Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Exploration of uracils: Pot and step economic production of pyridine core containing templates by multicomponent aza-Diels-Alder reaction

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General information

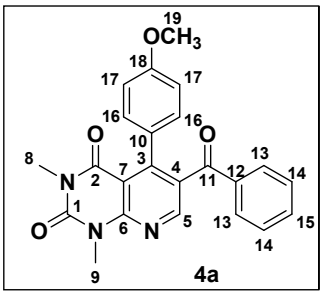
All the commercially available reagents were used as received. Melting points were measured with a Buchi M-560 melting point apparatus and are uncorrected. IR spectra were recorded on a SHIMADZU FTIR-8400 instrument. ^{1}H nuclear magnetic resonance (NMR) spectra were recorded on Avance DPX 300 MHz FT-NMR spectrometer using tetramethylsilane (TMS) as an internal standard. Chemical shifts (δ) are given from TMS (0 ppm) and coupling constants are expressed in Hertz (Hz). ^{13}C NMR spectra were recorded on an Avance DPX 75 MHz FT-NMR spectrometer and Chemical shifts (δ) are given from $CDCl_3$ (77.0 ppm). Mass spectra were recorded on ESQUIRE 3000 Mass spectrometer. All experiments were monitored by thin layer chromatography (TLC). TLC was performed on a pre-coated silica gel plates (Merck). After elution, plate was visualized under UV illumination at 254 nm for UV active materials. Further visualization was achieved by stating $KMnO_4$ and warming in a hot air oven. Column chromatography was performed on silica gel (100-200 mesh, Merck) using ethyl acetate-hexane as eluent.

Experimental data

General procedure for the synthesis of pyrido[2,3-*d*]pyrimidines

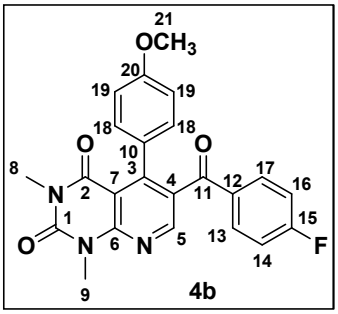
Mixture of vinyl uracil (**1**, 1 mmol), aromatic aldehydes (**2**, 1 mmol) and acetophenones (**3**, 1 mmol) with 10 mol% Na_2CO_3 is vigorously stirred in DMF (5 mL) at 153 ^{o}C under air till the reaction goes to completion. After the reaction is complete, as indicated by TLC, the solvent is distilled off under reduced pressure. The crude product mixture was dissolved in ethyl acetate and directly column chromatographed using ethyl acetate: hexane 1:2 as the eluent to get pure products **4a-4r**.

Characterization data of the Products



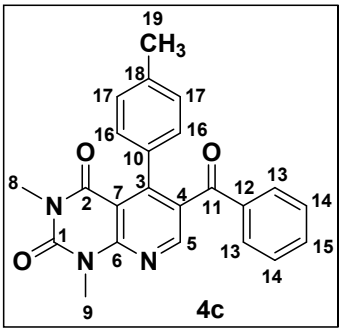
6-benzoyl-5-(4-methoxyphenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4a)

Pale yellow solid; mp 209-211 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.66 (s, 1H, H-5), 7.49-6.69 (m, 9H, ArH), 3.82 (s, 3H, H-19), 3.72 (s, 3H, H-9), 3.38 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.4 (C-11), 162.0 (C-18), 160.2 (C-6), 159.5 (C-2), 152.7 (C-1), 151.3 (C-3), 151.1 (C-5), 137.3 (C-12), 133.3 (C-10), 132.9 (C-15), 129.8 (C-13), 129.3 (C-16), 128.2 (C-14), 127.8 (C-4), 113.1 (C-17), 107.8 (C-7), 55.0 (C-19), 30.3 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2958.2, 2924.5, 2850.8, 1715.4, 1665.2; MS (GCMS, *m/z*) 401 $[M]^+$; Anal. Calcd. for $C_{23}H_{19}N_3O_4$: C, 68.82; H, 4.77; N, 10.47; O, 15.94. Found: C, 68.80; H, 4.70; N, 10.45; O, 15.91.



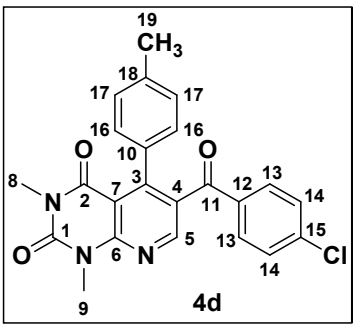
6-(4-fluorobenzoyl)-5-(4-methoxyphenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4b)

Reddish yellow solid; mp 135-137 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.65 (s, 1H, H-5), 7.55-6.71 (m, 8H, ArH), 3.81 (s, 3H, H-21), 3.73 (s, 3H, H-9), 3.38 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 193.9 (C-11), 167.3 (C-15), 163.9 (C-20), 160.2 (C-6), 159.5 (C-2), 152.7 (C-1), 152.4 (C-3), 151.3 (C-5), 133.6 (C-13), 132.6 (C-17), 132.0 (C-10), 131.9 (C-12), 129.8 (C-18), 127.7 (C-4), 115.6 (C-14), 115.3 (C-16), 113.1 (C-19), 107.7 (C-7), 55.1 (C-21), 30.4 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2959.2, 2927.4, 2853.4, 2837.1, 1715.7, 1668.2; MS (GCMS, *m/z*) 419 $[M]^+$; Anal. Calcd. for $C_{23}H_{18}FN_3O_4$: C, 65.87; H, 4.33; N, 10.02; O, 15.26. Found: C, 65.80; H, 4.31; N, 10.00; O, 15.21.



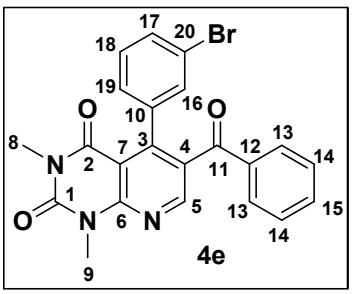
6-benzoyl-1,3-dimethyl-5-*p*-tolylpyrido[2,3-*d*]pyrimidine-2,4-dione (4c)

White solid; mp 183-185 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.65 (s, 1H, H-5), 7.54-6.94 (m, 9H, ArH), 3.81 (s, 3H, H-9), 3.37 (s, 3H, H-8), 2.25 (s, 3H, H-19); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.1 (C-11), 160.1 (C-6), 153.1 (C-2), 152.5 (C-1), 151.3 (C-3), 151.1 (C-5), 138.0 (C-10), 137.3 (C-12), 133.3 (C-4), 132.8 (C-15), 132.7 (C-18), 129.5 (C-13), 128.3 (C-14), 128.2 (C-17), 128.0 (C-16), 107.8 (C-7), 30.3(C-9), 28.6 (C-8), 21.3 (C-19); IR ($CHCl_3$, cm^{-1}) 2923.4, 2850.8, 1716.0, 1666.3; MS (GCMS, *m/z*) 385 $[M]^+$; Anal. Calcd. for $C_{23}H_{19}N_3O_3$: C, 71.67; H, 4.97; N, 10.90; O, 12.45. Found: C, 71.63; H, 4.95; N, 10.88; O, 12.44.



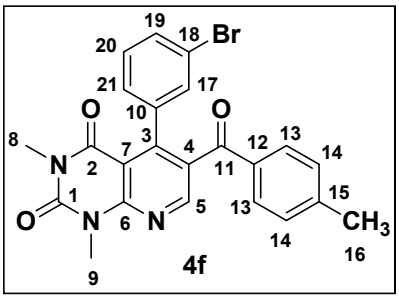
6-(4-chlorobenzoyl)-1,3-dimethyl-5-*p*-tolylpyrido[2,3-*d*]pyrimidine-2,4-dione (4d)[§]

Yellow solid; mp 140-141 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.64 (s, 1H, H-5), 7.56-6.94 (m, 8H, ArH), 3.81 (s, 3H, H-9), 3.37 (s, 3H, H-8), 2.26 (s, 3H, H-21); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 193.7 (C-11), 160.1 (C-6), 152.9 (C-2), 152.6 (C-1), 151.2 (C-3), 151.1 (C-5), 138.2 (C-15), 133.7 (C-10), 132.6 (C-18), 132.4 (C-12), 132.1 (C-17), 132.0 (C-13), 128.3 (C-13), 128.1 (C-14), 115.6 (C-16), 115.3 (C-17), 107.8 (C-7), 30.3 (C-9), 28.6 (C-8), 21.3 (C-19); IR ($CHCl_3$, cm^{-1}) 2924.2, 2851.9, 1716.6, 1667.4, 1583.1; MS (GCMS, *m/z*) 419 $[M]^+$; Anal. Calcd. for $C_{23}H_{18}ClN_3O_3$: C, 65.79; H, 4.32; N, 10.01; O, 11.43. Found: C, 65.78; H, 4.30; N, 10.01; O, 11.39.



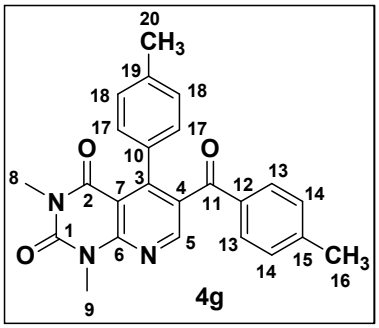
6-benzoyl-5-(3-bromophenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4e)

White solid; mp 232-234 °C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.64 (s, 1H, H-5), 7.41-6.91 (m, 9H, ArH), 3.74 (s, 3H, H-9), 3.29 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.7 (C-11), 159.9 (C-6), 152.6 (C-2), 151.8 (C-1), 151.0 (C-3), 150.9 (C-5), 137.7 (C-10), 137.2 (C-16), 133.5 (C-12), 132.3 (C-15), 131.2 (C-18), 131.1 (C-17), 129.3 (C-13), 129.0 (C-19), 128.3 (C-14), 126.7 (C-20), 121.6 (C-4), 107.5 (C-7), 30.3 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2923.3, 2852.9, 1713.1, 1667.3; MS (GCMS, *m/z*) 449 $[M]^+$; Anal. Calcd. for $C_{22}H_{16}BrN_3O_3$: C, 58.68; H, 3.58; N, 9.33; O, 10.66. Found: C, 58.60; H, 3.55; N, 9.32; O, 10.65.



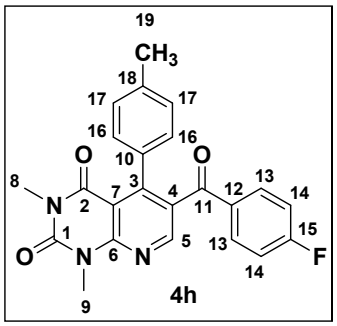
5-(3-bromophenyl)-1,3-dimethyl-6-(4-methylbenzoyl)pyrido[2,3-*d*]pyrimidine-2,4-dione (4f)

Pale yellow solid; mp 265-267 °C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.63 (s, 1H, H-5), 7.36-6.94 (m, 8H, ArH), 3.74 (s, 3H, H-9), 3.30 (s, 3H, H-8), 2.30 (s, 3H, H-16); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.2 (C-11), 159.9 (C-6), 152.4 (C-2), 151.6 (C-1), 151.0 (C-3), 150.8 (C-5), 144.7 (C-15), 137. (C-10), 134.7 (C-17), 132.5 (C-20), 131.0 (C-19), 129.8 (C-13), 129.5 (C-14), 129.1 (C-12), 127.7 (C-21), 126.6 (C-18), 121.5 (C-4), 107.6 (C-7), 30.3 (C-9), 28.6 (C-8), 21.7 (C-16); IR ($CHCl_3$, cm^{-1}) 2922.9, 2852.9, 1712.9, 1676.9; MS (GCMS, *m/z*) 463 $[M]^+$; Anal. Calcd. for $C_{23}H_{18}BrN_3O_3$: C, 59.50; H, 3.91; N, 9.05; O, 10.34. Found: C, 59.48; H, 3.90; N, 9.00; O, 10.31.



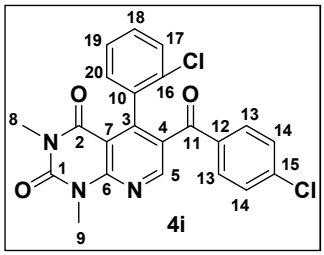
1,3-dimethyl-6-(4-methylbenzoyl)-5-*p*-tolylpyrido[2,3-*d*]pyrimidine-2,4-dione (4g)

White solid; mp 178-179 °C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.56 (s, 1H, H-5), 7.41-6.88 (m, 8H, ArH), 3.74 (s, 3H, H-9), 3.30 (s, 3H, H-8), 2.29 (s, 3H, H-16), 2.19 (s, 3H, H-20); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.5 (C-11), 160.2 (C-6), 153.1 (C-2), 152.4 (C-1), 151.2 (C-3), 151.1 (C-5), 144.5 (C-15), 137.9 (C-10), 134.7 (C-19), 132.9 (C-12), 132.8 (C-4), 129.8 (C-13), 129.0 (C-17), 128.3 (C-18), 127.9 (C-14), 108.0 (C-7), 30.3 (C-9), 28.6 (C-8), 21.7 (C-16), 21.3 (C-20); IR ($CHCl_3$, cm^{-1}) 2923.5, 2850.8, 1716.3, 1668.9; MS (GCMS, *m/z*) 399 $[M]^+$; Anal. Calcd. for $C_{24}H_{21}N_3O_3$: C, 72.16; H, 5.30; N, 10.52; O, 12.02. Found: C, 72.13.48; H, 5.27; N, 10.51; O, 12.00.



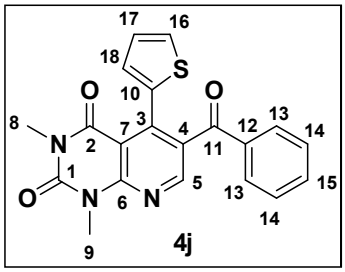
6-(4-fluorobenzoyl)-1,3-dimethyl-5-*p*-tolylpyrido[2,3-*d*]pyrimidine-2,4-dione (4h)

White solid; mp 170-173 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.64 (s, 1H, H-5), 7.46-6.93 (m, 8H, ArH), 3.81 (s, 3H, H-9), 3.37 (s, 3H, H-8), 2.26 (s, 3H, H-19); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.0 (C-11), 160.1 (C-15), 153.0 (C-6), 152.7 (C-2), 151.3 (C-1), 151.1 (C-3), 149.8 (C-5), 138.3 (C-10), 135.6 (C-18), 132.6 (C-12), 132.3 (C-4), 130.7 (C-13), 128.5 (C-17), 128.4 (C-16), 128.1 (C-14), 107.8 (C-7), 30.3 (C-9), 28.6 (C-8), 21.3 (C-19); IR ($CHCl_3$, cm^{-1}) 2924.6, 2851.9, 1716.6, 1669.6; MS (GCMS, *m/z*) 403 $[M]^+$; Anal. Calcd. for $C_{23}H_{18}FN_3O_3$: C, 68.48; H, 4.50; N, 10.42; O, 11.90. Found: C, 68.40; H, 4.46; N, 10.38; O, 11.87.



6-(4-chlorobenzoyl)-5-(2-chlorophenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4i)

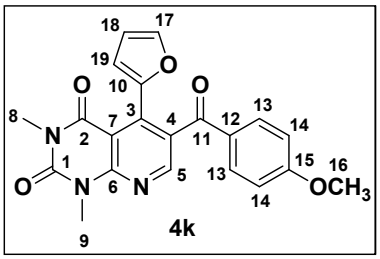
Yellowish orange solid; mp 193-195 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.74 (s, 1H, H-5), 7.55-7.05 (m, 8H, ArH), 3.82 (s, 3H, H-9), 3.38 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 193.2 (C-11), 159.8 (C-6), 152.5 (C-2), 152.4 (C-1), 151.0 (C-3), 149.5 (C-5), 140.0 (C-15), 135.3 (C-10), 134.8 (C-16), 132.1 (C-12), 131.3 (C-18), 130.7 (C-13), 129.8 (C-17), 129.2 (C-20), 128.9 (C-19), 128.6 (C-14), 126.4 (C-4), 108.3 (C-7), 30.3 (C-9), 28.7 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.6, 2853.3, 1717.6, 1668.2; MS (GCMS, *m/z*) 439 $[M]^+$; Anal. Calcd. for $C_{22}H_{15}Cl_2N_3O_3$: C, 60.02; H, 3.43; N, 9.54; O, 10.90. Found: C, 60.00; H, 3.41; N, 9.53; O, 10.87.



6-benzoyl-1,3-dimethyl-5-(thiophen-2-yl)pyrido[2,3-*d*]pyrimidine-2,4-dione (4j)

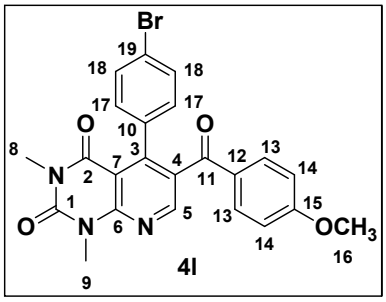
White solid; mp 210-211 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.67 (s, 1H, H-8), 7.56-6.84 (m, 8H), 3.81 (s, 3H, H-12), 3.40 (s, 3H, H-11); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.8 (C-11), 159.8 (C-6), 152.6 (C-2), 151.4

(C-1), 151.0 (C-5), 145.4 (C-3), 136.9 (C-10), 135.4 (C-12), 133.6 (C-15), 133.4 (C-16), 129.7 (C-13), 128.8 (C-17), 128.2 (C-14), 128.0 (C-16), 126.4 (C-4), 108.3 (C-7), 30.4 (C-9), 28.7 (C-8); IR ($CHCl_3$, cm^{-1}) 2923.8, 2853.6, 1714.8, 1663.8; MS (GCMS, *m/z*) 377 $[M]^+$; Anal. Calcd. for $C_{20}H_{15}N_3O_3S$: C, 63.65; H, 4.01; N, 11.13; O, 12.72. Found: C, 63.60; H, 4.00; N, 11.10; O, 12.69.



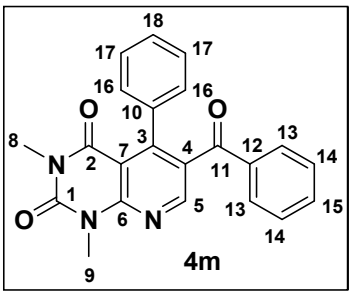
5-(furan-2-yl)-6-(4-methoxybenzoyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4k)

White solid; mp 168-169 °C; ^1H NMR ($CDCl_3$, 300 MHz) δ 8.58 (s, 1H, H-5), 7.37-6.63 (m, 7H, ArH), 3.74 (s, 3H, H-16), 3.66 (s, 3H, H-9), 3.30 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.3 (C-11), 160.1 (C-15), 159.6 (C-6), 152.8 (C-2), 152.5 (C-1), 151.3 (C-10), 151.1 (C-5), 139.7 (C-3), 135.6 (C-17), 132.4 (C-12), 130.6 (C-13), 129.9 (C-14), 128.5 (C-19), 127.6 (C-4), 113.1 (C-18), 107.7 (C-7), 55.1 (C-16), 30.4 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.3, 2853.0, 1715.8, 1666.7; MS (GCMS, *m/z*) 391 $[M]^+$; Anal. Calcd. for $C_{21}H_{17}N_3O_5$: C, 64.45; H, 4.38; N, 10.74; O, 20.44. Found: C, 64.40; H, 4.35; N, 10.70; O, 20.39.



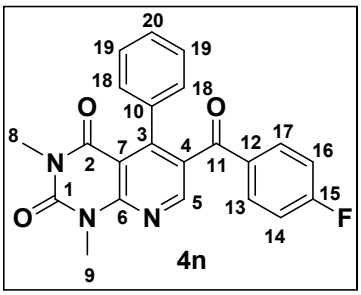
5-(4-bromophenyl)-6-(4-methoxybenzoyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4l)

White solid; mp 216-217 °C; ^1H NMR ($CDCl_3$, 300 MHz) δ 8.63 (s, 1H, H-5), 7.57-6.82 (m, 8H, ArH), 3.85 (s, 3H, H-16), 3.81 (s, 3H, H-9), 3.37 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 192.8 (C-11), 164.1 (C-15), 160.2 (C-6), 152.3 (C-2), 151.3 (C-1), 151.2 (C-3), 151.0 (C-5), 134.8 (C-10), 132.6 (C-12), 132.1 (C-13), 130.8 (C-17), 130.0 (C-19), 129.5 (C-18), 122.6 (C-4), 113.8 (C-14), 107.7 (C-7), 55.6 (C-16), 30.3 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.6, 2853.4, 1715.8, 1596.5, 1579.2; MS (GCMS, *m/z*) 479 $[M]^+$; Anal. Calcd. for $C_{23}H_{18}BrN_3O_4$: C, 57.51; H, 3.78; N, 8.75; O, 13.32. Found: C, 57.48; H, 3.71; N, 8.70; O, 13.30.



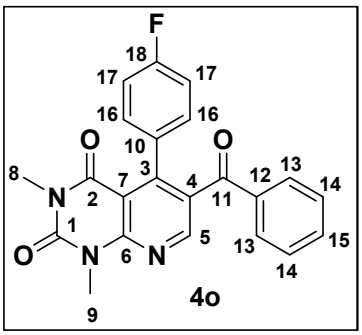
6-benzoyl-1,3-dimethyl-5-phenylpyrido[2,3-*d*]pyrimidine-2,4-dione (4m)

White solid; mp 238-240 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.61 (s, 1H, H-5), 7.45-7.00 (m, 10H, ArH), 3.75 (s, 3H, H-9), 3.29 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.1 (C-11), 160.1 (C-6), 152.7 (C-2), 152.5 (C-1), 151.4 (C-3), 151.1 (C-5), 137.3 (C-10), 135.7 (C-12), 133.4 (C-15), 132.6 (C-4), 129.4 (C-18), 128.3 (C-13), 128.2 (C-14), 128.1 (C-17), 127.4 (C-16), 107.7 (C-7), 30.3 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.2, 2850.8, 1715.0, 1659.9; MS (GCMS, *m/z*) 371 $[M]^+$; Anal. Calcd. for $C_{22}H_{17}N_3O_3$: C, 71.15; H, 4.61; N, 11.31; O, 12.92. Found: C, 71.09; H, 4.57; N, 11.30; O, 12.90.



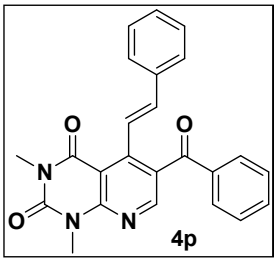
6-(4-fluorobenzoyl)-1,3-dimethyl-5-phenylpyrido[2,3-*d*]pyrimidine-2,4-dione (4n)

White solid; mp 212-213 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.61 (s, 1H, H-5), 7.45-6.78 (m, 9H, ArH), 3.74 (s, 3H, H-9), 3.29 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.0 (C-11), 164.0 (C-15), 160.1 (C-6), 152.6 (C-2), 151.7 (C-1), 151.5 (C-3), 151.0 (C-5), 137.2 (C-10), 133.6 (C-13), 132.6 (C-12), 131.6 (C-17), 130.1 (C-20), 130.0 (C-4), 129.4 (C-19), 128.4 (C-18), 114.9 (C-14), 114.6 (C-16), 107.8 (C-7), 30.4 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.1, 2853.3, 1716.1, 1665.7; MS (GCMS, *m/z*) 389 $[M]^+$; Anal. Calcd. for $C_{22}H_{16}FN_3O_3$: C, 67.86; H, 4.14; N, 10.79; O, 12.33. Found: C, 67.80; H, 4.11; N, 10.70; O, 12.32.



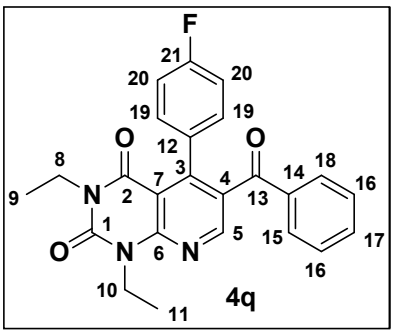
6-benzoyl-5-(4-fluorophenyl)-1,3-dimethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4o)

Off white solid; mp 211-213 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.70 (s, 1H, H-5), 7.50-7.07 (m, 9H, ArH), 3.82 (s, 3H, H-9), 3.37 (s, 3H, H-8); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.0 (C-11), 160.1 (C-18), 152.7 (C-6), 152.5 (C-2), 151.4 (C-1), 151.1 (C-3), 144.8 (C-5), 137.3 (C-10), 135.7 (C-15), 133.4 (C-12), 129.4 (C-13), 128.3 (C-17), 128.2 (C-4), 128.1 (C-16), 127.5 (C-14), 107.7 (C-7), 30.3 (C-9), 28.6 (C-8); IR ($CHCl_3$, cm^{-1}) 2924.3, 2853.8, 1715.9, 1666.8; MS (GCMS, *m/z*) 389 $[M]^+$; Anal. Calcd. for $C_{22}H_{16}FN_3O_3$: C, 67.86; H, 4.14; N, 10.79; O, 12.33. Found: C, 67.80; H, 4.11; N, 10.75; O, 12.30.



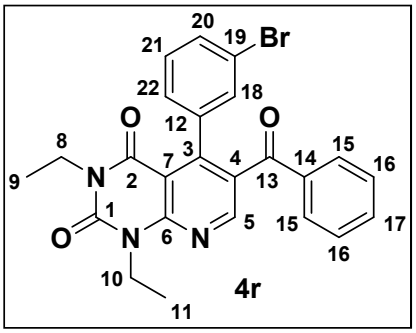
6-benzoyl-1,3-dimethyl-5-styrylpyrido[2,3-*d*]pyrimidine-2,4-dione (4p)

Pale yellow solid; mp 222-223 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.73 (s, 1H, H-8), 7.89-7.84 (d, J = 16 Hz, 1H, H-24), 7.63-7.30 (m, 10H, ArH), 6.53-6.48 (d, J = 16 Hz, 1H, H-15), 3.80 (s, 3H, H-12), 3.48 (s, 3H, H-11); IR ($CHCl_3$, cm^{-1}) 2924.2, 2856.3, 1713.7, 1662.0, 1578.9; MS (GCMS, *m/z*) 397 $[M]^+$; Anal. Calcd. for $C_{24}H_{19}N_3O_3$: C, 72.53; H, 4.82; N, 10.57; O, 12.08. Found: C, 72.50; H, 4.80; N, 10.51; O, 12.02.



6-benzoyl-1,3-diethyl-5-(4-fluorophenyl)pyrido[2,3-*d*]pyrimidine-2,4-dione (4q)

White solid; mp 98-100 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.68 (s, 1H, H-5), 7.52-6.84 (m, 9H, ArH), 4.55-4.48 (q, J = 6.9 Hz, 2H, H-10), 4.05-3.98 (q, J = 6.9 Hz, 2H, H-8), 1.42-1.38 (t, J = 6.9 Hz, 3H, H-11), 1.22-1.18 (t, J = 7 Hz, 3H, H-9); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 195.2 (C-13), 159.8 (C-21), 152.2 (C-6), 151.7 (C-2), 151.6 (C-1), 145.0 (C-3), 150.1 (C-5), 137.2 (C-12), 133.5 (C-14), 132.6 (C-17), 131.8 (C-4), 130.1 (C-15), 130.0 (C-19), 129.3 (C-15), 128.3 (C-16), 114.9 (C-20), 114.6 (C-19), 107.9 (C-7), 38.6 (C-10), 37.2 (C-8), 13.2 (C-11), 12.9 (C-9); IR ($CHCl_3$, cm^{-1}) 2923.6, 2851.5, 1715.2, 1668.3; MS (GCMS, *m/z*) 417 $[M]^+$; Anal. Calcd. for $C_{24}H_{20}FN_3O_3$: C, 69.05; H, 4.83; N, 10.07; O, 11.50. Found: C, 69.00; H, 4.80; N, 10.01; O, 11.46.



6-benzoyl-5-(3-bromophenyl)-1,3-diethylpyrido[2,3-*d*]pyrimidine-2,4-dione (4r)

White solid; mp 182-184 ^{o}C; ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.70 (s, 1H, H-5), 7.52-7.03 (m, 9H, ArH), 4.54-4.49 (q, J = 7 Hz, 2H, H-10), 4.04-4.00 (q, J = 7 Hz, 2H, H-8), 1.41-1.38 (t, J = 7 Hz, 3H, H-11), 1.21-

1.19 (t, J = 7 Hz, 3H, H-9); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 194.7 (C-13), 159.5 (C-6), 152.2 (C-2), 151.8 (C-3), 150.8 (C-1), 150.0 (C-5), 137.8 (C-12), 137.2 (C-14), 133.5 (C-18), 132.2 (C-17), 131.2 (C-21), 131.1 (C-20), 129.3 (C-15), 128.9 (C-22), 128.3 (C-16), 126.8 (C-19), 121.6 (C-4), 107.7 (C-7), 38.6 (C-10), 37.2 (C-8), 13.2 (C-11), 12.9 (C-9); IR ($CHCl_3$, cm^{-1}) 2923.5, 2851.3, 1716.4, 1669.6; MS (GCMS, *m/z*) 479 $[M]^+$; Anal. Calcd. for $C_{24}H_{20}BrN_3O_3$: C, 60.26; H, 4.21; N, 8.78; O, 10.03. Found: C, 60.21; H, 4.16; N, 8.70; O, 10.00.

NMR Spectra of the Products

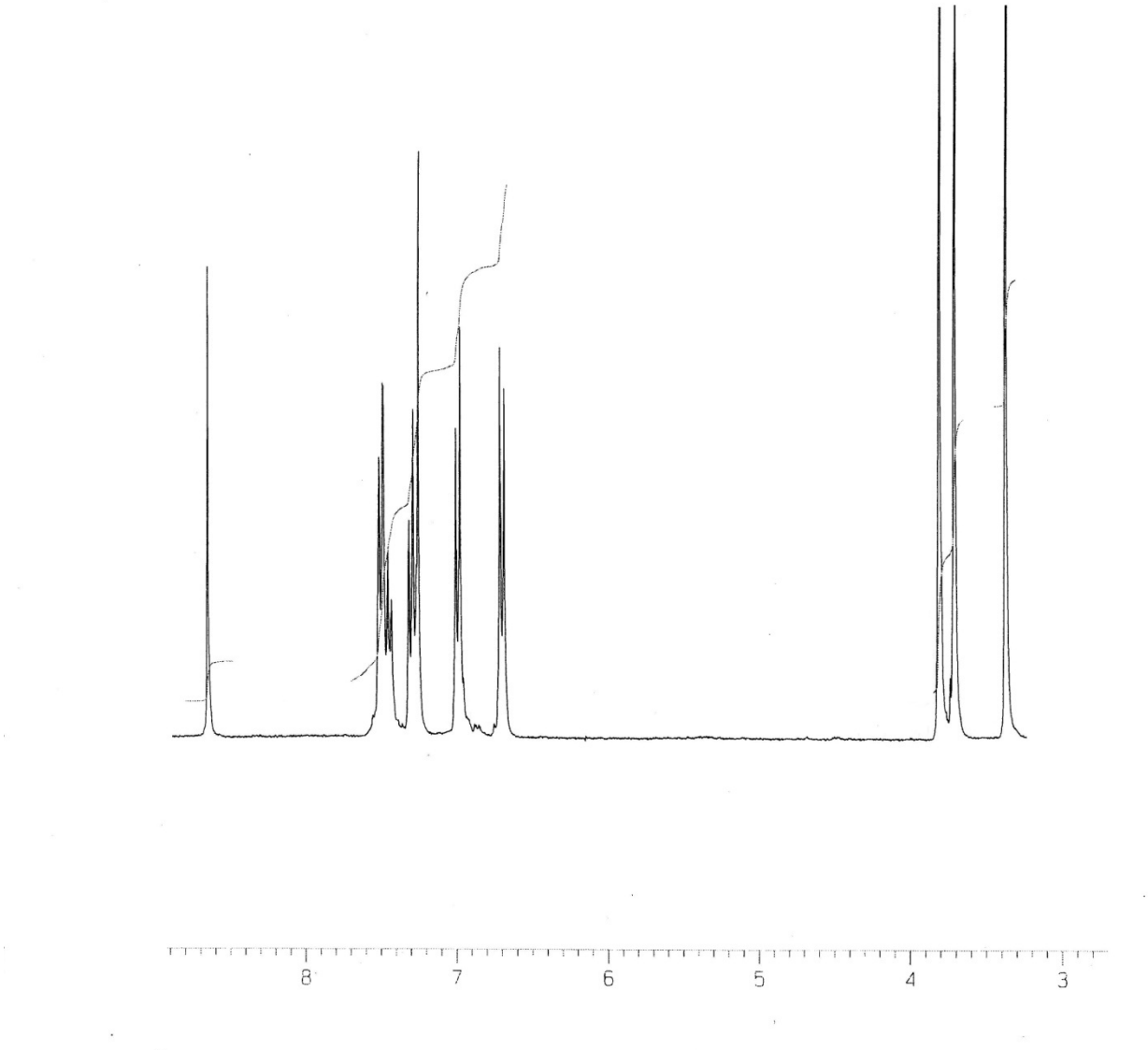


Fig S-1: ^1H NMR Spectrum of Product **4a**

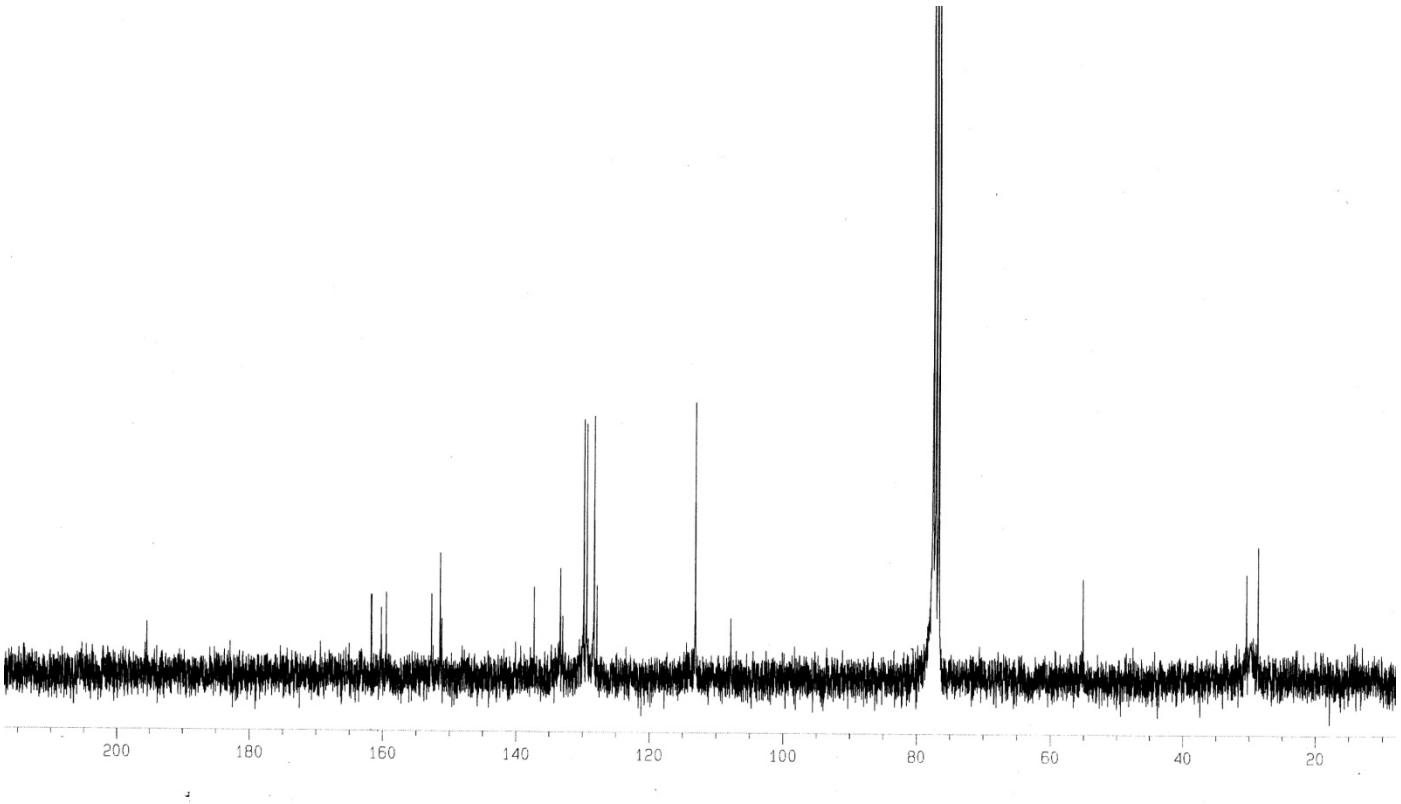


Fig S-2: ^{13}C NMR Spectrum of Product **4a**

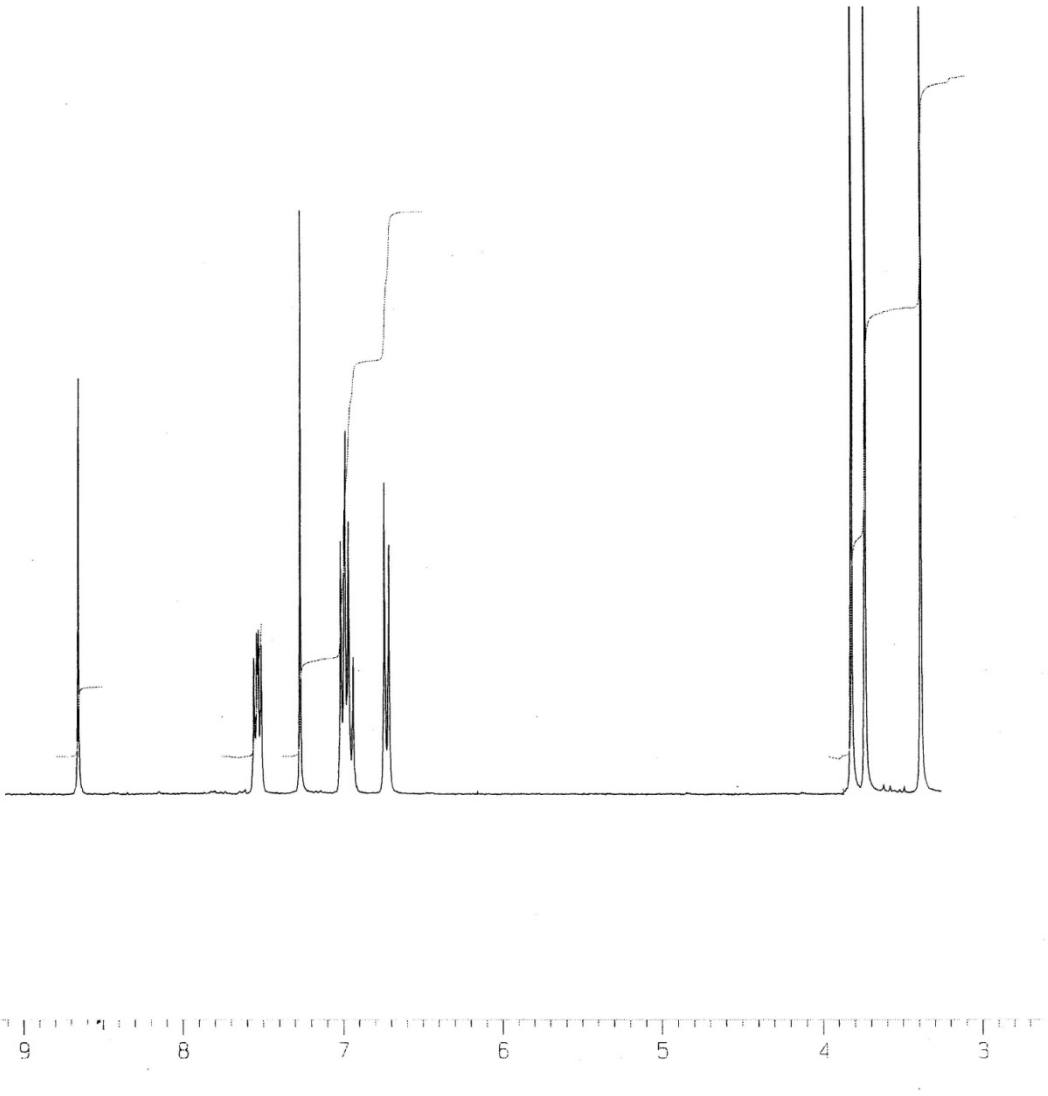


Fig S-3: ^{1}H NMR Spectrum of Product **4b**

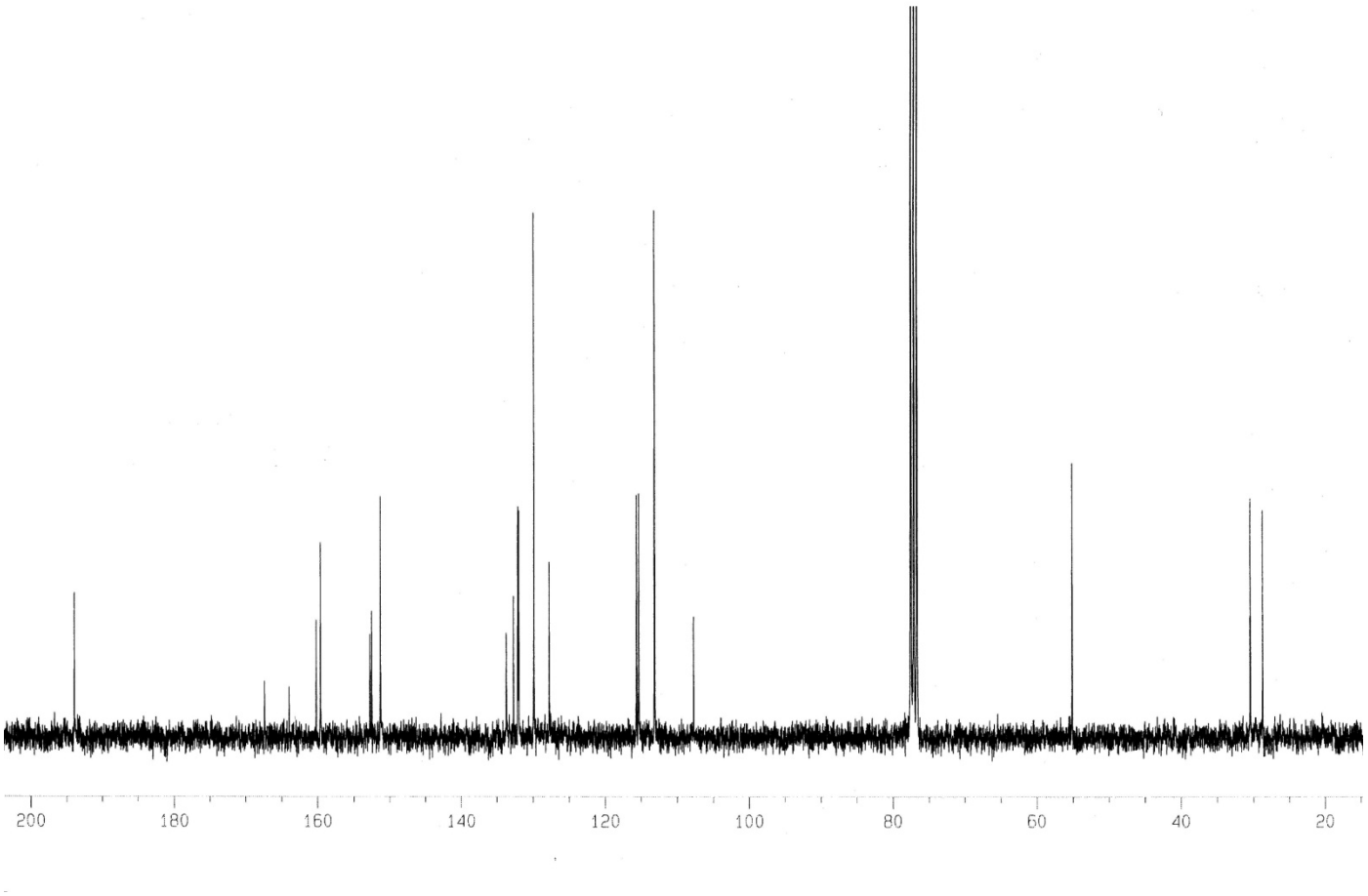


Fig S-4: ^{13}C NMR Spectrum of Product **4b**

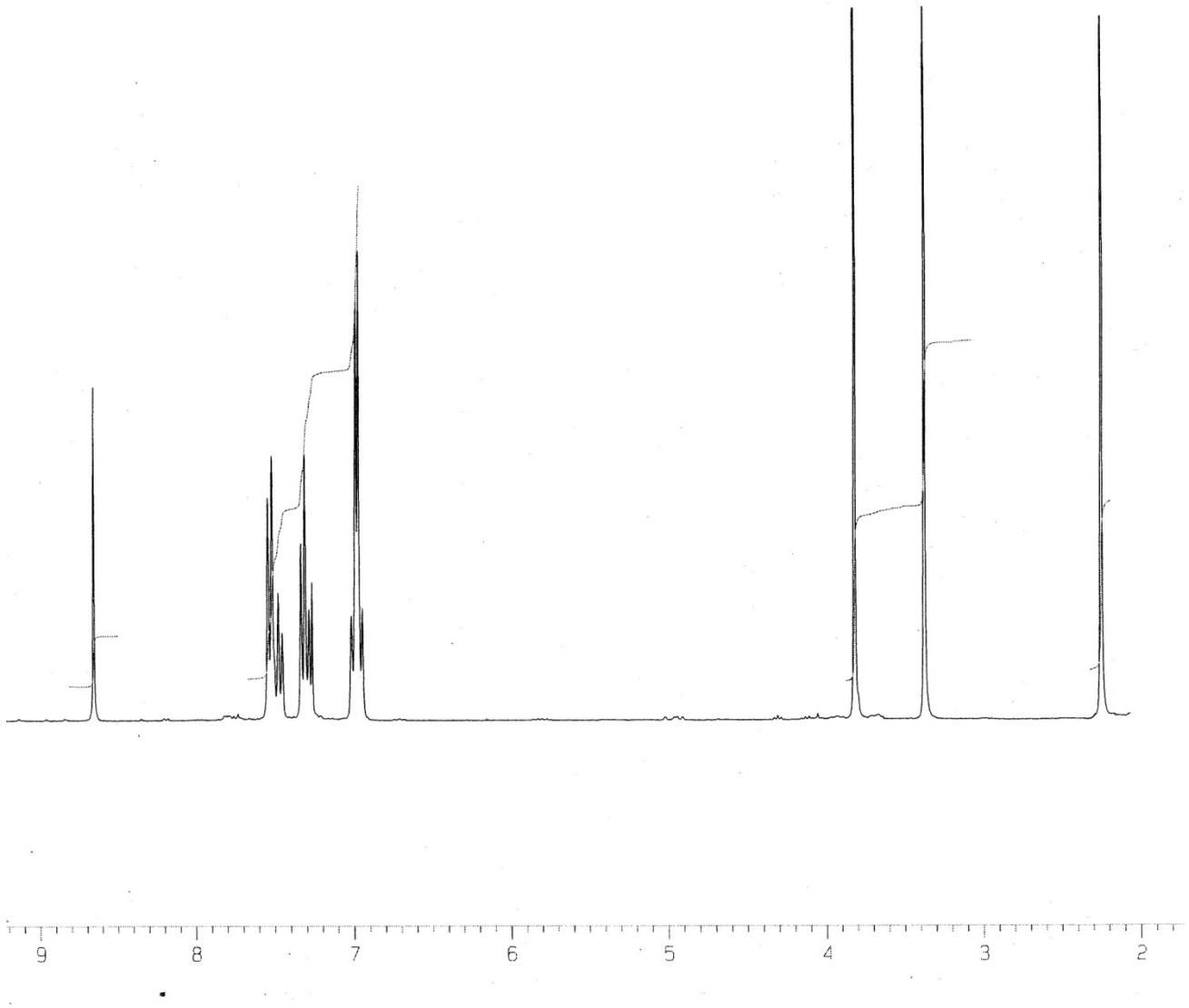


Fig S-5: ^{1}H NMR Spectrum of Product **4c**

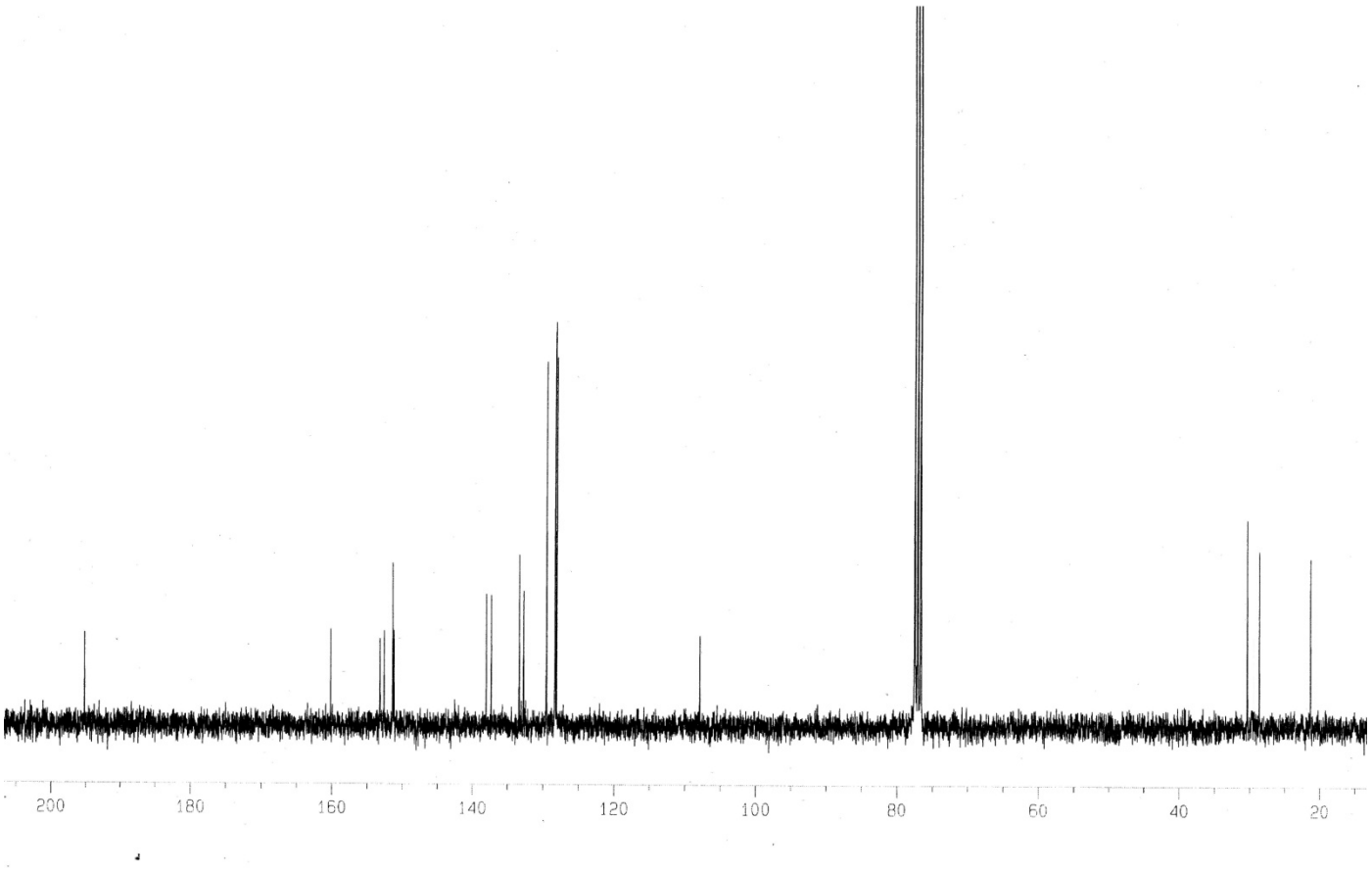


Fig S-6: ^{13}C NMR Spectrum of Product **4c**

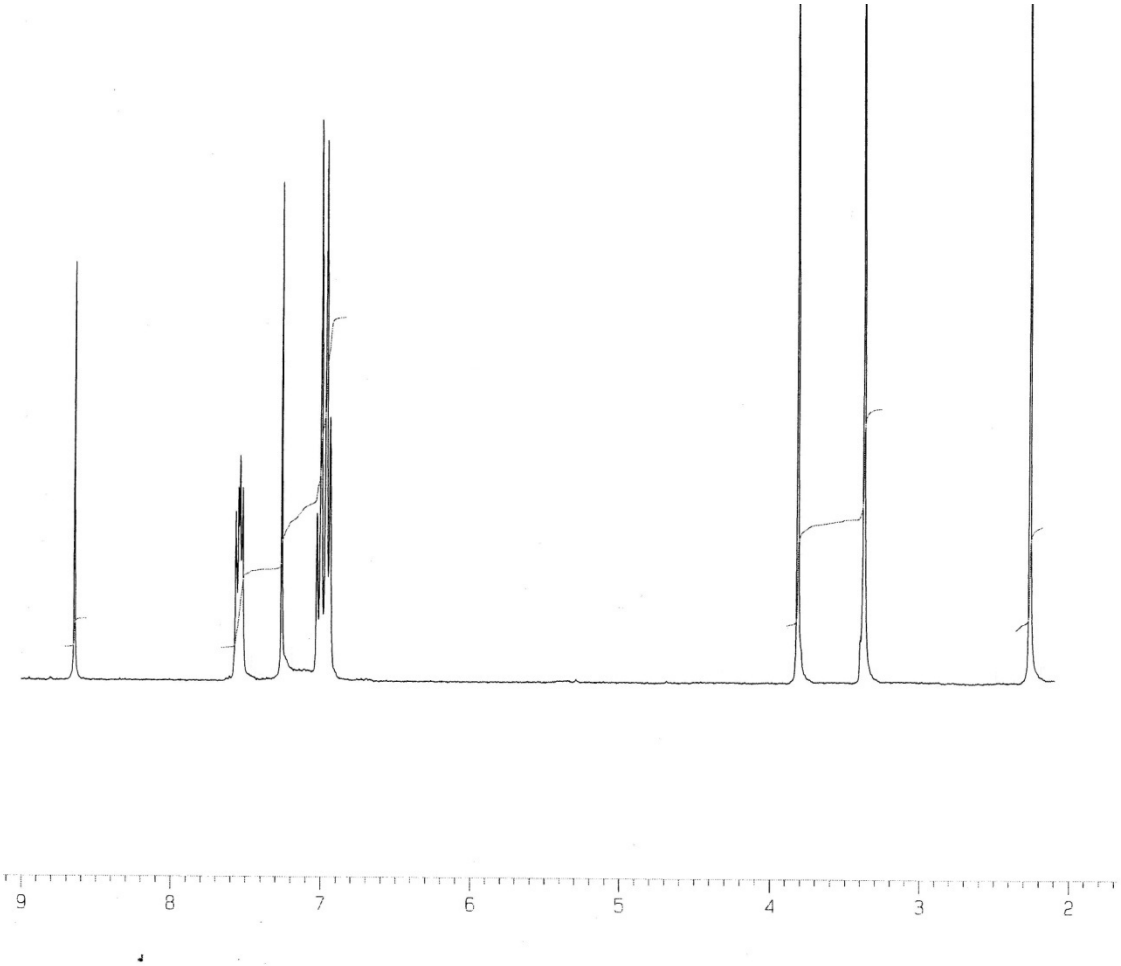


Fig S-7: ^{1}H NMR Spectrum of Product **4d**

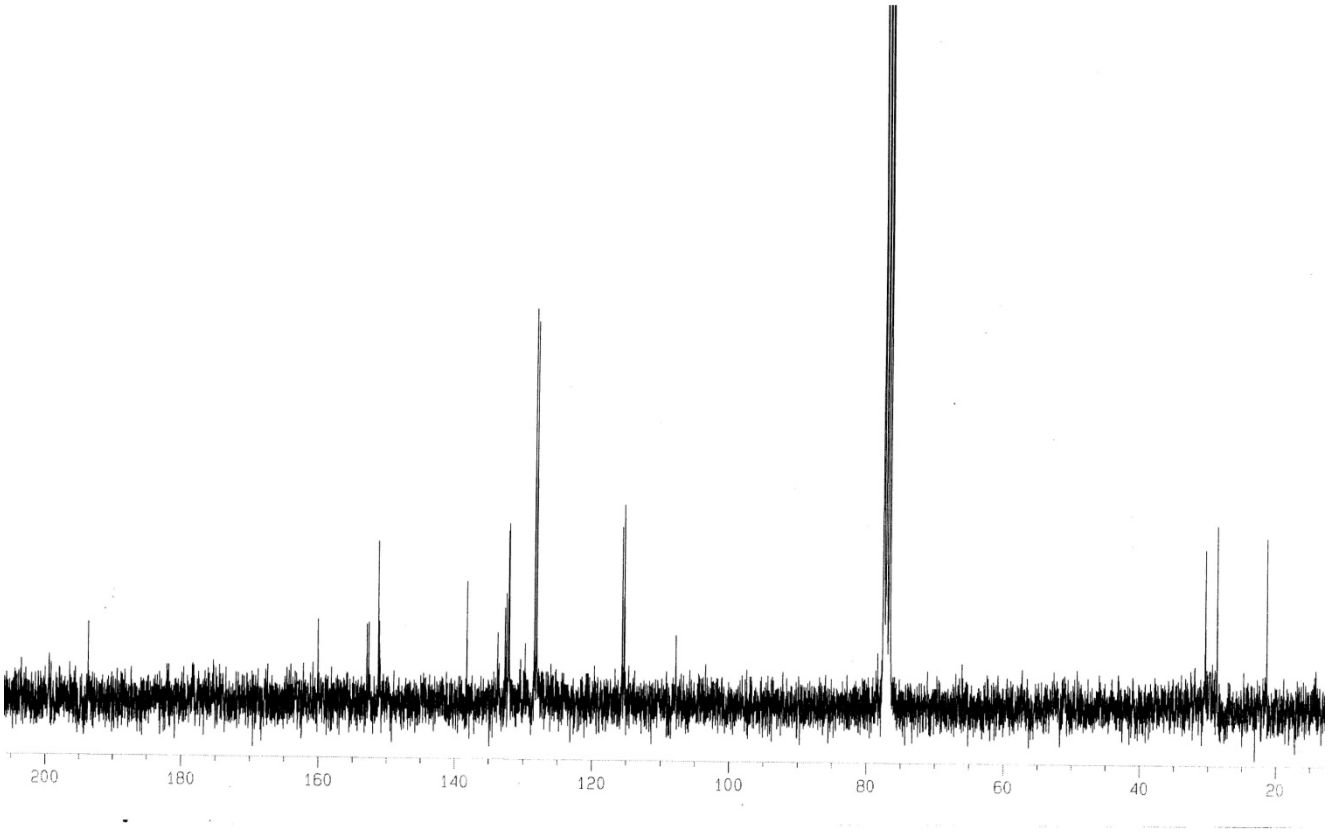


Fig S-8: ^{13}C NMR Spectrum of Product **4d**

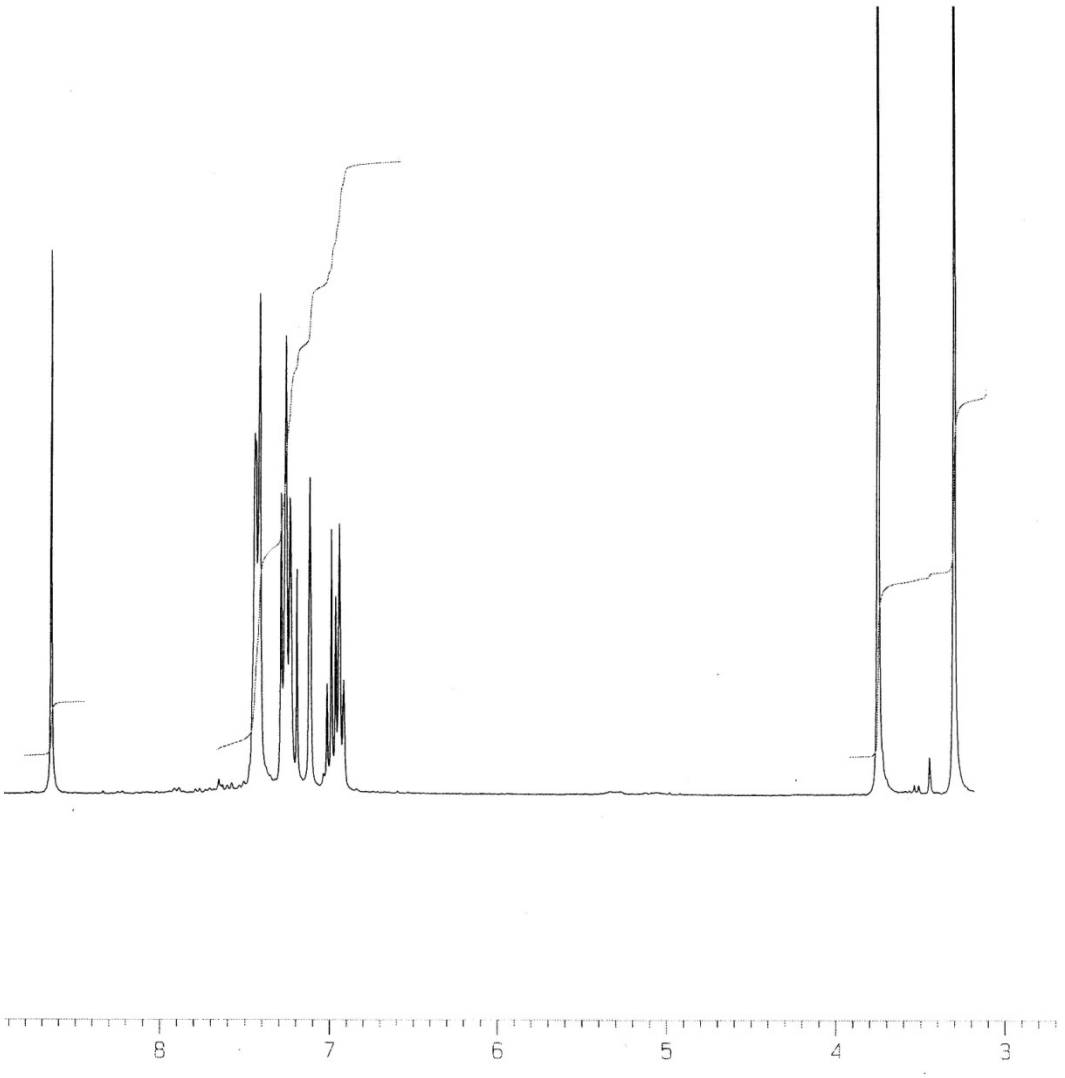


Fig S-9: ^{1}H NMR Spectrum of Product **4e**

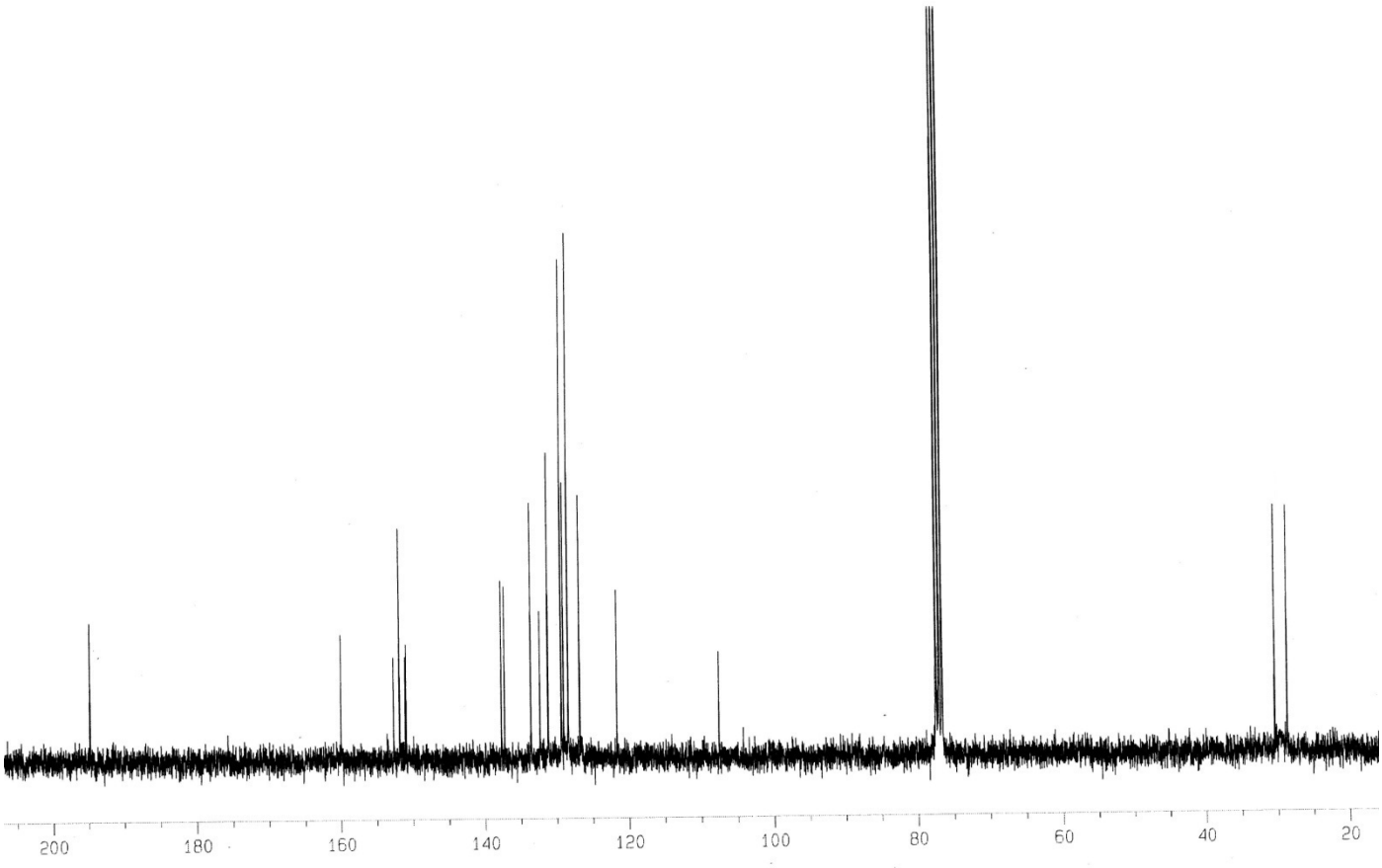


Fig S-10: ^{13}C NMR Spectrum of Product **4e**

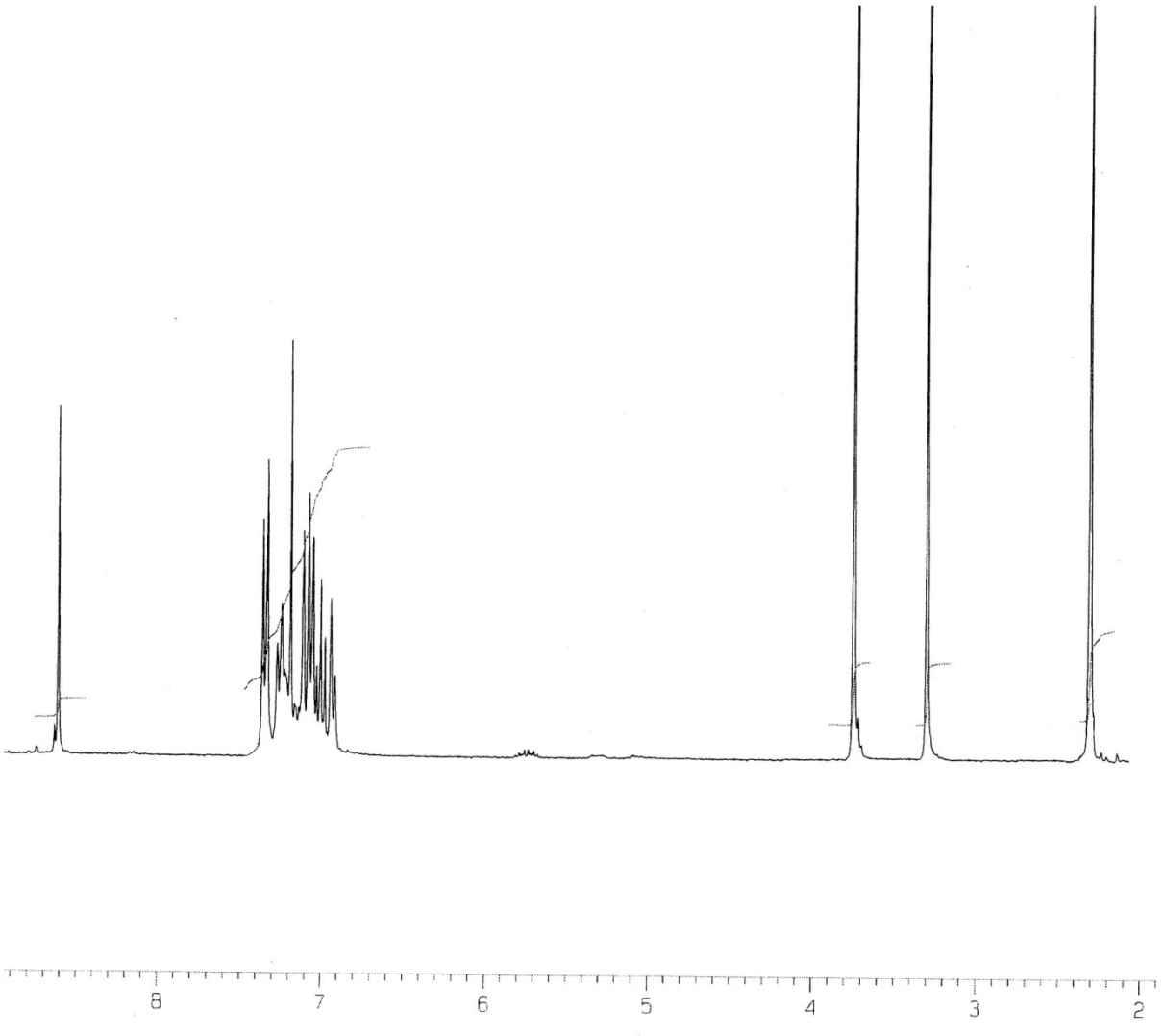


Fig S-11: ^{1}H NMR Spectrum of Product **4f**

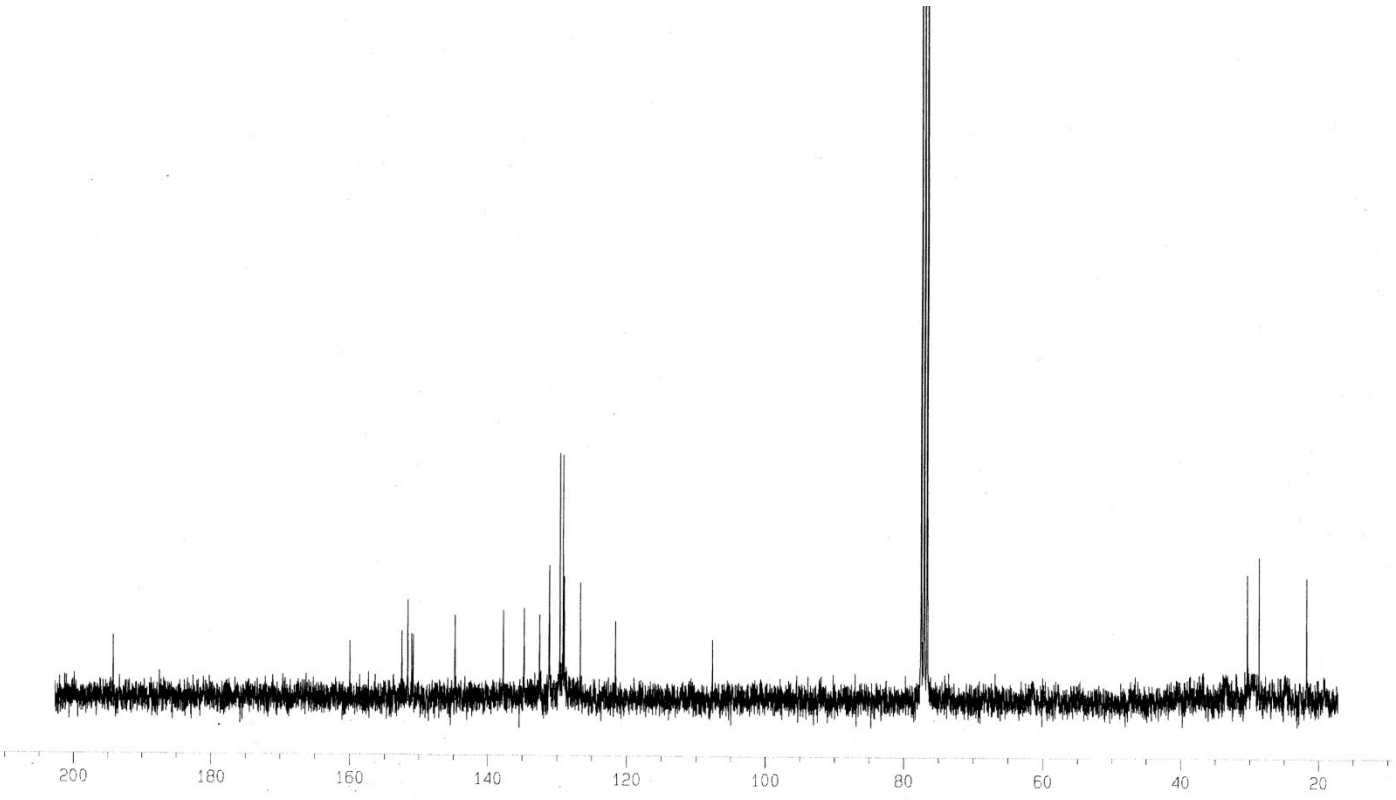


Fig S-12: ^{13}C NMR Spectrum of Product **4f**

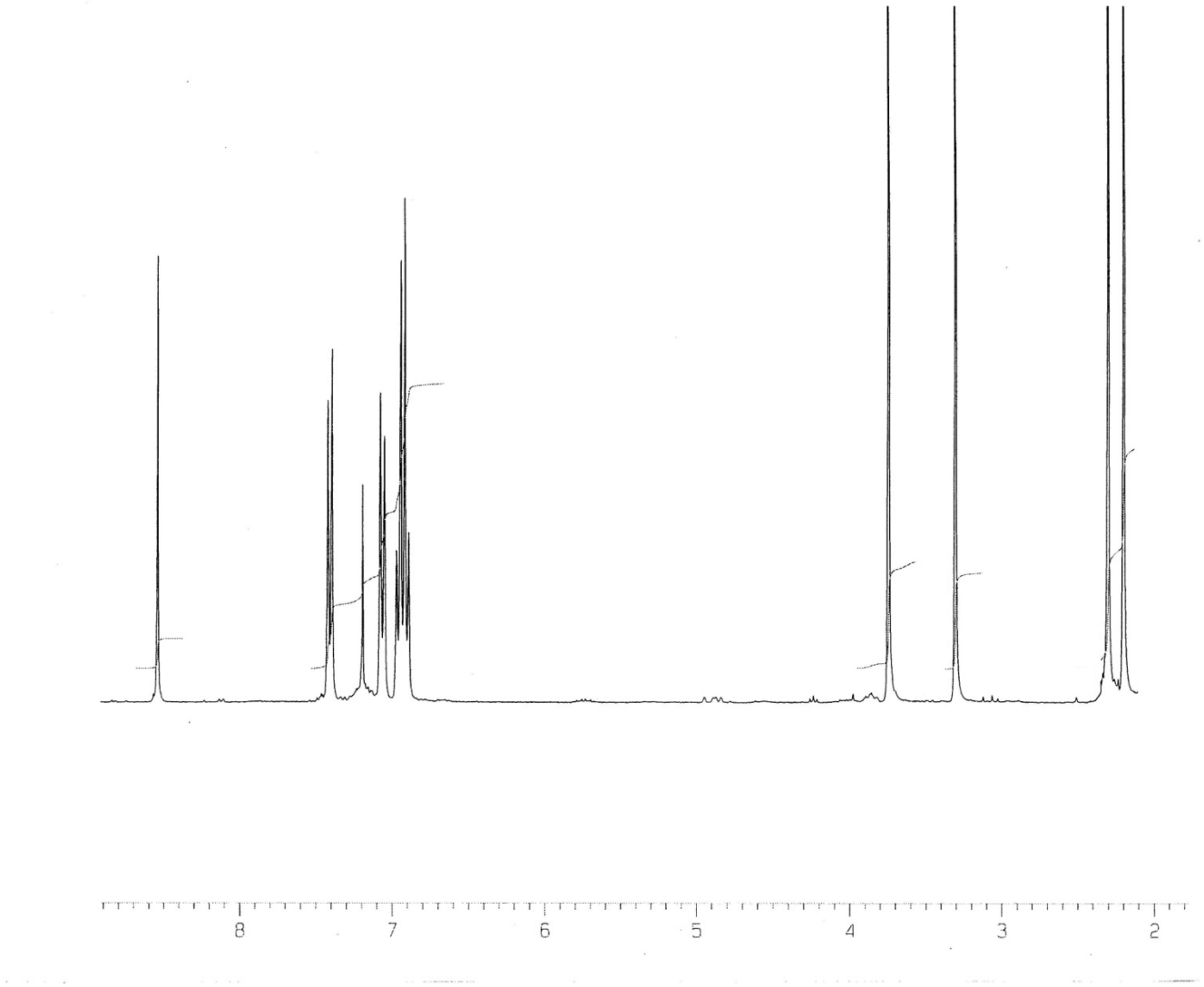


Fig S-13: ^{1}H NMR Spectrum of Product **4g**

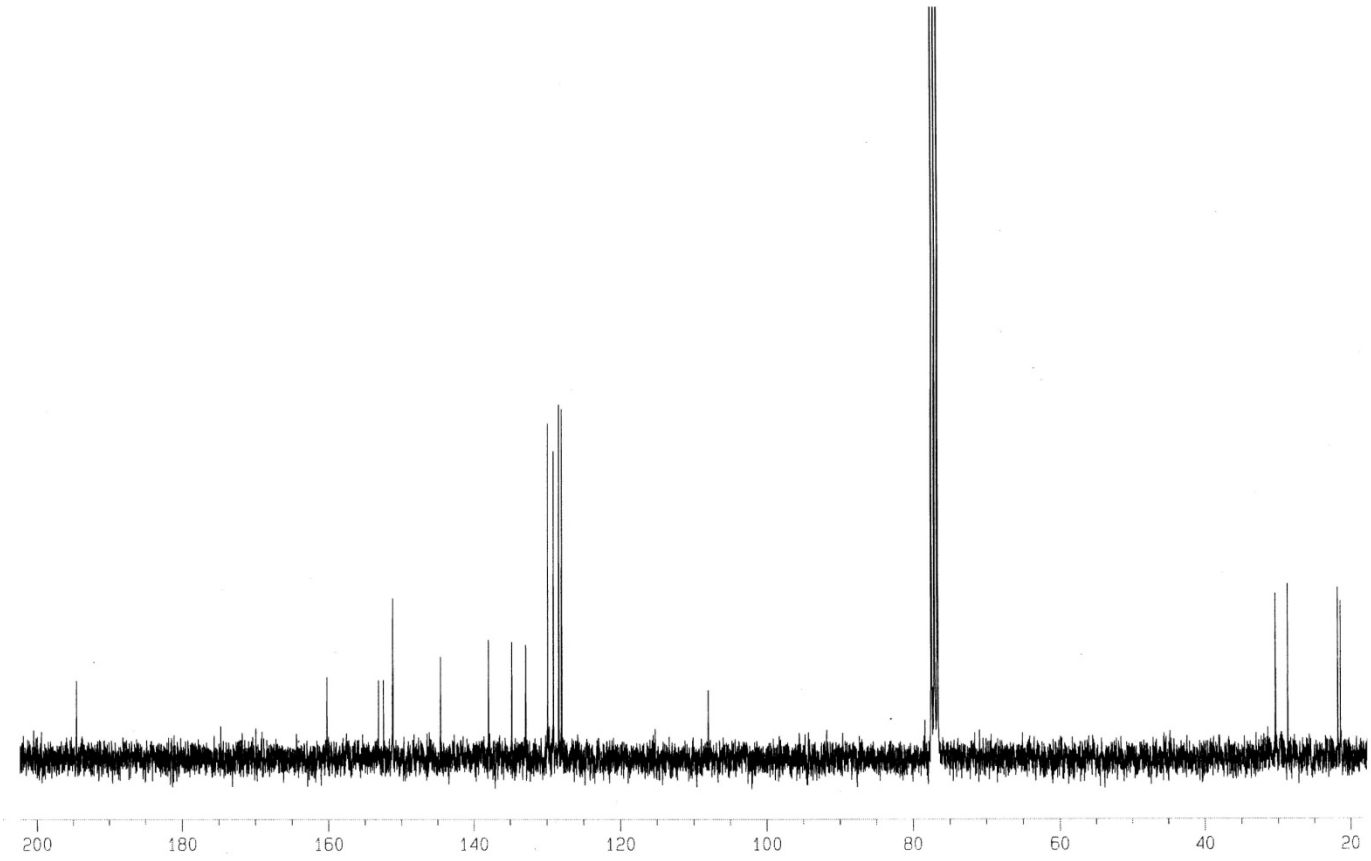


Fig S-14: ^{13}C NMR Spectrum of Product **4g**

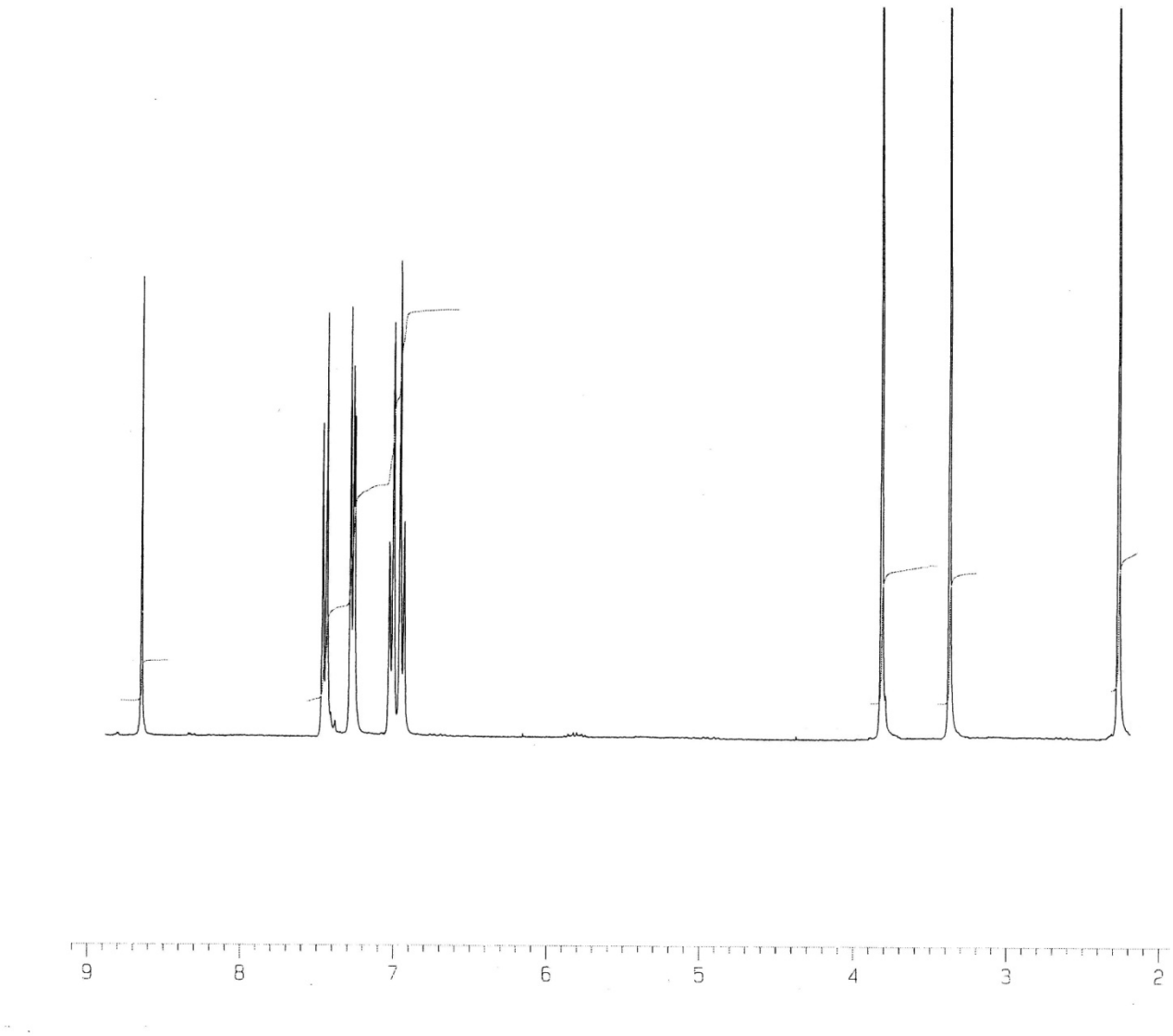


Fig S-15: ^{1}H NMR Spectrum of Product **4h**

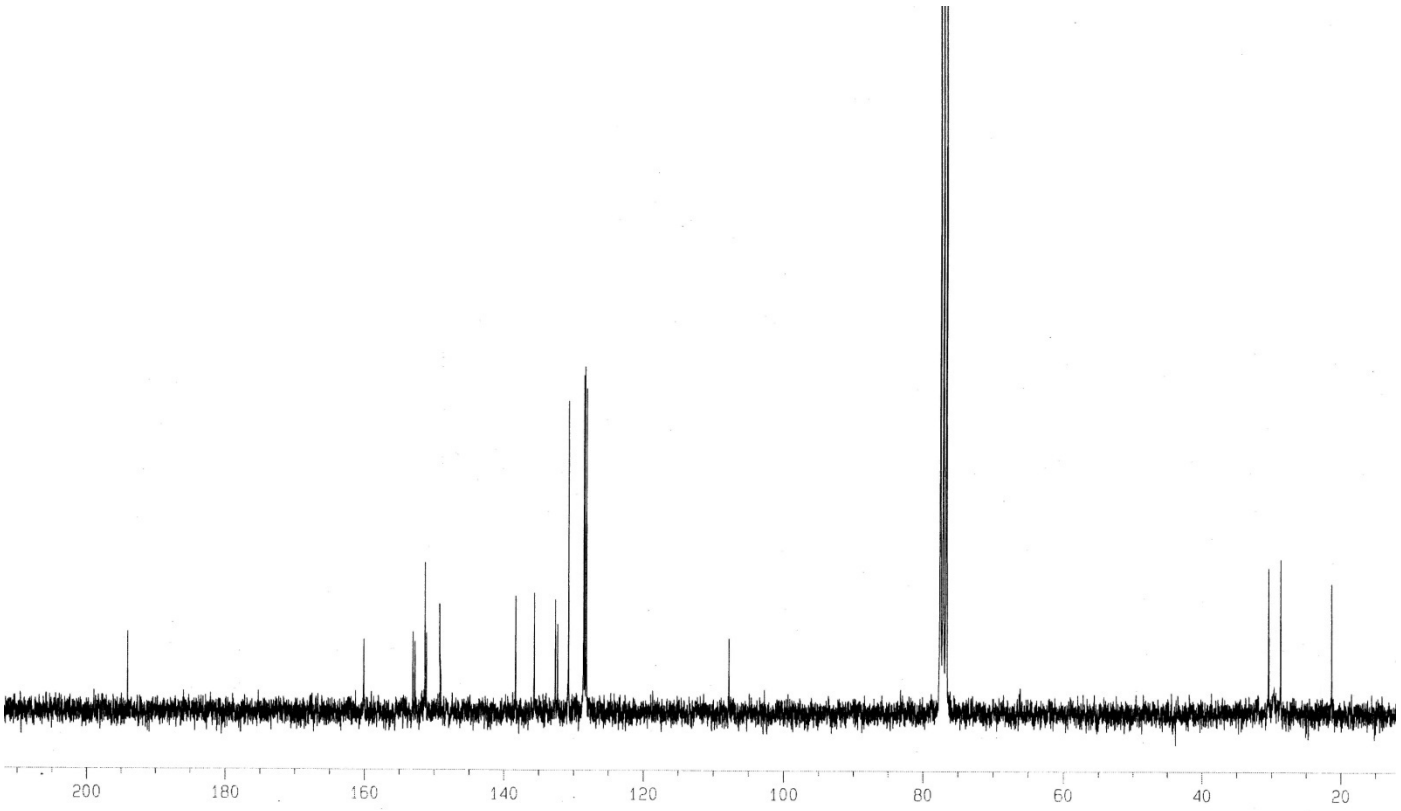


Fig S-16: ^{13}C NMR Spectrum of Product **4h**

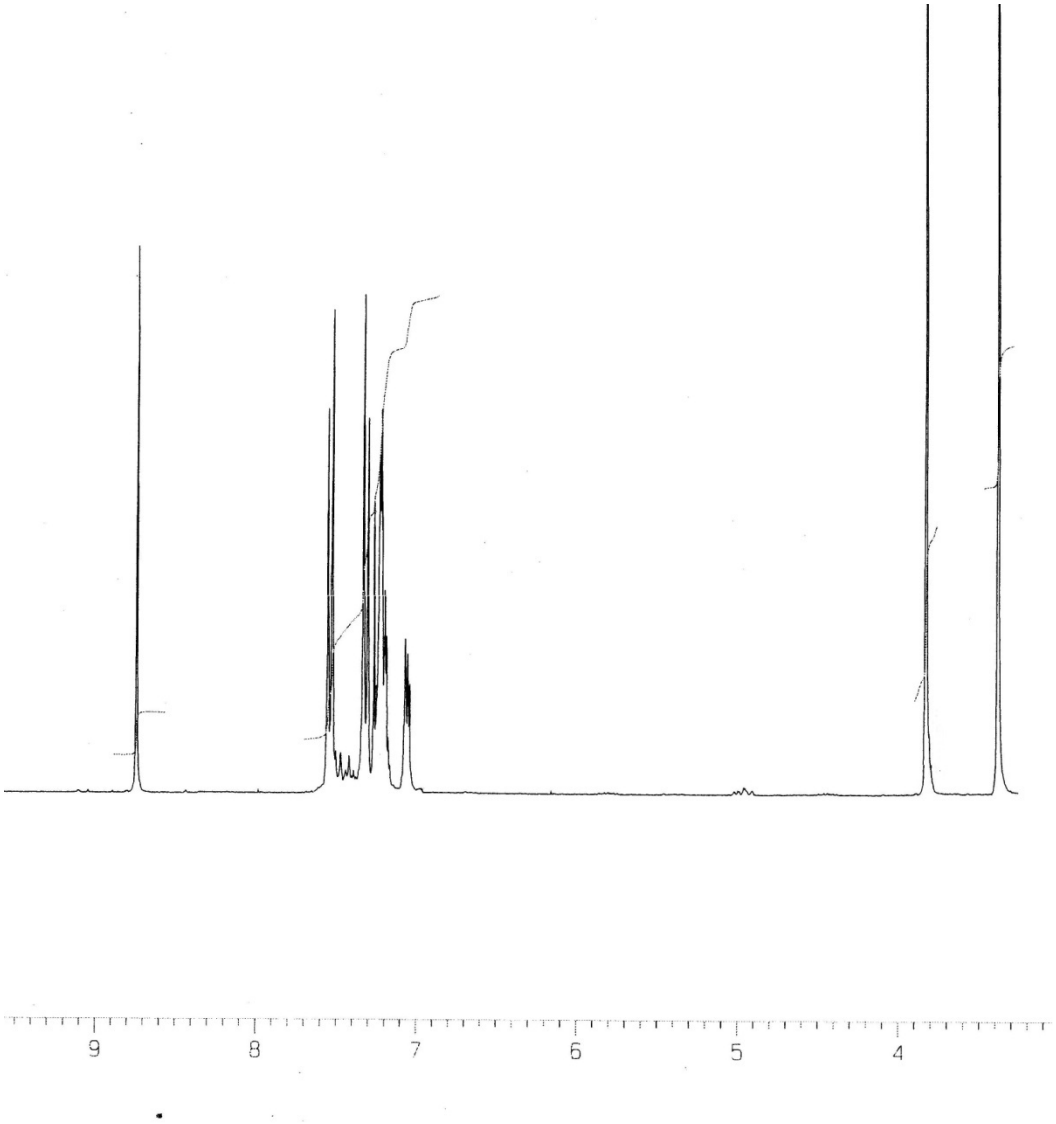


Fig S-17: ^{1}H NMR Spectrum of Product **4i**

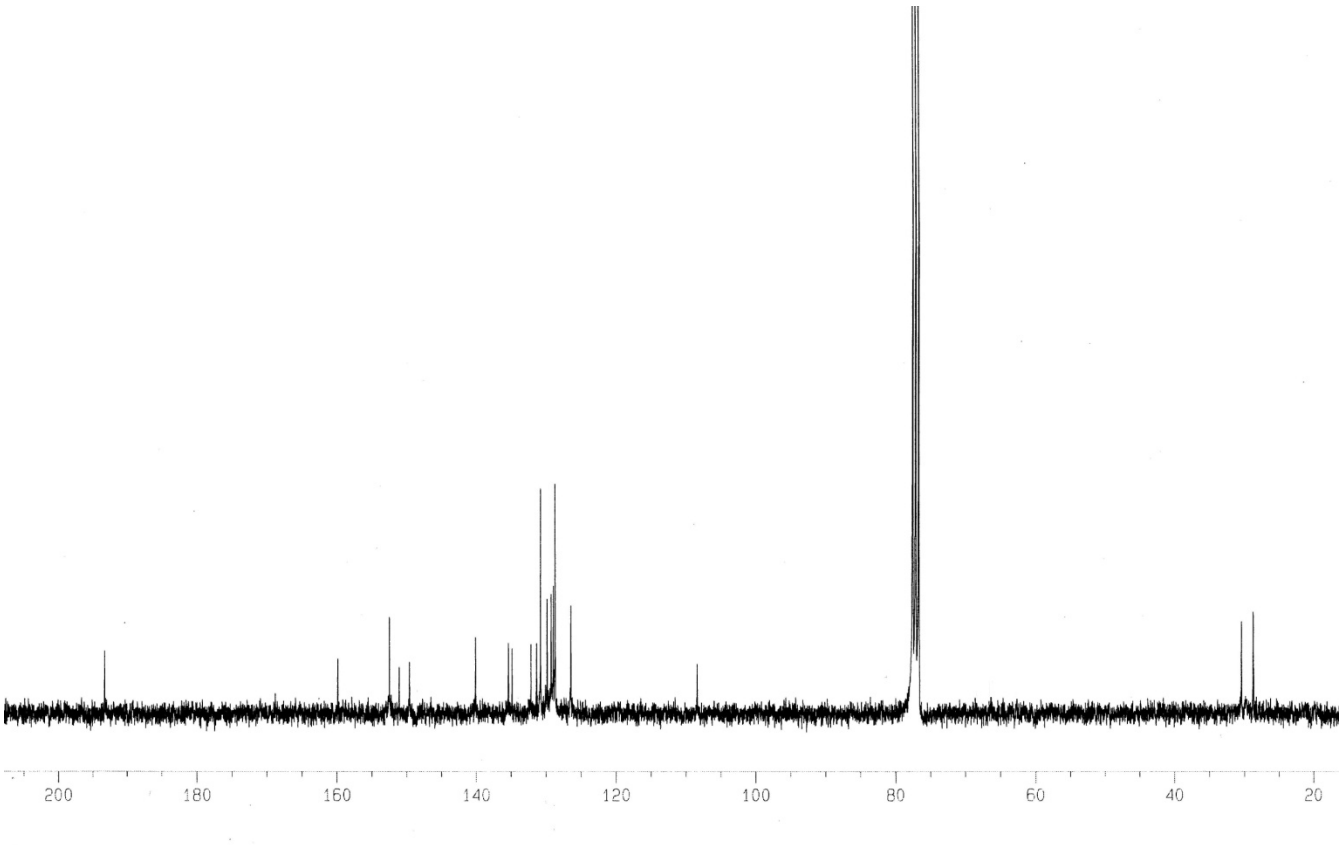


Fig S-18: ^{13}C NMR Spectrum of Product **4i**

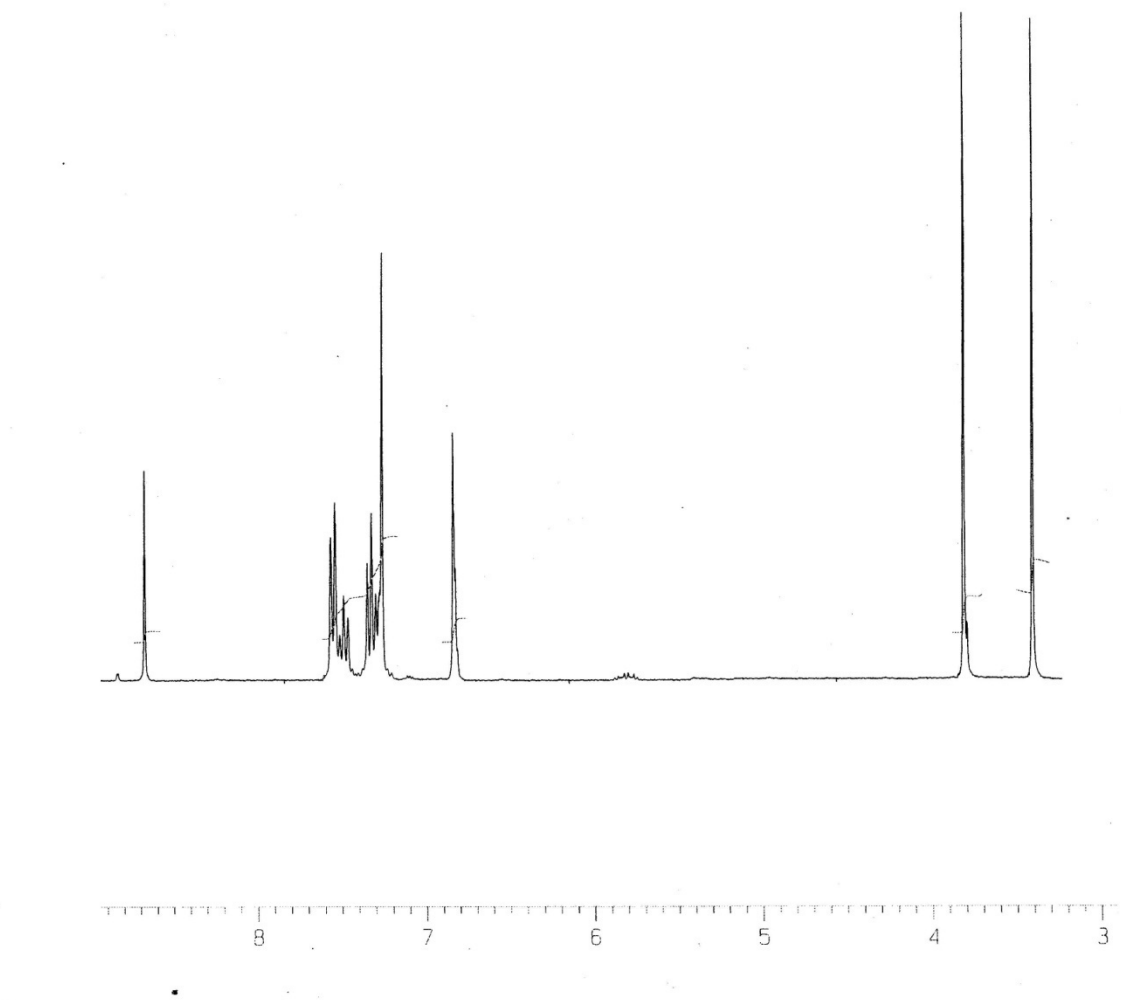


Fig S-19: ^{1}H NMR Spectrum of Product **4j**

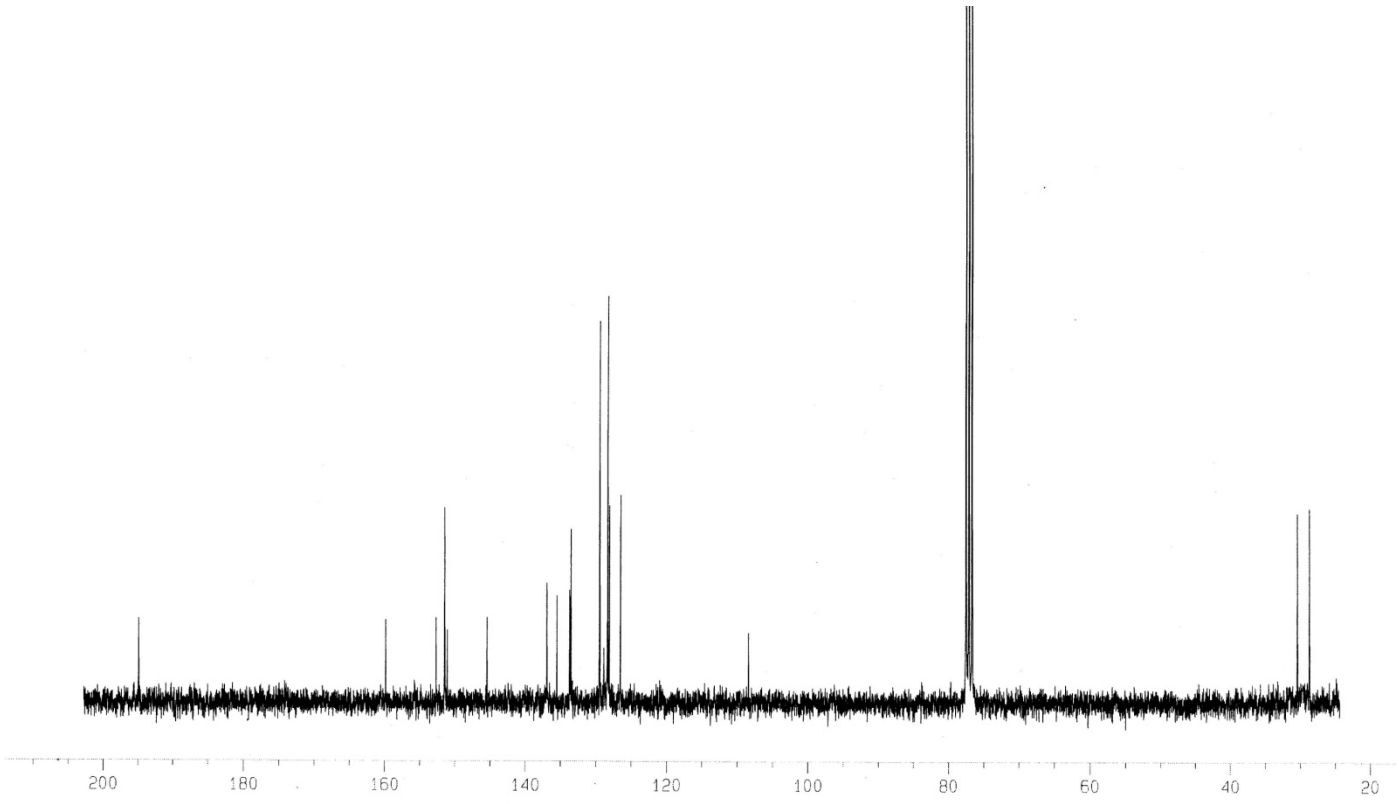


Fig S-20: ^{13}C NMR Spectrum of Product **4j**

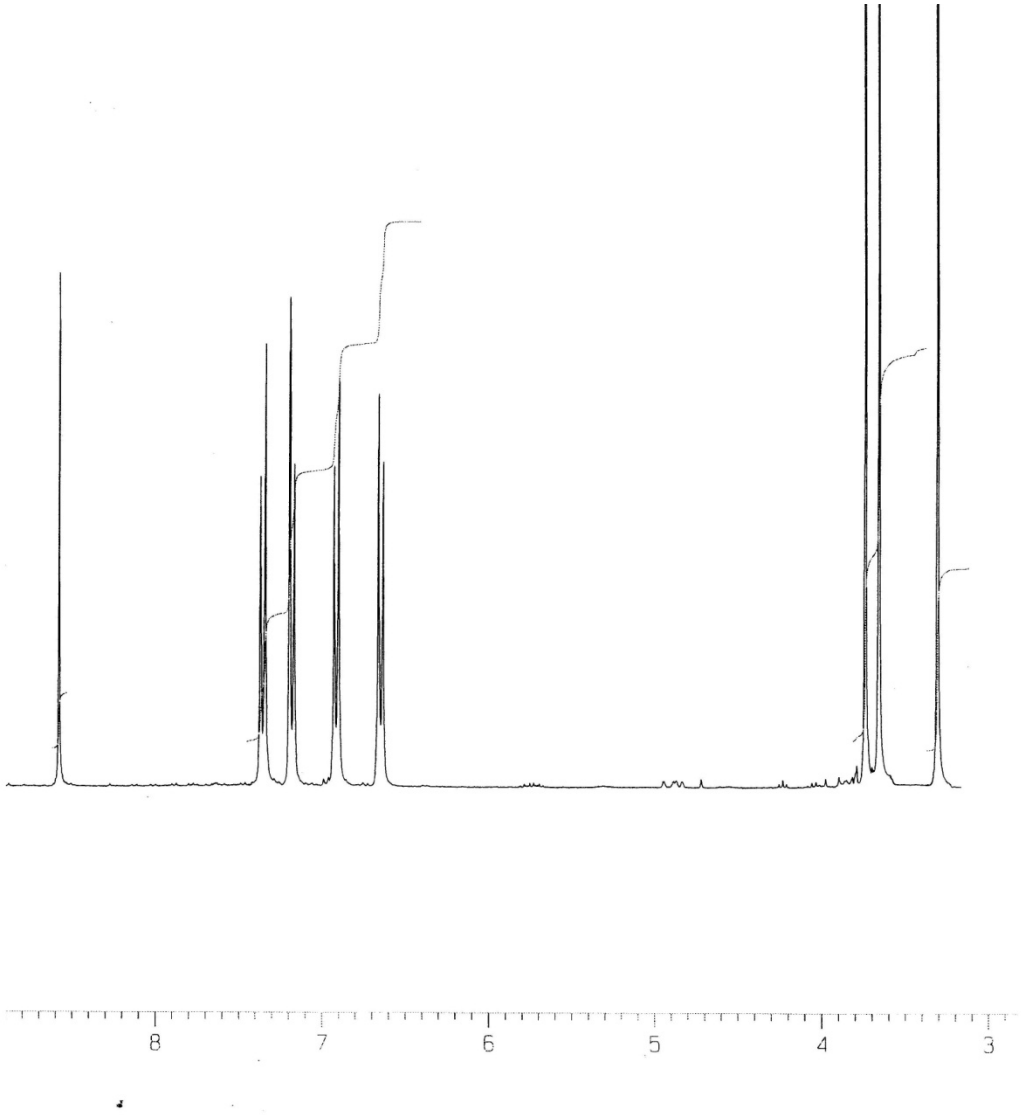


Fig S-21: ^{1}H NMR Spectrum of Product **4k**

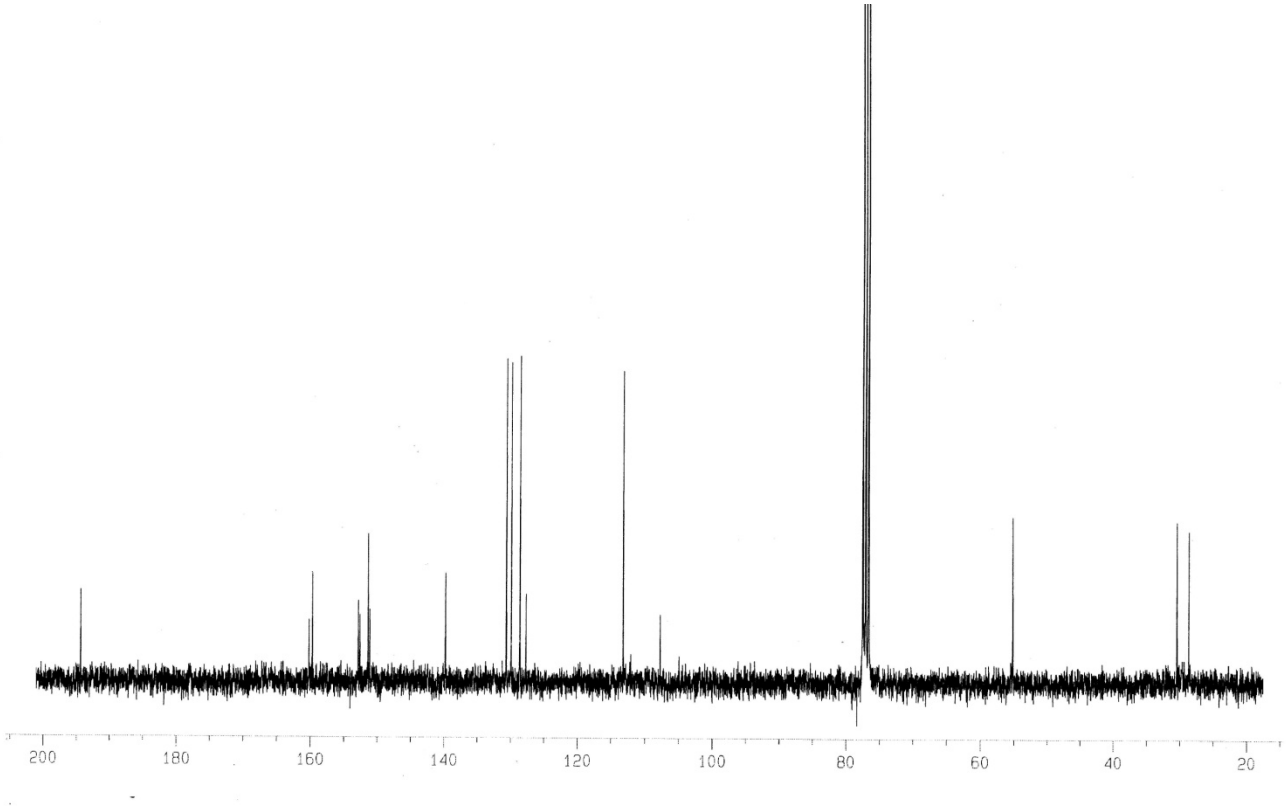


Fig S-22: ^{13}C NMR Spectrum of Product **4k**

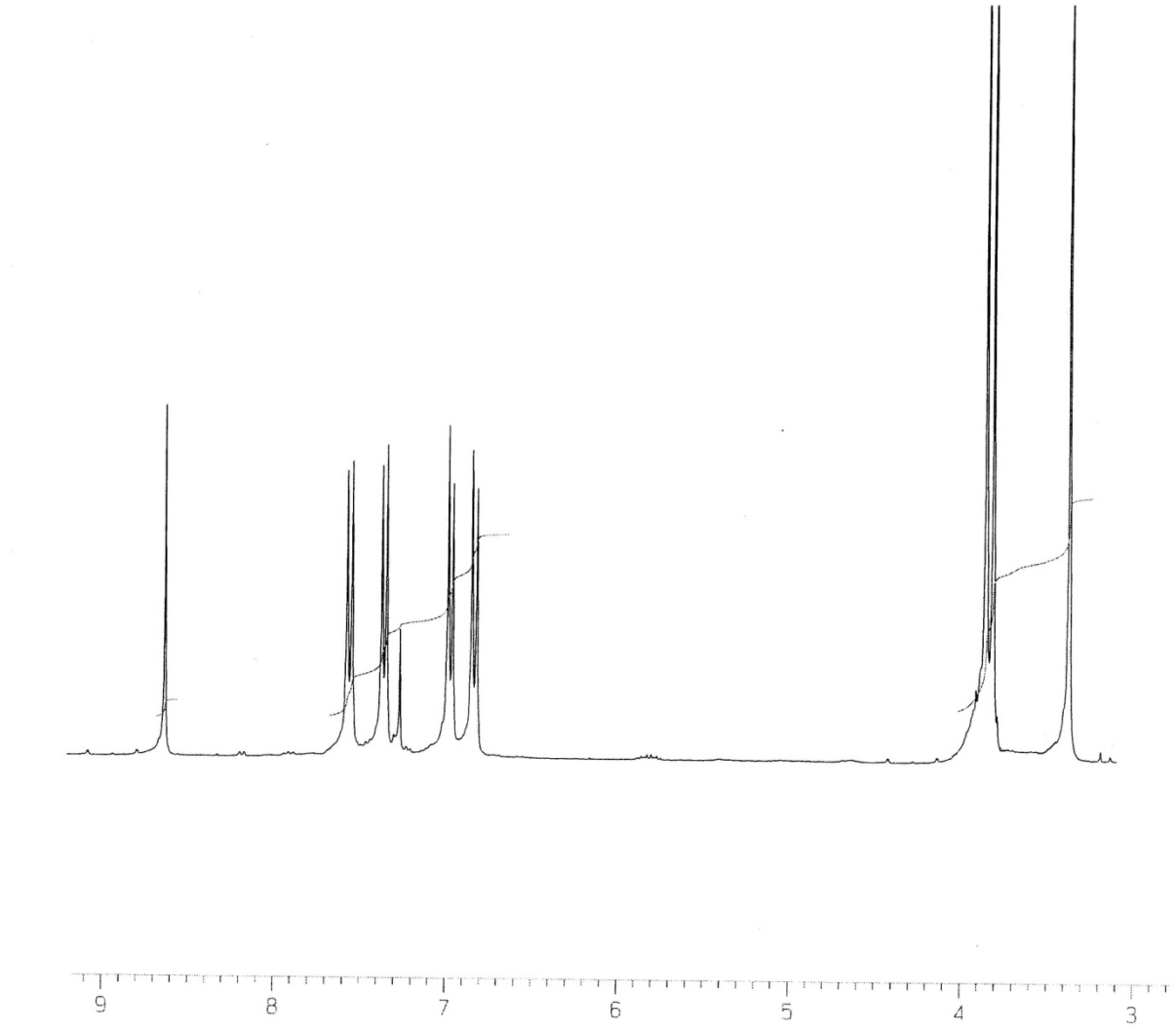


Fig S-23: ^{1}H NMR Spectrum of Product **4l**

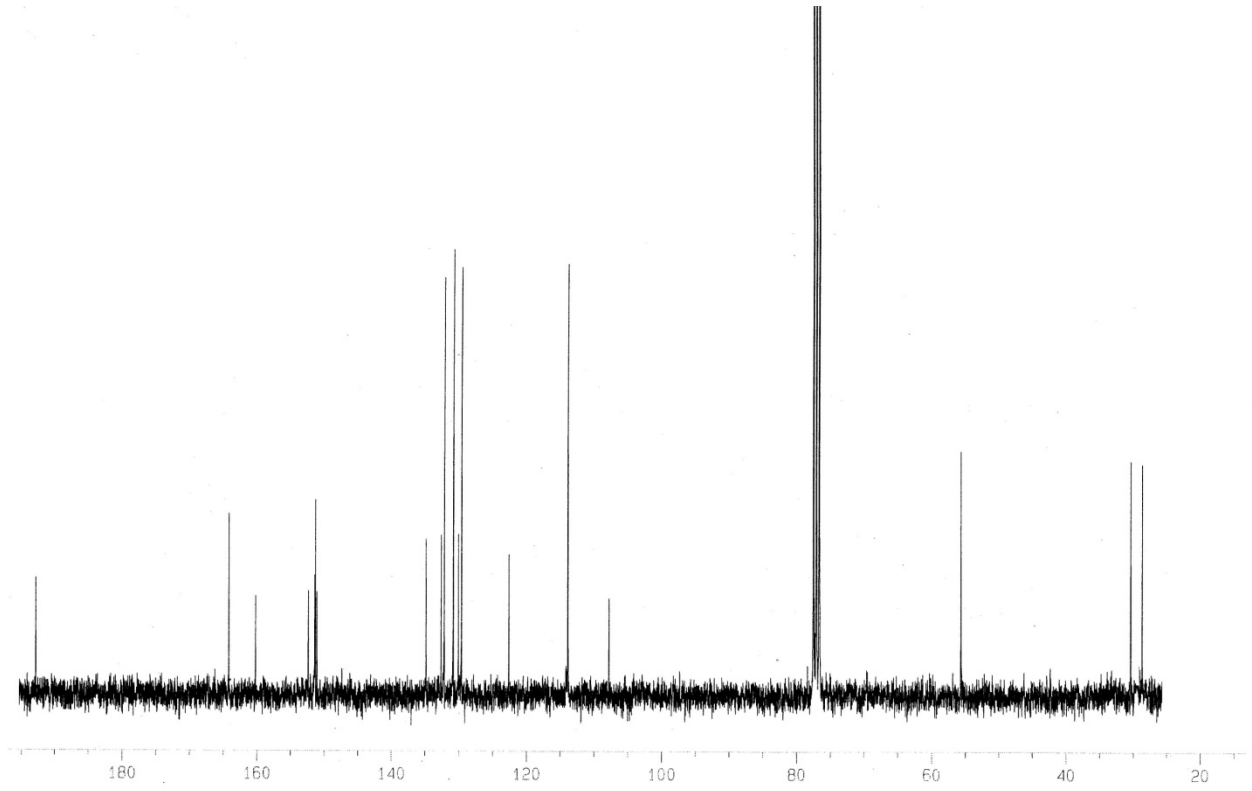


Fig S-24: ^{13}C NMR Spectrum of Product **4l**

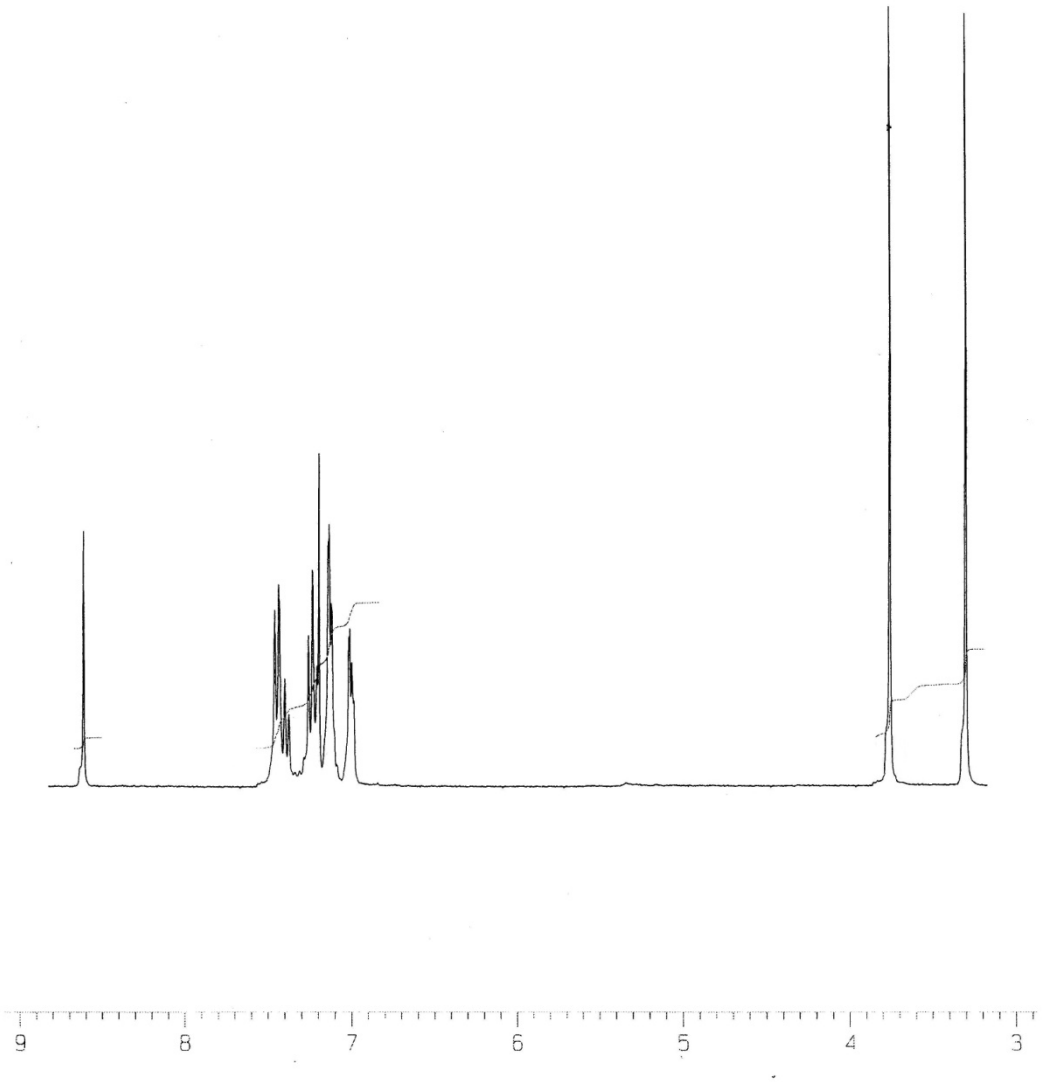


Fig S-25: ^{1}H NMR Spectrum of Product **4m**

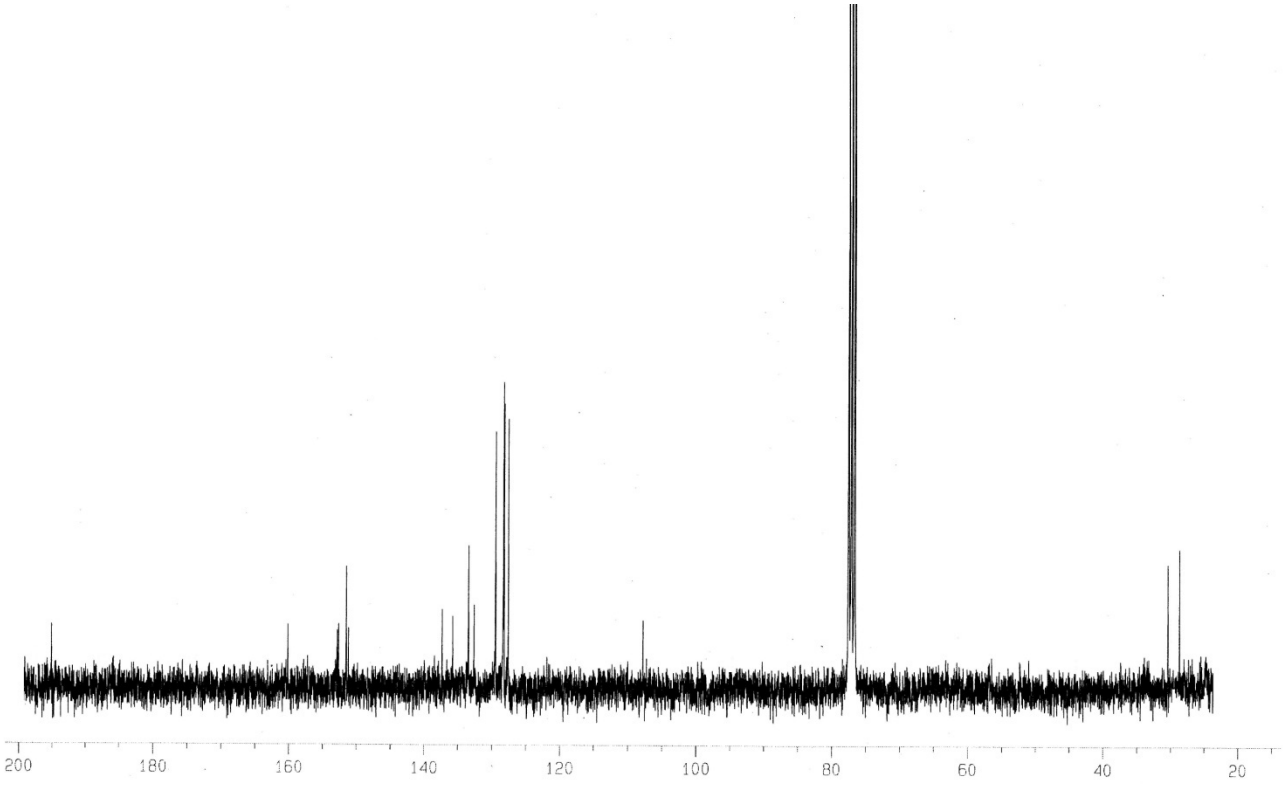


Fig S-26: ^{13}C NMR Spectrum of Product **4m**

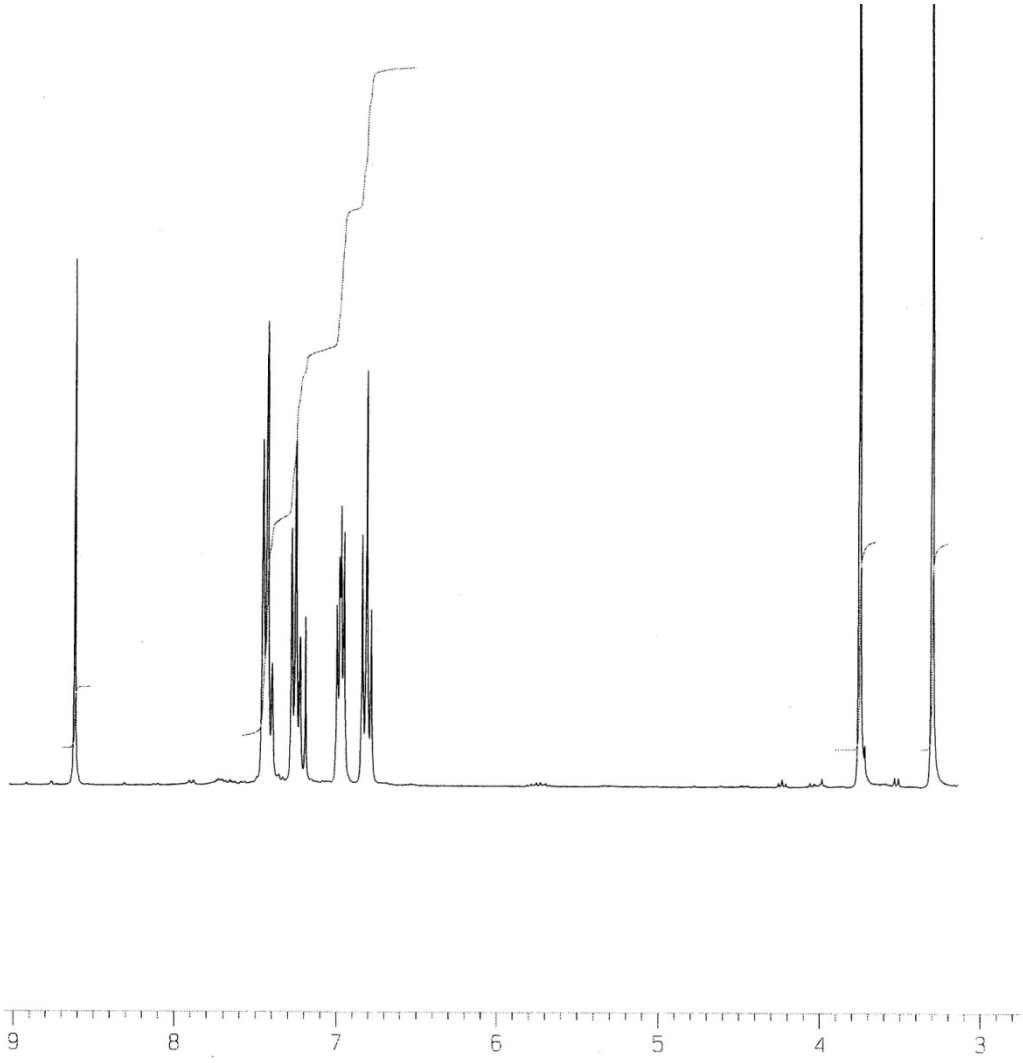


Fig S-27: ^{1}H NMR Spectrum of Product **4n**

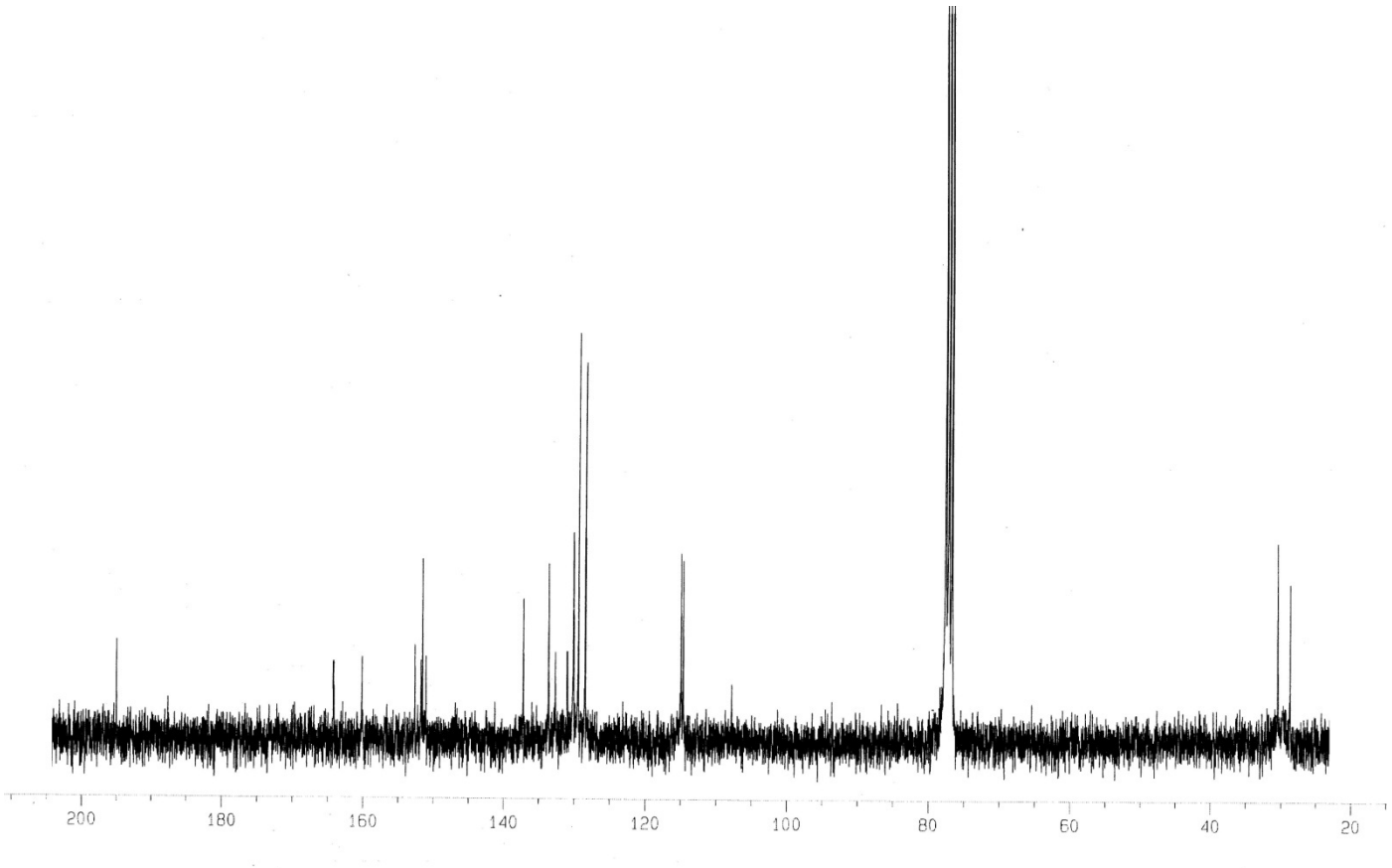


Fig S-28: ^{13}C NMR Spectrum of Product **4n**

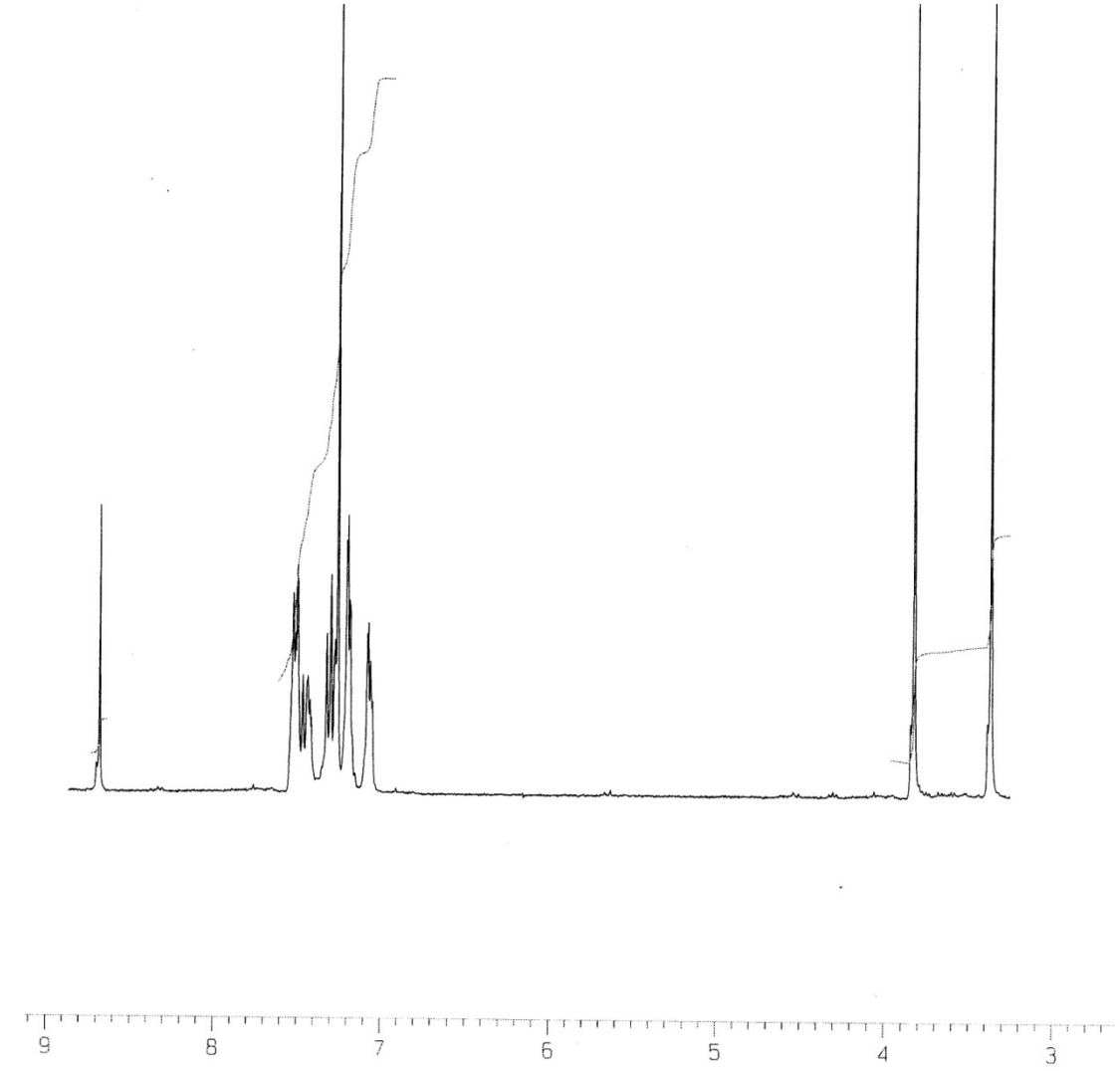


Fig S-29: ^{1}H NMR Spectrum of Product **4o**

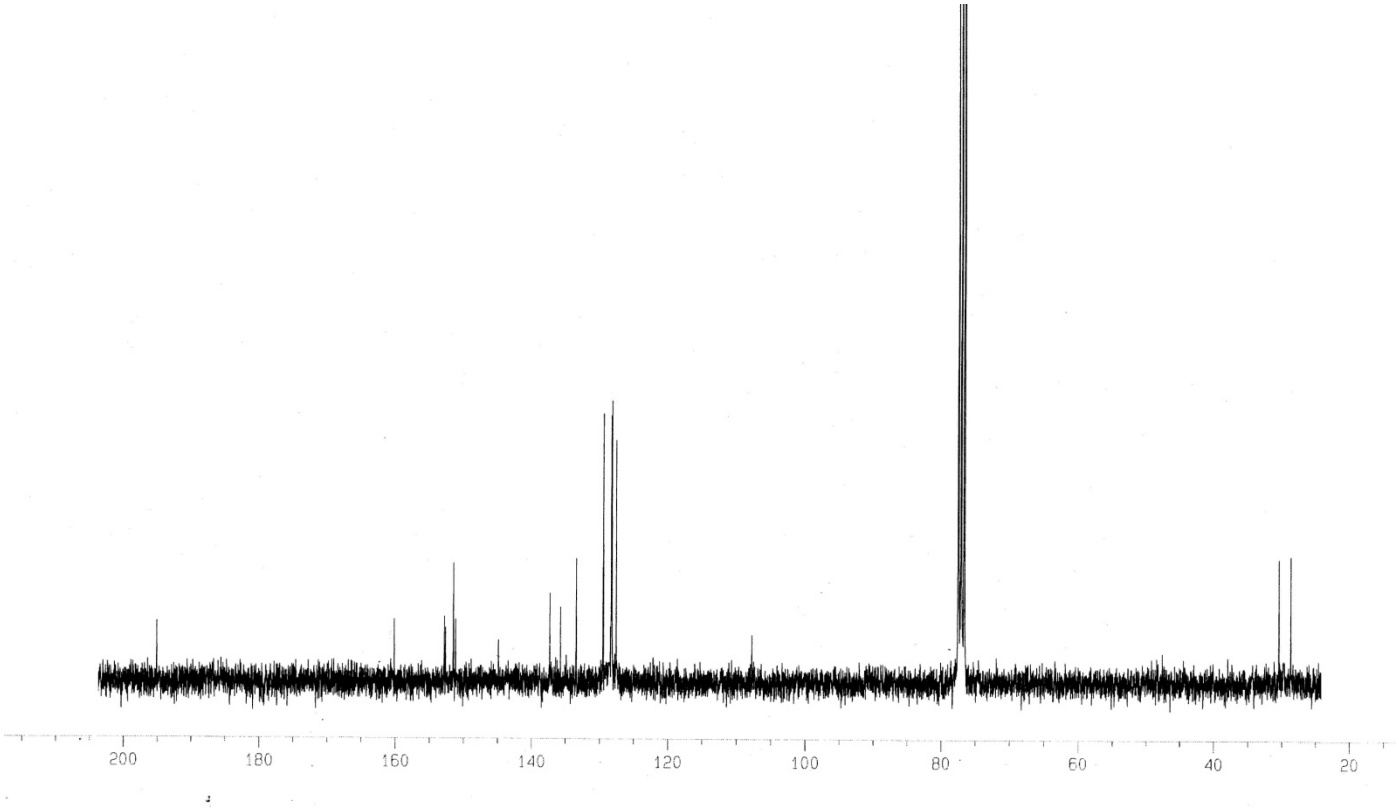


Fig S-30: ^{13}C NMR Spectrum of Product **4o**

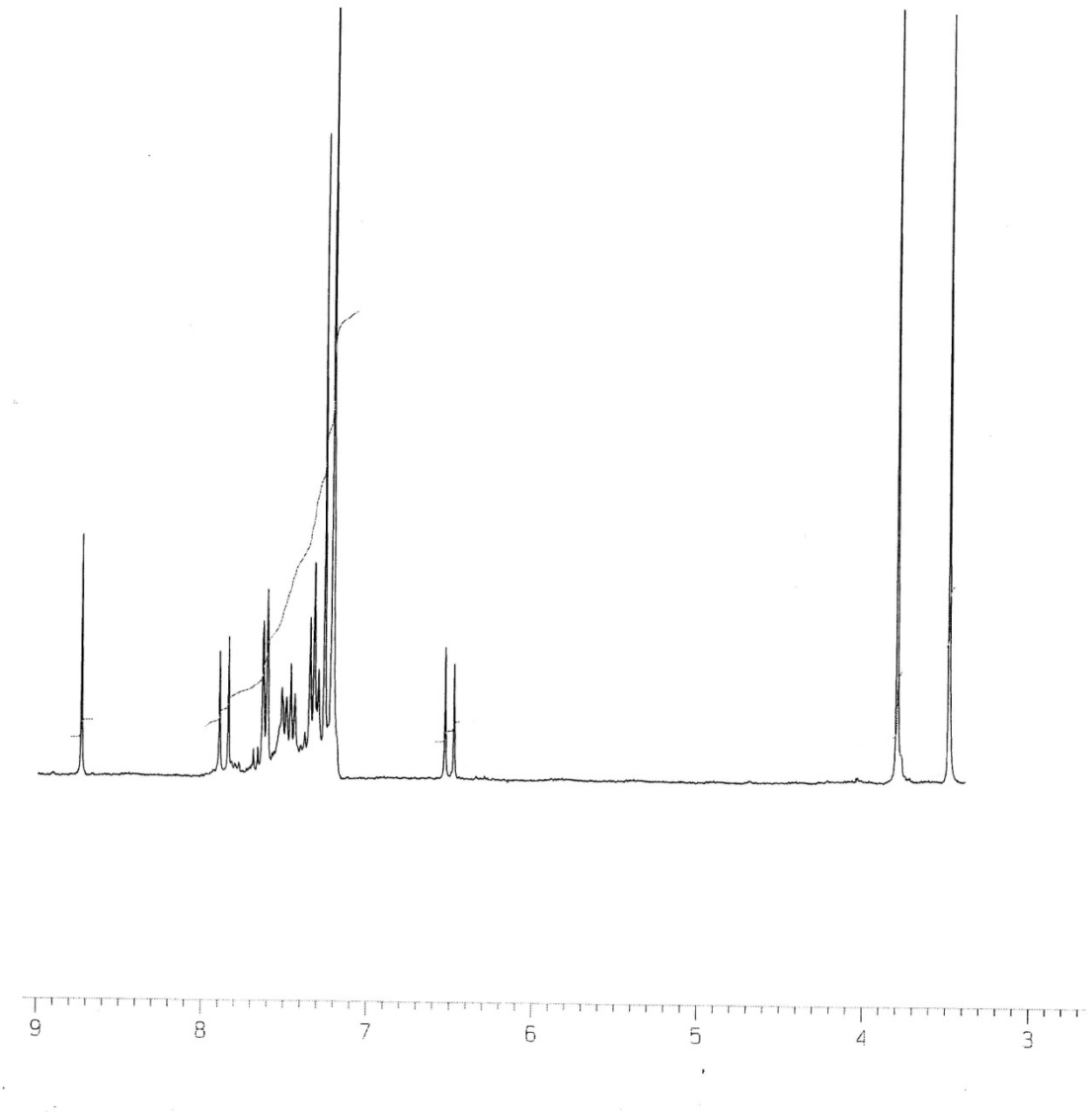


Fig S-31: ^{1}H NMR Spectrum of Product **4p**

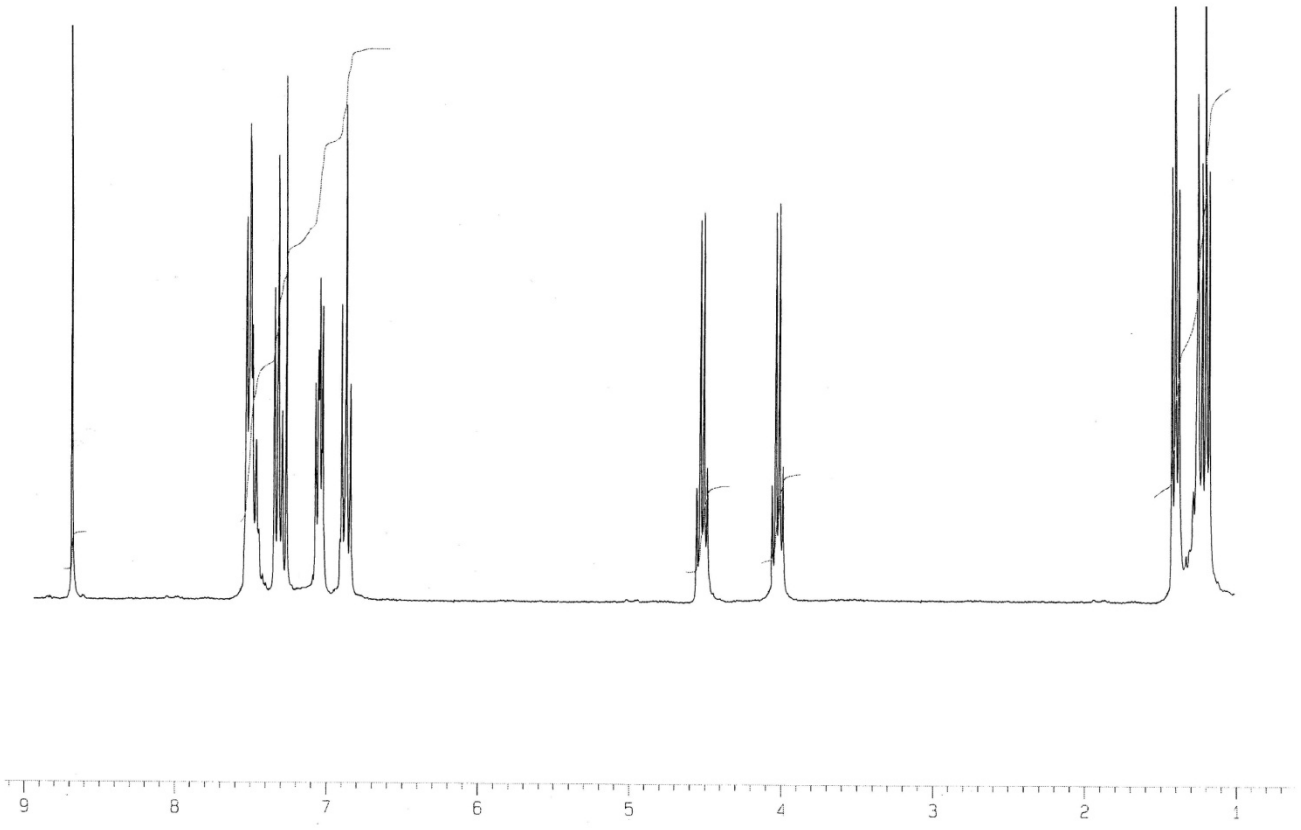


Fig S-32: ^{1}H NMR Spectrum of Product **4q**

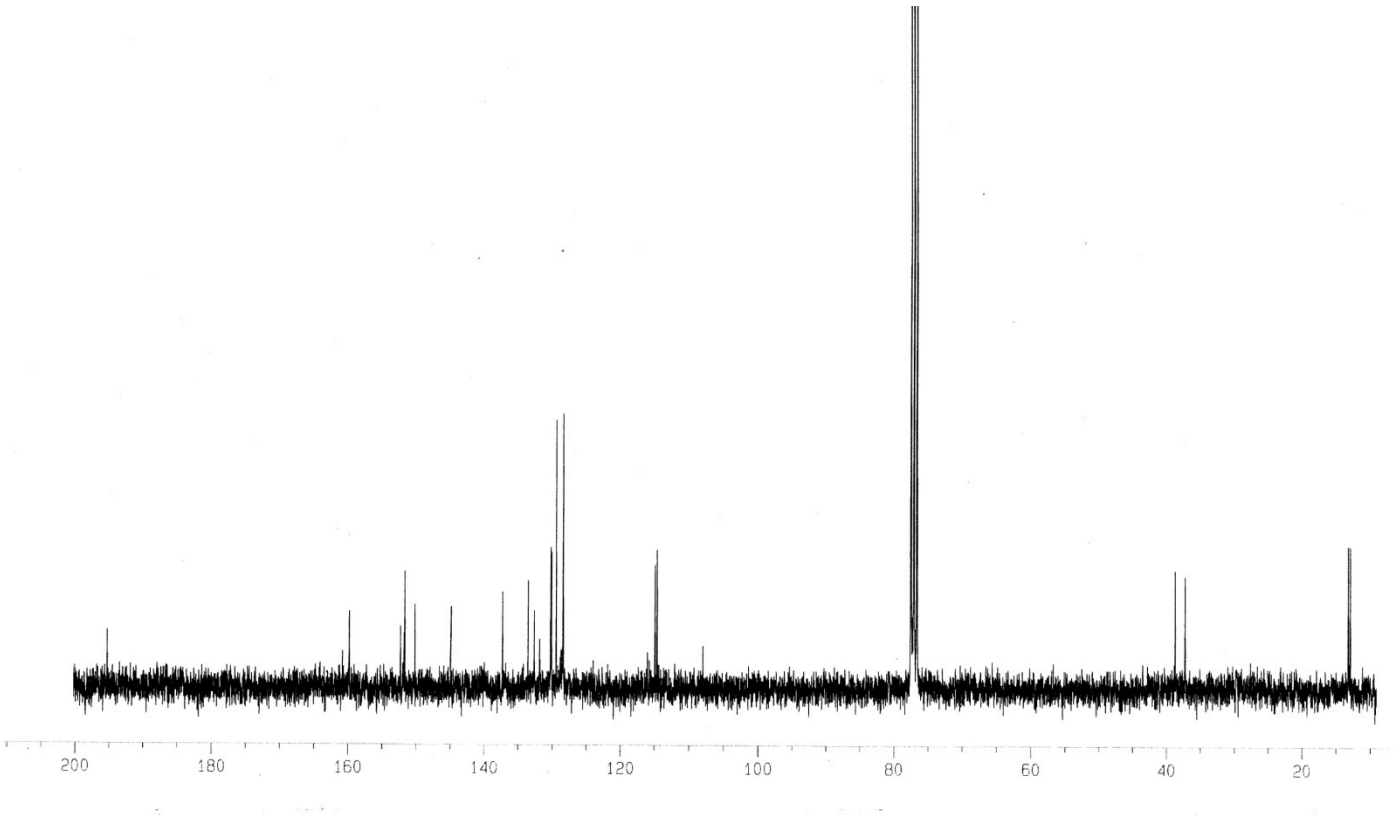


Fig S-33: ^{13}C NMR Spectrum of Product **4q**

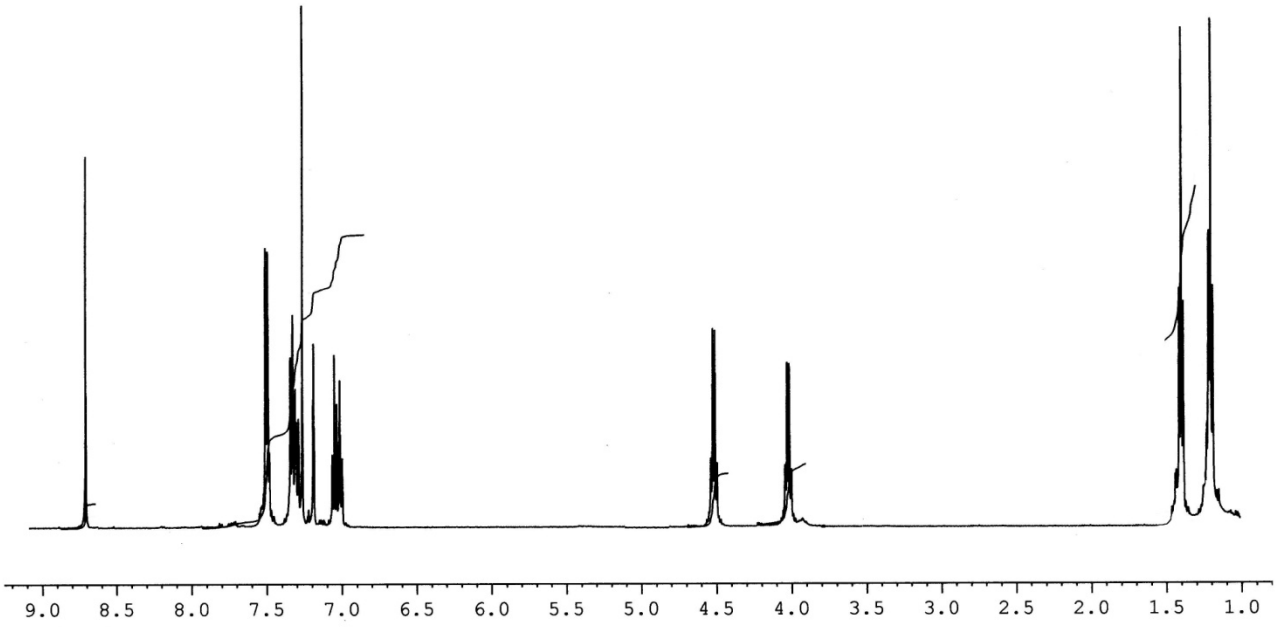


Fig S-34: ^{1}H NMR Spectrum of Product **4r**

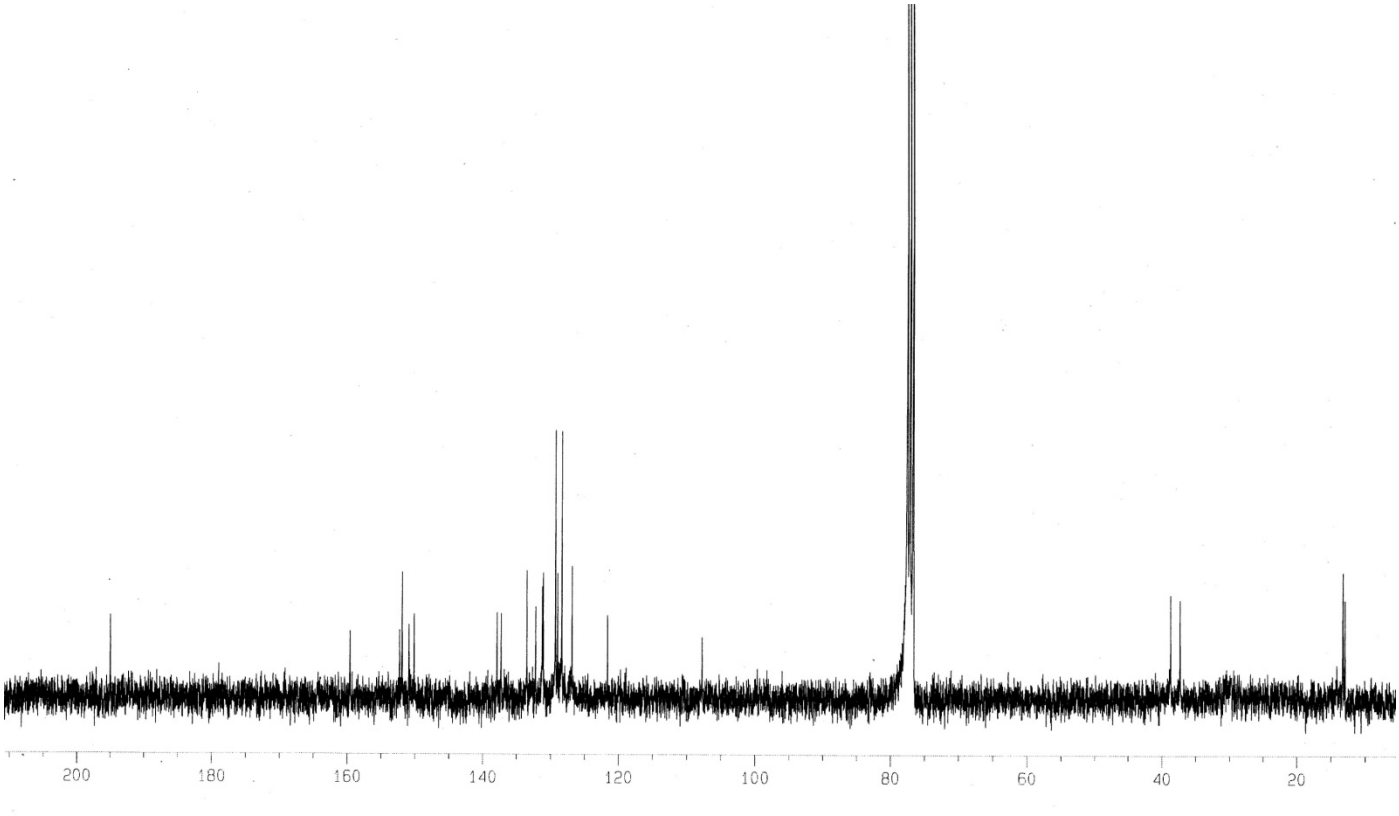


Fig S-35: ^{13}C NMR Spectrum of Product **4r**

§ ^{13}C spectra of compound **4d** shows one carbon peak less than expected which may be due to the partial solubility of the compound in $CDCl_3$ and because of hindered carbon.