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Electronic Supporting Information

Solvent tailored $Pd_3P_{0.95}$ nano catalyst for amide-nitrile inter-conversion, hydration of nitriles and transfer hydrogenation of >C=O bond

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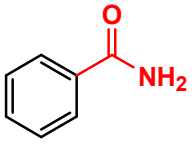
S1. Solubility of Complex and $Pd_3P_{0.95}$ (QD/Ps):

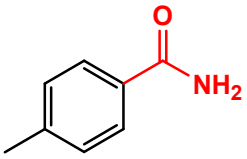
The complex $Pd(PPh_3)_2Cl_2$ shows good solubility in DMF, DMSO, $PhCH_3$,CH_3CN, $CHCl_3$ and CH_2Cl_2. It has been found sparingly soluble in CH_3OH and diethyl ether and negligibly in hexane. On the other hand $Pd_3P_{0.95}$ QD and $Pd_3P_{0.95}$ NPs have been found insoluble in DMF, DMSO, EtOH, H_2O, $CHCl_3$, CH_3CN, CH_2Cl_2,diethyl ether, hexane and CH_3OH. The complex as well as catalyst can be stored for three to four months in vacuo under desiccators.

S2. NMR Data of Compounds 2a-2j, 4a-4j and 6a-6k:

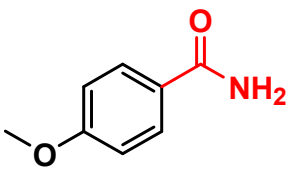
The NMR spectral data of compounds **2a- 2j**, **4a-4j**and **6a-6k**were found as reported in literature.[2-7]



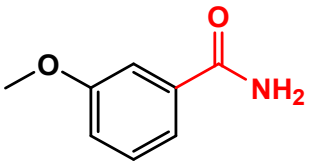
Benzamide (2a):[1]White solid (0.11 g, 92%). ^1H NMR (300 MHz, $CDCl_3$, 25 °C vsMe_4Si):δ7.82 (d, *J* = 6 Hz, 2H), 7.56-7.53 (m, 1H), 7.51-7.42 (m, 2H), 6.04 (bs, 2H).$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$,25 °C vsMe_4Si):δ 169.41, 133.38, 131.99, 128.62, 127.33.



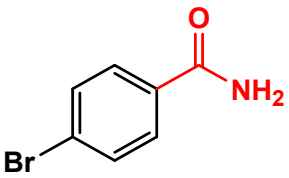
4-Methyl-benzamide (2b):[1]White solid (0.12 g, 86%). ^1H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 10.8 Hz, 2H), 6.10 (bs, 2H), 2.40 (s, 3H).$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ169.51, 142.48, 130.50, 129.24, 127.35, 21.44.



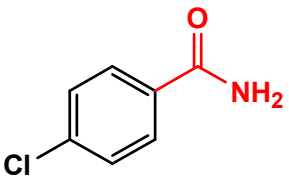
4-Methoxy-benzamide (2c):[1]White solid (0.13 g, 84%). ^1H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ7.71 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 5.83 (bs, 2H), 3.79 (s, 3H).$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 168.96, 162.60, 129.27, 125.59, 113.79, 55.41.



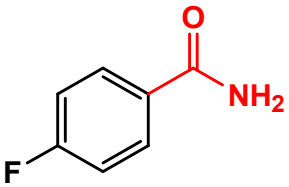
3-Methoxy-benzamide (2d):[1]White solid (0.11 g, 73%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.42 (s, 1H), 7.37-7.35 (m, 2H), 7.10-7.07 (m, 1H), 6.07 (bs, 2H), 3.87 (s, 3H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ169.31, 159.86, 134.81, 129.59, 119.16, 118.26, 112.60, 55.44.



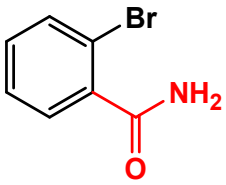
4-Bromo-benzamide (2e):[1]White solid (0.18 g, 91%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.59 (d, J = 8.7, 2H), 5.82 (bs, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 168.24, 132.13, 131.91, 128.95, 126.84.



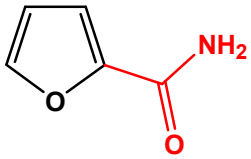
4-Chloro-benzamide (2f):[1]White solid (0.14 g, 90%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.43 (d, J = 8.4, 2H), 6.01 (bs, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 168.29, 138.36, 131.69, 128.92, 128.80.



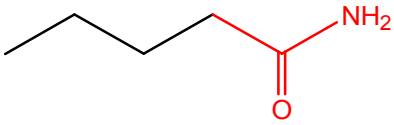
4-Fluoro-benzamide (2g):[1]White solid (0.12 g, 87%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.86-7.81 (m, 2H), 7.15-7.10 (t, *J* = 8.4, 2H), 6.06 (bs, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ168.36, 166.72, 129.81, 129.69, 115.83.



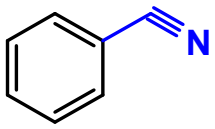
2-Bromo-benzamide (2h):[1]White solid (0.15 g, 74%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ7.66-7.61 (t, *J* = 7.5Hz, 2H), 7.41-7.36 (m, 1H), 7.33-7.28 (m, 1H), 6.24 (bs, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ169.31, 136.67, 133.56, 131.63, 129.90, 127.57, 119.18.



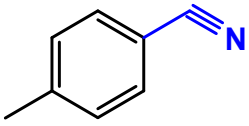
Furan-2-carbamide (2i):[1,4]Light yellow solid (0.083 g, 75%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ7.49 (s, 1H), 7.19 (s, 1H), 6.54 (s, 1H), 6.23-5.82 (bs, 2H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 160.08, 147.42, 144.40, 115.26, 112.31.



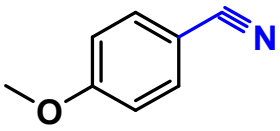
Pentanamide (2j):[1]White solid (0.075 g, 75%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ5.82 (bs, 2H), 2.28-2.23 (t,*J* = 7.52H), 1.69-1.59 (m, 2H), 1.45-1.33 (m, 2H), 0.97-0.92 (t,*J* = 7.2, 2H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 163.53, 35.62, 27.59, 22.33, 13.75.



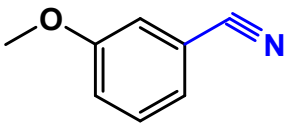
Benzonitrile (4a):[2]Colourless oil (0.091 g, 89%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 7.68 – 7.58 (m, 3H), 7.47 (t, *J* = 7.8 Hz, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ132.48, 132.13, 128.82, 118.50, 112.00.



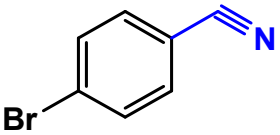
4-Methyl-benzonitrile (4b):[2]Colourless oil (0.10 g, 85%).[1]H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ7.50 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2H), 2.41 (s, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 143.48, 131.72, 129.60, 118.87, 109.00, 21.52.



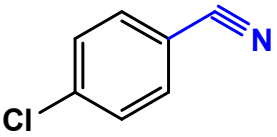
4-Methoxy-benzonitrile (4c):[2]White solid (0.11 g, 82%).[1]H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ7.52 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 162.64, 133.71, 119.05, 114.55, 103.68, 55.33.



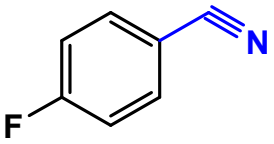
3-Methoxy-benzonitrile (4d):[2]Colourless oil (0.095 g, 72%). ^1H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 7.48-7.37 (m, 1H), 7.26-7.24 (m, 1H), 7.16-7.18 (m, 2H), 3.84 (s, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 159.38, 130.10, 124.15, 119.00, 118.45, 116.61, 112.93, 55.25.



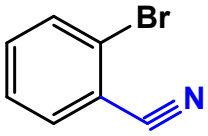
4-Bromo-benzonitrile (4e):[2]White solid (0.16 g, 88%). ^1H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 7.65-7.62 (m, 2H), 7.54-7.51 (m, 2H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 133.26, 132.47, 127.83, 117.88, 111.08.



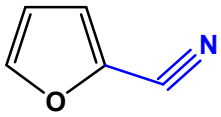
4-Chloro-benzonitrile (4f):[3]White solid (0.12 g, 86%).[1]H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ 7.60 (d, *J* = 9.0 Hz, 2H), 7.47 (d, *J* = 9.0, 2H).$^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ139.54, 133.35, 129.67, 117.93, 110.77.



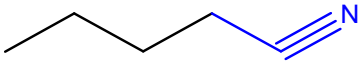
4-Fluoro-benzonitrile (4g):[4]White solid (0.10 g, 83%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 7.72-7.67 (m, 2H), 7.22-7.16 (m, 2H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ166.65, 134.54, 117.94, 116.62, 108.51.



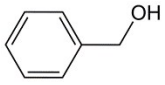
2-Bromo-benzonitrile (4h):[3]White solid (0.13 g, 71%).^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 7.71-7.65 (m, 2H), 7.48-7.43 (m, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 134.20, 133.85, 133.07, 127.57, 125.13, 117.01, 115.66.



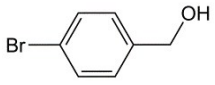
2-Furonitrile (4i):[4,5]Yellowoil (0.067 g, 72%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si):δ7.70 (s, 1H), 7.12 (s, 1H), 6.49 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 148.02, 144.45, 114.89, 112.51, 112.05.



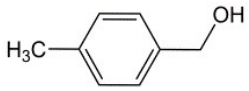
Pentanenitrile (4j):[6]Colourless oil (0.058 g, 70%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 2.32 (t,*J* =6.9,2H), 1.67-1.57 (m, 2H), 1.50-1.42 (m, 2H), 0.93 (t,*J* =7.2,3H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 °C vs Me_4Si): δ 119.65, 27.11, 21.60, 16.58, 12.98.



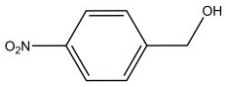
Phenylmethanol (6a):[7]Colourlessliquid (0.104 g, 97%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): *δ* (ppm): 1.93 (s, br 1H), 4.66 (s, 2H), 7.24-7.36 (m,5H), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): *δ* (ppm)65.33, 127.00, 127.65, 128.57, 140.88.



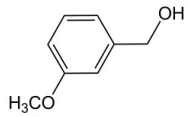
(4-bromophenyl)methanol (6b):[7]White solid (0.173 g, 97%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ(ppm): 1.60 (s, br, 1H), 4.66 (s, 2H), 7.24 (d, 2H, J = 9 Hz), 7.48 (d, 2H, J = 9 Hz), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 64.60, 121.46, 128.58, 131.64, 139.79.



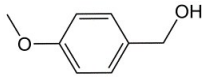
***p*-Tolylmethanol (6c)**:[7]White solid (0.112 g, 92%). ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 1.63 (s, br, 1H), 2.35 (s, 3H), 4.64 (s, 2H), 7.17 (d, 2H, J = 9 Hz), 7.26 (d, 2H, J = 9 Hz), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 21.13, 65.30, 127.12, 129.25, 137.41, 137.93



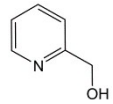
(4-Nitrophenyl)methanol (6d):[7]Yellow solid (0.140 g, 96%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 1.96 (br, 1H), 4.85 (s, 2H), 7.54 (d, 2H, J = 9 Hz), 8.23 (d, 2H, J = 9 Hz), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 64.00, 123.73, 127.00, 147.32, 148.16.



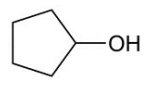
(3-methoxyphenyl)methanol (6e):[7]Colourlessliquid (0.131 g, 95%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 2.14 (s, br, 1H), 3.79 (s, 3H), 4.64 (s, 2H), 7.26 (t, 1H, J = 9 Hz), 6.80-6.93 (m, 3H), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 55.23, 65.17, 112.28, 113.25, 119.13, 129.59, 142.58, 159.83



(4-methoxyphenyl)methanol (6f):[7]Colourlessliquid (0.131 g, 95%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 2.17 (br, s, 1H), 3.78 (s, 3H), 4.56 (s, 2H), 6.86 (d, 2H, J = 8.4 Hz), 7.25 (d, 2H, J = 8.4 Hz), ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 55.29, 64.88, 113.94, 128.63, 133.20, 159.16

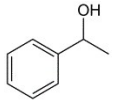


pyridine-2-ylmethanol (6g):[7] Yellowliquid (0.102 g, 94%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm): 1.65 (br, 1H), 4.77 (s, 2H), 7.21 (m, 2H), 7.66-7.71 (m, 1H), 8.57 (d, 1H),

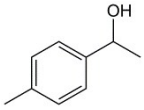


$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 64.33, 120.72, 122.25, 136.79, 148.46, 159.71.

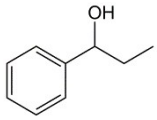
cyclopentanol (6h):[7] Colorless liquid (0.077 g, 90%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.55-1.58 (m, 4H) 1.75-1.78 (m, 4H), 2.03 (br, s, 1H), 4.31-4.34 (m, 1H), $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 23.26, 35.52, 73.96.



1-phenylethanol (6i):[7] Colorless liquid (0.108 g, 89%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.43 (d, 3H, J = 6.3 Hz), 2.56 (s, 1H), 4.78-4.80 (m, 1H), 7.22-7.31 (m, 5H), $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 25.16, 70.29, 125.46, 127.41, 128.48, 145.92.



1-(*p*-tolyl)ethanol (6j):[7] Colorless liquid (0.116 g, 86%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 1.47 (d, 3H, J = 6.3 Hz), 1.87 (s, 1H), 2.33 (s, 3H), 4.84-4.87 (m, 1H), 7.15 (d, 2H, J = 7.8 Hz), 7.26 (d, 2H, J = 7.8 Hz)$^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 21.07, 25.07, 70.24, 125.35, 129.16, 137.14, 142.89.



1-phenylpropan-1-ol (6k):[7]Colorless liquid (0.112 g, 83%).^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 0.90 (t, 3H, J = 7.29), 1.67-1.84 (m, 2H), 2.12 (br, 1H), 4.55 (t, 1H, J = 6.12 Hz), 7.29-7.33 (m, 5H), $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 25 ºC, TMS): δ (ppm) 10.14, 31.87, 76.00, 126.01, 127.48, 128.39, 144.62.

S3. SEM–EDX Data:

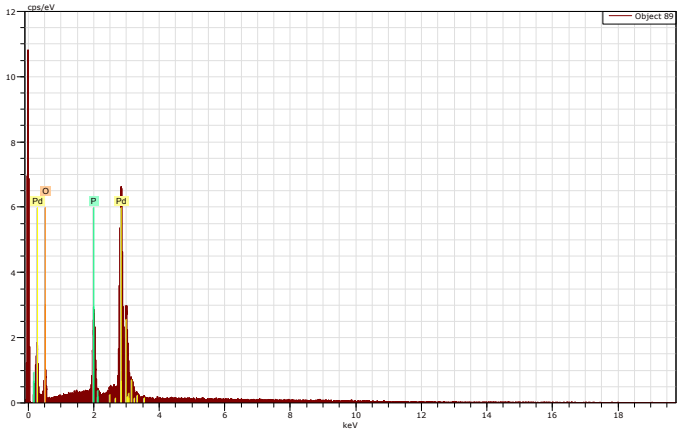


Figure S1. SEM-EDX of $Pd_3P_{0.95}$ QDs.

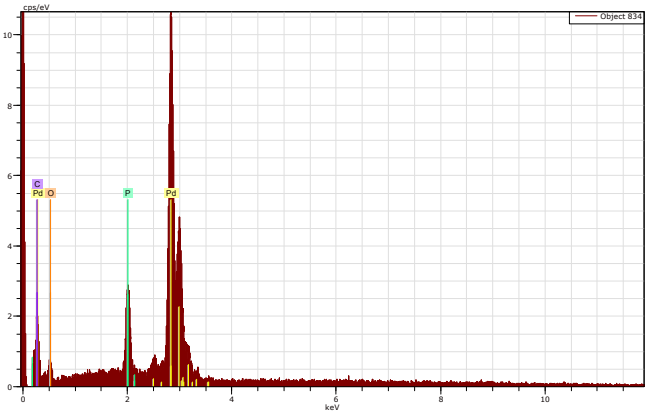


Figure S2. SEM-EDX of $Pd_3P_{0.95}$ NPs.

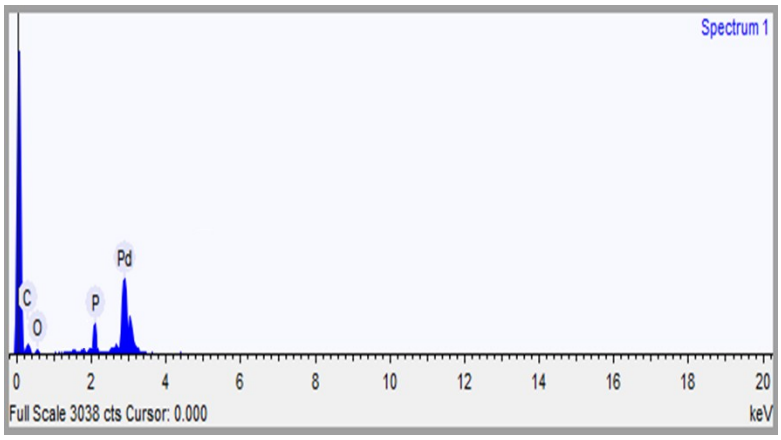


Figure S3. SEM-EDX of $Pd_3P_{0.95}$ QDs after 3rd reaction cycle.

S4. Powder–XRD Data

The powder X-ray diffraction pattern of $Pd_3P_{0.95}$ QDs and NPs (Figure 2a,2b, and S3) was indexed on the basis of a orthorhombic unit cell[6] (JCPDS # 89-3046) with the d values (*hkl*): 2.77 (210), 2.69 (121), 2.58 (201), 2.44 (211), 2.36 (102), 2.32 (220), 2.25 (112), 2.23 (031), 2.12 (221), 2.09 (131), 1.99 (122), 1.90 (230), 1.85 (301), 1.51 (123), 1.42 (401).

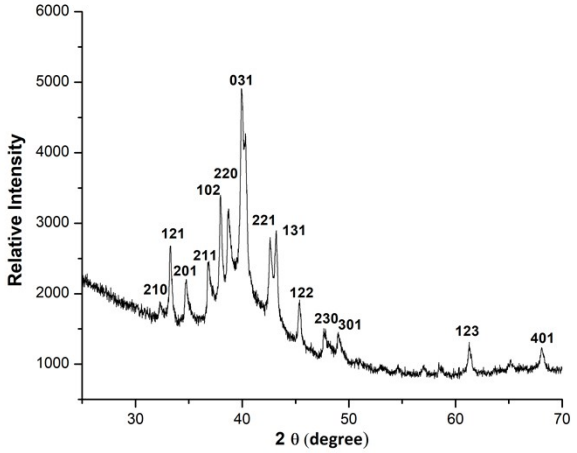


Figure S4. PXRD of $Pd_3P_{0.95}$ QDs after 3rd reaction cycle.

S5. X-ray photoelectron spectra

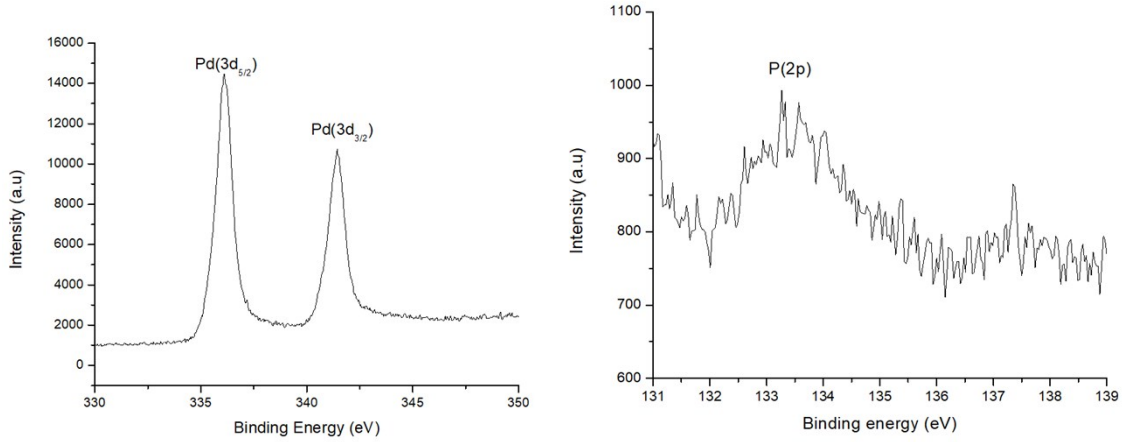


Figure S5. X-ray photoelectron spectra for recycled $Pd_3P_{0.95}$QDs

S6. Size Distribution Curve:

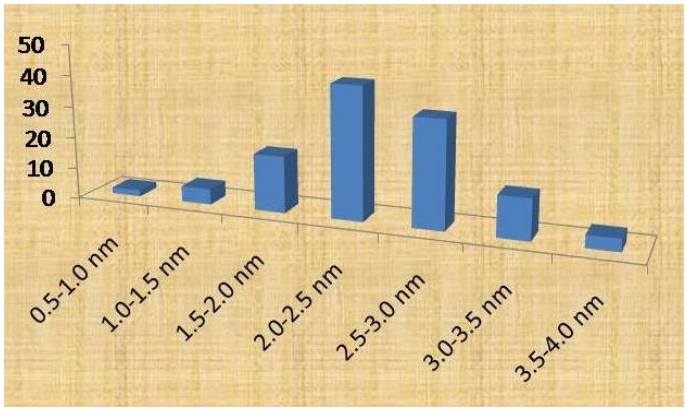


Figure S6. Size distribution curve of $Pd_3P_{0.95}$ QDs.

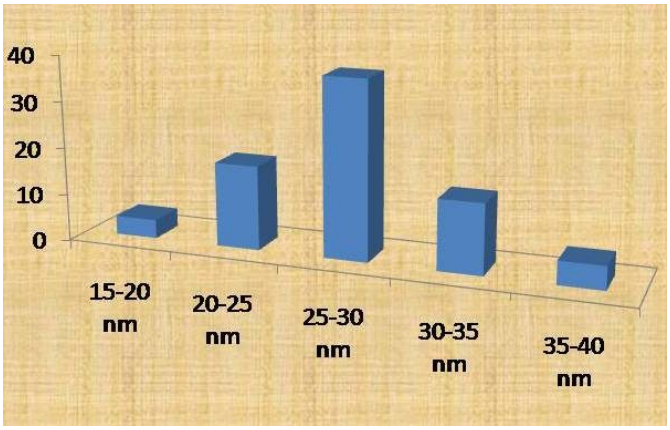


Figure S7. Size distribution curve of $Pd_3P_{0.95}$ NPs.

S7. Temperature Dependant P^{31} NMR Spectra

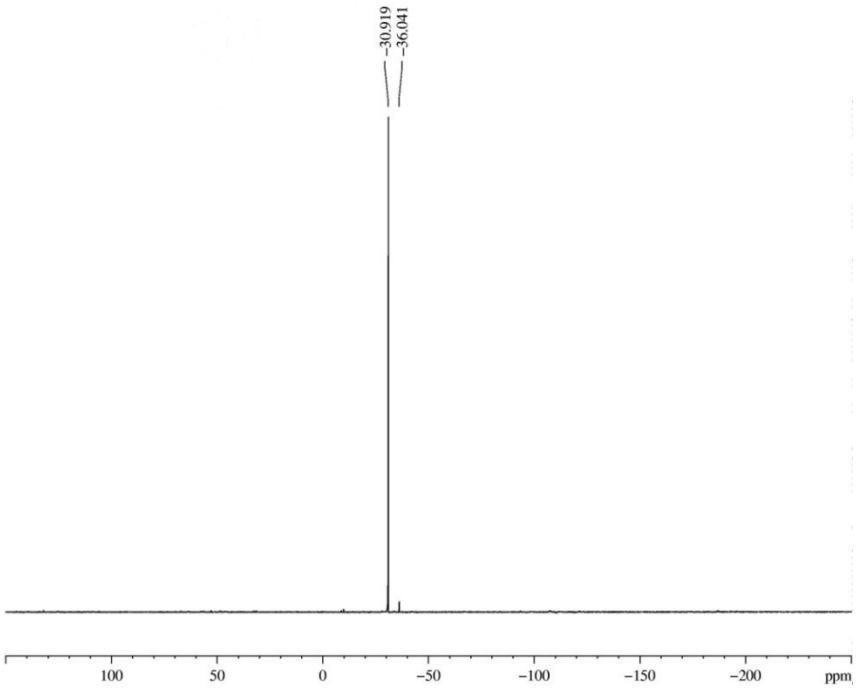


Figure S8. $P^{31}\{^1H\}$ NMR of TOP.

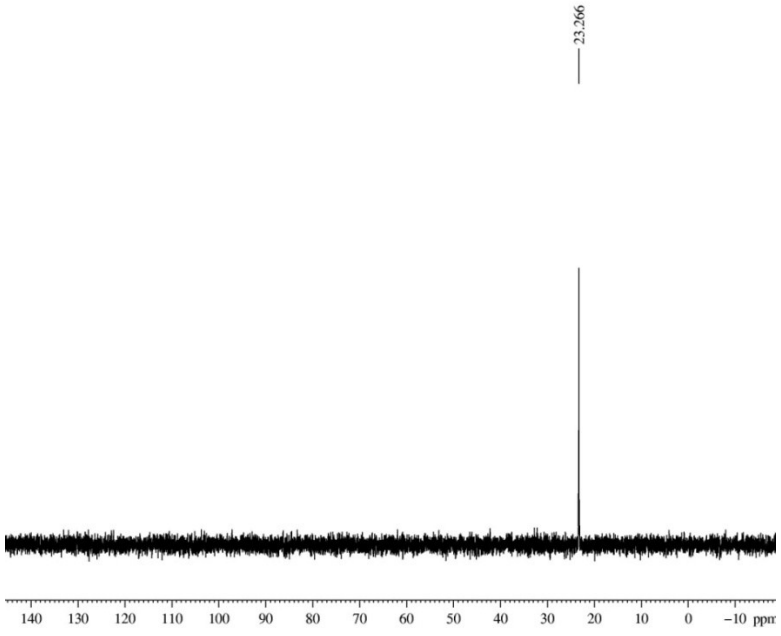


Figure S9. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ complex.

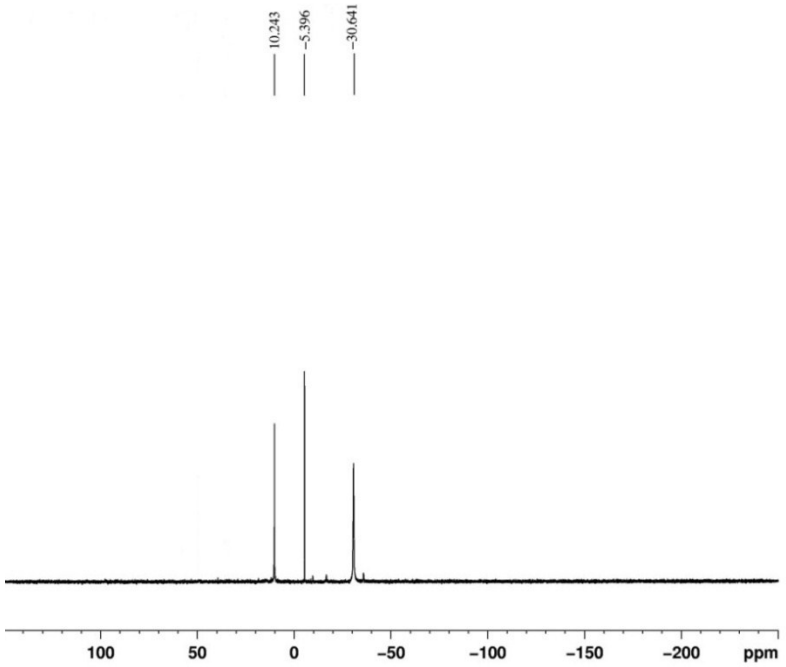


Figure S11. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in TOP at 100 °C.

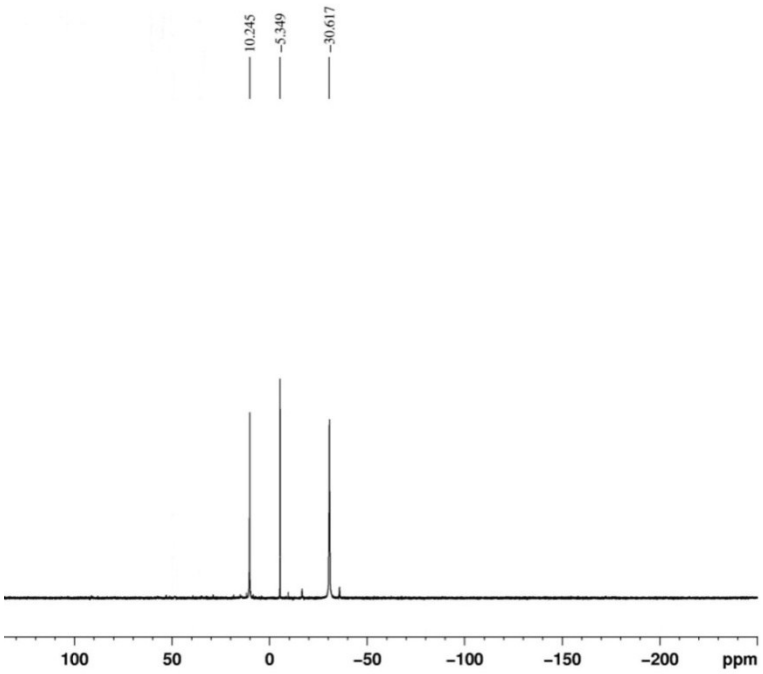


Figure S12. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in TOP at 220 °C.

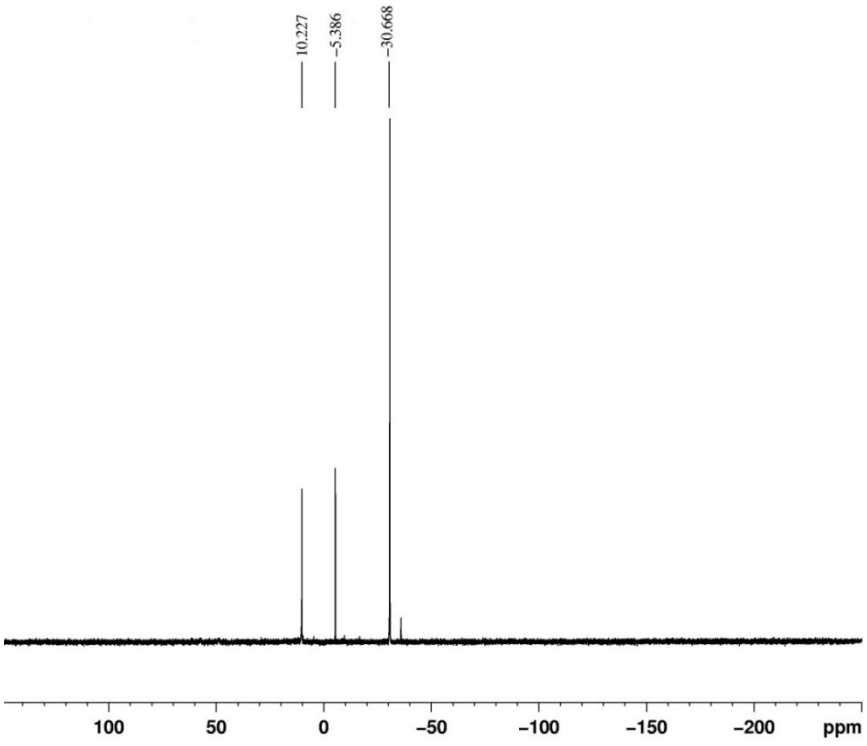


Figure S13. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in TOP at 270 °C.

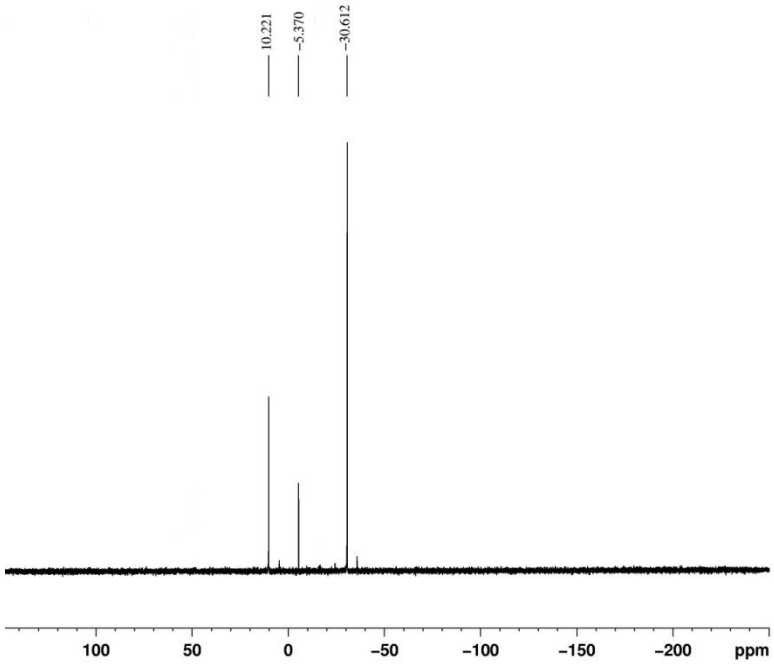


Figure S14. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in TOP at 280 °C.

Figure S15. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in OA+ODE at RT.

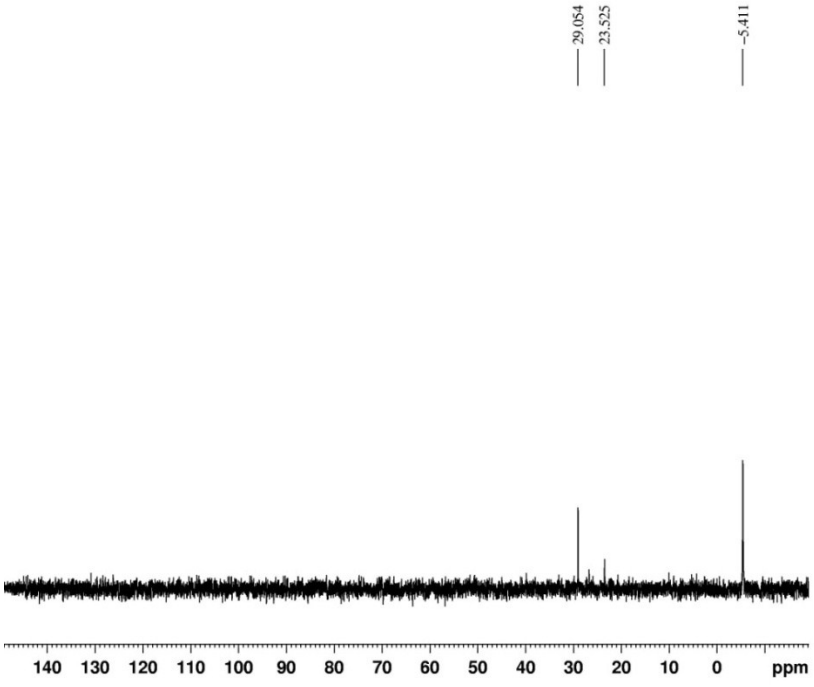
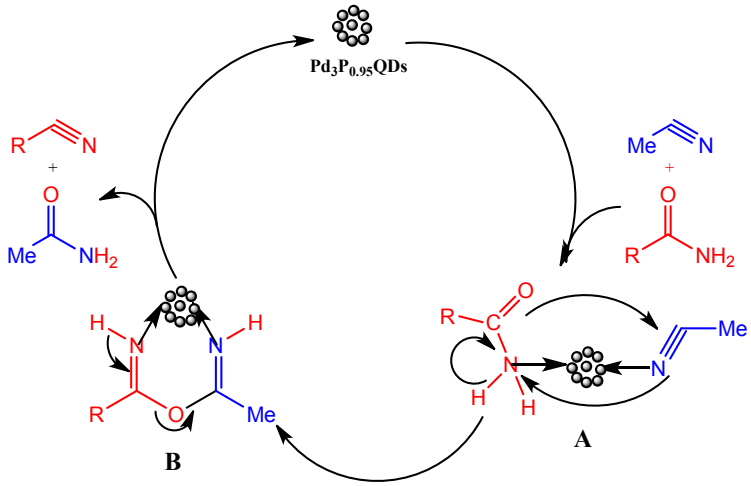


Figure S16. $P^{31}\{^1H\}$ NMR of $[Pd(PPh_3)_2Cl_2]$ in OA+ODE at 200 °C.

S8. Tentative mechanism of amide-nitrile interconversion



Scheme S1. Tentative mechanism of amide-nitrile interconversion with $Pd_3P_{0.95}$ QDs.

Table S1. Comparison of activity with other catalyst for hydration of nitriles

S. No.	Catalyst	Solvent	Time (h)	Catalyst Loading (mol%)	T (°C)	Reusability
1[8]	$Pd(OAc)_2$ + TBA-SiW10	DMF+ H_2O	5-48	5	90	
2[9]	Pd/C	H_2O	24	2-3	120-135	3
3[10a]	Ag NPs	H_2O	1-6	0.3		3
4[10b]	AgHAP	H_2O			140-280	4
5[11]	Os-NHCs Catalyst	H_2O/2 Propanol with base	0.5-24	3		
6[12a]	[{Au(IPr)}$_2$(m-OH)]X	THF: H_2O	2	2	140	1
7[12b]	[(IPr)Au(NTf_2)]	THF: H_2O	2	2	140	
8[13]	CeO_2	H_2O+Acetone /H_2O+Isopropyl alcohol	0.25-24			
9[14]	MnO_2	H_2O	2-20 (min)	600		
10[15]	NiNPs/HT (hydrotalcite-clay supported)	H_2O	10-24		150-170	1
12[20]	Ag NPs	H_2O + Toluene	1-6		150-170	5
13	$Pd_3P_{0.95}$ (Present work)	Water	4 h	2 mol %	90	4

Table S2. Comparison of activity with other catalyst for TH of carbonyl compounds

S. No.	Catalyst	H-Source	Time (h)	Catalyst Loading (mol%)	Temperature (°C)	Reusability
1[16]	Ru/C	2 Propanol	10	5	120-200	
2[17]	Pd/Fe_2O_3	2 Propanol	7.5	10	180	
3[18]	Pd/Urea-MCF catalyst	Ammonium formate	12-24	10	60	10
4[19]	Polyurea-encapsulated palladium	Formic acid	18-48	10	24	5
5[20]	Silica-supported mesoporous Rh catalysts	Sodium formate	1	4	40	3
6	$Pd_3P_{0.95}$ (Present work)	2-Propanol	3	1	80	6

S9. References

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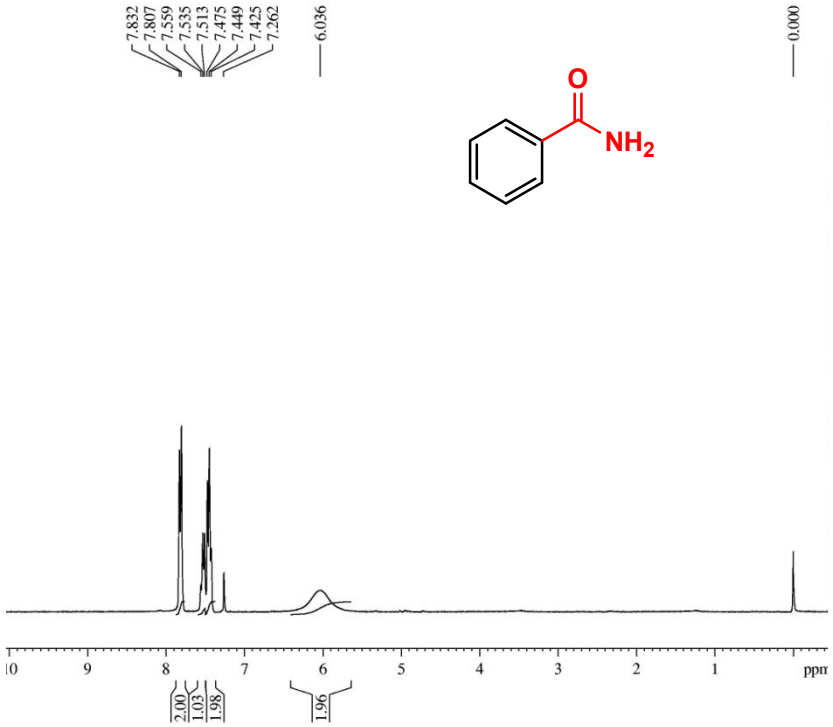
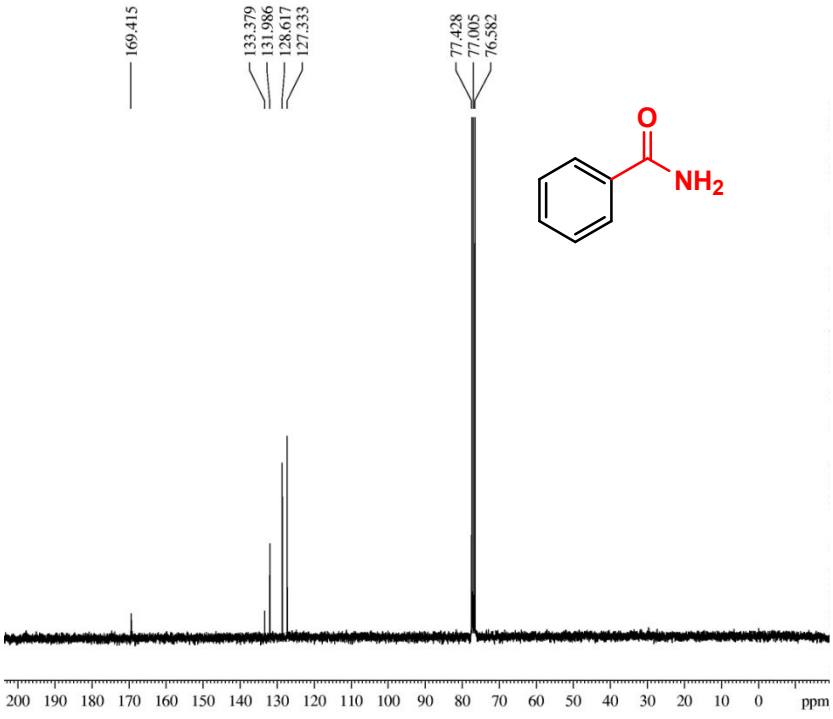
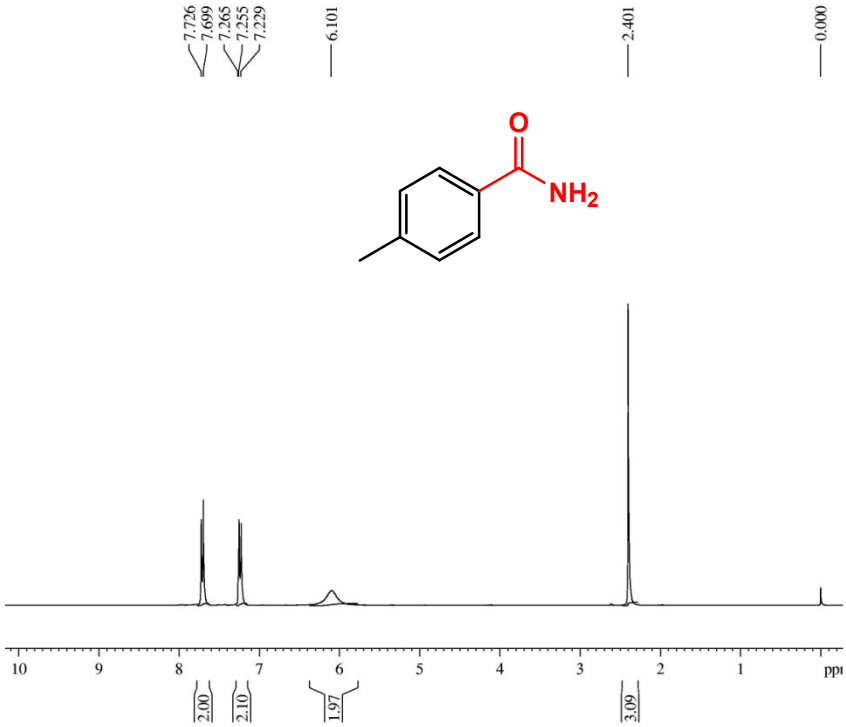
S10. NMR spectral data of compounds



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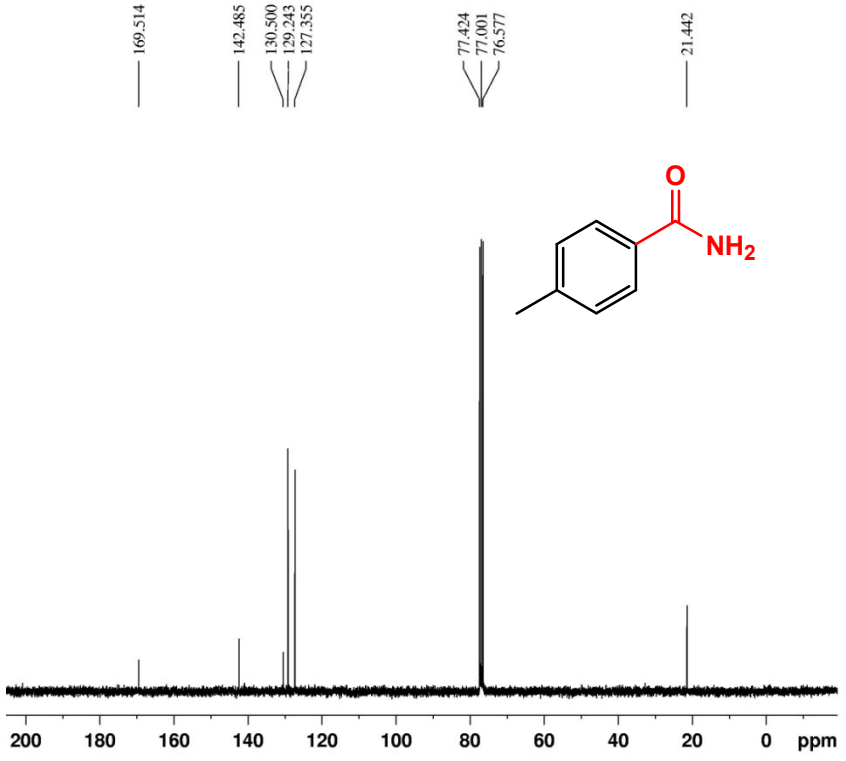
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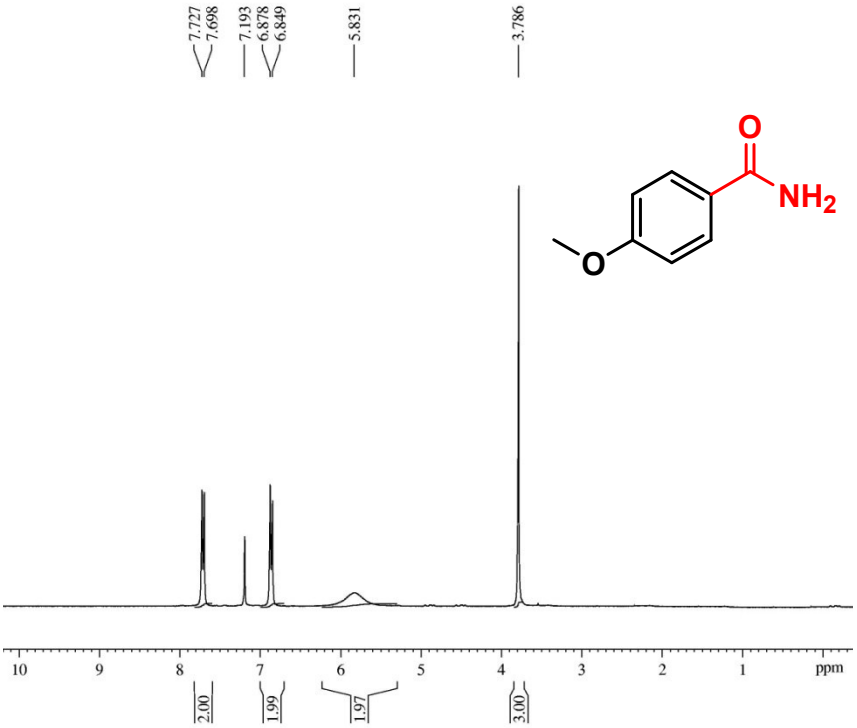
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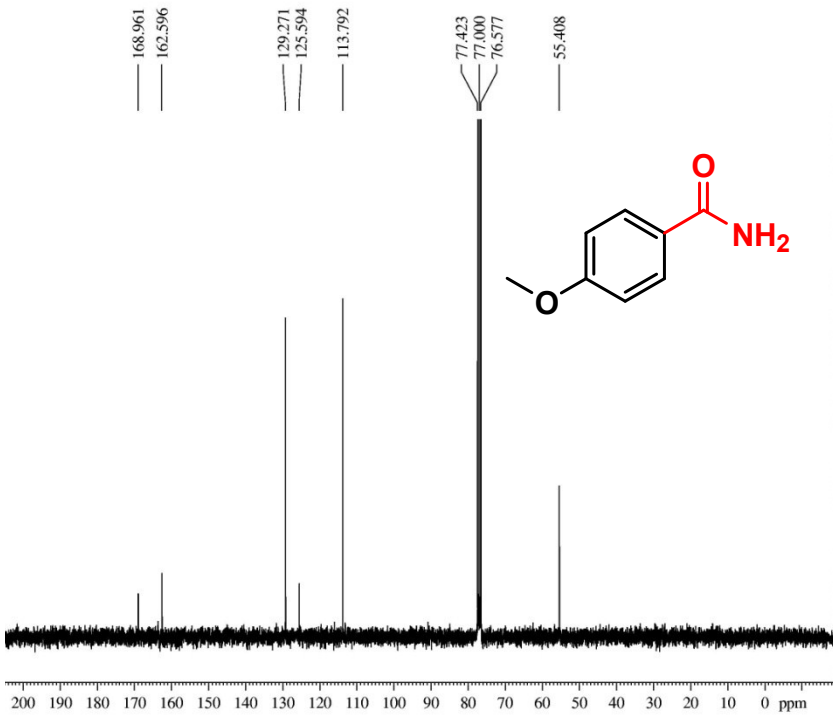
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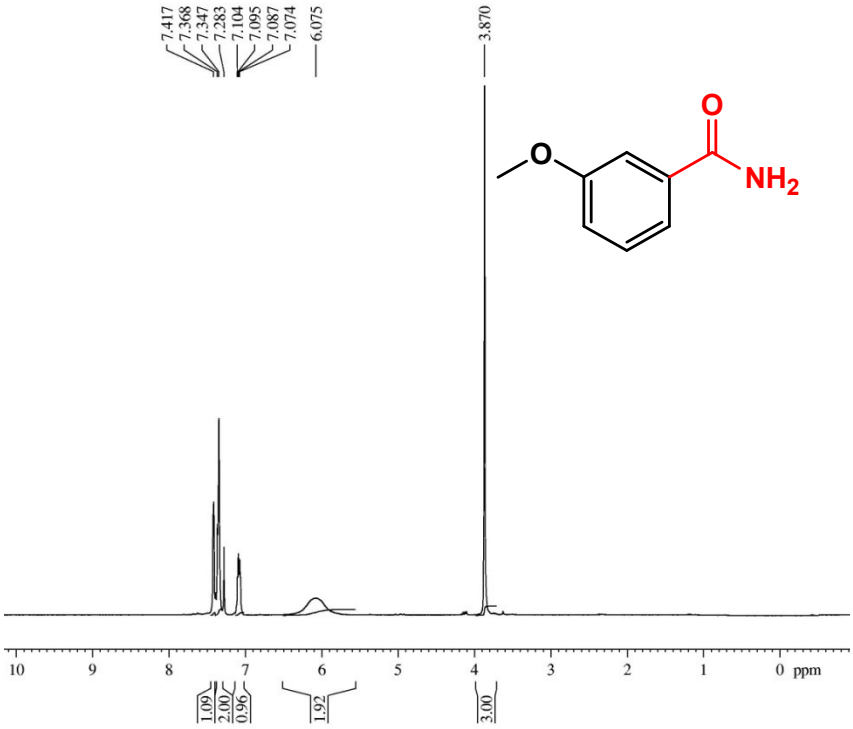
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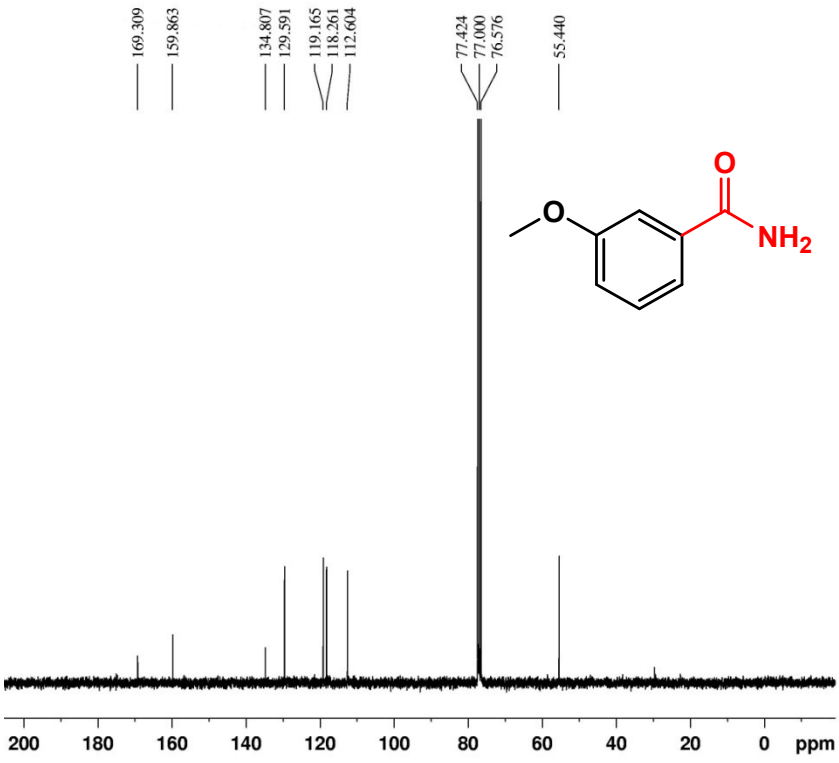
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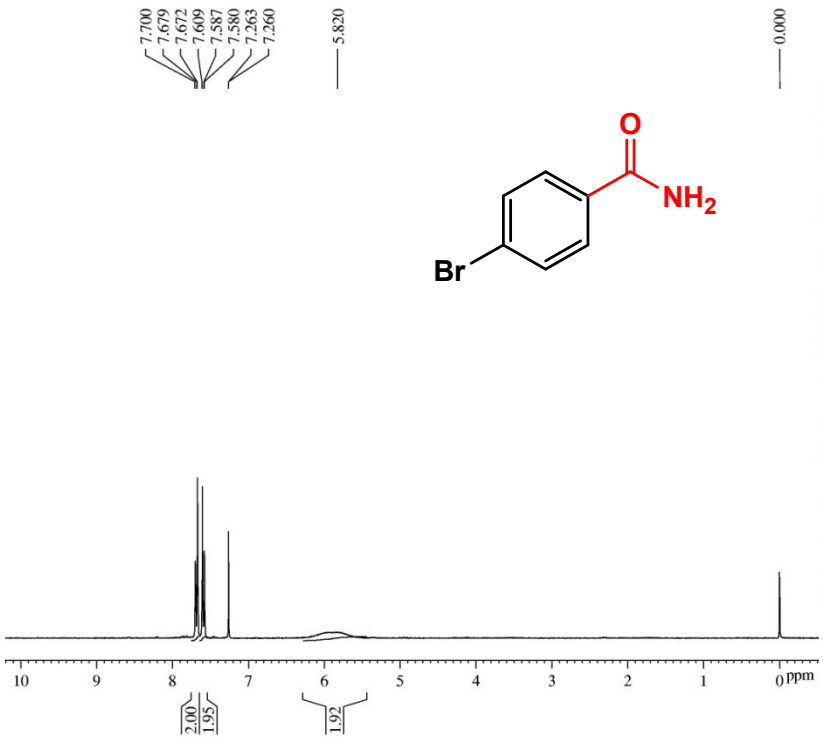
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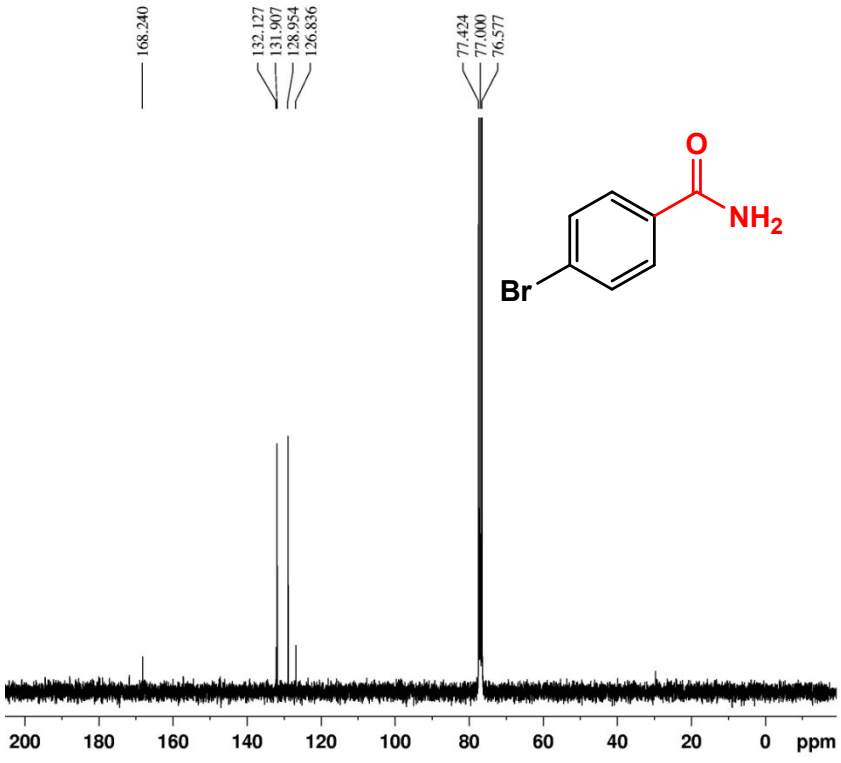
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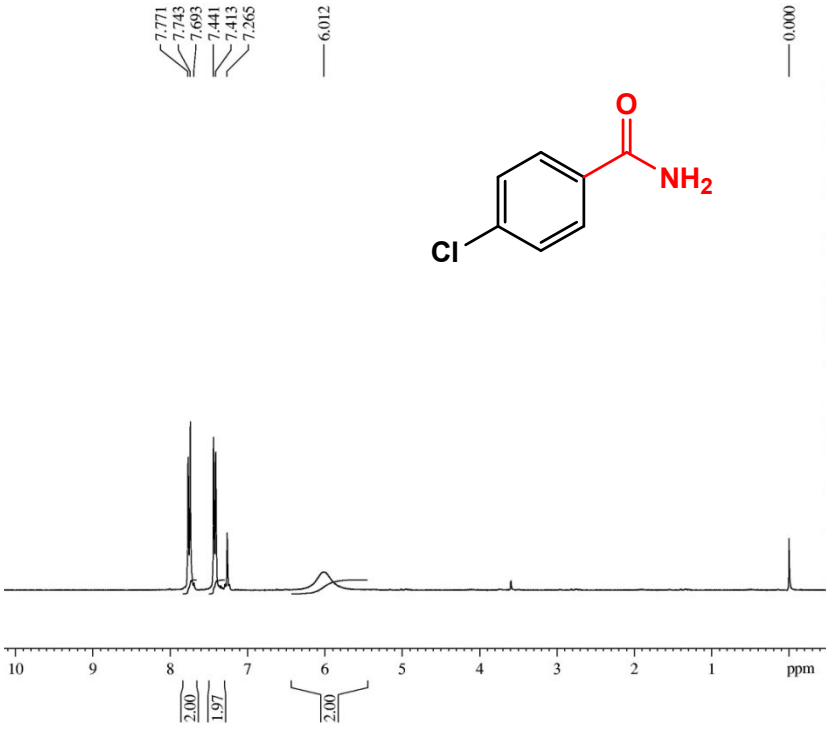
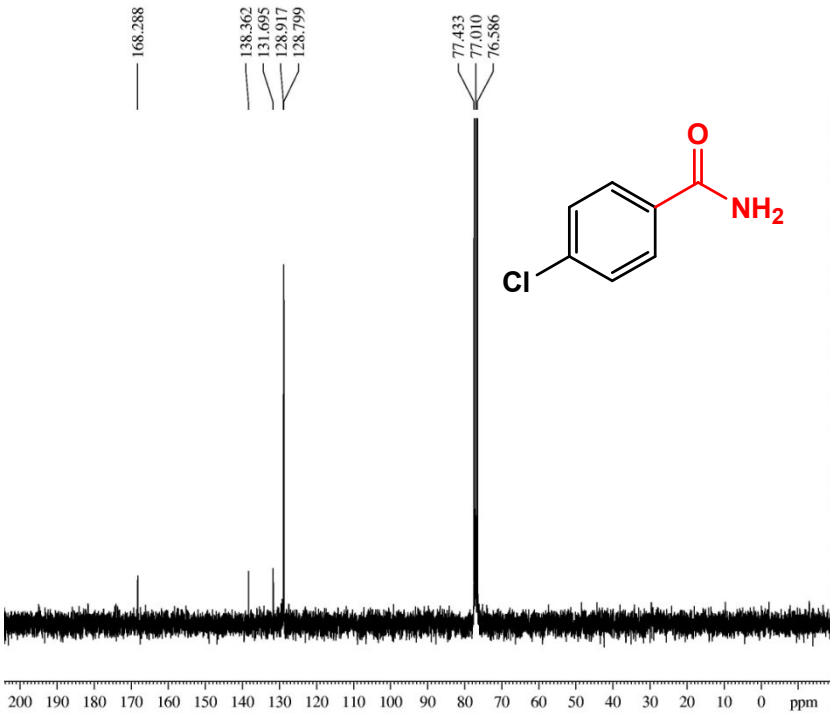
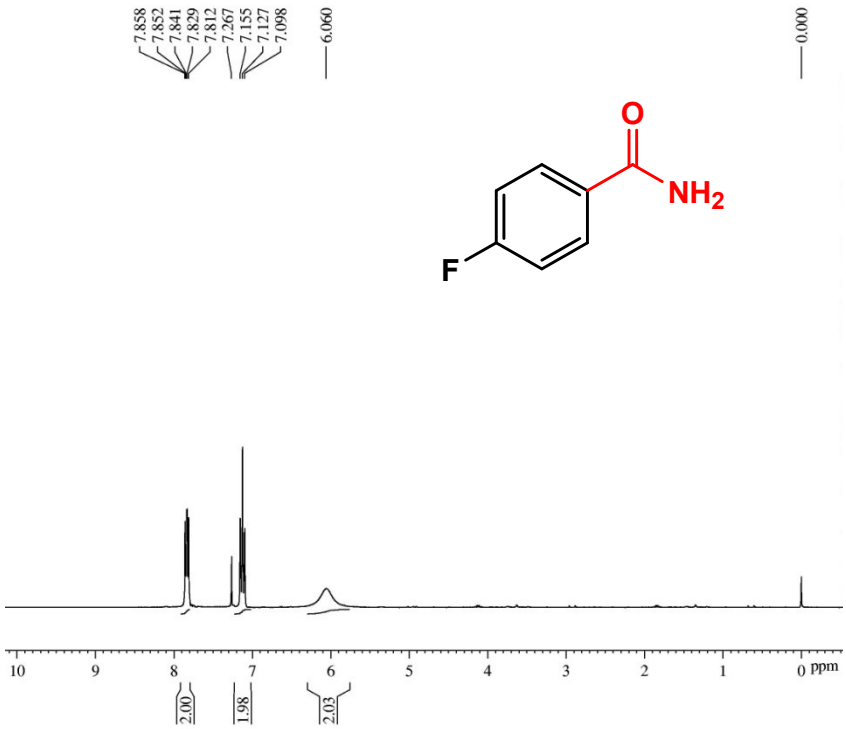
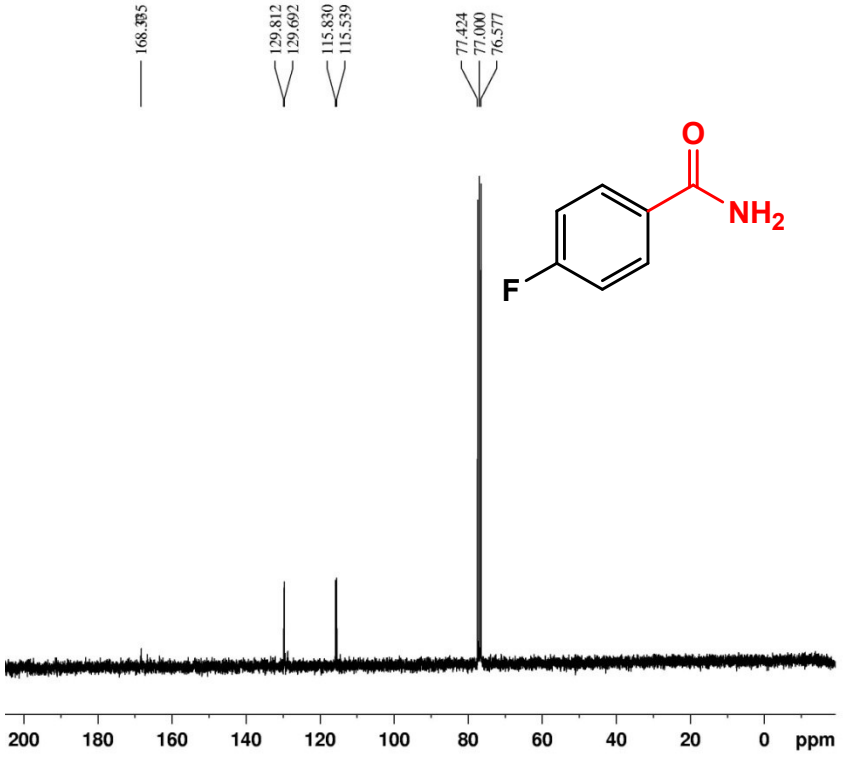
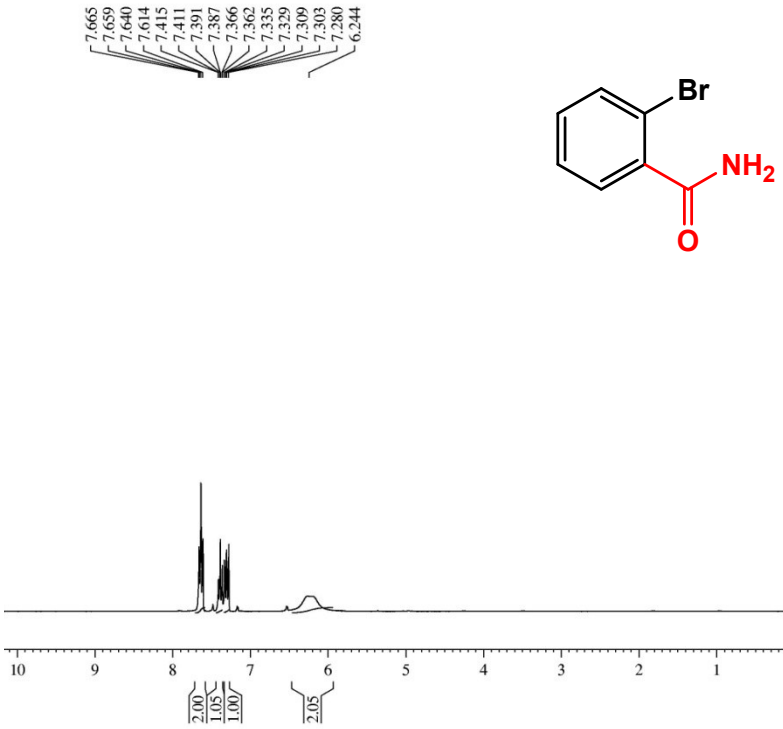
ppm

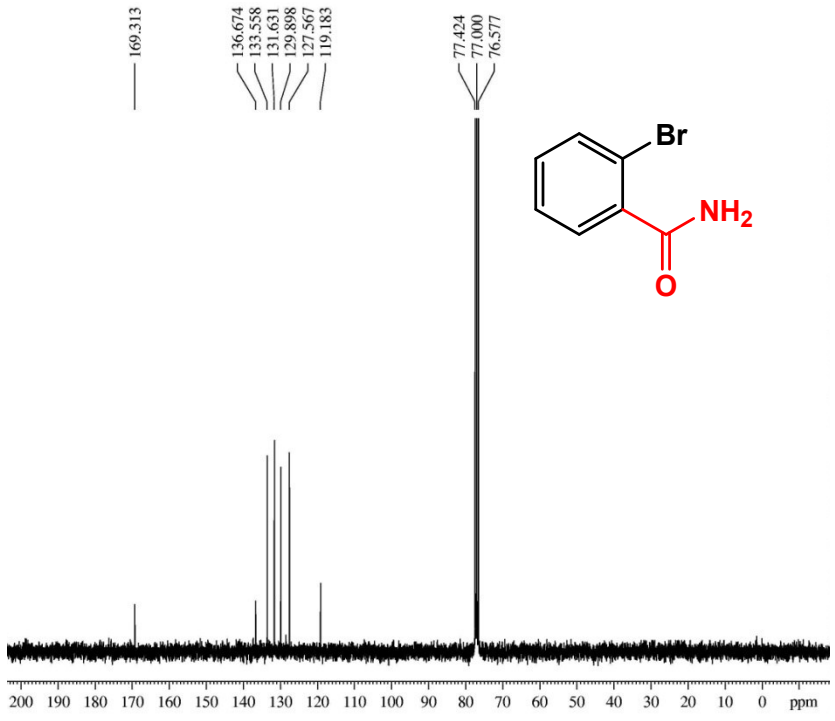

7.771
7.743
7.693
7.441
7.413
7.265
6.012
0.000
O
NH2
Cl
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.97
2.00

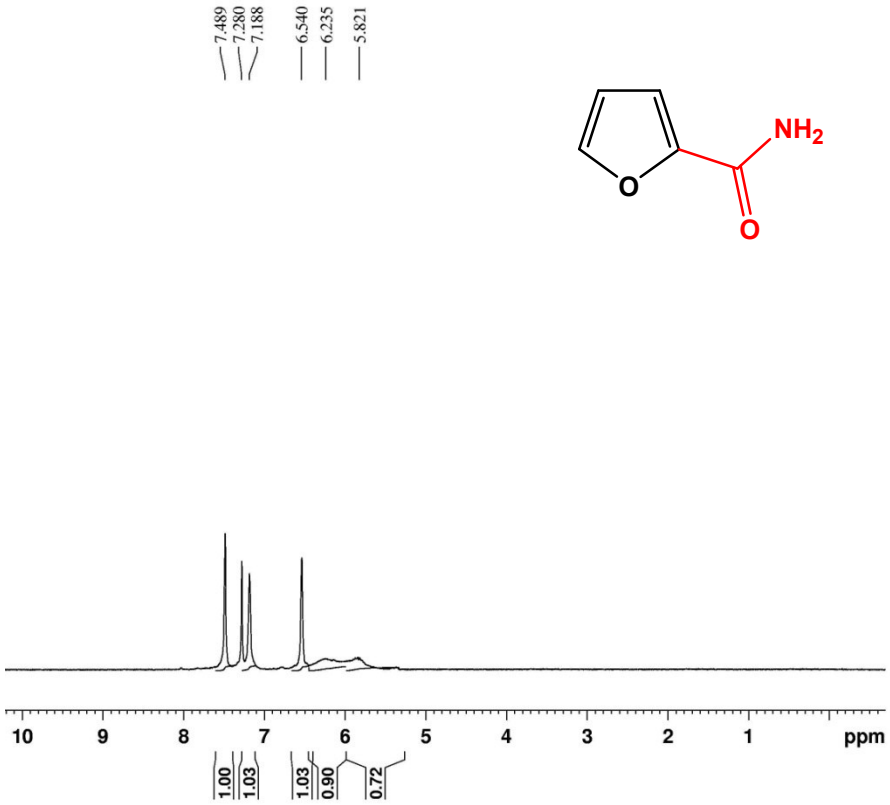

168.288
138.362
131.695
128.917
128.799
77.433
77.010
76.586
O
NH2
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

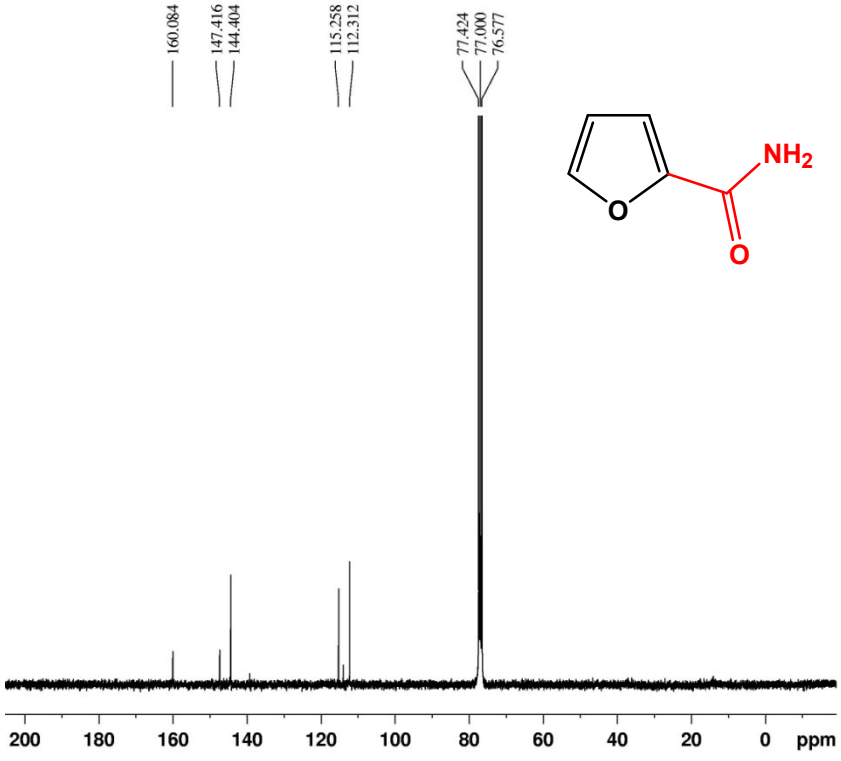

7.858
7.852
7.841
7.829
7.812
7.267
7.155
7.127
7.098
6.060
0.000
O
NH2
F
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.98
2.03

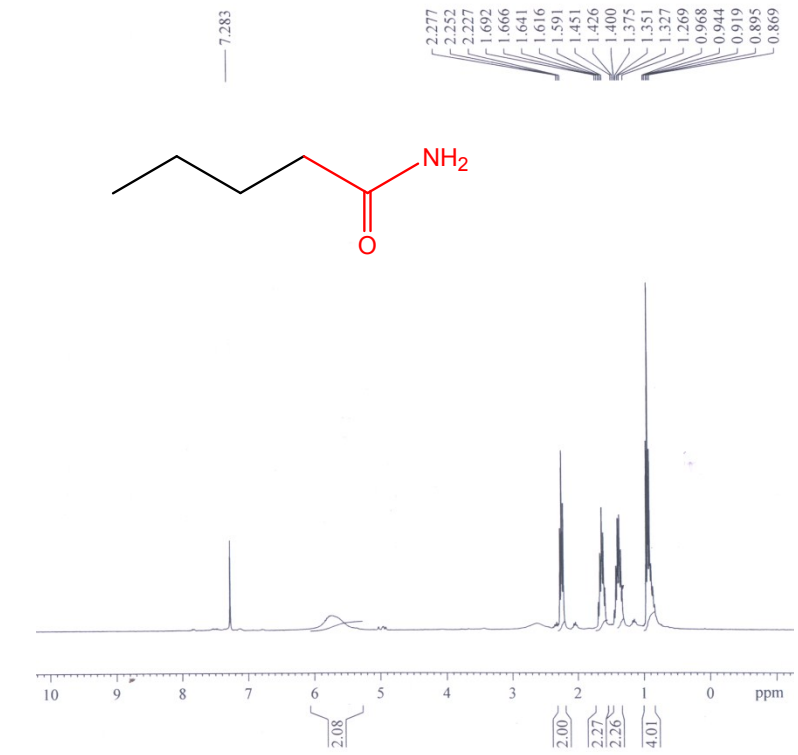

168.385
129.812
129.692
115.830
115.539
77.424
77.000
76.577
O
NH2
F
200
180
160
140
120
100
80
60
40
20
0 ppm

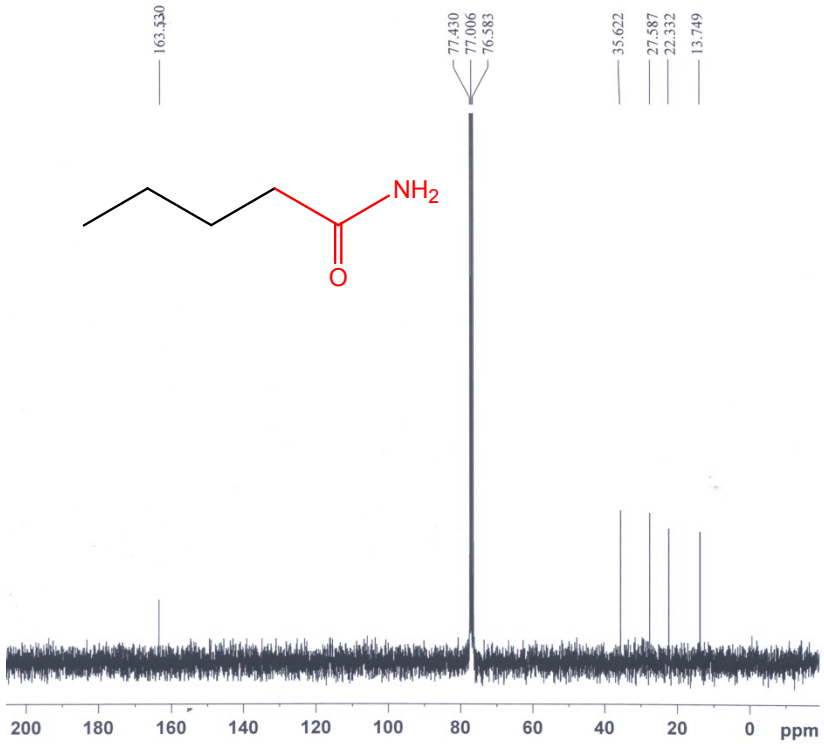

7.665
7.659
7.640
7.614
7.415
7.411
7.391
7.387
7.366
7.362
7.335
7.329
7.309
7.303
7.280
6.244
Br
NH2
O
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.05
1.00
2.05

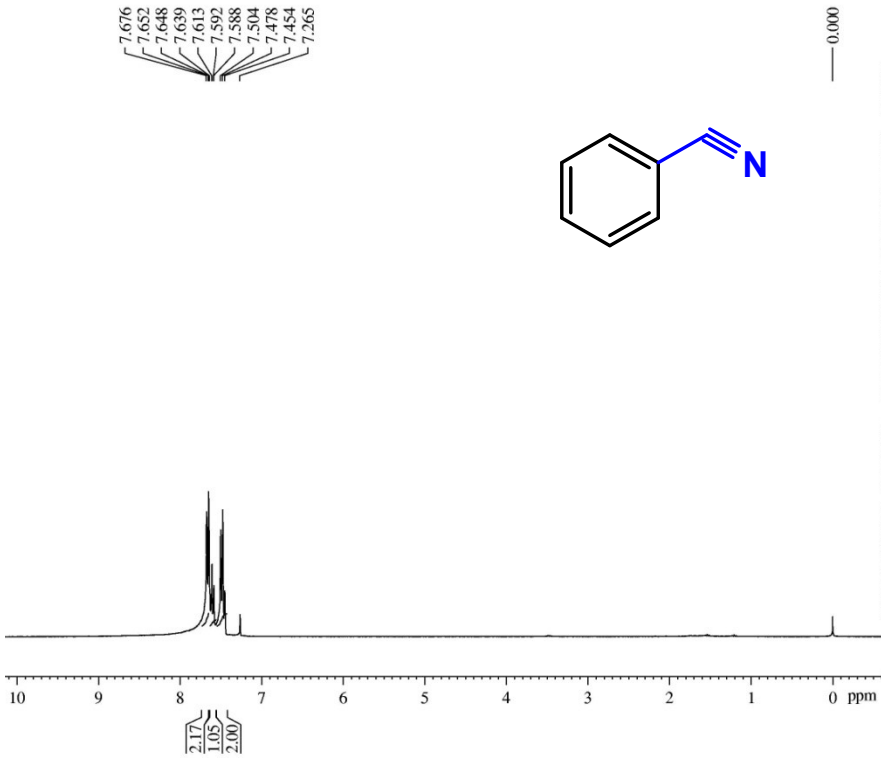

169.313
136.674
133.558
131.631
129.898
127.567
119.183
77.424
77.000
76.577
Br
NH2
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

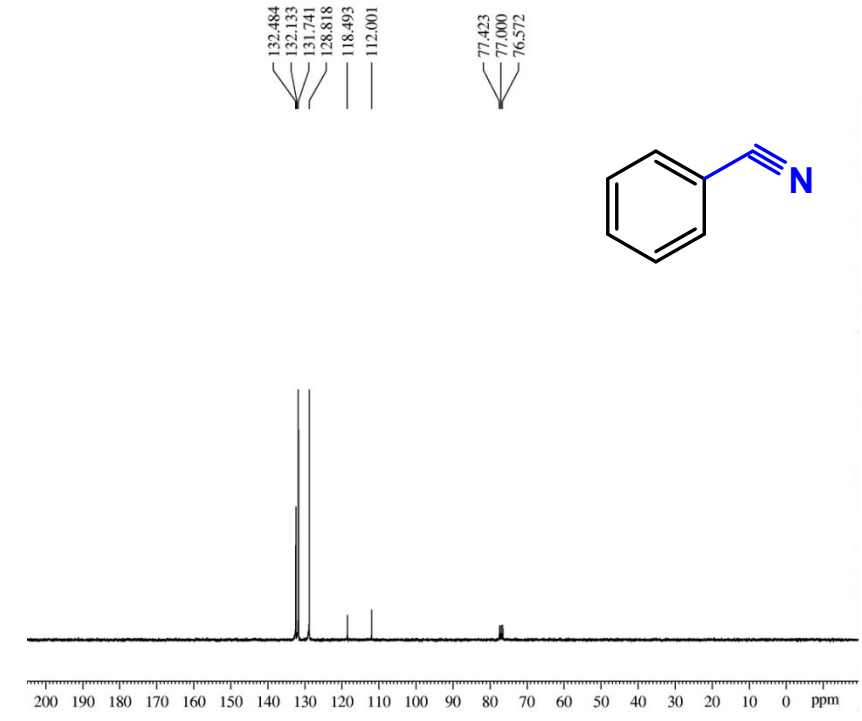

7.489
7.280
7.188
6.540
6.235
5.821
NH2
O
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.03
0.90
0.72

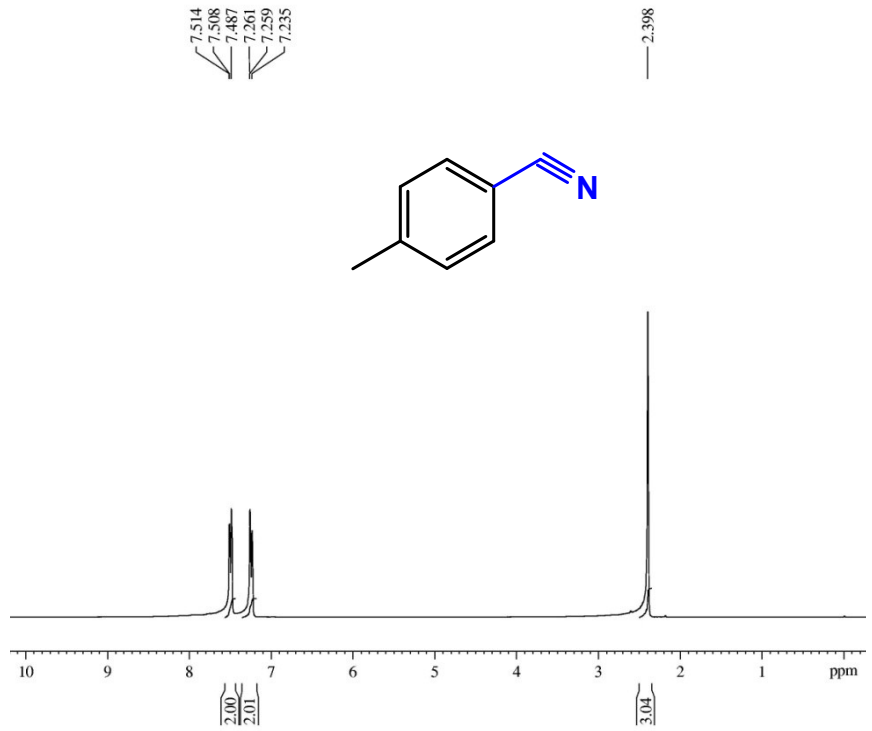

160.084
147.416
144.404
115.258
112.312
77.424
77.000
76.577
NH2
O
O
200
180
160
140
120
100
80
60
40
20
0
ppm

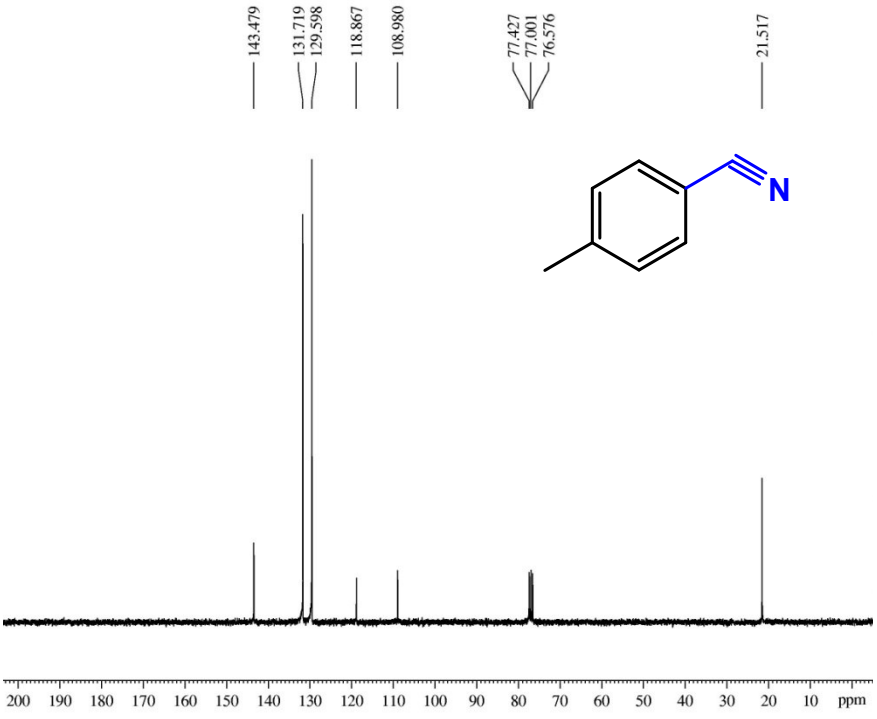

7.283
2.277
2.252
2.227
1.692
1.666
1.641
1.616
1.591
1.451
1.426
1.400
1.375
1.351
1.327
1.269
0.968
0.944
0.919
0.895
0.869
NH2
O
10
9
8
7
6
5
4
3
2
1
0
ppm
2.08
2.00
2.27
2.26
4.01

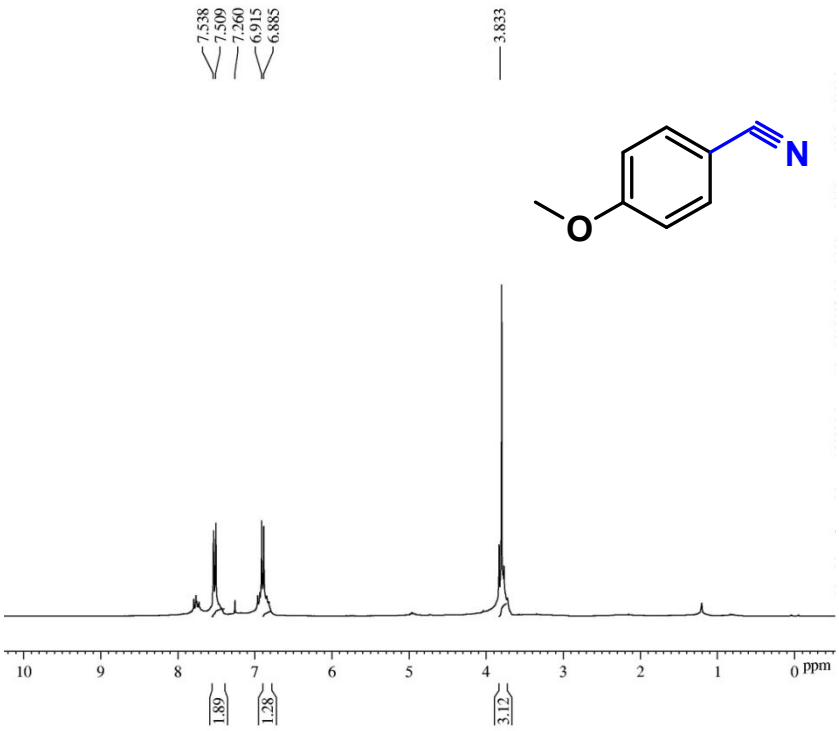

163.530
77.430
77.006
76.583
35.622
27.587
22.332
13.749
NH2
O
200
180
160
140
120
100
80
60
40
20
0
ppm

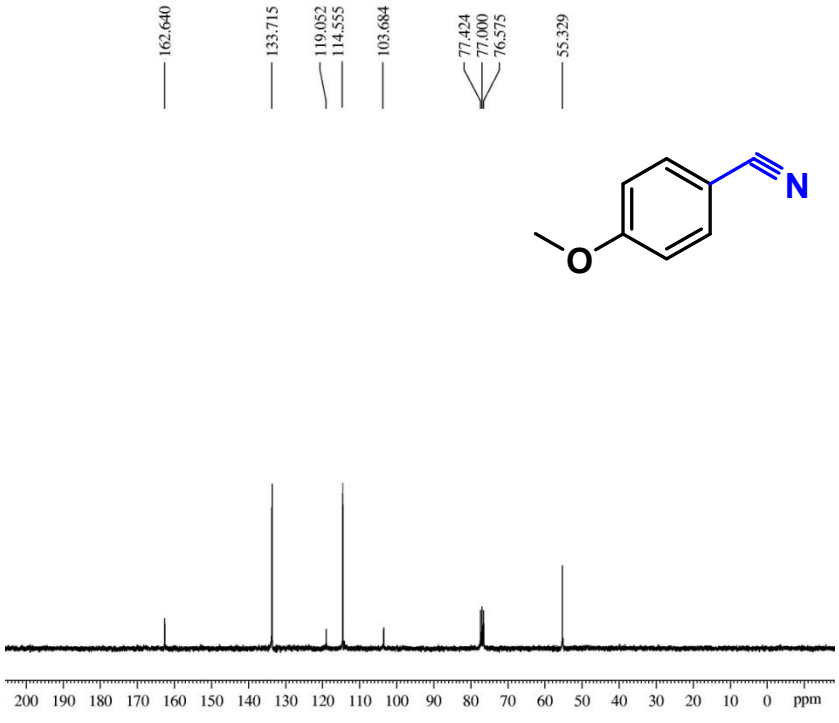

7.676
7.652
7.648
7.639
7.613
7.592
7.588
7.504
7.478
7.454
7.265
0.000
N
10 9 8 7 6 5 4 3 2 1 0 ppm
2.17
1.05
2.00

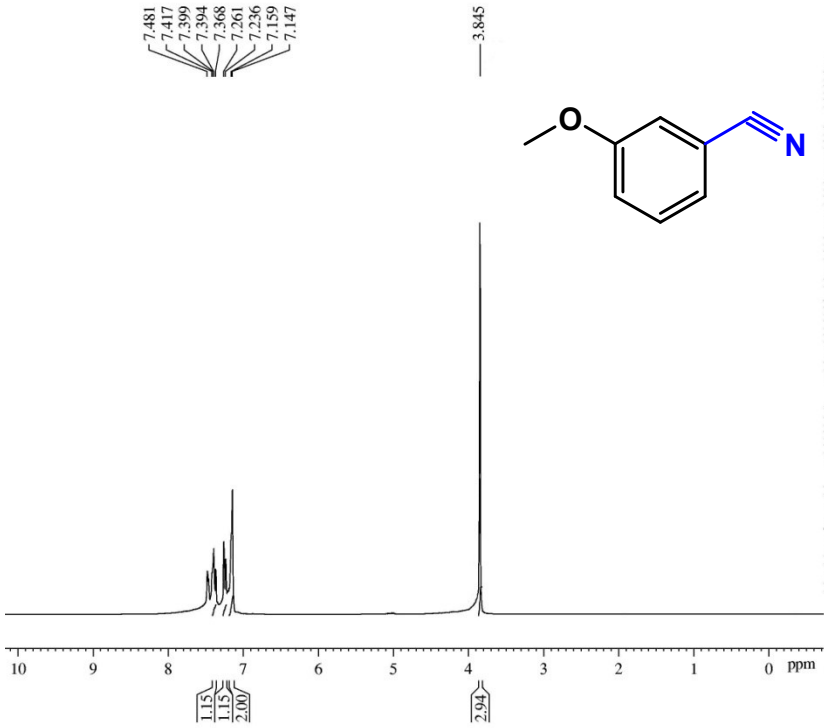

132.484
132.133
131.741
128.818
118.493
112.001
77.423
77.000
76.572
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

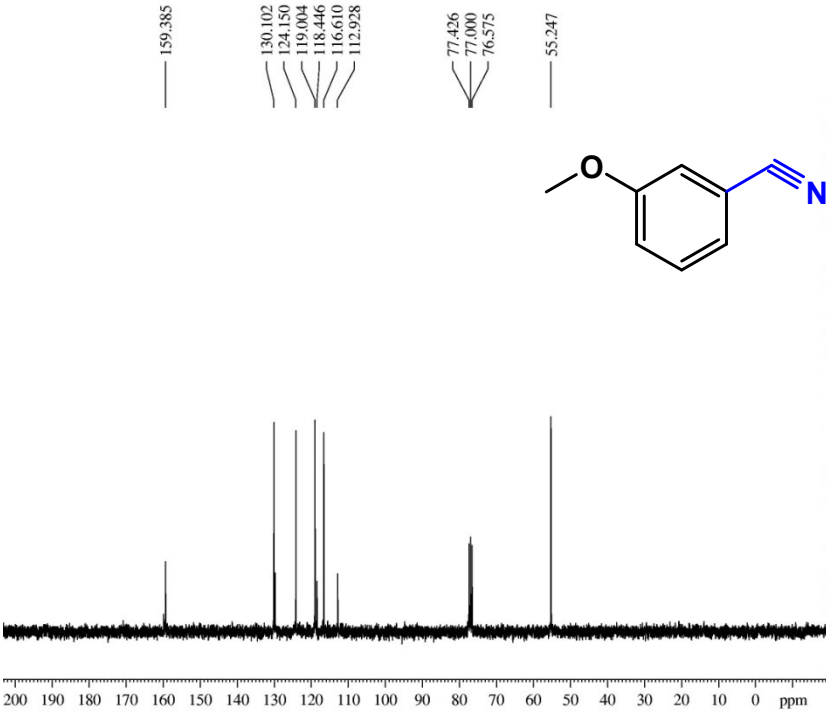

7.514
7.508
7.487
7.261
7.259
7.235
2.398
N
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
3.04

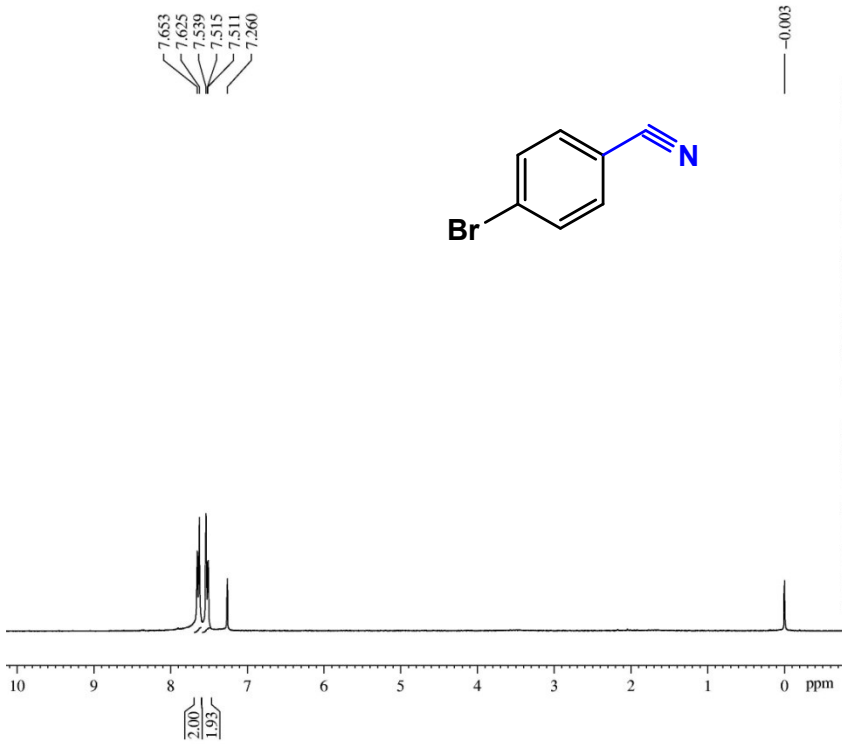

143.479
131.719
129.598
118.867
108.980
77.427
77.001
76.576
21.517
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

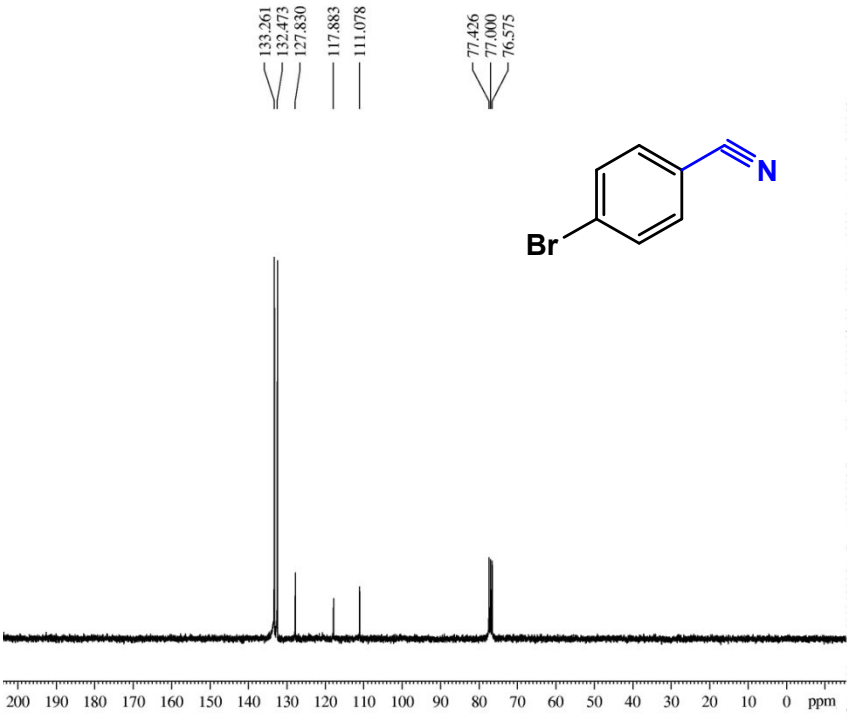

7.538
7.509
7.260
6.915
6.885
3.833
N
O
10 9 8 7 6 5 4 3 2 1 0 ppm
1.89
1.28
3.12

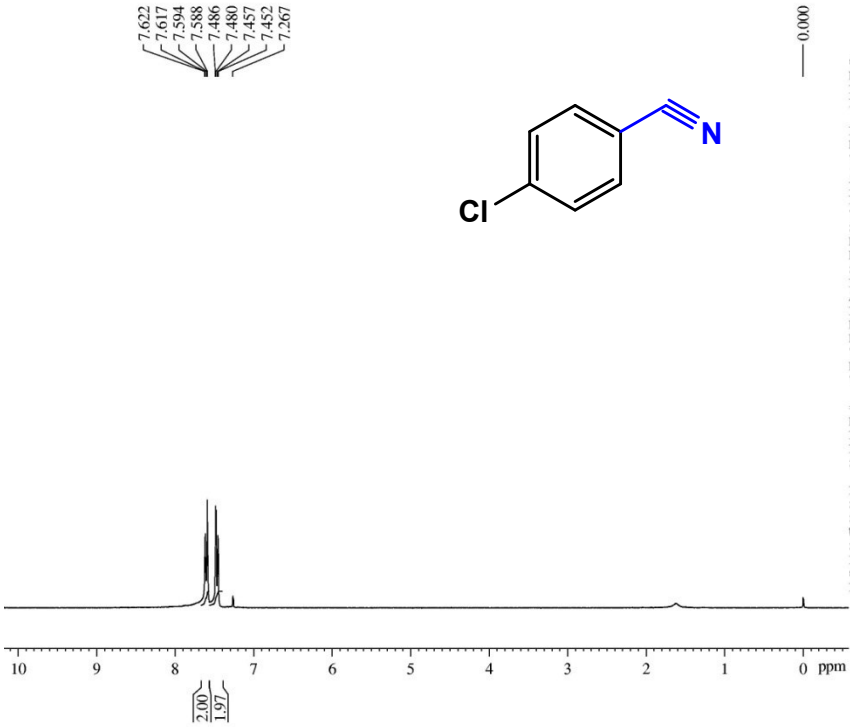

162.640
133.715
119.052
114.555
103.684
77.424
77.000
76.575
55.329
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

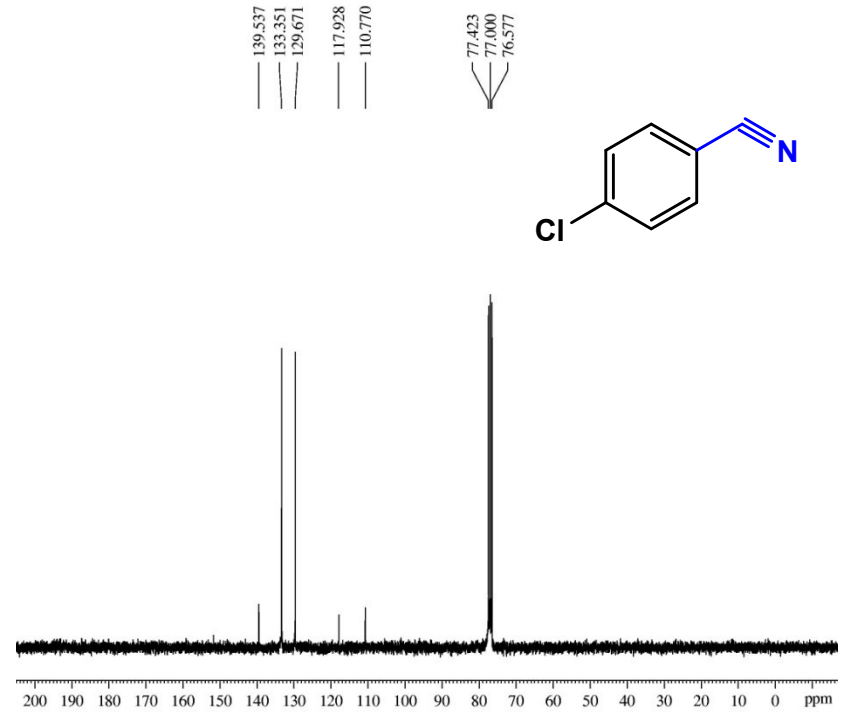

7.481
7.417
7.399
7.394
7.368
7.261
7.236
7.159
7.147
3.845
O
N
10 9 8 7 6 5 4 3 2 1 0 ppm
1.15
1.15
2.00
2.94

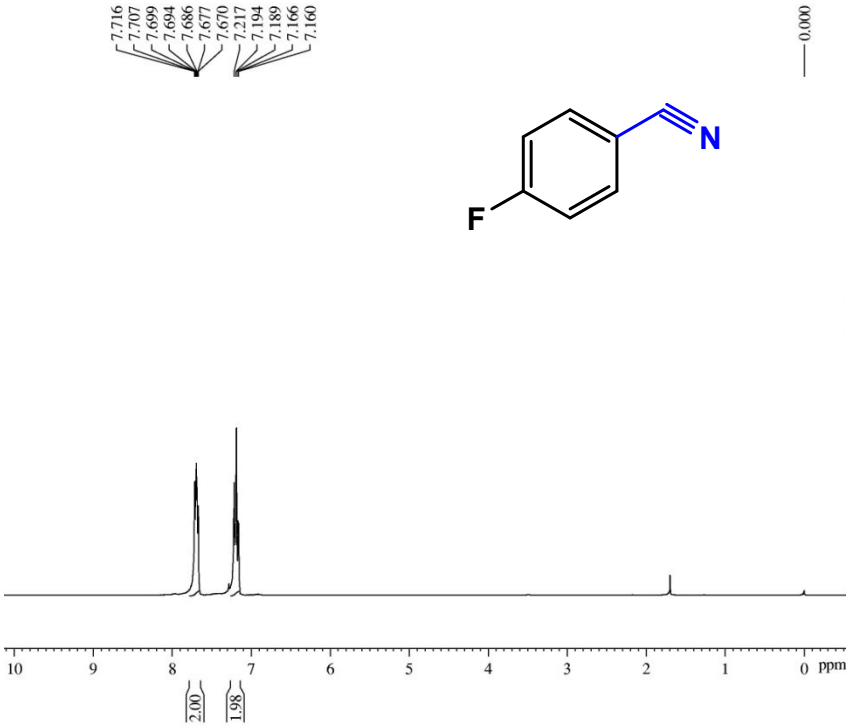

159.385
130.102
124.150
119.004
118.446
116.610
112.928
77.426
77.000
76.575
55.247
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

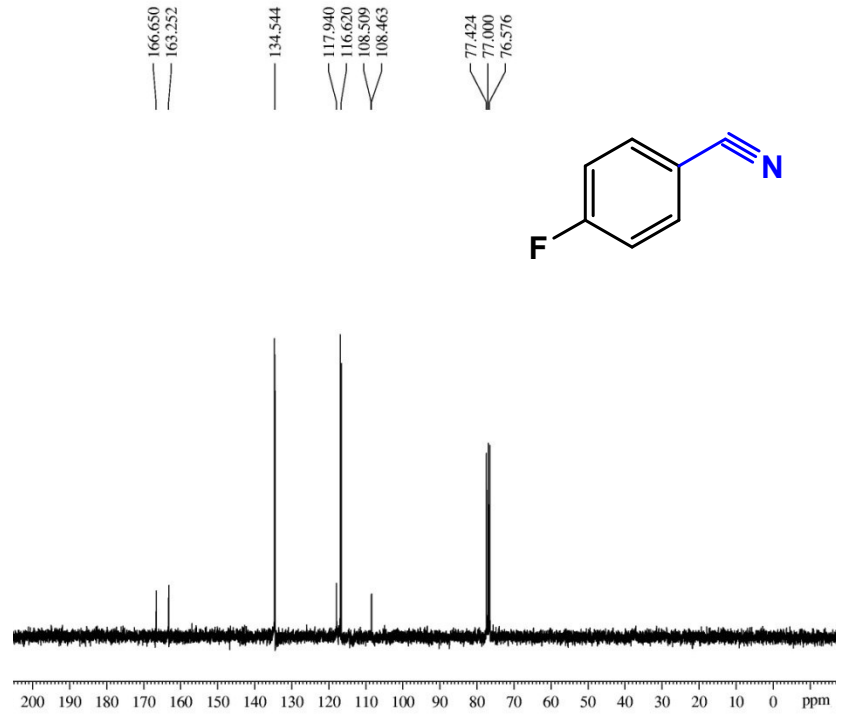

7.653
7.625
7.539
7.515
7.511
7.260
0.003
N
Br
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
1.93


133.261
132.473
127.830
117.883
111.078
77.426
77.000
76.575
N
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

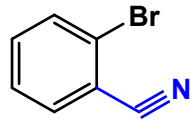

7.622
7.617
7.594
7.588
7.486
7.480
7.457
7.452
7.267
0.000
N
Cl
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.97

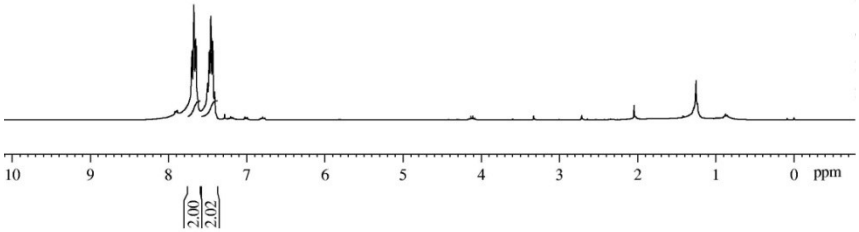

139.537
133.351
129.671
117.928
110.770
77.423
77.000
76.577
N
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

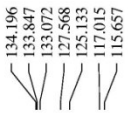

7.716
7.707
7.699
7.694
7.686
7.677
7.670
7.217
7.194
7.189
7.166
7.160
0.000
N
F
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.98


166.650
163.252
134.544
117.940
116.620
108.509
108.463
77.424
77.000
76.576
N
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

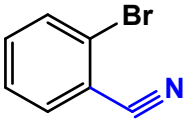

7.708
7.702
7.678
7.655
7.648
7.485
7.478
7.461
7.457
7.452
7.439
7.434

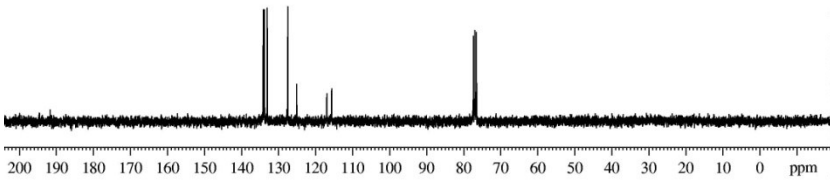

Br
N

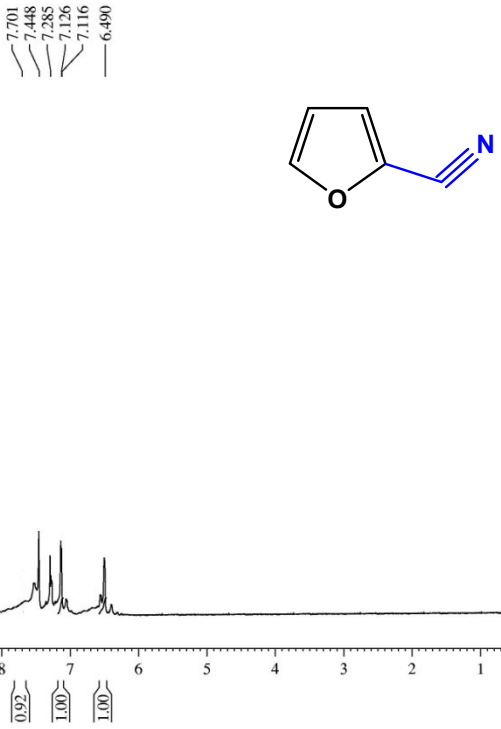

10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02

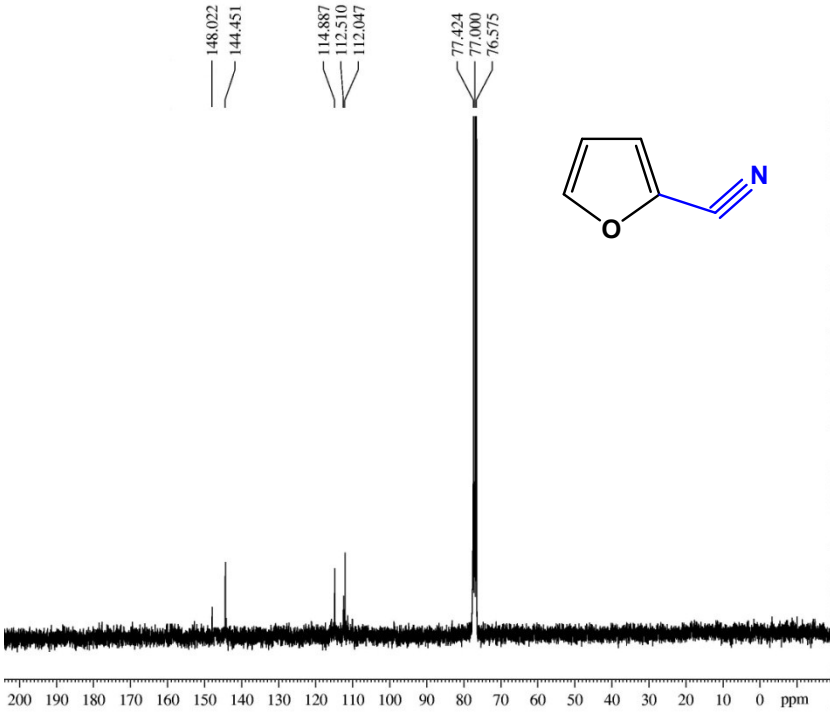

134.196
133.847
133.072
127.568
125.133
117.015
115.657

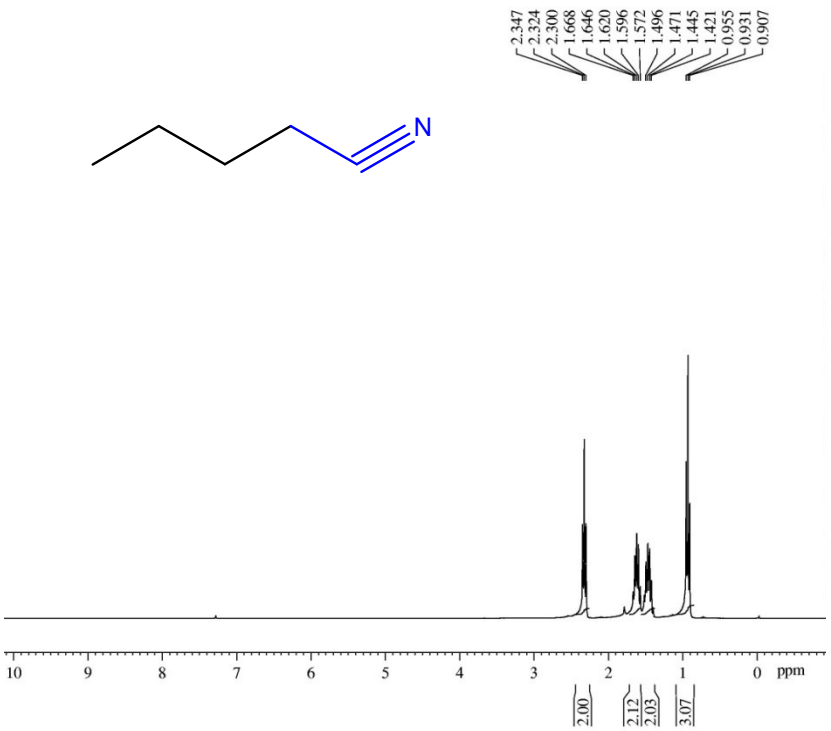

77.425
77.000
76.577

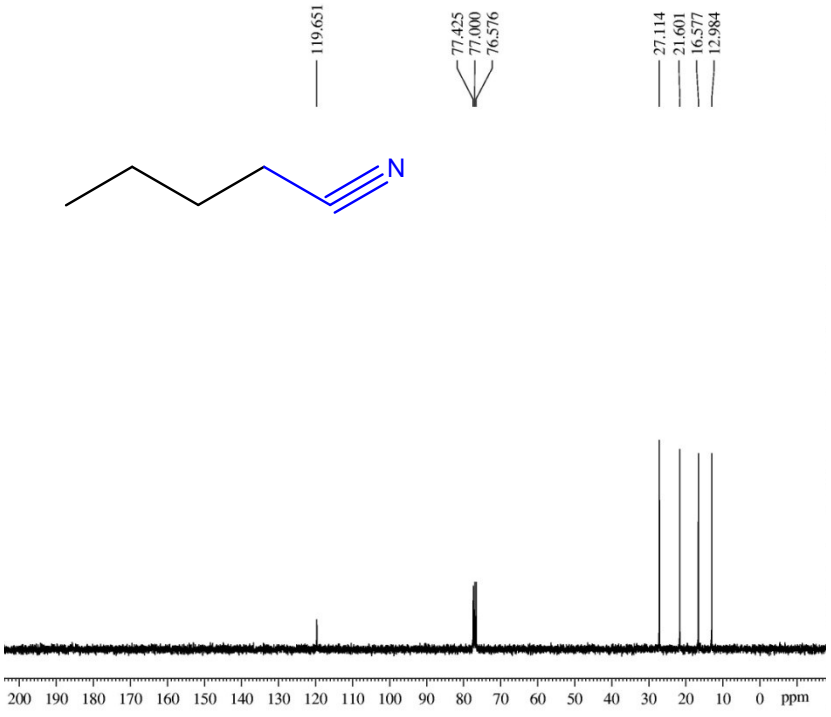

Br
N

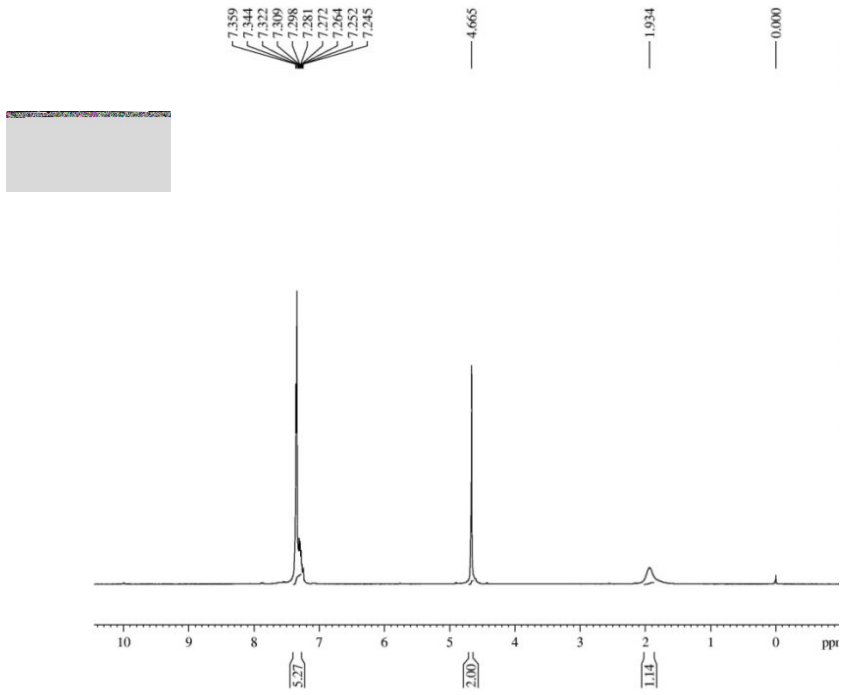

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

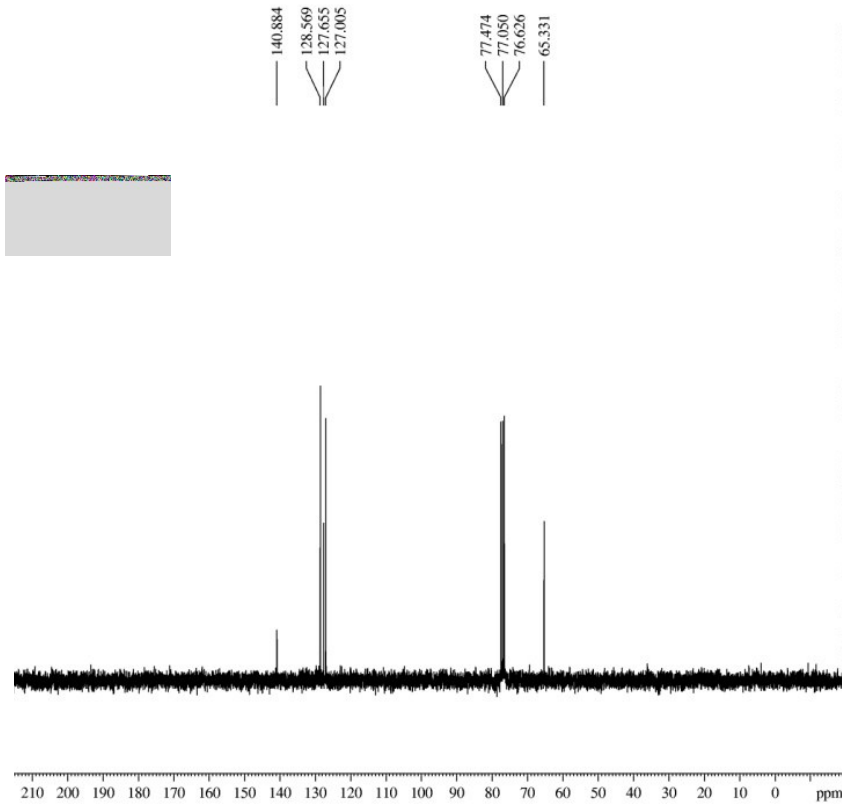

7.701
7.448
7.285
7.126
7.116
6.490
N
O
10 9 8 7 6 5 4 3 2 1 0 ppm
0.92
1.00
1.00

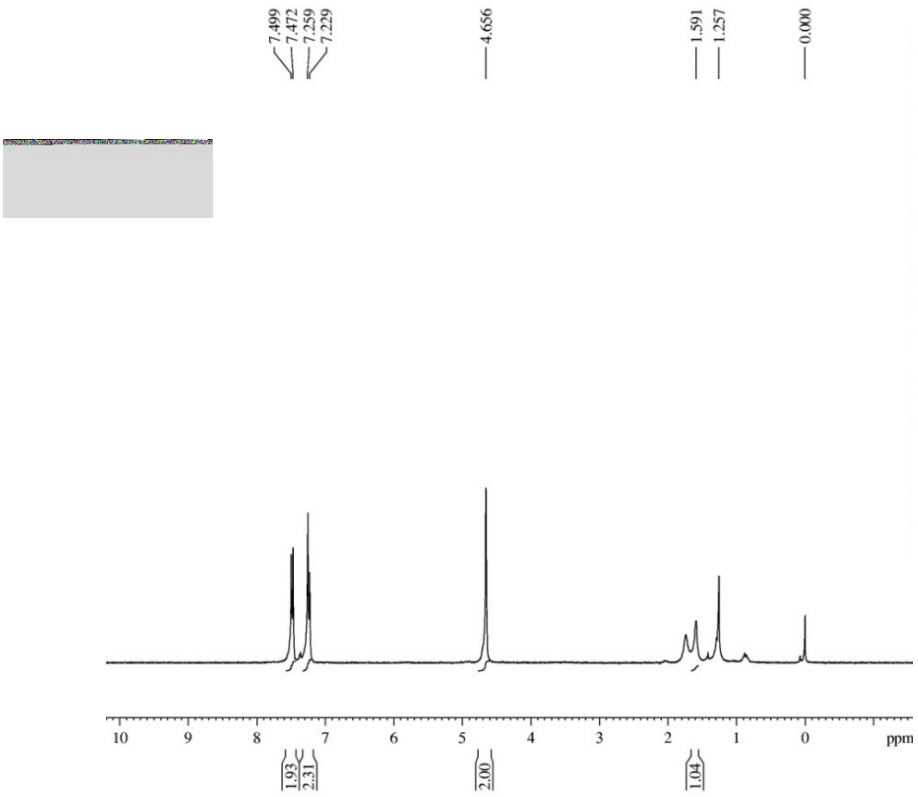

148.022
144.451
114.887
112.510
112.047
77.424
77.000
76.575
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

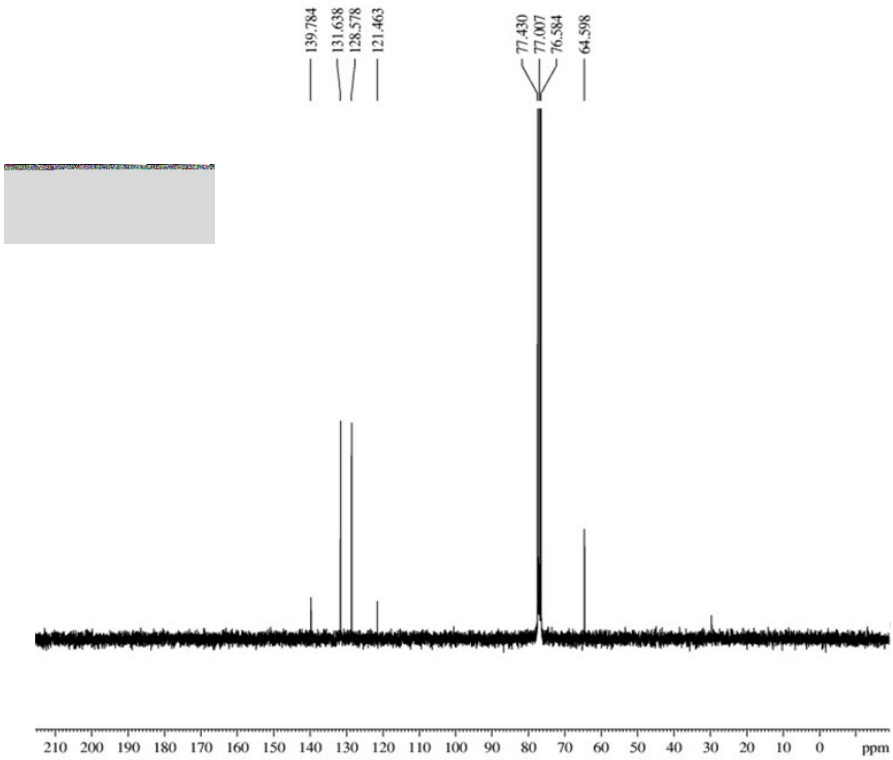

2.347
2.324
2.300
1.668
1.646
1.620
1.596
1.572
1.496
1.471
1.445
1.421
0.955
0.931
0.907
N
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.12
2.03
3.07

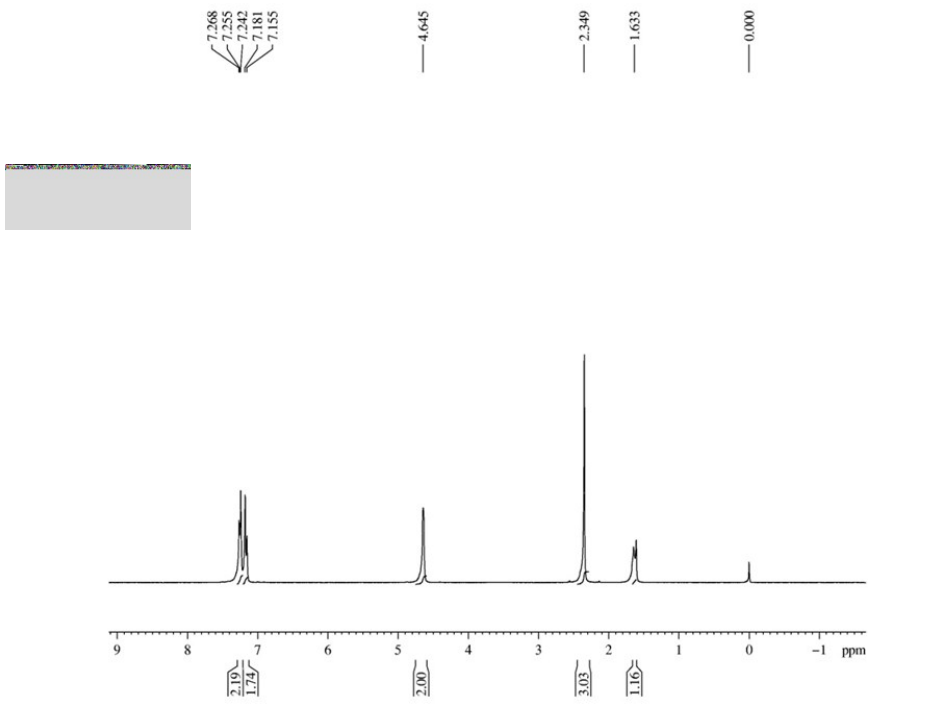

119.651
77.425
77.000
76.576
27.114
21.601
16.577
12.984
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

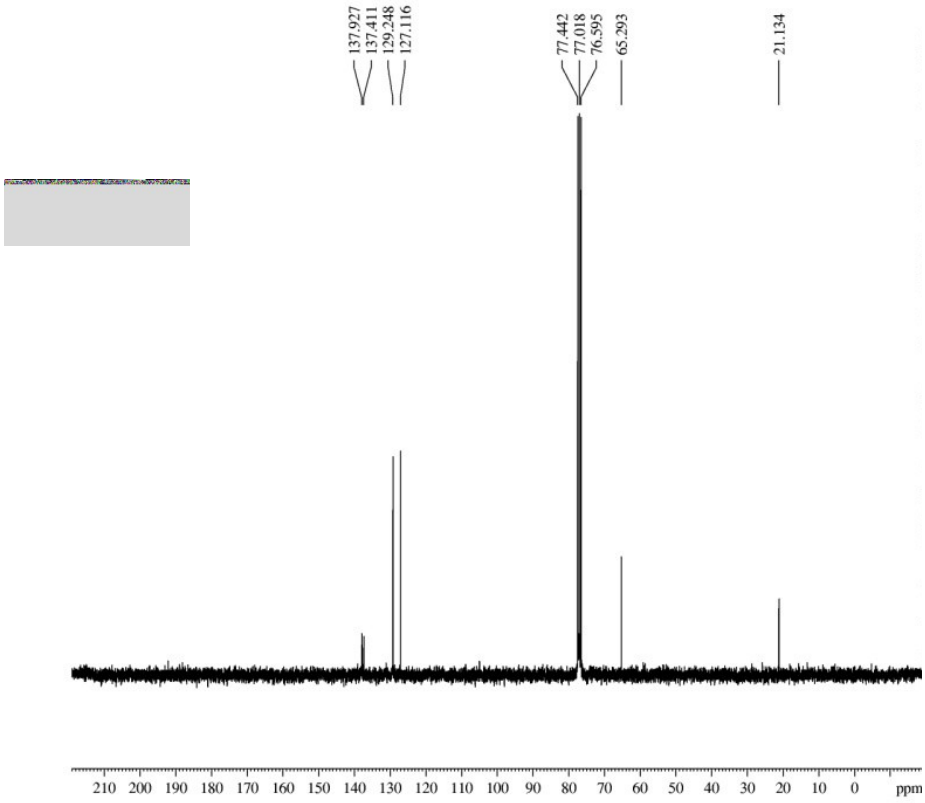

7.359
7.344
7.332
7.309
7.298
7.281
7.272
7.264
7.252
7.245
4.665
1.934
0.000
10
9
8
7
6
5
4
3
2
1
0
5.27
2.00
1.14

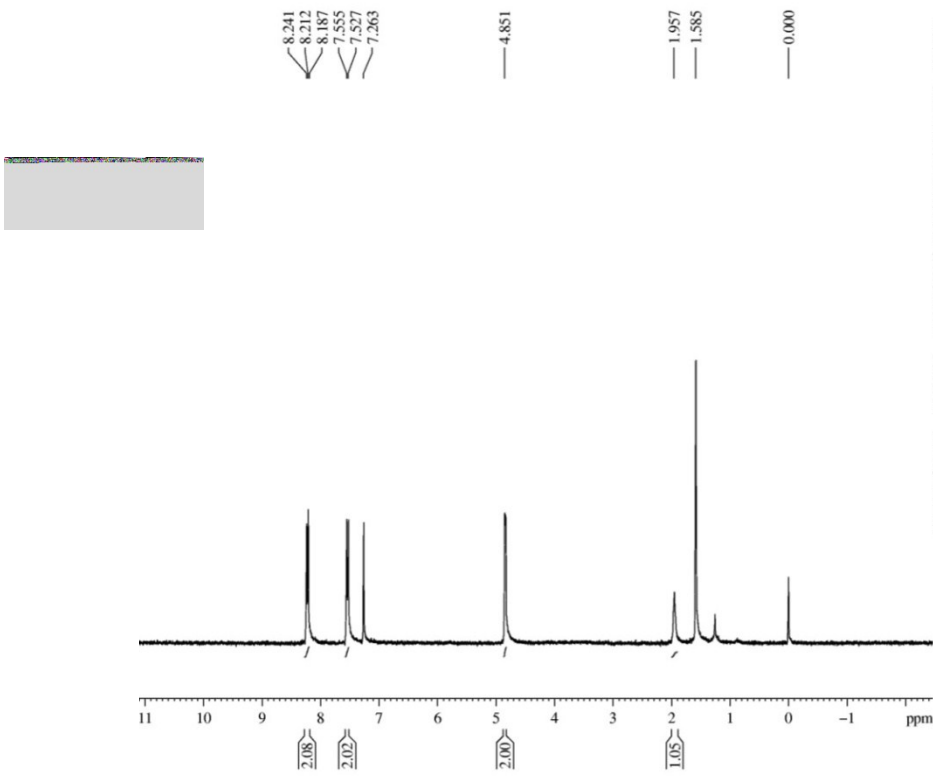

140.884
128.569
127.655
127.005
77.474
77.050
76.626
65.331
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

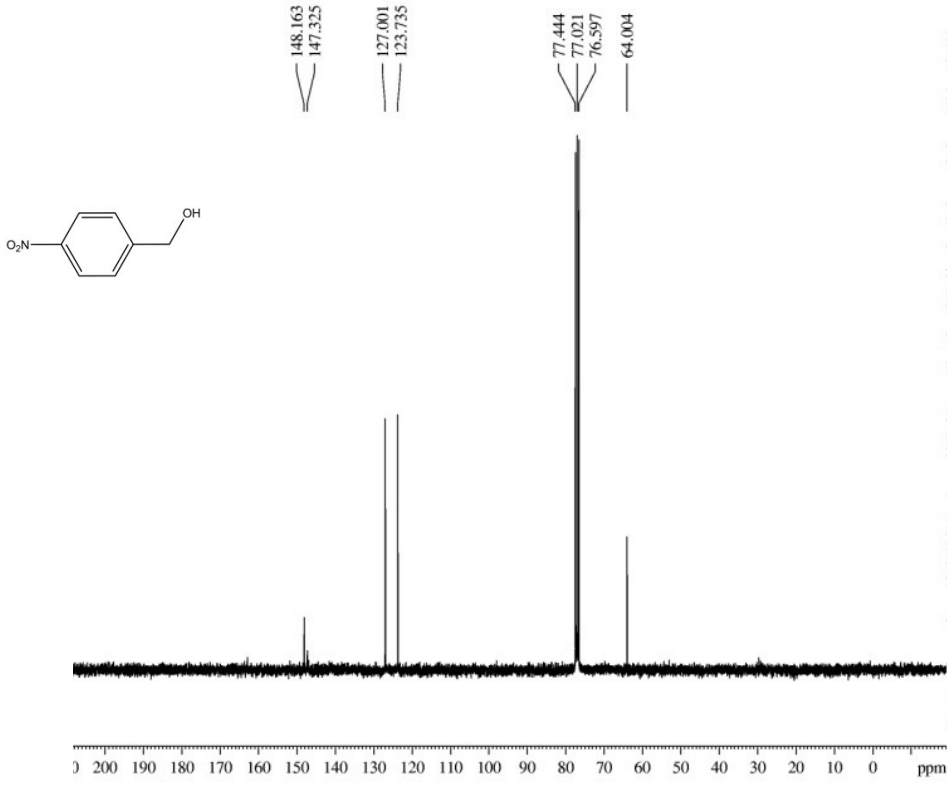

7.499
7.472
7.259
7.229
4.656
1.591
1.257
0.000
10 9 8 7 6 5 4 3 2 1 0 ppm
1.93
2.31
2.00
1.04

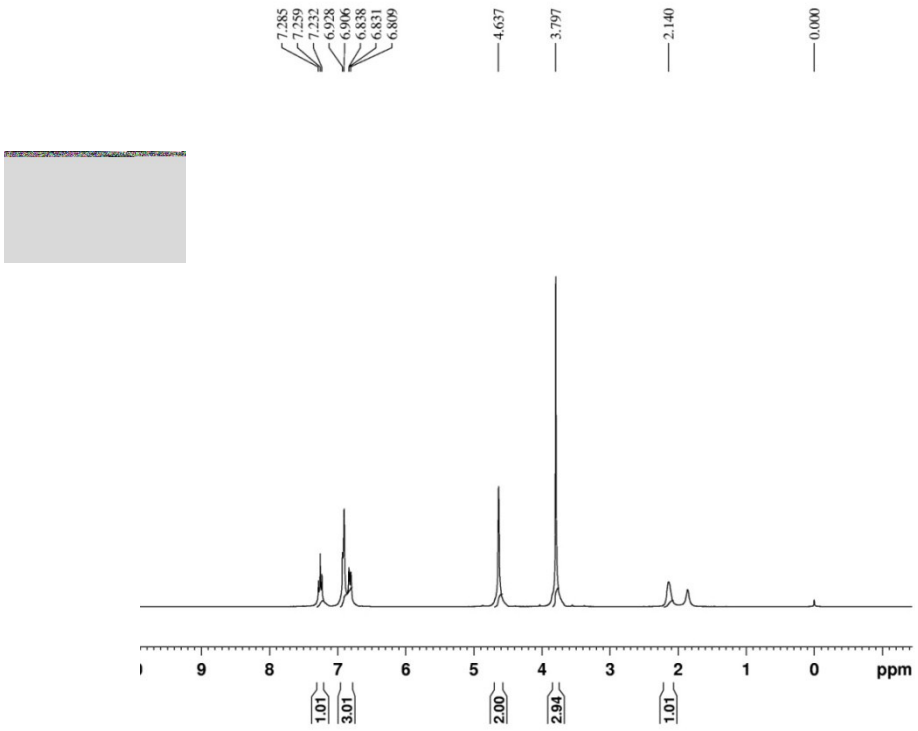

139.784
131.638
128.578
121.463
77.430
77.007
76.584
64.598
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

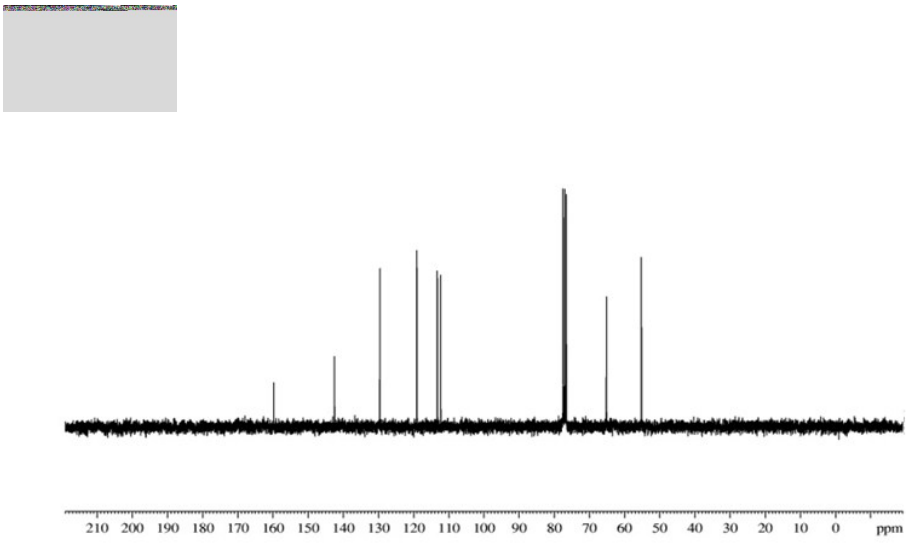

7.268
7.255
7.242
7.181
7.155
4.645
2.349
1.633
0.000
9
8
7
6
5
4
3
2
1
0
−1
ppm
2.19
1.74
2.00
3.03
1.16

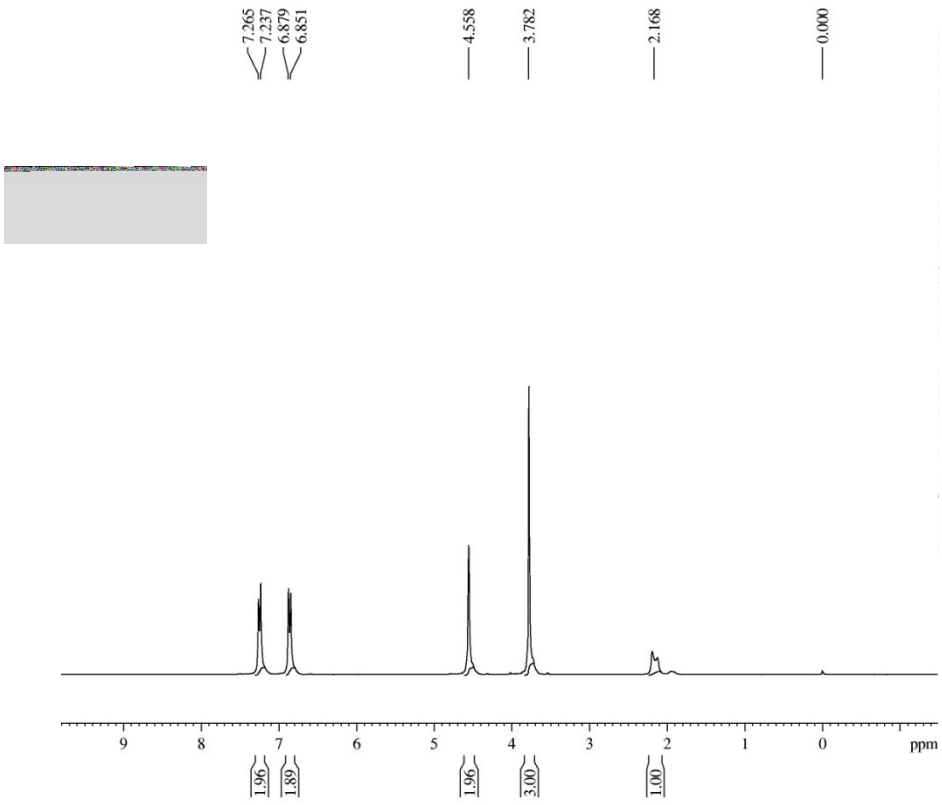

137.927
137.411
129.248
127.116
77.442
77.018
76.595
65.293
21.134
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

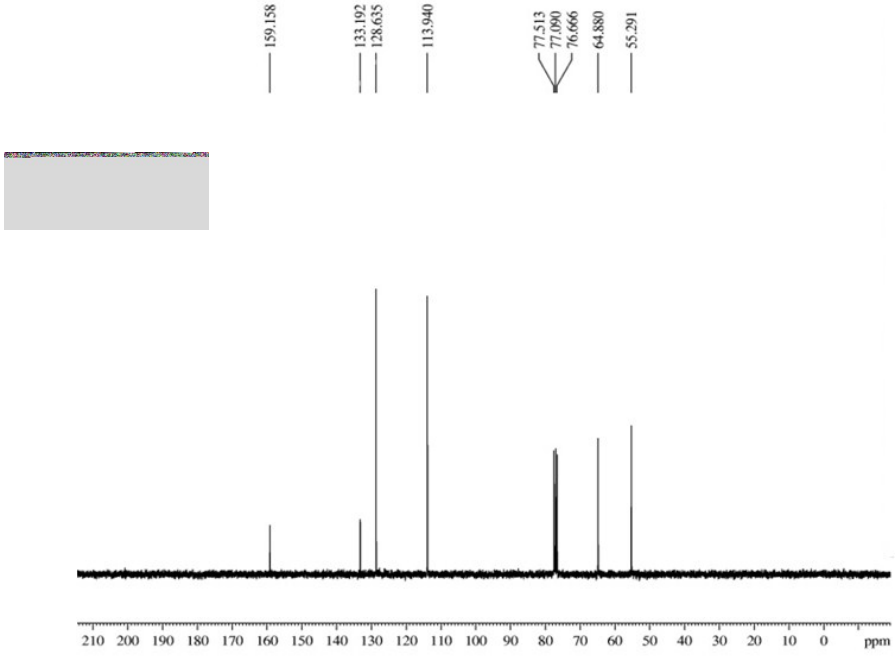

8.241
8.212
8.187
7.555
7.527
7.263
4.851
1.957
1.585
0.000
11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
2.08
2.02
2.00
1.05

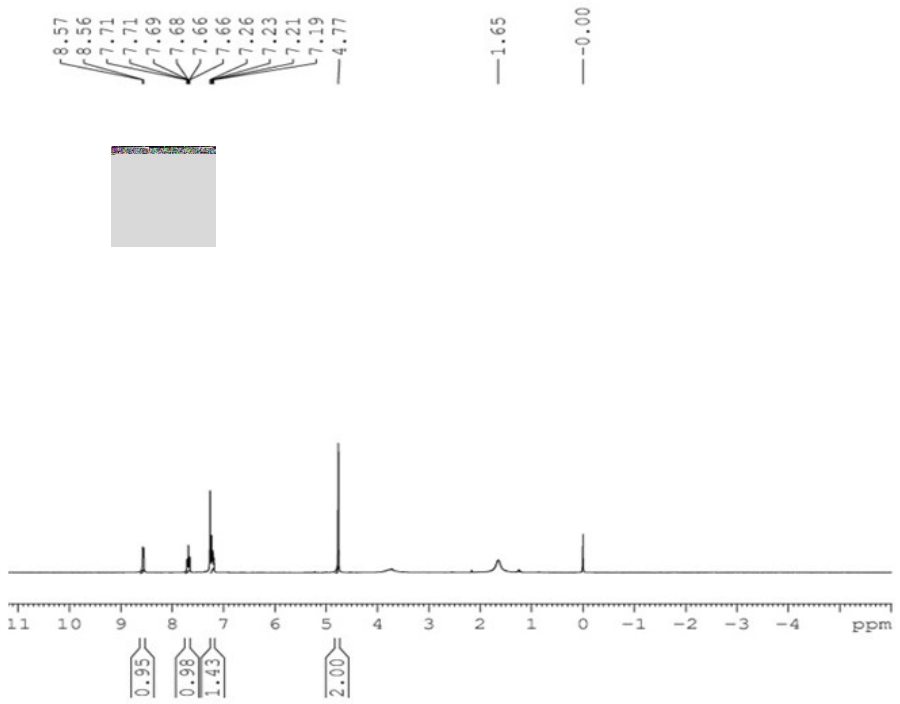

148.163
147.325
127.001
123.735
77.444
77.021
76.597
64.004
OH
O2N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

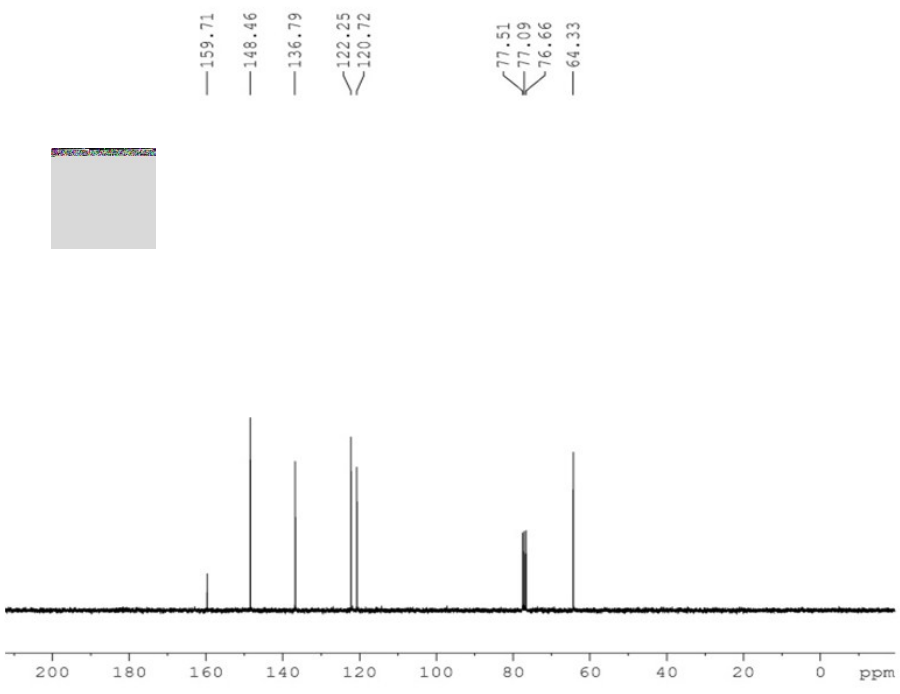

7.285
7.259
7.232
6.928
6.906
6.838
6.831
6.809
4.637
3.797
2.140
0.000
9
8
7
6
5
4
3
2
1
0
ppm
1.01
3.01
2.00
2.94
1.01

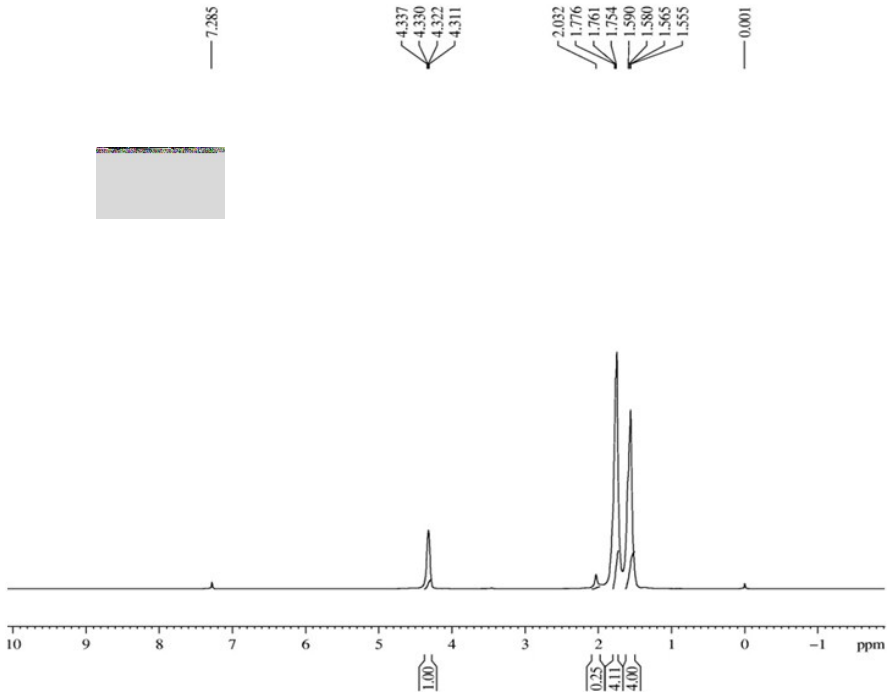

159.829
142.577
129.589
119.127
113.346
112.281
77.483
77.061
76.637
65.171
55.229
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

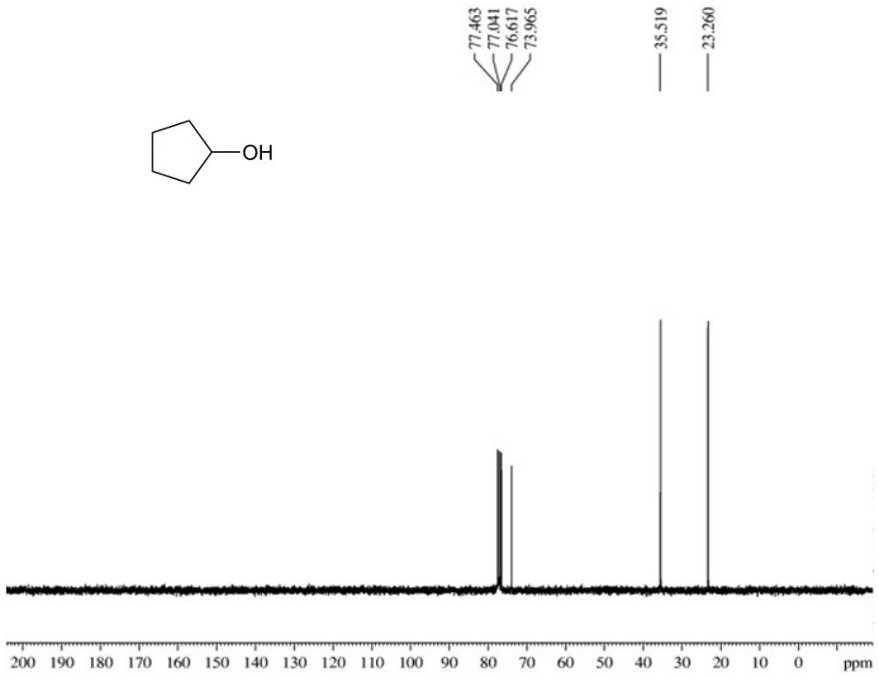

7.265
7.237
6.879
6.851
4.558
3.782
2.168
0.000
9
8
7
6
5
4
3
2
1
0
ppm
1.96
1.89
1.96
3.00
1.00

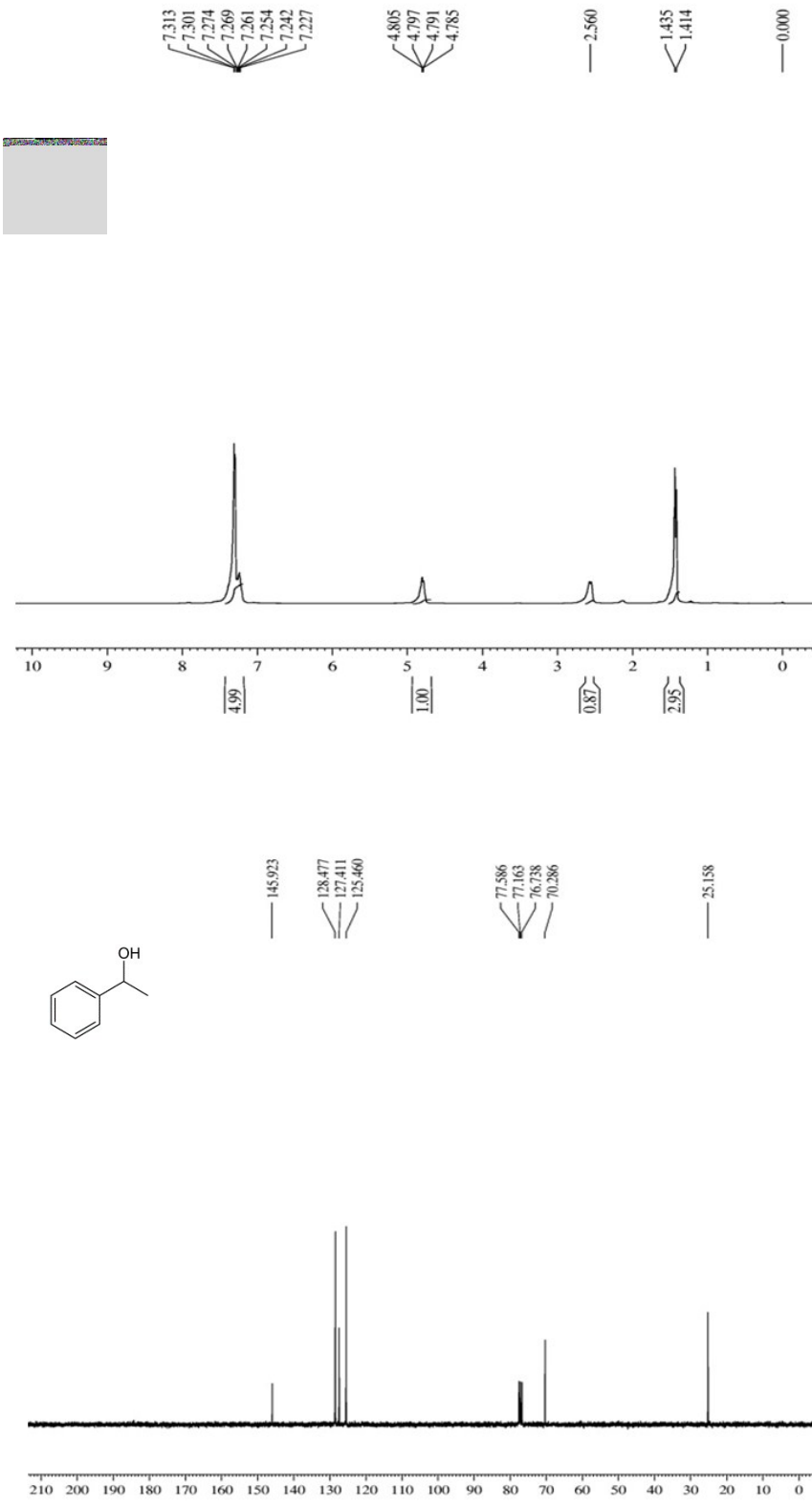

159.158
133.192
128.635
113.940
77.513
77.090
76.666
64.880
55.291
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

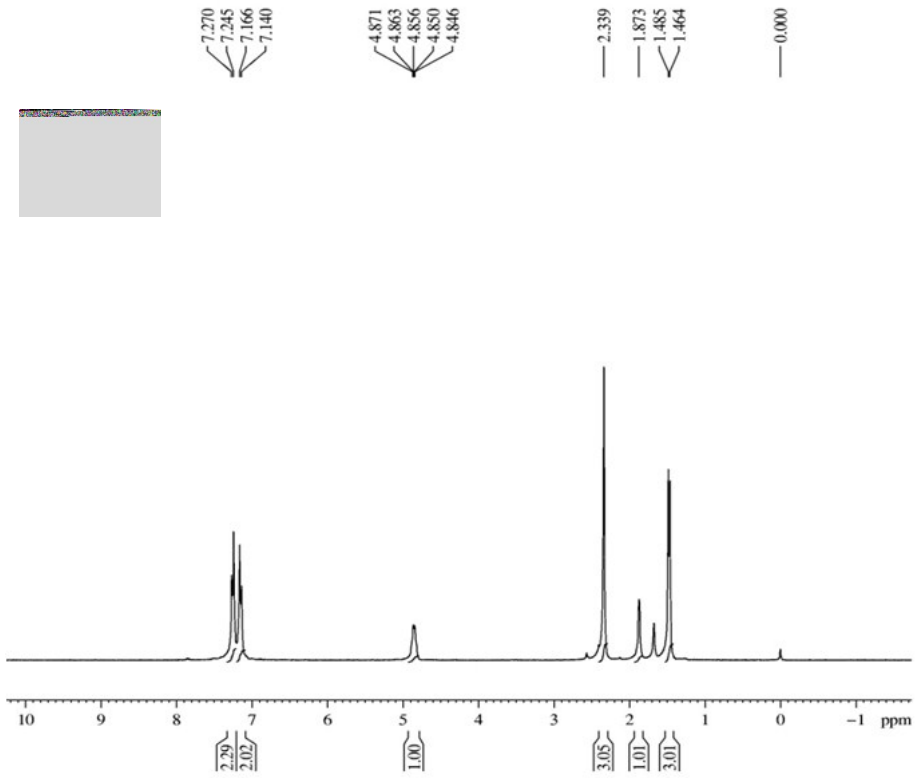

8.57
8.56
7.71
7.71
7.69
7.68
7.66
7.66
7.26
7.23
7.21
7.19
4.77
1.65
0.00
11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 −4 ppm
0.95
0.98
1.43
2.00

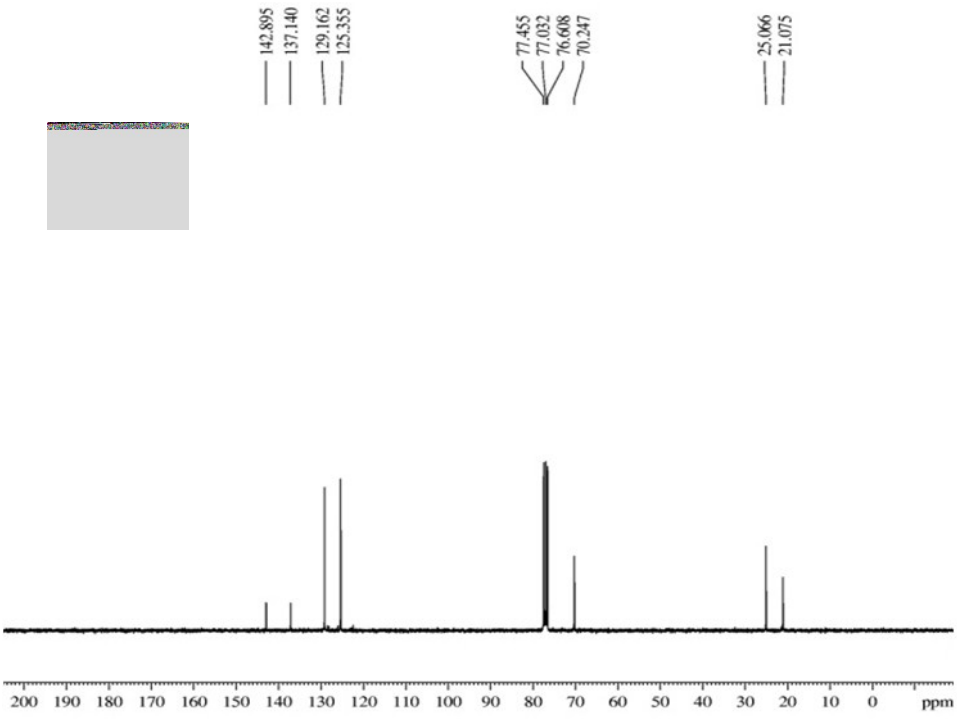

159.71
148.46
136.79
122.25
120.72
77.51
77.09
76.66
64.33
200 180 160 140 120 100 80 60 40 20 0 ppm

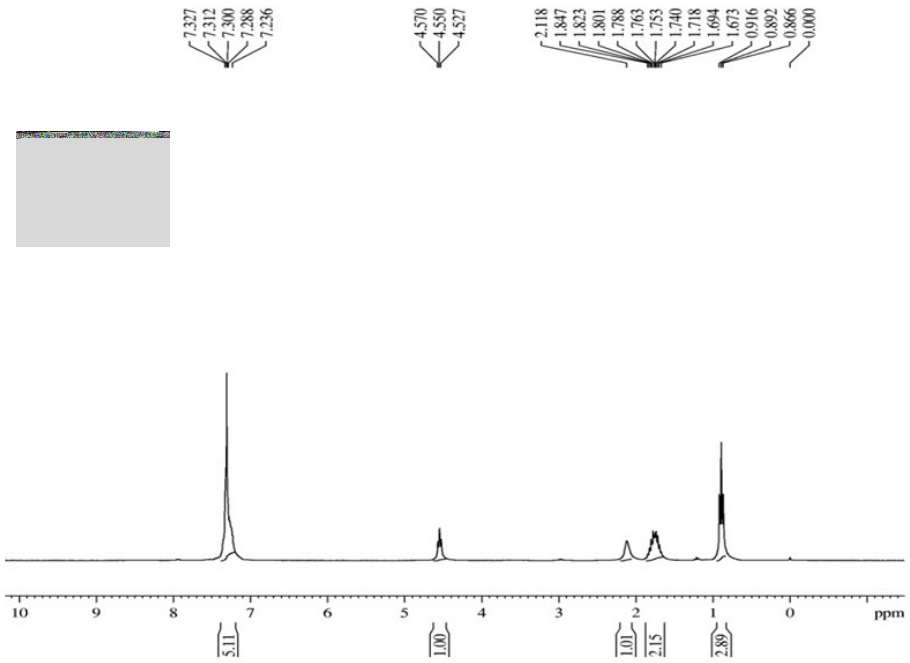

7.285
4.337
4.330
4.322
4.311
2.032
1.776
1.761
1.754
1.590
1.580
1.565
1.555
0.001
10 9 8 7 6 5 4 3 2 1 0 −1 ppm
1.00
0.25
4.11
4.00

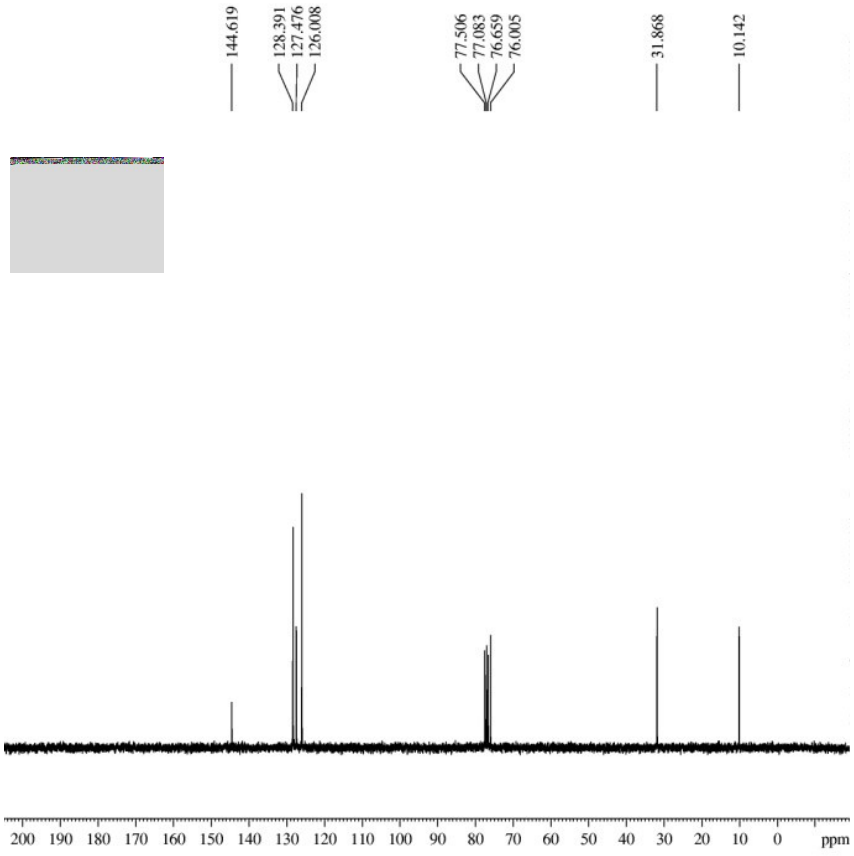

77.463
77.041
76.617
73.965
35.519
23.260
OH
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.313
7.301
7.274
7.269
7.261
7.254
7.242
7.227
4.805
4.797
4.791
4.785
2.560
1.435
1.414
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm
4.99
1.00
0.87
2.95
145.923
128.477
127.411
125.460
77.586
77.163
76.738
70.286
25.158
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.270
7.245
7.166
7.140
4.871
4.863
4.856
4.850
4.846
2.339
1.873
1.485
1.464
0.000
10 9 8 7 6 5 4 3 2 1 0 −1 ppm
2.29
2.02
1.00
3.05
1.01
3.01


142.895
137.140
129.162
125.355
77.455
77.032
76.608
70.247
25.066
21.075
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.327
7.312
7.300
7.288
7.236
4.570
4.550
4.527
2.118
1.847
1.823
1.801
1.788
1.763
1.753
1.740
1.718
1.694
1.673
0.916
0.892
0.866
0.000
10 9 8 7 6 5 4 3 2 1 0 ppm
5.11
1.00
1.01
2.15
2.89


144.619
128.391
127.476
126.008
77.506
77.083
76.659
76.005
31.868
10.142
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm