

SUPPORTING INFORMATION

for

Exploiting a Silver–Bismuth Hybrid Material as Heterogeneous Noble Metal Catalyst for Decarboxylations and Decarboxylative Deuterations of Carboxylic Acids under Batch and Continuous Flow Conditions

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1. Additional Figures and Tables

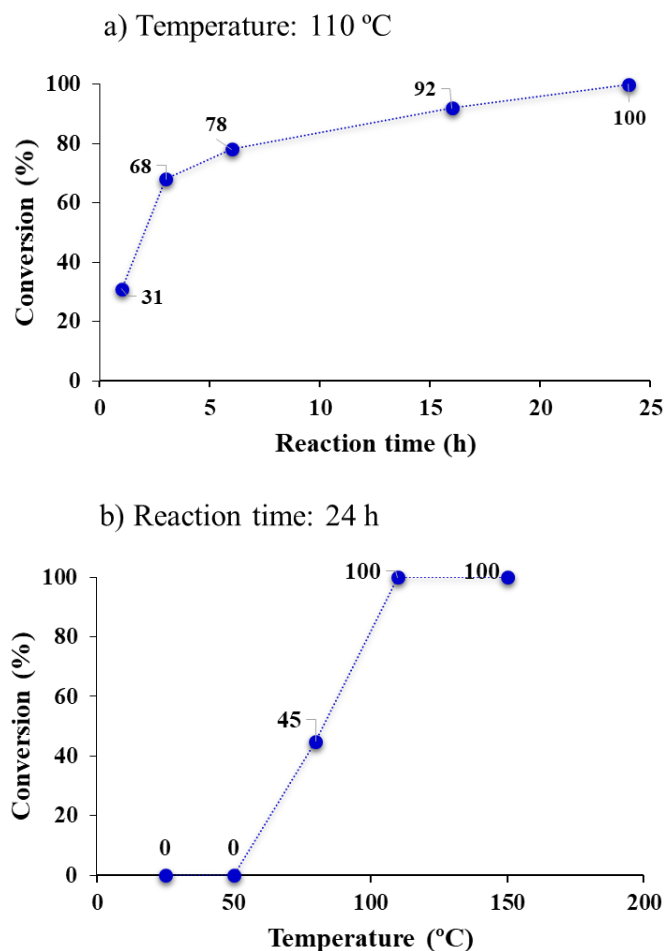


Fig. S1 Investigation of the effects of the temperature (a) and reaction time (b) on the AgBi-HM-catalyzed decarboxylation of 2-nitrobenzoic acid. (Reaction conditions: 0.15 M substrate concentration, 5 mol% catalyst, 15 mol% of KOH as base, DMF as solvent.)

Table S1 Investigation of the effects the substrate concentration in the AgBi-HM-catalyzed decarboxylation of 2-nitrobenzoic acid under batch conditions.

Entry	c (M)	Conversion (%) ^a	Selectivity (%) ^a	
			A	B
1	0.25	63	100	0
2	0.2	86	100	0
3	0.15	100	100	0
4	0.1	100	100	0

^aDetermined by ¹H NMR analysis of the crude product.

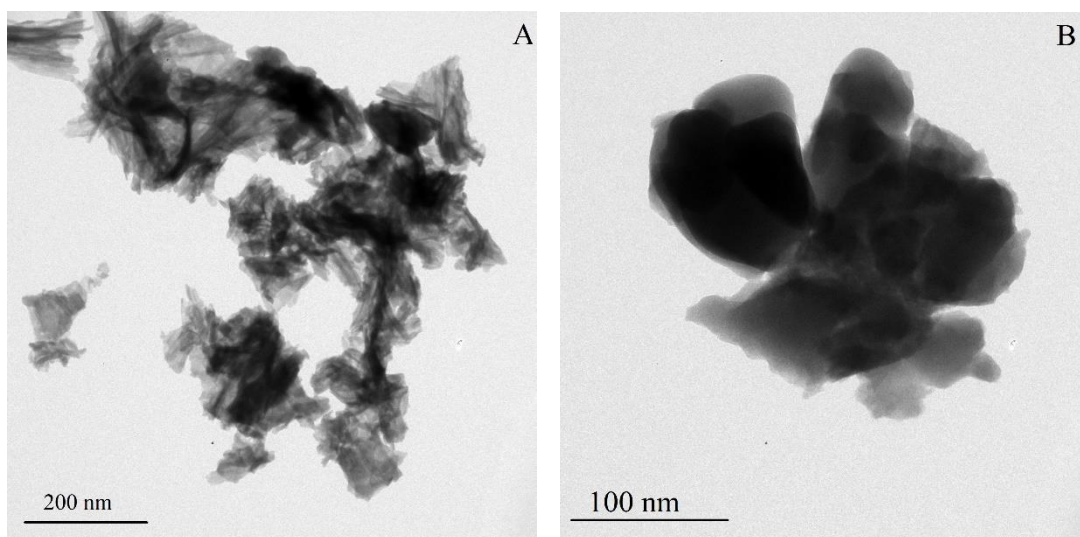


Fig. S2 TEM images: as-prepared AgBi-HM sample (A), AgBi-HM sample used in flow scale-out (B).

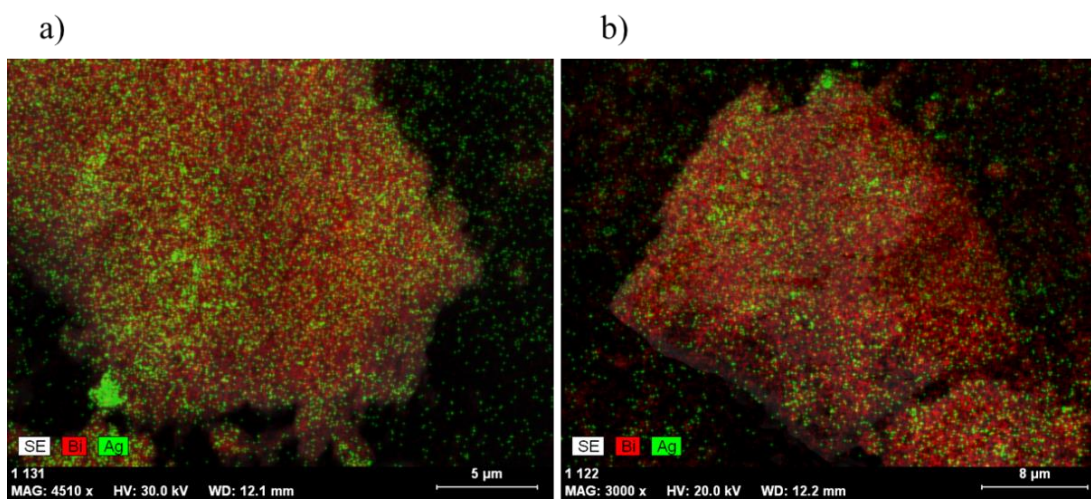
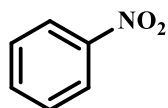


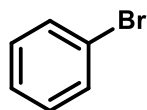
Fig. S3 SEM-EDX results of AgBi-HM catalyst samples used a) in batch process b) in flow scale-out process.

2. Analytical Data of the Reaction Products



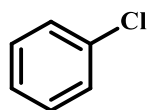
nitrobenzene

^1H NMR (500 MHz, CDCl_3): δ = 8.22-8.21 (d, J = 8.38 Hz, 2H), 7.72- 7.69 (t, J =7.38 Hz, 1H), 7.56-7.53 (t, J = 8.38 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3): 148.2, 134.3, 129.3, 123.4. NMR data is in agreement with the published data.¹ MS (EI) m/z = 51, 65, 77, 93, 123



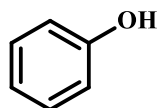
bromobenzene

^1H NMR (500 MHz, CDCl_3): δ = 7.87-7.85 (dd, J = 7.63 Hz, 1H), 7.68-7.66 (dd, J = 7.63 Hz, 1H), 7.39-7.31 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 134.5, 132.7, 131.4, 127.1. NMR data is in agreement with the published data.² MS (EI) m/z = 51, 63, 77, 84, 100, 157



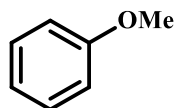
chlorobenzene

^1H NMR (500 MHz, CDCl_3): δ = 7.48-7.33 (m, 3+2H); ^{13}C NMR (125 MHz, CDCl_3): 132.8, 131.6, 131.2, 126.6. NMR data is in agreement with the published data.² MS (EI) m/z = 51, 61, 77, 113



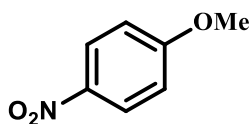
phenol

^1H NMR (500 MHz, CDCl_3): δ = 7.24-7.21 (t, J = 7.27 Hz, 2H), 6.91-6.83 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 155.4, 129.6, 120.7, 115.3. NMR data is in agreement with the published data.³ MS (EI) m/z = 51, 65, 78, 94



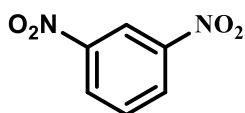
anisole

^1H NMR (500 MHz, CDCl_3): δ = 7.80-7.78 (m, 1H), 7.48-7.43 (m, 1H), 6.99-6.96 (m, 3H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 159.1, 131.6, 120.1, 112.4, 55.9. NMR data is in agreement with the published data.⁴ MS (EI) m/z = 51, 65, 78, 93, 108



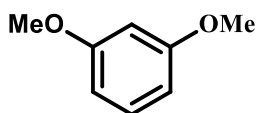
4-nitroanisole

^1H NMR (500 MHz, CDCl_3): δ = 8.22-8.19 (d, J = 9.24 Hz, 2H), 6.98-6.94 (d, J = 9.24 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3): 164.6, 141.6, 125.9, 114.0, 56.2. NMR data is in agreement with the published data.⁵ MS (EI) m/z = 63, 77, 92, 95, 107, 123, 137, 153



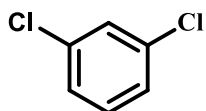
1,3-dinitrobenzene

^1H NMR (500 MHz, CDCl_3): δ = 9.10-9.07 (m, 1H), 8.59-8.57 (m, 2H), 7.83-7.79 (t, J =8.45 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): 148.6, 130.7, 128.8, 119.0. NMR data is in agreement with the published data.⁶ MS (EI) m/z = 51, 64, 75, 83, 85, 92, 122, 168



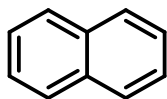
1,3-dimethoxybenzene

^1H NMR (500 MHz, CDCl_3): δ = 7.29-7.26 (t, J =8.47 Hz 1H), 6.56-6.54 (d, J =8.47 Hz, 2 H), 6.52-6.51 (m, 1H), 3.79 (s, 6H); ^{13}C NMR (125 MHz, CDCl_3): 157.4, 131.0, 104.1, 100.2, 56.0. NMR data is in agreement with the published data.² MS (EI) m/z = 51, 52, 65, 78, 95, 109, 138



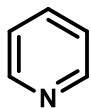
1,3-dichlorobenzene

^1H NMR (500 MHz, CDCl_3): δ = 7.44-7.42 (m, 1H), 7.32-7.30 (m, 3H); ^{13}C NMR (125 MHz, CDCl_3): 132.6, 131.1, 128.8, 127.0. NMR data is in agreement with the published data.⁷ MS (EI) m/z = 55, 75, 83, 111, 145, 148



naphthalene

^1H NMR (500 MHz, CDCl_3): δ = 8.04-8.03 (d, J = 8.12 Hz, 4H), 7.63-7.62 (d, J =8.12 Hz, 4H); ^{13}C NMR (125 MHz, CDCl_3): 133.7, 128.5, 126.2. NMR data is in agreement with the published data.⁷ MS (EI) m/z = 51, 63, 83, 102, 127, 128



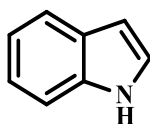
pyridine

^1H NMR (500 MHz, CDCl_3): δ = 8.61-8.59 (m, 2H); 7.66-7.62 (m, 1H); 7.35-7.24 (m, 2H);
 ^{13}C NMR (125 MHz, CDCl_3): 149.8, 135.8, 123.7. NMR data is in agreement with the
published data.⁶ MS (EI) m/z = 51, 52, 64, 78, 79



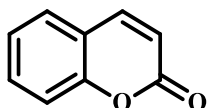
thiophene

^1H NMR (500 MHz, CDCl_3): δ = 7.34-7.33 (m, 2H), 7.12-7.11 (m, 2H); ^{13}C NMR (125 MHz,
 CDCl_3): 126.9, 125.2. NMR data is in agreement with the published data.⁴ MS (EI) m/z = 58,
84



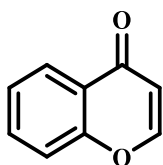
1H-indole

^1H NMR (500 MHz, CDCl_3): δ = 8.56 (s, 1H), 7.64-7.63 (d, J = 7.83 Hz, 1H) 7.37-7.35 (d, J =
7.83 Hz, 1H), 7.19-7.08 (m, 3H), 6.53-6.52 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 135.9,
127.9, 124.3, 121.8, 120.6, 119.8, 111.2, 102.3; NMR data is in agreement with the published
data.⁸ MS (EI) m/z = 117, 116, 90, 89, 64, 63



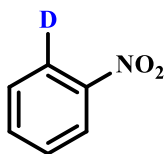
2H-chromen-2-one

^1H NMR (500 MHz, CDCl_3): δ = 7.72-7.70 (d, J = 9.61 Hz, 1H), 7.55-7.48 (m, 2H), 7.35-7.26
(m, 2H), 6.44-6.42 (d, J = 9.61 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3): 160.8, 154.1, 143.4,
131.8, 127.9, 124.4, 118.8, 116.9, 116.8; NMR data is in agreement with the published data.⁸
MS (EI) m/z = 146, 118, 90, 89, 64, 63



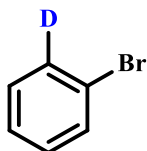
4H-1-benzopyran-4-one

^1H NMR (500 MHz, CDCl_3): δ = 8.22-8.21 (m, 1H), 7.87-7.86 (m, 1H), 7.69-7.68 (m, 1H),
7.45-7.38 (m, 2H), 6.36-6.35 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3): 177.7, 155.4, 154.8,
134.0, 125.8, 125.3, 125.0, 118.2, 113.0; NMR data is in agreement with the published data.⁸
MS (EI) m/z = 146, 120, 118, 92, 90, 74, 63



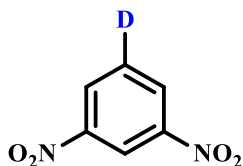
2-nitro-1-deuterobenzene

^1H NMR (500 MHz, DMSO- d_6): δ = 7.90-7.88 (m, 1H), 7.83-7.82 (m, 1H), 7.76-7.68 (m, 2H); ^{13}C NMR (125 MHz, DMSO- d_6): 148.2, 135.6, 130.2, 123.7. NMR data is in agreement with the published data.⁹ MS (EI) m/z = 51, 65, 77, 93, 123



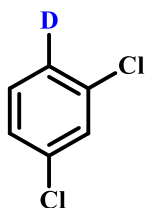
2-bromo-1-deuterobenzene

^1H NMR (500 MHz, DMSO- d_6): δ = 7.63-7.61 (d, J = 8.14 Hz, 2H), 7.41-7.38 (t, J =7.76 Hz, 1H), 7.33-7.30 (m, 1H); ^{13}C NMR (125 MHz, DMSO- d_6): 133.6, 131.8, 130.1, 127.9. NMR data is in agreement with the published data.² MS (EI) m/z = 51, 63, 77, 84, 155



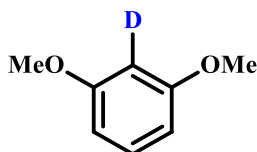
3,5-dinitro-1-deuterobenzene

^1H NMR (500 MHz, DMSO- d_6): δ = 8.94-8.93 (d, J = 2.18 Hz, 2H), 8.88-8.87 (t, J = 2.18 Hz, 1H); ^{13}C NMR (125 MHz, DMSO- d_6): 148.2, 140.6, 128.9, 120.2. NMR data is in agreement with the published data.² MS (EI) m/z = 51, 64, 75, 83, 92, 122, 168



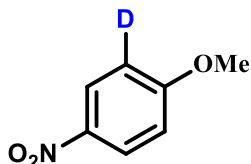
2,4-dichloro-1-deuterobenzene

^1H NMR (500 MHz, DMSO- d_6): δ = 7.66-7.64 (d, J = 8.17 Hz, 1H), 7.56-7.52 (m, 1H), 7.42-7.40 (d, J = 8.17 Hz, 1H); ^{13}C NMR (125 MHz, DMSO- d_6): 135.2, 131.4, 129.8, 127.4. NMR data is in agreement with the published data.² MS (EI) m/z = 55, 75, 83, 111, 145, 148



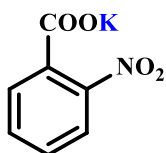
2,6-dimethoxy-1-deuterobenzene

^1H NMR (500 MHz, DMSO- d_6): δ = 7.32-7.29 (t, J = 8.37 Hz, 1H), 6.71-6.70 (d, J = 8.37 Hz, 2H), 3.79 (s, 6H); ^{13}C NMR (125 MHz, DMSO- d_6): 156.9, 130.8, 114.8, 104.6, 56.1. NMR data is in agreement with the published data.⁹ MS (EI) m/z = 52, 65, 78, 95, 109, 138



2-methoxy-5-nitro-1-deuterobenzene

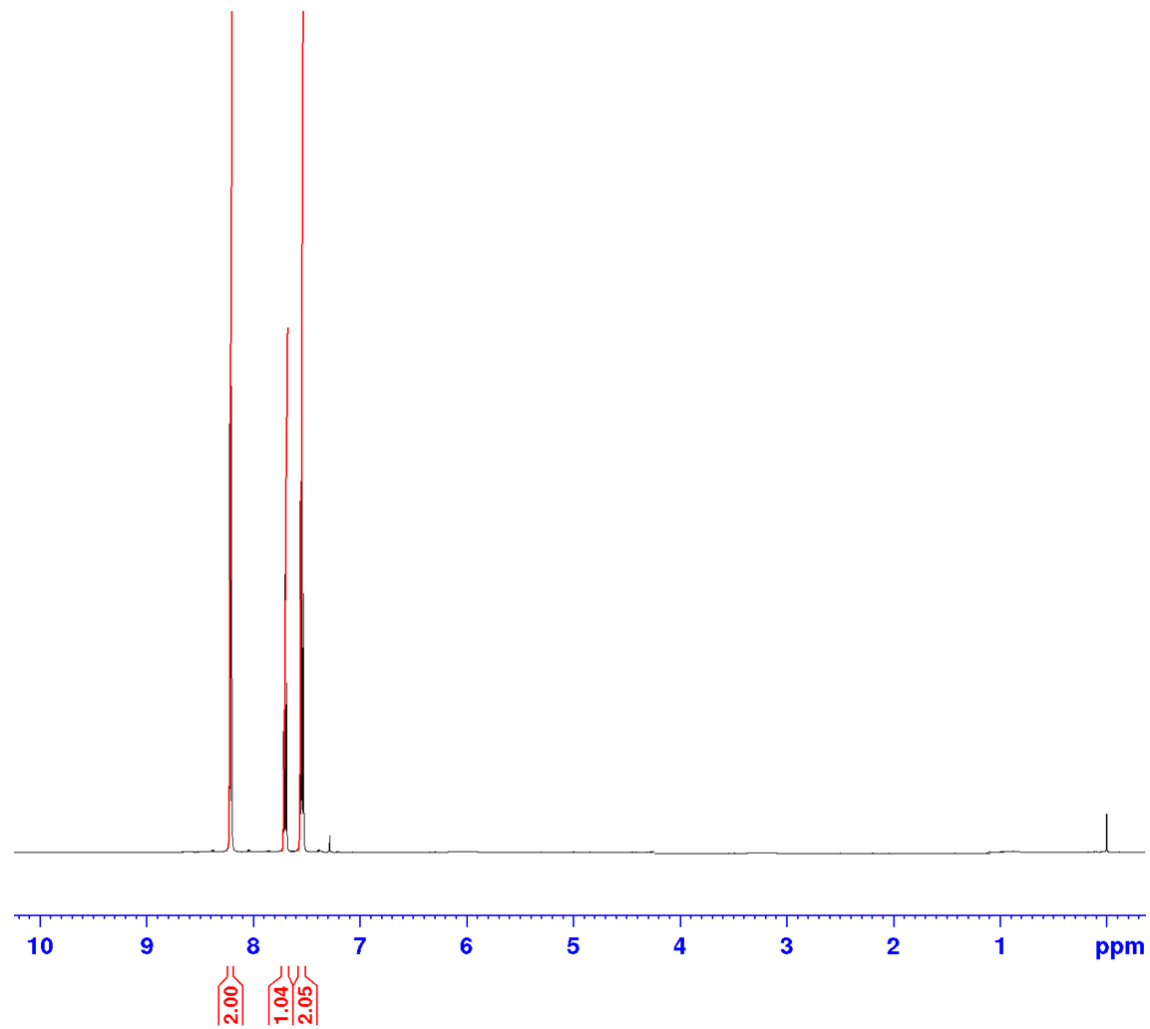
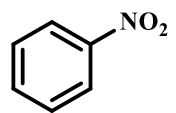
^1H NMR (500 MHz, DMSO- d_6): δ = 7.87-7.86 (d, J = 8.81 Hz, 1H), 7.05-7.01 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6): 162.9, 138.1, 126.2, 126.1, 114.3, 113.8, 56.4. NMR data is in agreement with the published data.¹⁰ MS (EI) m/z = 63, 77, 92, 95, 107, 123, 137, 153

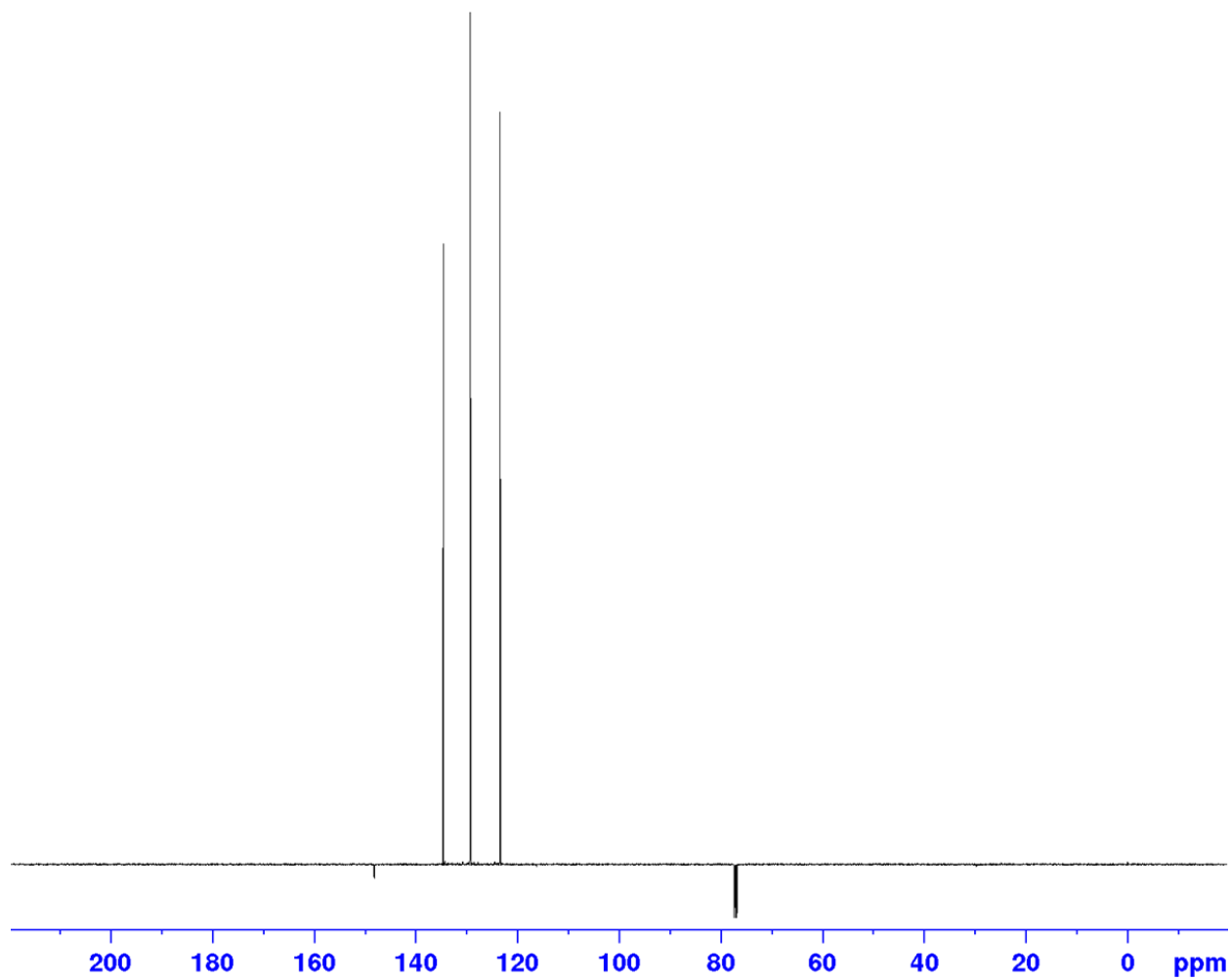
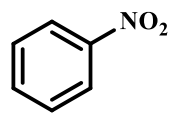


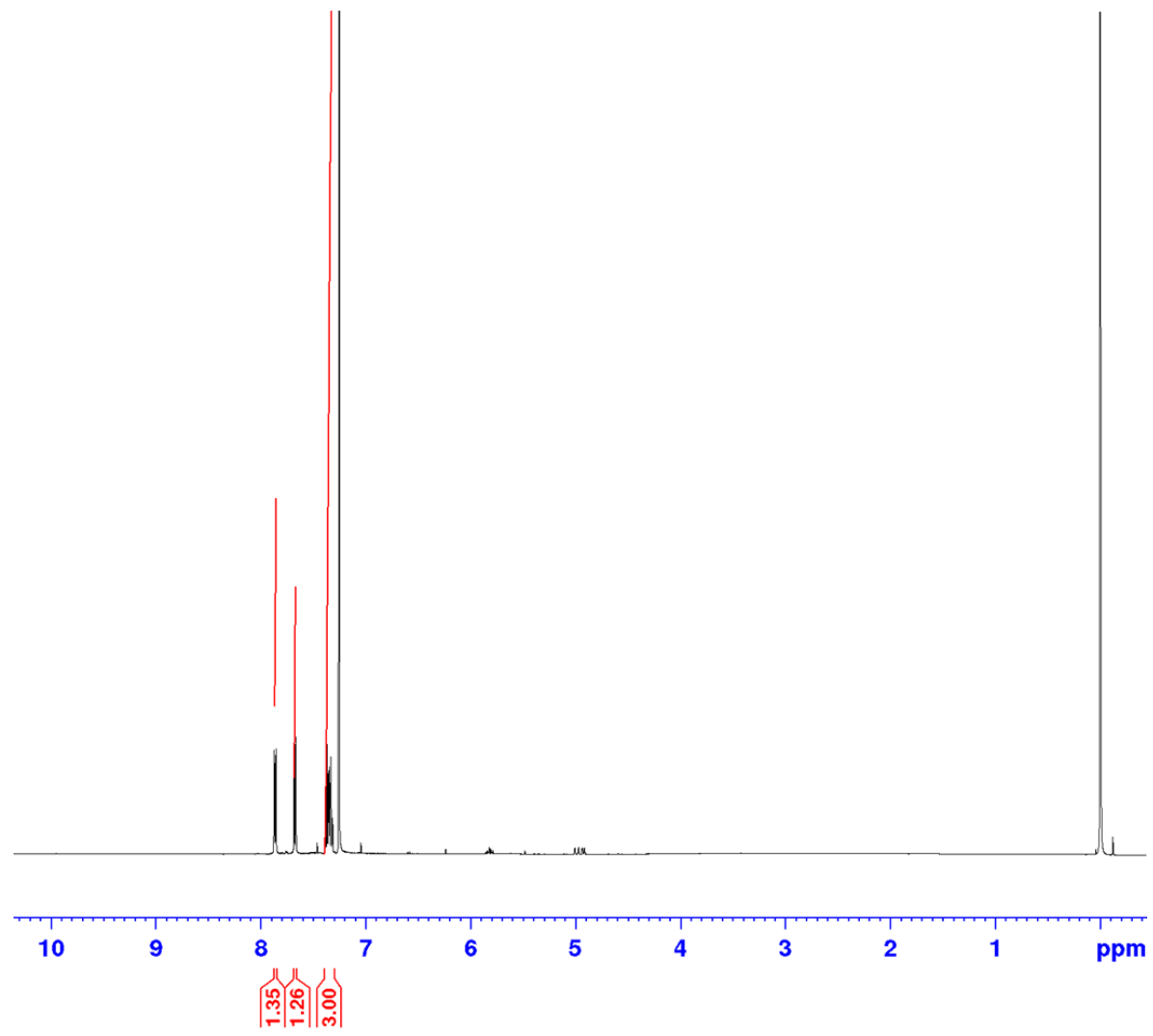
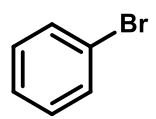
potassium-2-nitrobenzoate

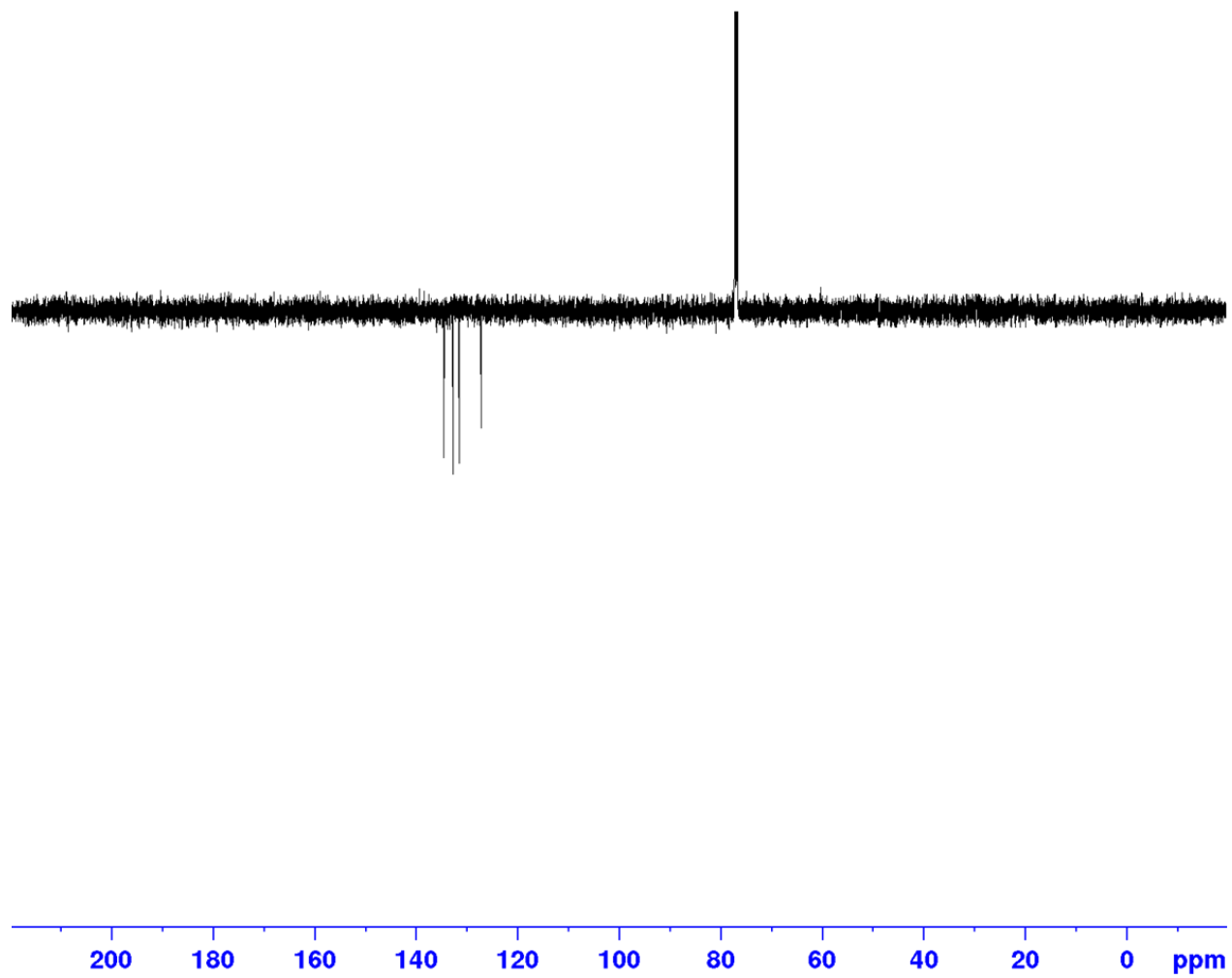
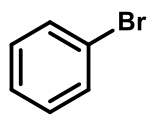
^1H NMR (500 MHz, DMSO- d_6): δ = 7.69-7.67 (d, J = 7.99 Hz, 1H), 7.23-7.19 (m, 1H), 6.74-6.72 (d, J = 7.99 Hz, 1H), 6.51-6.48 (m, 1H). NMR data is in agreement with the published data.¹¹ MS (EI) m/z = 57, 77, 86, 91, 105, 115, 145, 161, 177, 205

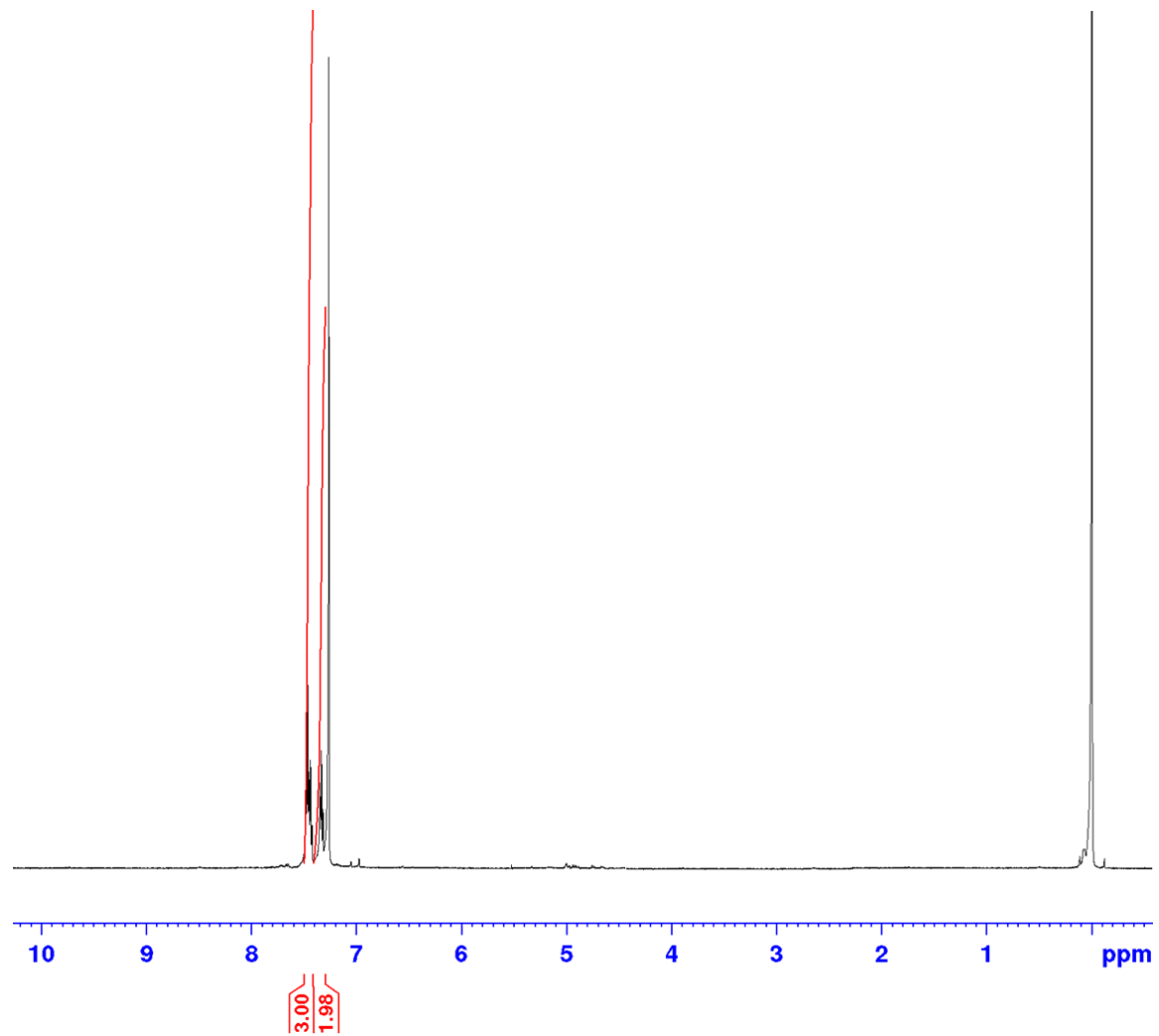
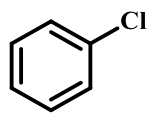
3. Collection of NMR Spectra

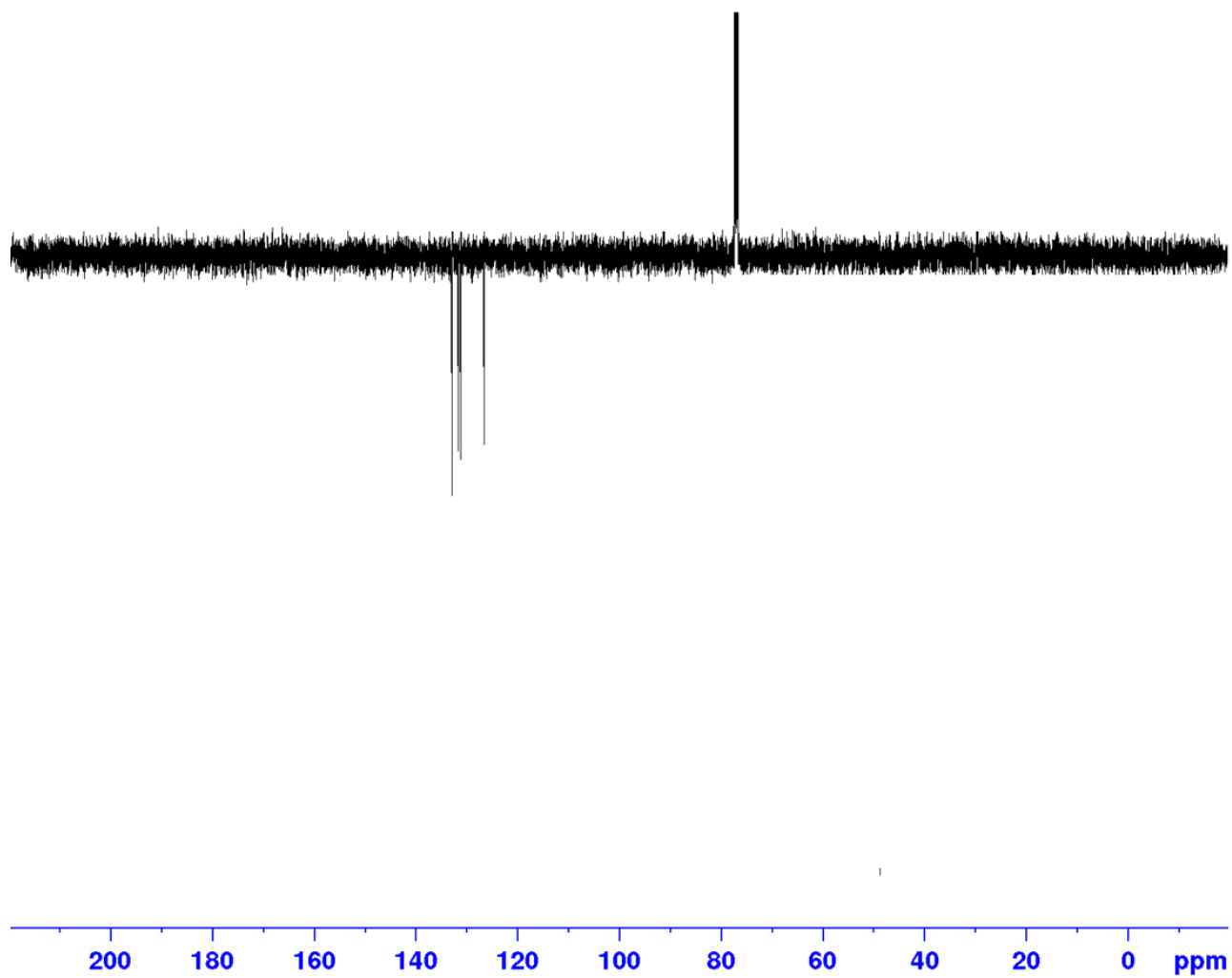
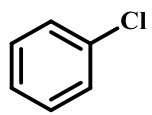


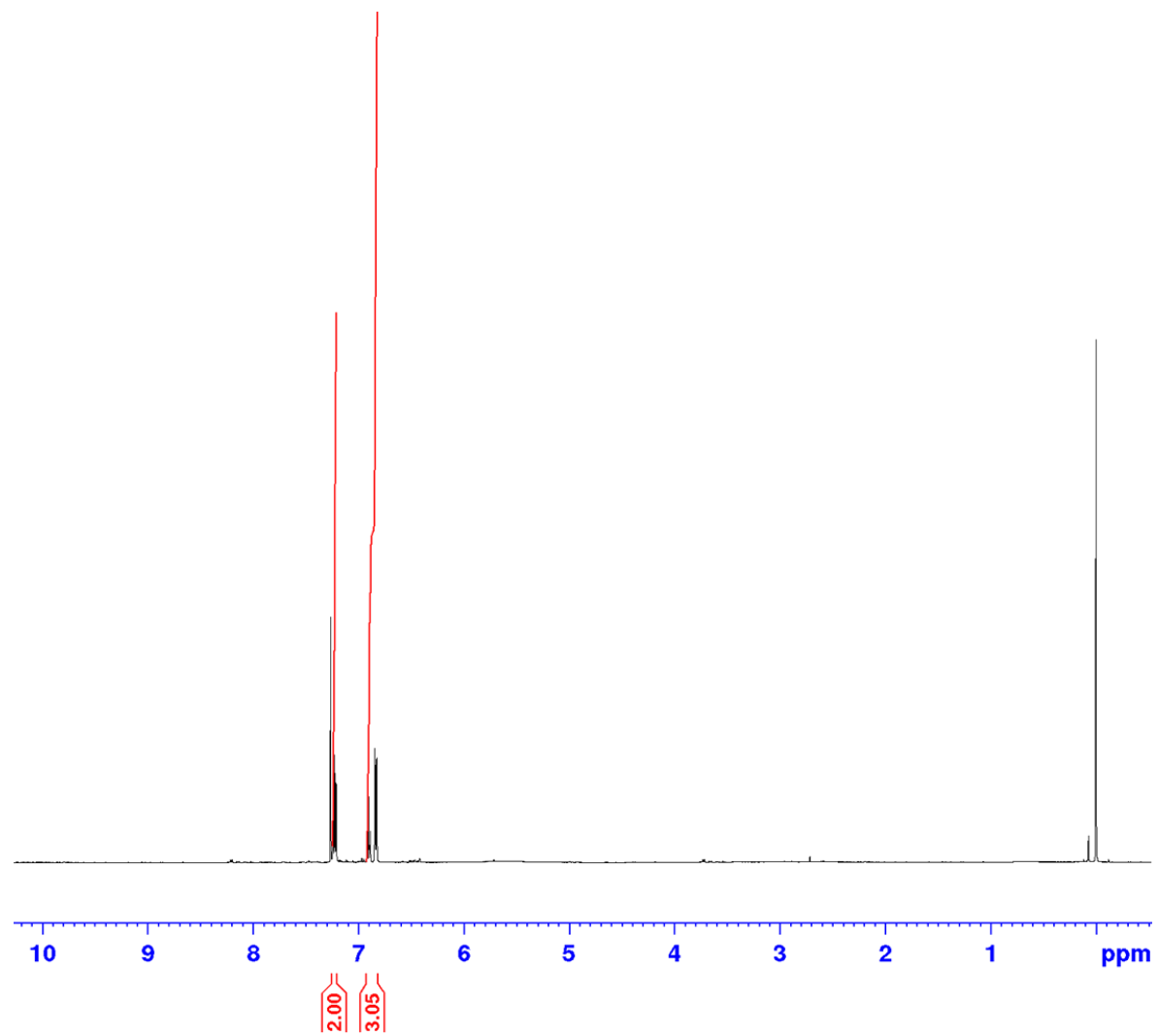
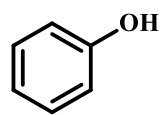


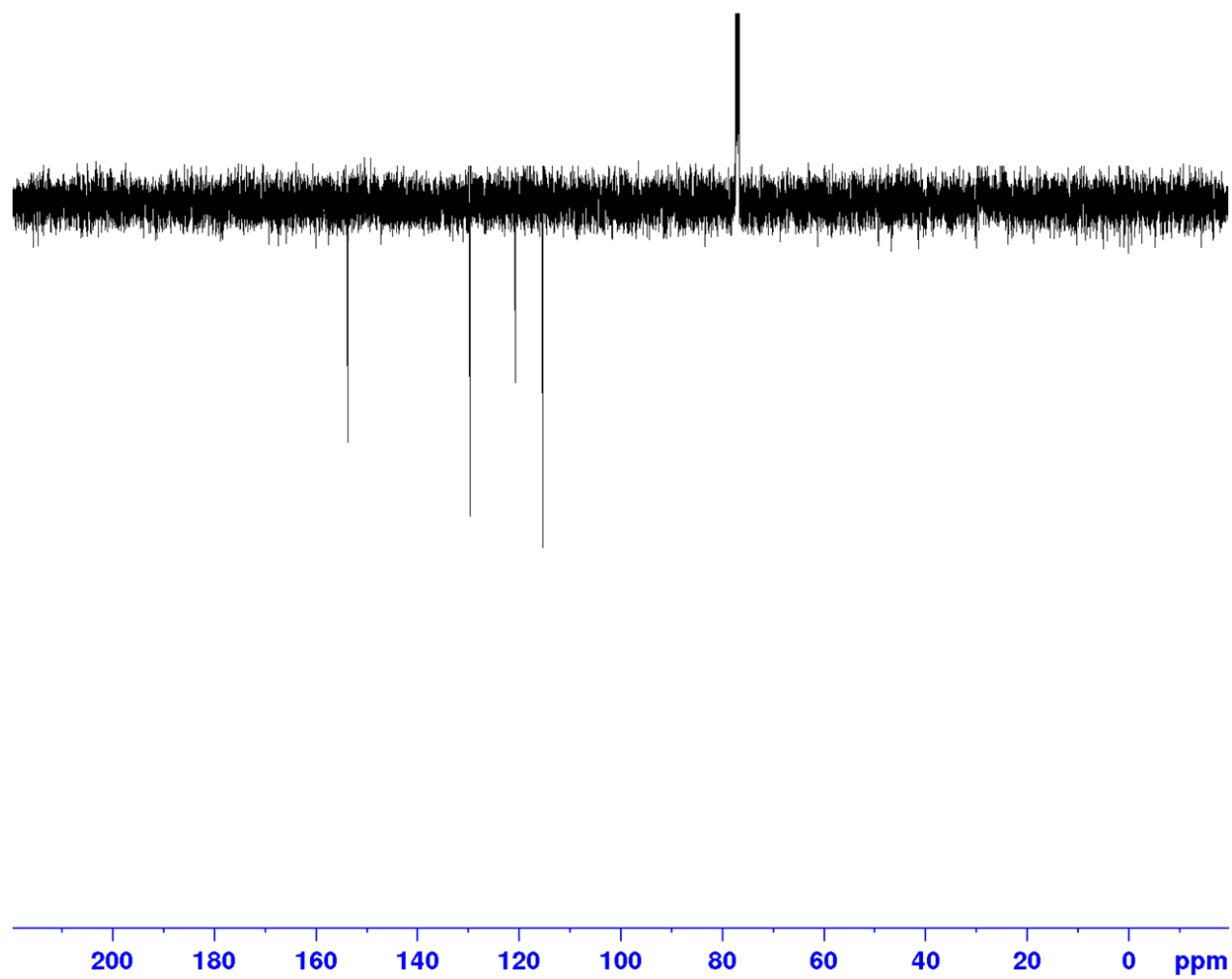
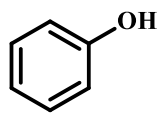


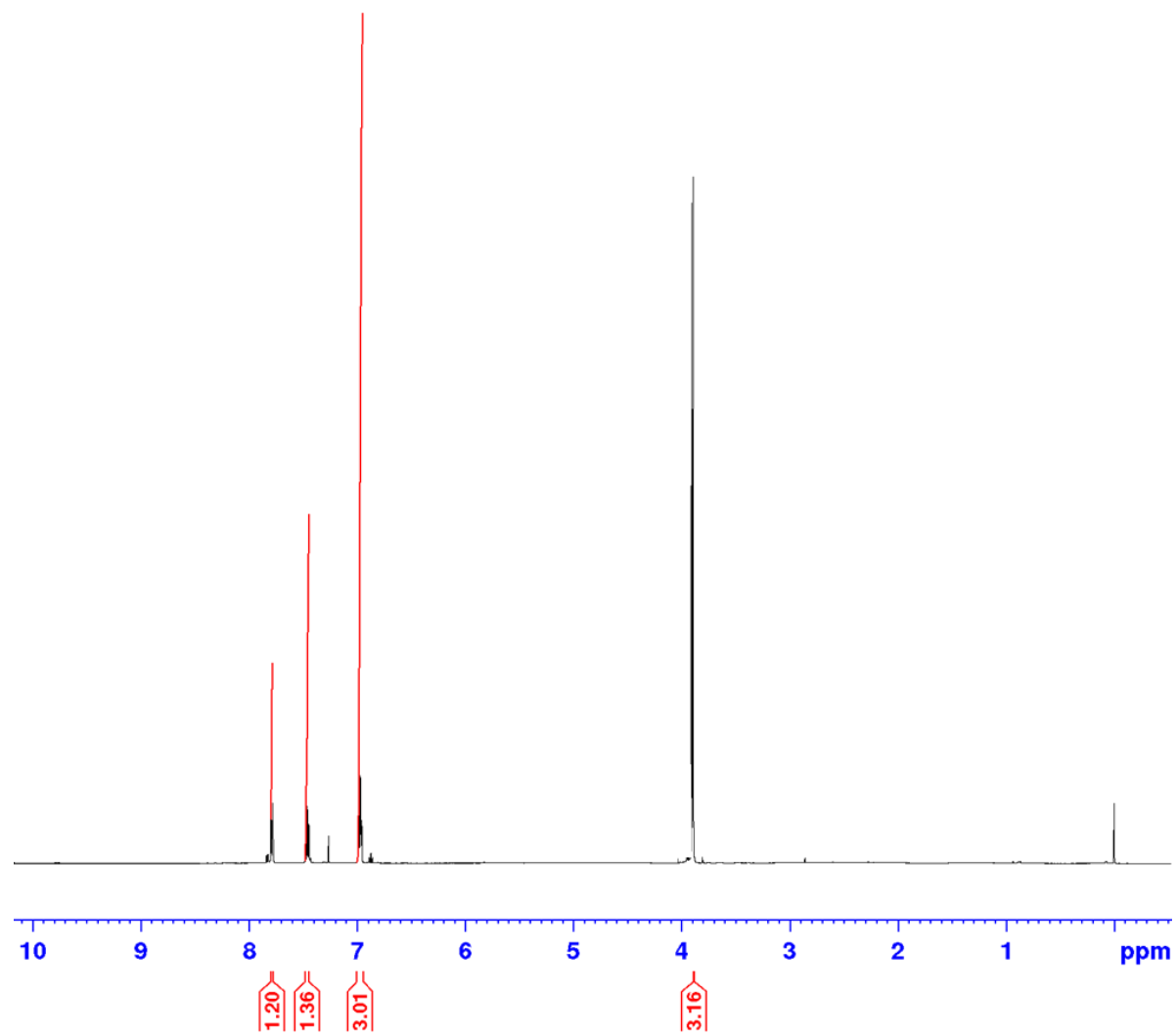
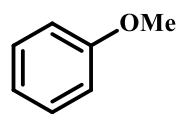


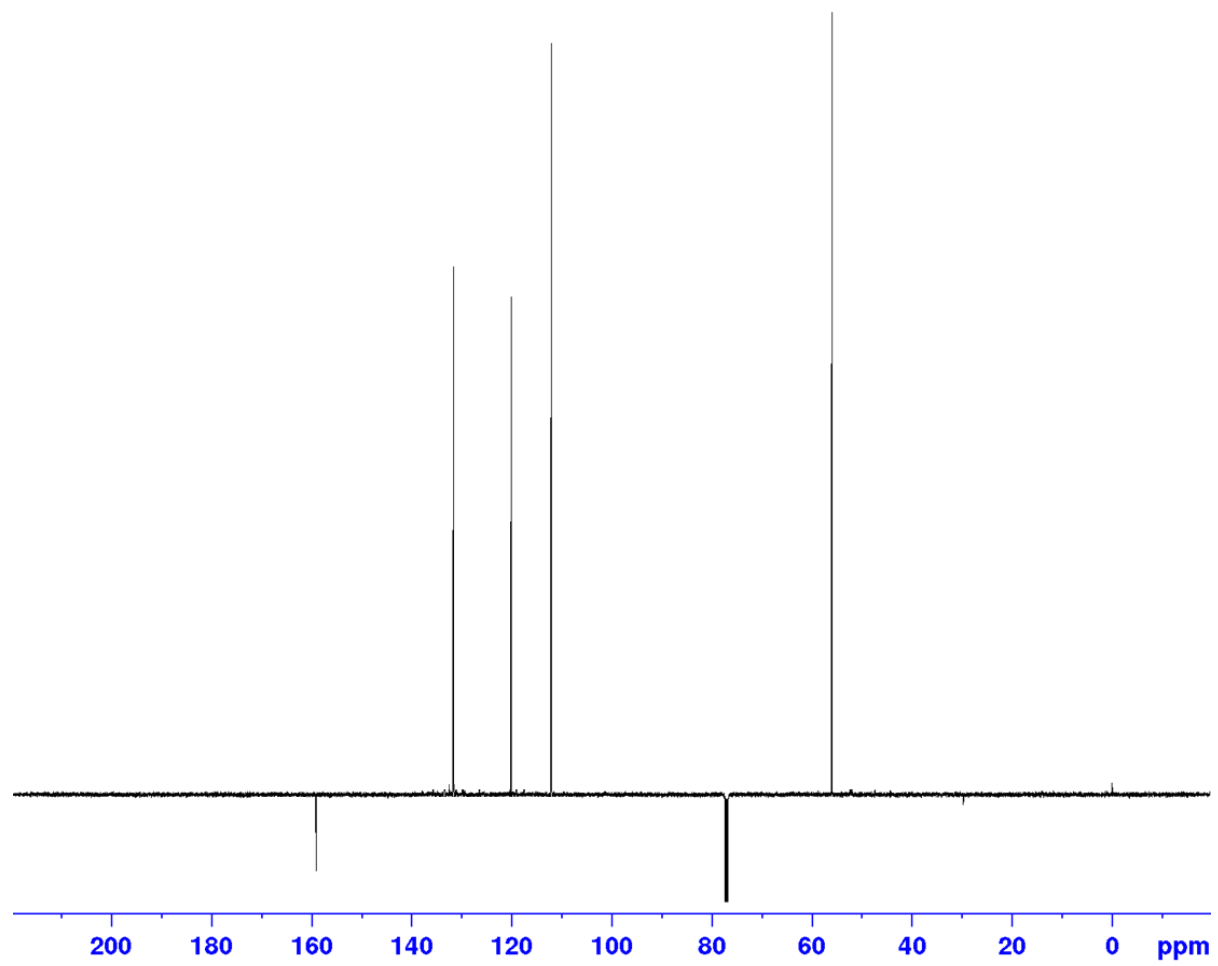
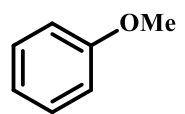


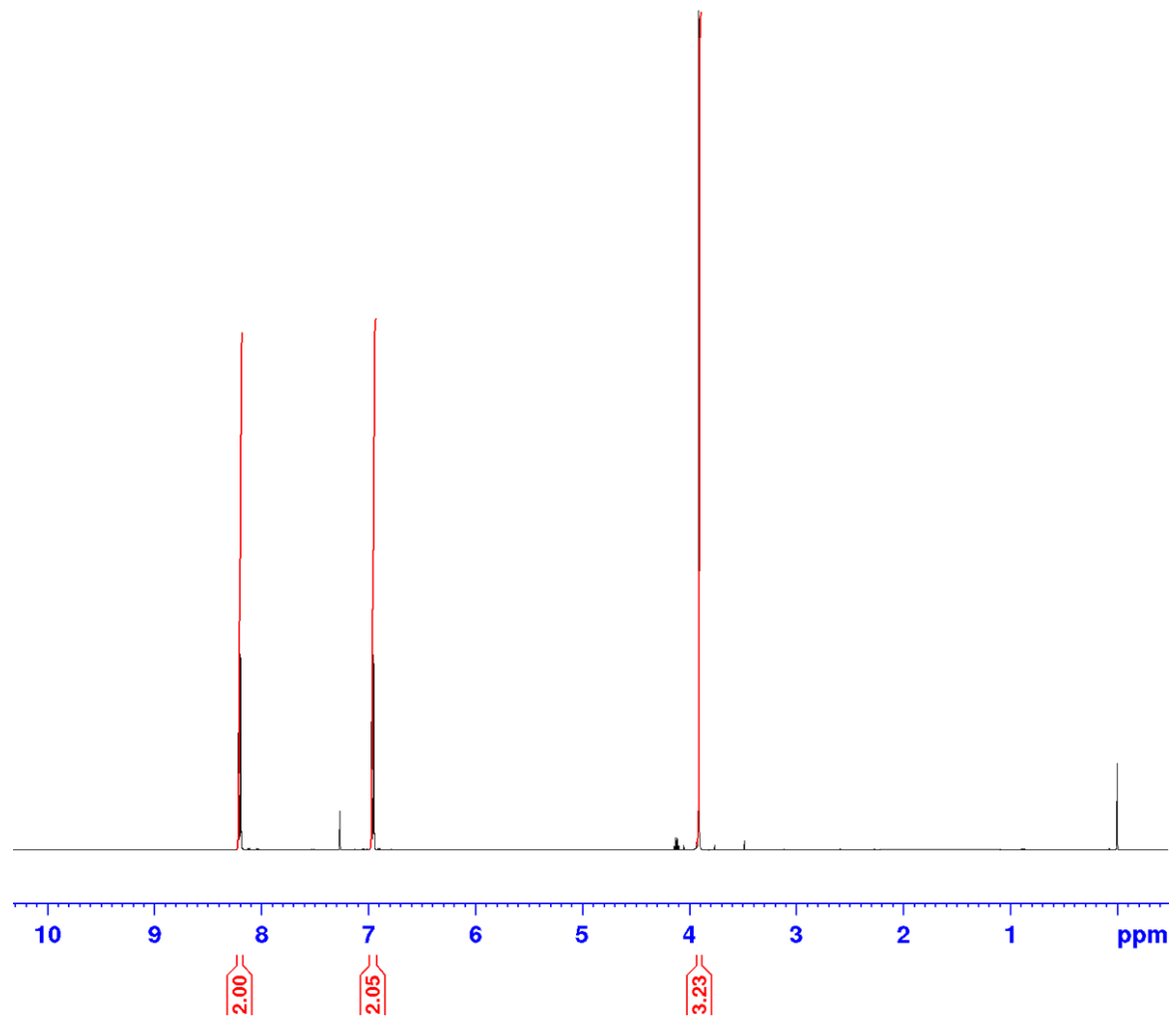
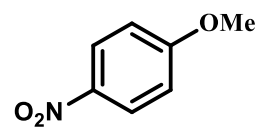


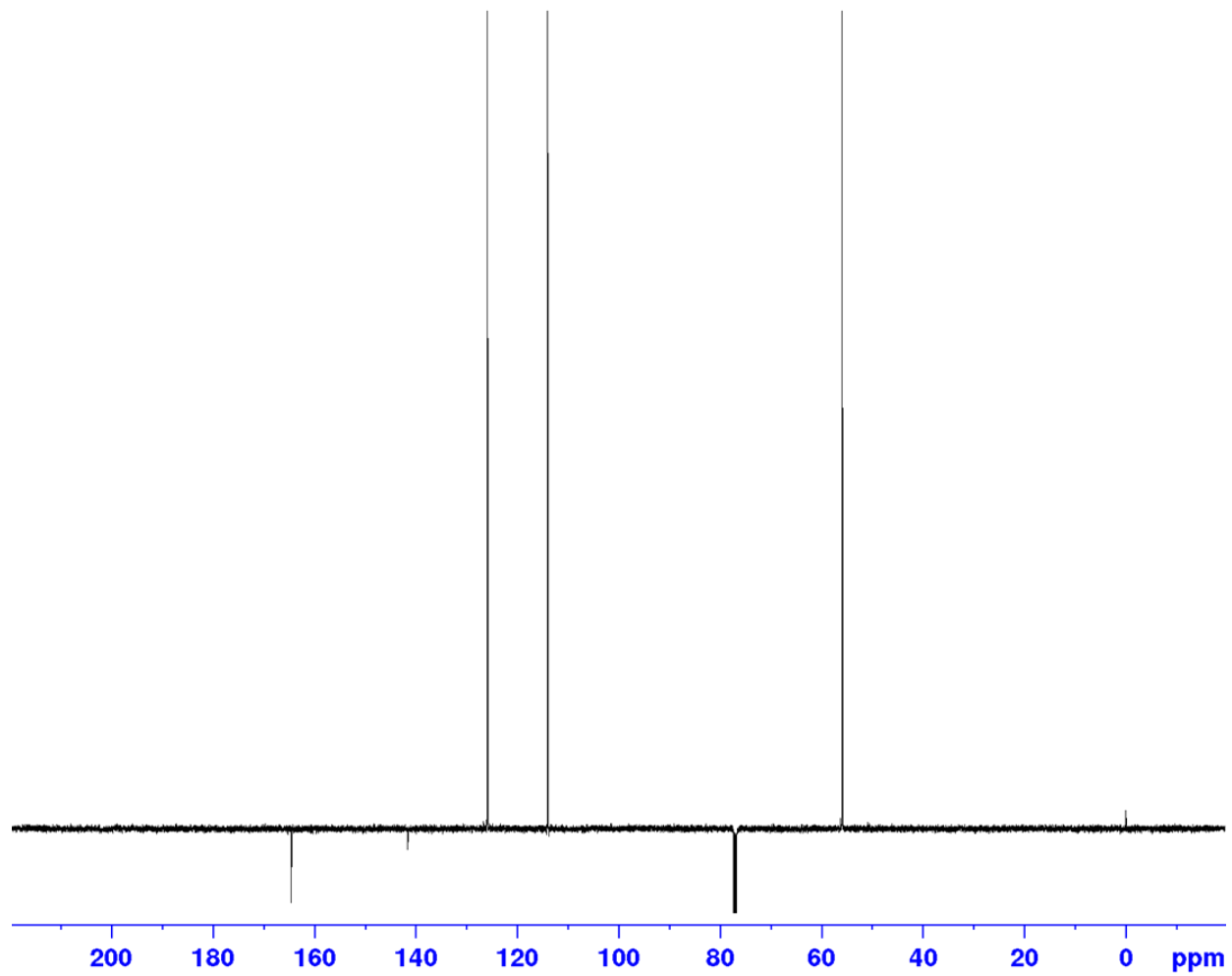
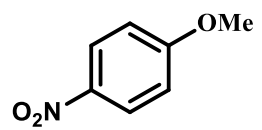


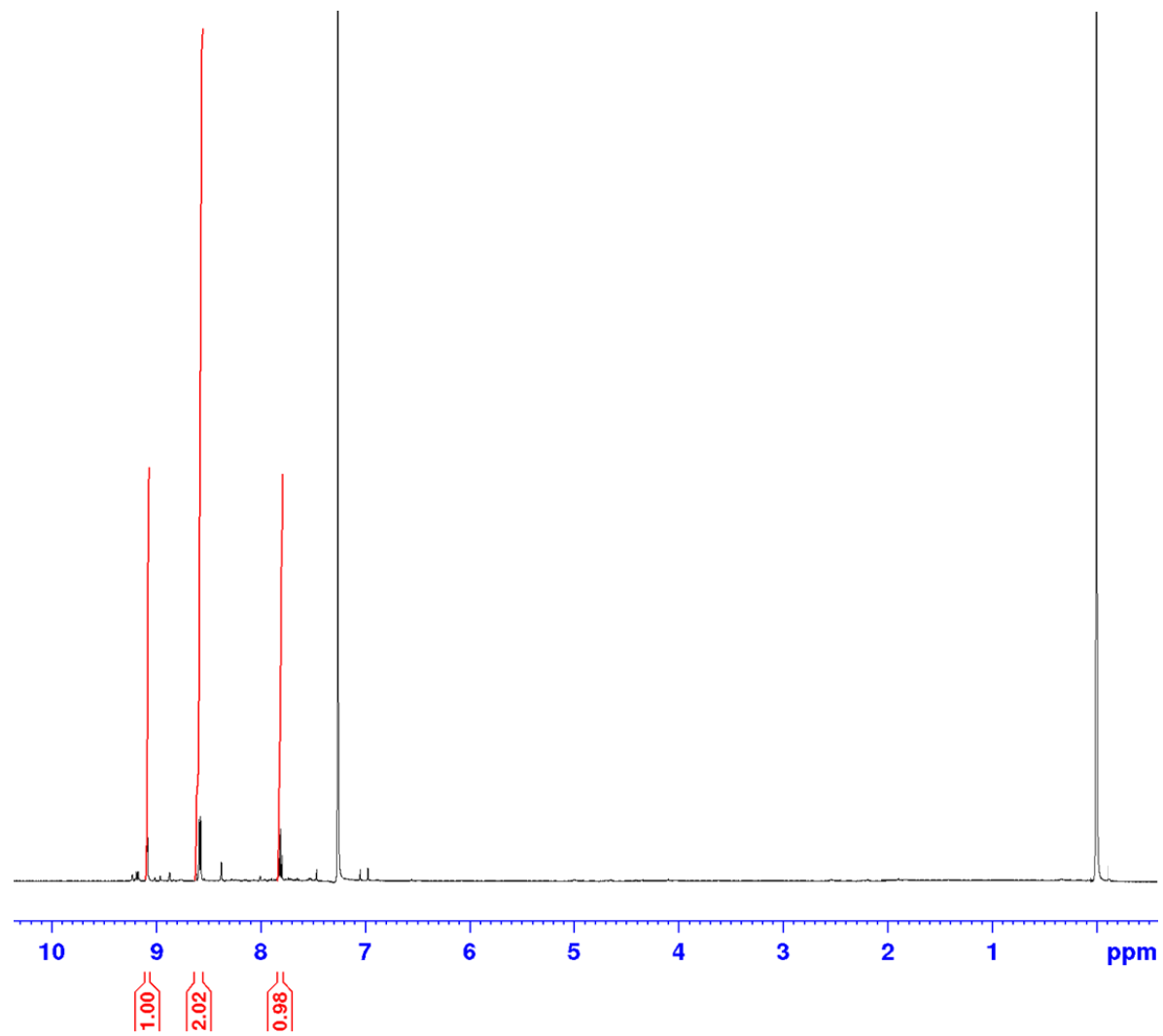
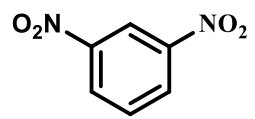


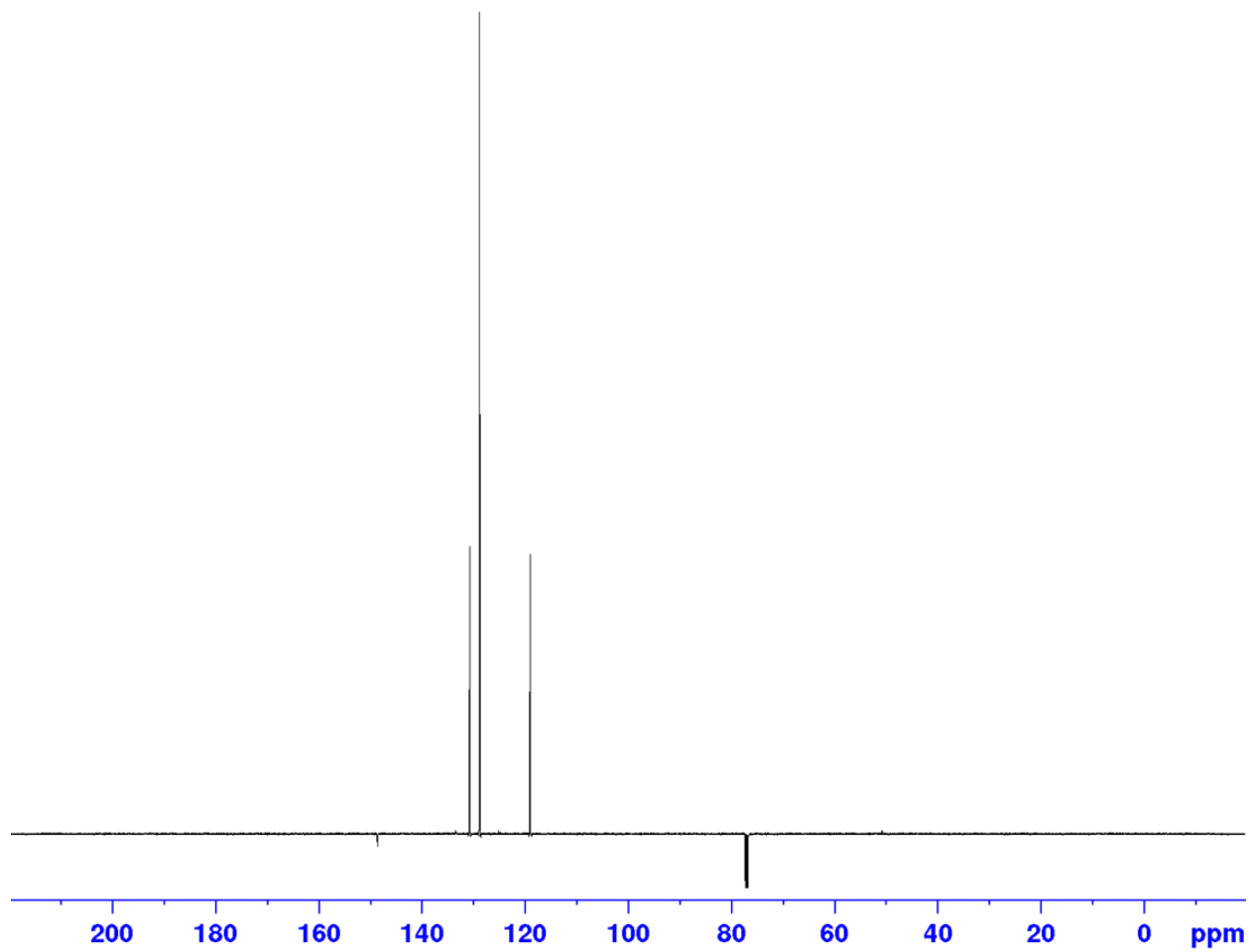
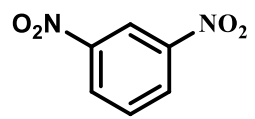


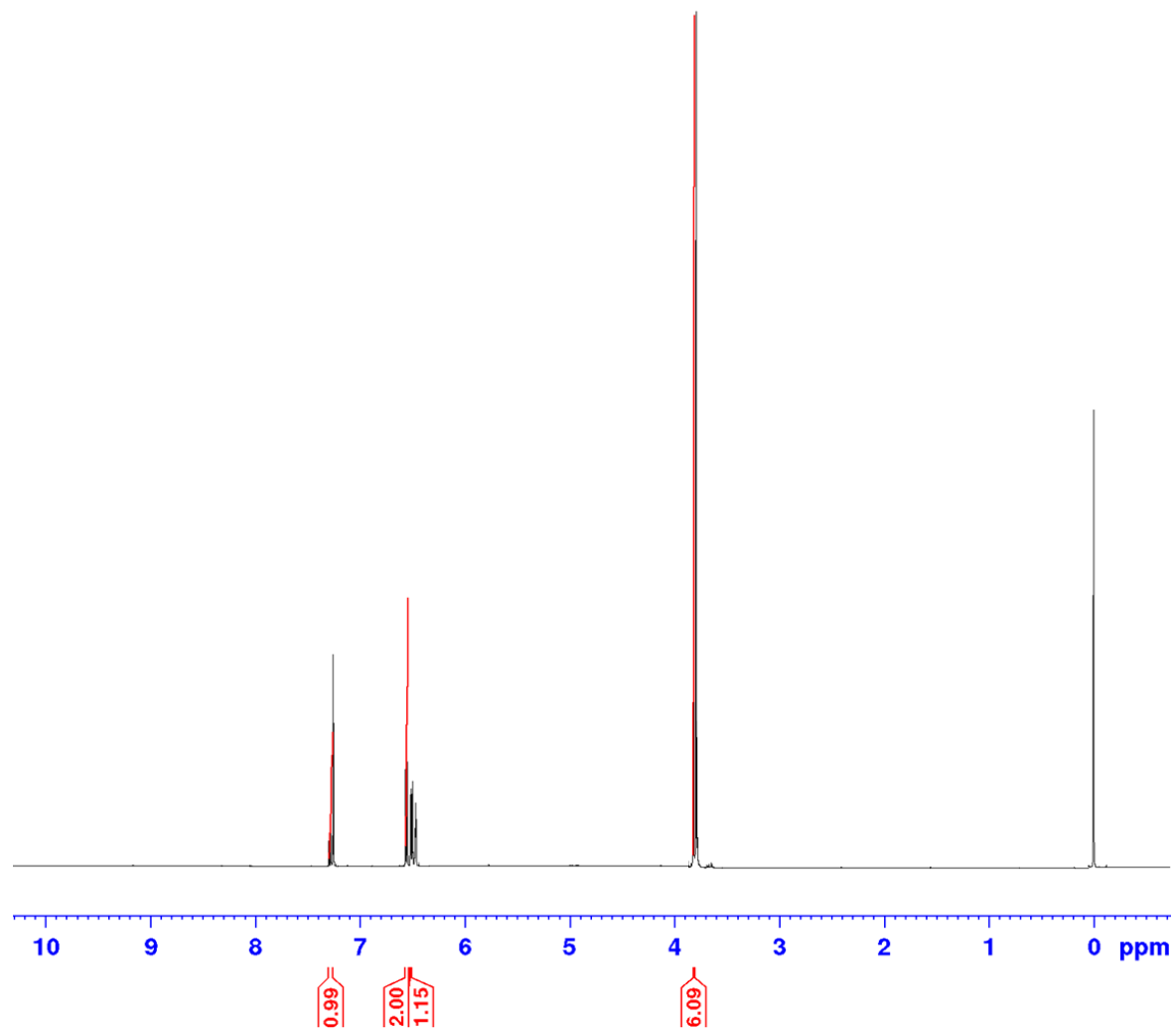
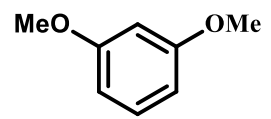


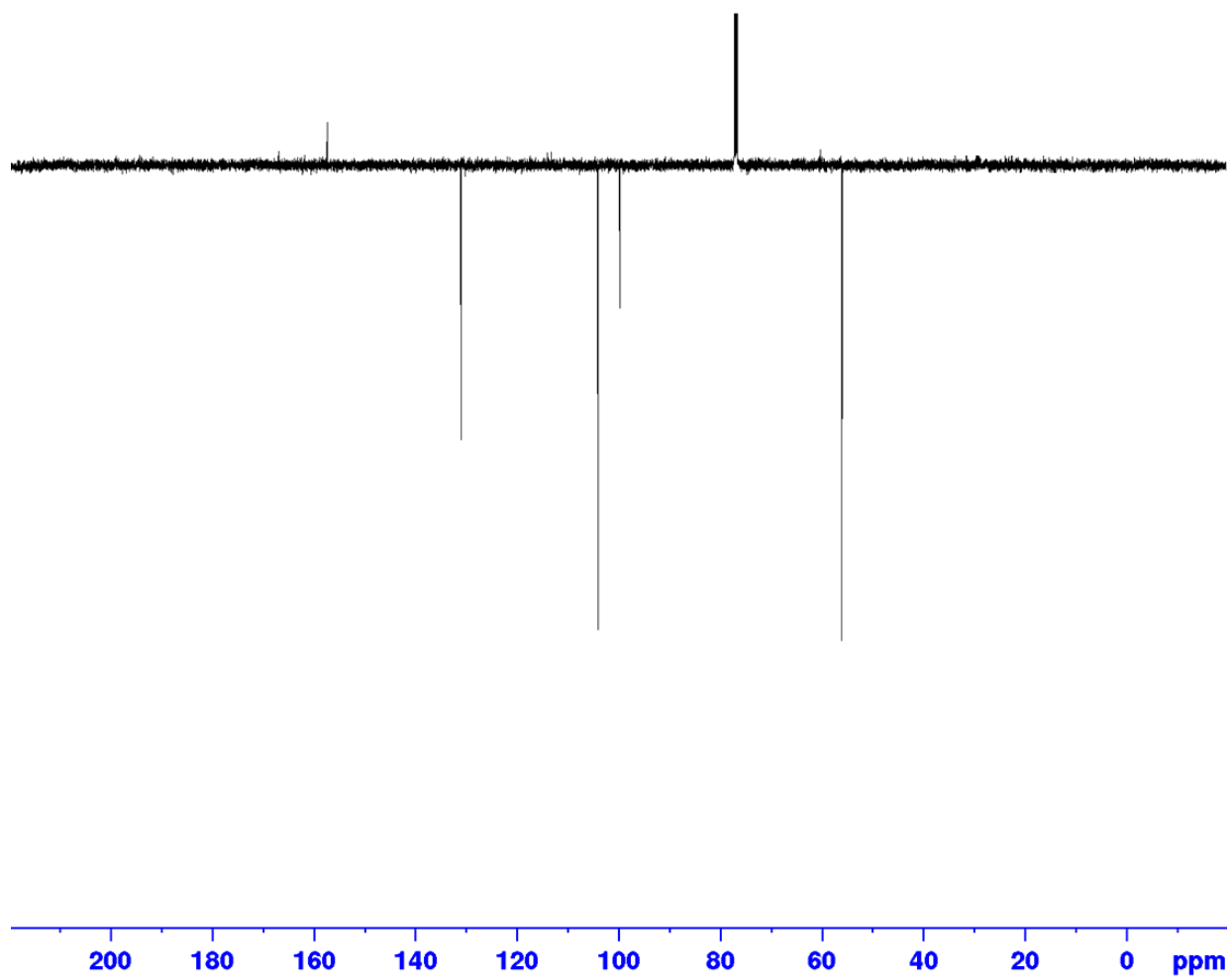
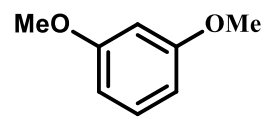


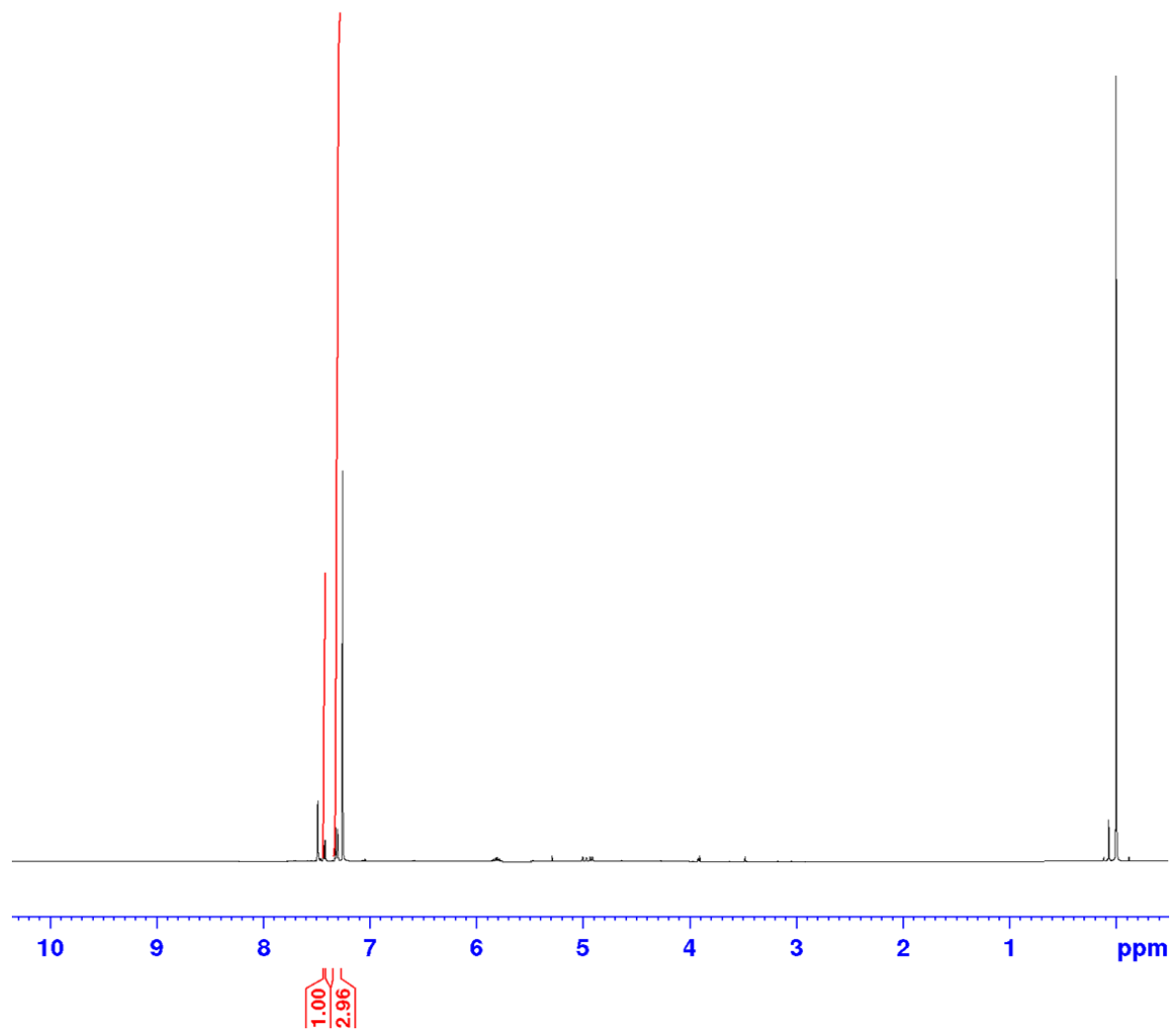
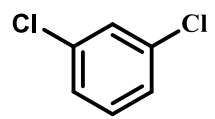


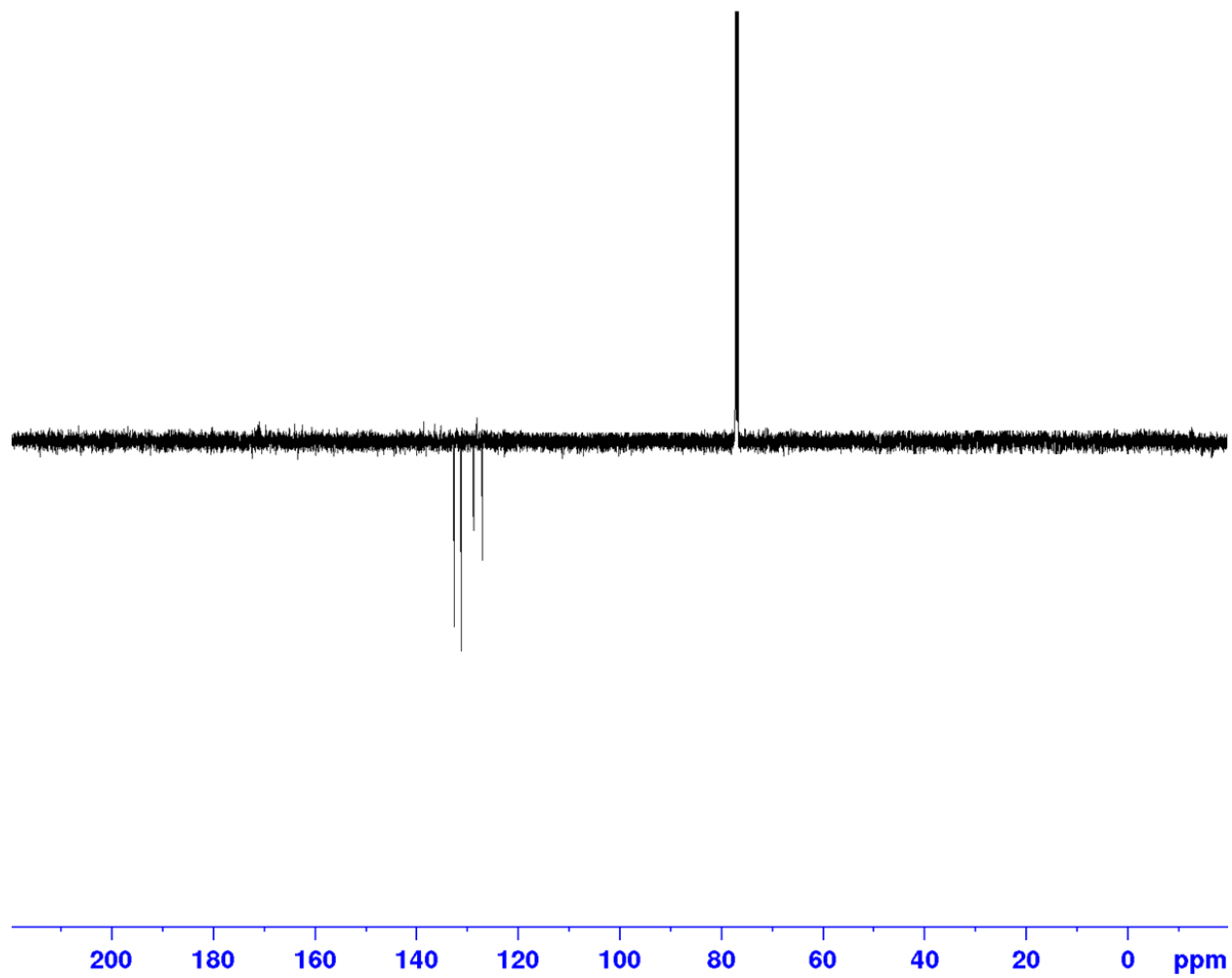
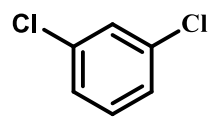


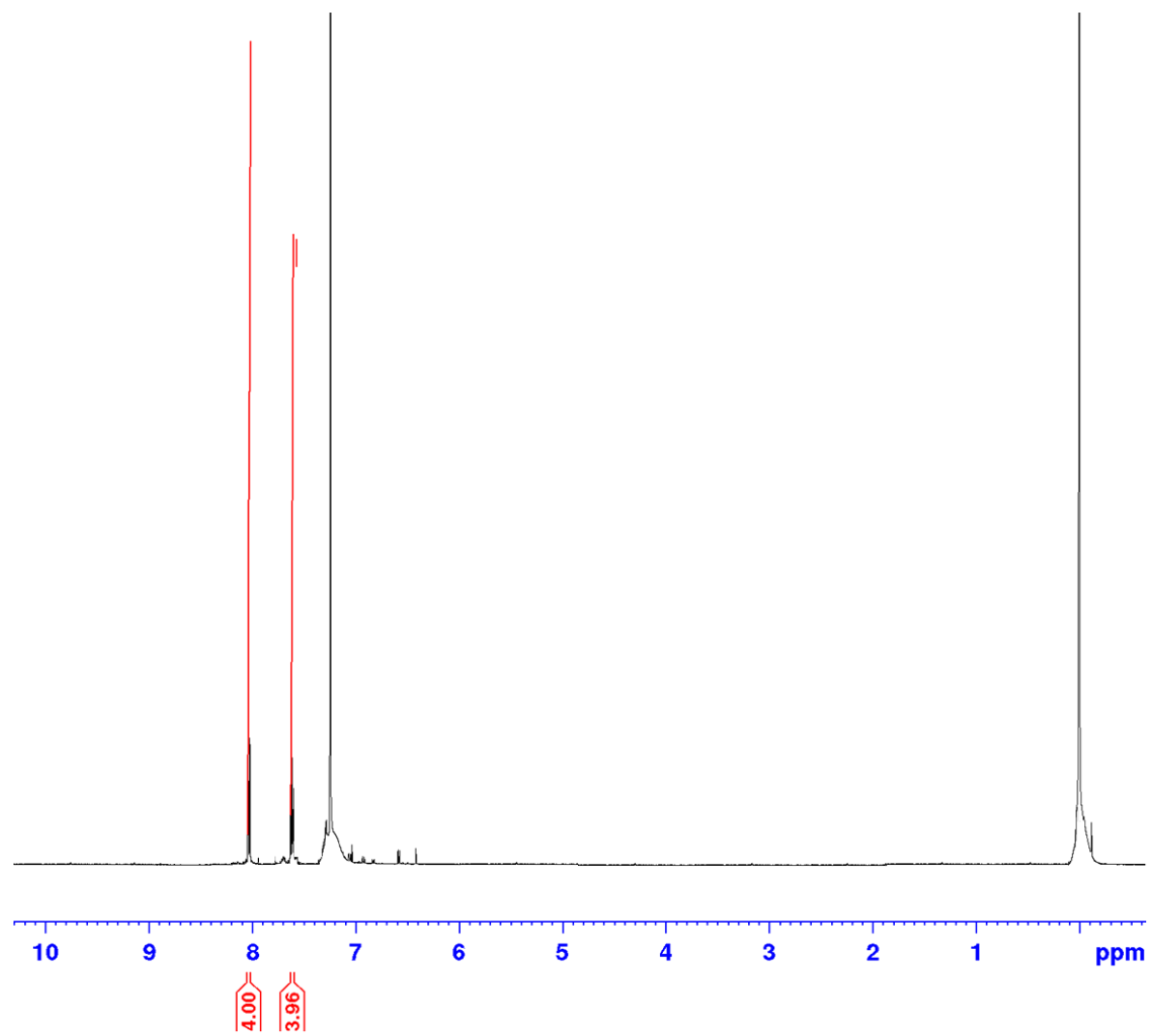
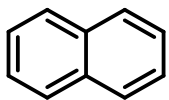


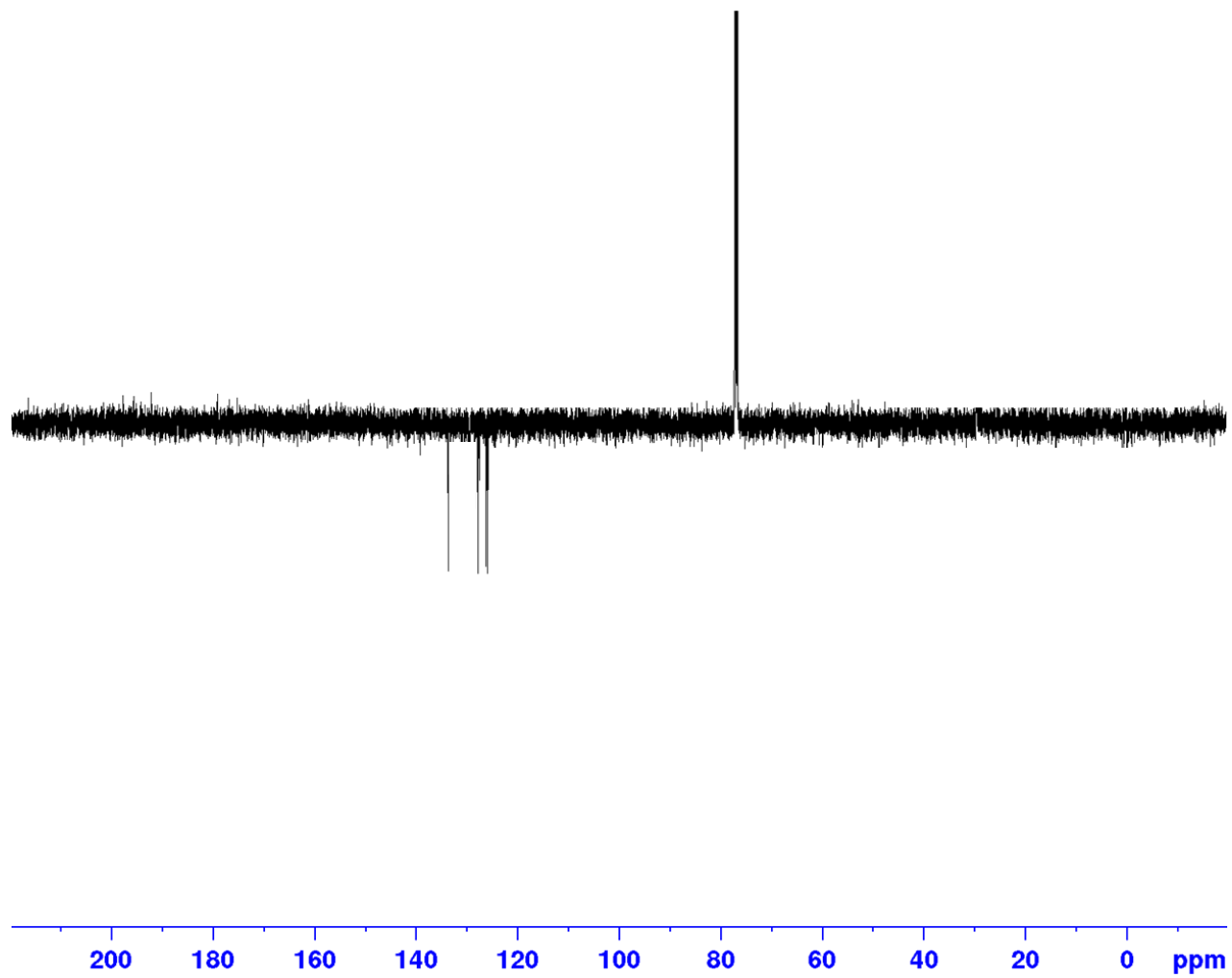
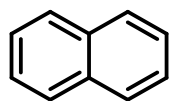


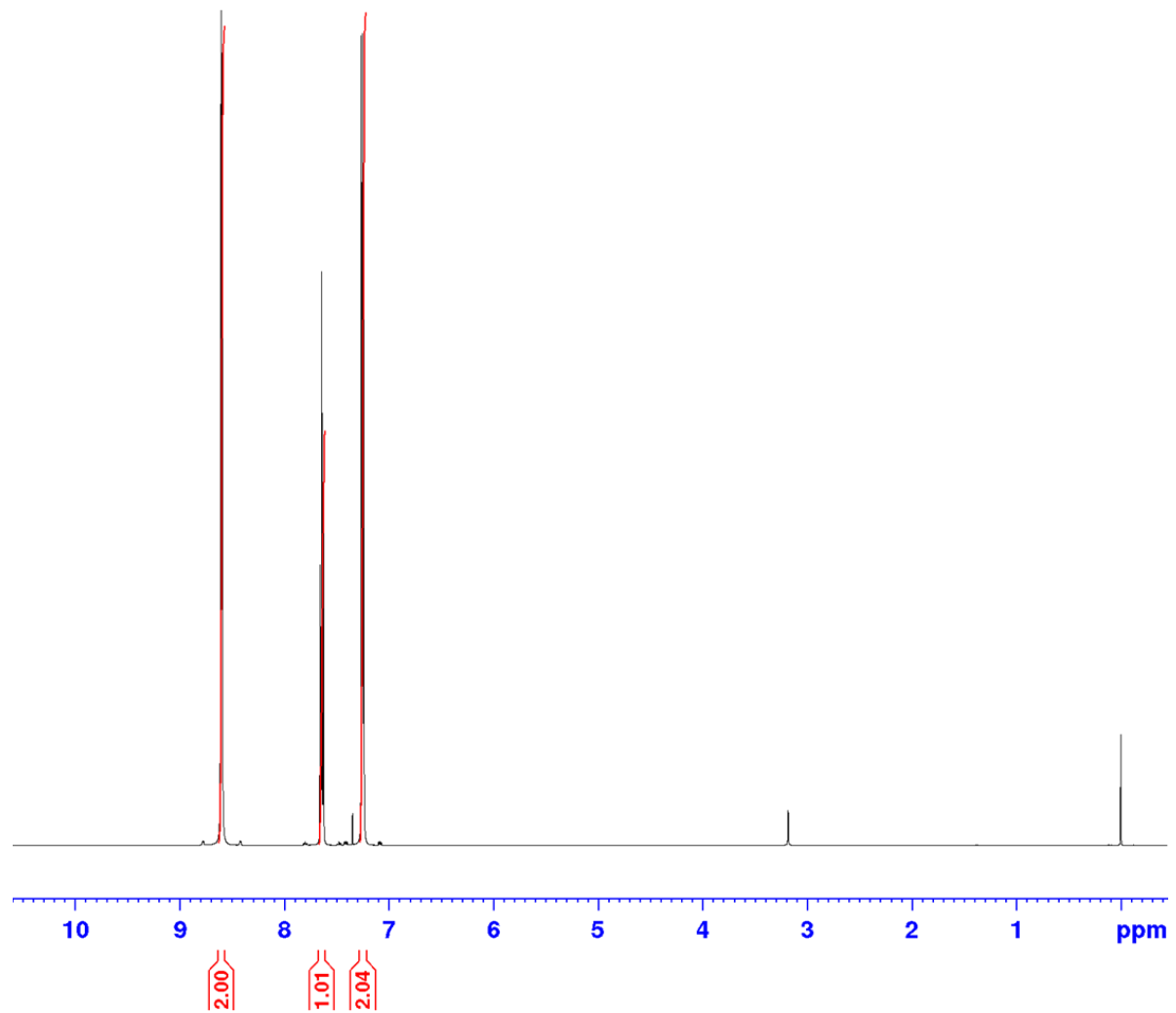
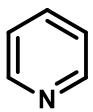


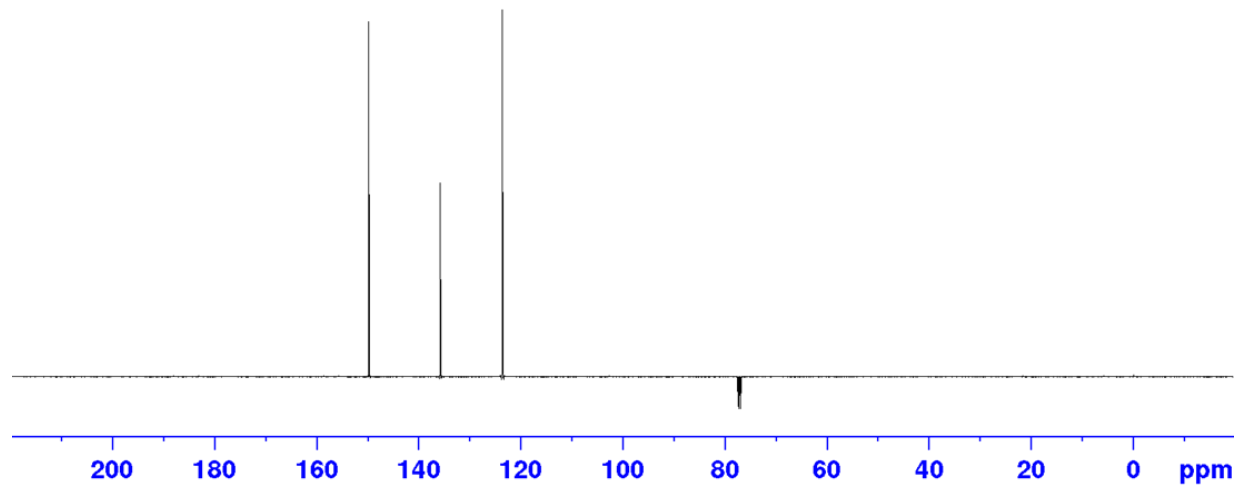
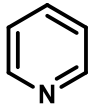


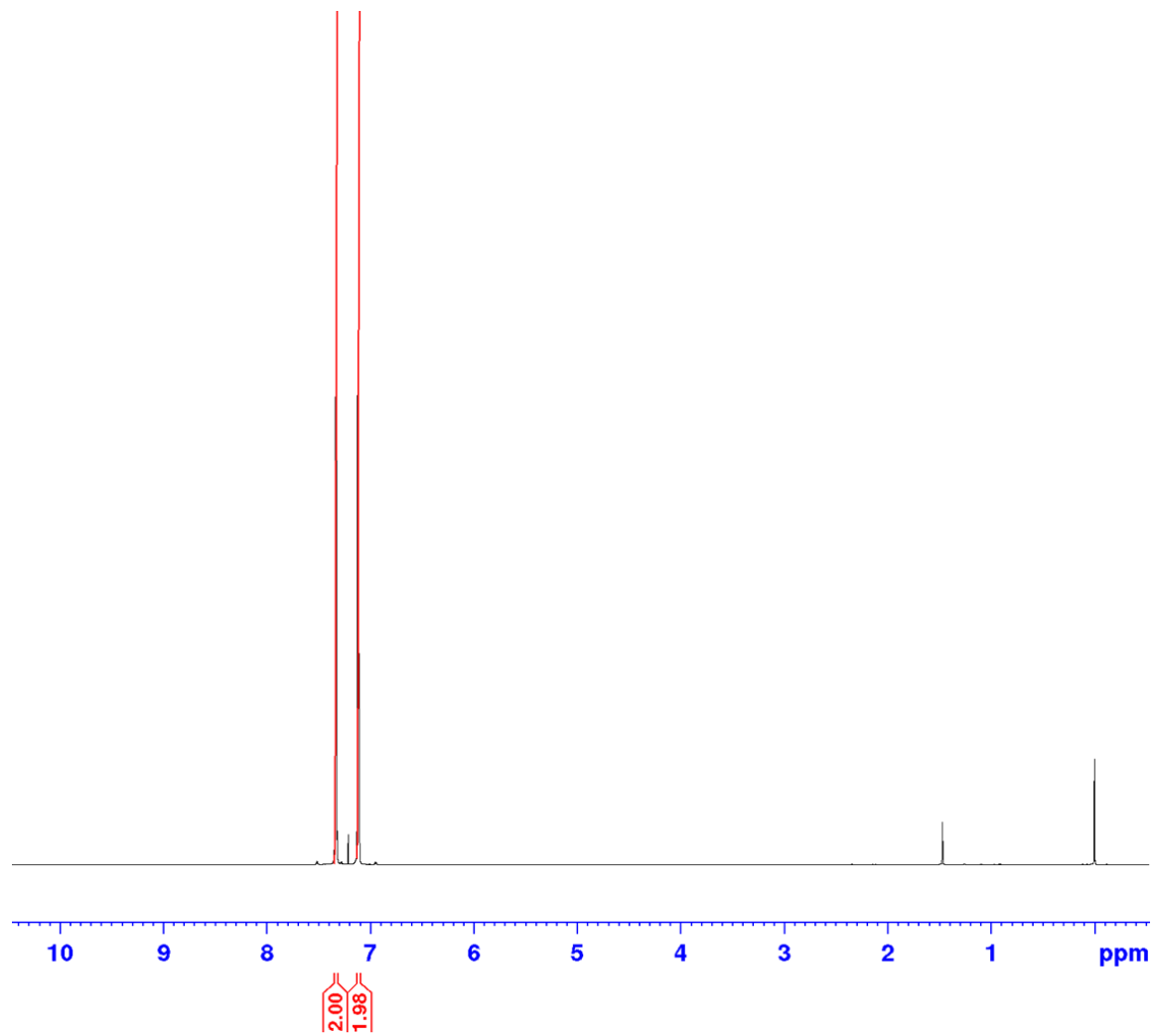


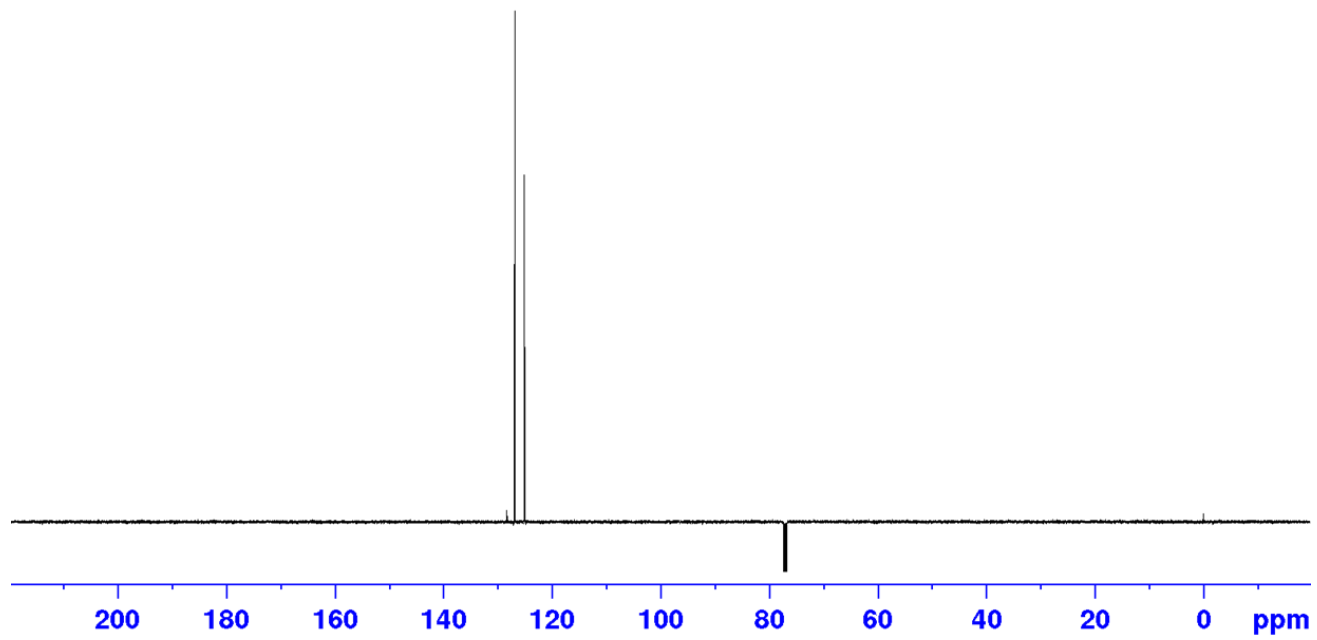


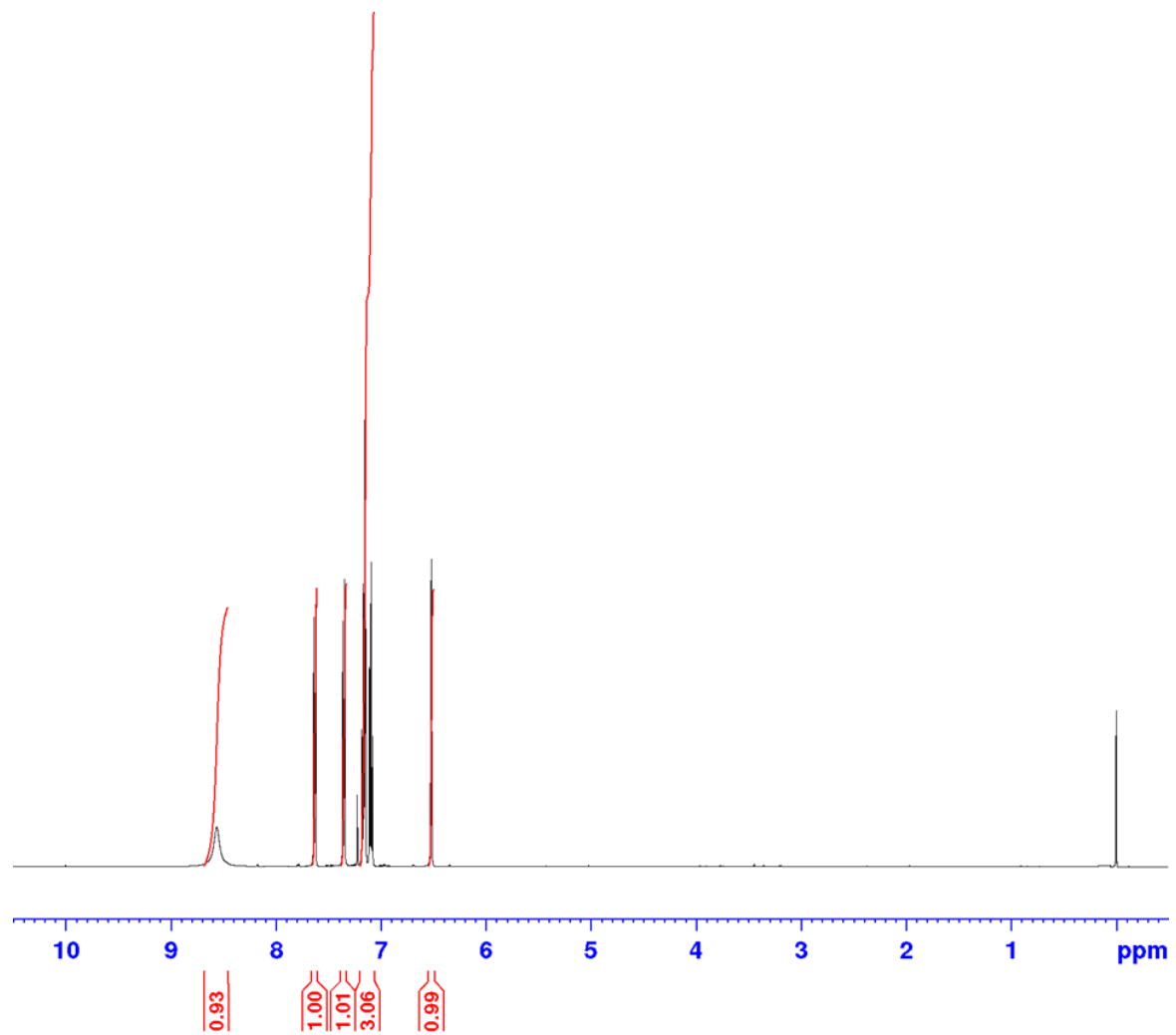
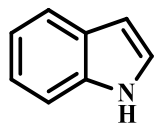


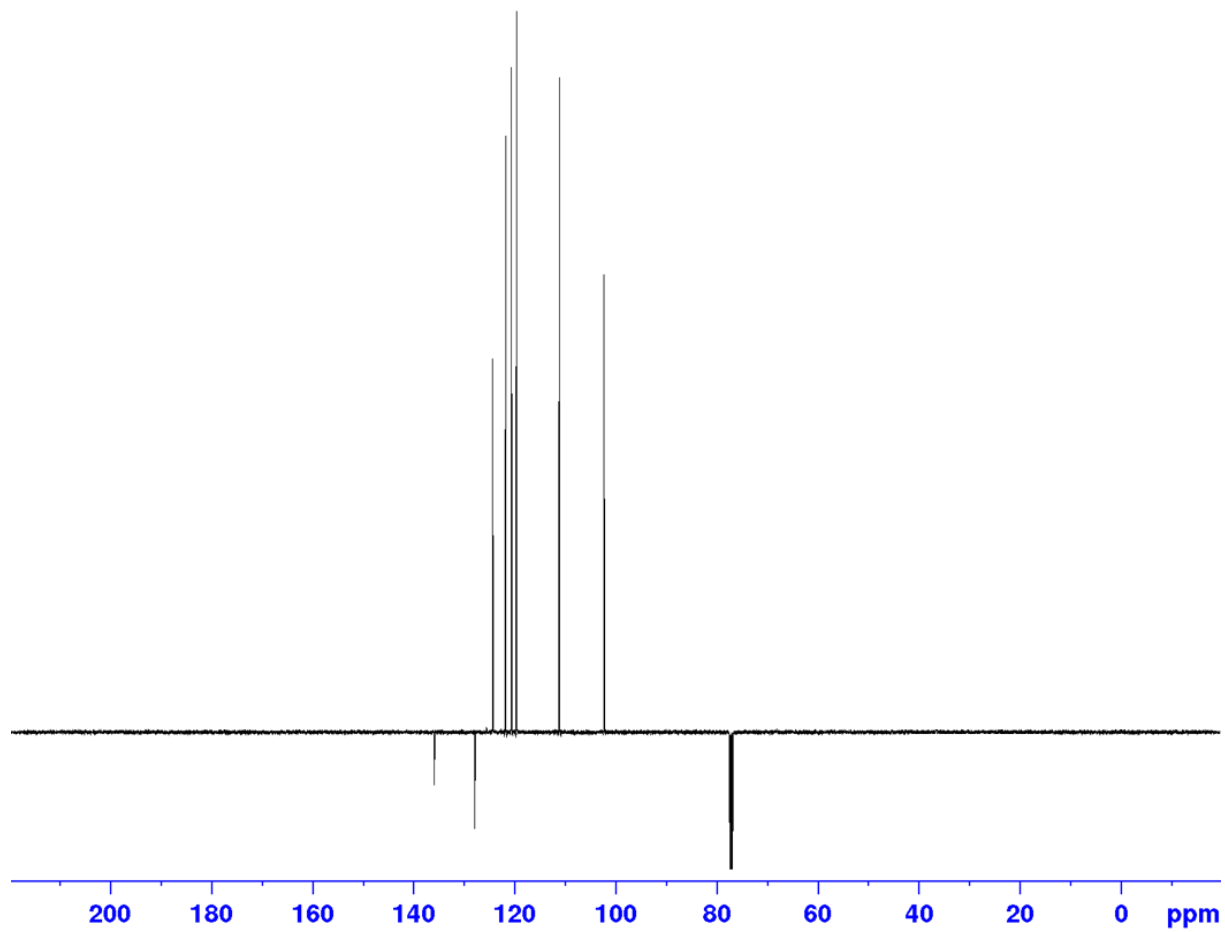
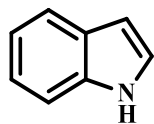


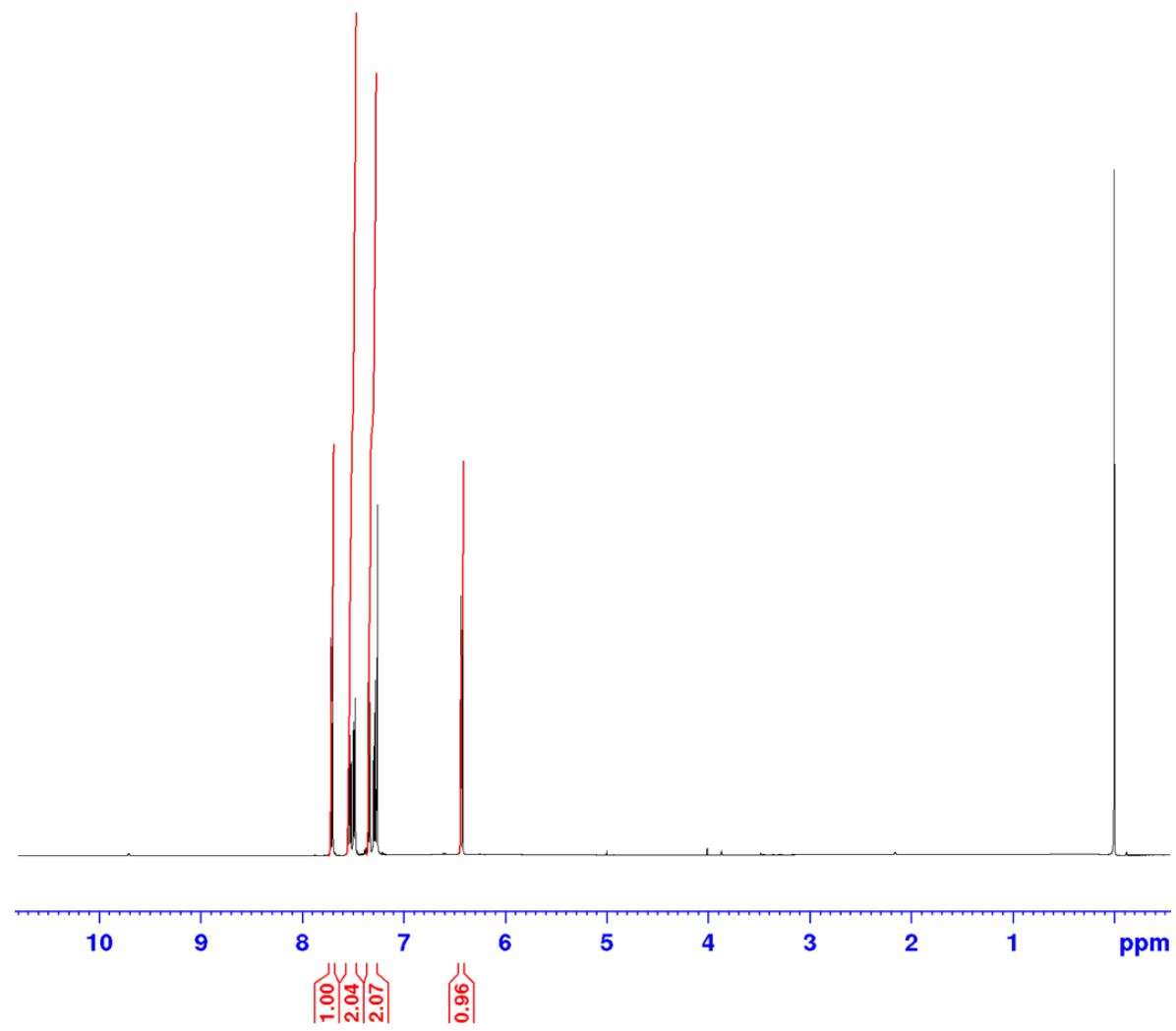
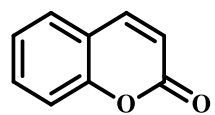


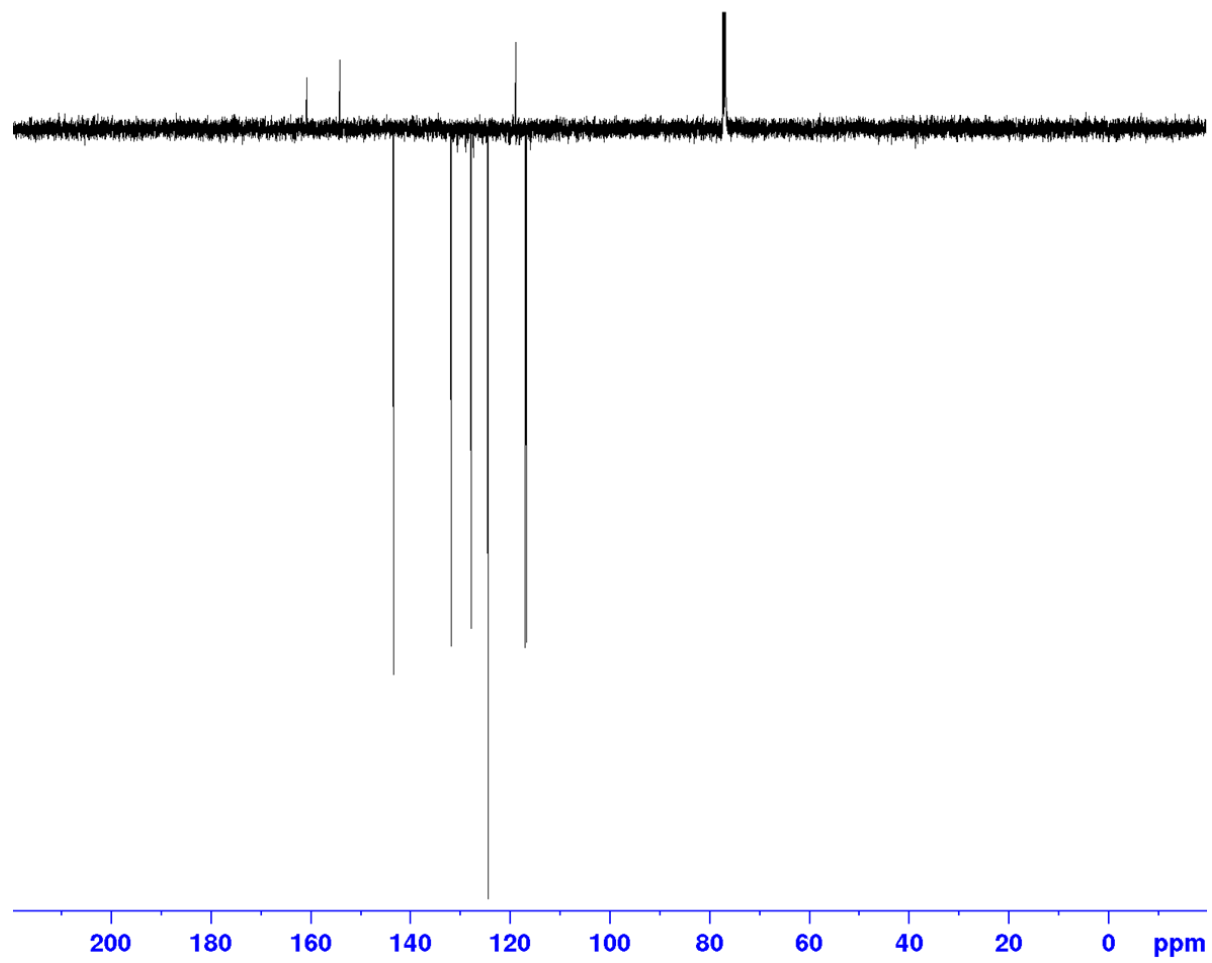
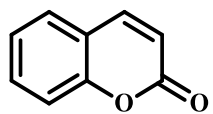


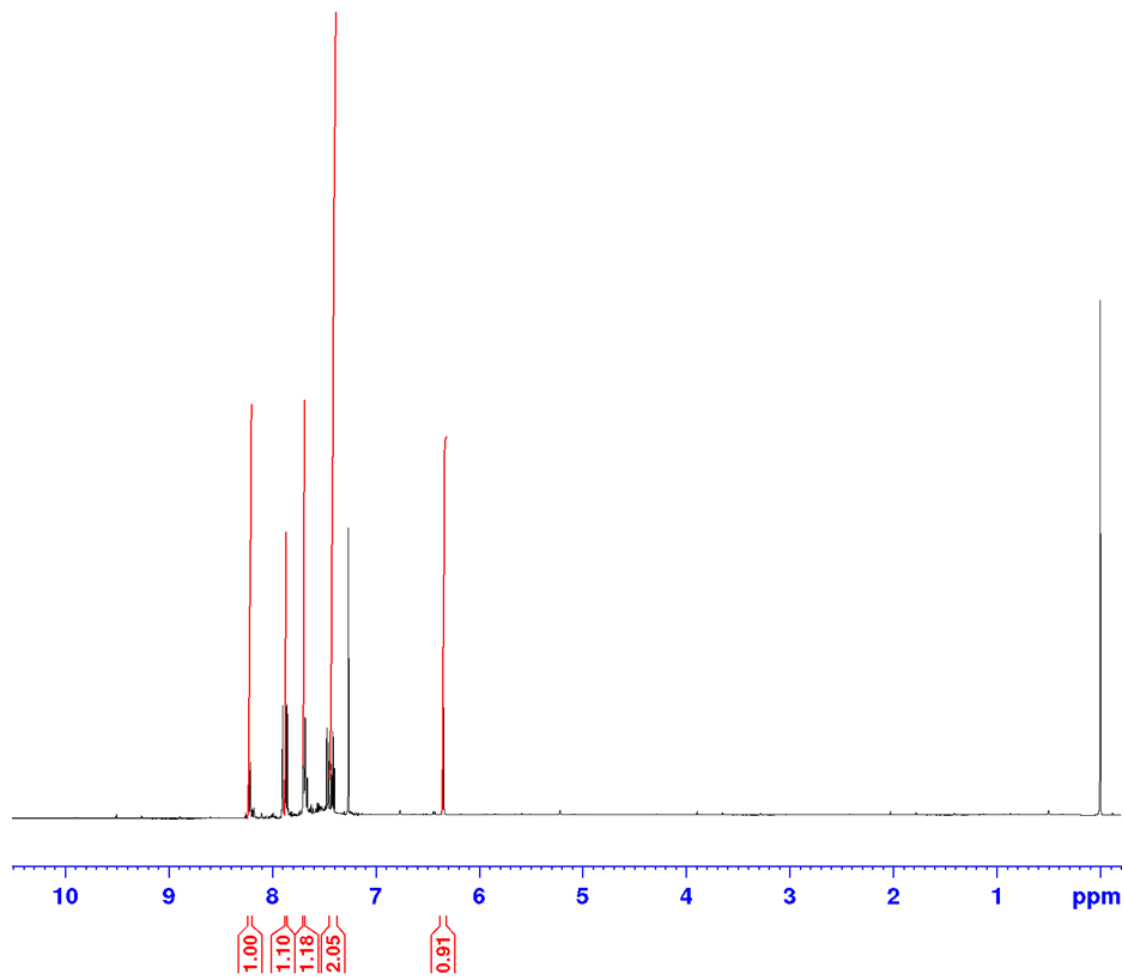
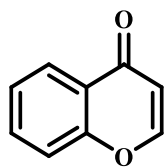


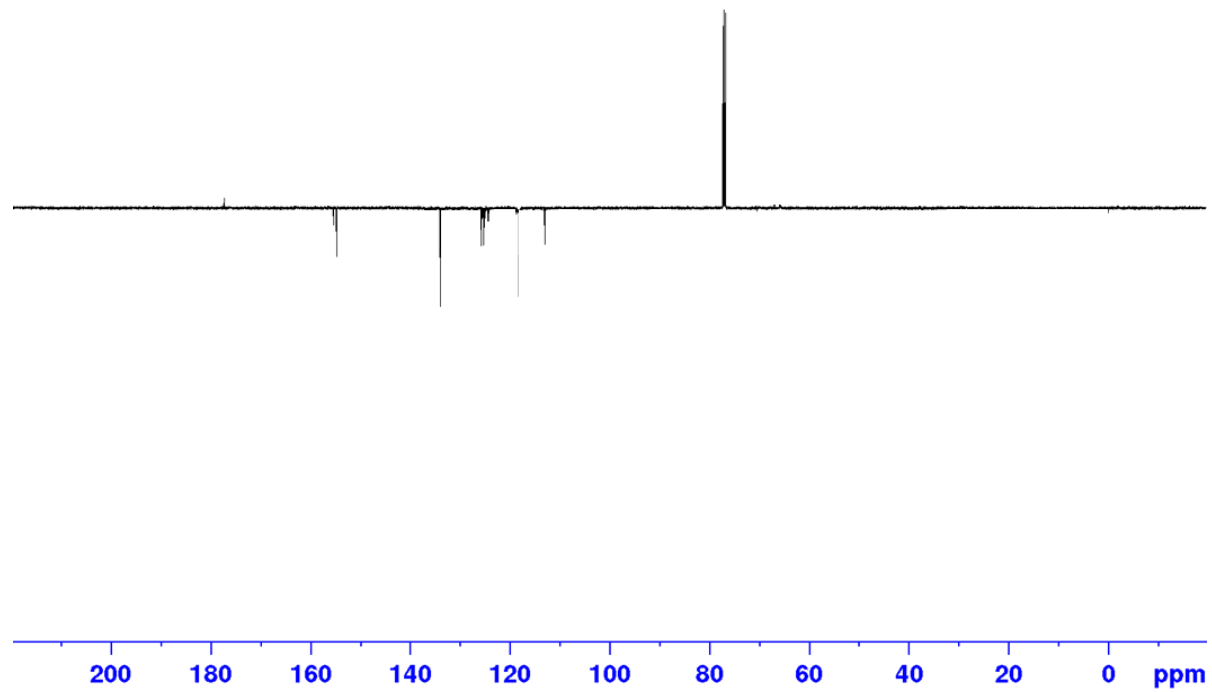
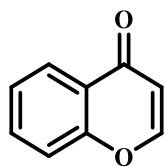


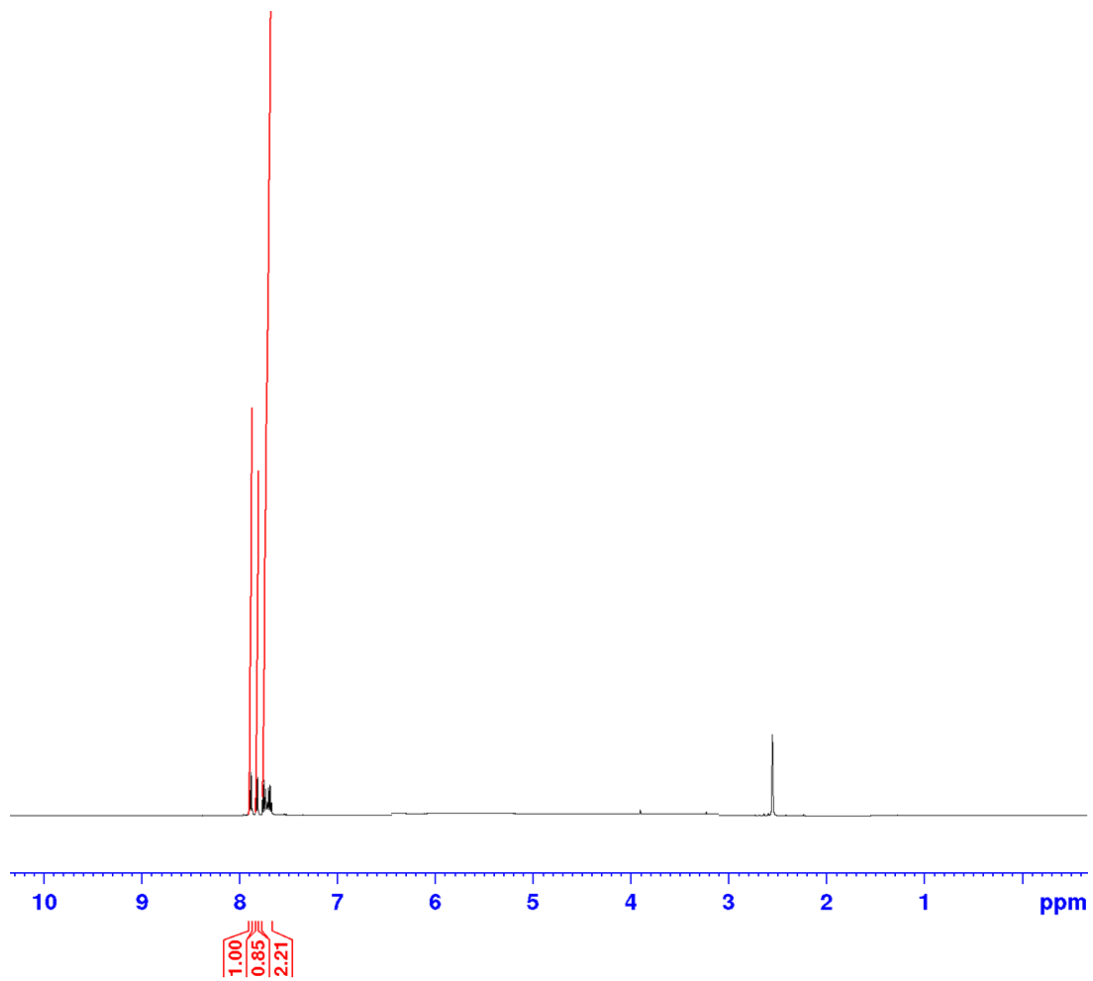
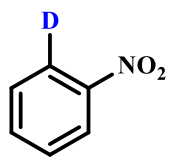


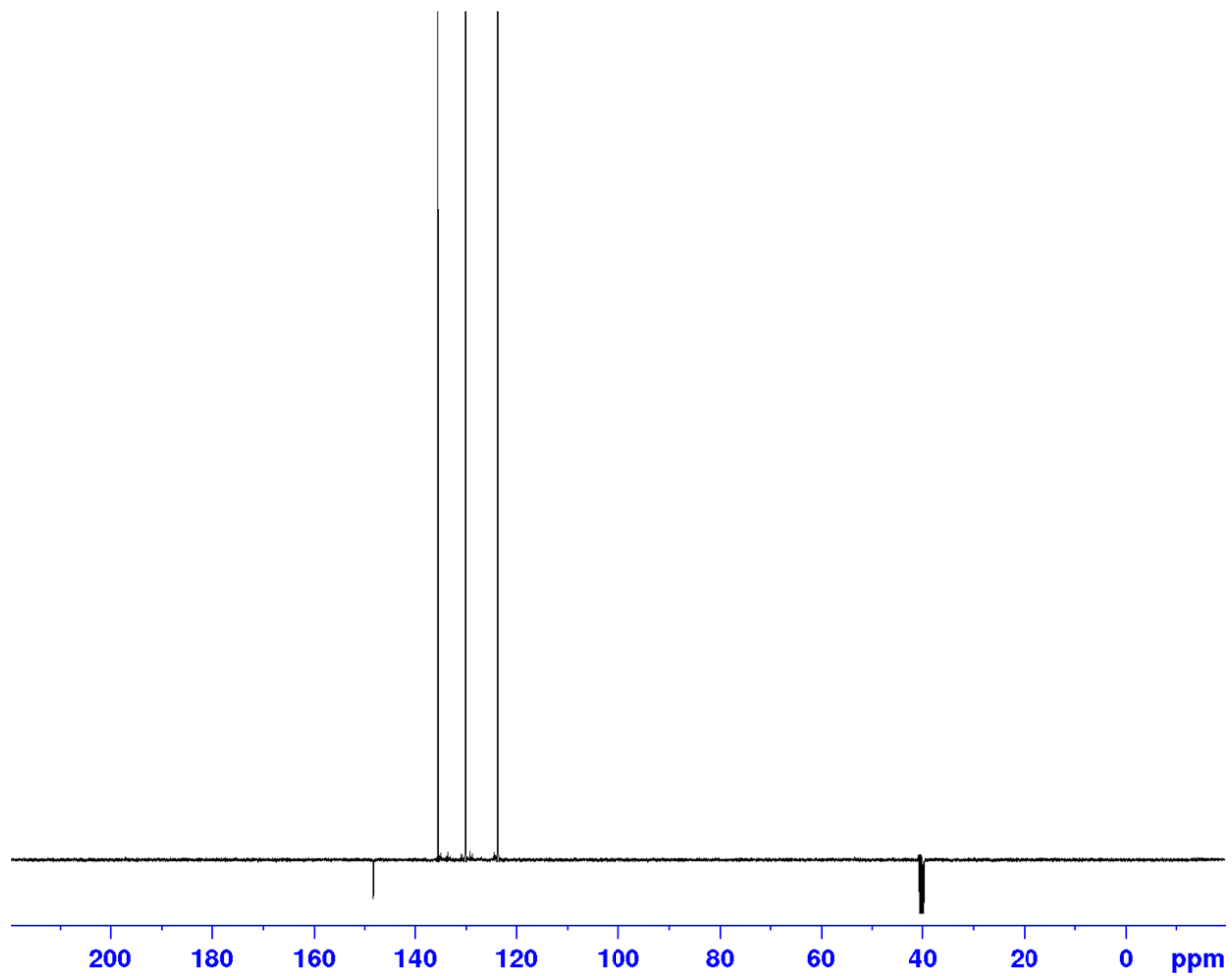
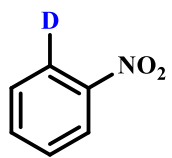


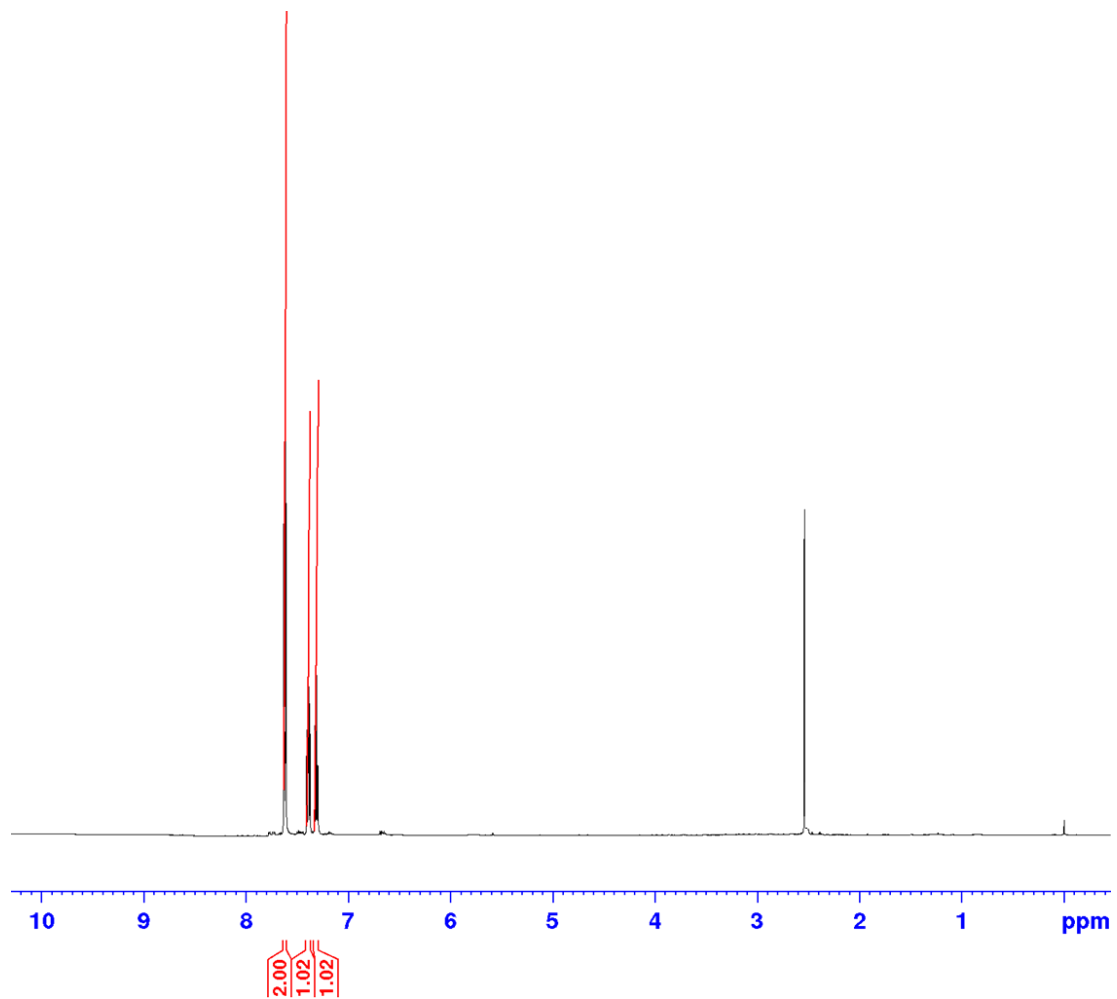
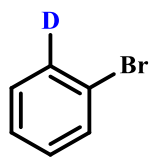


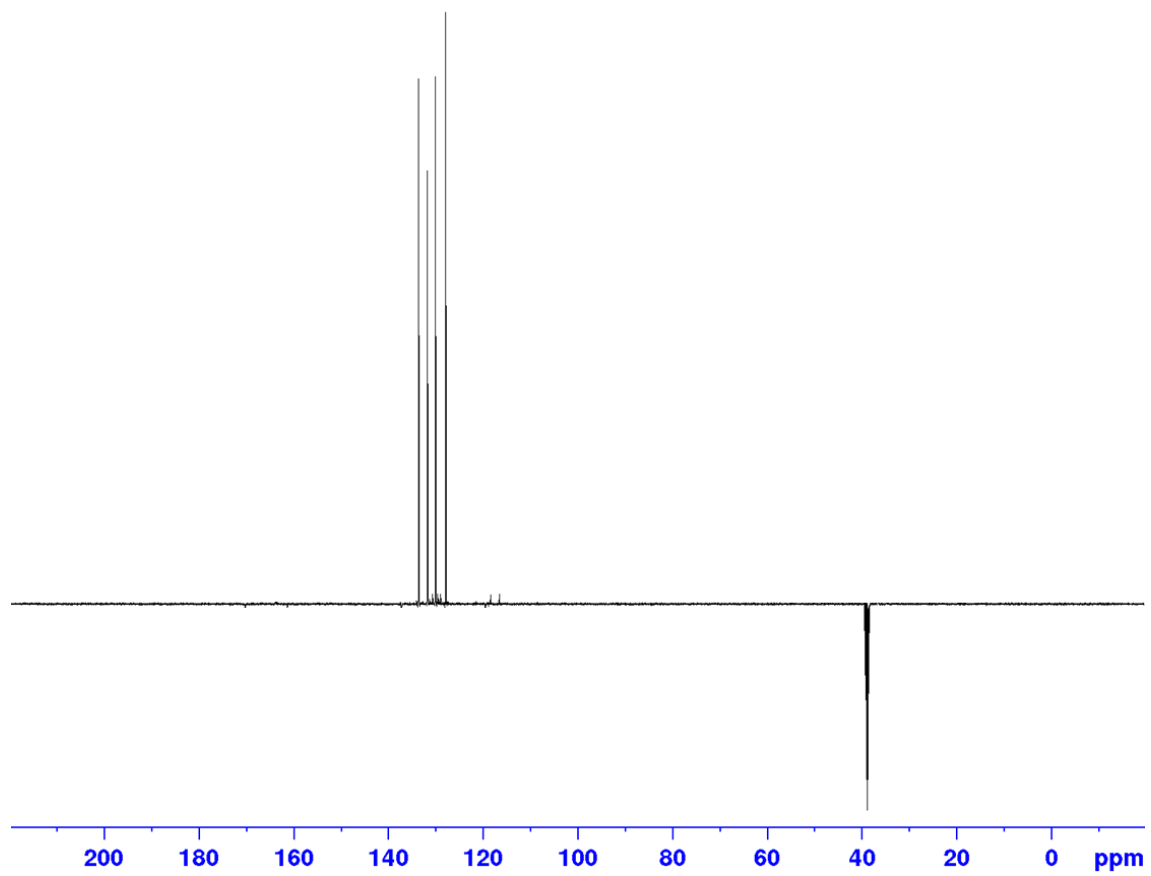
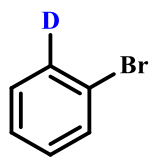


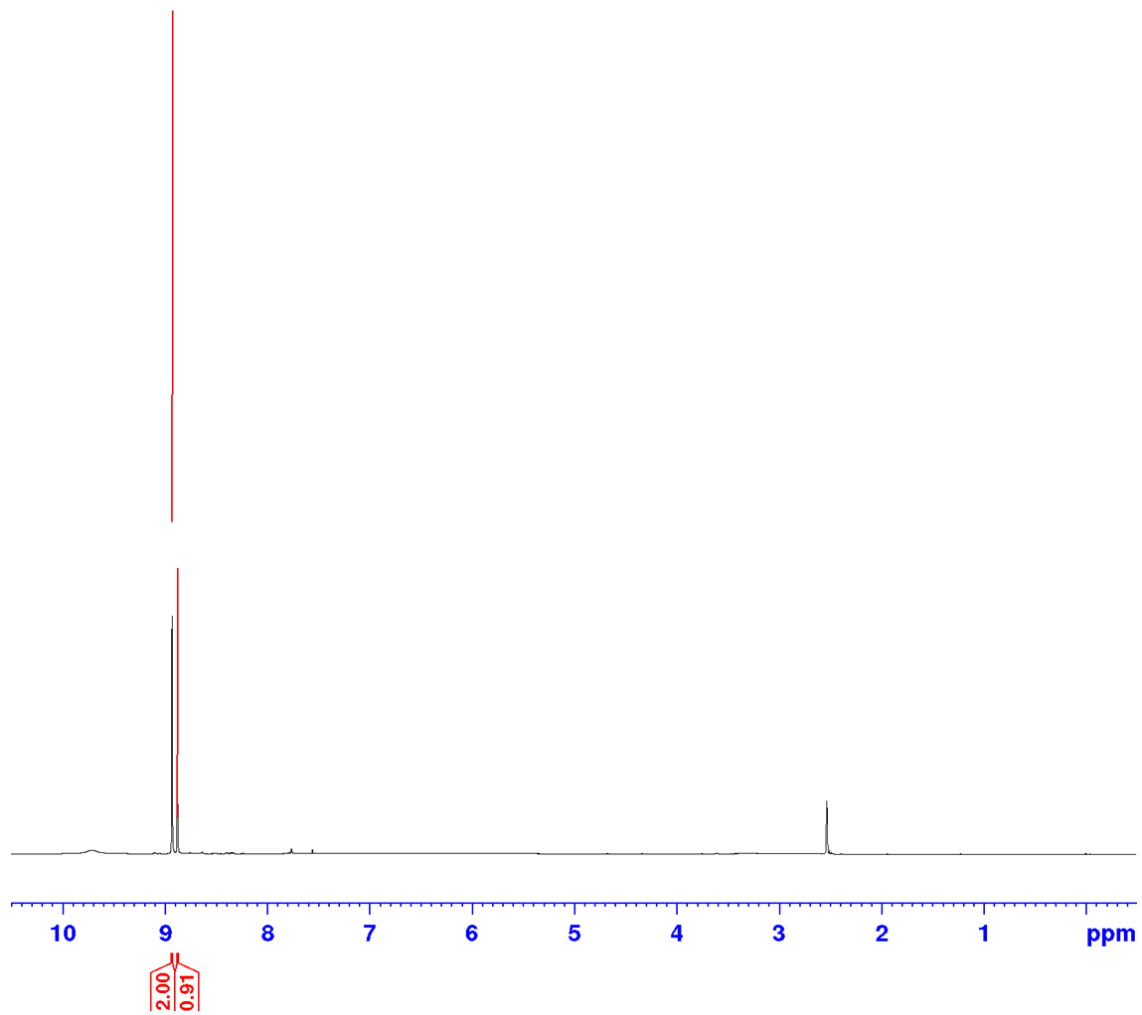
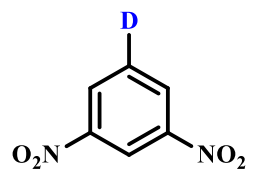


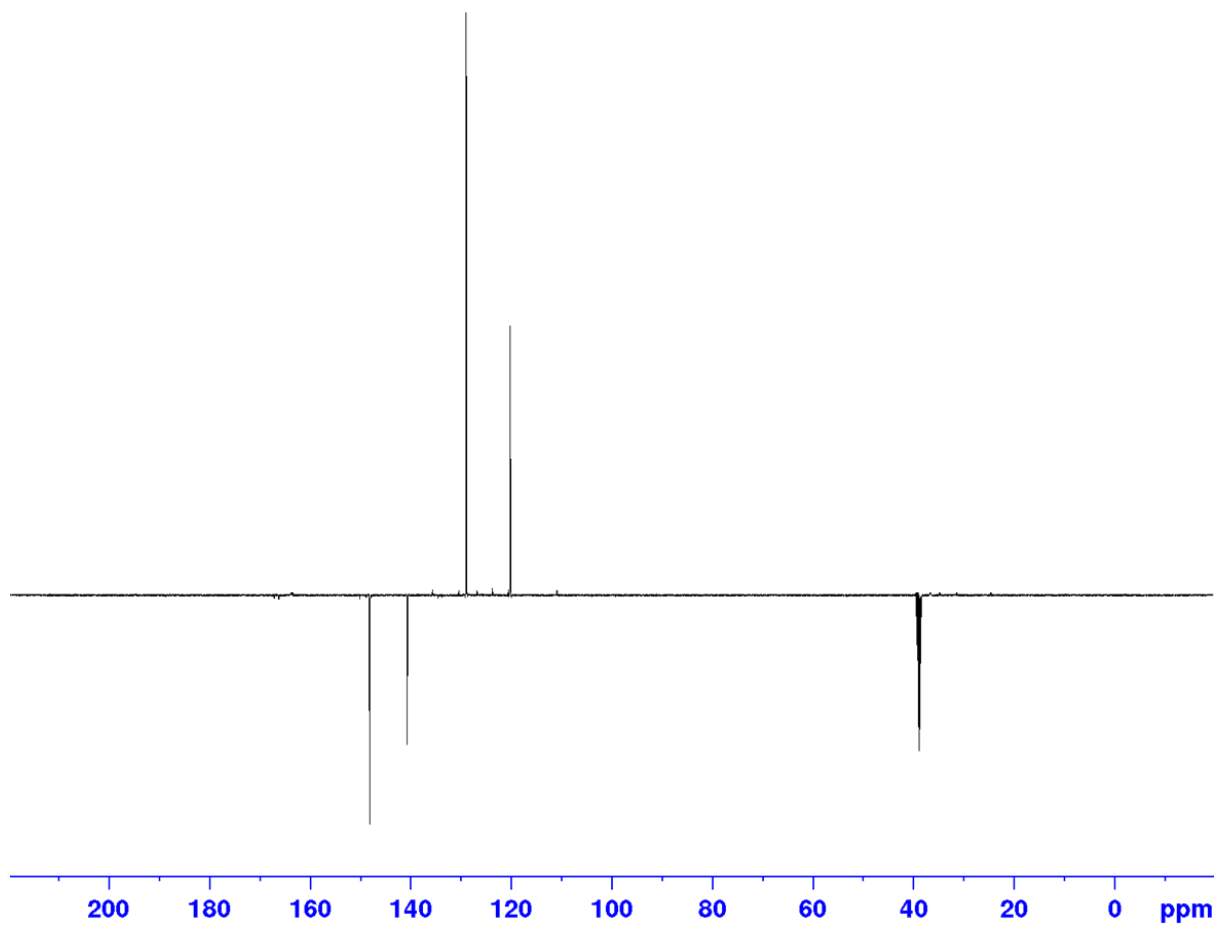
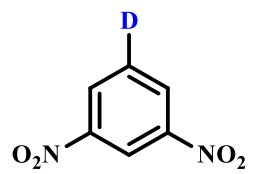


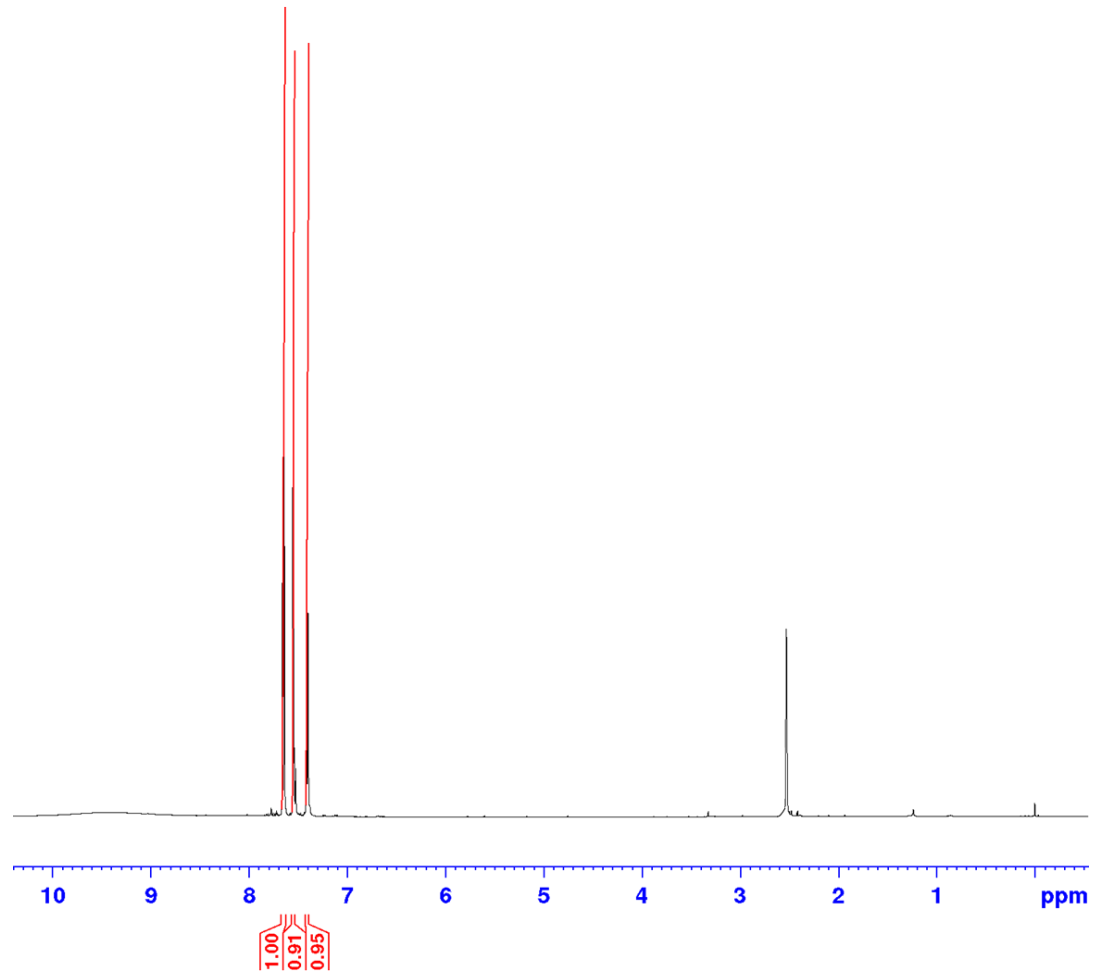
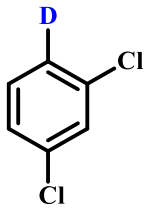


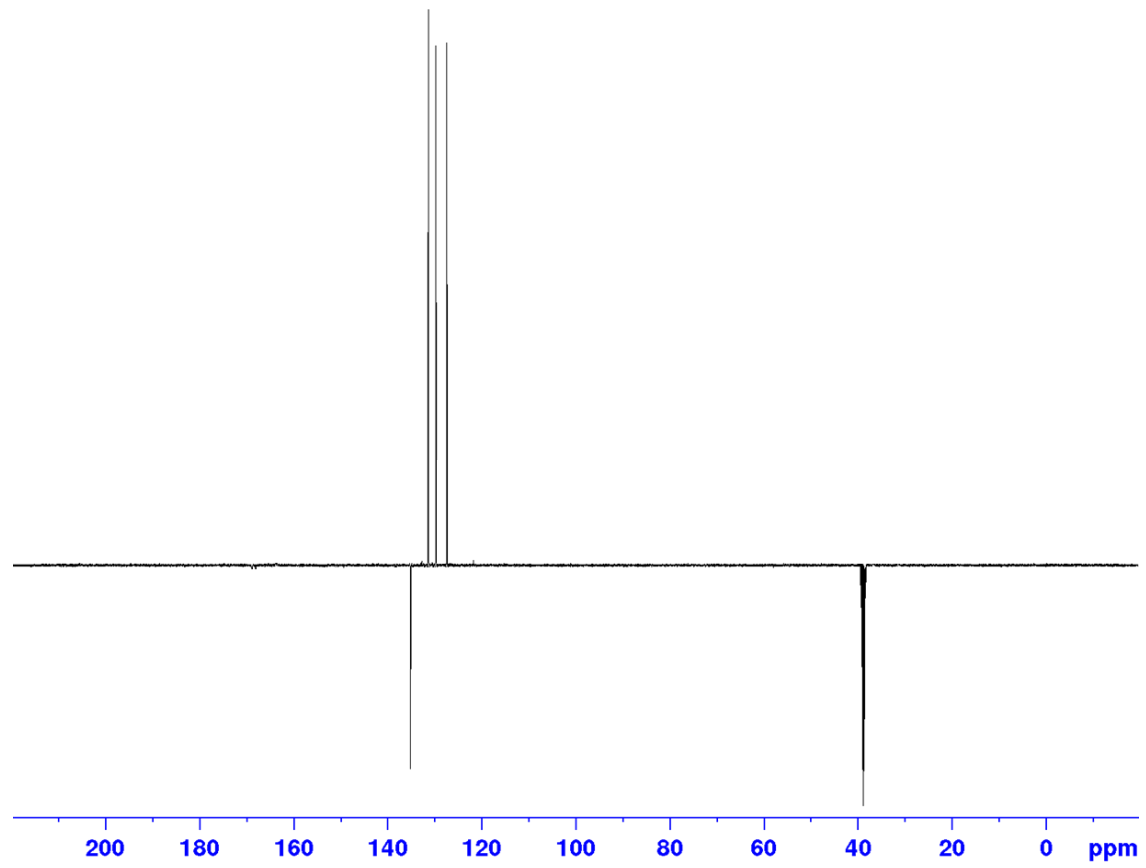
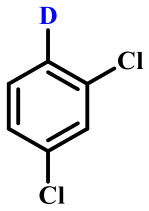


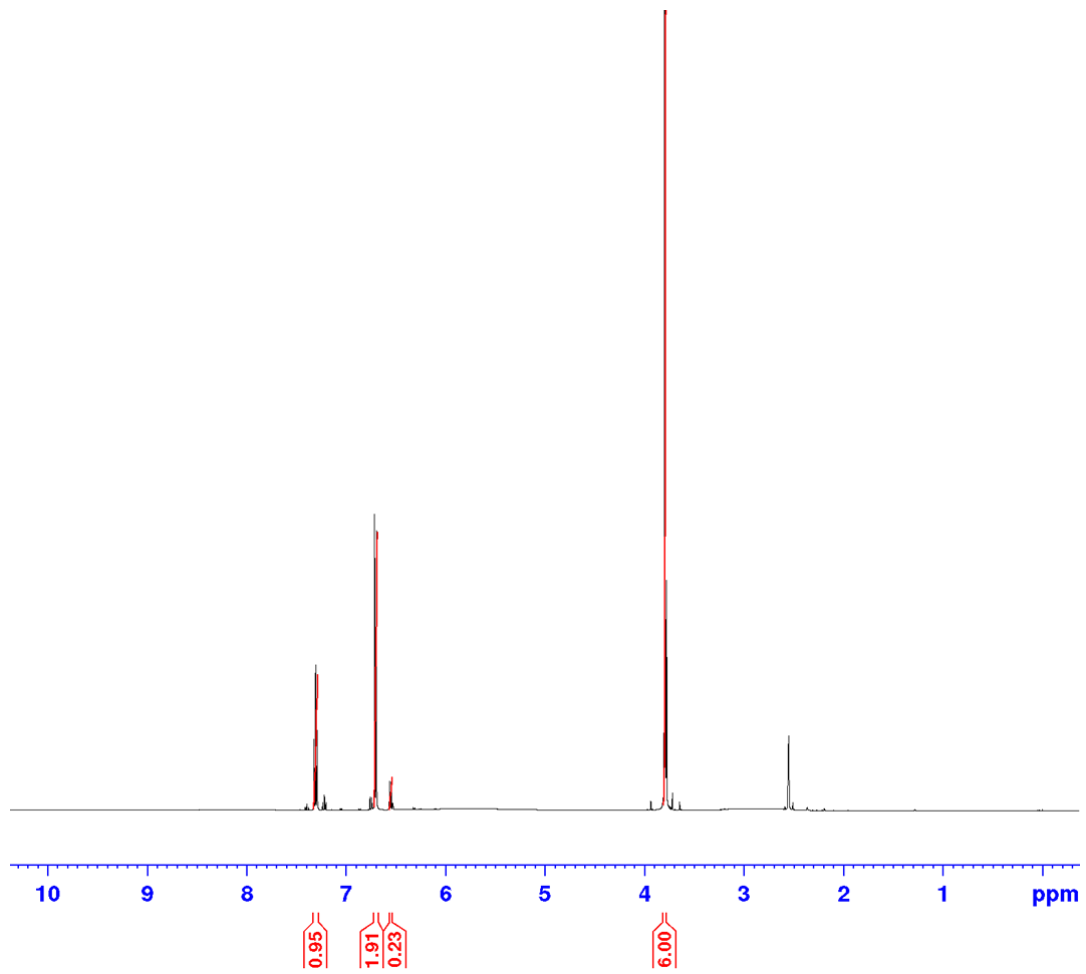
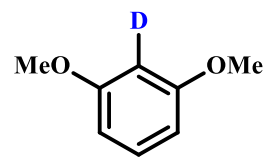


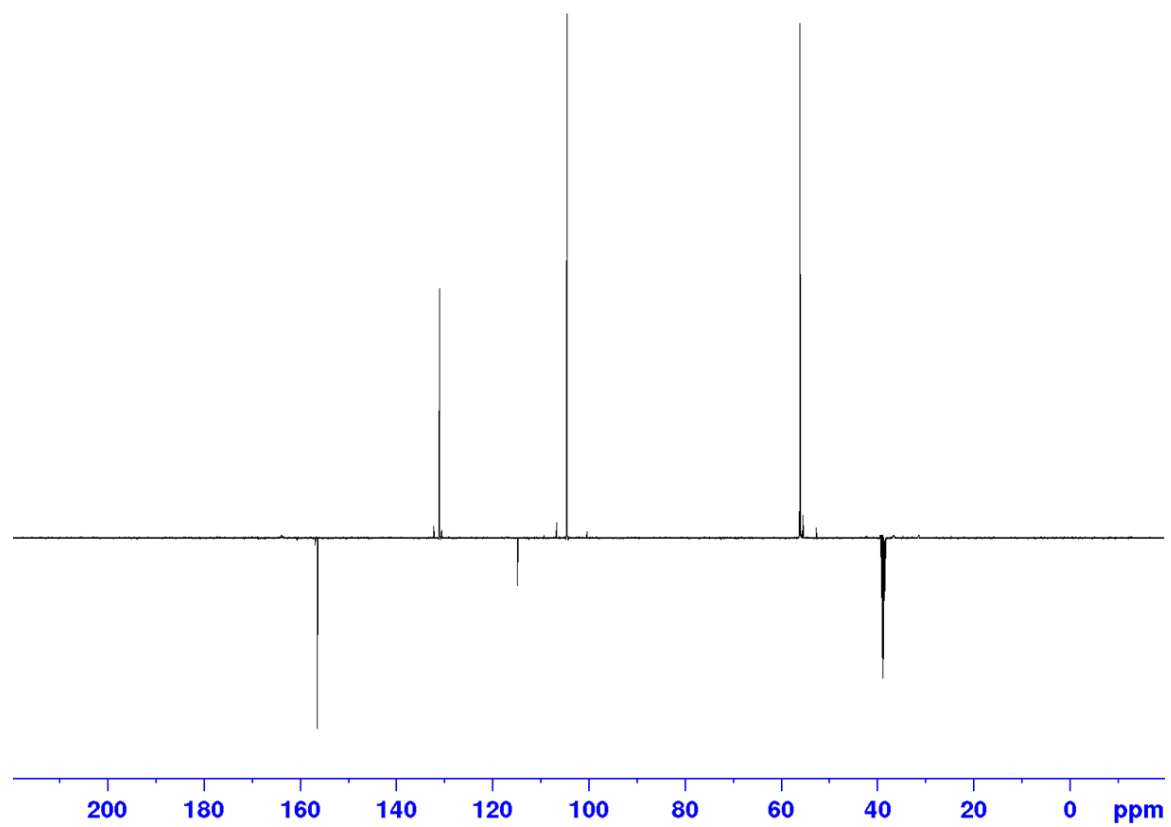
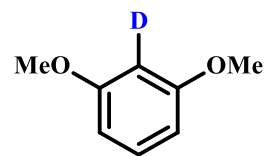


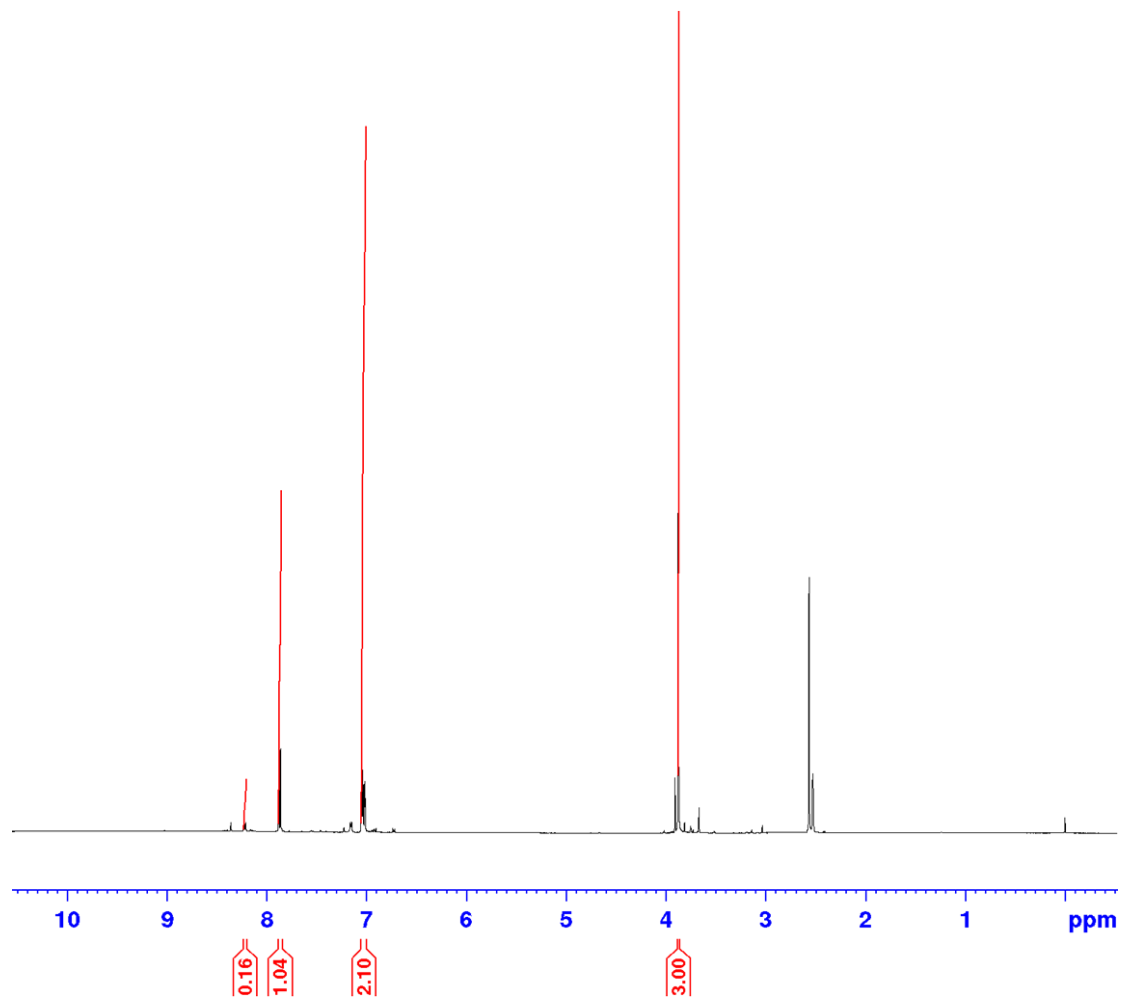
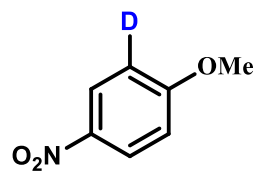


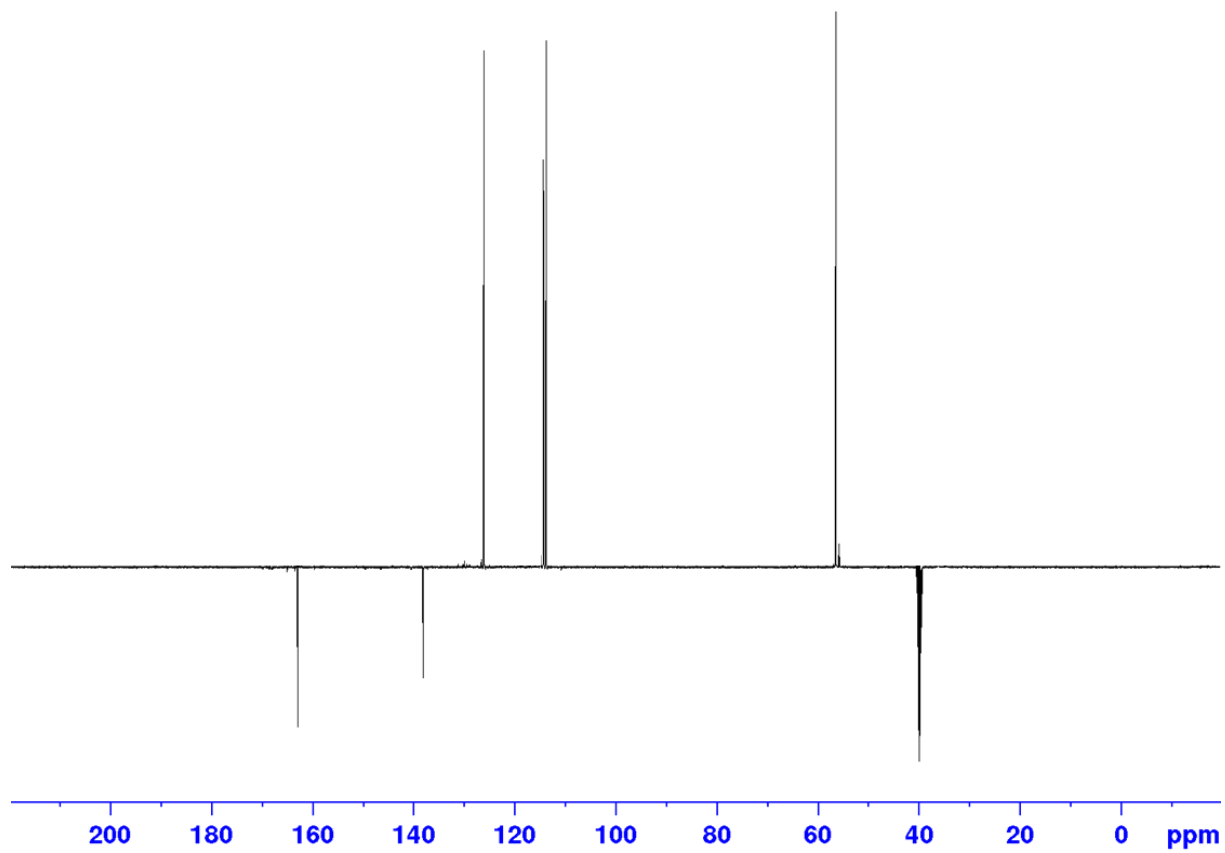
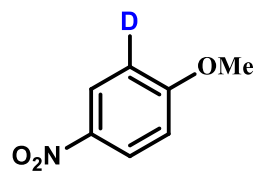


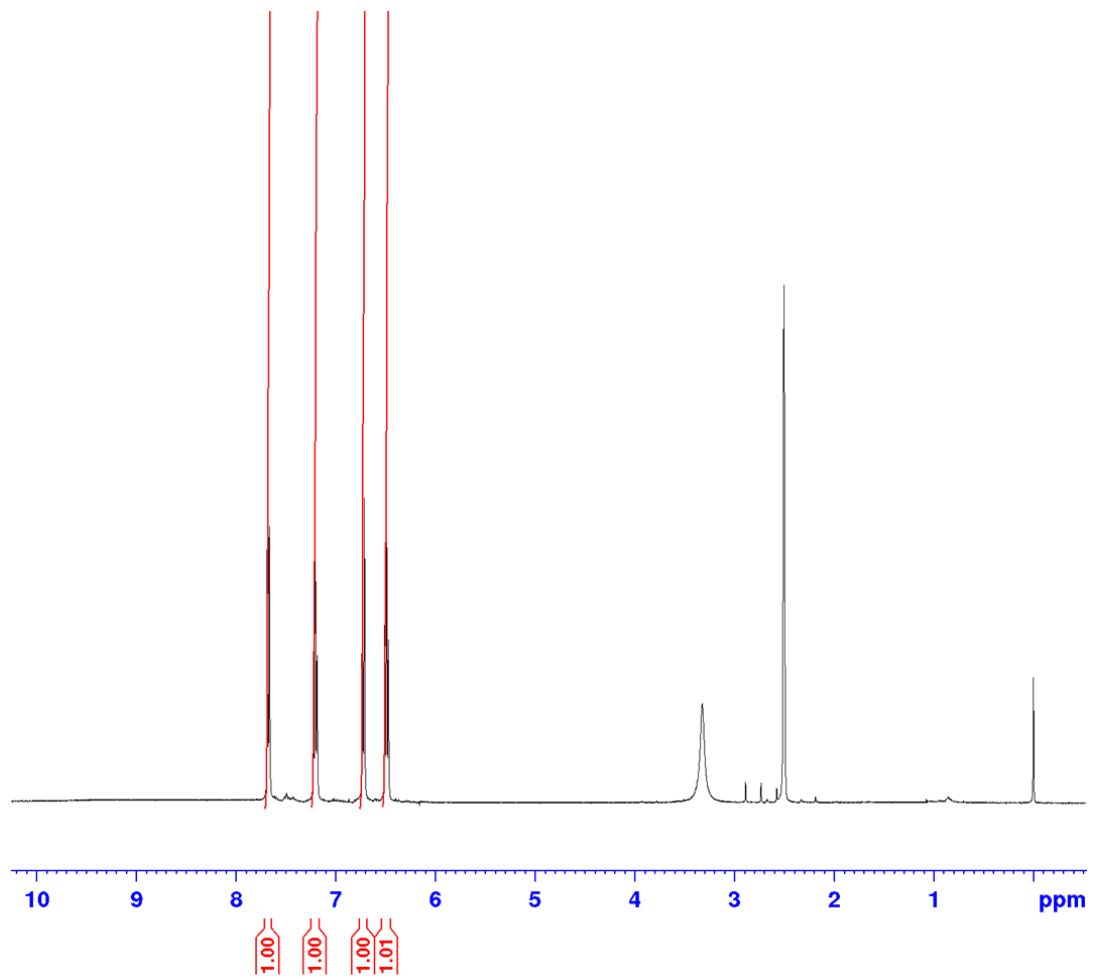
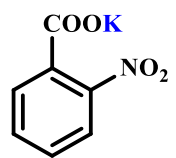












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