) Injection ID=b910a27b7a8042c297de8aba7ac74a3f Scan=2339 Scan Type=+ c EI Full ms [50.00-350.0



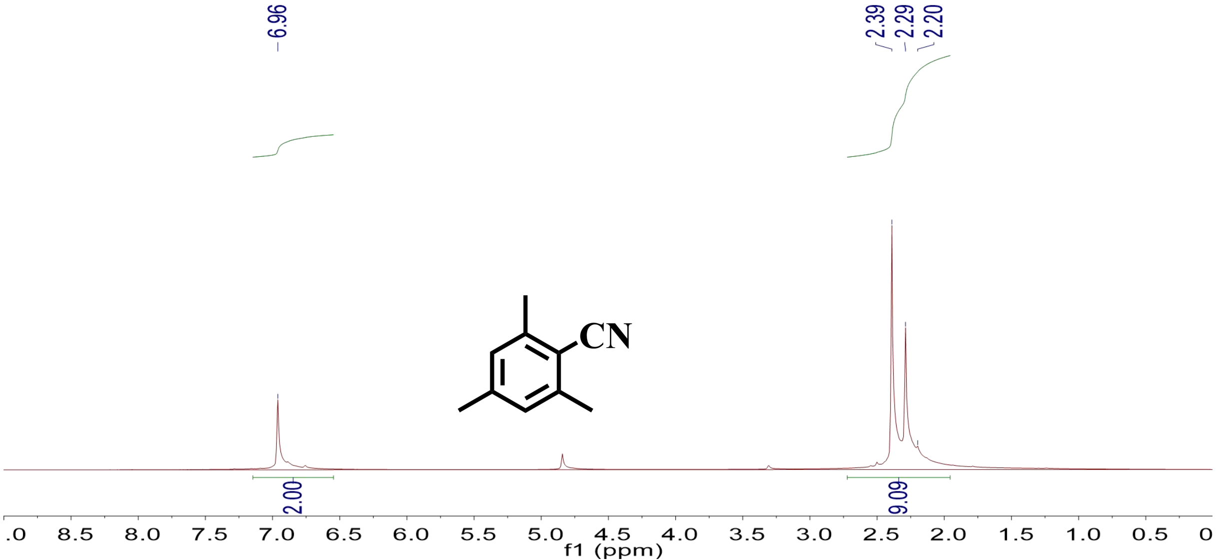
7.90
7.73
7.73
7.26
Br
CN
Br
1.13
2.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

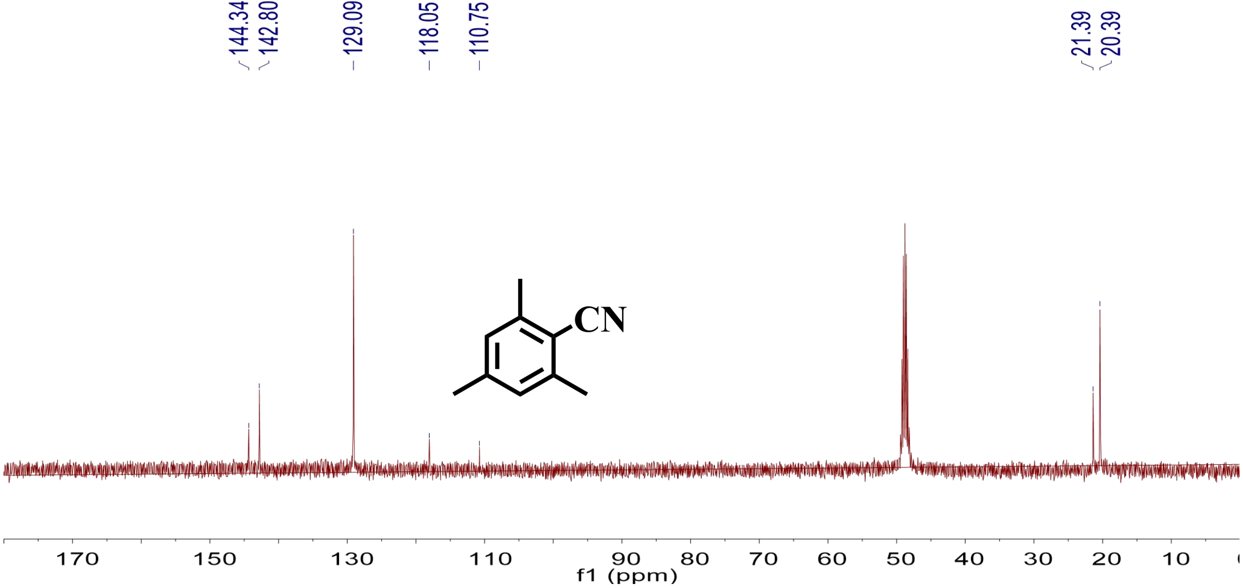


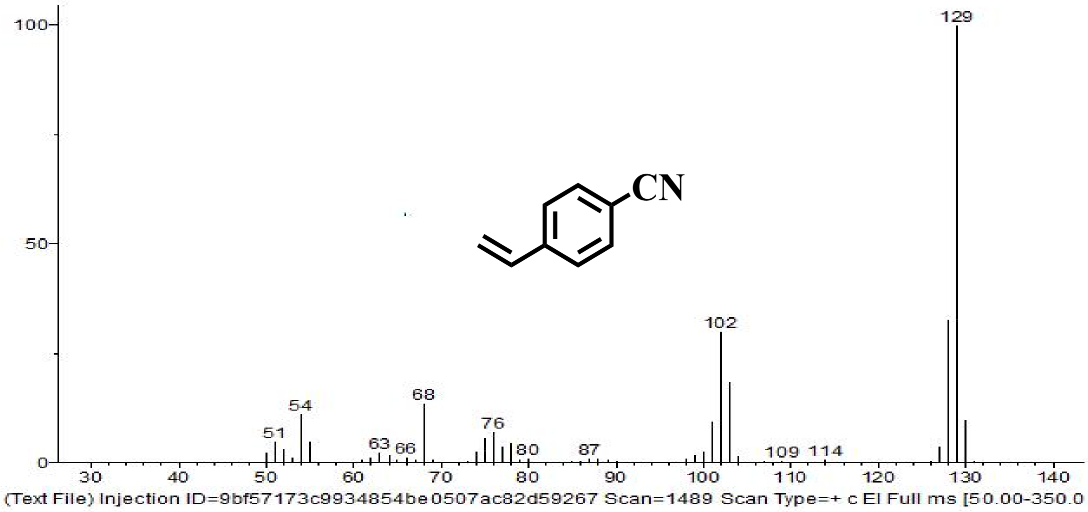
138.85
133.47
123.61
115.94
115.45
Br
CN
Br
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

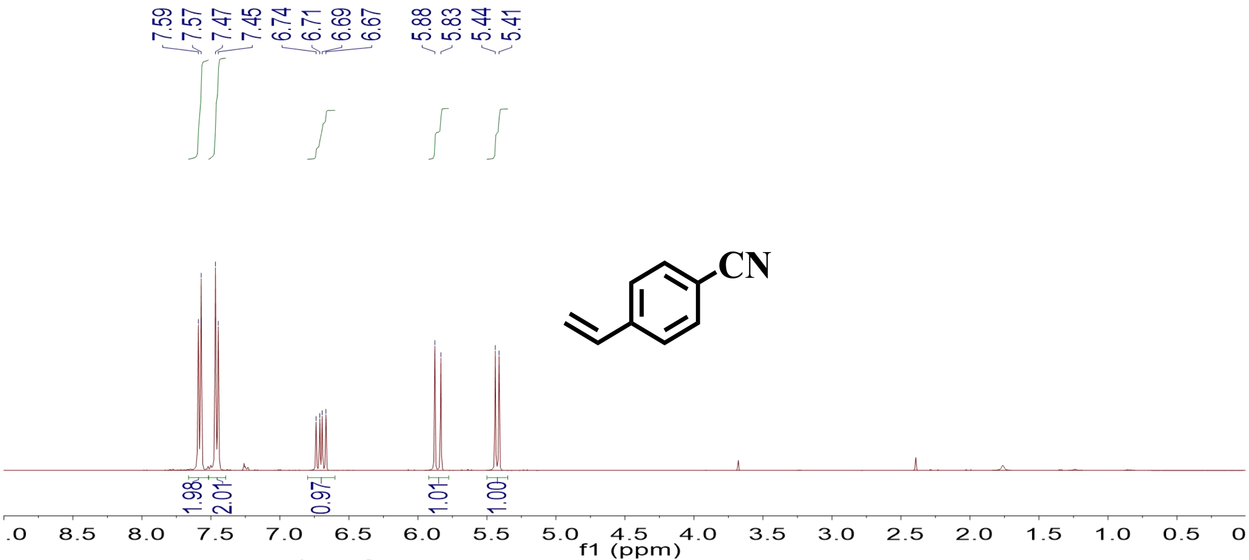


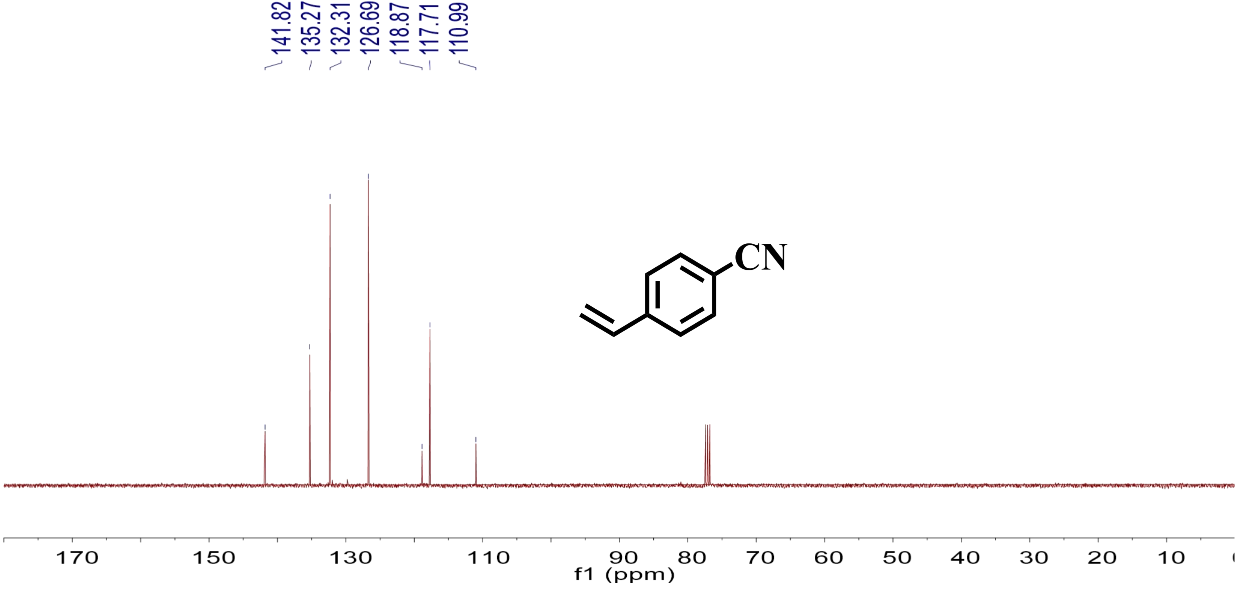
(Text File) Injection ID=ee7c32754be04e18a6c03e73fcf5f630 Scan=1720 Scan Type=+ c EI Full ms [50.00-350.00]

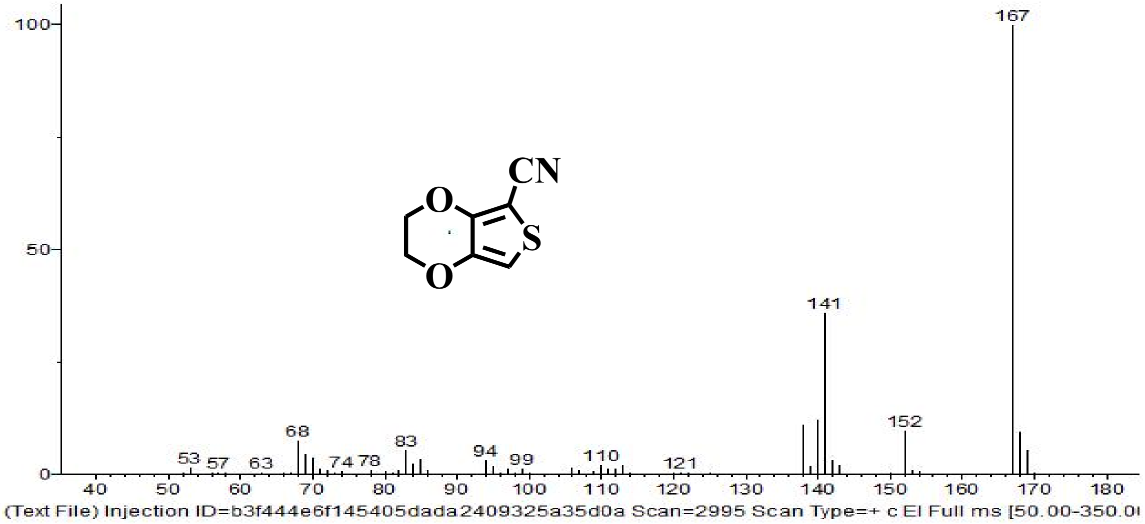


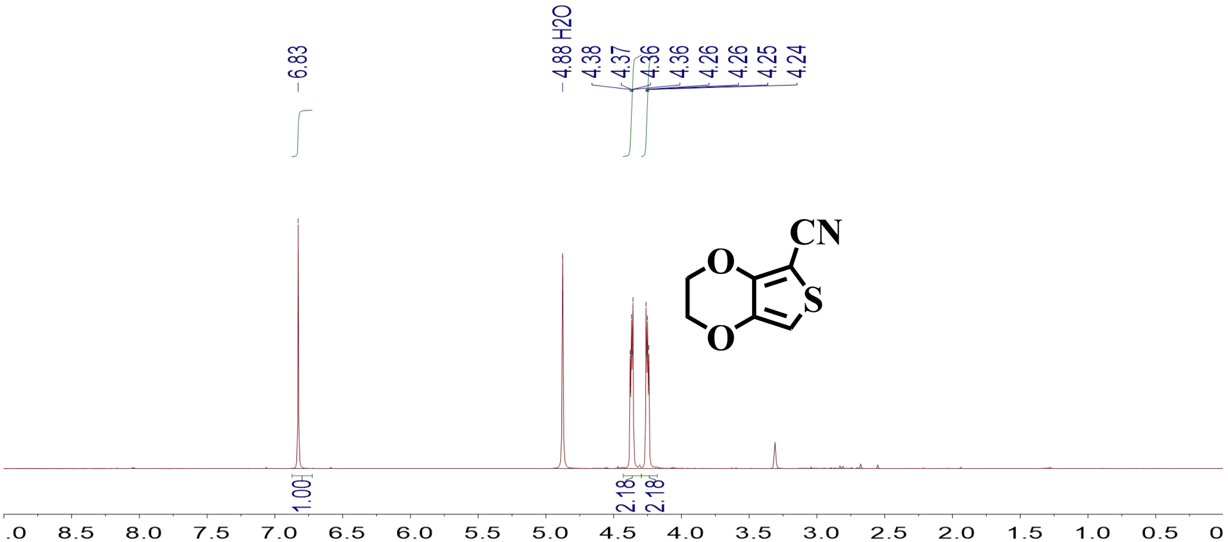


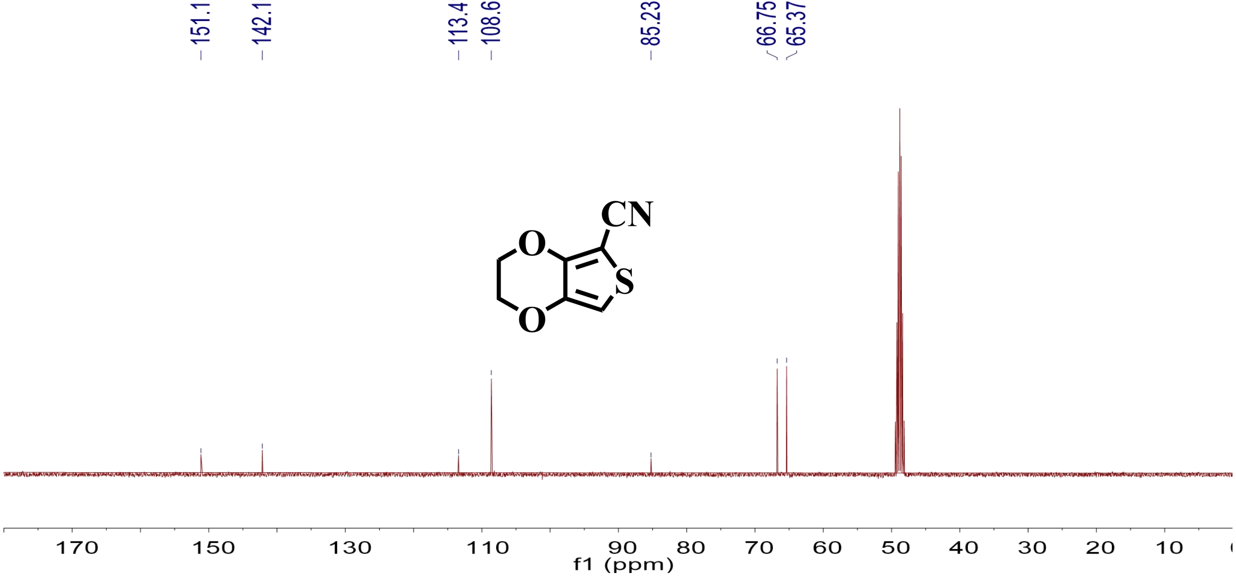

100
50
0
129
102
68
54
76
51
63
66
80
87
109
114
30
40
50
60
70
80
90
100
110
120
130
140
CN
(Text File) Injection ID=9bf57173c9934854be0507ac82d59267 Scan=1489 Scan Type=+ c EI Full ms [50.00-350.0

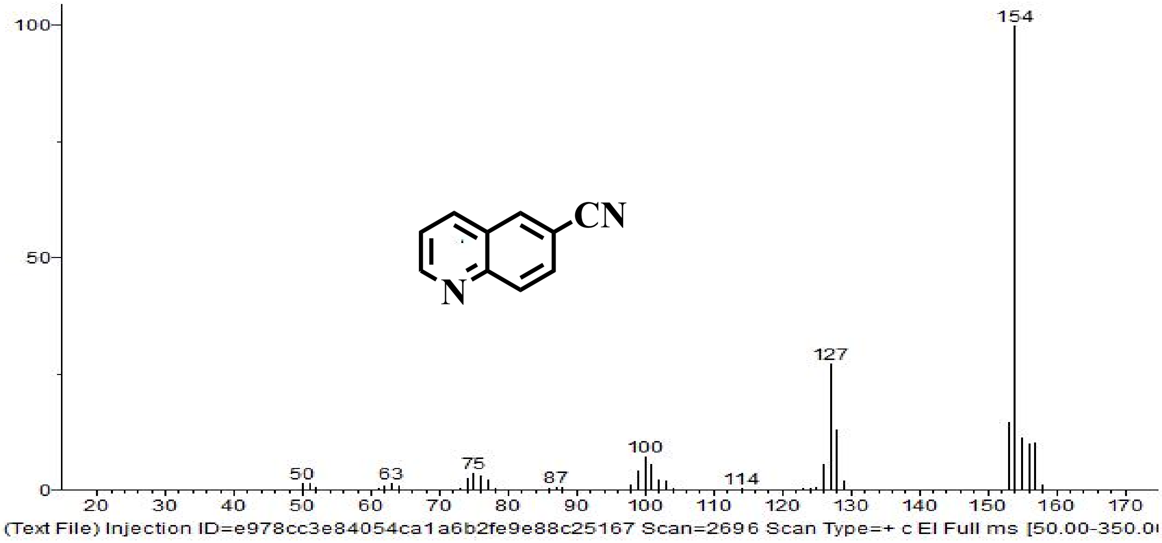

7.59
7.57
7.47
7.45
6.74
6.71
6.69
6.67
5.88
5.83
5.44
5.41
CN
1.98
2.01
0.97
1.01
1.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

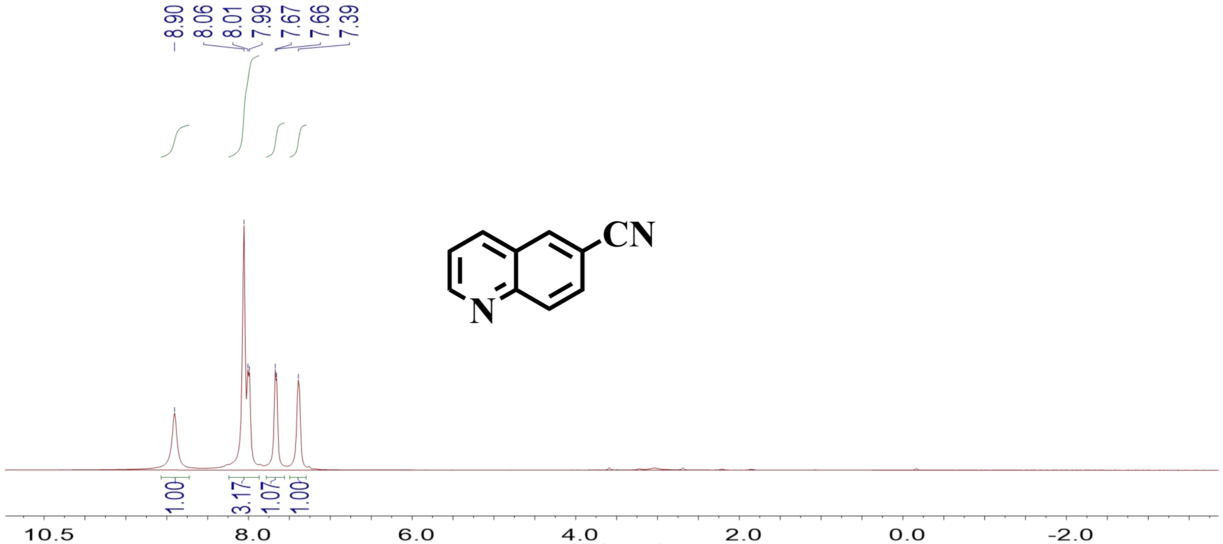

141.82
135.27
132.31
126.69
118.87
117.71
110.99
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

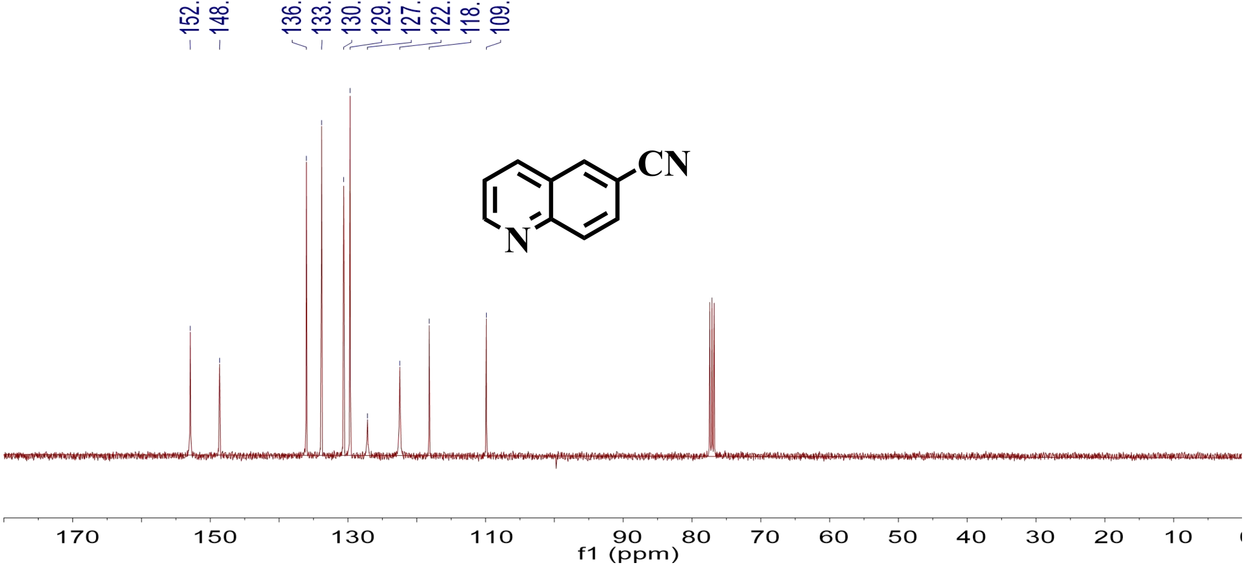

100
50
0
167
141
152
68
83
94
99
110
121
53
57
63
74
78
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
CN
O
O
S
(Text File) Injection ID=b3f444e6f145405dada2409325a35d0a Scan=2995 Scan Type=+ c EI Full ms [50.00-350.0

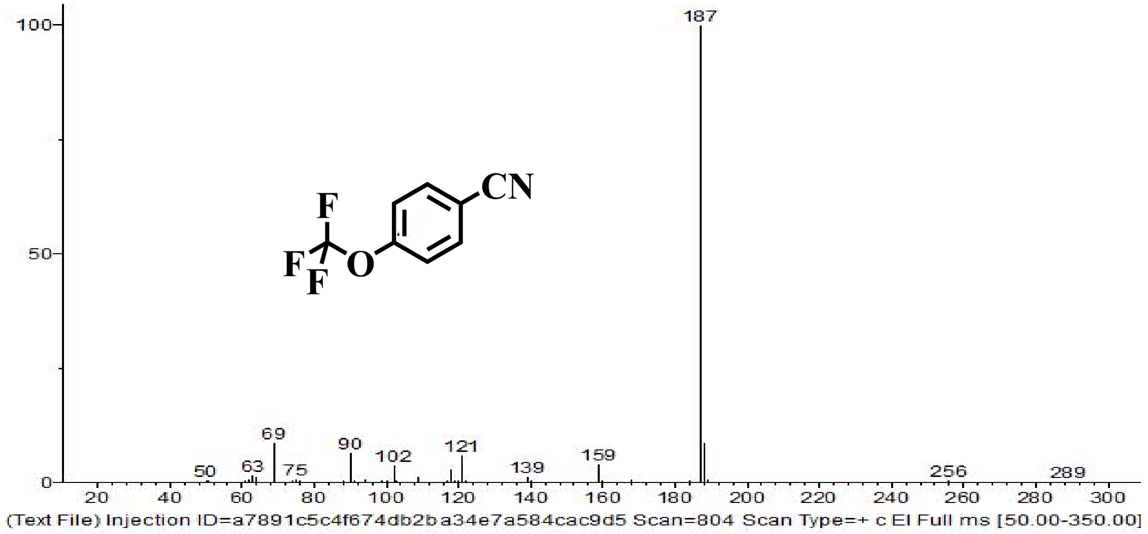

6.83
4.88 H2O
4.38
4.37
4.36
4.36
4.26
4.26
4.25
4.24
1.00
2.18
2.18
CN
O
O
S
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

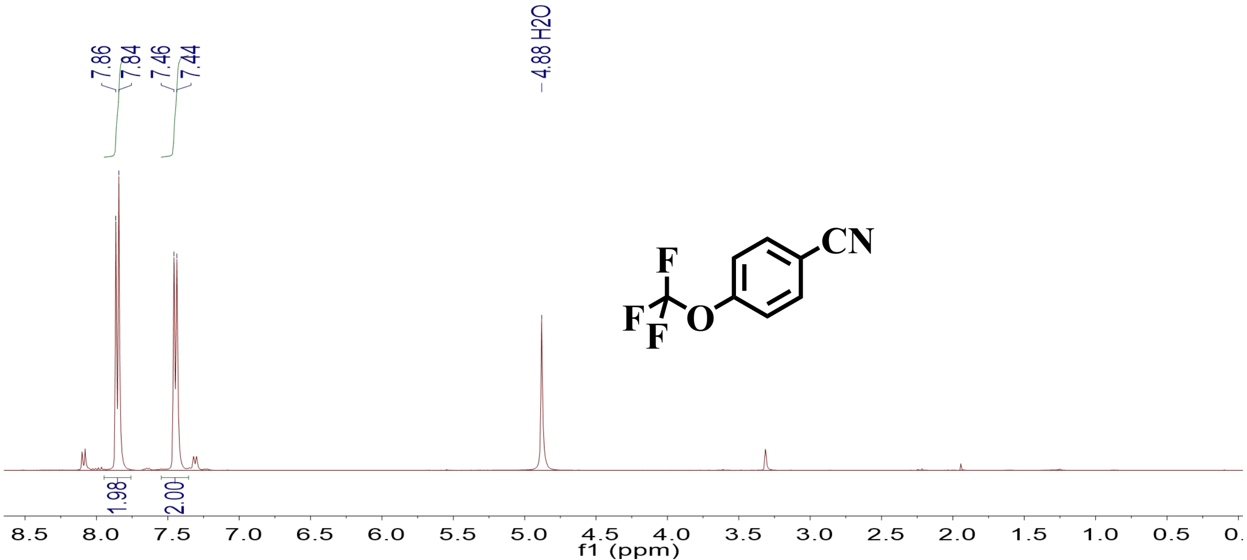

151.14
142.16
113.41
108.61
85.23
66.75
65.37
CN
O
O
S
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

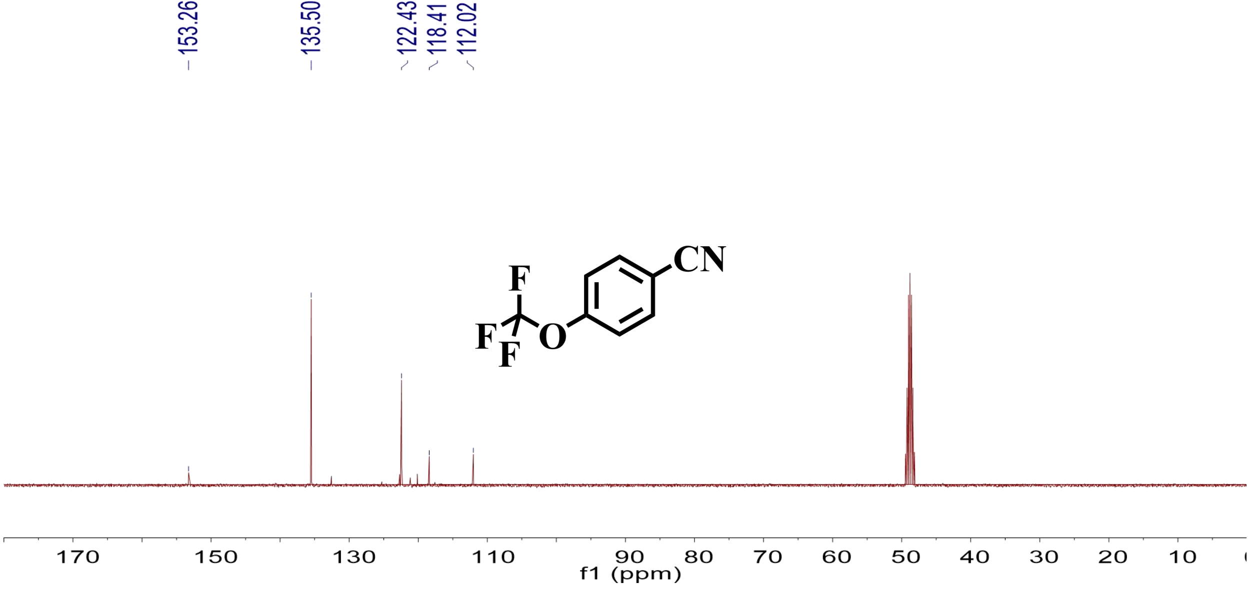

100
50
0
154
127
100
114
87
75
63
50
CN
N
20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170
(Text File) Injection ID=e978cc3e84054ca1a6b2fe9e88c25167 Scan=2696 Scan Type=+ c EI Full ms [50.00-350.0

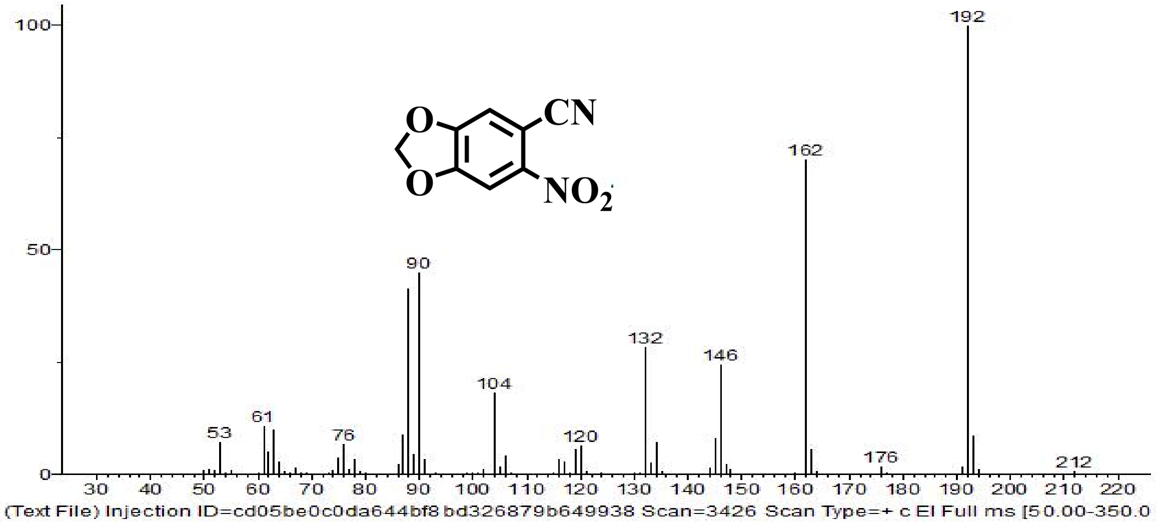

8.90
8.06
8.01
7.99
7.67
7.66
7.39
CN
N
1.00
3.17
1.07
1.00
10.5
8.0
6.0
4.0
2.0
0.0
-2.0
f1 (ppm)


152.91
148.65
136.04
133.83
130.62
129.69
127.16
122.47
118.19
109.88
CN
N
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

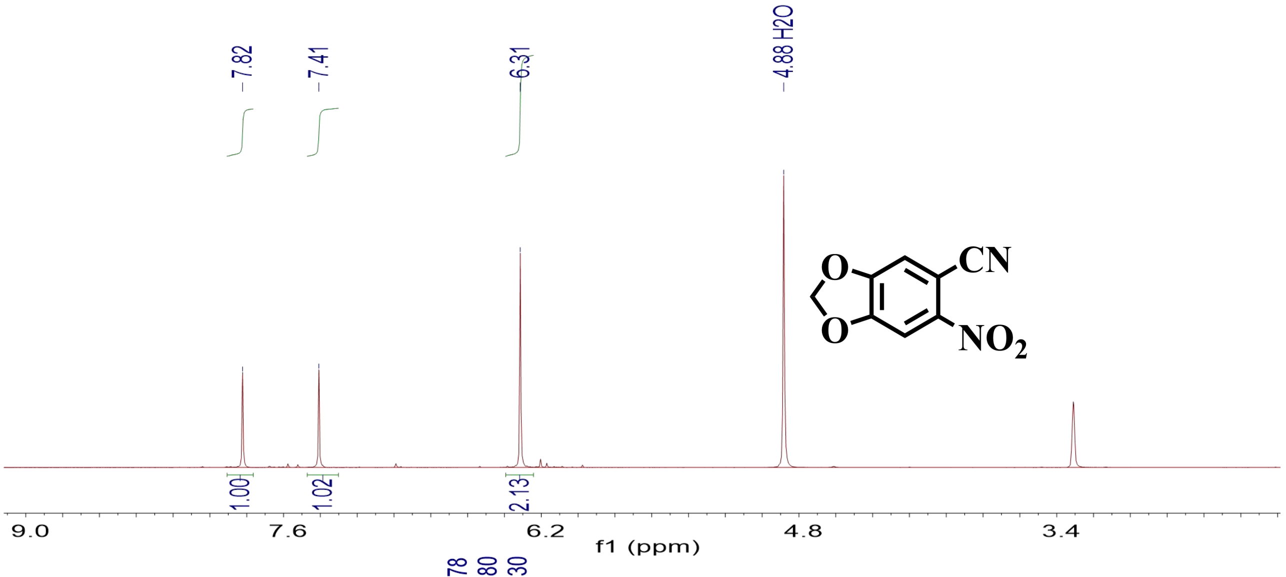

100
50
0
187
69
90
102
121
139
159
50
63
75
256
289
CN
F
F
F
O
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
(Text File) Injection ID=a7891c5c4f674db2ba34e7a584cac9d5 Scan=804 Scan Type=+ c EI Full ms [50.00-350.00]


7.86
7.84
7.46
7.44
4.88 H2O
CN
F
F
F
O
1.98
2.00
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.
f1 (ppm)

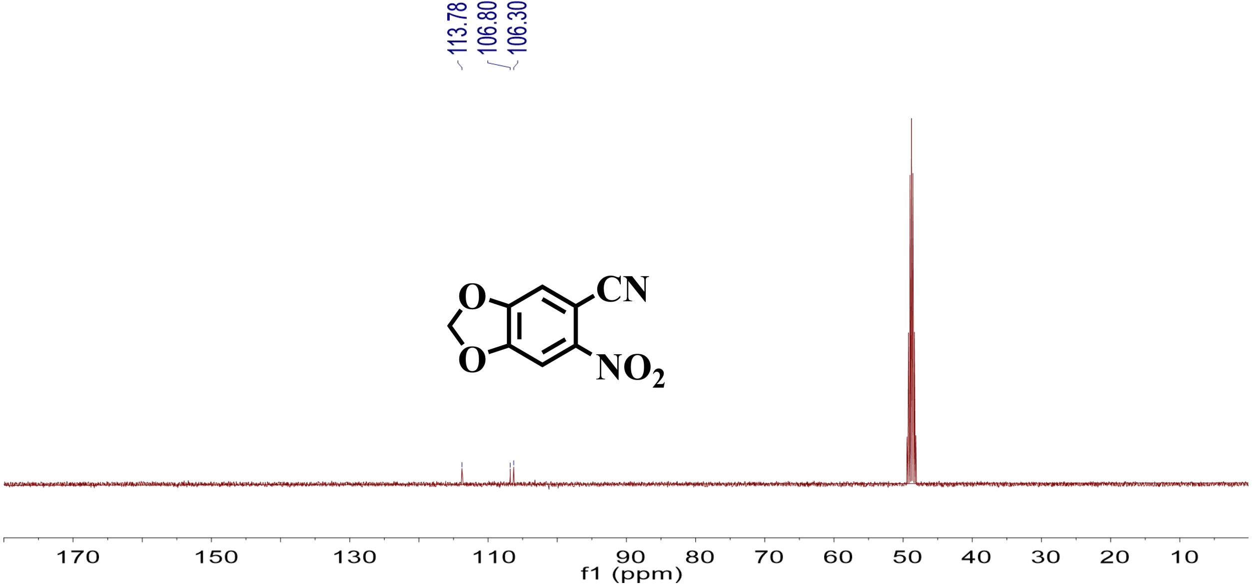

153.26
135.50
122.43
118.41
112.02
CN
F
F
F
O
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)



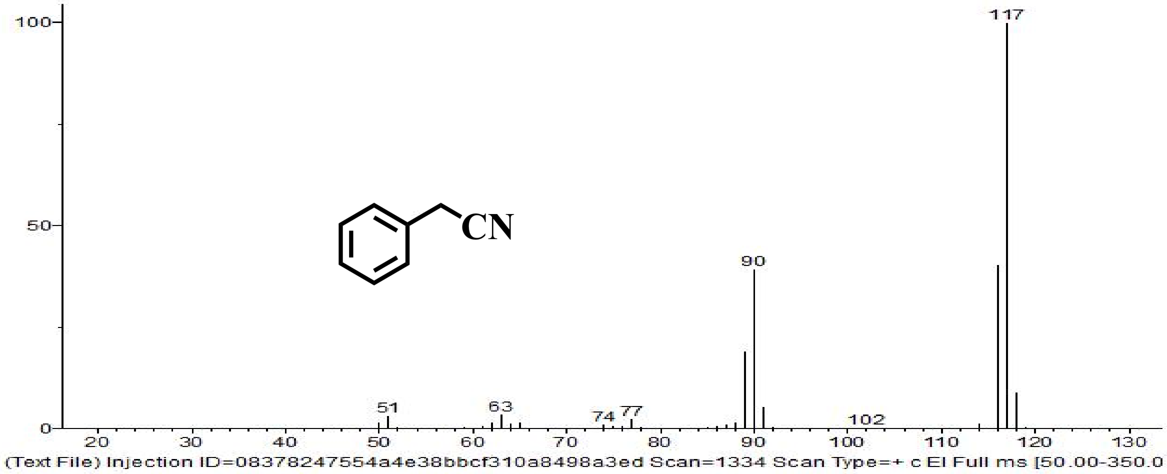
100
50
0
192
162
90
132
146
104
61
53
76
120
176
212
CN
O
O
NO2
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220
(Text File) Injection ID=cd05be0c0da644bf8 bd326879b649938 Scan=3426 Scan Type=+ c EI Full ms [50.00-350.0

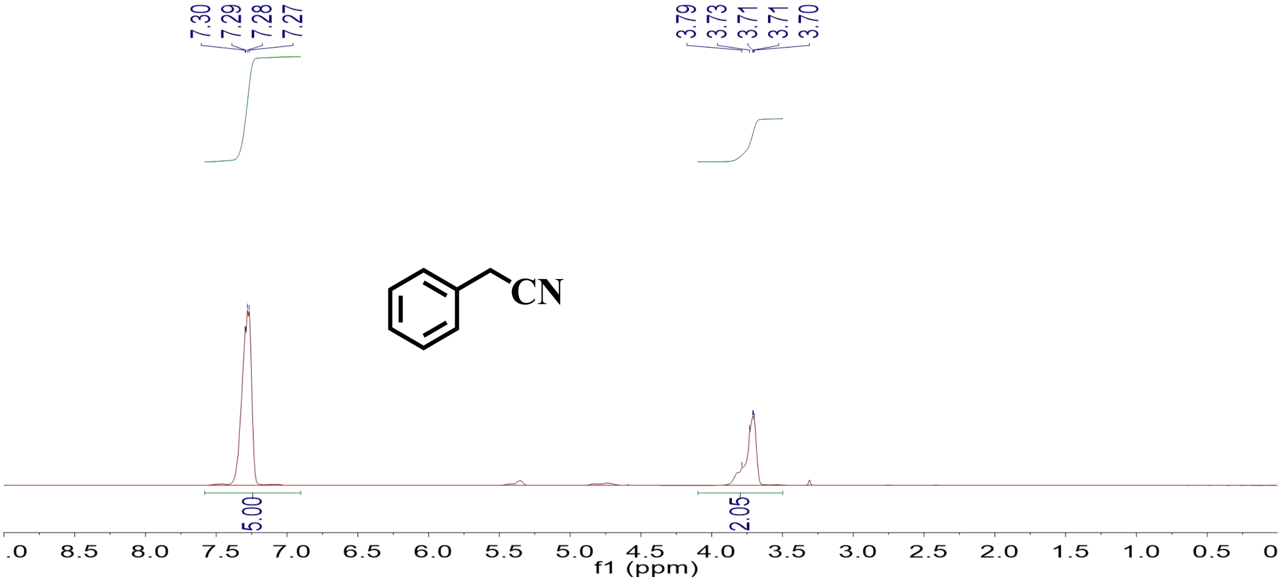


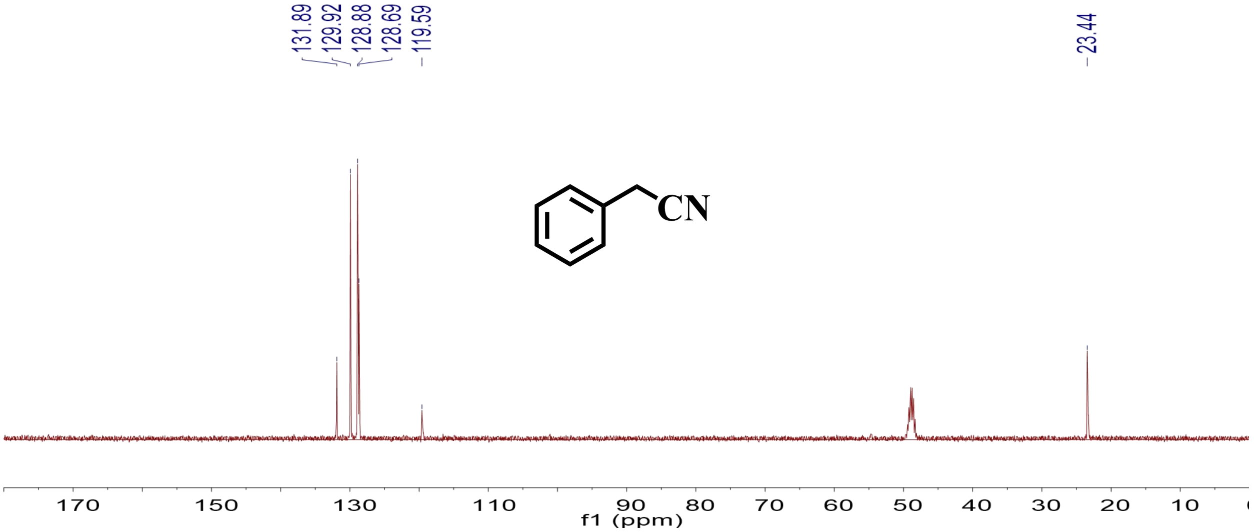
7.82
7.41
6.31
4.88 H2O
CN
O
O
NO2
1.00
1.02
2.13
9.0
7.6
6.2
4.8
3.4
f1 (ppm)

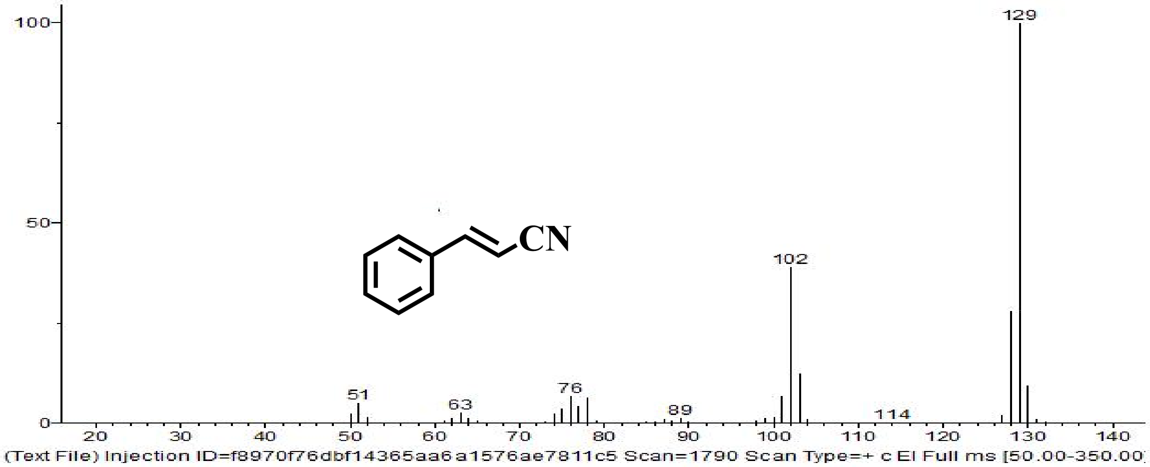


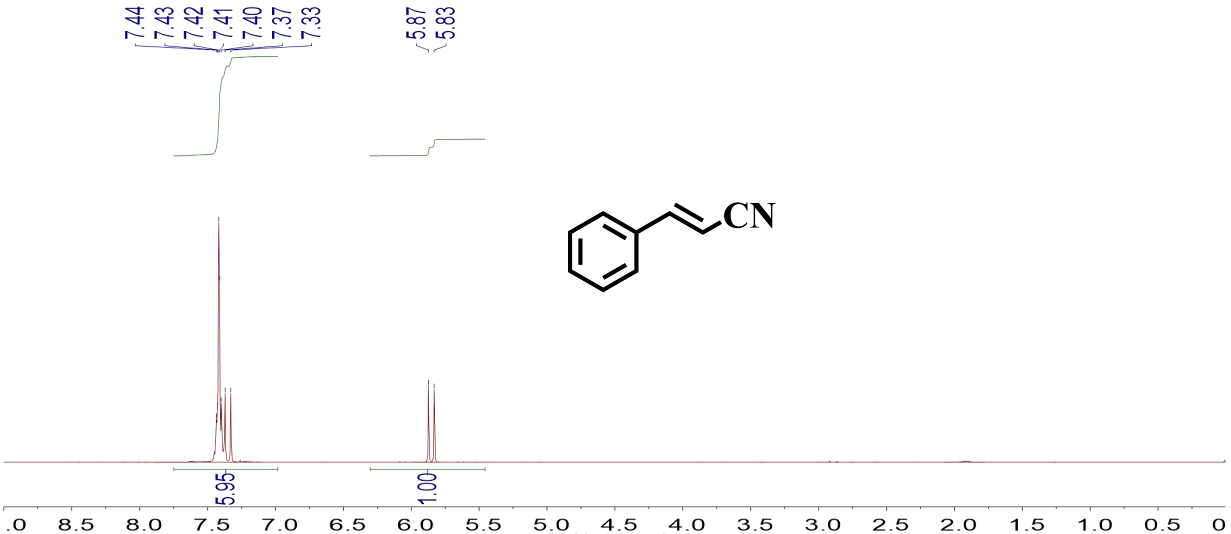
113.78
106.80
106.30
CN
O
O
NO2
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

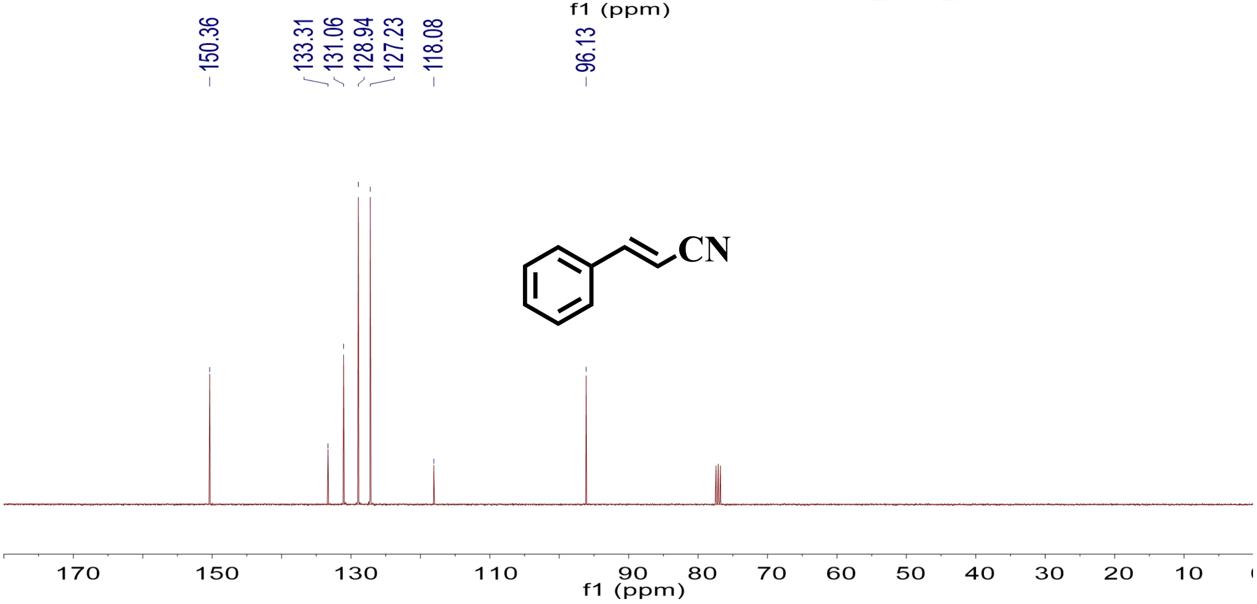

100
50
0
20
30
40
50
60
70
80
90
100
110
120
130
51
63
74
77
90
102
117
CN
(Text File) Injection ID=08378247554a4e38bbcf310a8498a3ed Scan=1334 Scan Type=+ c EI Full ms [50.00-350.0

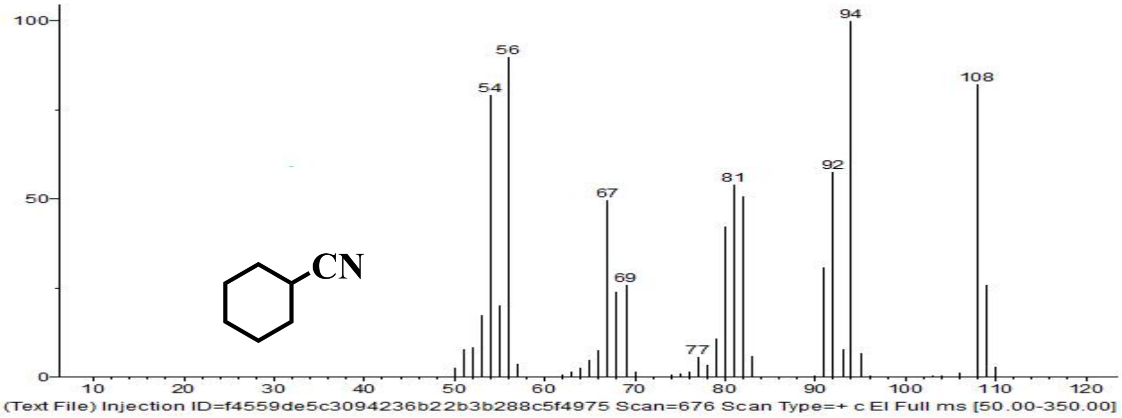

7.30
7.29
7.28
7.27
3.79
3.73
3.71
3.71
3.71
3.70
CN
5.00
2.05
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)

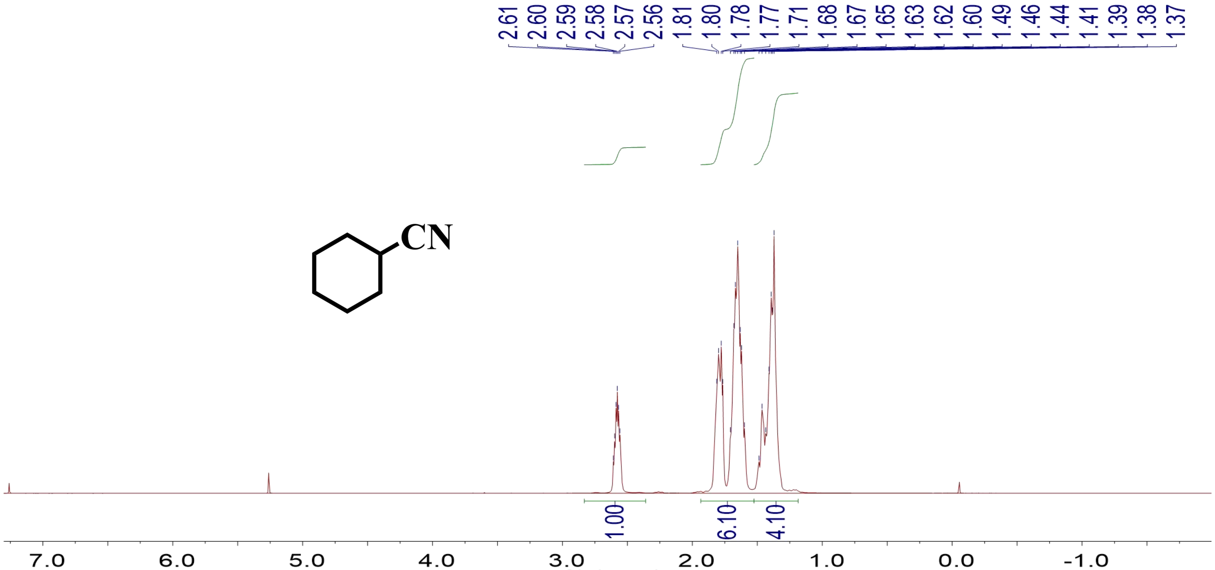

131.89
129.92
128.88
128.69
119.59
23.44
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

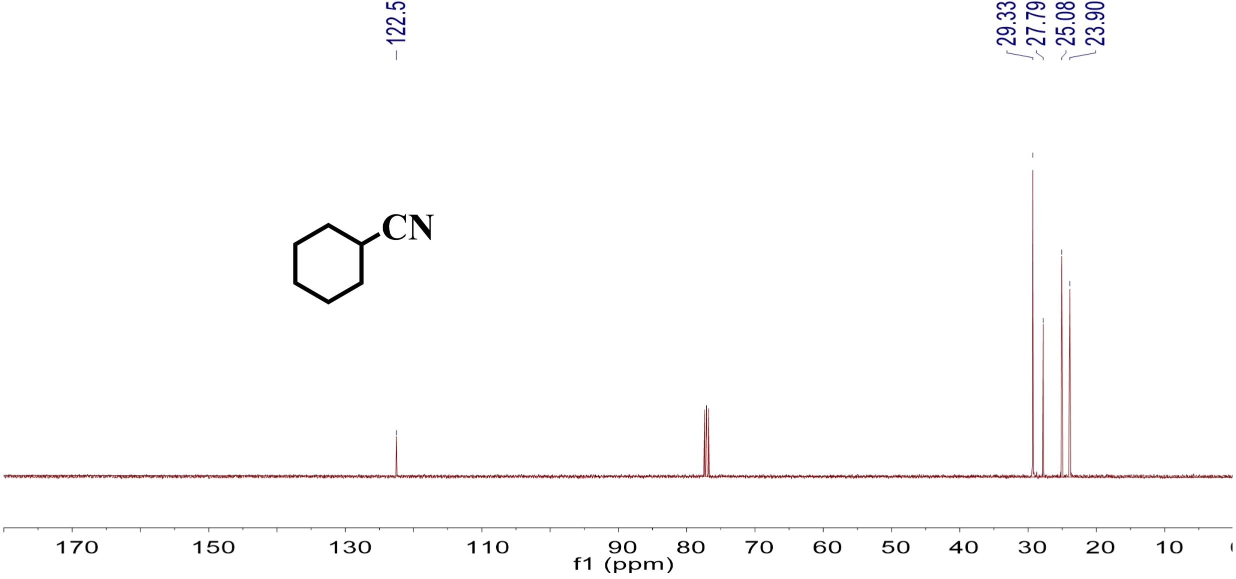

100
50
0
129
102
51
63
76
89
114
CN
20 30 40 50 60 70 80 90 100 110 120 130 140
(Text File) Injection ID=f8970f76dbf14365aa6a1576ae7811c5 Scan=1790 Scan Type=+ c EI Full ms [50.00-350.00]

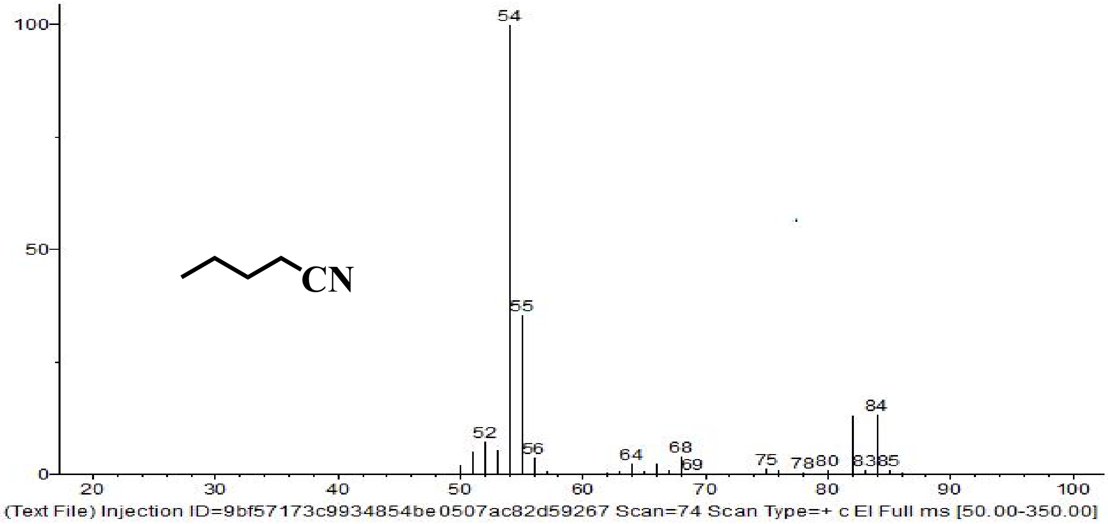

7.44
7.43
7.42
7.41
7.40
7.37
7.33
5.87
5.83
CN
5.95
1.00
.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)

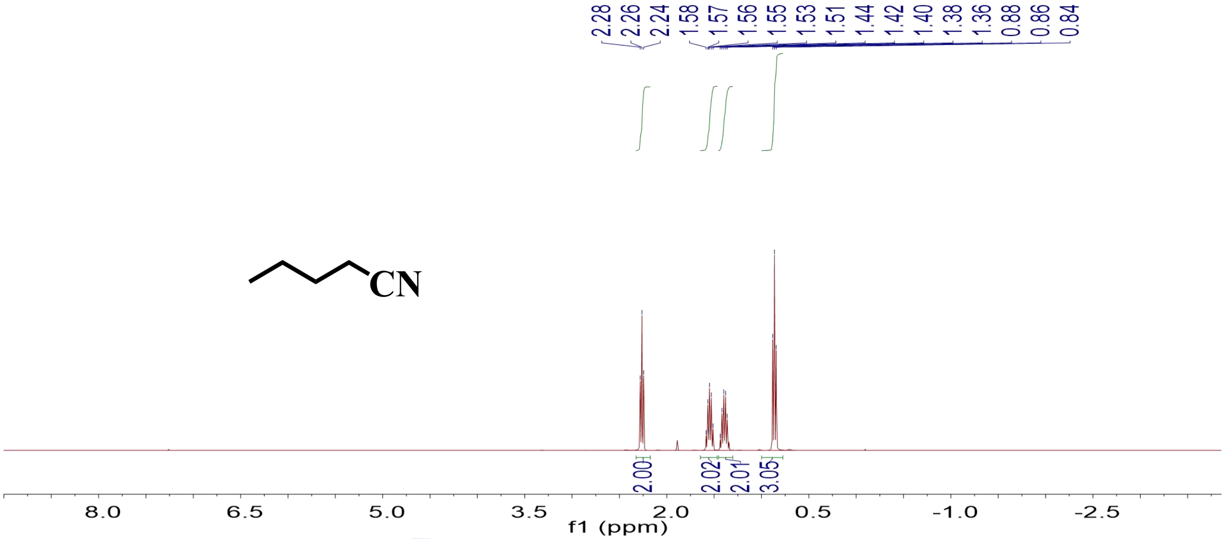

150.36
133.31
131.06
128.94
127.23
118.08
96.13
CN
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

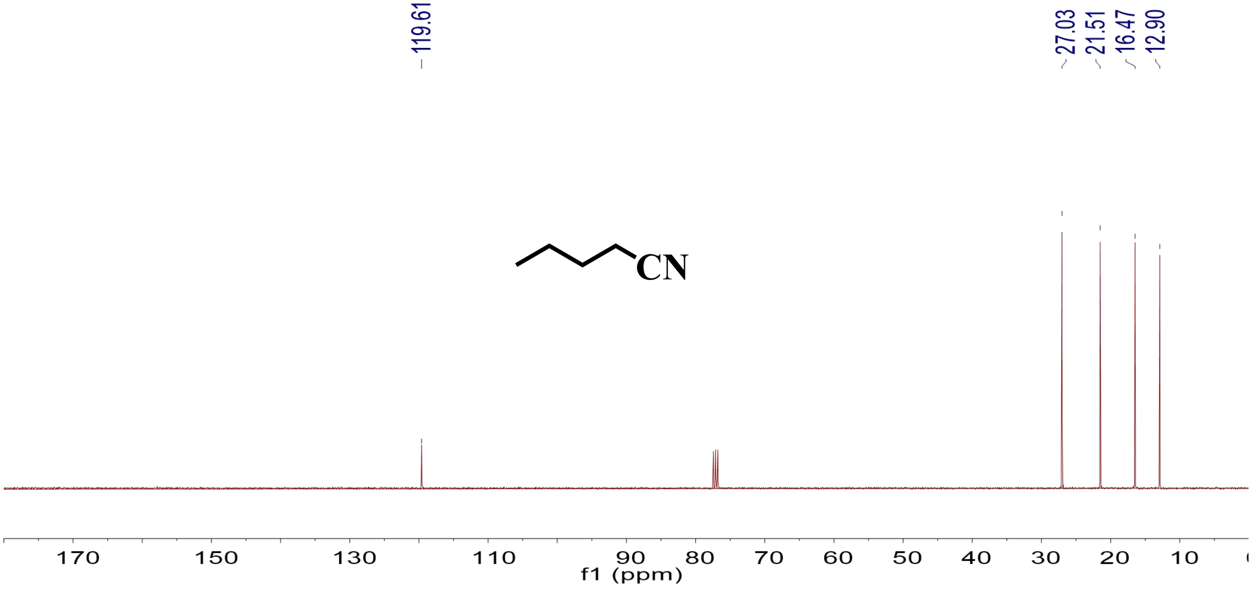

CN
100
50
0
54
56
67
69
77
81
92
94
108
10
20
30
40
50
60
70
80
90
100
110
120
(Text File) Injection ID=f4559de5c3094236b22b3b288c5f4975 Scan=676 Scan Type=+ c EI Full ms [50.00-350.00]

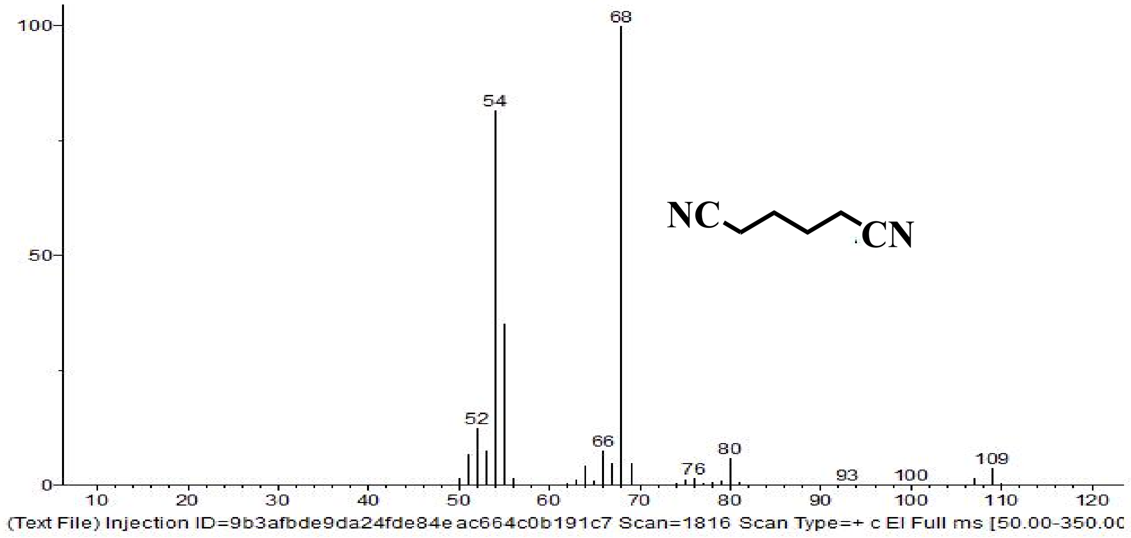

2.61
2.60
2.59
2.58
2.57
2.56
1.81
1.80
1.78
1.77
1.71
1.68
1.67
1.65
1.63
1.62
1.60
1.49
1.46
1.44
1.41
1.39
1.38
1.37
CN
1.00
6.10
4.10
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

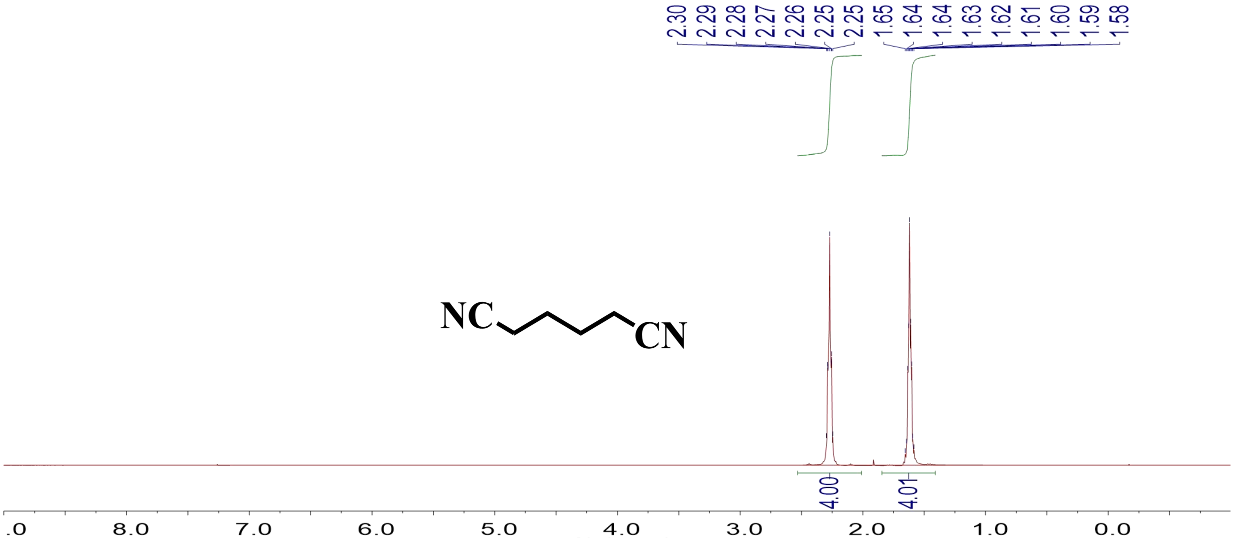

122.50
29.33
27.79
25.08
23.90
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

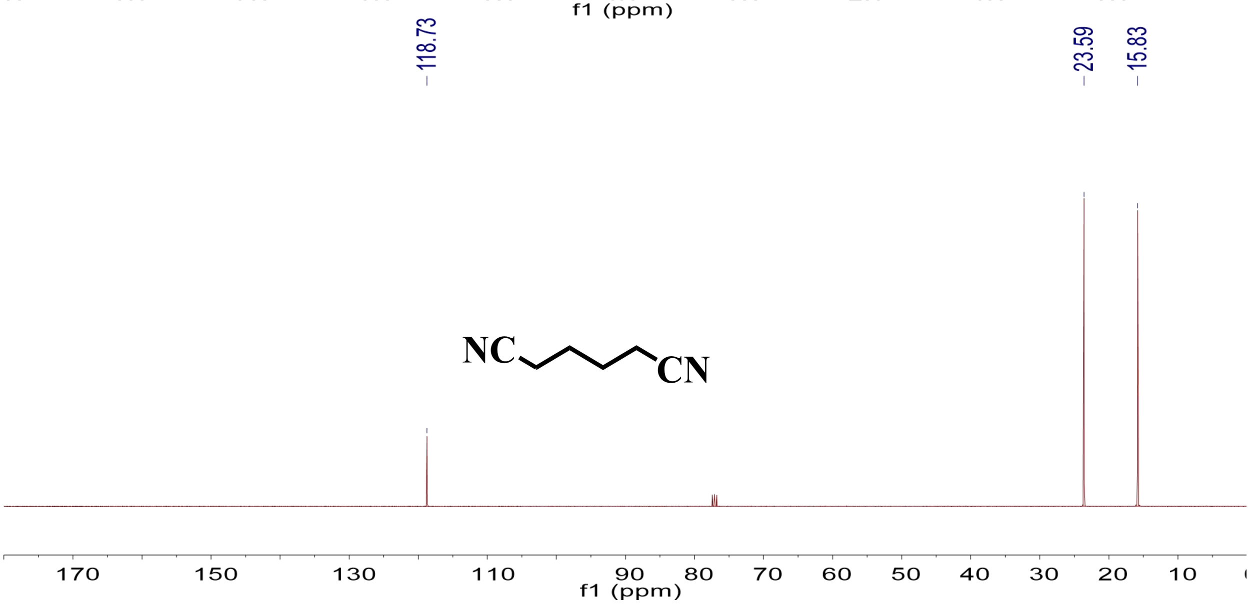

100
50
0
54
55
52
56
64
68
69
75
78
80
83
84
85
20
30
40
50
60
70
80
90
100
CN
(Text File) Injection ID=9bf57173c9934854be0507ac82d59267 Scan=74 Scan Type=+ c EI Full ms [50.00-350.00]

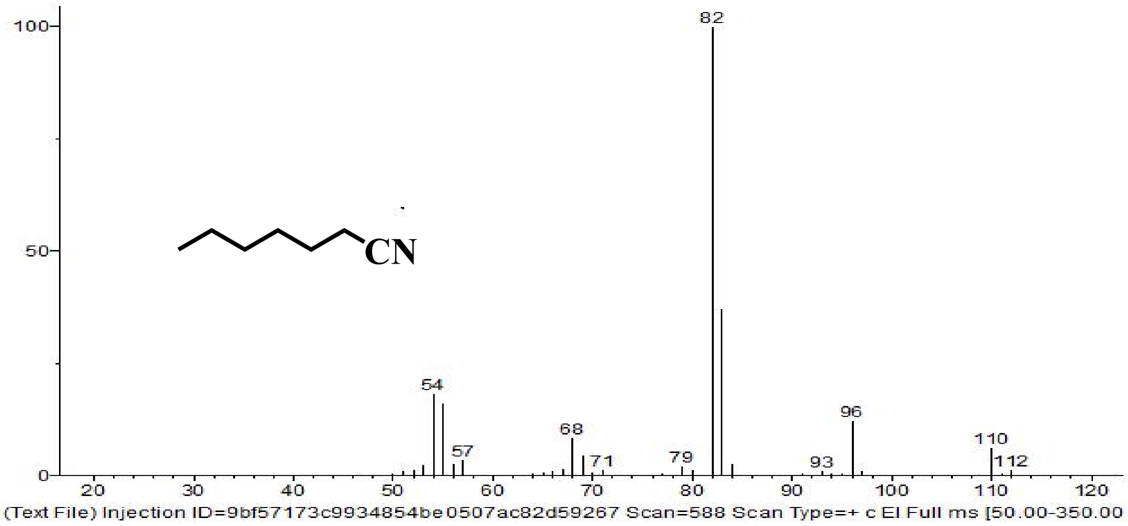

2.28
2.26
2.24
1.58
1.57
1.56
1.55
1.53
1.51
1.44
1.42
1.40
1.38
1.36
0.88
0.86
0.84
CN
2.00
2.02
2.01
3.05
8.0
6.5
5.0
3.5
2.0
0.5
-1.0
-2.5
f1 (ppm)


119.61
27.03
21.51
16.47
12.90
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)

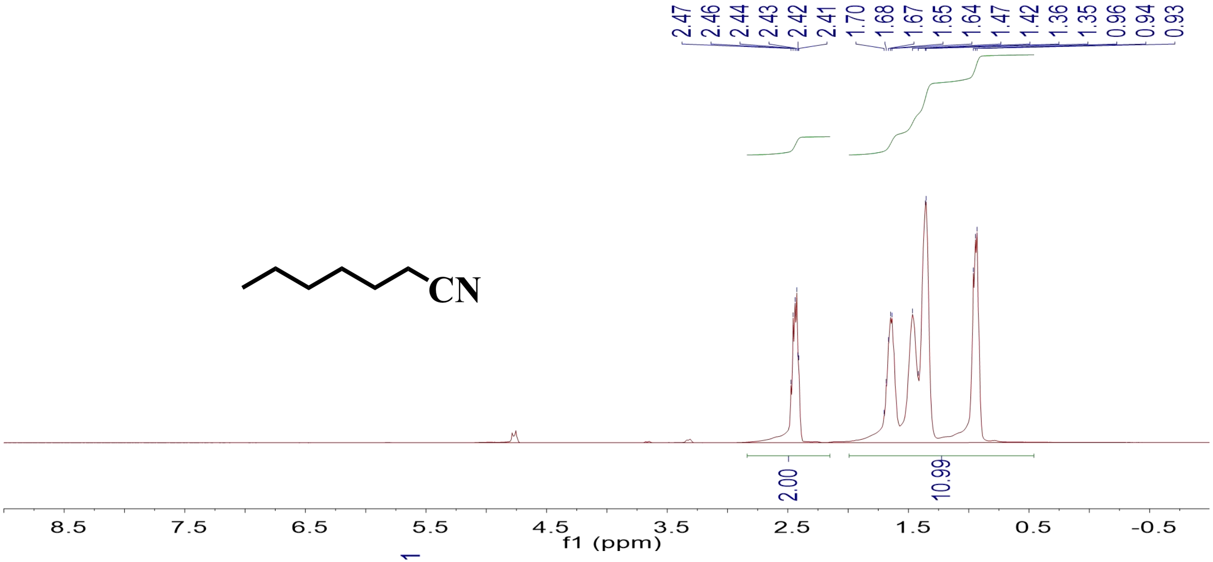

100
50
0
68
54
52
66
76
80
93
100
109
NC
CN
10
20
30
40
50
60
70
80
90
100
110
120
(Text File) Injection ID=9b3afbde9da24fde84e ac664c0b191c7 Scan=1816 Scan Type=+ c EI Full ms [50.00-350.0


2.30
2.29
2.28
2.27
2.26
2.25
2.25
1.65
1.64
1.64
1.63
1.62
1.61
1.60
1.59
1.58
NC
CN
4.00
4.01
.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

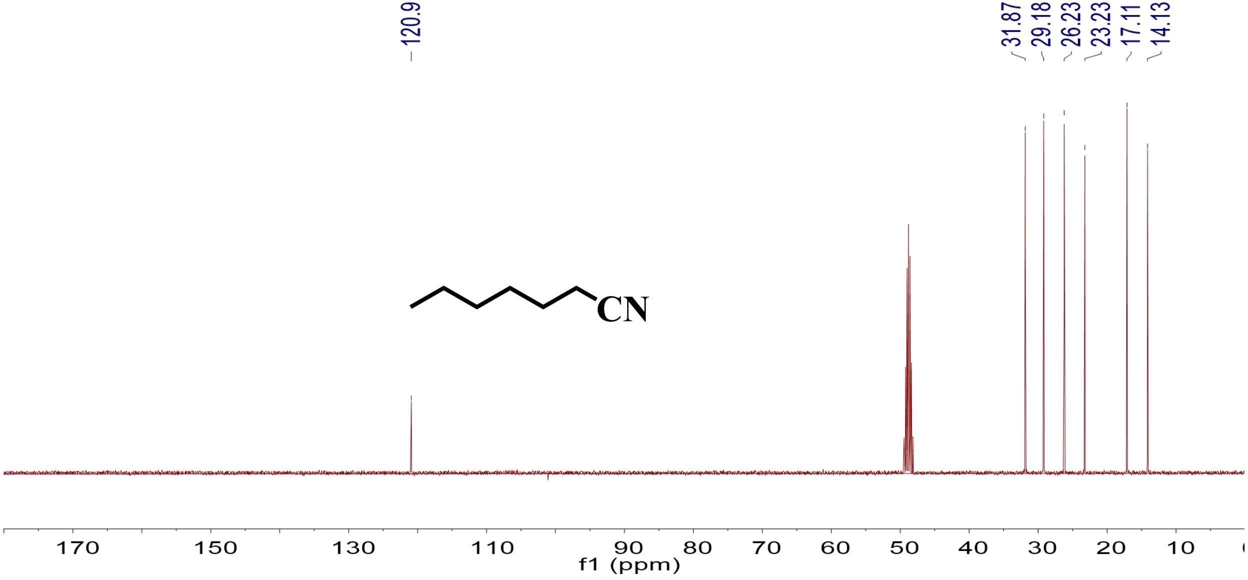

118.73
23.59
15.83
NC
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)



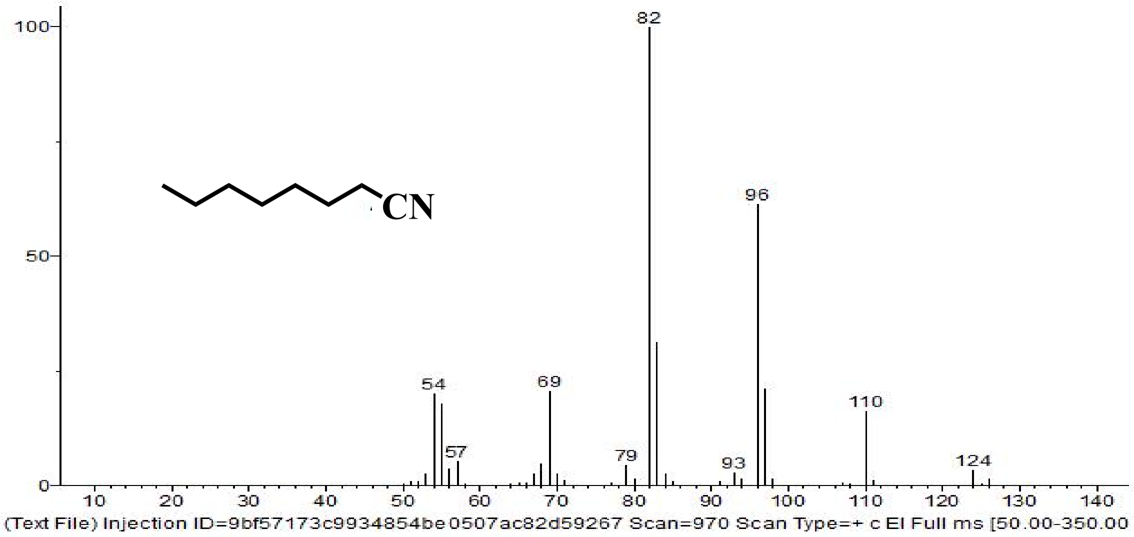
100
50
0
82
54
57
68
71
79
93
96
110
112
20
30
40
50
60
70
80
90
100
110
120
CN
(Text File) Injection ID=9bf57173c9934854be0507ac82d59267 Scan=588 Scan Type=+ c EI Full ms [50.00-350.00



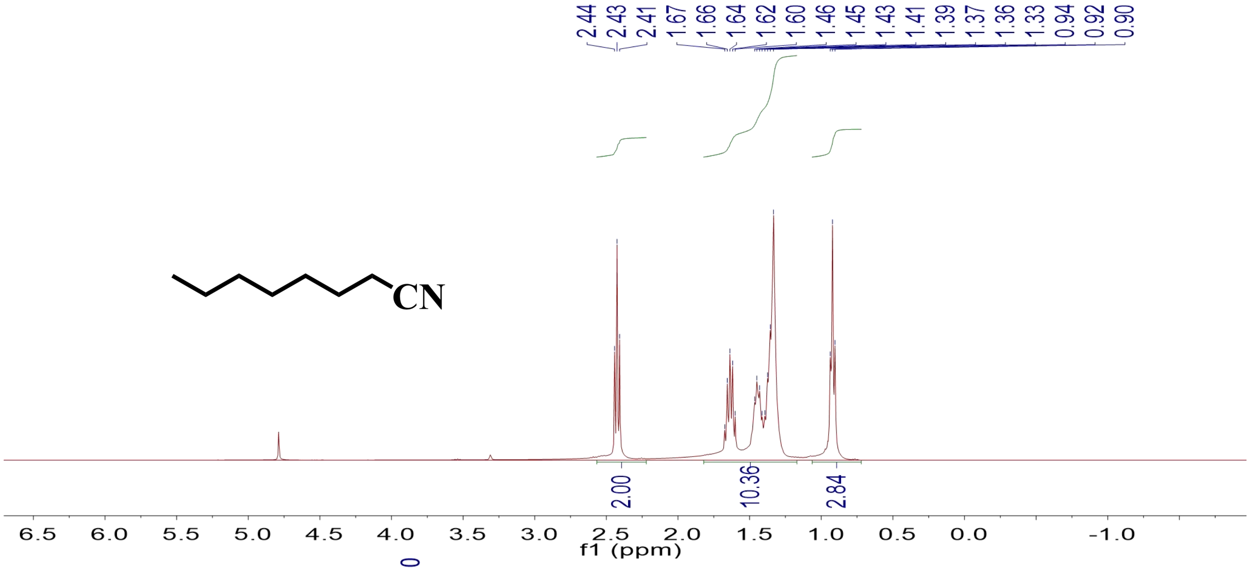
2.47
2.46
2.44
2.43
2.42
2.41
1.70
1.68
1.67
1.65
1.64
1.47
1.42
1.36
1.35
0.96
0.94
0.93
CN
2.00
10.99
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)



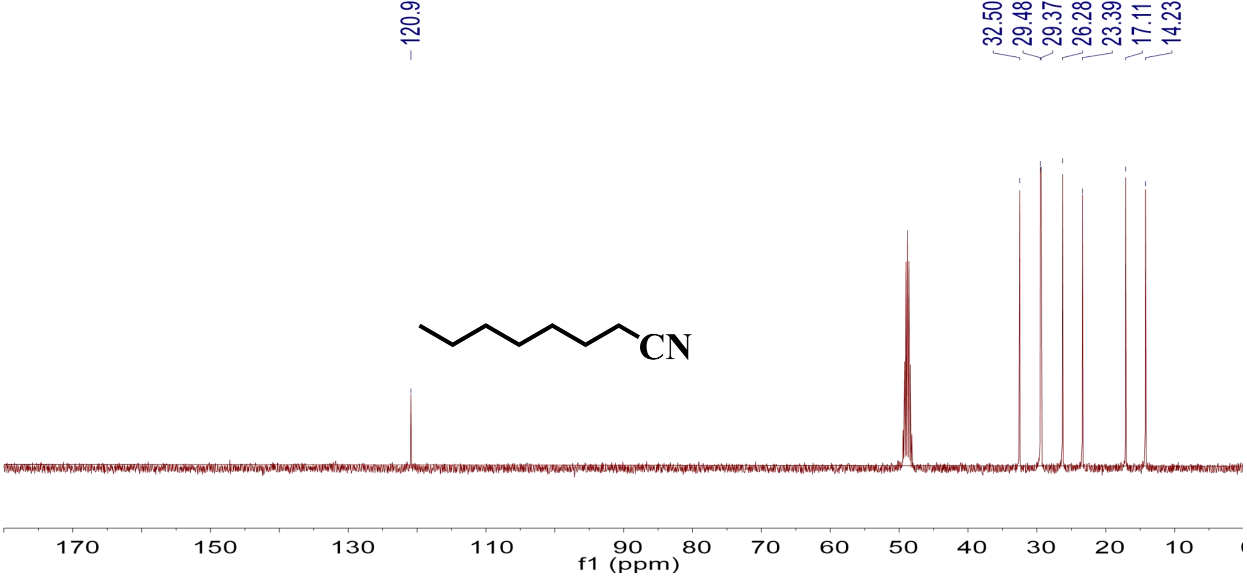
120.91
31.87
29.18
26.23
23.23
17.11
14.13
CN
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)



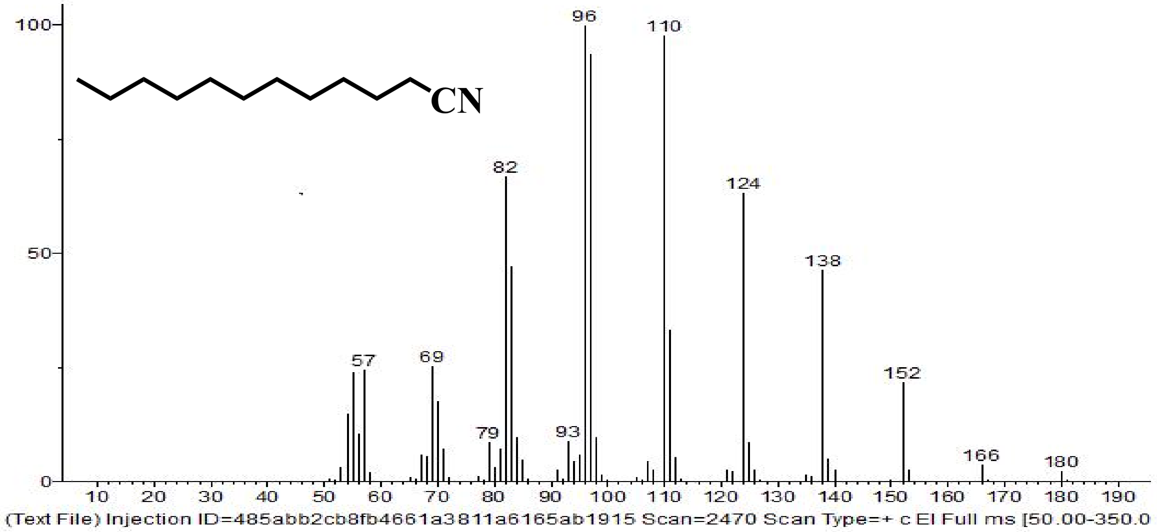
CN
100
50
0
82
96
54
69
57
79
93
110
124
10 20 30 40 50 60 70 80 90 100 110 120 130 140
(Text File) Injection ID=9bf57173c9934854be0507ac82d59267 Scan=970 Scan Type=+ c EI Full ms [50.00-350.00

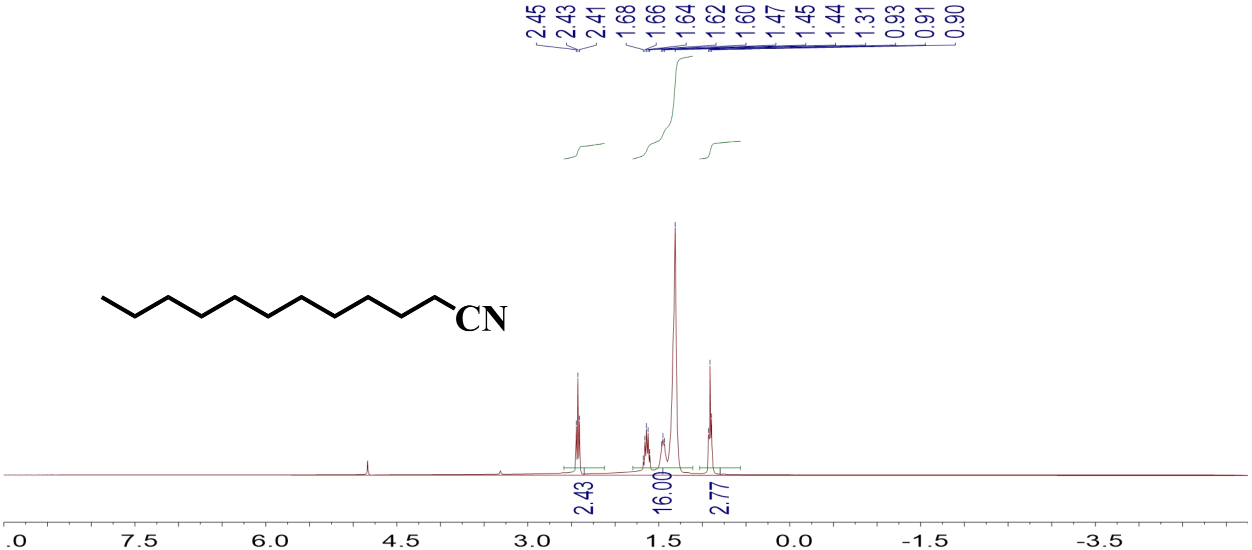


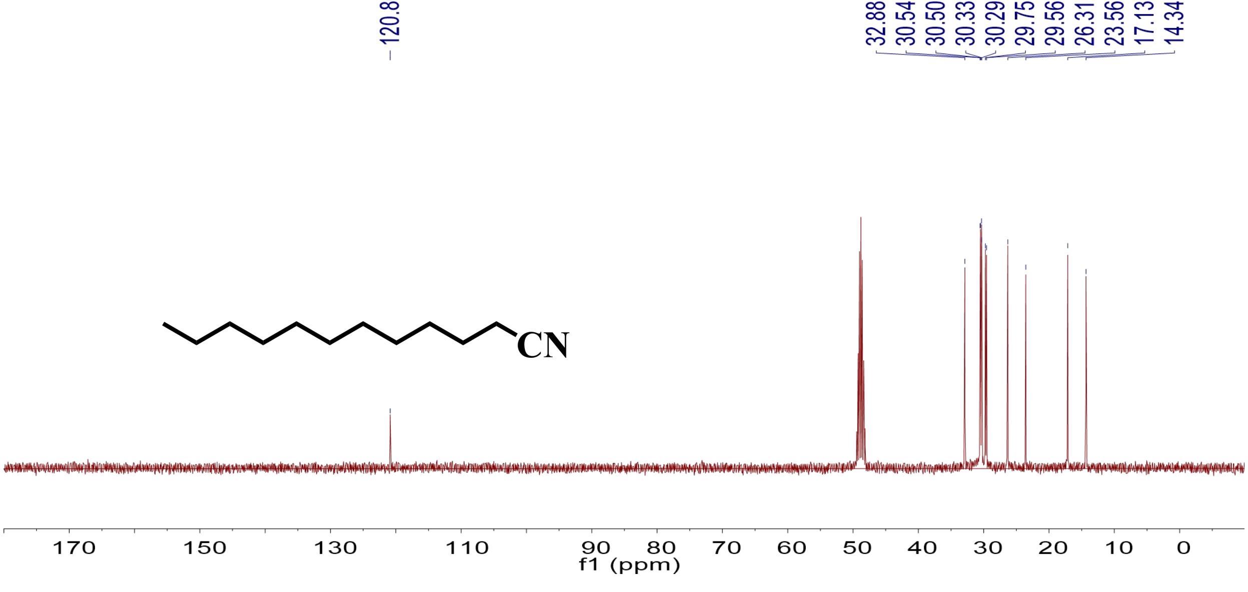
2.44
2.43
2.41
1.67
1.66
1.64
1.62
1.60
1.46
1.45
1.43
1.41
1.39
1.37
1.36
1.33
0.94
0.92
0.90
CN
2.00
10.36
2.84
6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)

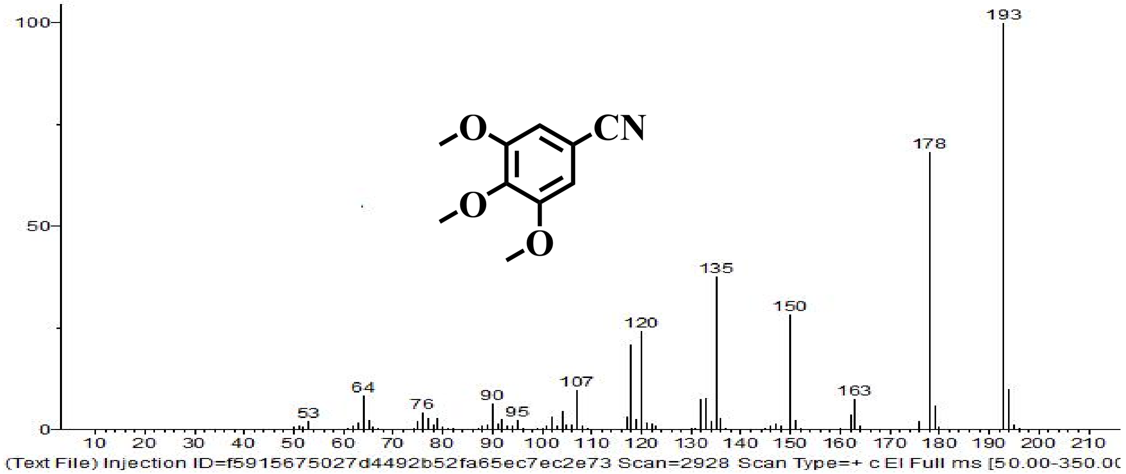


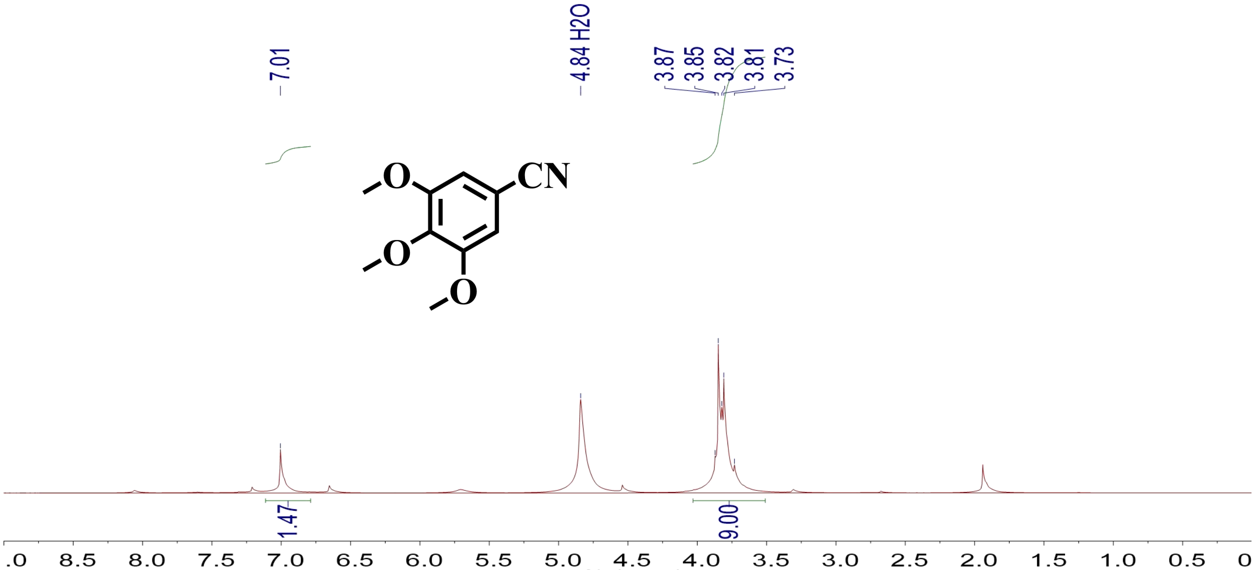
120.90
32.50
29.48
29.37
26.28
23.39
17.11
14.23
CN
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

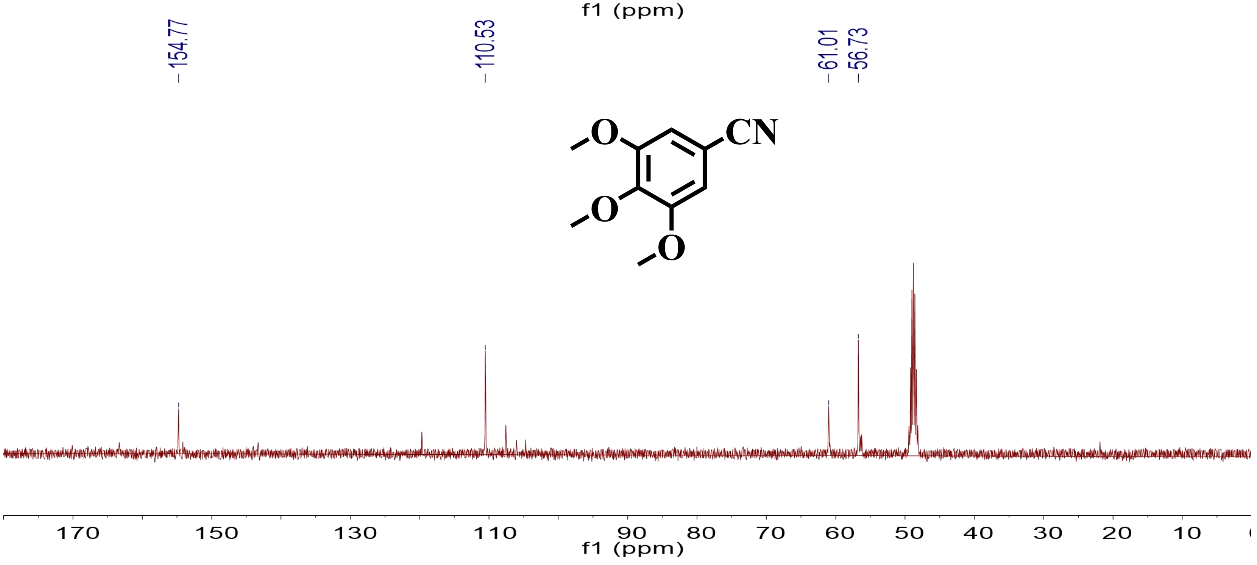

100
50
0
CN
96
110
82
124
138
57
69
152
79
93
166
180
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190
(Text File) Injection ID=485abb2cb8fb4661a3811a6165ab1915 Scan=2470 Scan Type=+ c EI Full ms [50.00-350.0

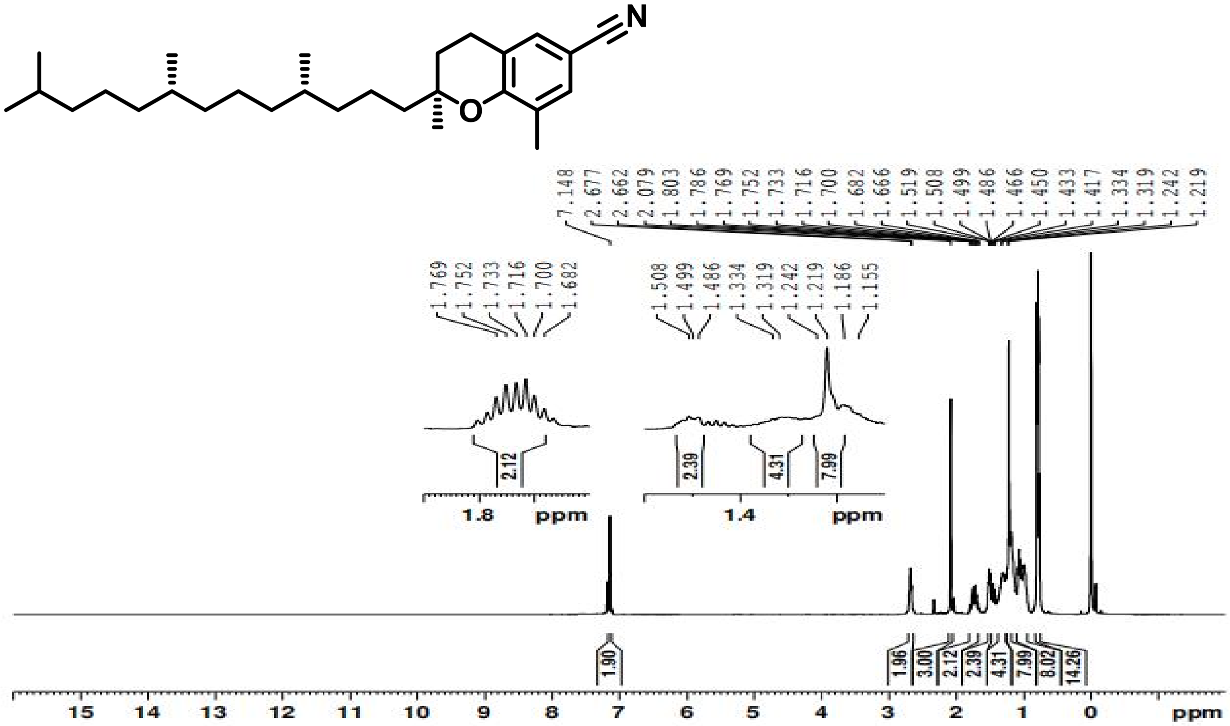

2.45
2.43
2.41
1.68
1.66
1.64
1.62
1.60
1.47
1.45
1.44
1.31
0.93
0.91
0.90
CN
2.43
16.00
2.77
.0 7.5 6.0 4.5 3.0 1.5 0.0 -1.5 -3.5
f1 (ppm)

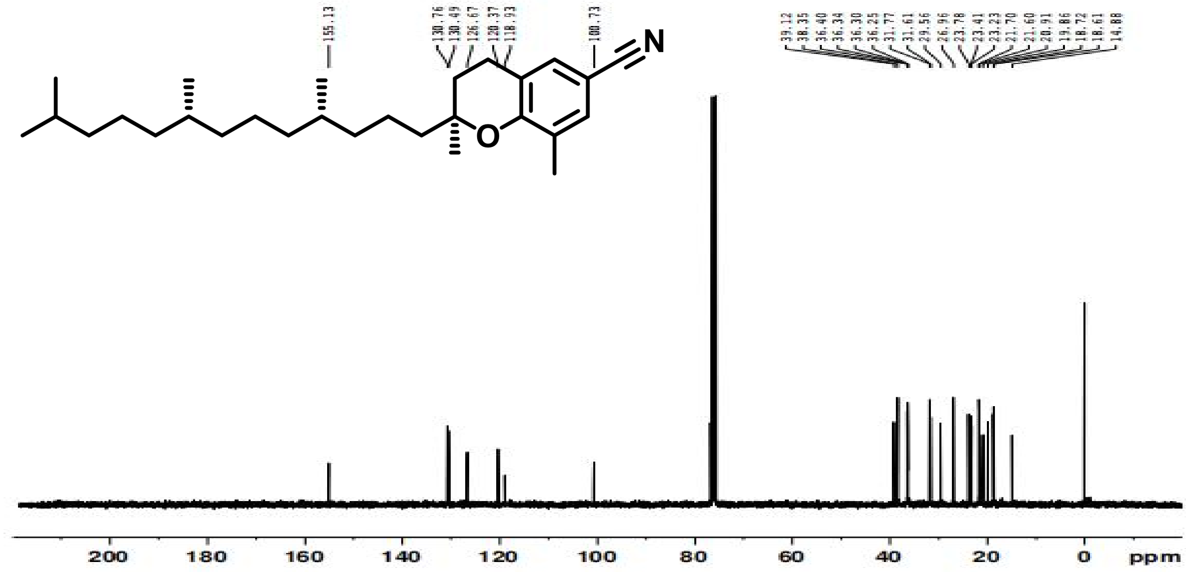

120.86
32.88
30.54
30.50
30.33
30.29
29.75
29.56
26.31
23.56
17.13
14.34
CN
170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


100
50
0
CN
O
O
O
193
178
135
150
120
107
163
64
76
90
95
53
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210
(Text File) Injection ID=f5915675027d4492b52fa65ec7ec2e73 Scan=2928 Scan Type=+ c EI Full ms [50.00-350.0


7.01
4.84 H2O
3.87
3.85
3.82
3.81
3.73
CN
O
O
O
1.47
9.00
.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
f1 (ppm)


154.77
110.53
61.01
56.73
CN
O
O
O
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)


N
O
7.148
2.677
2.662
2.079
1.803
1.786
1.769
1.752
1.733
1.716
1.700
1.682
1.666
1.519
1.508
1.499
1.486
1.466
1.450
1.433
1.417
1.334
1.319
1.242
1.219
1.769
1.752
1.733
1.716
1.700
1.682
2.12
1.8
ppm
1.508
1.499
1.486
1.334
1.319
1.242
1.219
1.186
1.155
2.39
4.31
7.99
1.4
ppm
1.90
1.96
3.00
2.12
2.39
4.31
7.99
8.02
14.26
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


N
O
155.13
130.76
130.49
126.67
120.37
118.93
100.73
39.12
38.35
36.40
36.34
36.30
36.25
31.77
31.61
29.56
26.96
23.78
23.41
23.23
21.70
21.60
20.91
19.86
18.72
18.61
14.88
200
180
160
140
120
100
80
60
40
20
0
ppm