Supplementary information

A Strategy for Generating Aryl Radicals from Arylborates by Using Organic Photoredox Catalysis: Photo-Meerwein Type Arylations of Electron-Deficient Alkenes

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Experimental Section

All reagents and solvents were used as received from commercial suppliers. IR spectra were recorded on an FT-IR spectrometer. ^{1}H NMR spectra were recorded in $CDCl_3$ containing tetramethylsilane as an internal standard, and were acquired on either a 300 or a 500 MHz spectrometer. ^{13}C NMR spectra were acquired on a 125 MHz spectrometer. High-resolution mass spectra were obtained using FAB mass spectrometer. The light source was a high-pressure (100 W) mercury arcs and 28W blue LED.

General procedures for the photoreaction of arylboronic acids 3 and acrylonitrile 4a

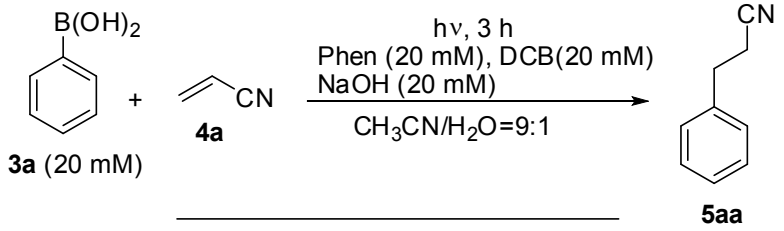
An aqueous CH_3CN solution (CH_3CN 36 mL, H_2O 4 mL) of arylboronic acids **3** (20 mM), NaOH (20 mM), Phen (10 mM), and DCB (10 mM) in Pyrex vessels (18 mm x 180 mm) was purged with argon for 10 min, and acrylonitrile **4a** (100 mM) was added under argon

atmosphere. The mixture was irradiated with 100 W high-pressure mercury lamp for 6 h, and then the solvent was removed under reduced pressure. The crude product was purified by silica-gel column chromatography using hexane/EtOAc as the eluents to yield adducts **5**. The photoreactions of alkyl- and alkenyl-boronic acids **6** were also carried out similarly.

Optimization in the photoreaction of phenylboronic acid 3a with 4a

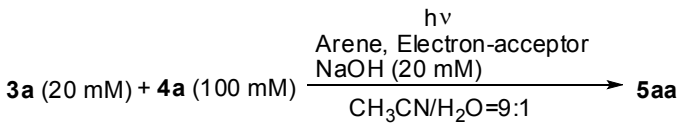
The effects of concentration of **4a**, photocatalyst, solvent, and base were investigated in the photoreaction of **3a** with **4a** as shown in Table S1-S3.

Table S1. Effect of concentration of **4a** in the photoreaction of **3a** with **4a**



Entry	**4a**/mM	Yield of **5aa**/%
1	20 (1 equiv.)	37
2	40 (2 equiv.)	51
3	60 (3 equiv.)	57
4	80 (4 equiv.)	66
5	100 (5 equiv.)	74
6	120 (6 equiv.)	63

Table S2. Effect of photocatalyst in the photoreaction of **3a** with **4a**



Entry	Arene (mM)	Electron-acceptor (mM)	Irradiation time/h	Yield of **5aa**/%
1	Phen (20)	DCB (20)	3	74
2	Phen (10)	DCB (10)	6	78
3	Phen (5)	DCB (5)	12	64
4	Biphenyl (20)	DCN (20)	3	48
5	Biphenyl (10)	DCN (10)	6	41
6	Biphenyl (5)	DCN (5)	12	56

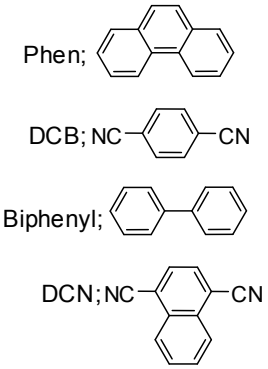
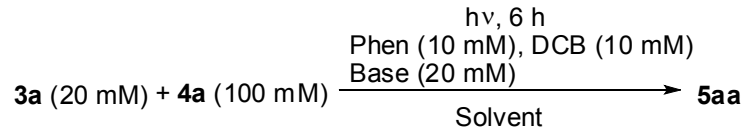
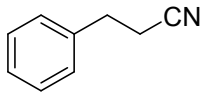


Table S3. Effects of solvent and base in the photoreaction of **3a** with **4a**

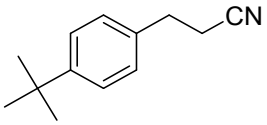


Entry	Solvent	Base	Yield of **5aa**/%
1	DMF/H_2O = 9:1	NaOH	26
2	DMSO/H_2O = 9:1	NaOH	11
3	EtOH/H_2O = 9:1	NaOH	25
4	MeOH/H_2O = 9:1	NaOH	49
5	CH_3COCH_3/H_2O = 9:1	NaOH	66
6	CH_3CN/H_2O = 9:1	NaOH	78
7	CH_3CN/H_2O = 8:2	NaOH	66
8	CH_3CN/H_2O = 7:3	NaOH	41
9	CH_3CN/H_2O = 9:1	LiOH	39
10	CH_3CN/H_2O = 9:1	KOH	48
11	CH_3CN/H_2O = 9:1	$(n\text{-Bu})_4N^{+-}OH$	21
12	CH_3CN (dry)	$(n\text{-Bu})_4N^{+-}OH$	0
13	CH_3CN/H_2O = 9:1	Na_2CO_3	50
14	CH_3CN/H_2O = 9:1	K_2CO_3	59
15	CH_3CN/H_2O = 9:1	Cs_2CO_3	61
16	CH_3CN/H_2O = 9:1	CH_3CO_2Na	32

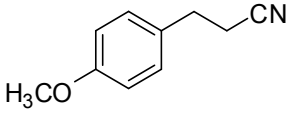
Characterization data for 5aa–wa, 7aa–ca, 5ab–af, 7bd, 7cd, and 8–11



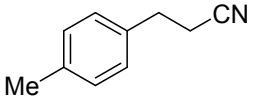
5aa Compound **5aa** has been previously reported.[1] Colorless oil, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.42–7.16 (m, 5H), 2.95 (t, J = 7.4 Hz, 2H), 2.61 (t, J = 7.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.2, 129.0, 128.4, 127.3, 119.3, 31.7, 19.5; GC-MS (M^+) 131.



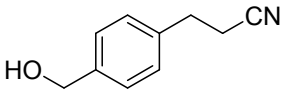
5fa Colorless oil, IR (KBr, cm^{-1}) 2964, 2246; ^1H NMR (300 MHz, $CDCl_3$): δ 7.36 (d, J = 6.4 Hz, 2H), 7.16 (d, J = 6.4 Hz, 2H), 2.93 (t, J = 7.4 Hz, 2H), 2.60 (t, J = 7.4 Hz, 2H), 1.31 (s, 9H);^{13}C NMR (125 MHz, $CDCl_3$): δ 150.2, 135.1, 128.1, 125.9, 119.5, 34.6, 31.4, 31.2, 19.5; HRMS (FAB) calcd for $(M+H)^+$ $C_{13}H_{18}N$, 188.1439; found, 188.1429.



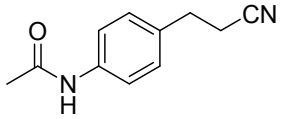
5ga Compound **5ga** has been previously reported.[1] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 7.16 (d, J = 8.7 Hz, 2H), 6.87 (d, J = 8.7 Hz, 2H), 3.80 (s, 3H), 2.90 (t, J = 7.3 Hz, 2H), 2.58 (t, J = 7.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.8, 130.2, 129.4, 119.3, 114.3, 55.4, 30.9, 19.8.



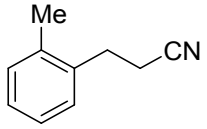
5ha Colorless oil, IR (neat, cm^{-1}) 3021, 2925, 2245; ^1H NMR (500 MHz, $CDCl_3$): δ 7.16–7.12 (m, 4H), 2.91 (t, J = 7.4 Hz, 2H), 2.58 (t, J = 7.4 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.9, 135.2, 129.6, 128.3, 119.4, 31.3, 21.2, 19.6; HRMS (FAB) calcd for $(M+H)^+$ $C_{10}H_{12}N$, 146.0970; found, 146.0965.



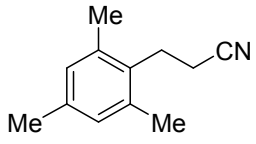
5ia White solid, mp 48 °C; IR (KBr, cm^{-1}) 3254, 3199, 2240; ^1H NMR (300 MHz, $CDCl_3$): δ 7.31 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 4.61 (s, 2H), 2.93 (t, J = 7.3 Hz, 2H), 2.59 (t, J = 7.3 Hz, 2H), 2.44 (s, 1H, OH); ^{13}C NMR (125 MHz, $CDCl_3$): δ 140.1, 137.4, 128.5, 127.6, 119.3, 64.6, 31.2, 19.5; HRMS (FAB) calcd for $(M+H)^+$ $C_{10}H_{12}NO$, 162.0919; found, 162.0899.



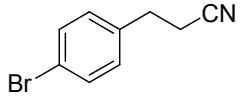
5ja White solid, mp 77 °C; IR (KBr, cm^{-1}) 3302, 3172, 2250, 1683; ^1H NMR (300 MHz, $CDCl_3$): δ 7.56 (s, 1H, NH), 7.48 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 2.92 (t, J = 7.3 Hz, 2H), 2.61 (t, J = 7.3 Hz, 2H), 2.16 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$): δ 168.6, 137.2, 133.9, 128.9, 120.4, 119.3, 31.0, 24.6, 19.6; HRMS (FAB) calcd for $(M+H)^+$ $C_{11}H_{13}N_2O$, 189.1028; found, 189.1033.



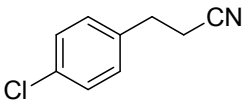
5ka Colorless oil; IR (neat, cm^{-1}) 2948, 2246; ^1H NMR (300 MHz, $CDCl_3$): δ 7.19–7.14 (m, 4H), 2.98 (t, J = 7.3 Hz, 2H), 2.58 (t, J = 7.3 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.3, 135.9, 130.6, 128.8, 127.5, 126.6, 119.3, 29.0, 19.3, 18.1; HRMS (FAB) calcd for $(M+H)^+$ $C_{10}H_{12}N$, 146.0970; found, 146.0954.



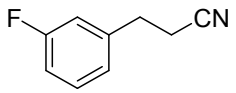
5la White solid, mp 82 °C; IR (KBr, cm^{-1}) 2966, 2921, 2240; ^1H NMR (300 MHz, $CDCl_3$): δ 6.79 (s, 2H), 2.93 (t, J = 7.5 Hz, 2H), 2.38 (t, J = 7.5 Hz, 2H), 2.23 (s, 3H), 2.18 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.6, 135.0, 130.8, 128.3, 118.4, 24.2, 19.8, 18.7, 15.7; HRMS (FAB) calcd for $(M+H)^+$ $C_{12}H_{16}N$, 174.1283; found, 174.1270.



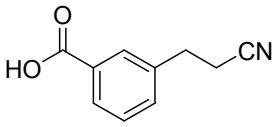
5na Compound **5na** has been previously reported.[2] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 7.47 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 8.4 Hz, 2H), 2.92 (t, J = 7.3 Hz, 2H), 2.61 (t, J = 7.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.0, 132.1, 130.1, 121.3, 118.9, 31.1, 19.3.



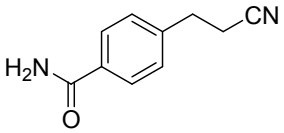
5ma Compound **5na** has been previously reported.[1] Colorless oil, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31 (d, *J* = 8.3 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 2H), 2.92 (t, *J* = 7.3 Hz, 2H), 2.60 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.7, 133.1, 129.9, 129.1, 119.1, 30.9, 19.3.



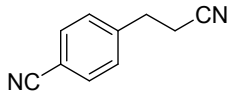
5oa Compound **5oa** has been previously reported.[1] Colorless oil, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34–7.26 (m, 1H), 7.03–6.92 (m, 3H), 2.95 (t, *J* = 7.3 Hz, 2H), 2.62 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.0 (d, *J* = 250.3 Hz), 140.5 (d, *J* = 7.3 Hz), 130.5 (d, *J* = 8.3 Hz), 124.1 (d, *J* = 3.0 Hz), 118.9, 115.4 (d, *J* = 21.3 Hz), 114.3 (d, *J* = 21.0 Hz), 31.3, 19.2.



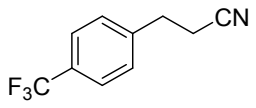
5pa White solid, mp 155 °C; IR (KBr, cm^{-1}) 3627, 3067, 2921, 2250, 1679; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 6.9 Hz, 1H), 7.97 (s, 1H), 7.51–7.46 (m, 2H), 3.03 (t, *J* = 7.4 Hz, 2H), 2.67 (t, *J* = 7.4 Hz, 2H) ^{13}C NMR (125 MHz, $CDCl_3$): δ 171.6, 138.5, 134.0, 130.0, 129.3, 118.8, 31.4, 19.3; HRMS (FAB) calcd for $(M+H)^+$ $C_{10}H_{10}NO_2$, 176.0712; found, 176.0706.



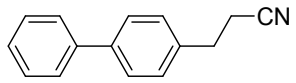
5qa White solid, mp 128 °C; IR (KBr, cm^{-1}) 3291, 3136, 2929, 2242, 1661, 1609; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.80 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 6.17 (brs, 1H, NH), 5.93 (brs, 1H, NH), 3.02 (t, *J* = 7.2 Hz, 2H), 2.66 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.0, 142.2, 132.5, 128.7, 128.1, 118.8, 31.4, 19.2; HRMS (FAB) calcd for $(M+H)^+$ $C_{10}H_{11}N_2O$, 175.0871; found, 175.0901.



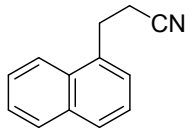
5ra Compound **5ra** has been previously reported.[3] White solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 3.03 (t, *J* = 7.2 Hz, 2H), 2.70 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.3, 132.8, 129.3, 118.6, 118.5, 111.5, 31.6, 19.0.



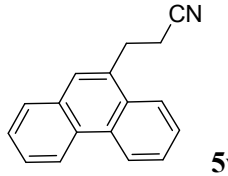
5sa Compound **5sa** has been previously reported.[3] Colorless oil, ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.60 (d, *J* = 7.7 Hz, 2H), 7.35 (d, J = 7.7 Hz, 2H), 3.01 (t, *J* = 7.3 Hz, 2H), 2.64 (t, *J* = 7.3 Hz, 2H) ^{13}C NMR (125 MHz, $CDCl_3$): δ 142.0, 129.5 (q, *J* = 32 Hz), 128.8, 126.0, 126.0, 124.1 (q, *J* = 270 Hz), 118.7, 31.4, 19.2.



5ta Compound **5ta** has been previously reported.[4] White solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59–7.54 (m, 4H), 7.46–7.40 (m, 2H), 7.37–7.28 (m, 3H), 2.98 (t, *J* = 7.4 Hz, 2H), 2.63 (t, *J* = 7.4 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 140.7, 140.3, 137.2, 128.9, 128.8, 127.7, 127.5, 127.2, 119.3, 31.3, 19.5.

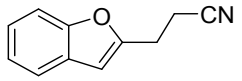


5ua Compound **5ua** has been previously reported.[5] Colorless oil, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93–7.88 (m, 2H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.59–7.49 (m, 2H), 7.47–7.39 (m, 2H), 3.44 (t, *J* = 7.5 Hz, 2H), 2.76 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.1, 134.0, 131.2, 129.3, 128.2, 126.7, 126.0, 125.7, 122.7, 119.3, 28.9, 18.6.

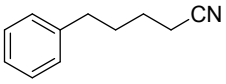


5va Compound **5va** has been previously reported.[6] White solid, ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.79–8.76 (m, 1H), 8.67 (d, *J* = 8.2 Hz, 1H), 8.00–7.97 (m, 1H), 7.89–7.86 (m, 1H), 7.72–7.61 (m, 5H), 3.51 (t, *J* = 7.5 Hz, 2H), 2.85 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR

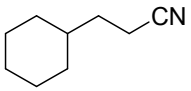
(150 MHz, $CDCl_3$): δ 132.0, 131.4, 130.9, 130.1, 130.0, 128.5, 127.2, 127.1, 127.0, 126.8, 126.7, 123.7, 123.3, 122.5, 119.2, 29.3, 18.1.



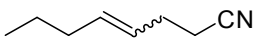
5wa Colorless oil, IR (neat, cm^{-1}) 2966, 2925, 2248; ^1H NMR (300 MHz, $CDCl_3$): δ 7.73–7.63 (m, 2H), 7.31–7.23 (m, 2H), 7.09 (s, 1H), 3.20 (t, *J* = 7.3 Hz, 2H), 2.70 (t, *J* = 7.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 140.8, 139.8, 139.4, 124.5, 124.3, 123.3, 122.4, 122.3, 118.6, 26.9, 19.3; HRMS (FAB) calcd for $(M+H)^+$ $C_{11}H_{10}NO$, 172.0762; found, 172.0782.



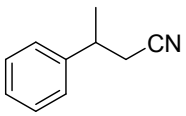
7aa Compound **7aa** has been previously reported.[1] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 7.32–7.26 (m, 2H), 7.23–7.16 (m, 3H), 2.66 (t, *J* = 7.3 Hz, 2H), 2.35 (t, *J* = 7.3 Hz, 2H), 1.85–1.63 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 141.3, 128.6, 128.5, 126.2, 119.7, 35.1, 30.4, 24.9, 17.2.



7ba Compound **7ba** has been previously reported.[7] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 2.35 (t, *J* = 7.4 Hz, 2H), 1.74–1.70 (m, 4H), 1.55 (q, *J* = 7.2 Hz, 2H), 1.43–1.34 (m, 1H), 1.32–1.12 (m, 3H), 0.96–0.84 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 120.2, 36.7, 32.6, 32.6, 26.4, 26.0, 14.7.

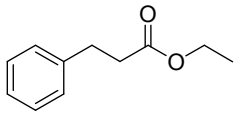


(E/Z mixture) **7ca** Compound **7ca** has been previously reported.[8] Colorless oil, ^1H NMR (500 MHz, $CDCl_3$): δ 5.61–5.54 (m, 1H), 5.45–5.37 (m, 1H), 2.41–2.31 (m, 4H), 2.06–1.98 (m, 2H), 1.44–1.35 (m, 2H), 0.94–0.88 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.1, 133.6, 125.8, 125.2, 119.5, 34.6, 29.4, 28.5, 23.3, 22.7, 22.4, 17.8, 17.7, 13.8, 13.7.

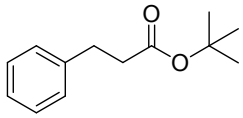


5ab Compound **5ab** has been previously reported.[9] Colorless oil, ^1H NMR

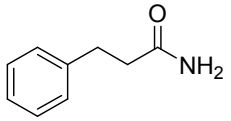
(300 MHz, $CDCl_3$): δ 7.40–7.23 (m, 5H), 3.23–3.113 (m, 1H), 2.66–2.51 (m, 2H), 1.46 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.2, 129.0, 127.4, 126.7, 118.7, 36.6, 26.5, 20.8.



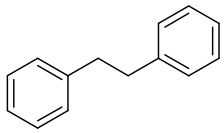
5ac Compound **5ac** has been previously reported.[3] Colorless oil, ^1H NMR (500 MHz, $CDCl_3$): δ 7.28 (t, *J* = 7.4 Hz, 2H), 7.20–7.18 (m, 3H), 4.12 (q, *J* = 7.3 Hz, 2H), 2.94 (t, *J* = 7.7 Hz, 2H), 2.61 (t, *J* = 7.7 Hz, 2H), 1.22 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 173.0, 140.7, 128.6, 128.4, 126.3, 60.5, 36.1, 31.1, 14.3.



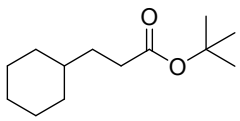
5ad Compound **5ad** has been previously reported.[10] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 7.24–7.19 (m, 2H), 7.14–7.12 (m, 3H), 2.84 (t, *J* = 7.5 Hz, 2H), 2.45 (t, *J* = 7.5 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.4, 140.9, 128.5, 128.4, 126.2, 80.4, 37.2, 31.2, 28.2.



5ae Compound **5ae** has been previously reported.[11] White solid, ^1H NMR (300 MHz, $CDCl_3$): δ 7.33–7.19 (m, 5H), 5.36 (brs, 2H, NH_2), 2.98 (t, *J* = 7.8 Hz, 2H), 2.54 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 174.4, 140.7, 128.7, 128.4, 126.4, 37.6, 31.5.

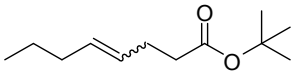


5af Compound **5af** has been previously reported.[9] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 7.20–7.06 (m, 10H), 2.82 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 142.0, 128.7, 128.6, 126.2, 38.2.

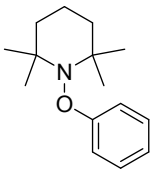


7bd Compound **7bd** has been previously reported.[12] Colorless oil, ^1H NMR (300 MHz, $CDCl_3$): δ 2.21 (t, *J* = 7.9 Hz, 2H), 1.71–1.68 (m, 5H), 1.51–1.40 (m, 12H),

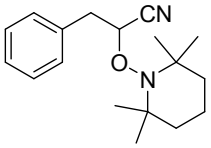
1.23–1.17 (m, 3H), 0.93–0.83 (m, 2H); ^{13}C NMR (125 MHz, CDCl3): δ 173.7, 79.9, 37.3, 33.3, 33.2, 33.1, 33.0, 32.6, 28.2, 28.1, 26.7, 26.6, 26.4, 26.3.



7cd Compound **7cd** has been previously reported.[12] Colorless oil,^{1}H NMR (500 MHz, $CDCl_3$): δ 5.45–5.36 (m, 2H), 2.31–2.25 (m, 4H), 2.02–1.91 (m, 2H), 1.42 (s, 9H), 1.39–1.30 (m, 2H), 0.90–0.85 (m, 3H) ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.8, 131.4, 131.1, 128.4, 127.9, 80.1, 35.7, 34.7, 29.3, 28.2, 23.1, 22.8, 22.7, 13.9, 13.7.



8 Compound **8** has been previously reported.[13] Colorless oil, ^{1}H NMR (300 MHz, CDCl3): δ 7.23–7.16 (m, 4H), 6.86–6.81 (m, 1H), 1.69–1.53 (m, 5H), 1.44–1.39 (m, 1H), 1.23 (s, 6H), 1.01 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.7, 128.8, 119.9, 114.0, 60.4, 39.9, 32.7, 20.5, 17.1; GC-MS (M^+) 233.



9 Compound **9** has been previously reported.[14] Colorless oil, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.36–7.25 (m, 5H), 4.79 (t, *J* = 6.7 Hz, 1H), 3.21–3.11 (m, 2H), 1.59–1.38 (m, 5H), 1.34–1.27 (m, 4H), 1.12–1.06 (m, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.8, 129.9, 128.6, 127.5, 119.3, 75.1, 61.1, 60.0, 40.1, 40.0, 39.5, 34.1, 33.7, 20.6, 20.4, 17.1; GC-MS (M^+) 286.

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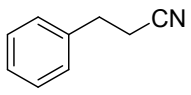
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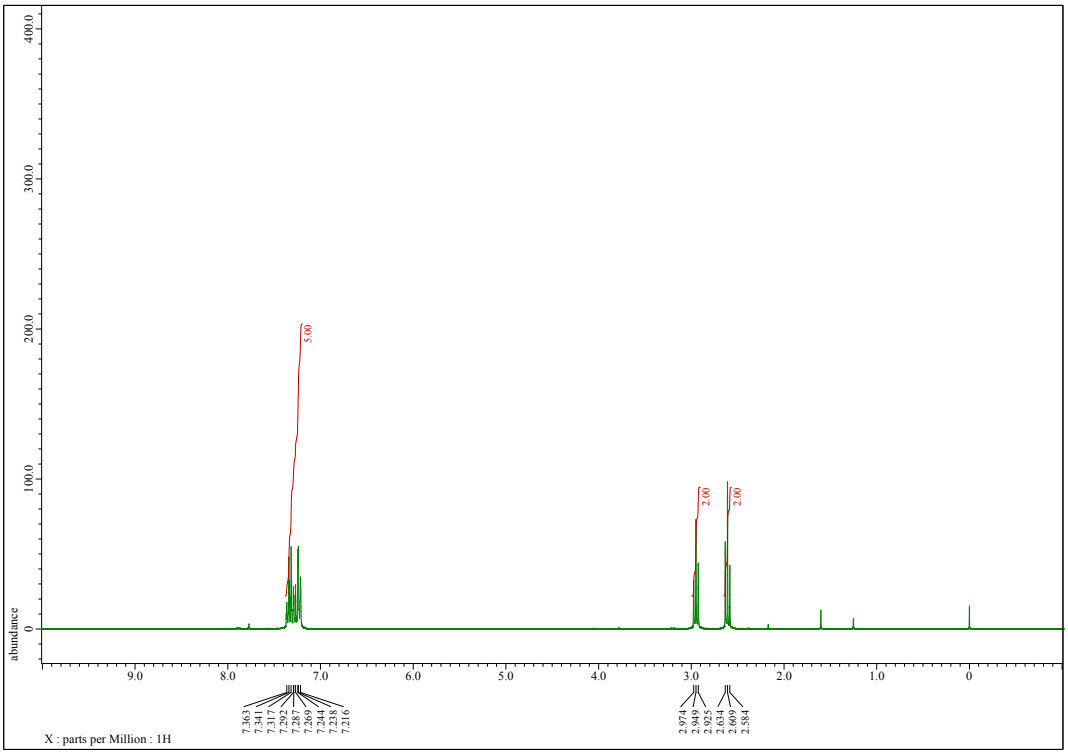
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7.216
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2.925
2.634
2.609
2.584
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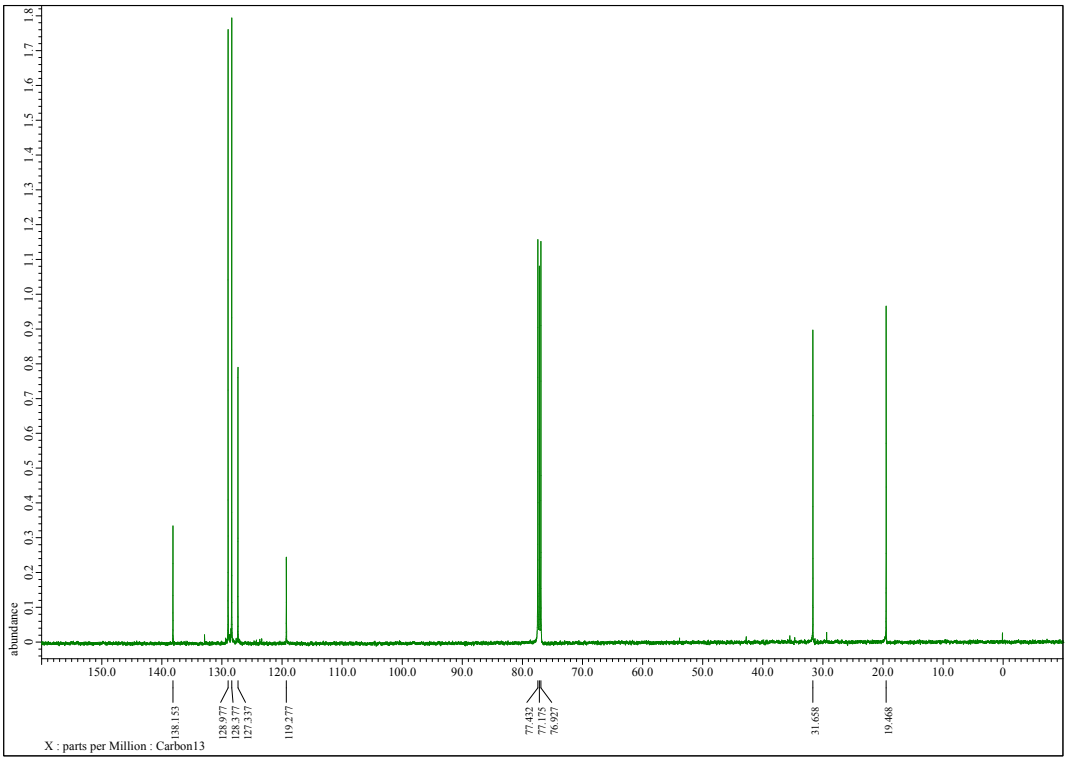
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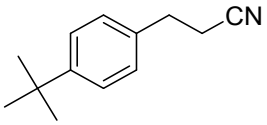
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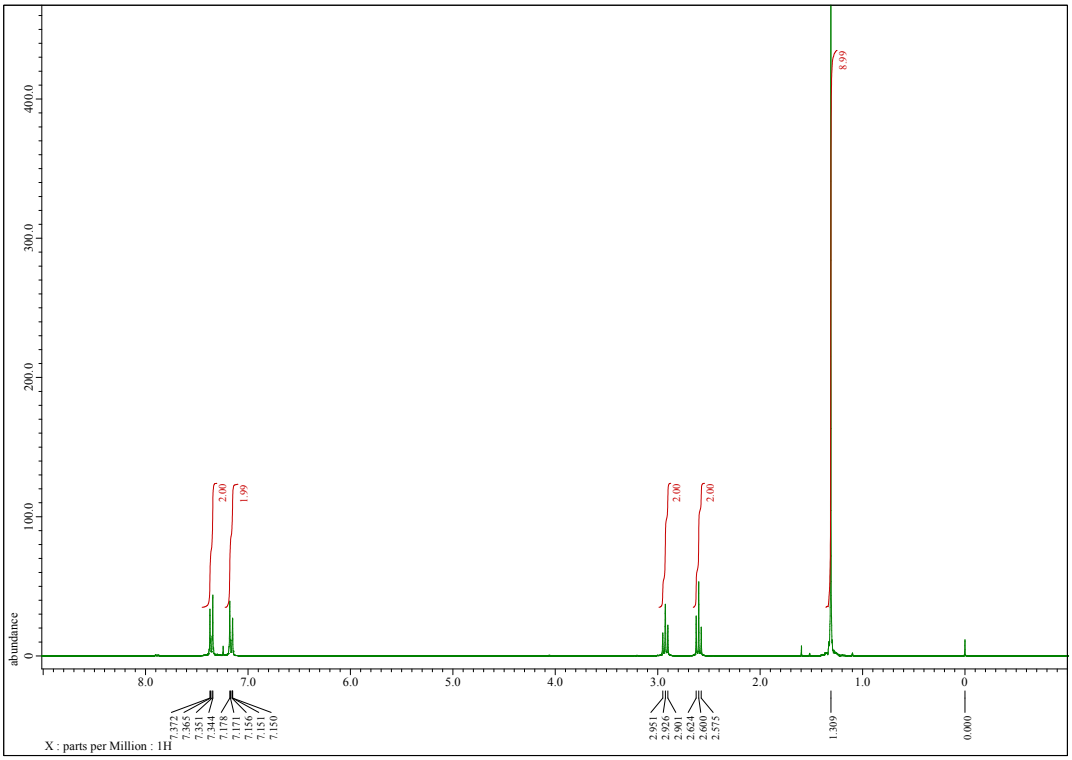
5fa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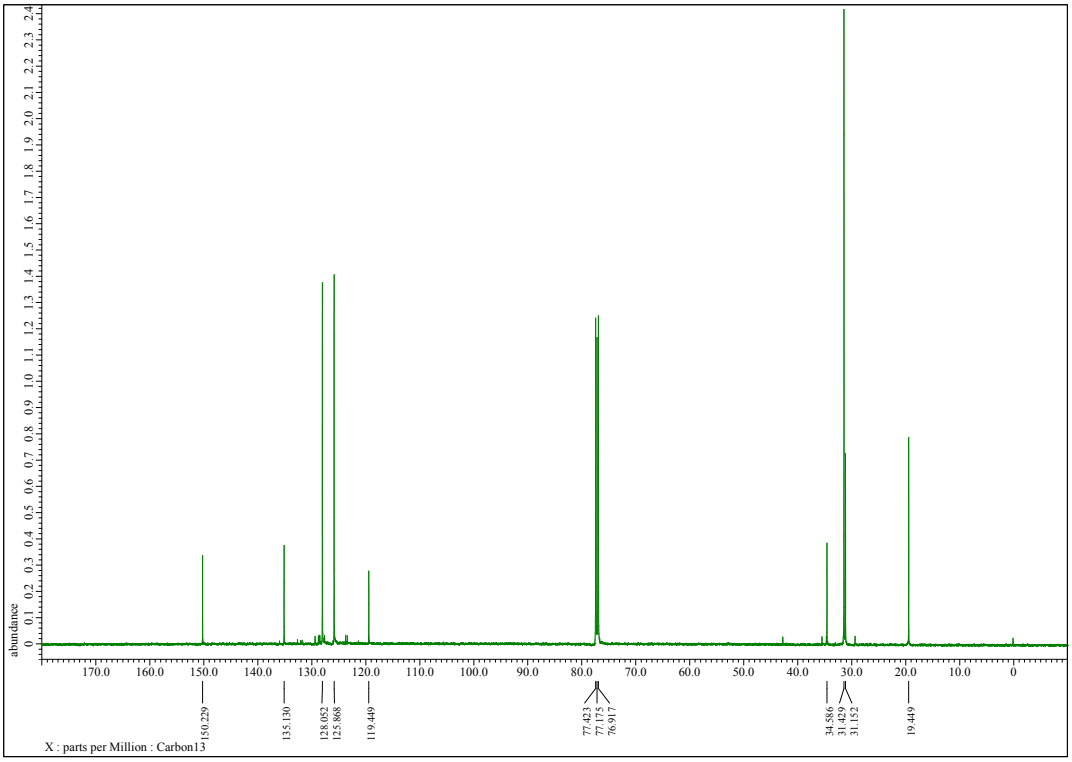
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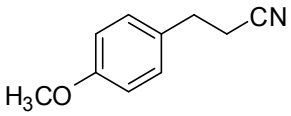
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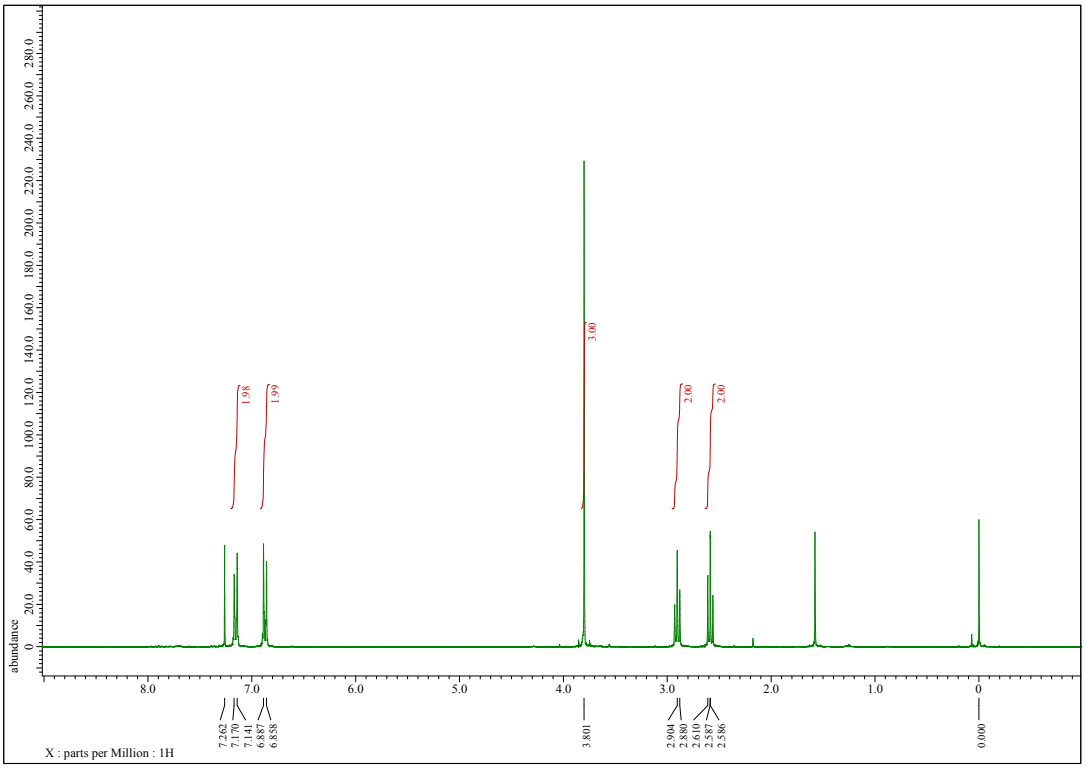
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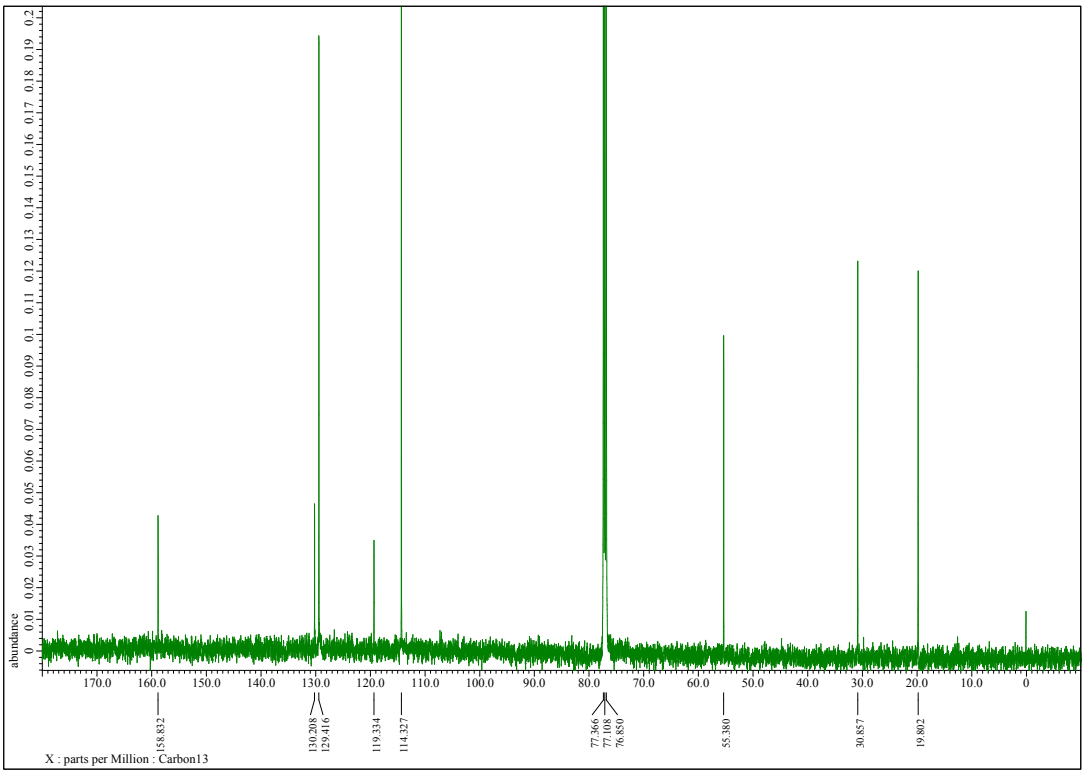
X : parts per Million : 1H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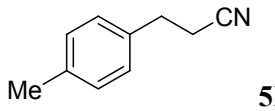
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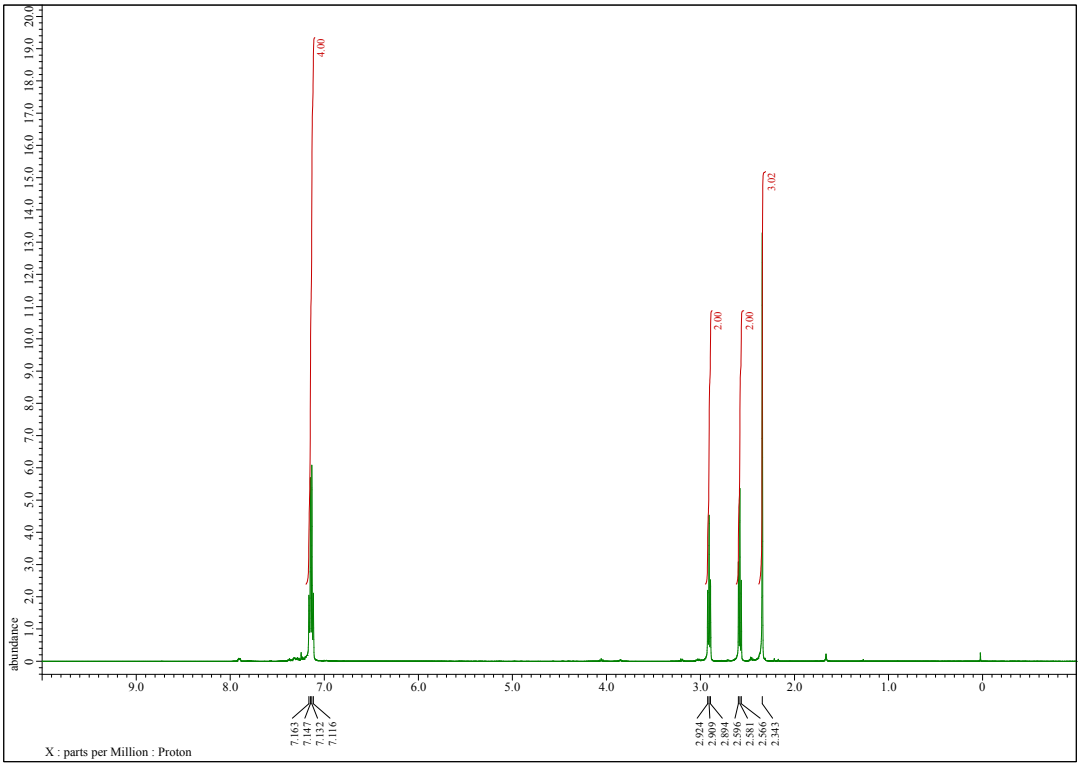
Me

5ha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2.00
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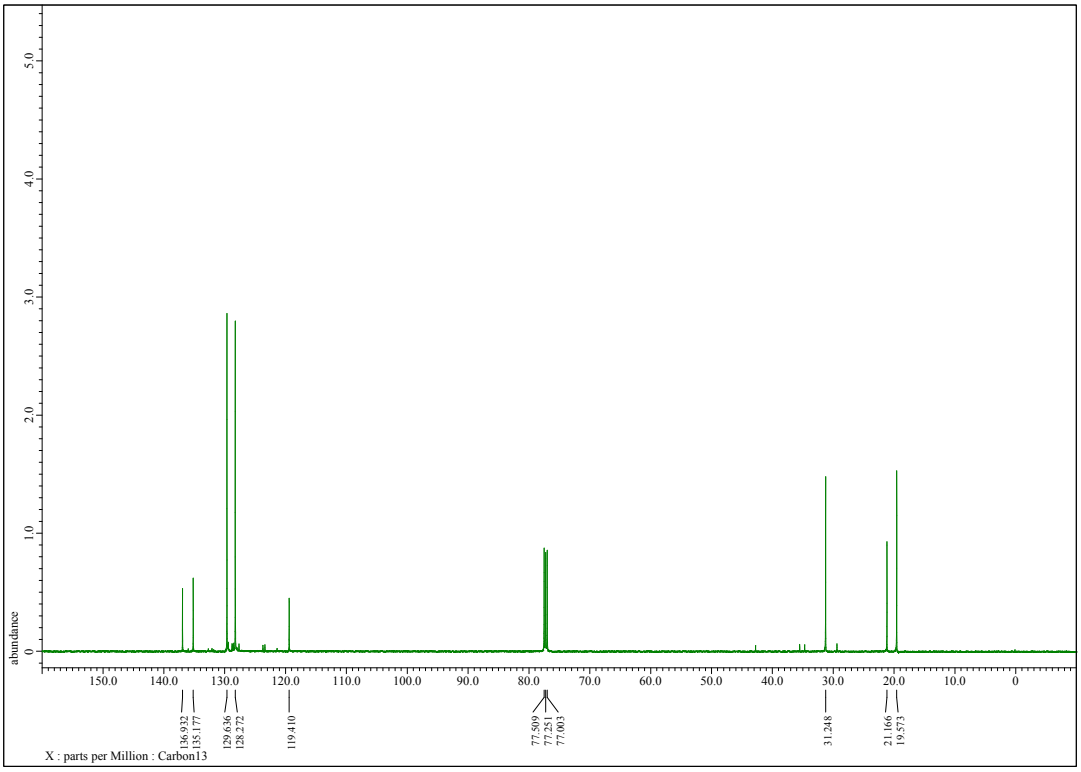
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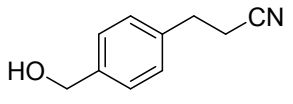
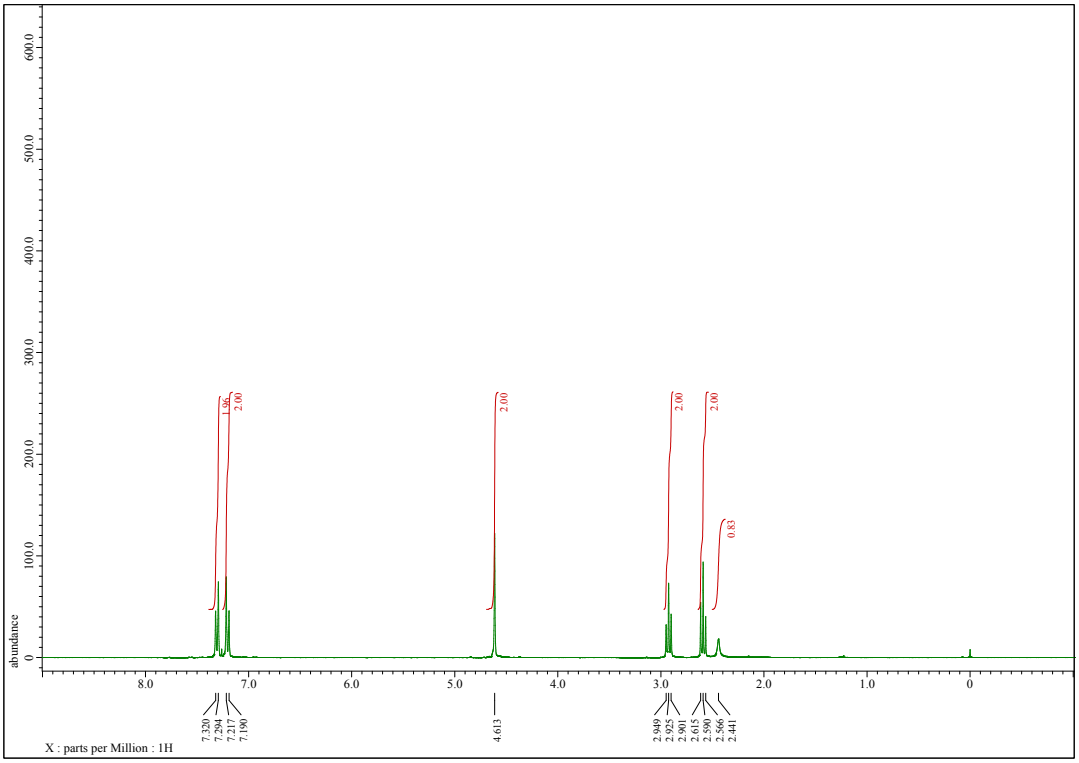

CN
HO

5ia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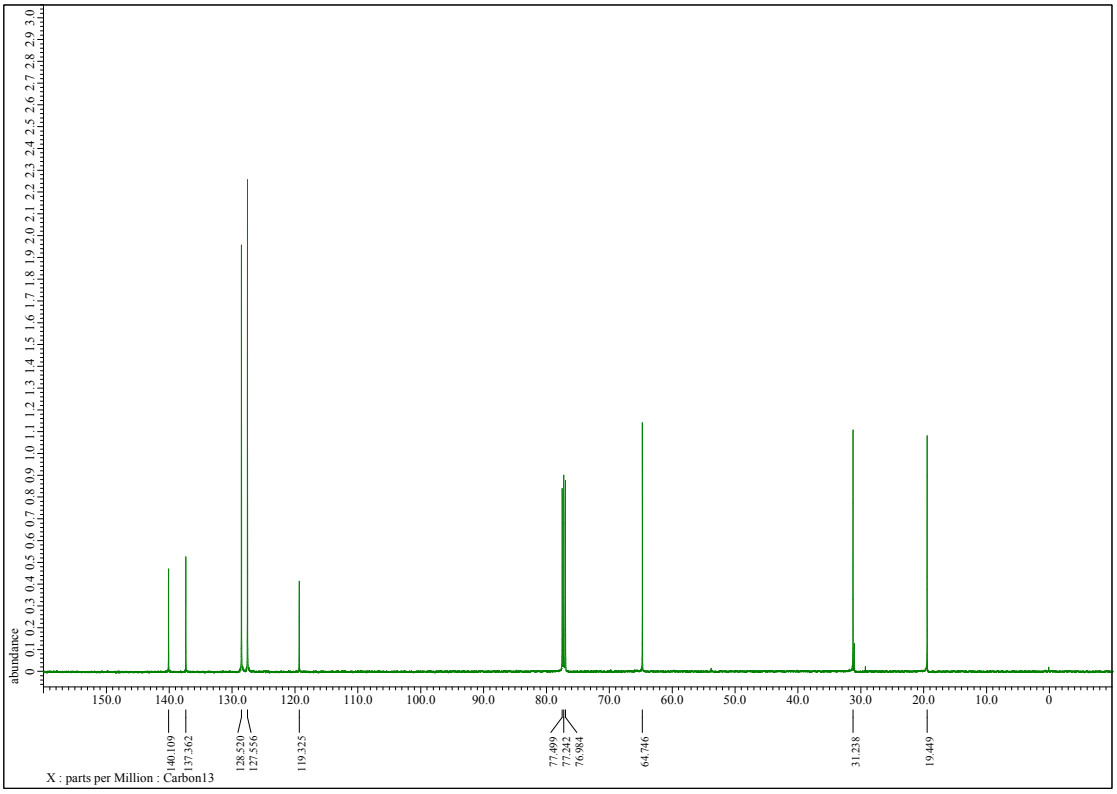
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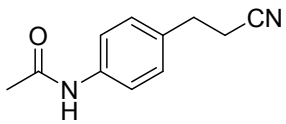
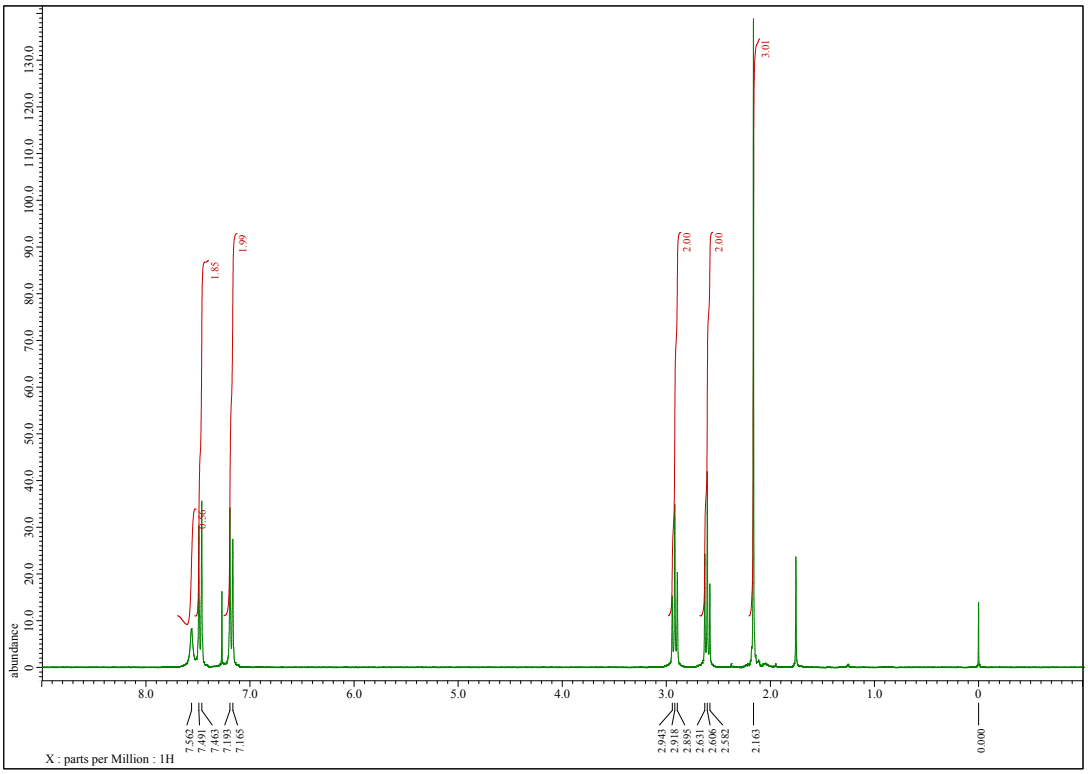

O
N
H
CN

5ja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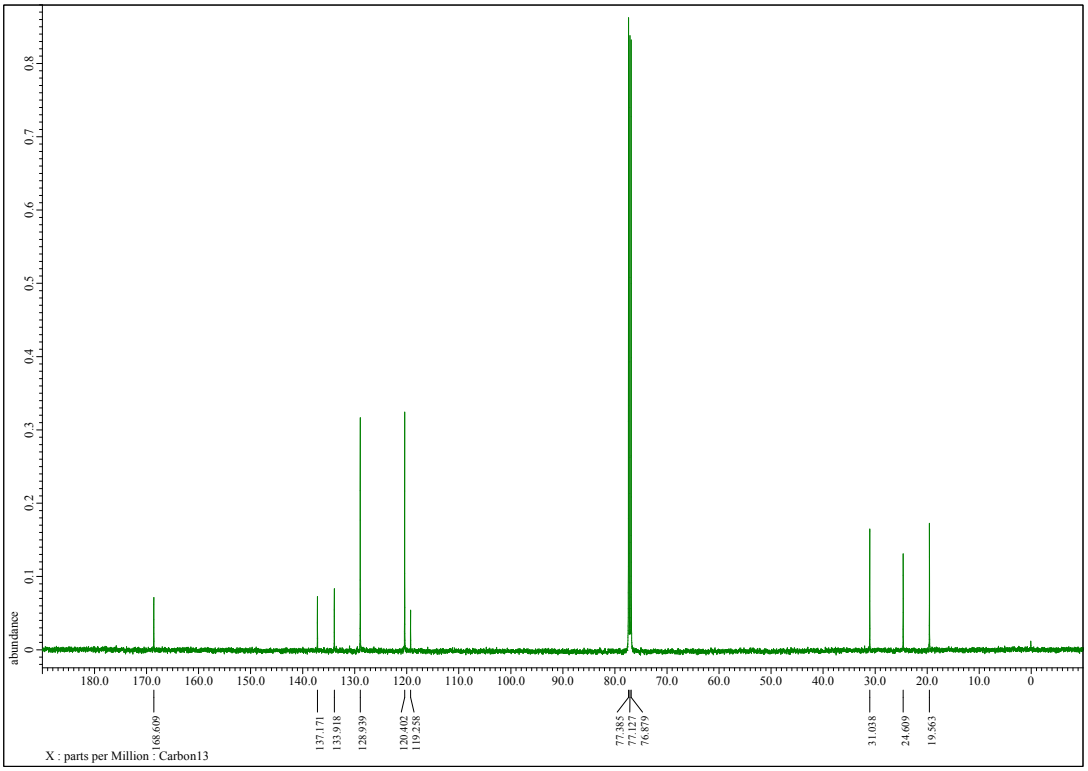
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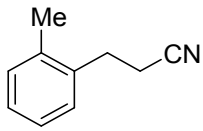
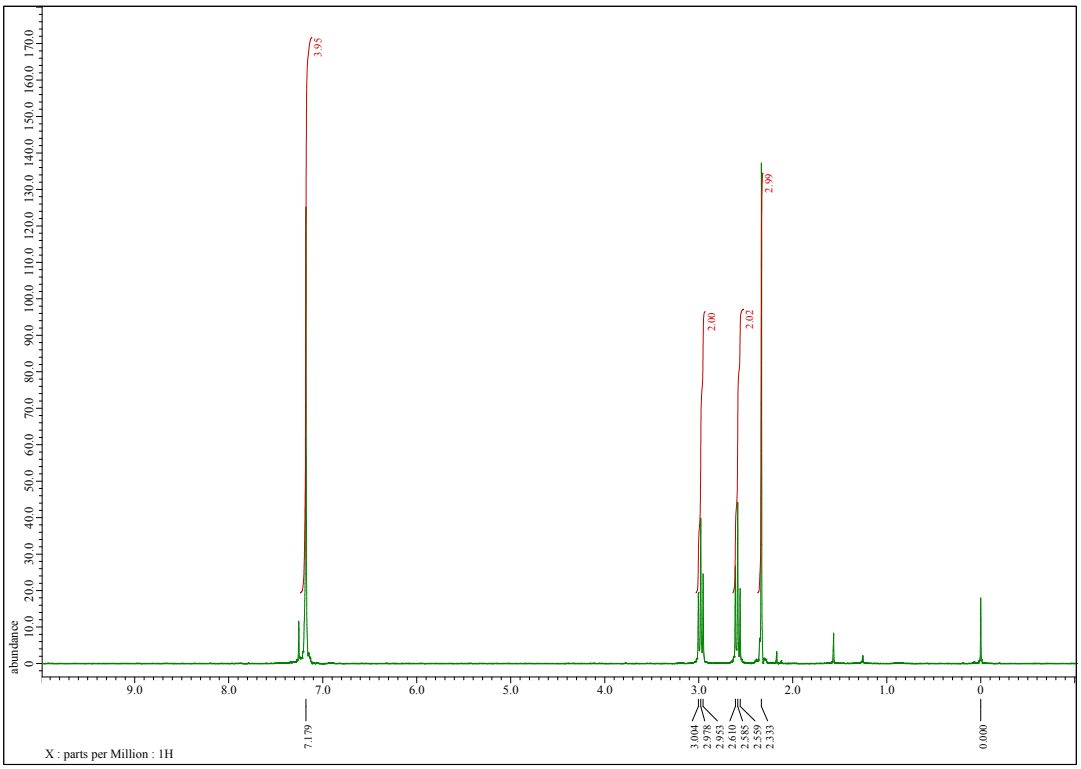

Me
CN

5ka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0
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3.004
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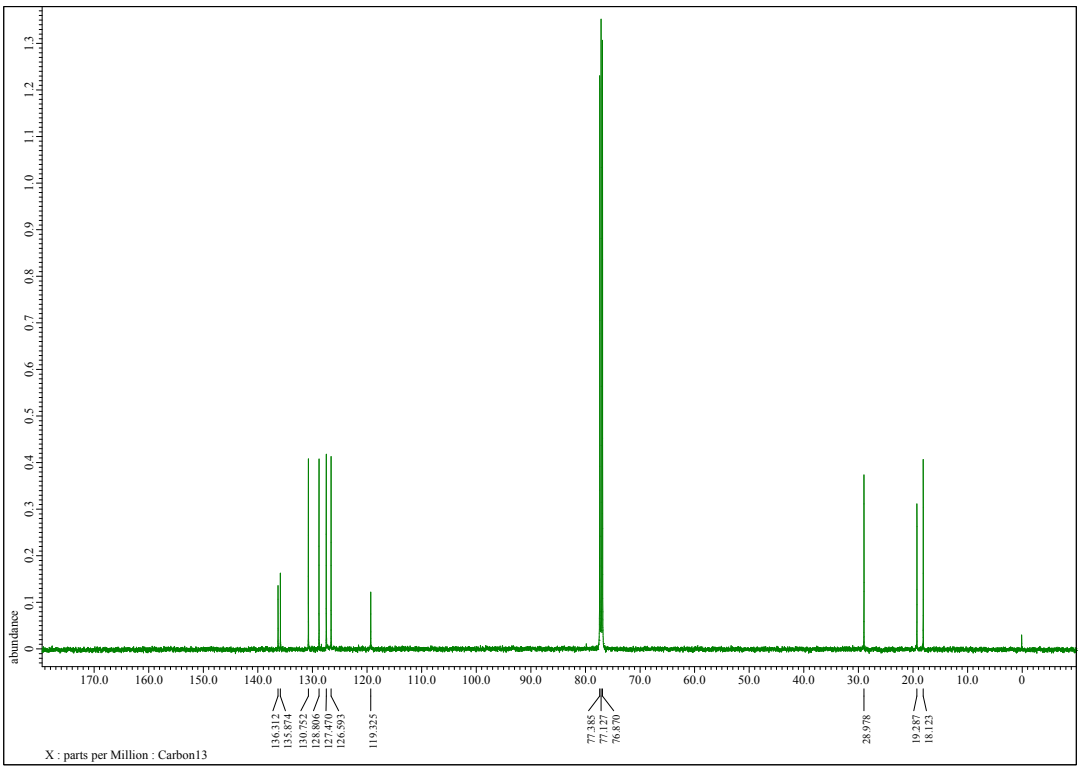
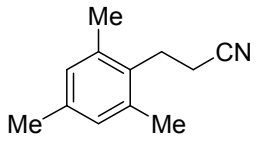
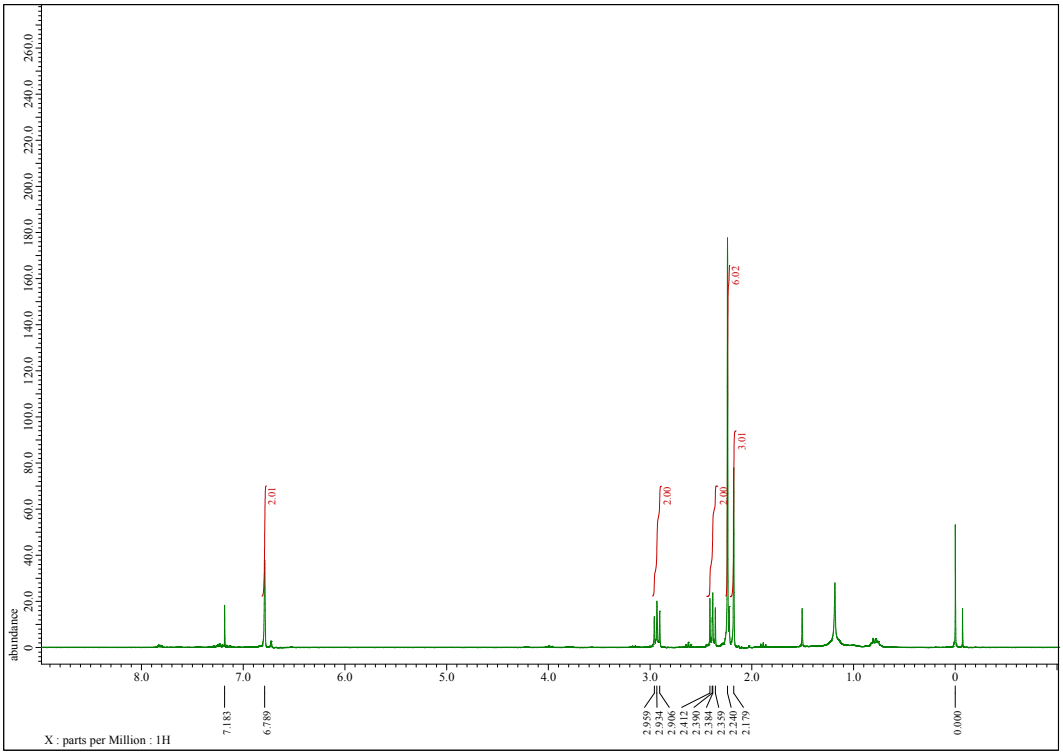
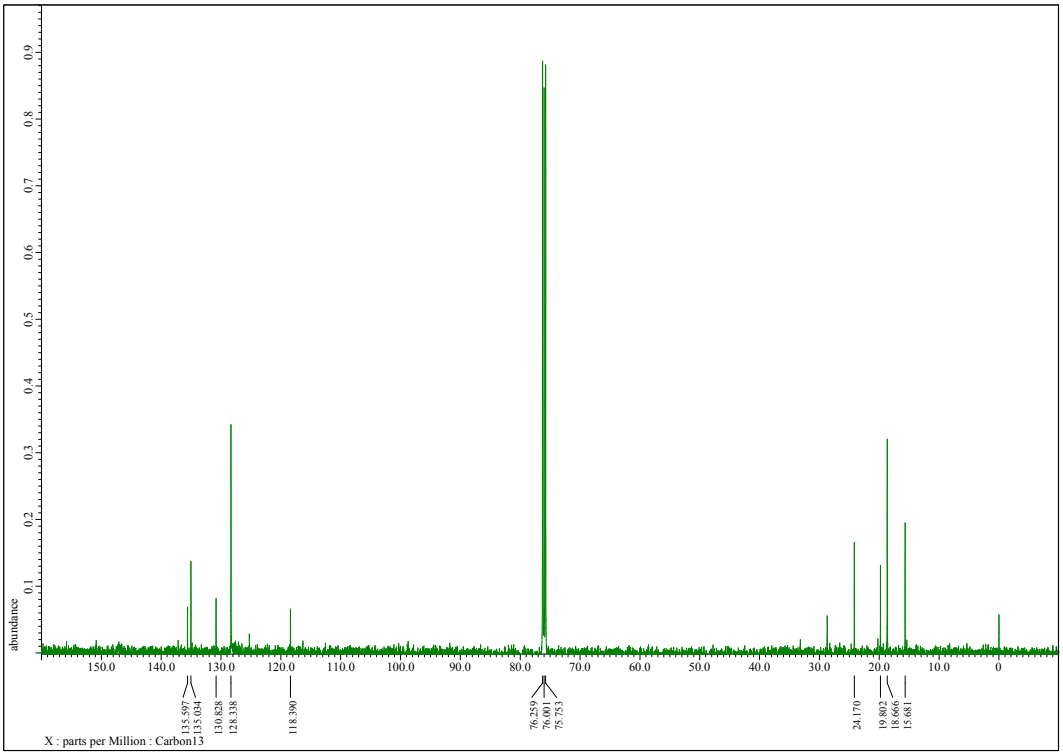
2.953
2.610
2.588
2.559
2.333
0.000
X : parts per Million : 1H

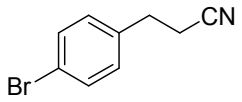

abundance
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
136.312
135.874
130.752
128.806
127.470
126.593
119.325
77.385
77.127
76.870
28.978
19.287
18.123
X : parts per Million : Carbon13


Me
CN
Me
Me

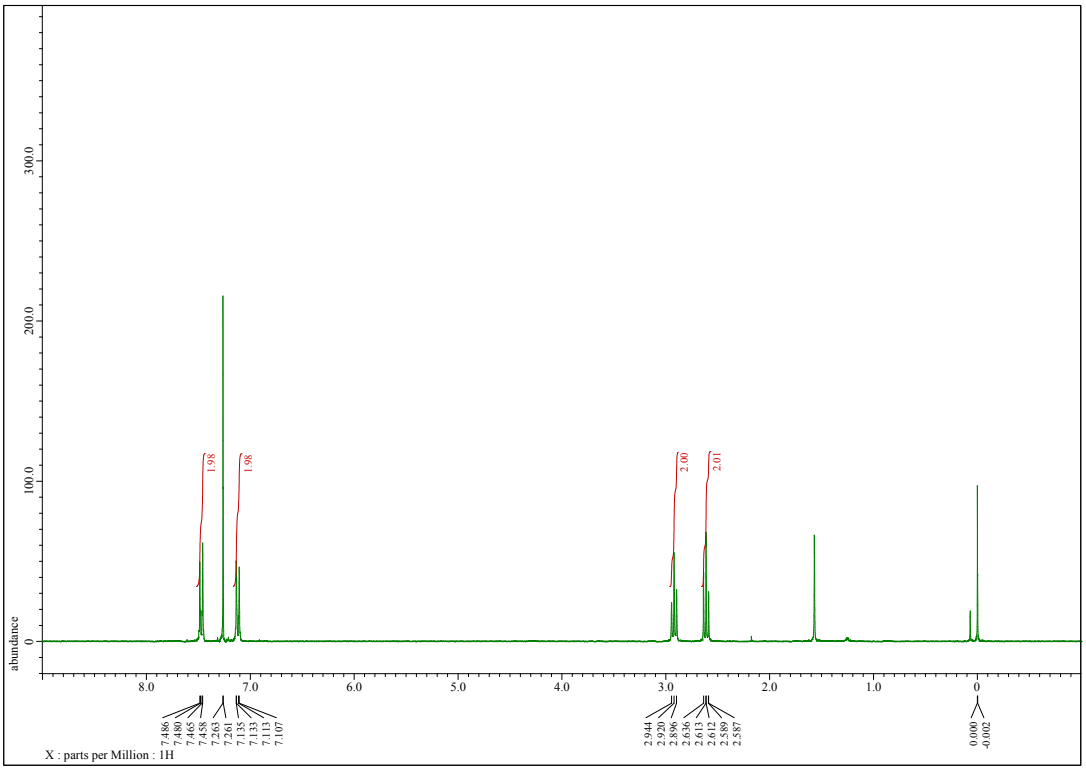
5la

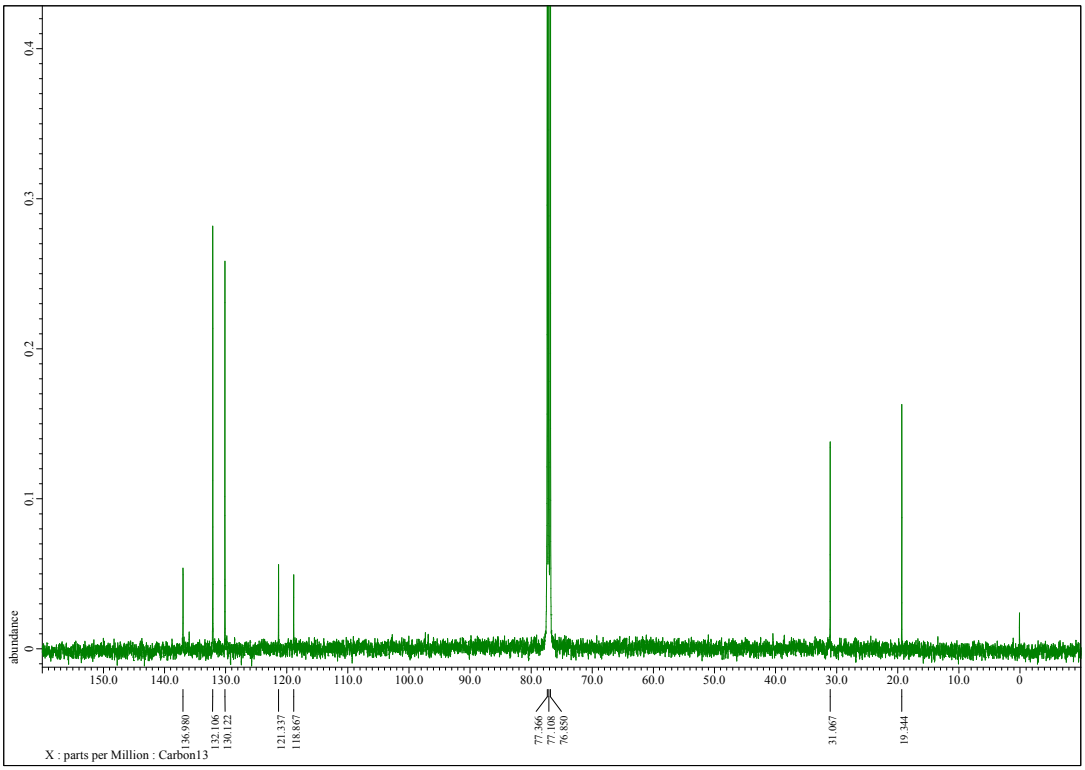

abundance
2.01
2.00
2.00
6.02
3.01
7.183
6.789
2.959
2.934
2.908
2.415
2.390
2.384
2.359
2.240
2.179
0.000
X : parts per Million : 1H

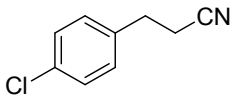

abundance
135.597
135.034
130.828
128.338
118.390
76.259
76.001
75.753
24.170
19.802
18.466
15.681
X : parts per Million : Carbon13


CN
Br

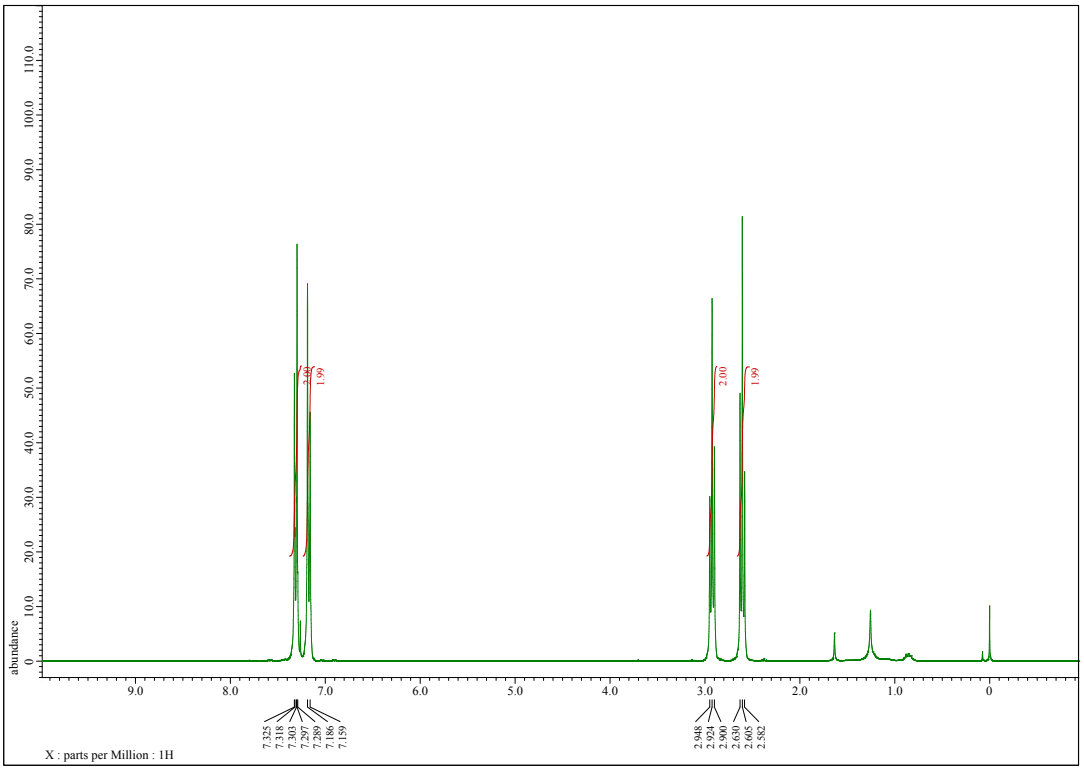
5na

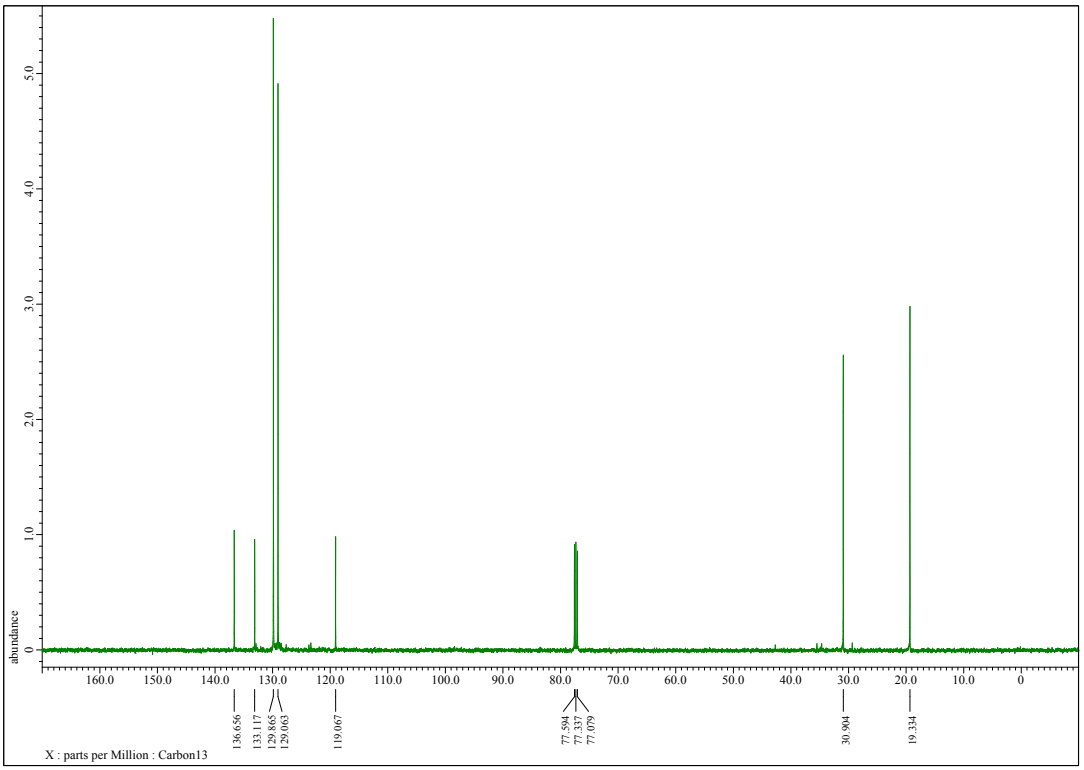

abundance
1.98
1.98
2.00
2.01
X : parts per Million : 1H

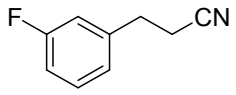

abundance
136.980
132.106
130.122
121.337
118.867
77.366
77.108
76.850
31.067
19.344
X : parts per Million : Carbon13


CN
Cl

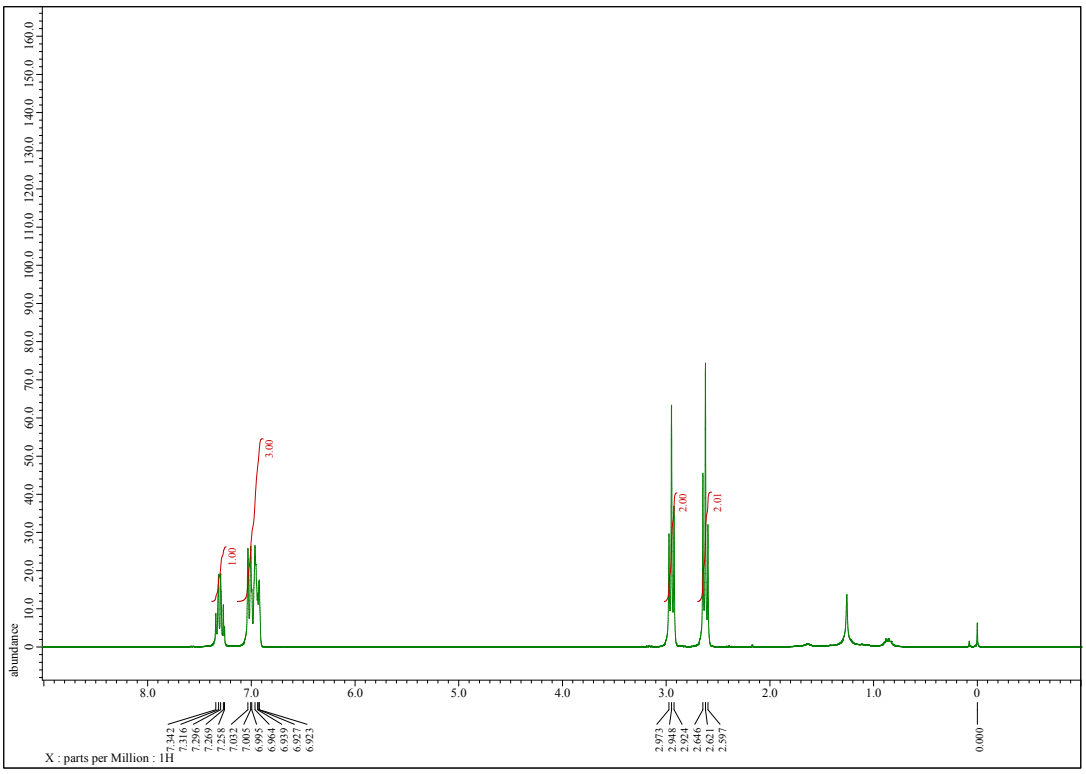
5ma

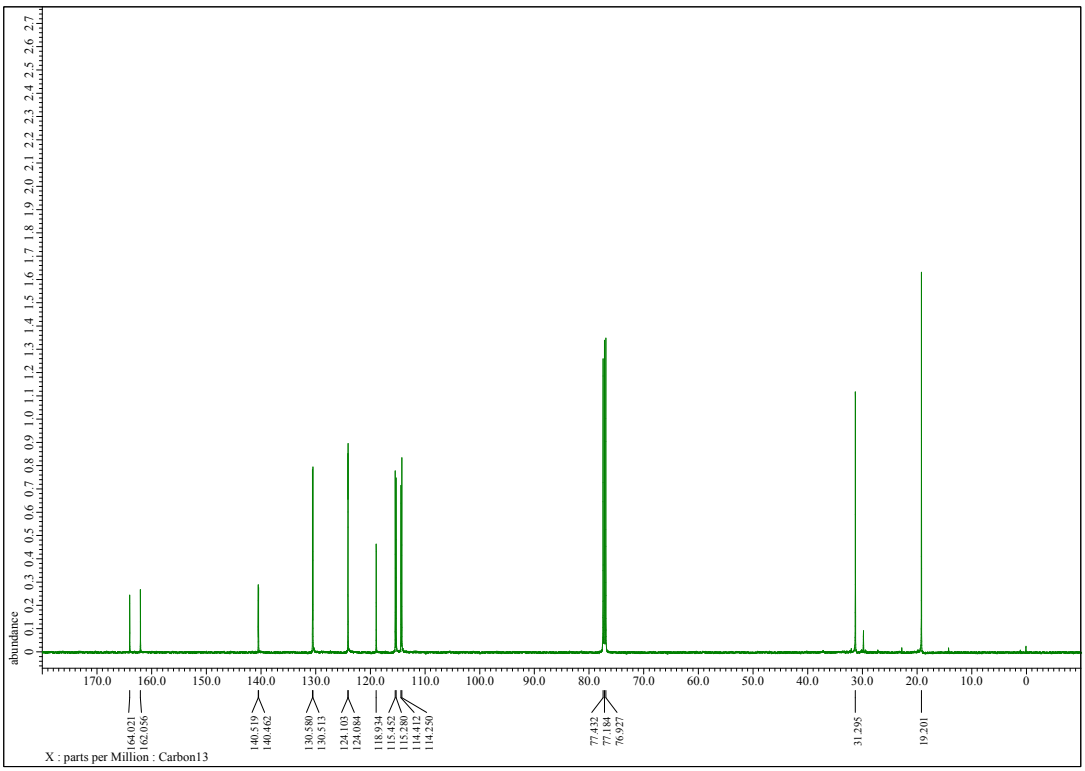

abundance
X : parts per Million : 1H
7.325
7.318
7.310
7.297
7.289
7.186
7.159
2.948
2.924
2.900
2.630
2.605
2.582
2.00
1.99
1.99

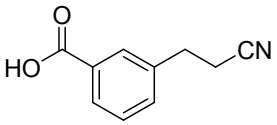

abundance
X : parts per Million : Carbon13
136.636
133.117
129.865
129.063
119.067
77.594
77.337
77.079
30.904
19.334


F
CN

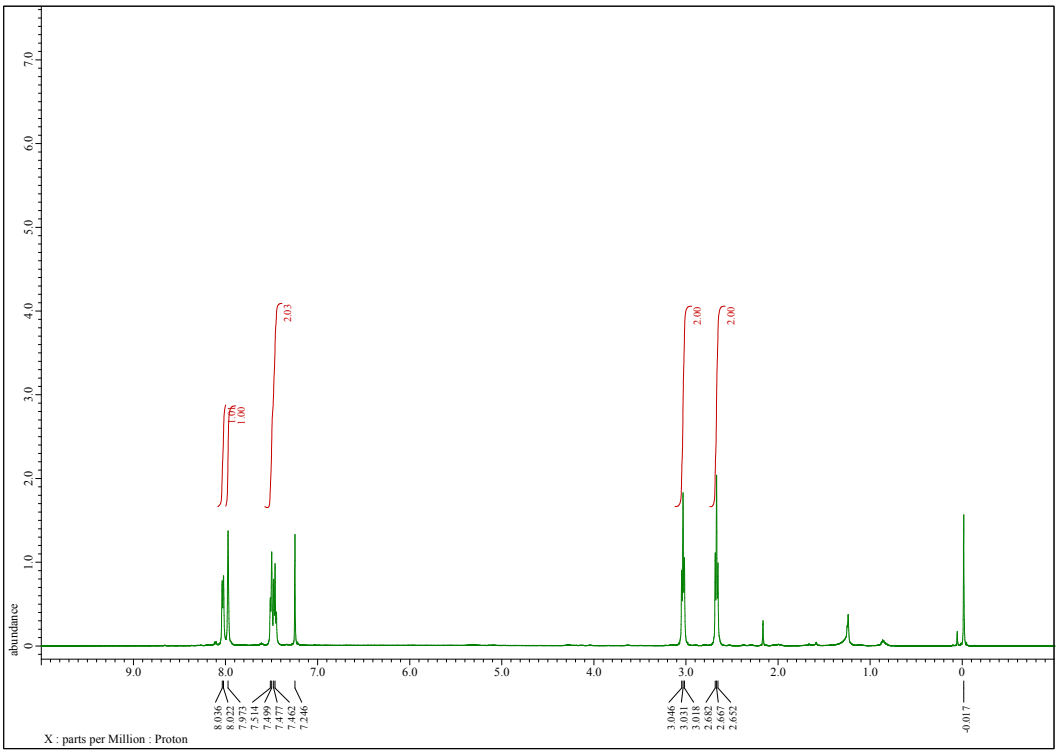
5oa

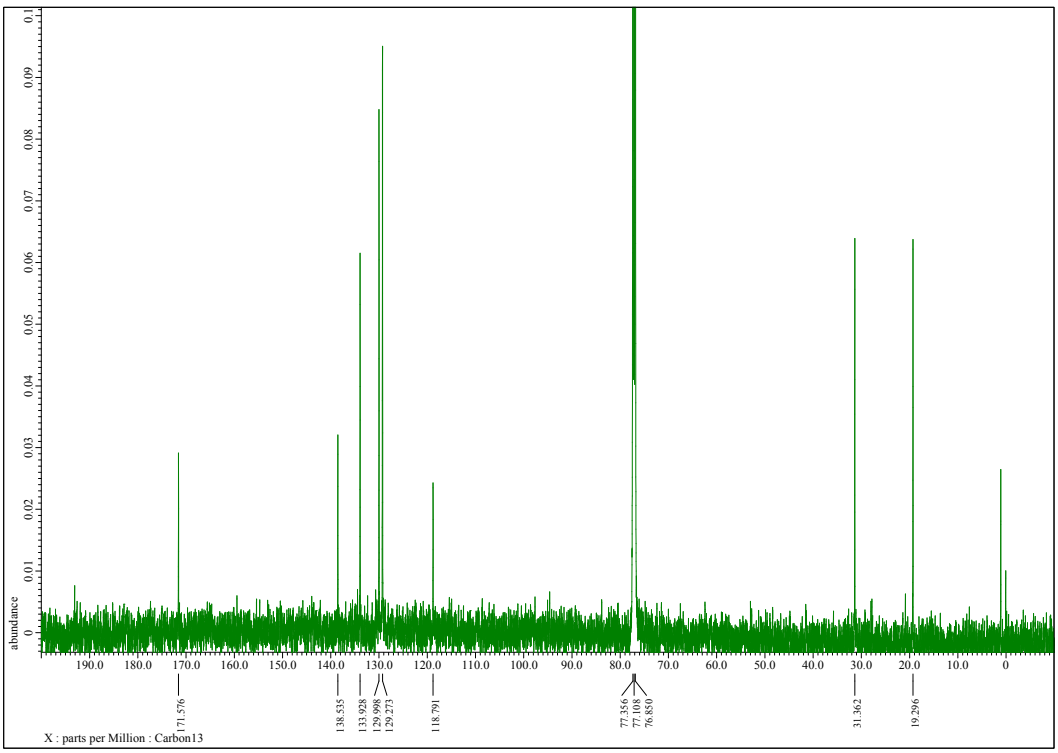

abundance
X : parts per Million : 1H
1.00
3.00
2.00
2.01
7.342
7.316
7.296
7.266
7.258
7.032
7.005
6.995
6.964
6.939
6.927
6.923
2.973
2.948
2.923
2.646
2.621
2.597
0.000

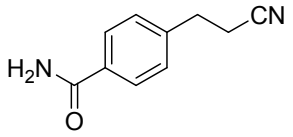

abundance
X : parts per Million : Carbon13
164.021
162.056
140.519
140.462
130.589
130.513
124.103
124.084
118.934
115.452
115.230
114.412
114.250
77.432
77.184
76.927
31.295
19.201


O
HO
CN

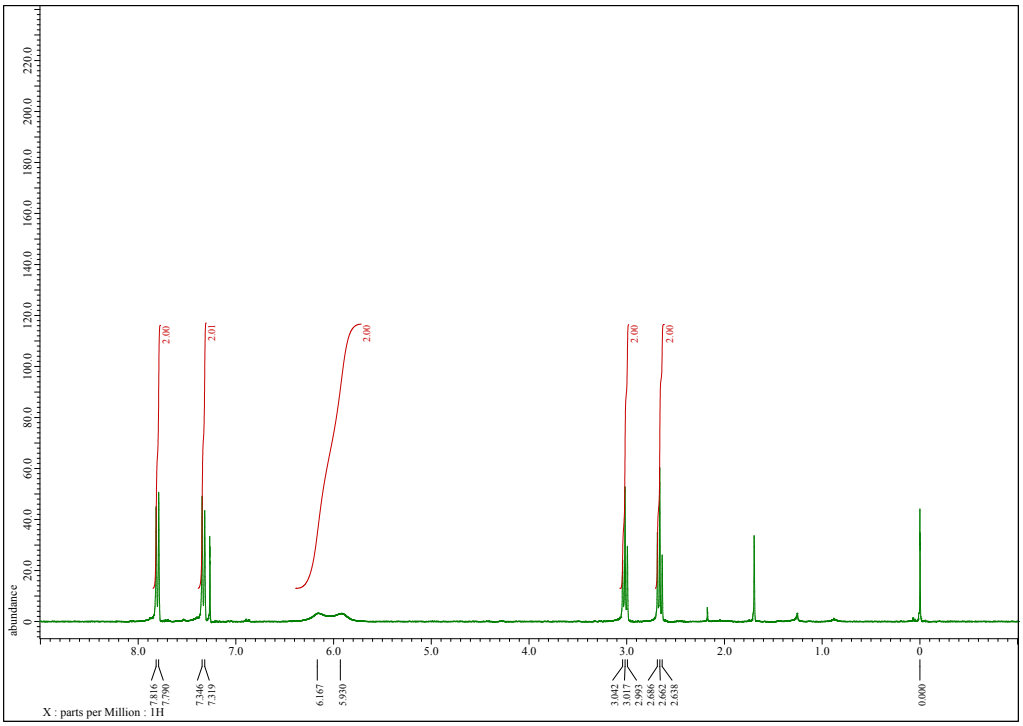
5pa

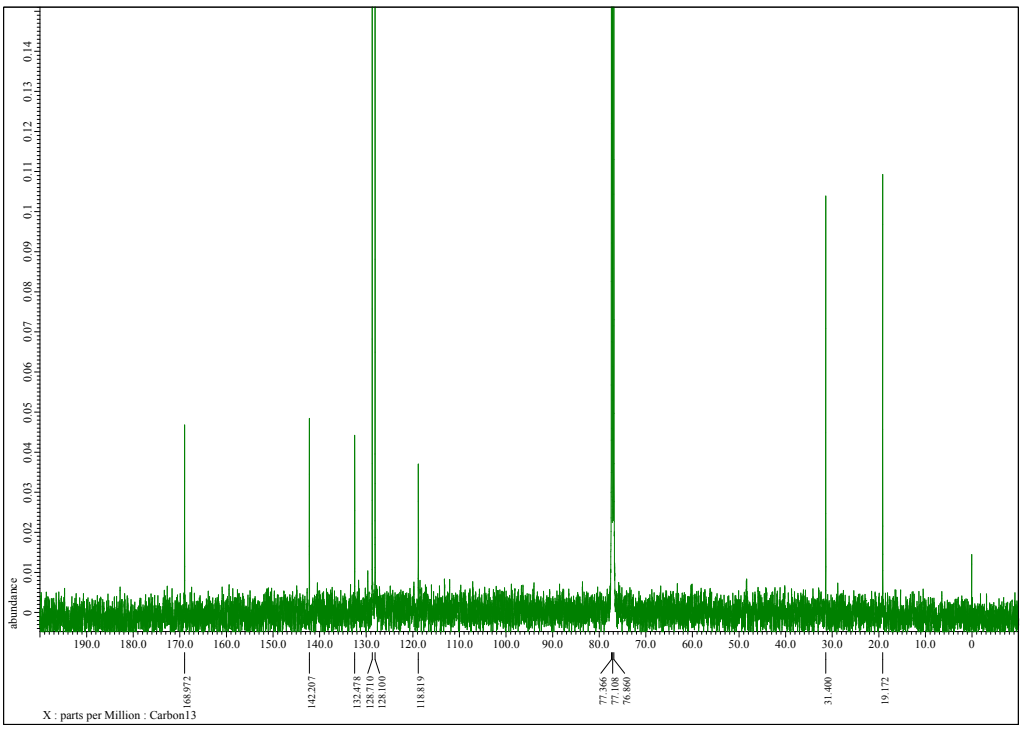

abundance
1.05
1.00
2.03
2.00
2.00
8.036
8.022
7.973
7.514
7.499
7.477
7.462
7.246
3.046
3.031
3.018
2.682
2.667
2.652
-0.017
X : parts per Million : Proton

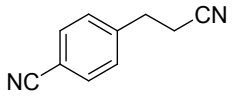

abundance
171.576
138.535
133.928
129.998
129.273
118.791
77.356
77.108
76.850
31.362
19.296
X : parts per Million : Carbon13


CN
H2N
O

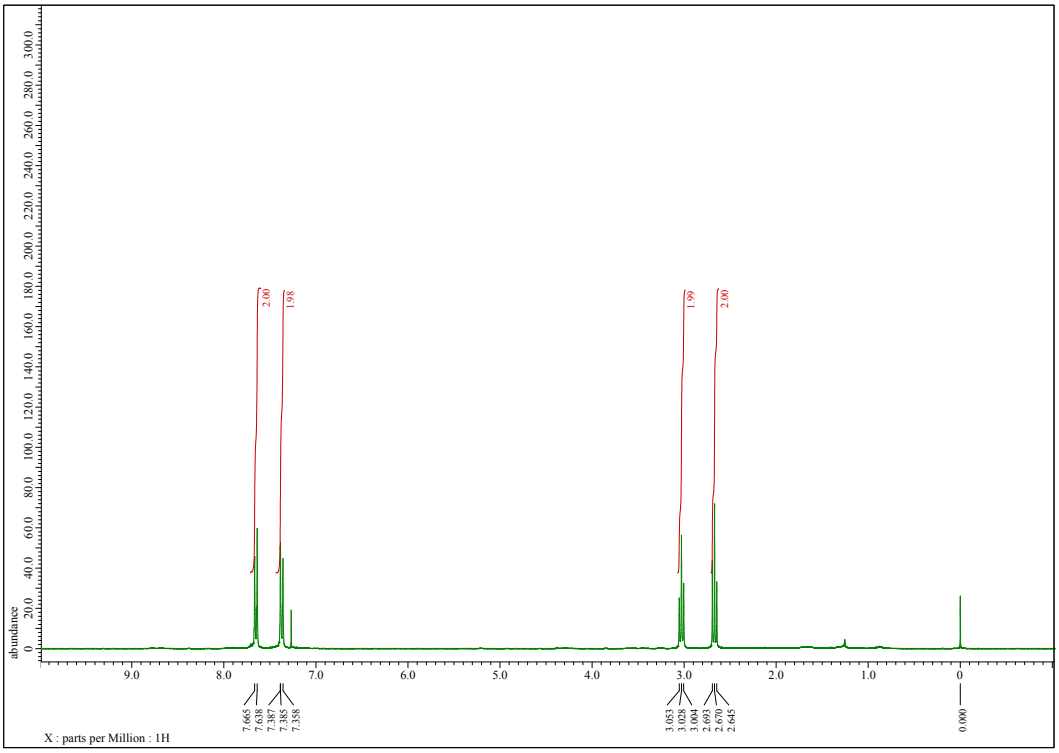
5qa

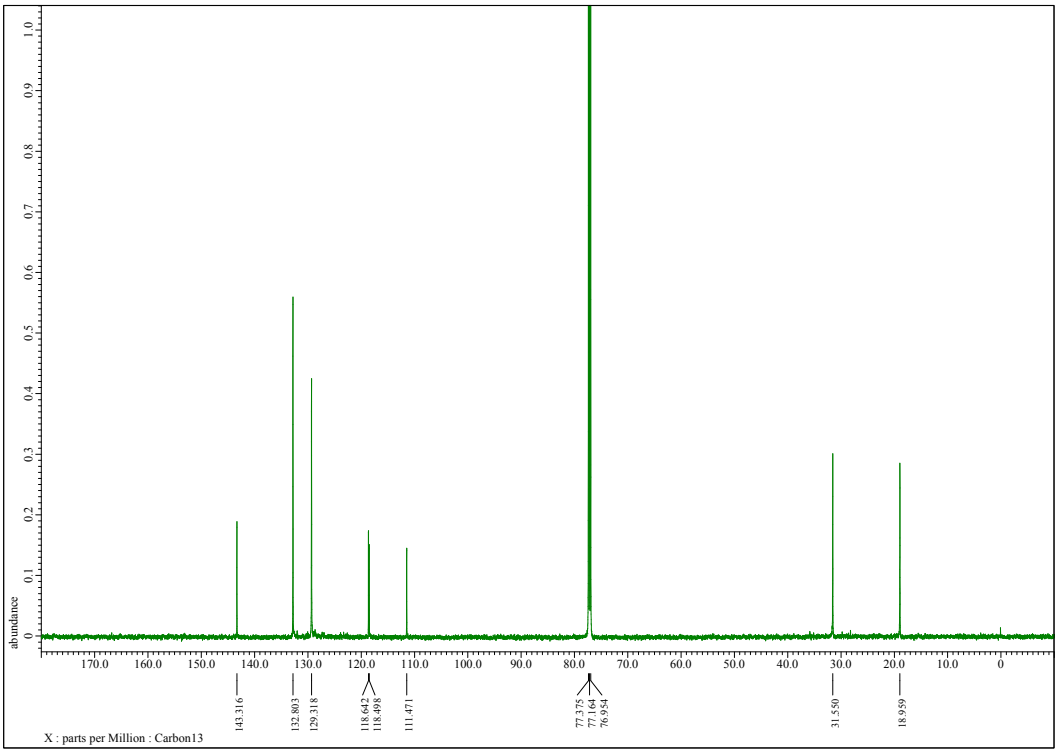

abundance
2.00
2.01
2.00
2.00
2.00
7.816
7.790
7.346
7.319
6.167
5.930
3.042
3.017
2.993
2.686
2.662
2.638
0.000
X : parts per Million : 1H

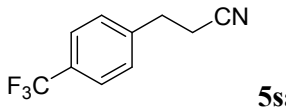

abundance
168.972
142.207
132.478
128.710
128.100
118.819
77.366
77.108
76.850
31.400
19.172
X : parts per Million : Carbon13


CN
NC

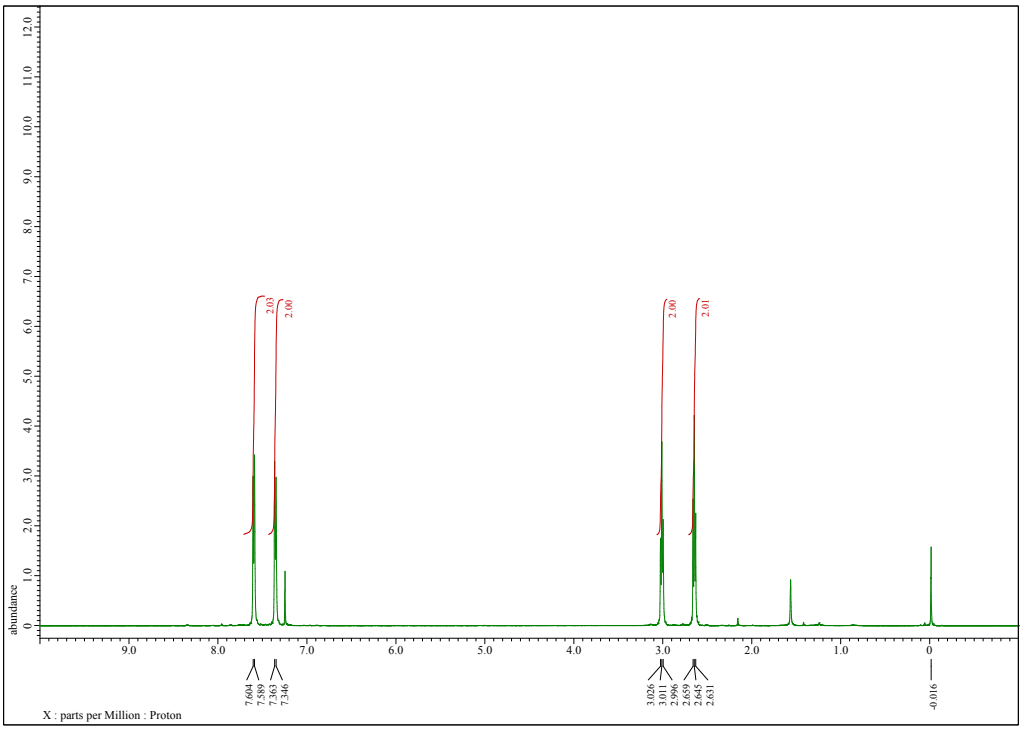
5ra

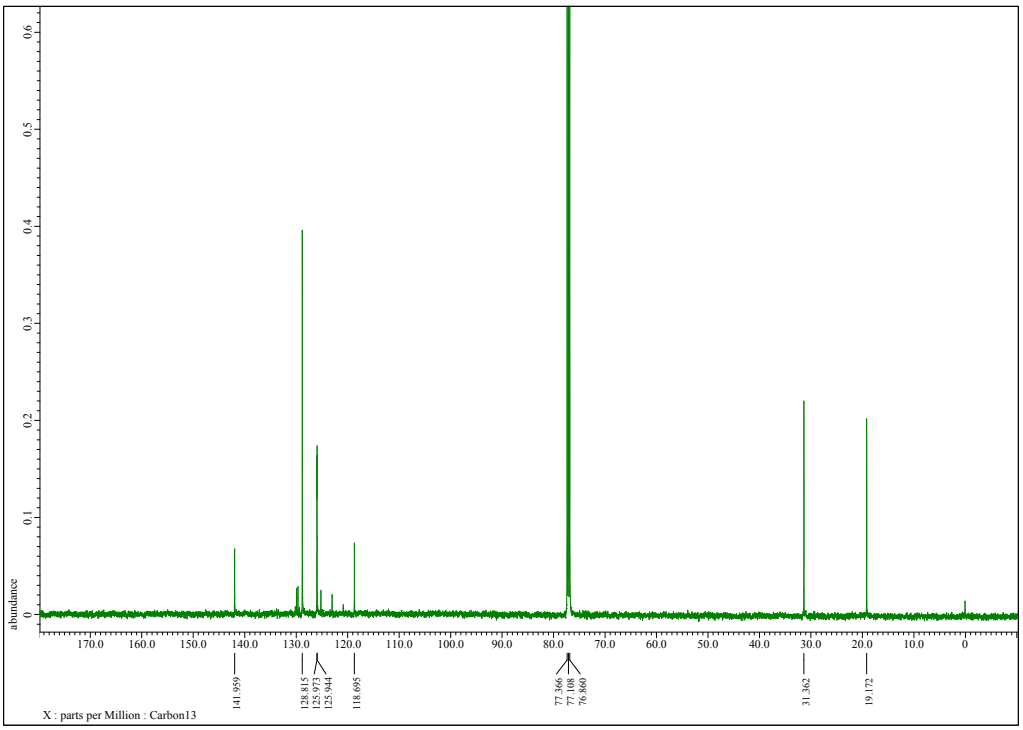

abundance
2.00
1.98
1.99
2.00
7.665
7.638
7.387
7.385
7.358
3.053
3.028
3.004
2.693
2.670
2.645
0.000
X : parts per Million : 1H

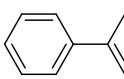

abundance
143.316
132.803
129.318
118.642
118.498
111.471
77.375
77.164
76.954
31.550
18.959
X : parts per Million : Carbon13


CN
F3C

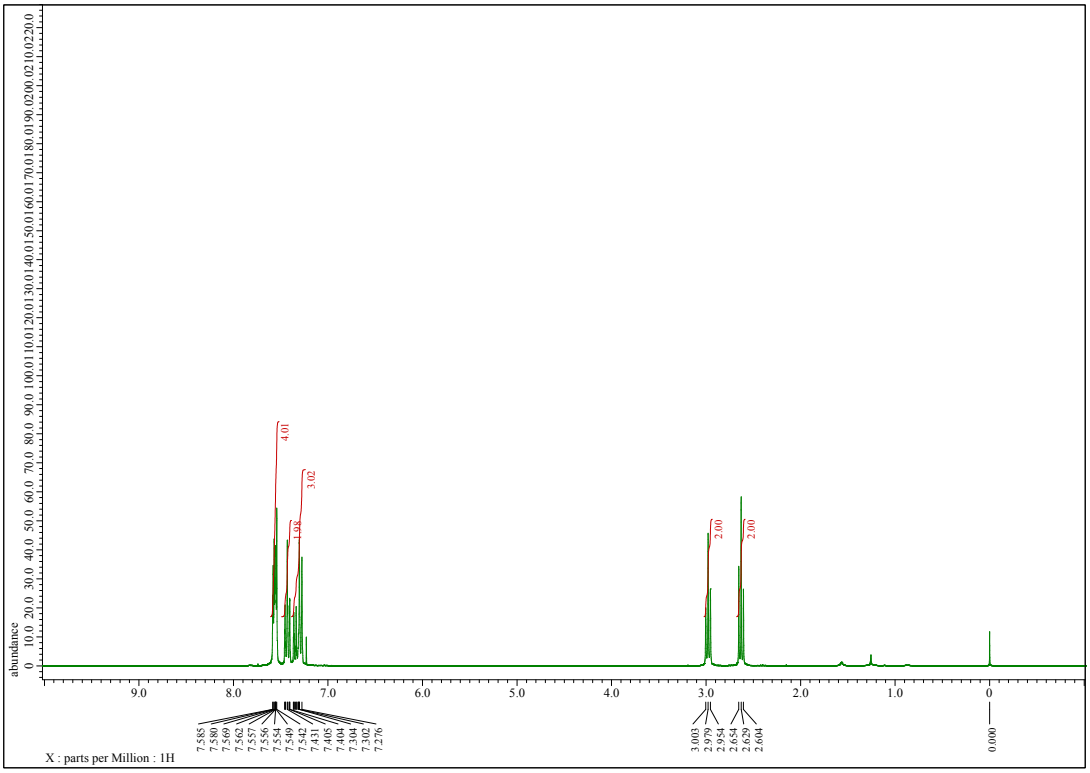
5sa

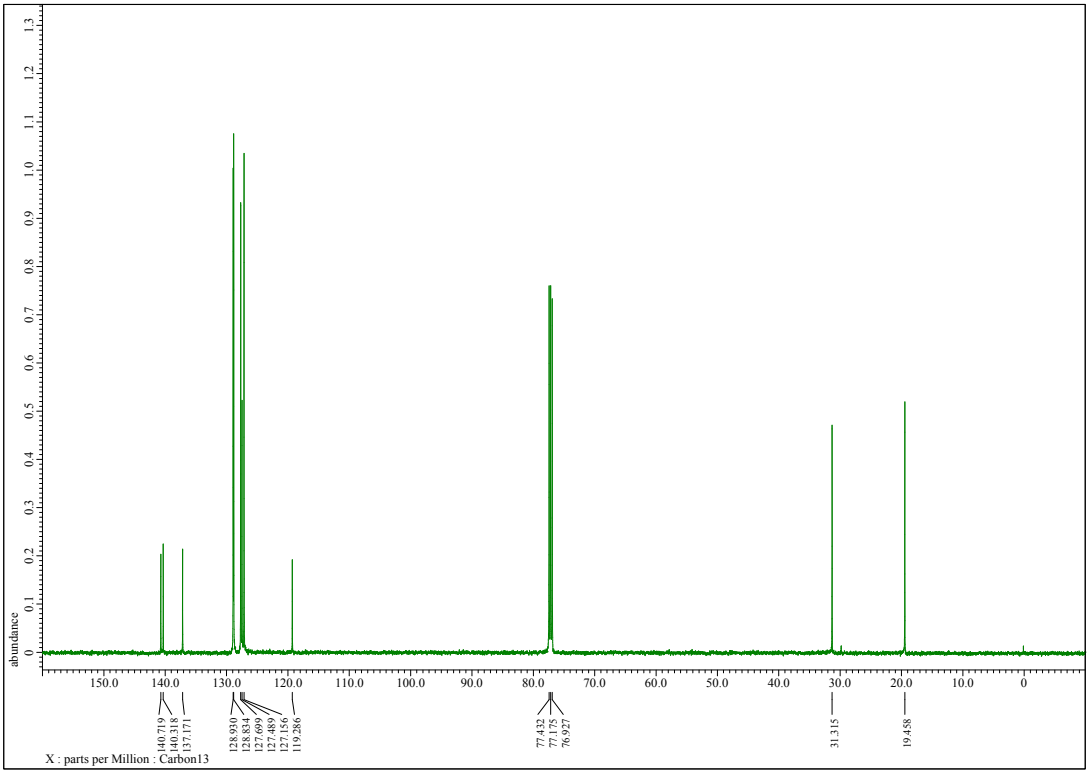

abundance
2.03
2.00
2.00
2.01
7.604
7.589
7.363
7.346
3.026
3.011
2.996
2.659
2.645
2.631
-0.016
X : parts per Million : Proton

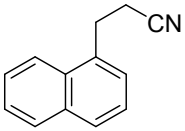

abundance
141.959
128.815
125.973
125.944
118.695
77.266
77.108
76.860
31.362
19.172
X : parts per Million : Carbon13


CN

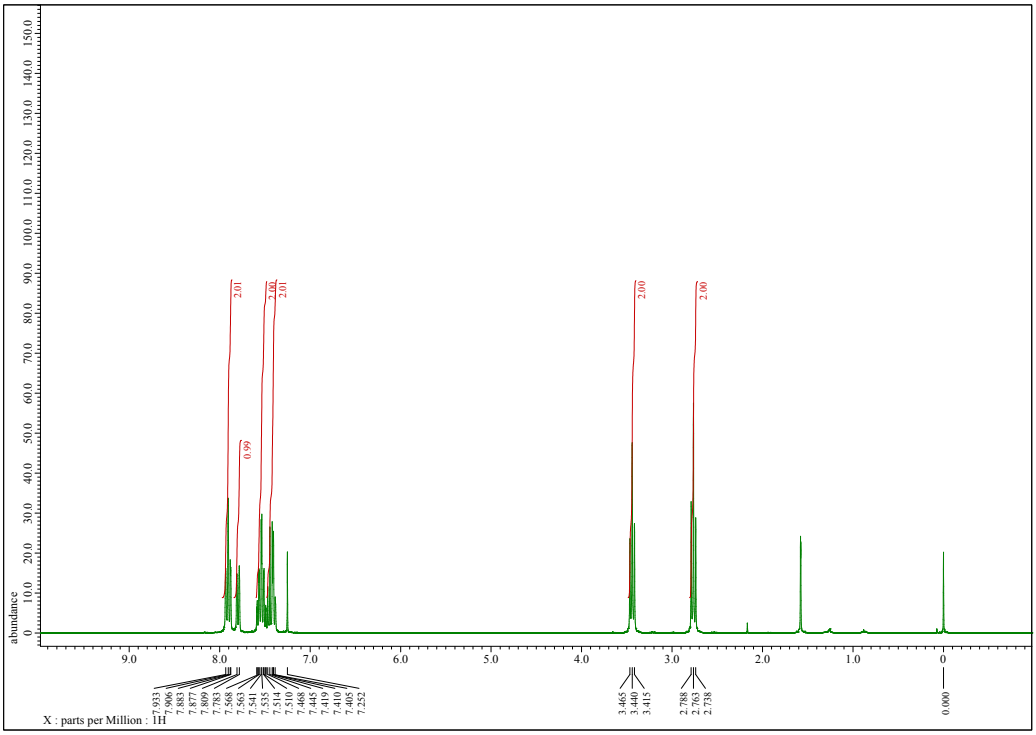
5ta

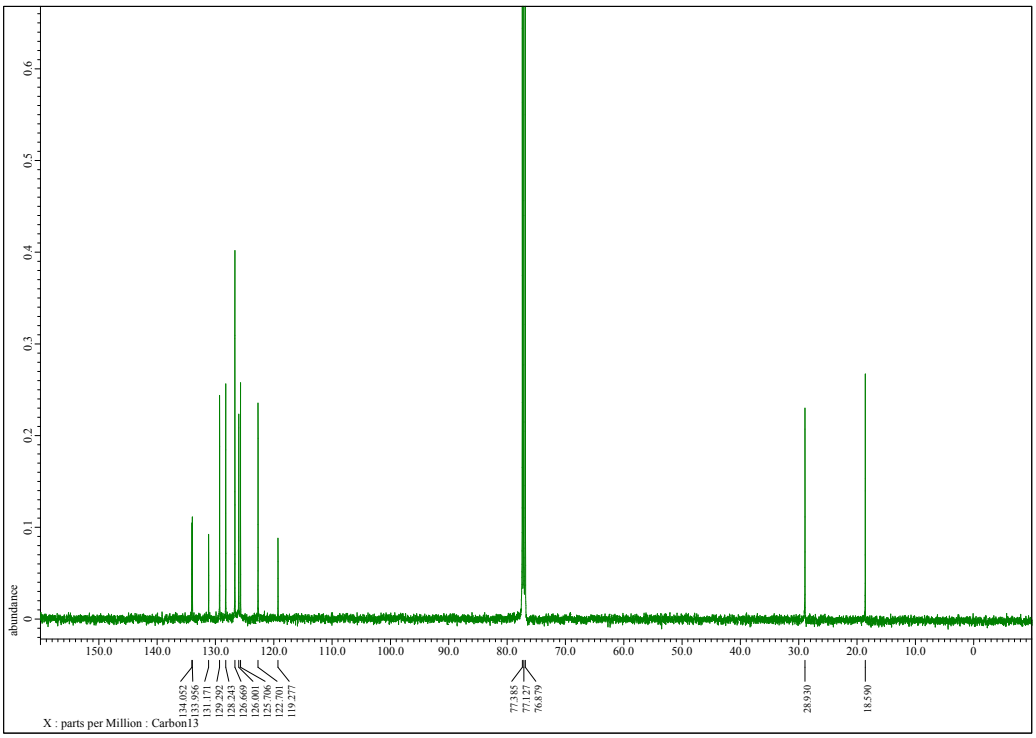

abundance
4.01
3.02
1.98
2.00
2.00
7.585
7.580
7.569
7.562
7.557
7.556
7.554
7.549
7.542
7.431
7.405
7.404
7.304
7.302
7.276
3.003
2.979
2.954
2.654
2.629
2.604
0.000
X : parts per Million : 1H

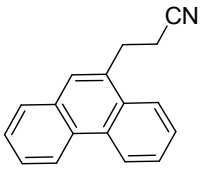

abundance
140.719
140.318
137.171
128.930
128.834
127.699
127.489
127.156
119.286
77.432
77.175
76.927
31.315
19.458
X : parts per Million : Carbon13


CN

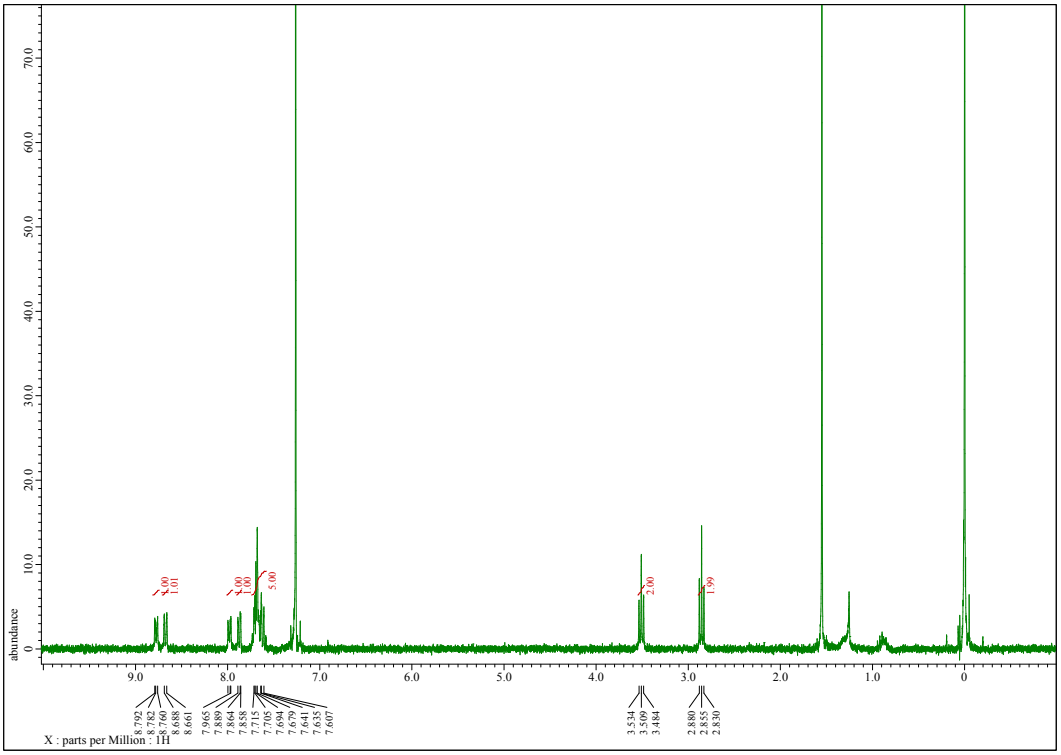
5ua

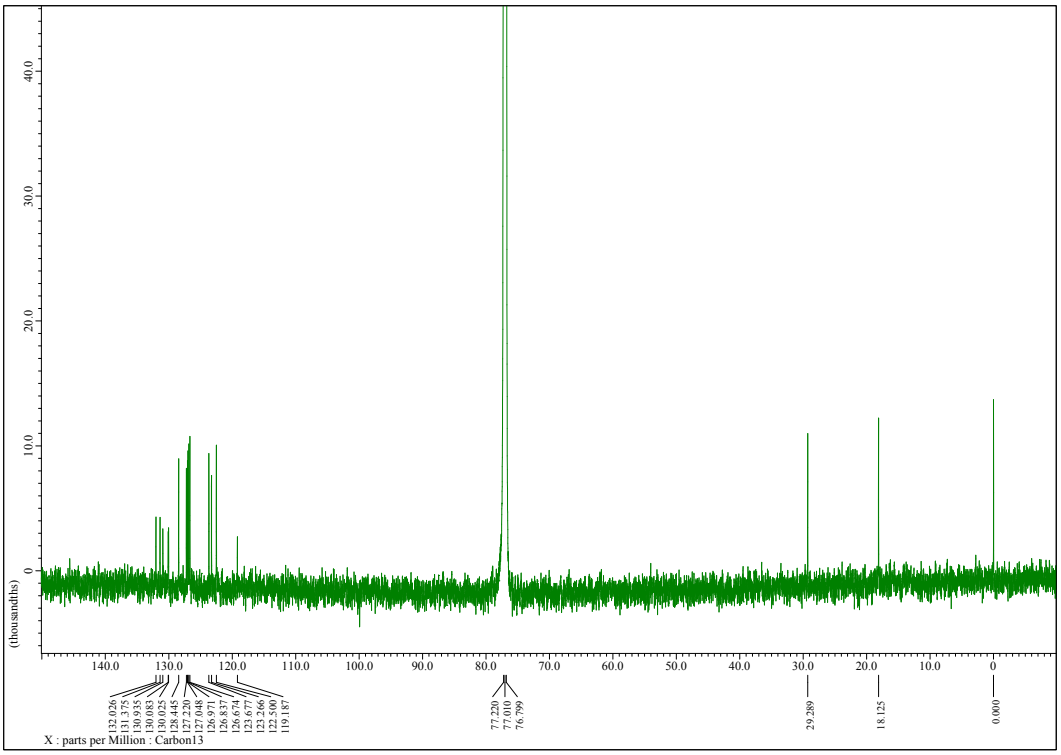

abundance
X : parts per Million : 1H
2.01
0.99
2.00
2.00
2.01
2.00
2.00
7.933
7.906
7.887
7.877
7.809
7.783
7.568
7.563
7.541
7.515
7.514
7.510
7.468
7.445
7.419
7.410
7.405
7.252
3.465
3.440
3.415
2.788
2.763
2.738
0.000

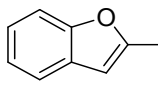

abundance
X : parts per Million : Carbon13
134.052
133.506
131.171
129.292
128.243
126.669
126.001
125.706
122.701
119.277
77.385
77.127
76.879
28.930
18.590


CN

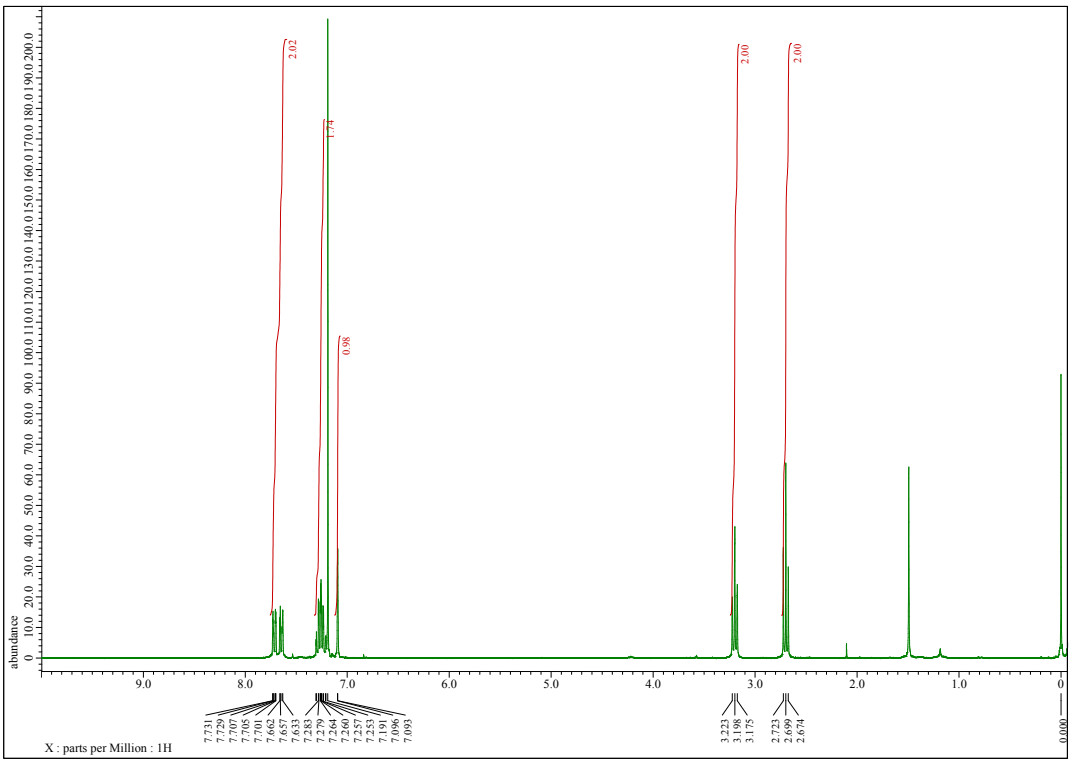
5va

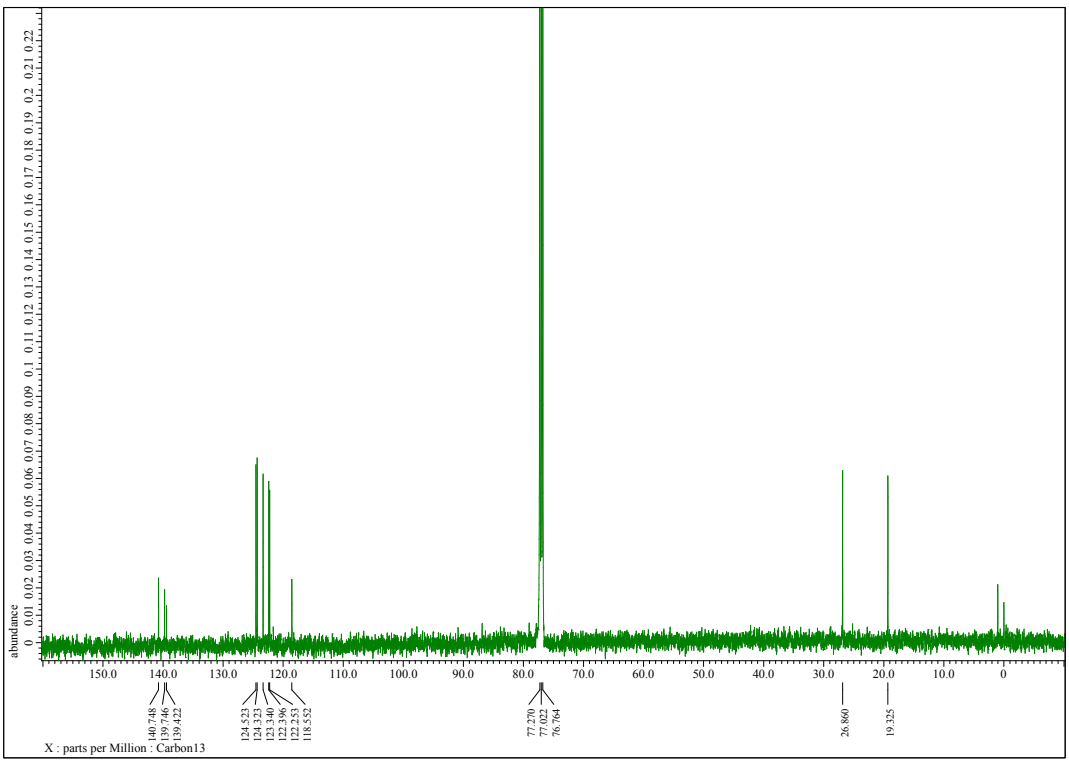

abundance
X : parts per Million : 1H

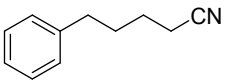

(thousandths)
X : parts per Million : Carbon13


O
CN

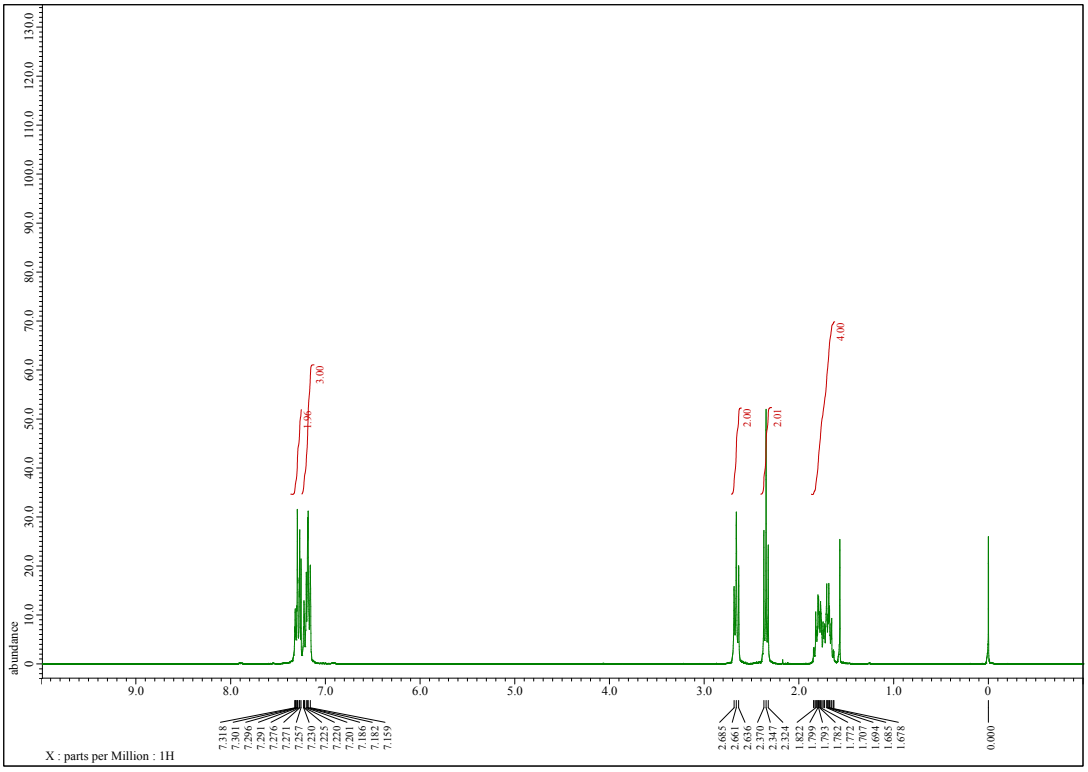
5wa

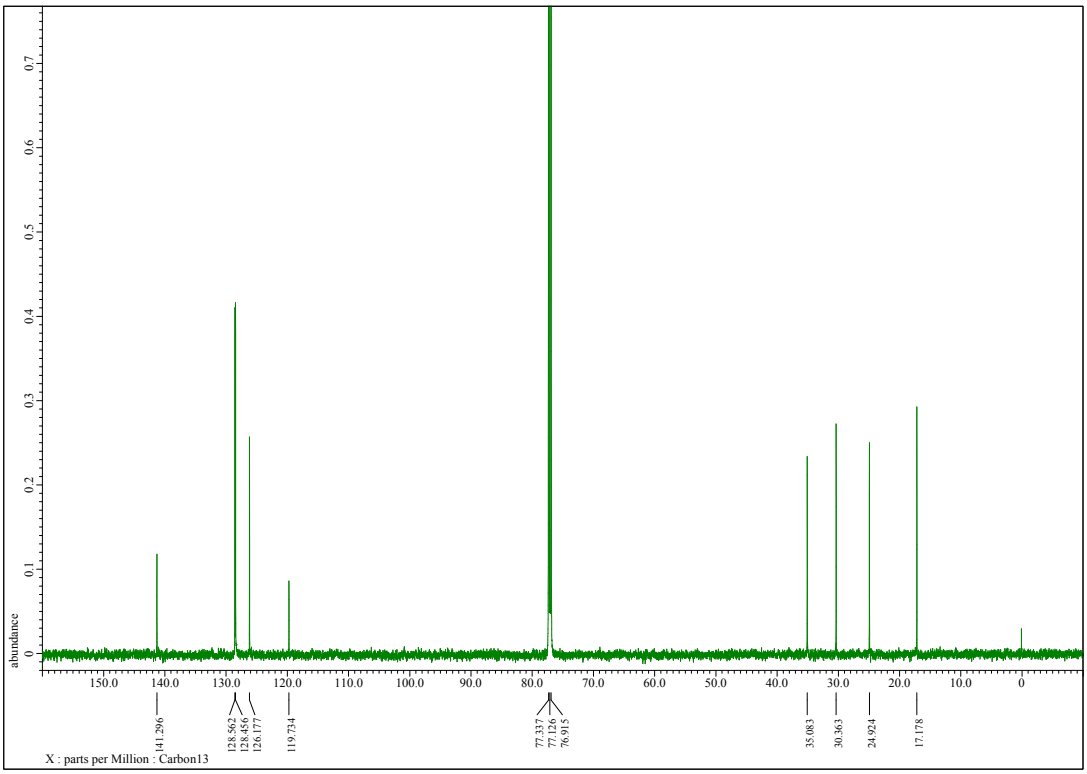

2.02
1.74
0.98
2.00
2.00
abundance
X : parts per Million : 1H

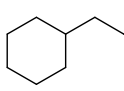

abundance
X : parts per Million : Carbon13


CN

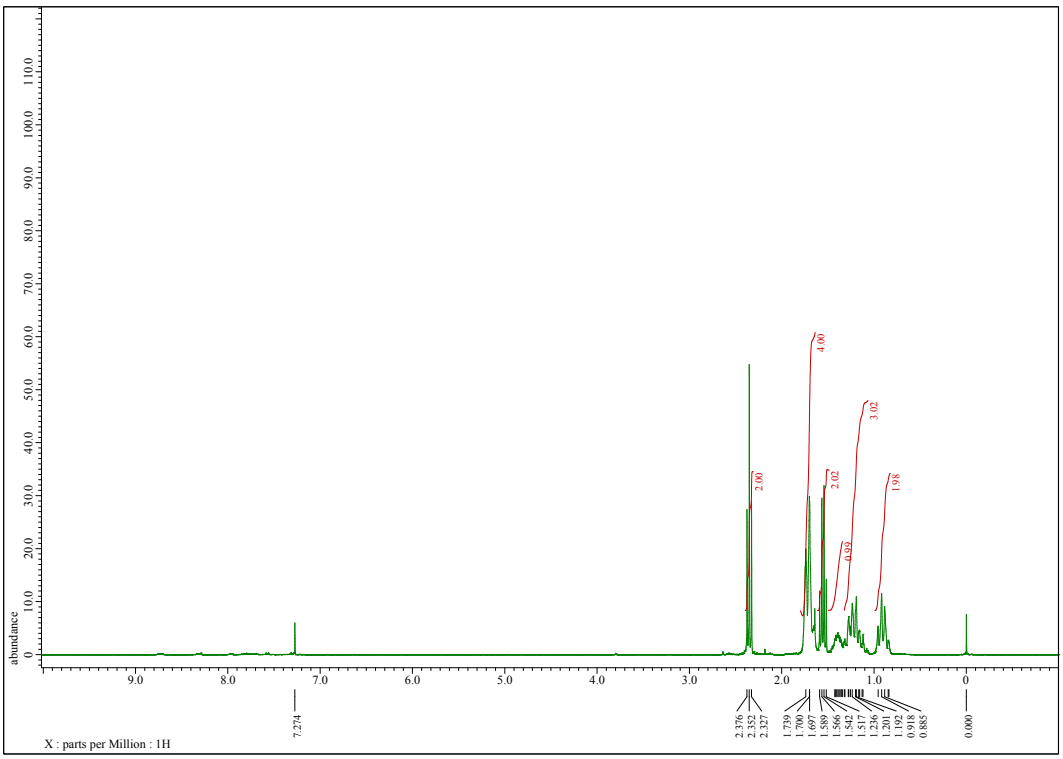
7aa

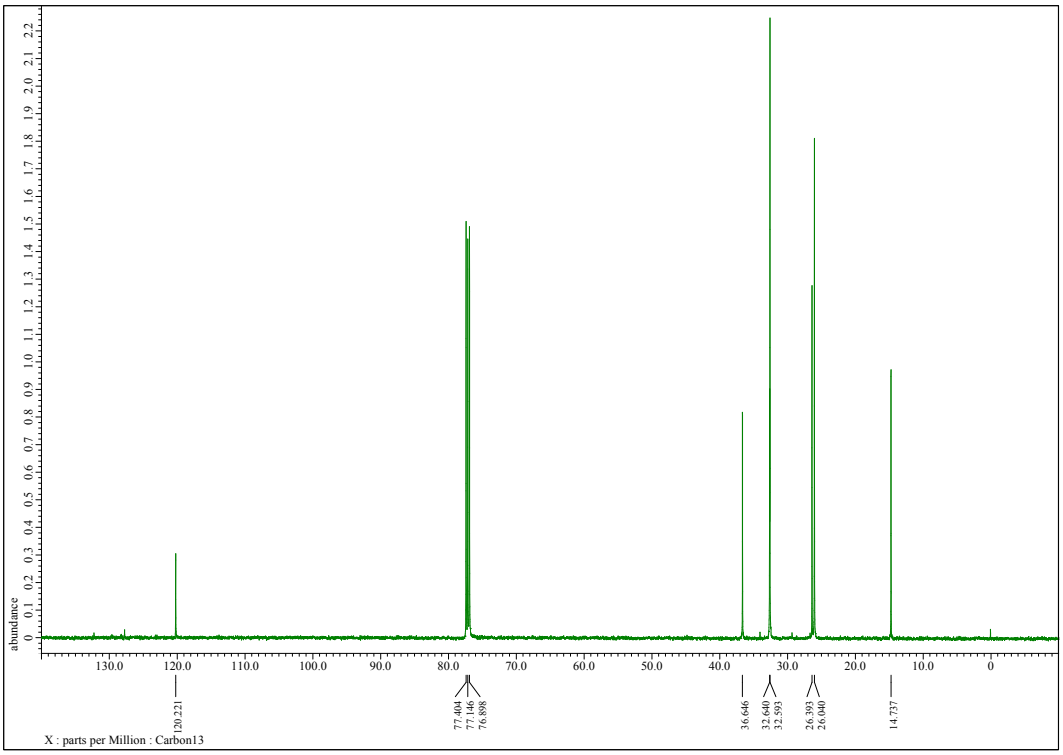

abundance
X : parts per Million : 1H
7.318
7.301
7.296
7.291
7.276
7.271
7.257
7.230
7.225
7.220
7.201
7.186
7.182
7.159
2.685
2.661
2.636
2.370
2.347
2.324
1.822
1.799
1.792
1.785
1.772
1.707
1.694
1.685
1.678
0.000
1.06
3.00
2.00
2.01
4.00

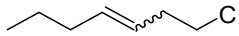

abundance
X : parts per Million : Carbon13
141.296
128.562
128.456
126.177
119.734
77.337
77.126
76.915
35.083
30.363
24.924
17.178


CN

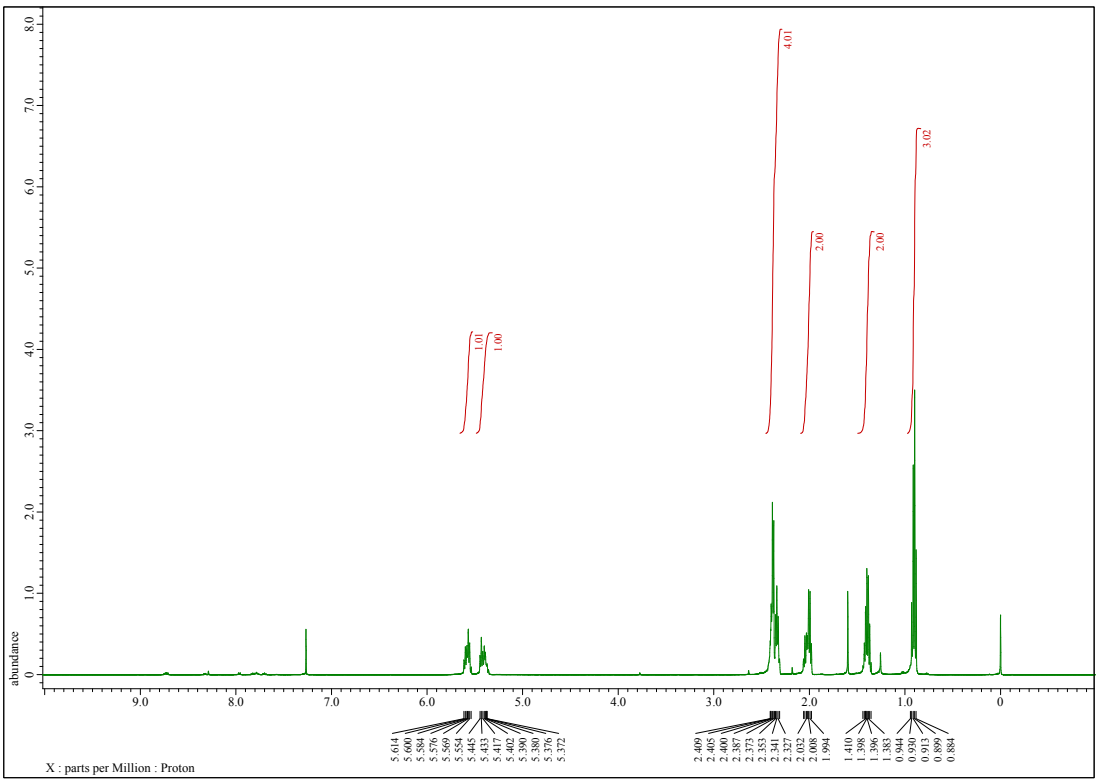
7ba

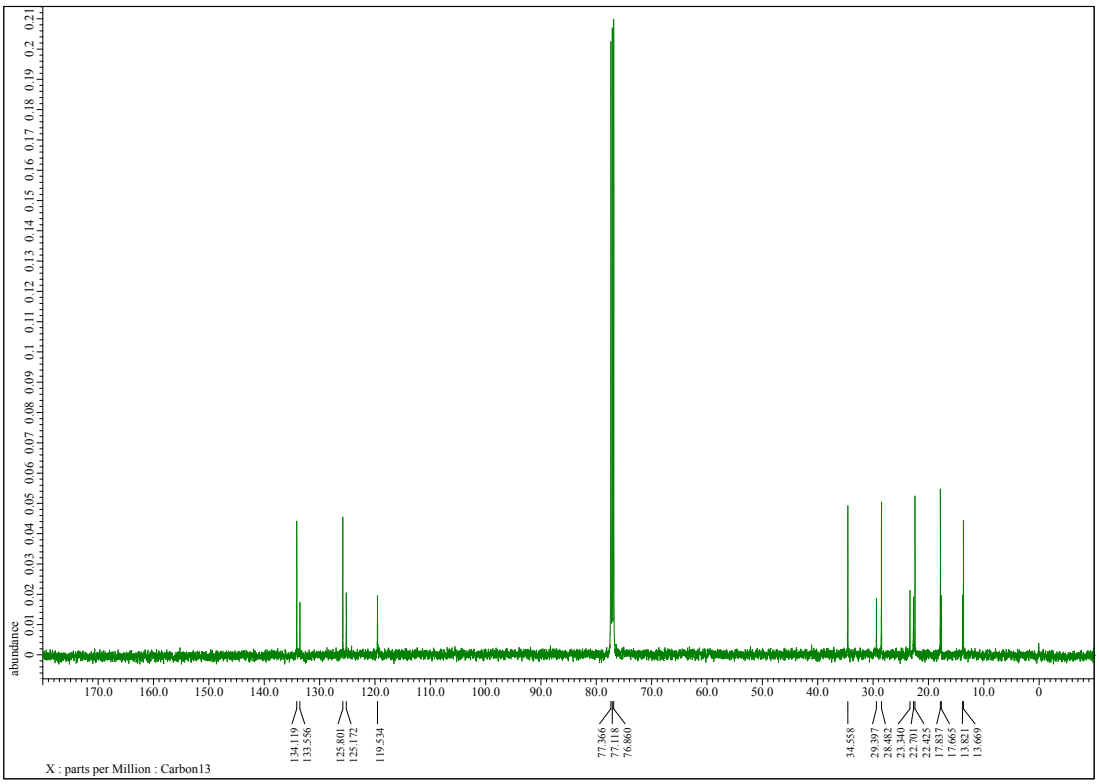

abundance
X : parts per Million : 1H
7.274
2.376
2.152
2.327
1.739
1.700
1.697
1.690
1.566
1.542
1.517
1.236
1.201
1.192
0.918
0.885
0.000
2.00
4.00
2.02
3.02
0.92
1.98

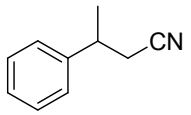

abundance
X : parts per Million : Carbon13
120.221
77.404
77.146
76.898
36.646
32.640
32.593
26.393
26.040
14.737


CN

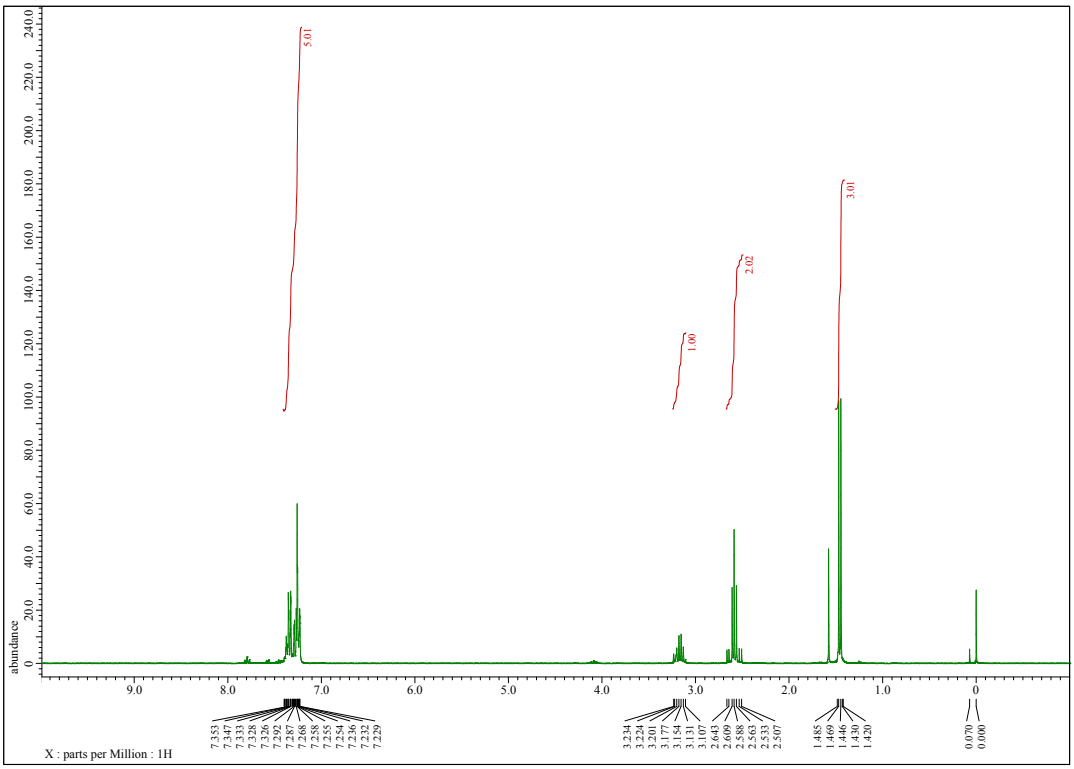
7ca

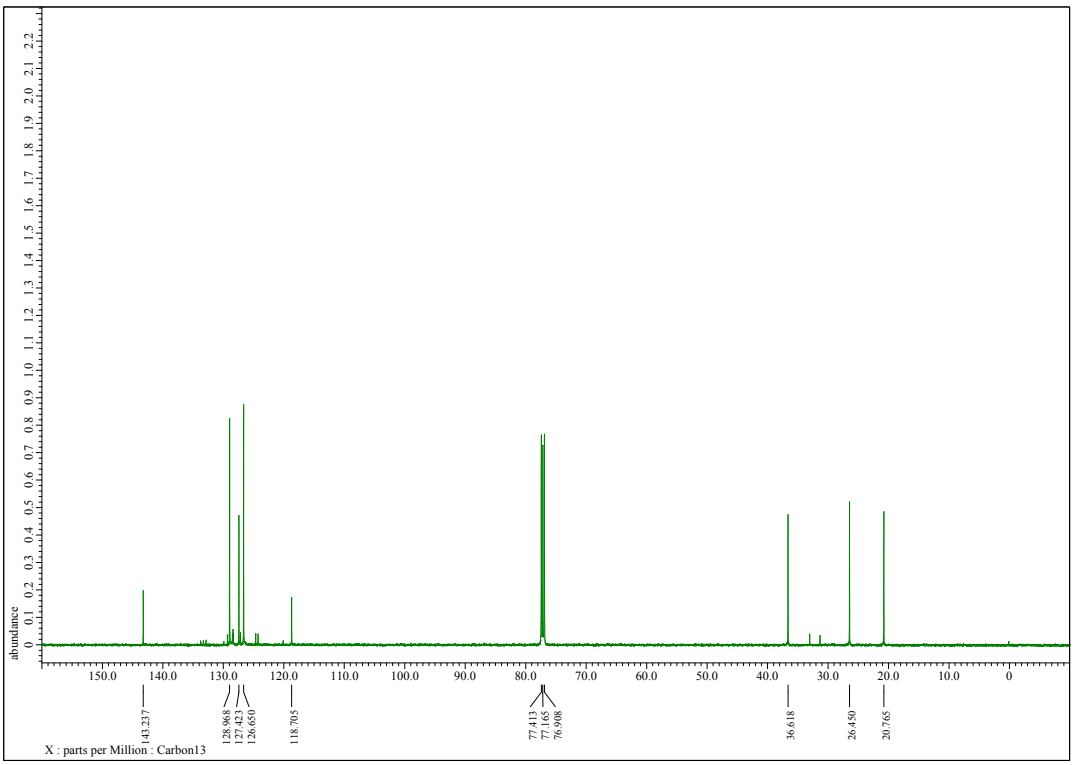

abundance
X : parts per Million : Proton
4.01
3.02
2.00
2.00
1.01
1.00

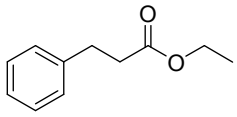

abundance
X : parts per Million : Carbon13
134.119
133.556
125.801
125.172
119.534
77.366
77.118
76.860
34.558
29.397
28.482
23.340
22.701
22.425
17.837
17.665
13.821
13.669


CN

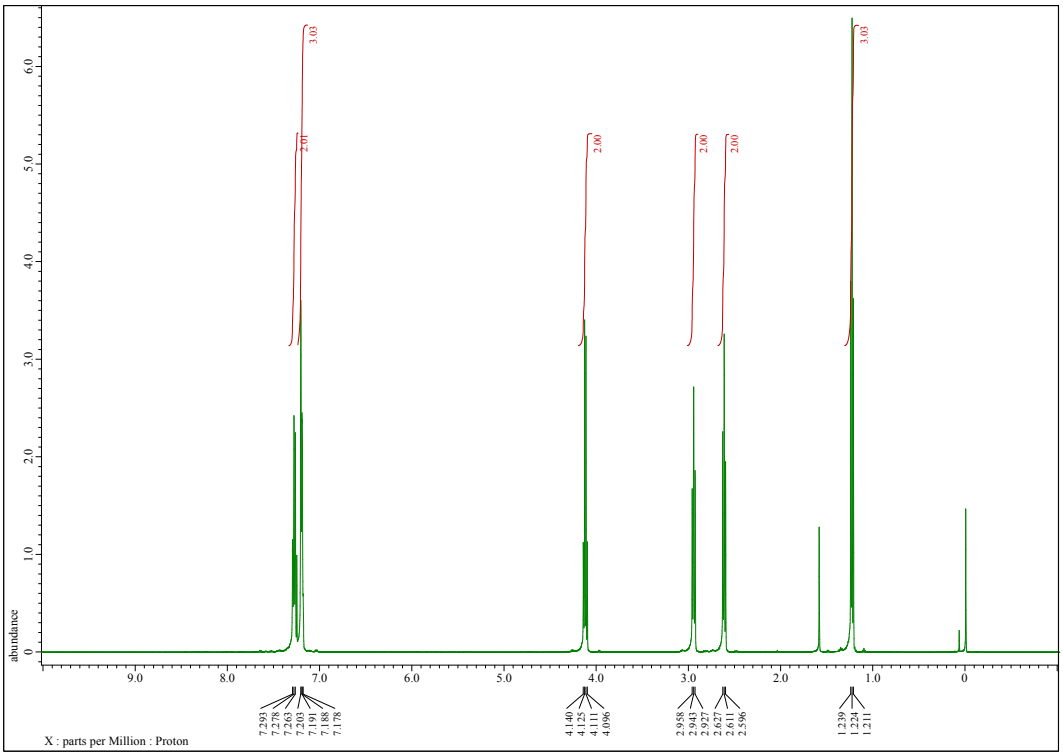
5ab

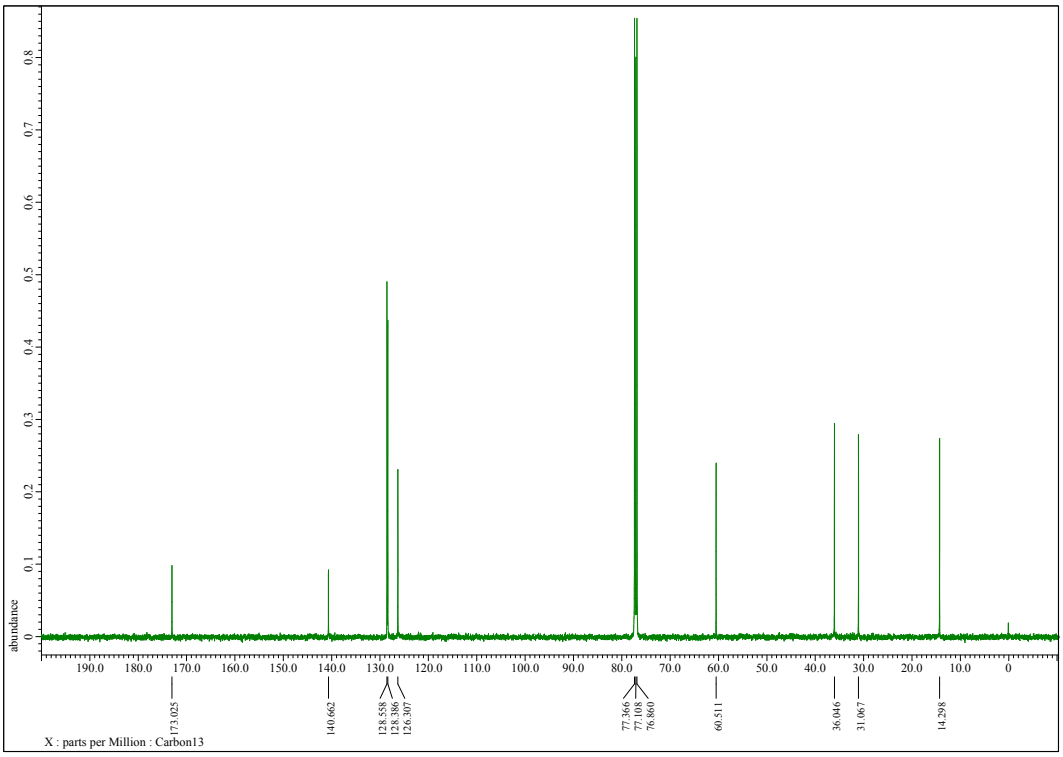

5.01
1.00
2.02
3.01
abundance
X : parts per Million : 1H

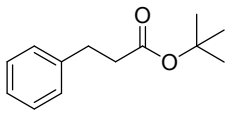

abundance
X : parts per Million : Carbon13



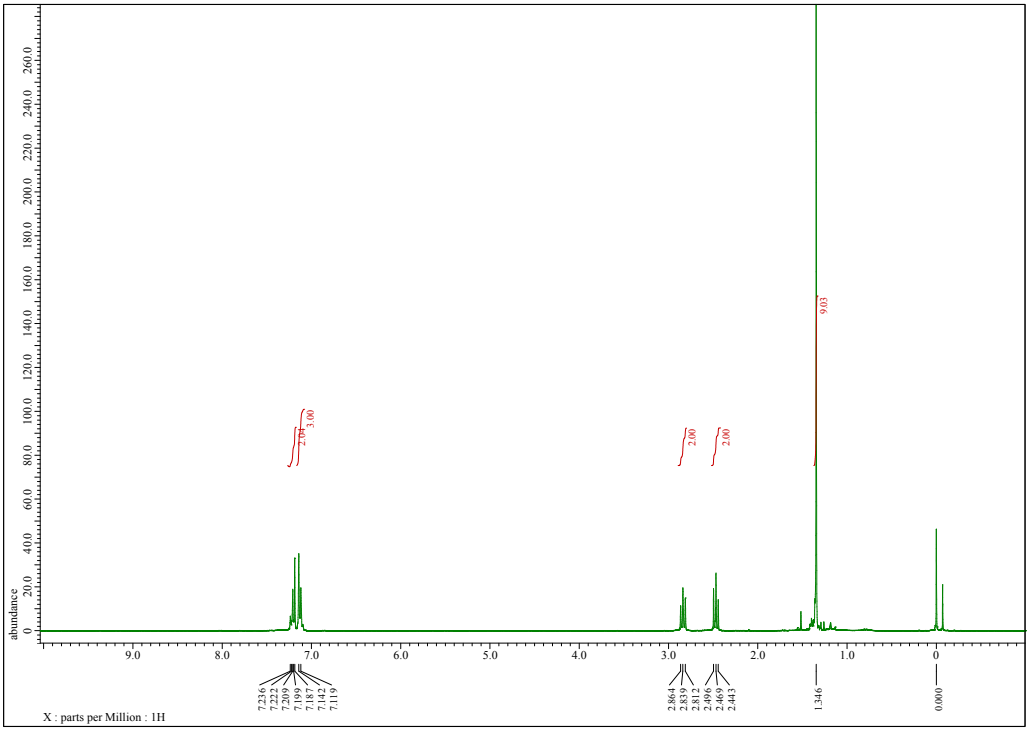
5ac

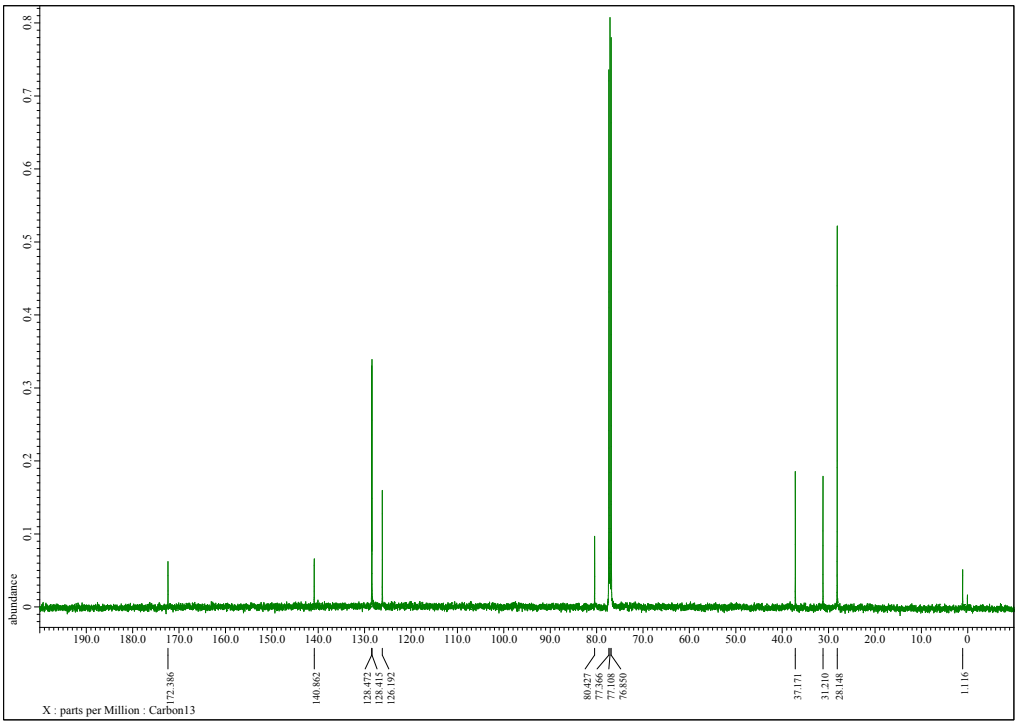

3.03
2.01
2.00
2.00
2.00
3.03
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.293
7.278
7.263
7.203
7.191
7.188
7.178
4.140
4.125
4.111
4.096
2.958
2.943
2.927
2.627
2.611
2.596
1.239
1.224
1.211
X : parts per Million : Proton

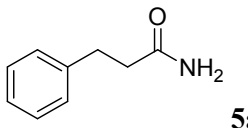

abundance
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
173.025
140.662
128.558
128.386
126.307
77.366
77.108
76.860
60.511
36.046
31.067
14.298
X : parts per Million : Carbon13



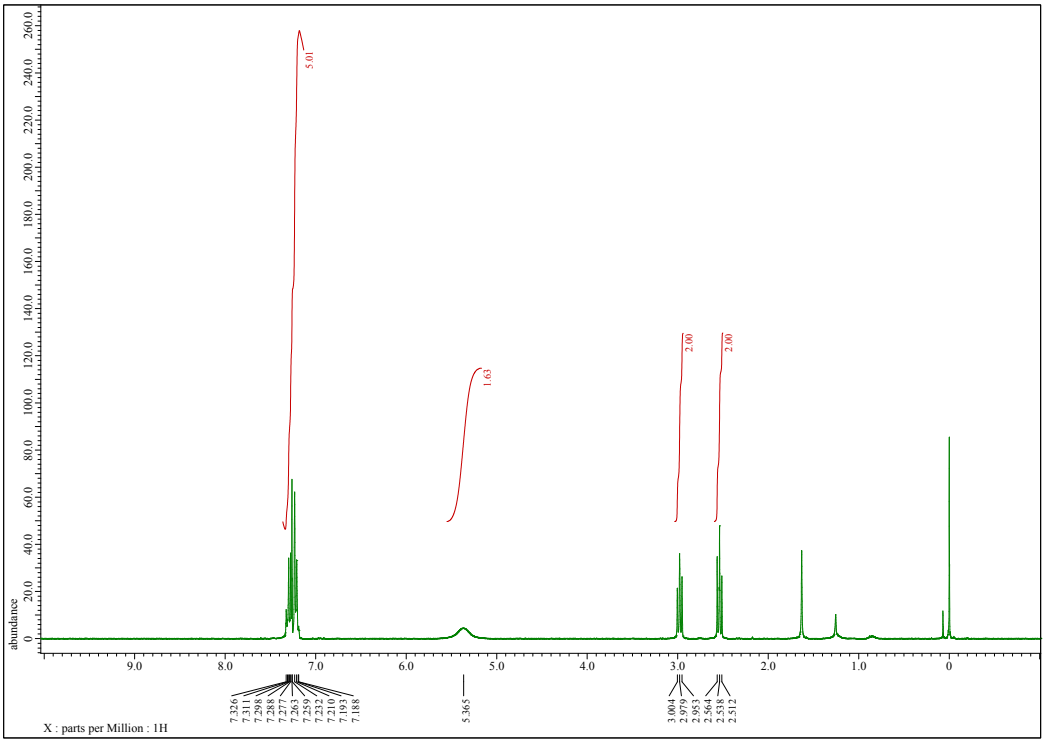
5ad

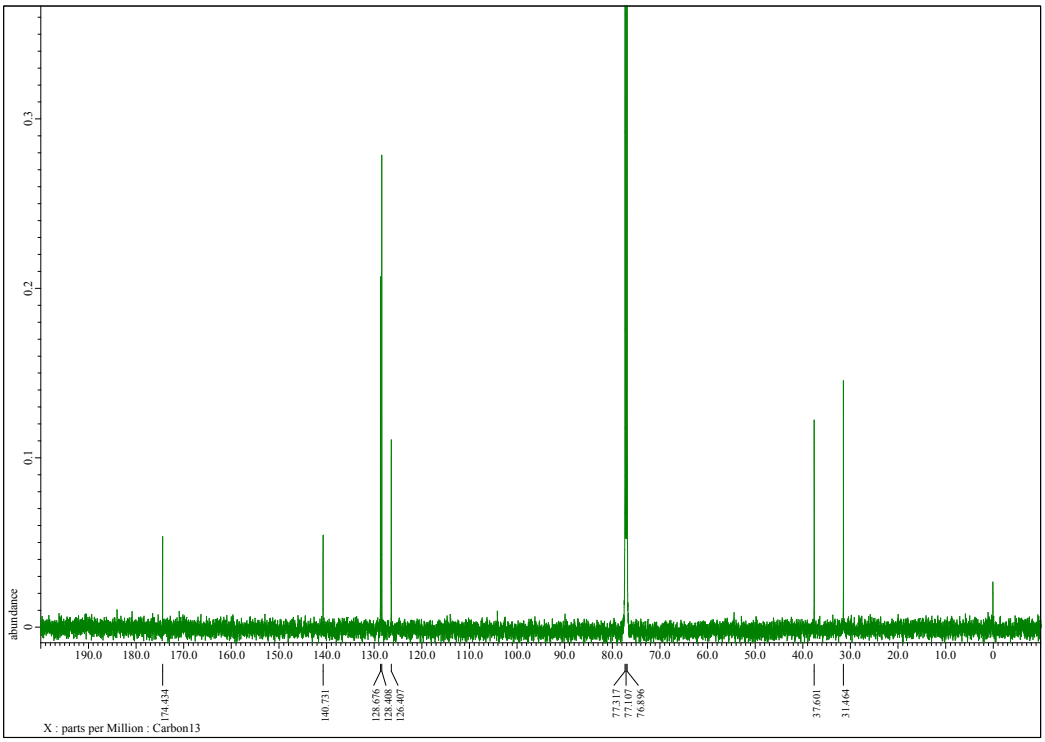

abundance
X : parts per Million : 1H
7.236
7.222
7.209
7.199
7.187
7.142
7.119
2.864
2.839
2.812
2.496
2.469
2.443
1.346
0.000
3.00
2.08
2.00
2.00
9.03

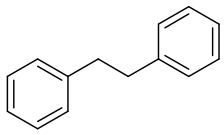

abundance
X : parts per Million : Carbon13
172.386
140.862
128.472
128.415
126.192
80.427
77.366
77.108
76.850
37.171
31.210
28.148
1.116


O
NH2

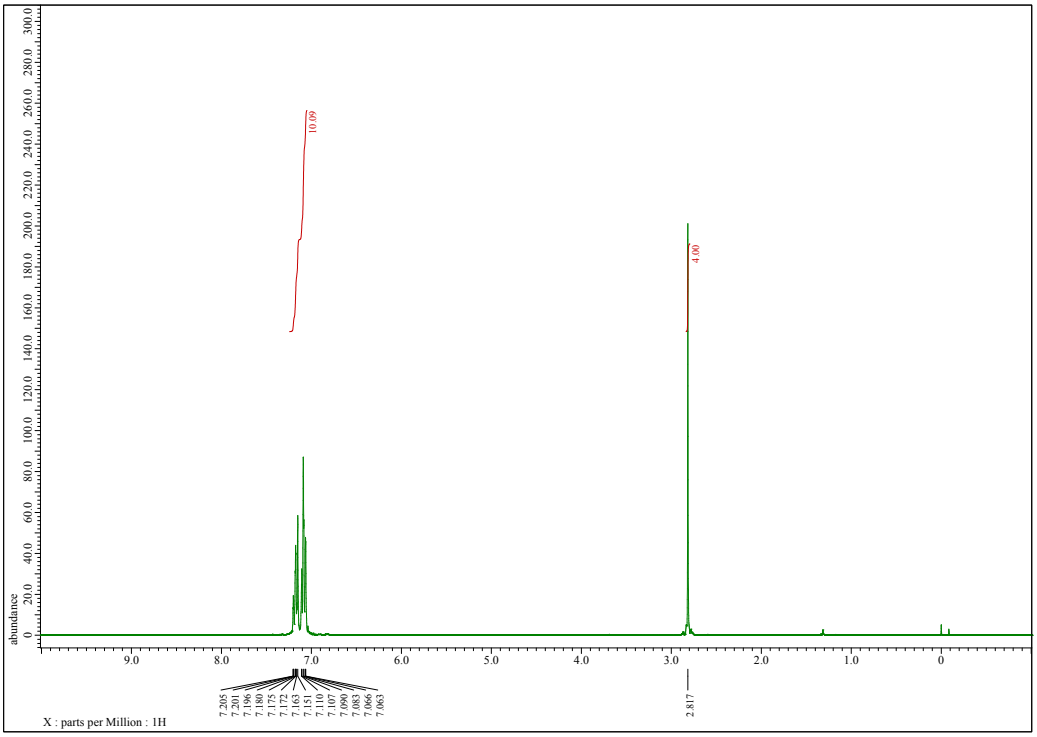
5ae

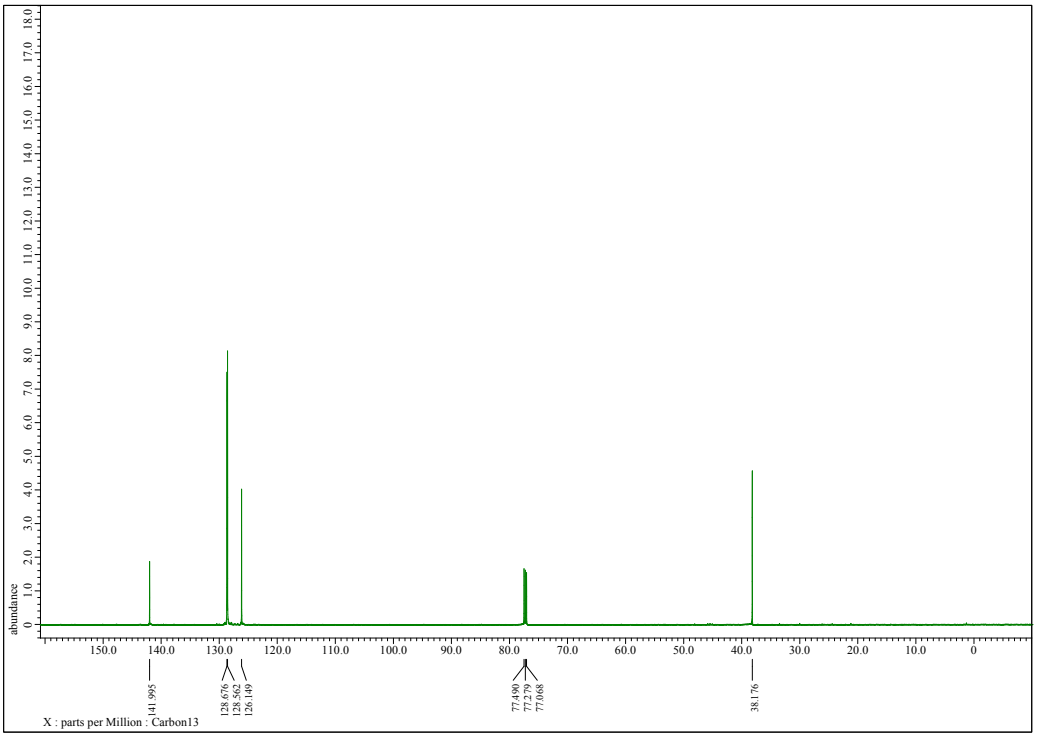

5.01
1.63
2.00
2.00
abundance
X : parts per Million : 1H

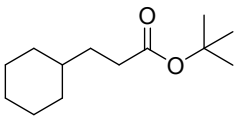

abundance
X : parts per Million : Carbon13



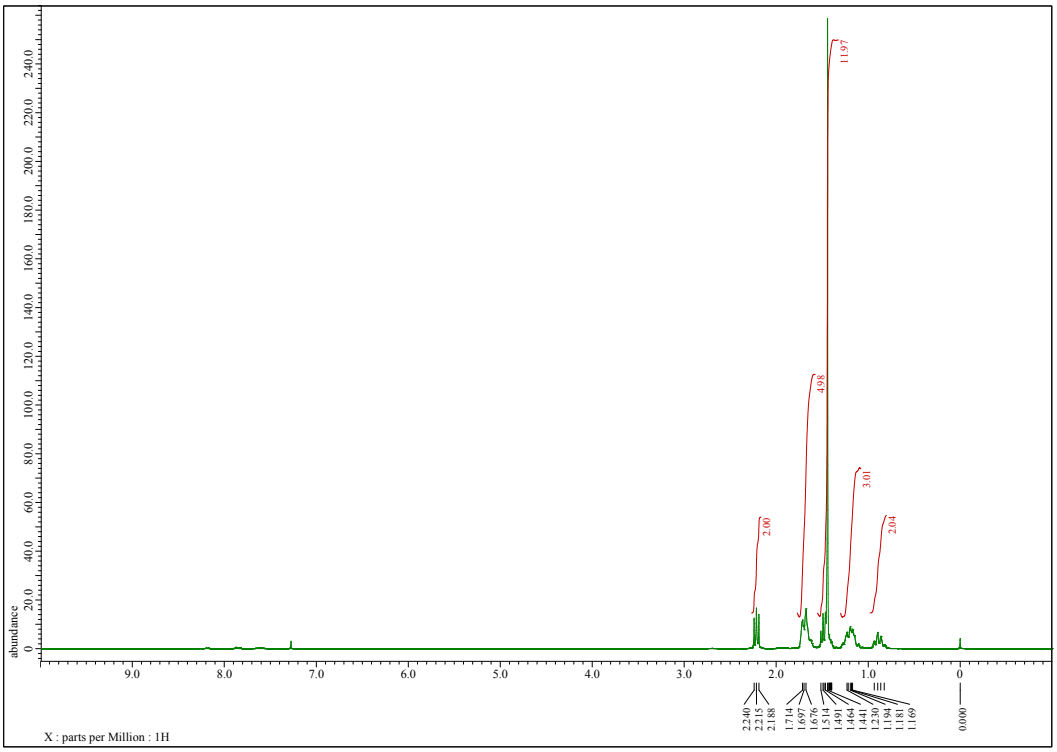
5af

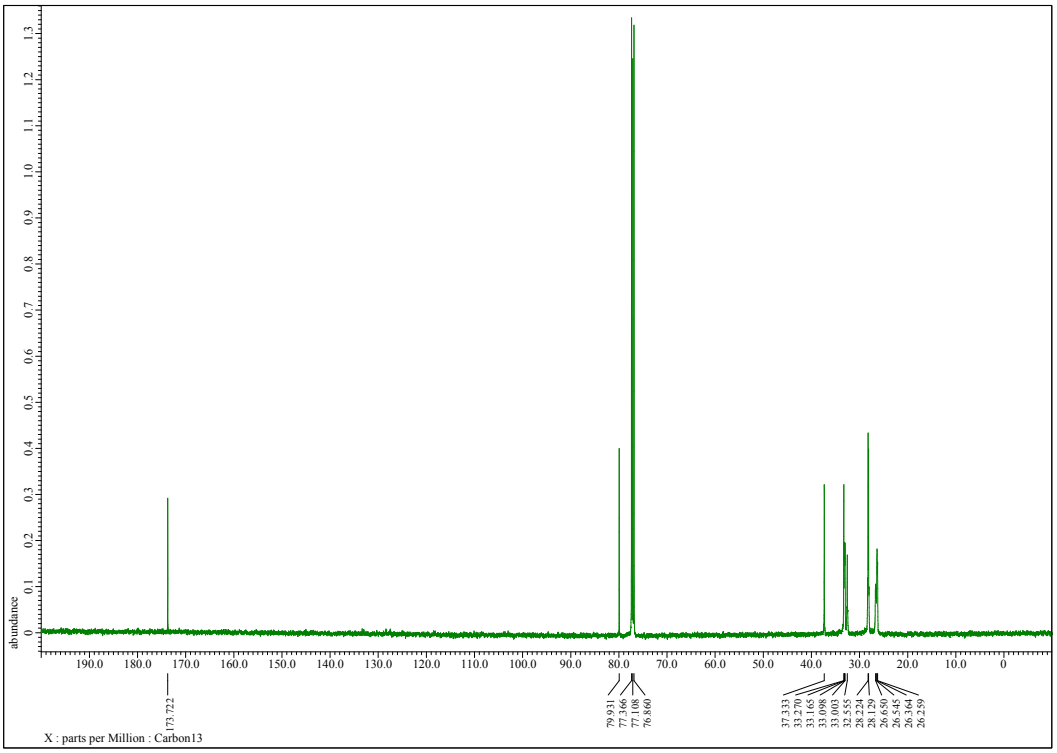

10.09
4.00
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.205
7.201
7.196
7.180
7.175
7.172
7.163
7.151
7.110
7.107
7.090
7.083
7.066
7.063
2.817
X : parts per Million : 1H

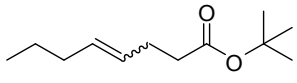

abundance
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
141.995
128.676
128.565
126.140
77.490
77.279
77.068
38.176
X : parts per Million : Carbon13



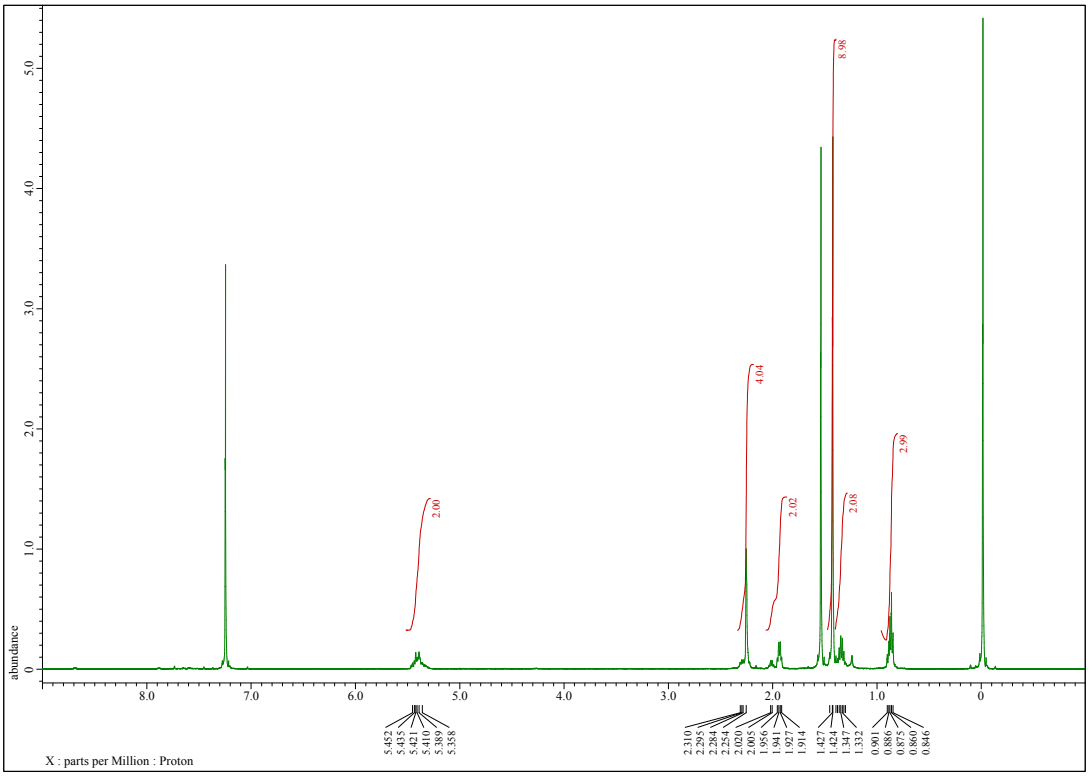
7bd

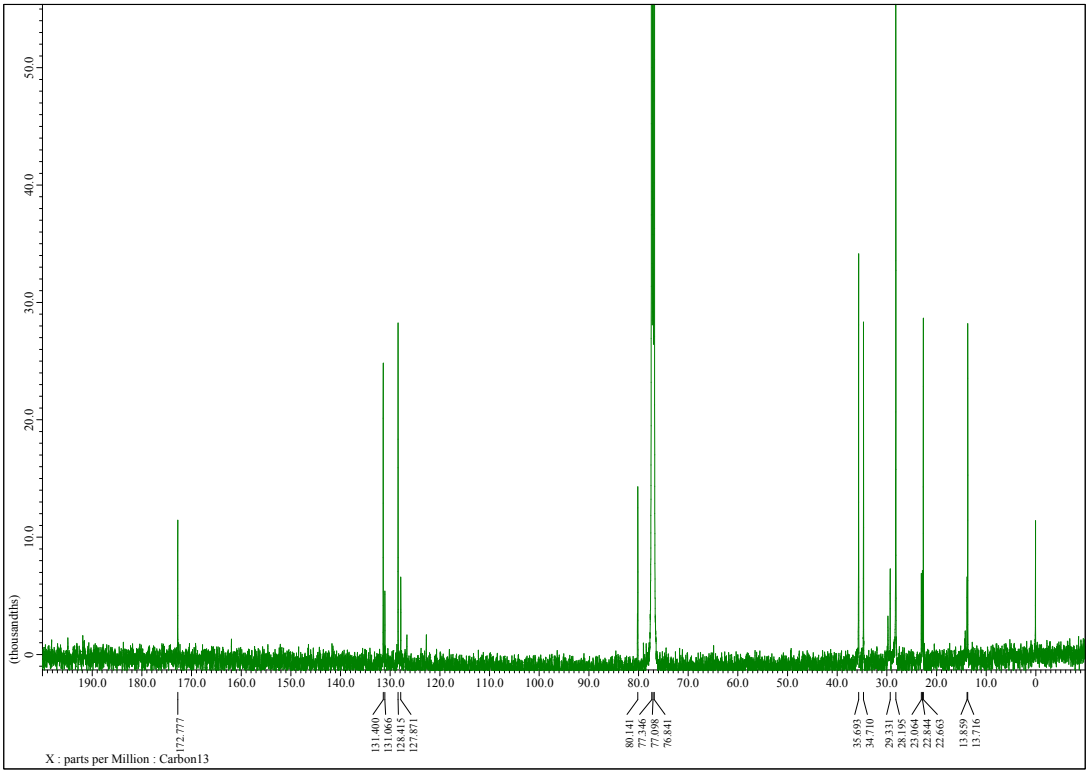

abundance
X : parts per Million : 1H
11.97
4.98
3.01
2.04
2.00

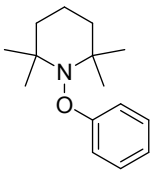

abundance
X : parts per Million : Carbon13
173.722
79.931
77.366
77.108
76.860
37.333
33.270
33.165
33.098
33.003
32.555
28.224
28.129
26.650
26.545
26.344
26.249



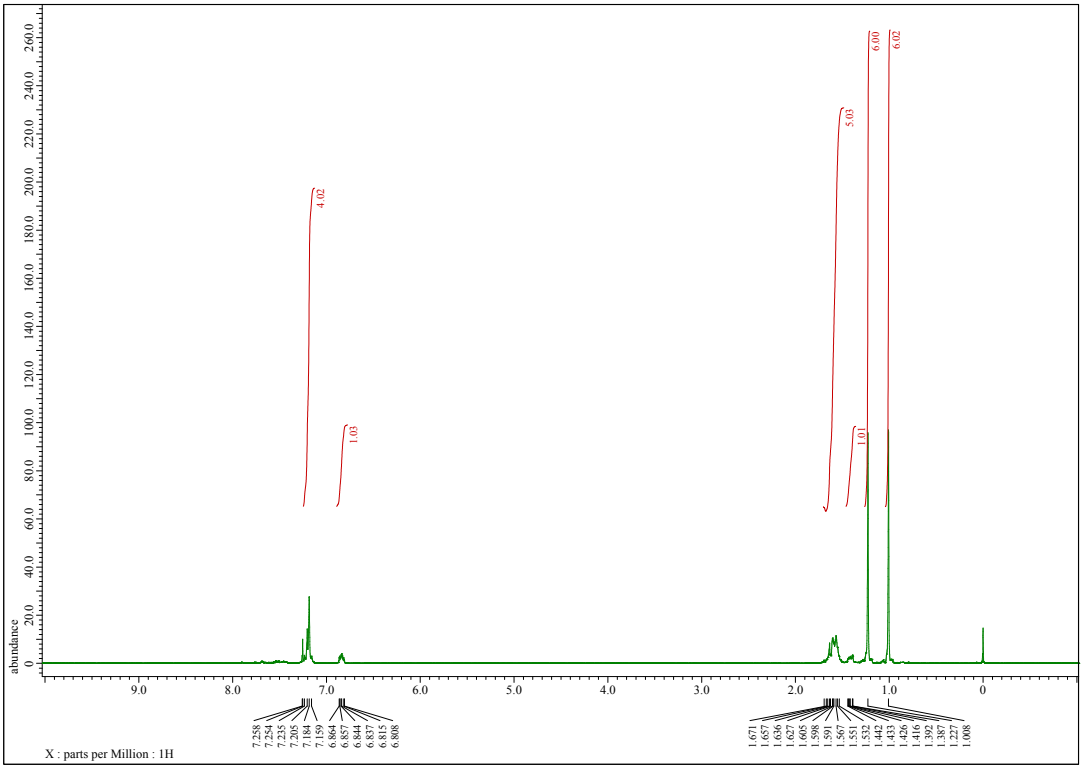
7cd

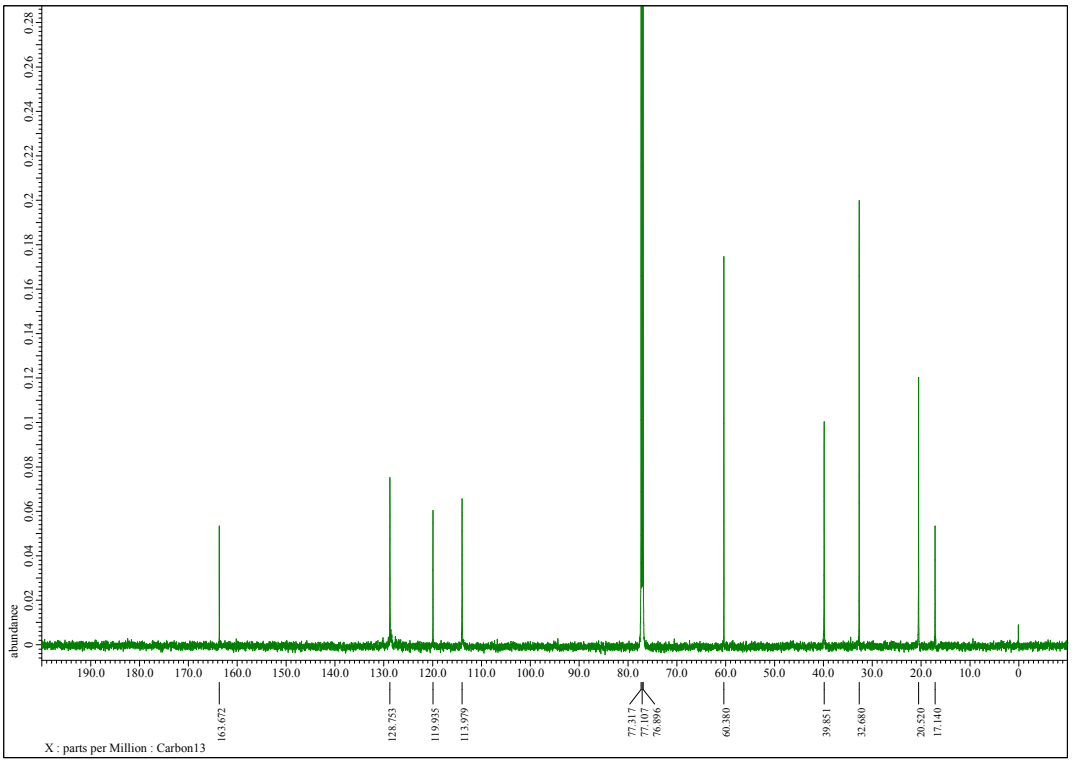

abundance
8.98
4.04
2.99
2.08
2.02
2.00
X : parts per Million : Proton

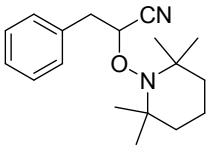

(thousandths)
172.777
131.400
131.066
128.415
127.871
80.141
77.346
77.098
76.841
35.693
34.710
29.331
28.195
23.064
22.844
22.663
13.859
13.716
X : parts per Million : Carbon13



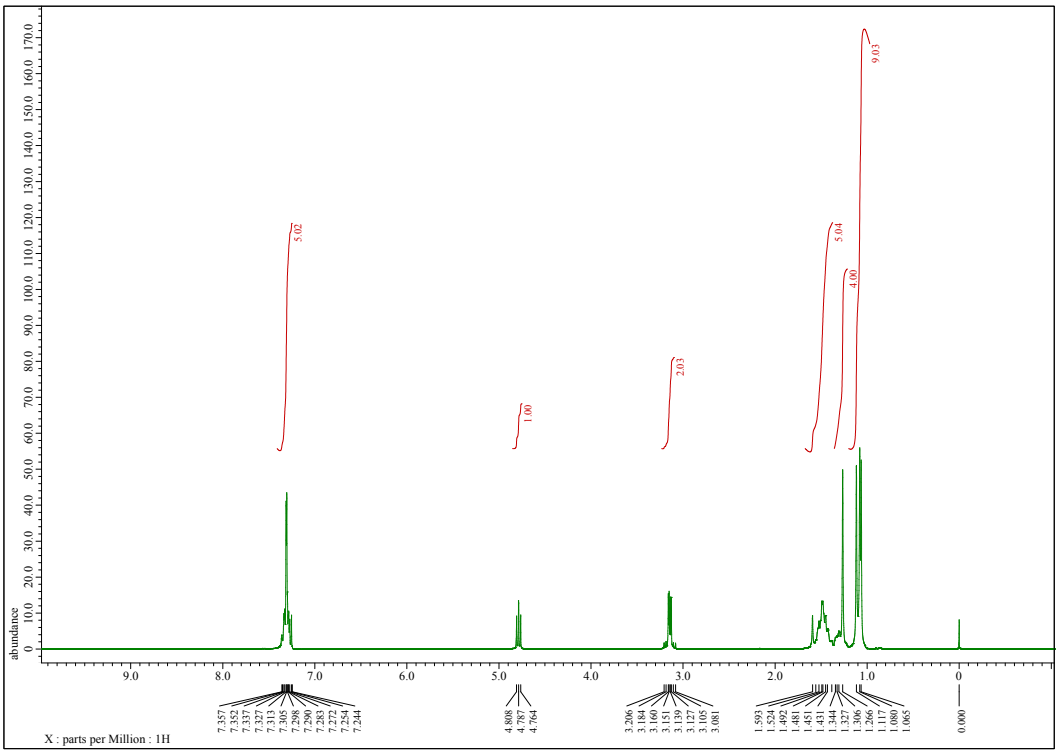
8

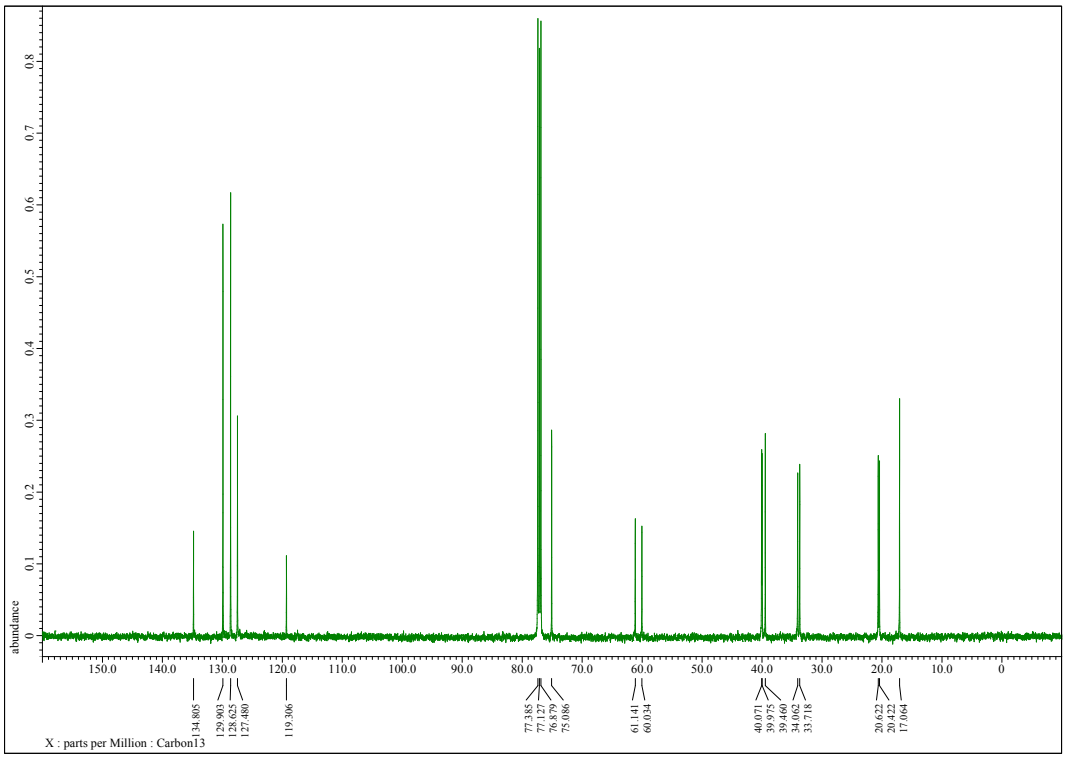

abundance
4.02
1.03
5.03
1.01
6.00
6.02
7.258
7.254
7.235
7.205
7.194
7.159
6.864
6.857
6.844
6.837
6.815
6.808
1.671
1.657
1.636
1.627
1.605
1.598
1.591
1.567
1.551
1.532
1.442
1.433
1.426
1.416
1.392
1.387
1.227
1.008
X : parts per Million : 1H

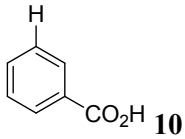

abundance
163.672
128.753
119.935
113.979
77.317
77.107
76.896
60.380
39.851
32.680
20.520
17.140
X : parts per Million : Carbon13


CN
O
N

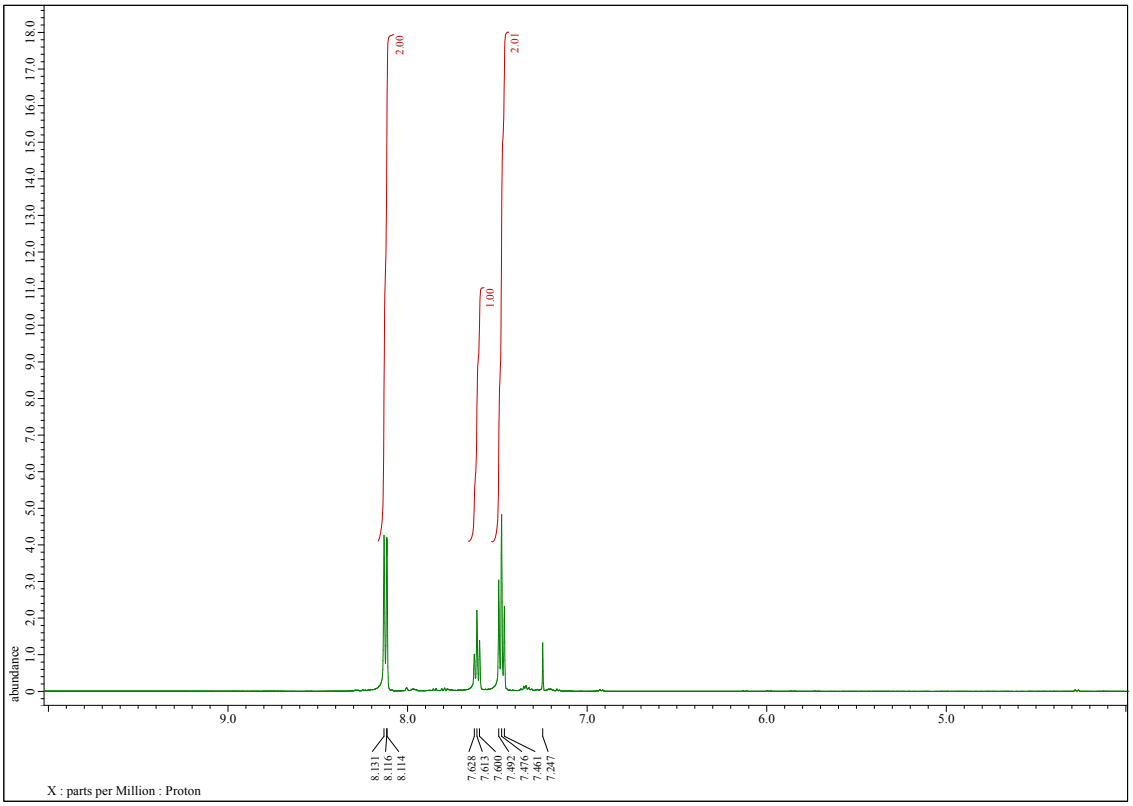
9

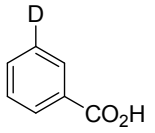

abundance
X : parts per Million : 1H
5.02
1.00
2.03
5.04
4.00
9.03


abundance
X : parts per Million : Carbon13

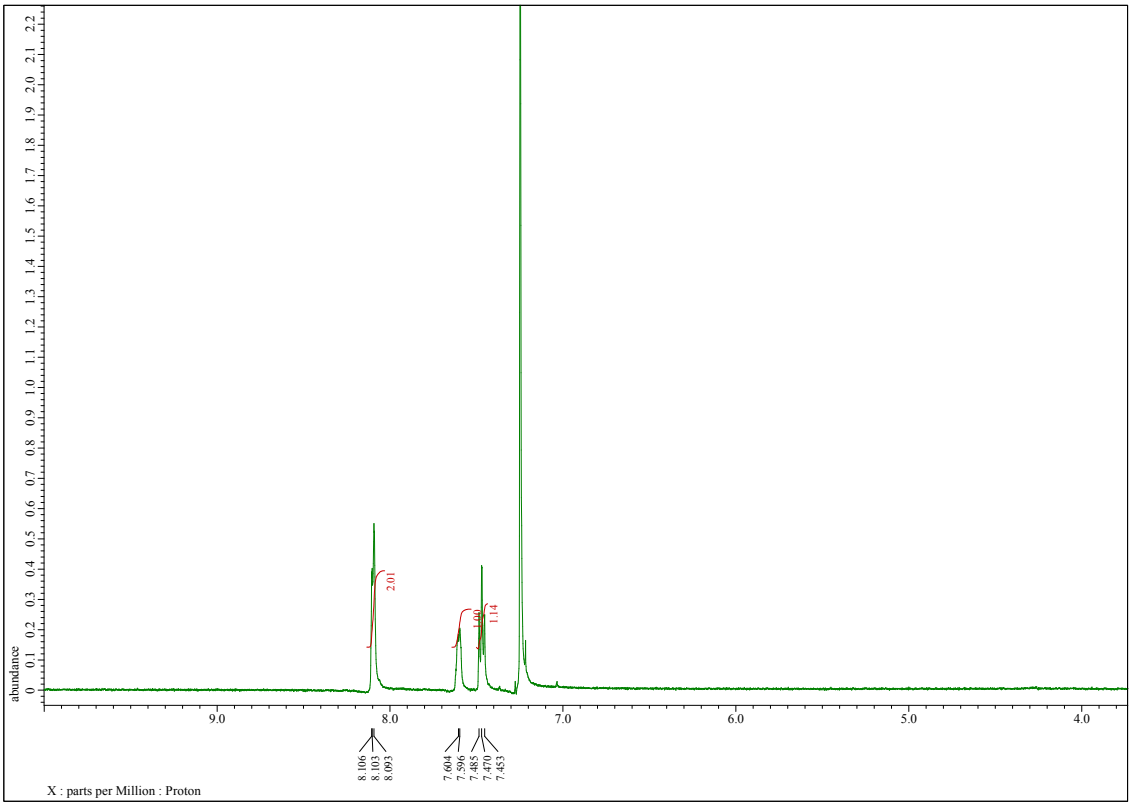

H
CO2H

10


2.00
2.01
1.00
abundance
9.0
8.0
7.0
6.0
5.0
8.131
8.116
8.114
7.628
7.613
7.600
7.492
7.476
7.461
7.247
X : parts per Million : Proton


D
CO2H

11


abundance
2.01
1.00
1.14
9.0
8.0
7.0
6.0
5.0
4.0
8.106
8.103
8.093
7.604
7.596
7.485
7.470
7.453
X : parts per Million : Proton