Supporting Information

Utilization of Nitriles as the Nitrogen Source: Practical and Economical Construction of 4-Aminopyrimidine and β-Enaminonitrile Skeleton

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1. General Information

Unless otherwise stated, the reaction was carried out in a Teflon screw-cap sealed tube (50 ml) under N_2 atmosphere. All the commercial liquid-nitriles were distilled before use. Other commercial-grade chemicals were used without further purification. DME were dried over Na and degassed before use. Flash chromatography was performed on silica gel (200-300 mesh). The single crystal data of compounds were collected by a Cu-Kα rotating anode source at 100 K, using a Supernova diffractometer with the ω-scan method. ESI-MS were obtained using a Bruker Impact II quardrupole time-of-flight mass spectrometer. The ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Avance III (400 MHz) and chemical shifts are expressed in δ ppm values with reference to tetramethylsilane (TMS) as internal standard. The NMR spectra were recorded in solvent of $CDCl_3$ except for the last compound **4ag**, which was recorded in d_6-DMSO. Product yields refer to isolated yields after column chromatography.

2. General Experimental Procedures

a) General experimental procedure for the synthesis of 4-aminopyrimidines

Alkyl nitrile **1** (0.20 mmol), aryl nitrile **2** (0.60 mmol), LiHMDS (0.20 mmol) and dried DME (1 ml) were mixed in a 50 mL Teflon screw-cap sealed tube. The tube was charged with N_2 and the mixture was vigorously stirred at 120 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane (20 mL), filtered through a pad of silica gel and further concentrated under reduced pressure. The crude product was purified on a silica gel column (200-300 mesh) eluted with petroleum ether/acetone (10 : 1 v/v) to afford products **3**.

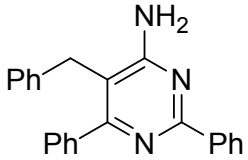
b) General experimental procedure for the synthesis of β-enaminonitriles

Alkyl nitrile **1** (0.20 mmol), aryl nitrile **2** (0.30 mmol), LiHMDS (0.20 mmol) and dried DME (1 ml) were mixed in a 50 mL Teflon screw-cap sealed tube. The tube was charged with N_2 and the mixture was vigorously stirred at 40 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane (20 mL), filtered through a pad of silica gel and further concentrated under reduced pressure. The crude product was purified on a silica gel column eluted with petroleum ether/acetone (8: 1 v/v) to afford products **4**.

c) General experimental procedure for the synthesis of variable substitution 4-aminopyrimidines

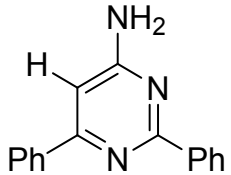
Alkyl nitrile **1** (0.20 mmol), aryl nitrile **2** (0.30 mmol), LiHMDS (0.20 mmol) and dried DME (1 ml) were mixed in a 50 mL Teflon screw-cap sealed tube. The tube was charged with N_2 and the mixture was vigorously stirred at 40 °C for 24 h. The intermediate **4a** was isolated on a silica column and mixed with a second portion of nitrile **2′** (0.3 mmol)/LiHMDS (0.20 mmol)/DME (1 ml) in a 50 mL Teflon screw-cap sealed tube. The tube was charged with N_2 again and the mixture was vigorously stirred at 120 °C for 24 h. After cooling to room temperature, the reaction mixture was diluted with dichloromethane (20 mL), filtered through a pad of silica gel. The crude product was purified on a silica gel column (200-300 mesh) eluted with petroleum ether/acetone (10 : 1 v/v) to afford the multi-substitution products **3**.

3. Characterization Data for the Products



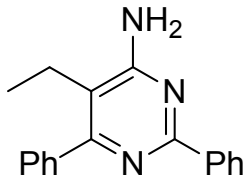
5-benzyl-2,6-diphenyl-4-aminopyrimidine (3a)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.65 (dt, *J* = 9.3, 3.3 Hz, 2H), 7.52 – 7.42 (m, 6H), 7.39 (t, *J* = 7.3 Hz, 2H), 7.31 (dd, *J* = 12.9, 5.6 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 2H), 4.91 (s, 2H), 4.05 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.21, 163.28, 162.27, 139.07, 138.17, 137.78, 130.11, 129.21, 128.88, 128.82, 128.31, 128.11, 127.86, 127.01, 110.04, 33.28. HRMS m/z (ESI) [M + H^+] calcd for $C_{23}H_{19}N_3$ + H^+: 338.1657. Found, 338.1652.



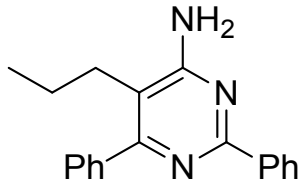
2,6-diphenyl-4-aminopyrimidine (3b)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 7.4, 2.2 Hz, 2H), 8.15 (dd, *J* = 7.3, 2.2 Hz, 2H), 7.62 – 7.44 (m, 6H), 6.74 (d, *J* = 2.0 Hz, 1H), 5.09 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.53, 164.24, 163.63, 138.44, 137.80, 130.50, 130.38, 128.83, 128.52, 128.38, 127.14, 98.58. HRMS m/z (ESI) [M + H^+] calcd for $C_{16}H_{13}N_3$ + H^+: 248.1187. found, 248.1182.



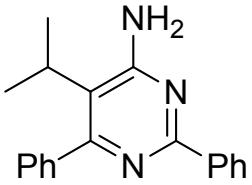
5-ethyl-2,6-diphenyl-4-aminopyrimidine (3c)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 – 8.41 (m, 2H), 7.68 – 7.58 (m, 2H), 7.58 – 7.43 (m, 6H), 5.33 (s, 2H), 2.53 (q, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.25, 162.74, 161.56, 139.74, 138.54, 130.04, 128.77, 128.61, 128.42, 128.34, 128.21, 114.28, 20.12, 12.83. HRMS m/z (ESI) [M + H^+] calcd for $C_{18}H_{17}N_3$ + H^+: 276.1500. found, 276.1495.



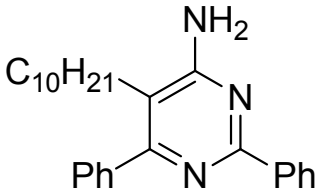
5-propyl-2,6-diphenyl-4-aminopyrimidine (3d)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.38 (m, 2H), 7.60 (d, *J* = 6.8 Hz, 2H), 7.50 (dd, *J* = 15.9, 6.7 Hz, 6H), 5.24 (s, 2H), 2.63 – 2.41 (m, 2H), 1.73 – 1.51 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.57, 162.74, 161.40, 139.77, 138.36, 129.93, 128.77, 128.44, 128.29, 128.21, 128.10, 112.96, 28.95, 21.48, 14.27. HRMS m/z (ESI) [M + H^+] calcd for $C_{19}H_{19}N_3$ + H^+: 290.1657. found, 290.1653.



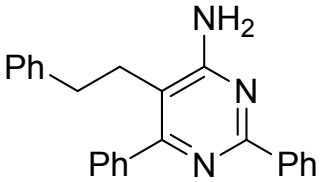
5-isopropyl-2,6-diphenyl-4-aminopyrimidine (3e)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.38 (m, 2H), 7.53 (tdd, *J* = 3.9, 2.7, 1.4 Hz, 2H), 7.51 – 7.42 (m, 6H), 5.30 (s, 2H), 3.37 – 3.24 (m, 1H), 1.29 (s, 3H), 1.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.72, 162.23, 161.14, 140.48, 138.22, 129.92, 128.63, 128.33, 128.26, 128.24, 128.10, 117.38, 27.07, 20.03. HRMS m/z (ESI) [M + H^+] calcd for $C_{19}H_{19}N_3$ + H^+: 290.1657. found, 290.1652.



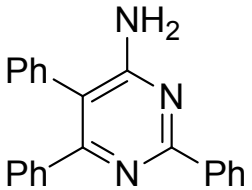
5-decyl-2,6-diphenyl-4-aminopyrimidine (3f)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.41 (m, 2H), 7.65 – 7.57 (m, 2H), 7.56 – 7.42 (m, 6H), 5.29 (s, 2H), 2.58 – 2.42 (m, 2H), 1.55 (dt, *J* = 22.8, 11.3 Hz, 2H), 1.32 (dd, *J* = 32.1, 13.9 Hz, 14H), 1.01 – 0.89 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.46, 162.72, 161.37, 139.75, 138.39, 129.90, 128.78, 128.44, 128.28, 128.19, 128.11, 113.15, 31.96, 29.66, 29.60, 29.55, 29.37, 29.21, 28.05, 26.80, 22.75, 14.21. HRMS m/z (ESI) [M + H^+] calcd for $C_{26}H_{33}N_3$ + H^+: 388.2752. found, 388.2747.



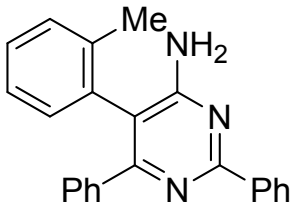
5-phenethyl-2,6-diphenyl-4-aminopyrimidine (3g)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.38 (m, 2H), 7.55 – 7.43 (m, 8H), 7.33 – 7.20 (m, 3H), 7.09 – 7.00 (m, 2H), 5.07 (s, 2H), 2.99 – 2.70 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.24, 162.66, 161.65, 140.80, 139.50, 138.22, 130.02, 128.68, 128.56, 128.47, 128.30, 128.25, 128.12, 126.39, 112.09, 34.28, 29.00. HRMS m/z (ESI) [M + H^+] calcd for $C_{24}H_{21}N_3$ + H^+: 352.1813. found, 352.1810.



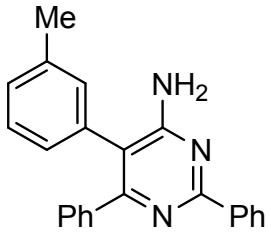
2,5,6-triphenyl-4-aminopyrimidine (3h)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (dt, *J* = 5.1, 3.2 Hz, 2H), 7.50 – 7.40 (m, 5H), 7.40 – 7.28 (m, 3H), 7.26 – 7.17 (m, 5H), 5.00 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.86, 162.32, 162.26, 138.77, 138.18, 135.13, 130.32, 130.21, 129.86, 129.38, 128.47, 128.31, 128.17, 127.98, 127.69, 114.34. HRMS m/z (ESI) [M + H^+] calcd for $C_{22}H_{17}N_3$ + H^+: 324.1500. found, 324.1495.



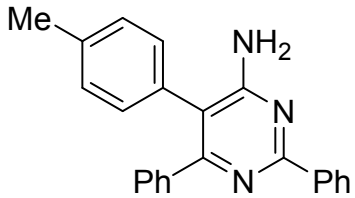
2,6-diphenyl-5-(*o*-tolyl)-4-aminopyrimidine (3i)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (dd, *J* = 7.1, 2.0 Hz, 2H), 7.59 – 7.46 (m, 5H), 7.35 – 7.18 (m, 7H), 4.96 (s, 2H), 2.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.02, 162.34, 161.83, 138.87, 138.22, 137.35, 134.14, 131.02, 130.68, 130.25, 129.31, 128.68, 128.57, 128.35, 128.17, 127.74, 126.89, 113.56, 19.55. HRMS m/z (ESI) [M + H$^+$] calcd for $C_{23}H_{19}N_3$ + H$^+$: 338.1657. Found, 338.1652.



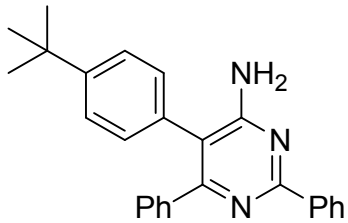
2,6-diphenyl-5-(*m*-tolyl)-4-aminopyrimidine (3j)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (dd, 2H), 7.57 – 7.45 (m, 5H), 7.32 – 7.21 (m, 4H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.10 (s, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 5.05 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.73, 162.40, 162.02, 139.08, 138.84, 138.25, 135.02, 130.72, 130.16, 129.86, 129.27, 128.74, 128.45, 128.30, 128.16, 127.66, 127.37, 114.47, 21.46.



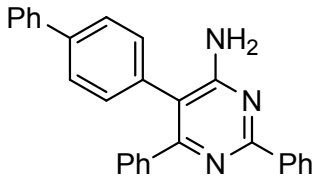
2,6-diphenyl-5-(*p*-tolyl)-4-aminopyrimidine (3k)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 – 8.39 (m, 2H), 7.54 – 7.45 (m, 5H), 7.31 – 7.18 (m, 5H), 7.15 (d, *J* = 8.1 Hz, 2H), 5.03 (s, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.69, 162.50, 162.16, 138.91, 138.24, 137.72, 131.93, 130.14, 130.10, 129.87, 128.39, 128.29, 128.14, 127.67, 114.33, 21.30. HRMS m/z (ESI) [M + H$^+$] calcd for $C_{23}H_{19}N_3$ + H$^+$: 338.1657. Found, 338.1652.



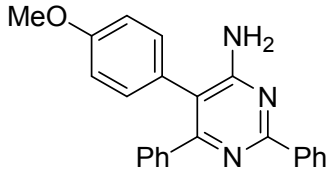
5-(4-(*tert*-butyl)phenyl)-2,6-diphenyl-4-aminopyrimidine (3l)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 – 8.44 (m, 2H), 7.53 – 7.44 (m, 5H), 7.44 – 7.38 (m, 2H), 7.31 – 7.22 (m, 3H), 7.20 (ddd, *J* = 8.4, 5.2, 1.8 Hz, 2H), 5.04 (s, 2H), 1.35 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.68, 162.52, 162.12, 151.03, 138.87, 138.26, 131.89, 130.13, 129.90, 129.87, 128.39, 128.29, 128.13, 127.60, 126.26, 114.31, 34.66, 31.32. HRMS m/z (ESI) [M + H$^+$] calcd for $C_{26}H_{25}N_3$ + H$^+$: 380.2126. found, 380.2120.



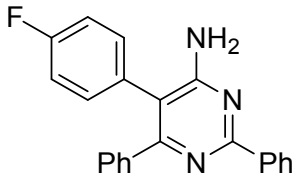
5-([1,1'-biphenyl]-4-yl)-2,6-diphenyl-4-aminopyrimidine (3m)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.48 (m, 2H), 7.70 – 7.61 (m, 4H), 7.55 – 7.45 (m, 7H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.26 (ddd, *J* = 8.8, 5.1, 3.2 Hz, 3H), 5.06 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.89, 162.34, 140.60, 140.22, 138.77, 138.16, 134.08, 130.75, 130.24, 129.90, 128.92, 128.52, 128.32, 128.18, 127.95, 127.77, 127.67, 126.98, 113.97.



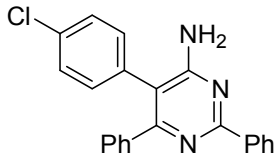
5-(4-methoxyphenyl)-2,6-diphenyl-4-aminopyrimidine (3n)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 – 8.46 (m, 2H), 7.53 – 7.45 (m, 5H), 7.31 – 7.23 (m, 3H), 7.20 – 7.14 (m, 2H), 6.99 – 6.82 (m, 2H), 5.04 (s, 2H), 3.85 (d, *J* = 6.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.67, 162.65, 162.27, 159.20, 138.92, 138.23, 131.45, 130.14, 129.85, 128.38, 128.30, 128.14, 127.71, 126.91, 114.84, 114.02, 55.28. HRMS m/z (ESI) [M + H^+] calcd for $C_{23}H_{19}ON_3$ + H^+: 354.1606. found, 354.1600.



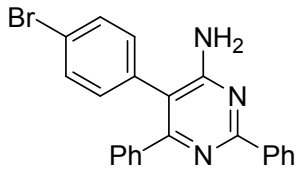
5-(4-fluorophenyl)-2,6-diphenyl-4-aminopyrimidine (3o)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (dd, *J* = 5.1, 2.3 Hz, 2H), 7.51 (dd, *J* = 6.9, 3.3 Hz, 3H), 7.47 – 7.42 (m, 2H), 7.31 – 7.20 (m, 5H), 7.13 – 7.06 (m, 2H), 5.06 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.56, 163.00, 162.61, 162.34, 161.09, 138.63, 138.07, 132.18, 132.10, 130.97, 130.93, 130.32, 129.80, 128.57, 128.34, 128.20, 127.80, 116.62, 116.41, 113.32. HRMS m/z (ESI) [M + H^+] calcd for $C_{22}H_{16}FN_3$ + H^+: 342.1406. found, 342.1402.



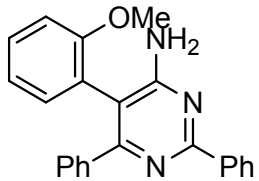
5-(4-chlorophenyl)-2,6-diphenyl-4-aminopyrimidine (3p)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 – 8.42 (m, 2H), 7.51 – 7.44 (m, 3H), 7.41 (ddd, *J* = 6.4, 5.3, 2.9 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.28 – 7.22 (m, 3H), 7.20 – 7.14 (m, 2H), 4.96 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.10, 162.58, 162.08, 138.48, 137.97, 134.00, 133.63, 131.75, 130.35, 129.79, 129.68, 128.65, 128.33, 128.18, 127.86, 113.10. HRMS m/z (ESI) [M + H^+] calcd for $C_{22}H_{16}ClN_3$ + H^+: 358.1111. found, 358.1106.



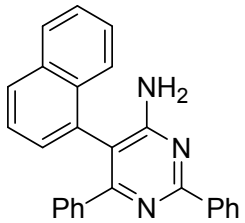
5-(4-bromophenyl)-2,6-diphenyl-4-aminopyrimidine (3q)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (dt, *J* = 4.9, 2.8 Hz, 2H), 7.56 – 7.47 (m, 5H), 7.43 (dt, *J* = 11.6, 5.6 Hz, 2H), 7.34 – 7.21 (m, 3H), 7.18 – 7.10 (m, 2H), 5.01 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.11, 162.52, 162.01, 138.46, 137.97, 134.13, 132.63, 132.06, 130.37, 129.80, 128.67, 128.35, 128.19, 127.88, 122.16, 113.11.



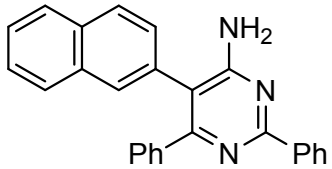
5-(2-methoxyphenyl)-2,6-diphenyl-4-aminopyrimidine (3r)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (dt, *J* = 5.2, 3.7 Hz, 2H), 7.52 – 7.44 (m, 5H), 7.35 (ddd, *J* = 9.1, 6.8, 2.7 Hz, 1H), 7.27 – 7.19 (m, 3H), 7.15 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.98 (dd, *J* = 7.5, 0.8 Hz, 1H), 6.94 (dd, *J* = 8.9, 4.6 Hz, 1H), 4.95 (s, 2H), 3.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.22, 162.91, 162.44, 157.21, 139.40, 138.34, 131.74, 130.06, 129.91, 129.04, 128.34, 128.25, 128.16, 127.53, 123.70, 121.39, 111.54, 111.09, 55.43.



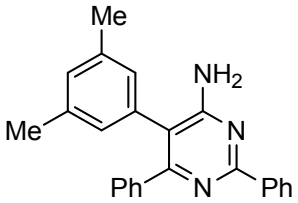
5-(naphthalen-1-yl)-2,6-diphen-4-aminoylpyrimidine (3s)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (dt, *J* = 5.1, 3.1 Hz, 2H), 7.93 (t, *J* = 7.9 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.78 (t, *J* = 10.4 Hz, 1H), 7.60 – 7.49 (m, 5H), 7.50 – 7.42 (m, 1H), 7.39 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.34 – 7.29 (m, 1H), 7.21 – 7.14 (m, 1H), 7.13 – 7.06 (m, 2H), 4.77 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.33, 162.64, 138.79, 138.14, 133.91, 132.48, 131.65, 130.32, 129.09, 128.91, 128.80, 128.77, 128.57, 128.36, 128.20, 127.64, 127.08, 126.48, 126.12, 125.13, 112.40. HRMS m/z (ESI) [M + H^+] calcd for $C_{26}H_{19}N_3$ + H^+: 374.1657. found, 374.1652.



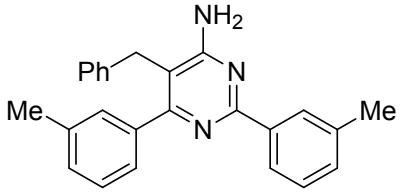
5-(naphthalen-2-yl)-2,6-diphenyl-4-aminopyrimidine (3t)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 – 8.49 (m, 2H), 7.92 – 7.79 (m, 4H), 7.58 – 7.47 (m, 7H), 7.29 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.26 – 7.14 (m, 3H), 5.04 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.92, 162.46, 162.38, 138.72, 138.17, 133.64, 132.70, 132.67, 130.25, 129.90, 129.21, 128.52, 128.33, 128.20, 128.13, 127.97, 127.86, 127.77, 126.56, 126.53, 114.18.



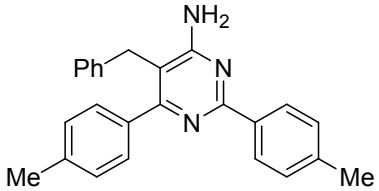
5-(3,5-dimethylphenyl)-2,6-diphenyl-4-aminopyrimidine (3u)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 – 8.42 (m, 2H), 7.61 – 7.44 (m, 5H), 7.33 – 7.18 (m, 4H), 6.96 (d, *J* = 9.2 Hz, 1H), 6.87 (s, 2H), 4.98 (s, 2H), 2.29 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.59, 162.43, 161.79, 138.92, 138.84, 138.27, 134.89, 130.10, 129.83, 129.60, 128.42, 128.28, 128.11, 127.79, 127.61, 114.58, 21.32.



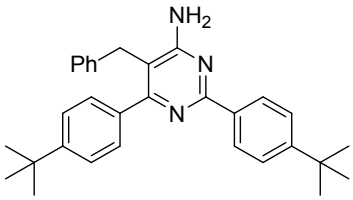
5-benzyl-2,6-di-*m*-tolyl-4-aminopyrimidine (3aa)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 – 8.17 (m, 2H), 7.47 (d, *J* = 15.5 Hz, 1H), 7.39 (dd, *J* = 14.0, 6.8 Hz, 4H), 7.35 – 7.26 (m, 4H), 7.24 (d, *J* = 7.4 Hz, 2H), 4.93 (s, 2H), 4.03 (s, 2H), 2.47 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.50, 163.20, 162.44, 139.06, 138.17, 138.04, 137.97, 137.87, 130.89, 129.60, 129.16, 128.69, 128.25, 128.11, 127.86, 126.94, 125.71, 125.34, 110.08, 33.30, 21.56. HRMS m/z (ESI) [M + H^+] calcd for $C_{25}H_{23}N_3$ + H^+: 366.1970. found, 366.1965.



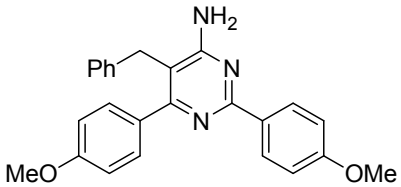
5-benzyl-2,6-di-*p*-tolyl-4-aminopyrimidine (3ab)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.37 (t, *J* = 7.3 Hz, 2H), 7.34 – 7.20 (m, 7H), 4.82 (s, 2H), 4.05 (s, 2H), 2.43 (d, *J* = 9.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.17, 163.19, 162.24, 140.11, 138.75, 137.95, 136.27, 135.47, 129.16, 129.02, 128.95, 128.75, 128.02, 127.86, 126.92, 109.62, 33.33, 21.50, 21.34. HRMS m/z (ESI) [M + H^+] calcd for $C_{25}H_{23}N_3$ + H^+: 366.1970. found, 366.1965.



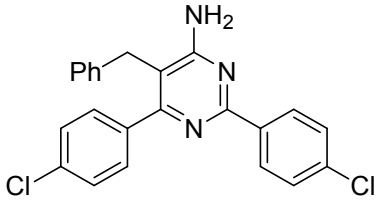
5-benzyl-2,6-bis(4-(*tert*-butyl)phenyl)-4-aminopyrimidine (3ac)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.2 Hz, 2H), 7.61 (d, *J* = 7.9 Hz, 2H), 7.47 (dd, *J* = 13.0, 8.3 Hz, 4H), 7.39 (t, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 7.1 Hz, 1H), 7.29 – 7.24 (m, 2H), 4.86 (s, 2H), 4.08 (s, 2H), 1.38 (d, *J* = 8.8 Hz, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.05, 163.24, 162.31, 153.18, 151.86, 138.05, 136.22, 135.53, 129.17, 128.59, 127.90, 127.84, 126.93, 125.24, 125.20, 109.57, 34.80, 34.73, 33.39, 31.33. HRMS m/z (ESI) [M + H^+] calcd for $C_{31}H_{35}N_3$ + H^+: 450.2909. found, 450.2904.



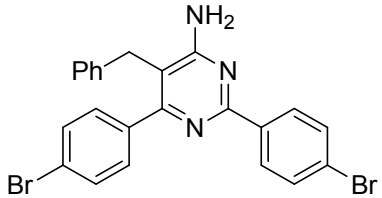
5-benzyl-2,6-bis(4-methoxyphenyl)-4-aminopyrimidine (3ad)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.38 (m, 2H), 7.61 (d, *J* = 8.8 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 2H), 7.03 – 6.89 (m, 4H), 4.76 (s, 2H), 4.05 (d, *J* = 11.3 Hz, 2H), 3.89 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.71, 163.28, 161.95, 161.40, 160.25, 138.04, 131.64, 130.98, 130.37, 129.68, 129.26, 127.91, 127.01, 113.71, 113.62, 108.98, 55.43, 33.43. HRMS m/z (ESI) [M + H^+] calcd for $C_{25}H_{23}O_2N_3$ + H^+: 398.1868. found, 398.1862.



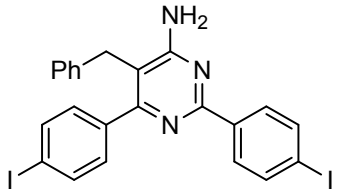
5-benzyl-2,6-bis(4-chlorophenyl)-4-aminopyrimidine (3ae)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.35 (m, 6H), 7.32 (t, *J* = 6.2 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 2H), 4.87 (s, 2H), 4.01 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.10, 163.34, 161.39, 137.32, 136.50, 136.41, 135.21, 130.24, 129.49, 129.40, 128.64, 128.58, 127.80, 127.27, 110.20, 33.27. HRMS m/z (ESI) [M + H^+] calcd for $C_{23}H_{17}Cl_2N_3$ + H^+: 406.0877. found, 406.0872.



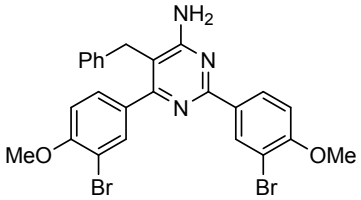
5-benzyl-2,6-bis(4-bromophenyl)-4-aminopyrimidine (3af)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.5 Hz, 2H), 7.58 (dd, *J* = 10.1, 8.6 Hz, 4H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 2H), 7.32 (t, *J* = 6.7 Hz, 1H), 7.22 (d, *J* = 7.3 Hz, 2H), 4.88 (s, 2H), 4.01 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.08, 163.28, 161.40, 137.73, 137.23, 136.88, 131.52, 131.46, 130.44, 129.70, 129.33, 127.72, 127.20, 124.90, 123.44, 110.18, 33.20. HRMS m/z (ESI) [M + H^+] calcd for $C_{23}H_{17}Br_2N_3$ + H^+: 496.9880. found, 496.9873.



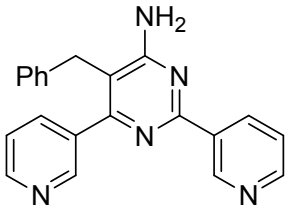
5-benzyl-2,6-bis(4-iodophenyl)-4-aminopyrimidine (3ag)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.5 Hz, 2H), 7.79 (dd, *J* = 11.6, 8.5 Hz, 4H), 7.41 – 7.30 (m, 5H), 7.21 (d, *J* = 7.2 Hz, 2H), 4.88 (s, 2H), 4.00 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.17, 163.27, 161.55, 138.32, 137.48, 137.23, 130.57, 129.82, 129.32, 127.72, 127.20, 110.23, 97.20, 95.33, 33.21.



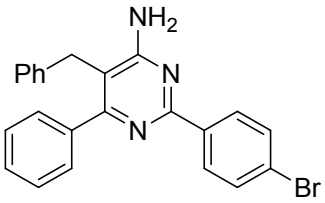
5-benzyl-2,6-bis(3-bromo-4-methoxyphenyl)-4-aminopyrimidine (3ah)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 2.0 Hz, 1H), 8.41 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.88 (d, *J* = 2.1 Hz, 1H), 7.55 – 7.47 (m, 1H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.31 (t, *J* = 5.8 Hz, 1H), 7.22 (d, *J* = 7.2 Hz, 2H), 6.98 (d, *J* = 8.7 Hz, 1H), 6.91 (d, *J* = 8.5 Hz, 1H), 4.85 (s, 2H), 4.03 (s, 2H), 3.98 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.38, 163.23, 160.72, 157.44, 156.46, 137.51, 134.03, 133.08, 132.63, 131.98, 129.28, 128.97, 128.56, 127.74, 127.10, 111.66, 111.57, 111.27, 111.24, 109.58, 56.36, 33.24.



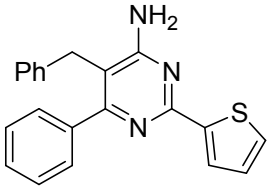
5-benzyl-2,6-di(pyridin-3-yl)-4-aminopyrimidine (3ai)

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 8.87 (t, *J* = 6.6 Hz, 1H), 8.75 – 8.65 (m, 3H), 8.02 – 7.90 (m, 1H), 7.40 (ddd, *J* = 9.8, 8.1, 5.4 Hz, 4H), 7.32 (t, *J* = 4.9 Hz, 1H), 7.23 (d, *J* = 7.0 Hz, 2H), 4.94 (d, *J* = 59.2 Hz, 2H), 4.05 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.36, 162.18, 160.70, 150.95, 150.08, 149.76, 149.57, 136.81, 136.31, 135.45, 134.48, 133.30, 129.41, 127.70, 127.36, 123.25, 111.08, 33.14. HRMS m/z (ESI) [M + H$^+$] calcd for $C_{21}H_{17}N_5$ + H$^+$: 340.1562. found, 340.1557.



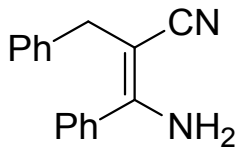
5-benzyl-2-(4-bromophenyl)-6-phenyl-4-aminepyrimidine (3aj)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.33 (m, 2H), 7.61 (dt, *J* = 8.2, 2.1 Hz, 3H), 7.59 – 7.57 (m, 1H), 7.44 (dd, *J* = 6.5, 3.7 Hz, 3H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 7.2 Hz, 2H), 4.84 (s, 2H), 4.04 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.24, 163.23, 161.28, 138.87, 137.60, 137.09, 131.41, 129.74, 129.23, 128.94, 128.74, 128.32, 127.81, 127.06, 124.74, 110.32, 33.28.



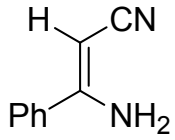
5-benzyl-6-phenyl-2-(thiophen-2-yl)-4-aminopyrimidine (3ak)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 3.6 Hz, 1H), 7.61 (dd, *J* = 6.6, 2.8 Hz, 2H), 7.46 – 7.40 (m, 4H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 5.0 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.16 – 7.10 (m, 1H), 4.83 (s, 2H), 4.02 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.12, 163.04, 159.01, 143.98, 138.67, 137.71, 129.20, 128.92, 128.79, 128.27, 128.22, 127.92, 127.81, 127.01, 109.71, 33.26.



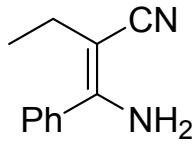
3-amino-2-benzyl-3-phenylacrylonitrile (4a)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.57 (m, 2H), 7.49 – 7.41 (m, 3H), 7.40 – 7.34 (m, 4H), 7.33 – 7.26 (m, 1H), 4.43 (s, 2H), 3.60 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.51, 137.73, 136.06, 130.33, 128.91, 128.76, 128.04, 128.03, 126.94, 123.41, 78.15, 34.51. HRMS m/z (ESI) [M + H$^+$] calcd for $C_{16}H_{14}N_2$ + H$^+$: 235.1235. found, 235.1228.



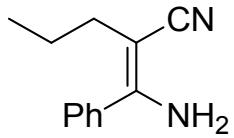
3-amino-3-phenylacrylonitrile (4b)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (q, *J* = 2.0 Hz, 1H), 7.52 (t, *J* = 2.0 Hz, 1H), 7.51 – 7.48 (m, 1H), 7.47 (t, *J* = 1.8 Hz, 1H), 7.46 – 7.43 (m, 1H), 5.16 – 4.84 (m, 2H), 4.28 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.52, 135.37, 130.99, 129.04, 126.02, 119.50, 63.82. HRMS m/z (ESI) [M + Na$^+$] calcd for $C_9H_8N_2$ + Na$^+$: 167.0585. found, 167.0580.



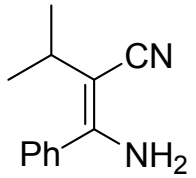
2-(amino(phenyl)methylene)butanenitrile (4c)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.56 (m, 2H), 7.47 – 7.42 (m, 3H), 4.33 (s, 2H), 2.29 – 2.16 (m, 2H), 1.27 (dd, *J* = 9.6, 5.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.56, 136.38, 130.07, 128.71, 127.96, 122.32, 81.94, 21.06, 12.25. HRMS m/z (ESI) [M + Na$^+$] calcd for $C_{11}H_{12}N_2$ + Na$^+$: 195.0898. found, 195.0893.



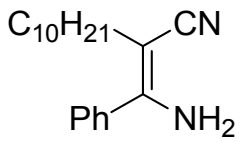
2-(amino(phenyl)methylene)pentanenitrile (4d)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.54 (m, 2H), 7.47 – 7.39 (m, 3H), 4.53 – 4.22 (m, 2H), 2.20 – 2.10 (m, 2H), 1.75 – 1.62 (m, 2H), 1.05 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.22, 136.47, 130.04, 128.67, 127.99, 122.79, 80.19, 29.85, 21.12, 13.79. HRMS m/z (ESI) [M + Na$^+$] calcd for $C_{12}H_{14}N_2$ + Na$^+$: 209.1049. found, 209.1054.



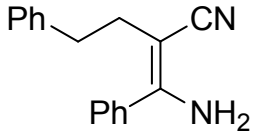
2-(amino(phenyl)methylene)-3-methylbutanenitrile (4e)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.54 (m, 2H), 7.48 – 7.40 (m, 3H), 4.34 (s, 2H), 2.55 (hept, *J* = 6.8 Hz, 1H), 1.25 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.55, 136.66, 130.01, 128.68, 128.07, 120.91, 88.05, 26.49, 21.24. HRMS m/z (ESI) [M + Na$^+$] calcd for $C_{12}H_{14}N_2$ + Na$^+$: 209.1049. found, 209.1054.



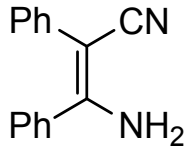
2-(amino(phenyl)methylene)dodecanenitrile (4f)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.54 (m, 2H), 7.50 – 7.40 (m, 3H), 4.32 (s, 2H), 2.22 – 2.14 (m, 2H), 1.71 – 1.63 (m, 2H), 1.47 – 1.26 (m, 14H), 0.91 (t, *J* = 6.8 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 155.88, 136.44, 130.05, 128.69, 127.99, 122.64, 80.73, 31.93, 29.63, 29.49, 29.35, 27.94, 27.80, 22.71, 14.15. HRMS m/z (ESI) [M + Na^+] calcd for $C_{19}H_{28}N_2$ + Na^+: 307.2150. found, 307.2145.



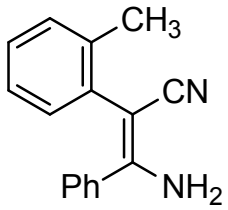
2-(amino(phenyl)methylene)-4-phenylbutanenitrile (4g)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.49 (m, 2H), 7.46 – 7.40 (m, 3H), 7.39 – 7.25 (m, 5H), 4.14 (s, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.48 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.85, 141.09, 136.40, 130.15, 128.70, 128.64, 128.62, 127.96, 126.39, 122.75, 79.36, 34.14, 30.43. HRMS m/z (ESI) [M + Na^+] calcd for $C_{17}H_{16}N_2$ + Na^+: 271.1211. found, 271.1206.



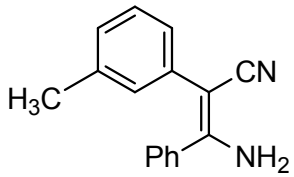
3-amino-2,3-diphenylacrylonitrile (4h)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.69 (m, 2H), 7.55 (ddd, *J* = 5.2, 3.7, 1.8 Hz, 2H), 7.53 – 7.44 (m, 5H), 7.36 – 7.30 (m, 1H), 4.92 (d, *J* = 73.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.97, 136.03, 133.99, 130.64, 129.45, 128.89, 128.68, 128.07, 127.52, 122.17, 81.96. HRMS m/z (ESI) [M + Na^+] calcd for $C_{15}H_{12}N_2$ + Na^+: 243.0898. found, 243.0893.



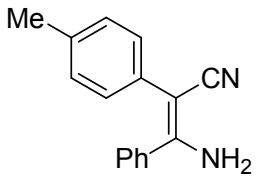
3-amino-3-phenyl-2-(*o*-tolyl)acrylonitrile (4i)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 2H), 7.54 – 7.49 (m, 3H), 7.43 – 7.39 (m, 1H), 7.36 – 7.29 (m, 3H), 4.41 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.35, 138.18, 135.42, 131.94, 131.11, 130.78, 130.61, 128.88, 128.74, 128.02, 126.91, 121.46, 80.72, 19.50. HRMS m/z (ESI) [M + Na^+] calcd for $C_{16}H_{14}N_2$ + Na^+: 257.1054. found, 257.1049.



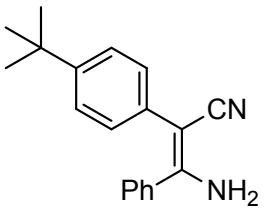
3-amino-3-phenyl-2-(*m*-tolyl)acrylonitrile (4j)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.67 (m, 2H), 7.54 – 7.46 (m, 3H), 7.40 – 7.33 (m, 3H), 7.14 (dd, *J* = 5.6, 2.4 Hz, 1H), 4.83 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.91, 139.29, 136.09, 133.87, 130.57, 129.35, 129.28, 128.86, 128.30, 128.06, 125.55, 122.31, 81.94, 21.48.



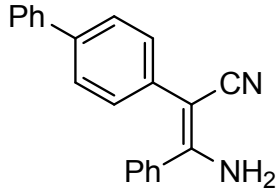
3-amino-3-phenyl-2-(*p*-tolyl)acrylonitrile (4k)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.68 (m, 2H), 7.53 – 7.47 (m, 3H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.7 Hz, 2H), 4.78 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.68, 137.38, 136.10, 130.92, 130.54, 130.10, 128.85, 128.55, 128.06, 122.28, 81.90, 21.24. HRMS m/z (ESI) [M + Na^+] calcd for $C_{16}H_{14}N_2$ + Na^+: 257.1054. found, 257.1049.



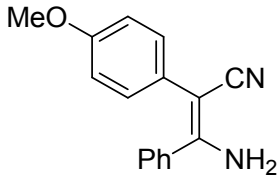
3-amino-2-(4-(*tert*-butyl)phenyl)-3-phenylacrylonitrile (4l)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.68 (m, 2H), 7.52 – 7.46 (m, 7H), 4.82 (s, 2H), 1.37 (s, 9H).^{13}C NMR (101 MHz, $CDCl_3$) δ 156.72, 150.56, 136.14, 130.96, 130.53, 128.85, 128.30, 128.08, 126.35, 125.09, 122.29, 81.83, 34.67, 31.30. HRMS m/z (ESI) [M + Na^+] calcd for $C_{19}H_{20}N_2$ + Na^+: 299.1524. found, 299.1520.



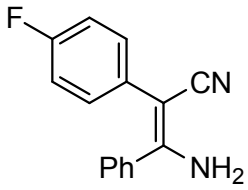
2-([1,1'-biphenyl]-4-yl)-3-amino-3-phenylacrylonitrile (4m)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.68 (m, 4H), 7.68 – 7.62 (m, 4H), 7.55 – 7.47 (m, 5H), 7.44 – 7.40 (m, 1H), 4.90 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.05, 140.37, 140.24, 136.05, 133.02, 130.70, 128.97, 128.92, 128.10, 128.07, 127.59, 127.03, 122.12, 81.70.



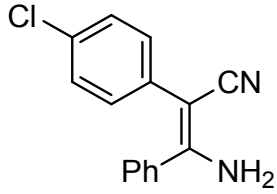
3-amino-2-(4-methoxyphenyl)-3-phenylacrylonitrile (4n)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.66 (m, 2H), 7.56 – 7.42 (m, 5H), 7.04 – 6.93 (m, 2H), 4.71 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.88, 156.51, 136.04, 130.51, 130.10, 128.85, 128.04, 125.96, 122.30, 114.84, 81.65, 55.39. HRMS m/z (ESI) [M + Na^+] calcd for $C_{16}H_{14}N_2O$+ Na^+: 273.1004. found, 273.0098.



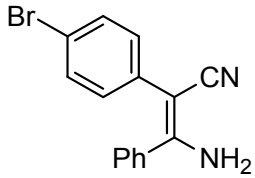
3-amino-2-(4-fluorophenyl)-3-phenylacrylonitrile (4o)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.68 (m, 2H), 7.57 – 7.47 (m, 5H), 7.23 – 7.10 (m, 2H), 4.75 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.62, 157.12, 135.76, 130.75, 130.72, 130.64, 129.80, 128.94, 8.01, 121.96, 116.60, 116.39, 81.01. HRMS m/z (ESI) [M + Na^+] calcd for $C_{15}H_{11}FN_2 + Na^+$: 261.0804. found, 261.0800.



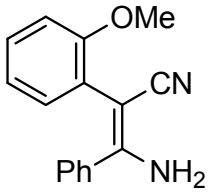
3-amino-2-(4-chlorophenyl)-3-phenylacrylonitrile (4p)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.67 (m, 2H), 7.58 – 7.47 (m, 5H), 7.46 – 7.41 (m, 2H), 4.82 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.29, 135.75, 133.21, 132.47, 130.83, 130.03, 129.65, 128.96, 128.02, 121.74, 80.97. HRMS m/z (ESI) [M + Na^+] calcd for $C_{15}H_{11}ClN_2 + Na^+$: 277.0508. found, 277.0503.



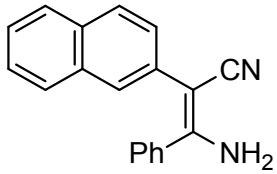
3-amino-2-(4-bromophenyl)-3-phenylacrylonitrile (4q)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 2H), 7.63 – 7.57 (m, 2H), 7.56 – 7.48 (m, 3H), 7.48 – 7.41 (m, 2H), 4.82 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.25, 135.75, 132.98, 132.61, 130.85, 130.32, 128.97, 128.01, 121.26, 81.06.



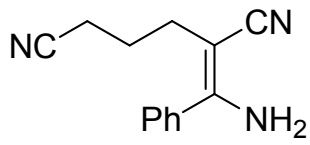
3-amino-2-(2-methoxyphenyl)-3-phenylacrylonitrile (4r)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.73 (m, 2H), 7.52 – 7.45 (m, 4H), 7.37 (td, *J* = 8.3, 1.7 Hz, 1H), 7.07 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.03 (dd, *J* = 6.3, 4.7 Hz, 1H), 4.58 (s, 2H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.53, 157.06, 136.05, 131.53, 130.40, 129.72, 128.74, 128.21, 122.08, 121.90, 121.37, 112.13, 78.34, 55.94.



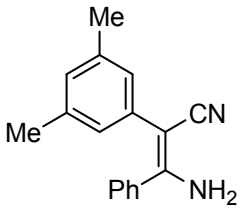
3-amino-2-(naphthalen-2-yl)-3-phenylacrylonitrile (4s)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.87 (dd, *J* = 9.4, 5.2 Hz, 2H), 7.80 – 7.74 (m, 2H), 7.68 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.59 – 7.50 (m, 5H), 5.00 (d, *J* = 68.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.18, 136.04, 133.74, 132.46, 131.40, 130.73, 129.27, 128.95, 128.11, 127.82, 127.78, 127.62, 126.67, 126.42, 126.32, 122.16, 82.14.



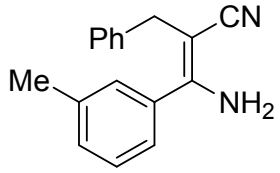
2-(amino(phenyl)methylene)hexanedinitrile (4t)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 – 8.23 (m, 2H), 7.53 – 7.38 (m, 3H), 4.92 (s, 2H), 3.00 (t, *J* = 7.8 Hz, 2H), 2.74 (dd, *J* = 9.3, 5.5 Hz, 2H), 2.16 (qd, *J* = 7.7, 4.9 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.20, 163.77, 159.54, 138.56, 129.78, 128.31, 128.01, 113.99, 34.30, 26.76, 21.60. HRMS m/z (ESI) [M + H^+] calcd for $C_{13}H_{13}N_3$ + H^+: 212.1188. found, 212.1182.



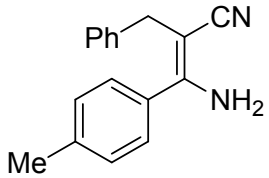
3-amino-2-(3,5-dimethylphenyl)-3-phenylacrylonitrile (4u)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 2H), 7.54 – 7.46 (m, 3H), 7.18 (s, 2H), 6.96 (s, 1H), 4.82 (s, 2H), 2.37 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.75, 139.08, 136.16, 133.75, 130.52, 129.22, 128.86, 128.05, 126.28, 122.33, 82.12, 21.35.



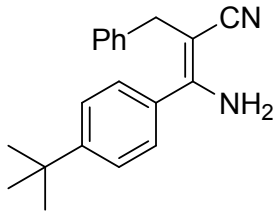
3-amino-2-benzyl-3-(*m*-tolyl)acrylonitrile (4aa)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 2.4 Hz, 2H), 7.37 (t, *J* = 5.0 Hz, 4H), 7.35 – 7.31 (m, 1H), 7.29 (dd, *J* = 7.4, 6.1 Hz, 2H), 4.38 (s, 2H), 3.62 (s, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.61, 138.54, 137.72, 136.01, 131.07, 128.92, 128.67, 128.53, 128.00, 126.93, 125.12, 123.33, 78.10, 34.58, 21.40. HRMS m/z (ESI) [M + Na^+] calcd for $C_{17}H_{16}N_2$ + Na^+: 271.1211. found, 271.1206.



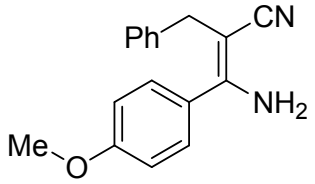
3-amino-2-benzyl-3-(*p*-tolyl)acrylonitrile (4ab)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.37 (t, *J* = 4.4 Hz, 4H), 7.29 (ddd, *J* = 12.8, 9.8, 6.0 Hz, 3H), 4.37 (s, 2H), 3.62 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.49, 140.57, 137.76, 133.14, 129.43, 128.91, 128.01, 127.88, 126.92, 123.51, 77.93, 34.61, 21.42. HRMS m/z (ESI) [M + Na^+] calcd for $C_{17}H_{16}N_2$ + Na^+: 271.1211. found, 271.1206.



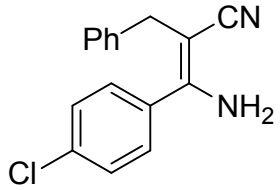
3-amino-2-benzyl-3-(4-(*tert*-butyl)phenyl)acrylonitrile (4ac)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.54 (m, 2H), 7.50 – 7.45 (m, 2H), 7.37 (d, *J* = 4.4 Hz, 4H), 7.32 – 7.26 (m, 1H), 4.42 (d, *J* = 35.2 Hz, 2H), 3.63 (s, 2H), 1.36 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.43, 153.63, 137.78, 133.06, 128.90, 128.00, 127.73, 126.91, 125.71, 123.60, 77.76, 34.86, 34.67, 31.23. HRMS m/z (ESI) [M + Na^+] calcd for $C_{20}H_{22}N_2$ + Na^+: 313.1680. found, 313.1675.



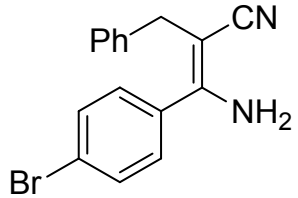
3-amino-2-benzyl-3-(4-methoxyphenyl)acrylonitrile (4ad)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.52 (m, 2H), 7.40 – 7.33 (m, 4H), 7.33 – 7.25 (m, 1H), 7.01 – 6.88 (m, 2H), 4.35 (s, 2H), 3.85 (s, 3H), 3.61 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.12, 157.18, 137.84, 129.48, 128.91, 128.21, 127.99, 126.91, 123.70, 114.08, 77.56, 55.40, 34.65. HRMS m/z (ESI) [M + Na^+] calcd for $C_{17}H_{16}ON_2$ + Na^+: 287.1160. found, 287.1155.



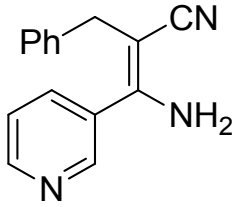
3-amino-2-benzyl-3-(4-chlorophenyl)acrylonitrile (4ae)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.4 Hz, 2H), 7.41 (dd, *J* = 7.8, 4.7 Hz, 2H), 7.36 (q, *J* = 6.8 Hz, 4H), 7.33 – 7.26 (m, 1H), 4.41 (s, 2H), 3.59 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.17, 137.43, 136.34, 134.38, 129.46, 129.05, 128.97, 128.00, 127.05, 122.98, 78.91, 34.49. HRMS m/z (ESI) [M + Na^+] calcd for $C_{16}H_{13}ClN_2$ + Na^+:291.0665. found, 291.0659.



3-amino-2-benzyl-3-(4-bromophenyl)acrylonitrile (4af)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.7, 2.1 Hz, 2H), 7.47 (dd, *J* = 8.7, 2.2 Hz, 2H), 7.41 – 7.32 (m, 4H), 7.32 – 7.26 (m, 1H), 4.41 (s, 2H), 3.59 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.18, 137.40, 134.85, 132.02, 129.68, 128.97, 128.01, 127.06, 124.64, 122.94, 78.94, 34.49. HRMS m/z (ESI) [M + Na^+] calcd for $C_{18}H_{13}BrN_2$ + Na^+: 335.0159. found, 335.0154.



3-amino-2-benzyl-3-(pyridin-3-yl)acrylonitrile (4ag)

^{1}H NMR (400 MHz, DMSO) δ 8.70 (d, *J* = 1.8 Hz, 1H), 8.65 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.96 – 7.89 (m, 1H), 7.49 (dd, *J* = 7.9, 4.9 Hz, 1H), 7.40 – 7.30 (m, 4H), 7.24 (pd, *J* = 5.5, 2.7 Hz, 1H), 6.82 (s, 2H), 3.57 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 160.74, 155.59, 153.90, 144.59, 141.30, 138.03, 133.62, 133.45, 131.46, 128.63, 128.53, 81.42, 37.87.

4. The Characterization of $MePhSO_2$-SPhMe

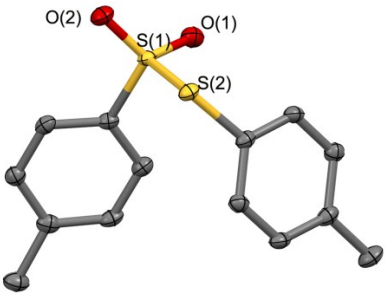
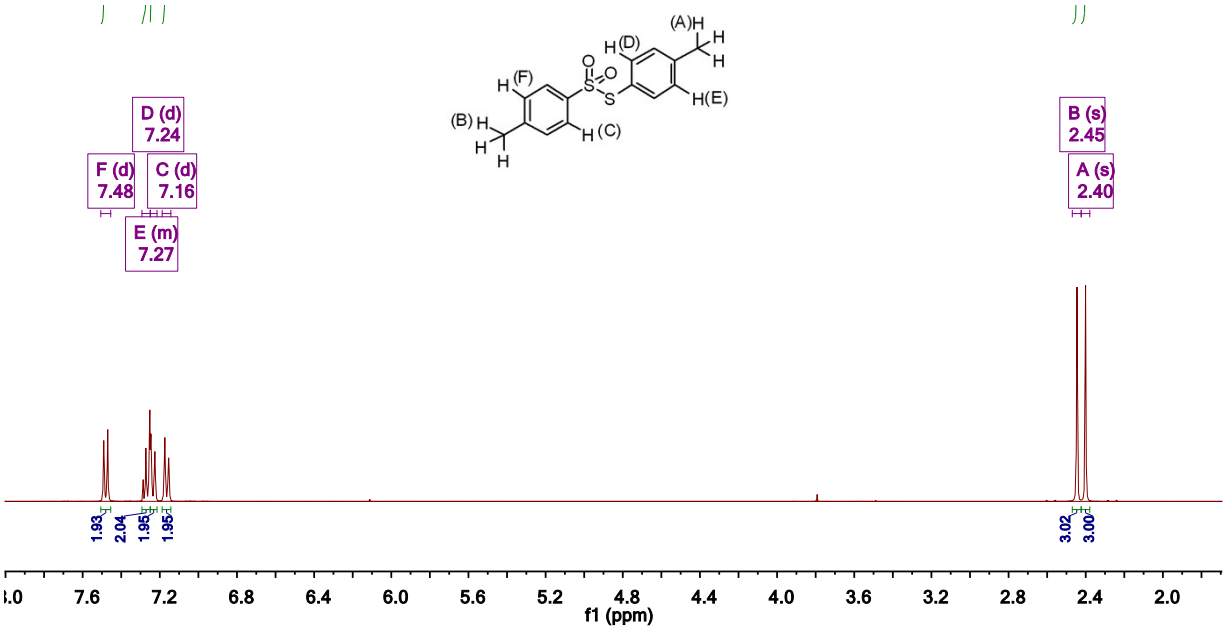
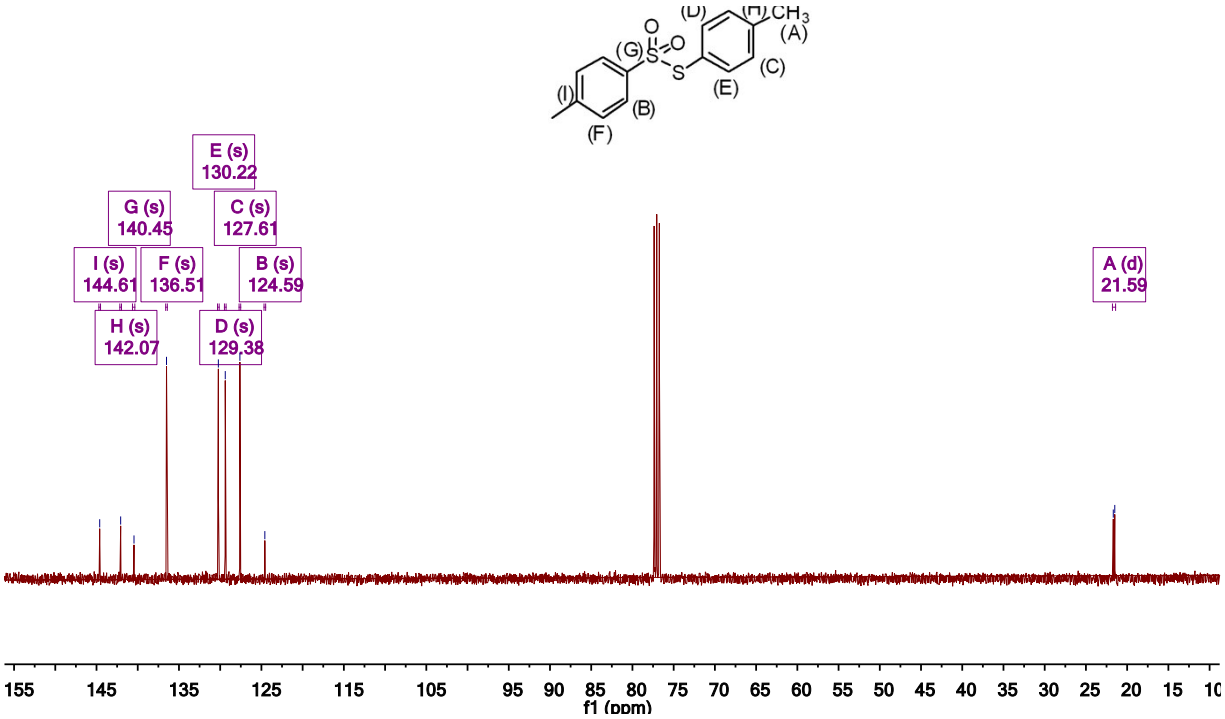
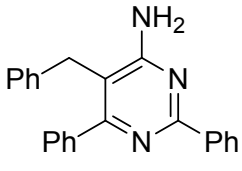


Figure S1. The structure of $MePhSO_2$-SPhMe (Refcode: BILCOO)

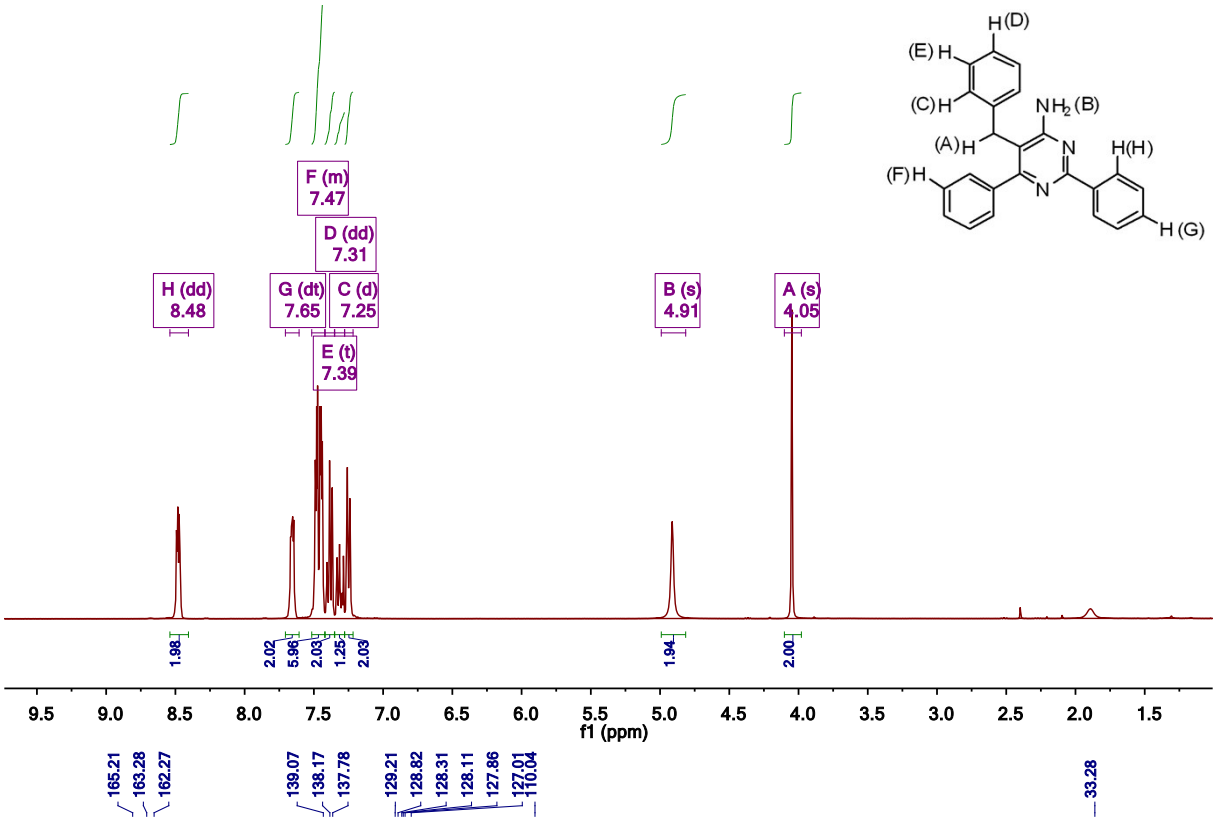


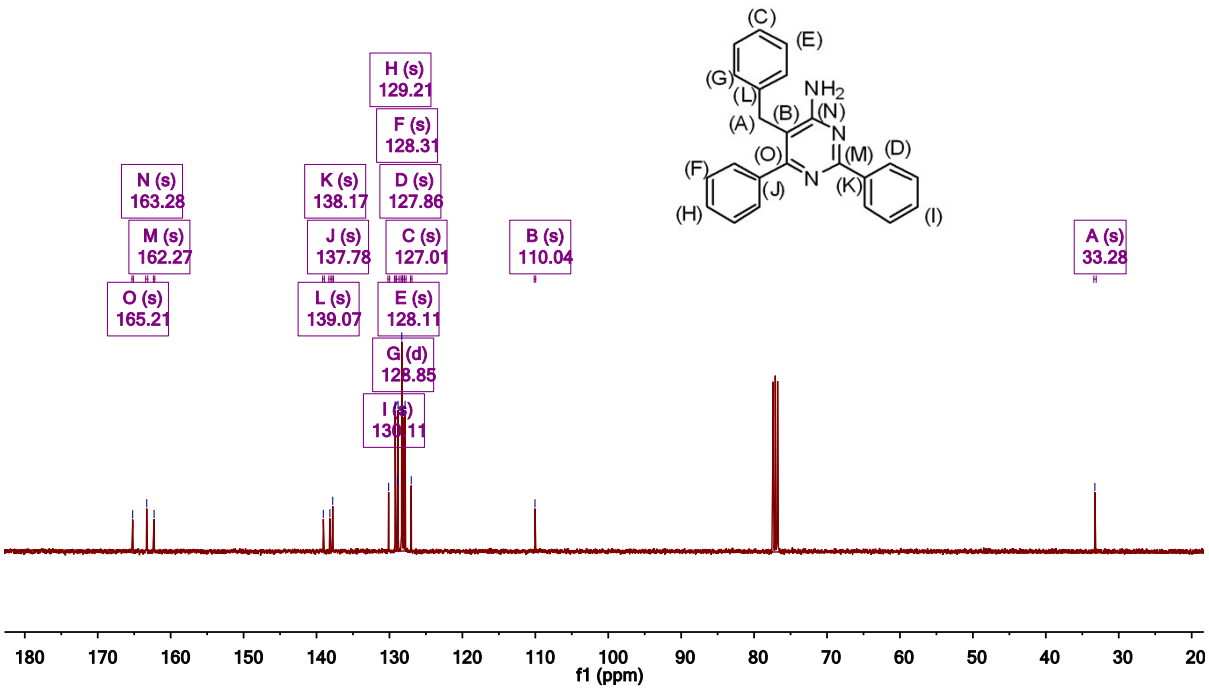


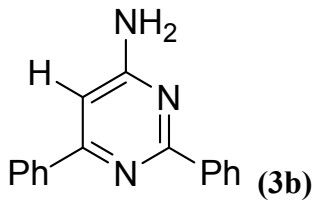
5. ^{1}H NMR and ^{13}C NMR of Products



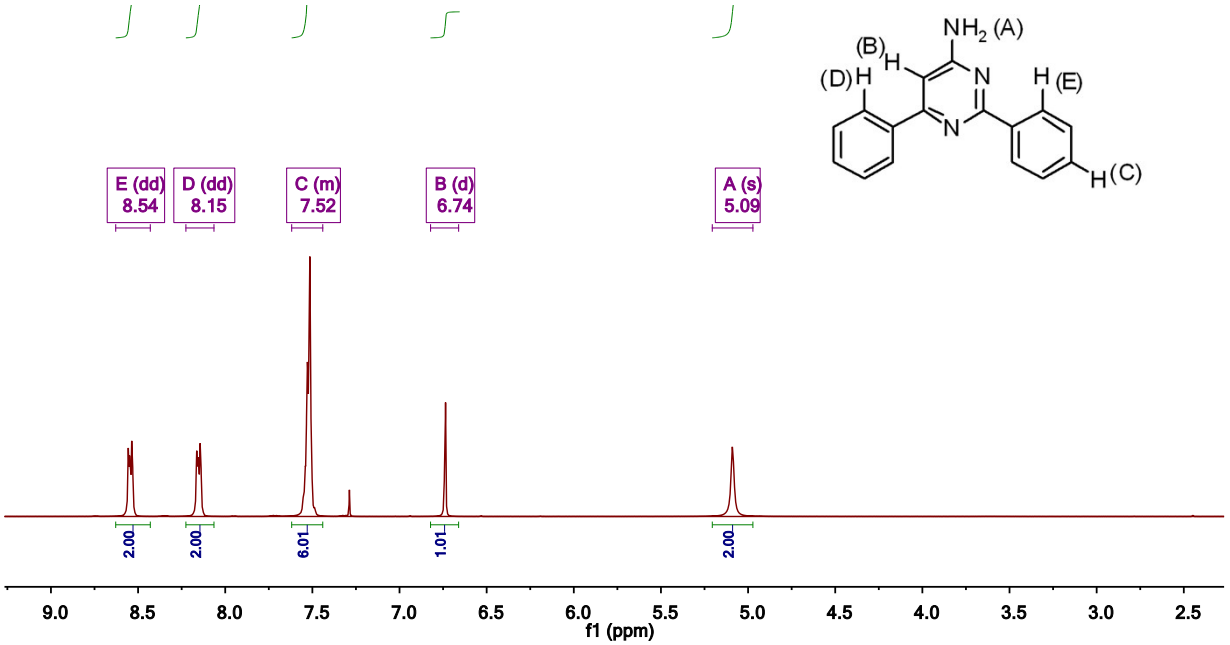
(3a)

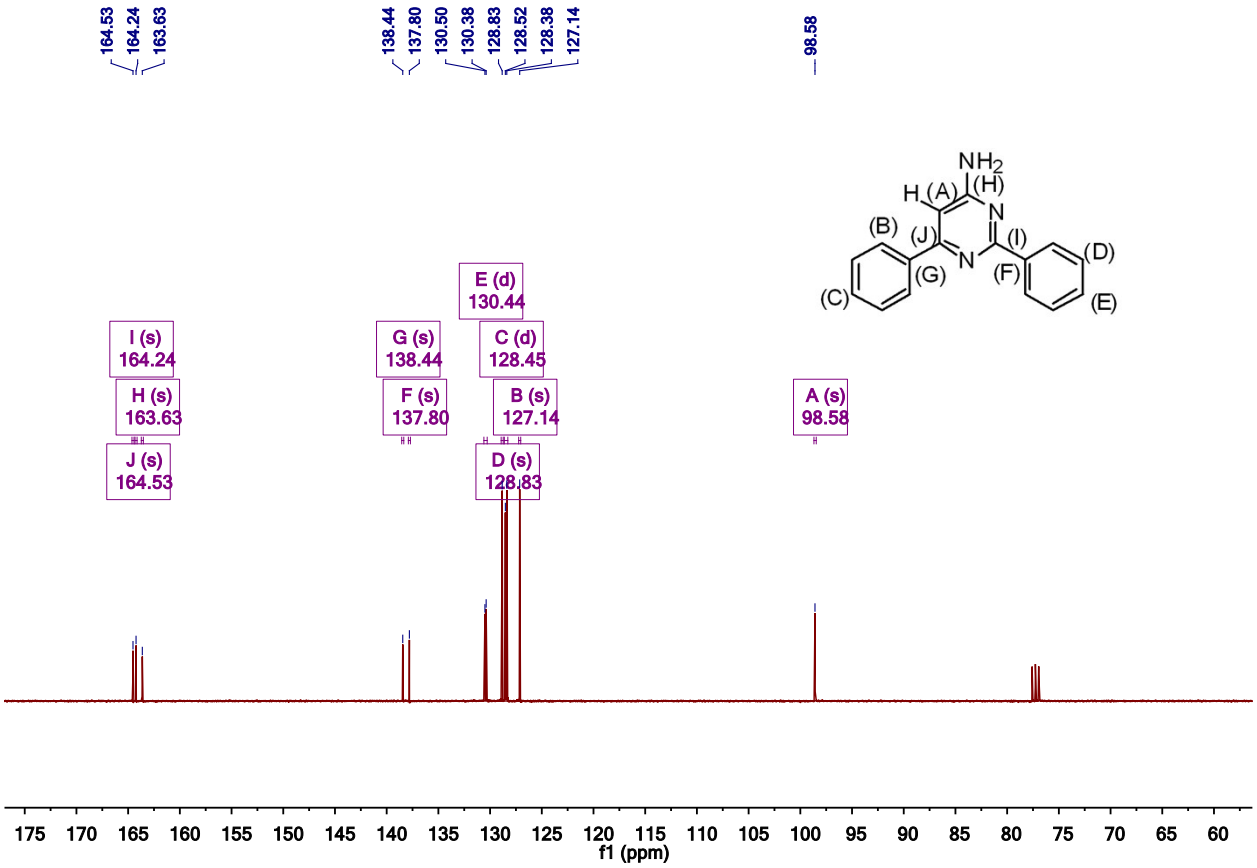


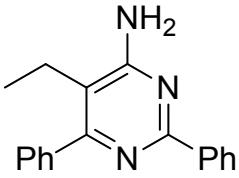



NH2
H
N
Ph
N
Ph

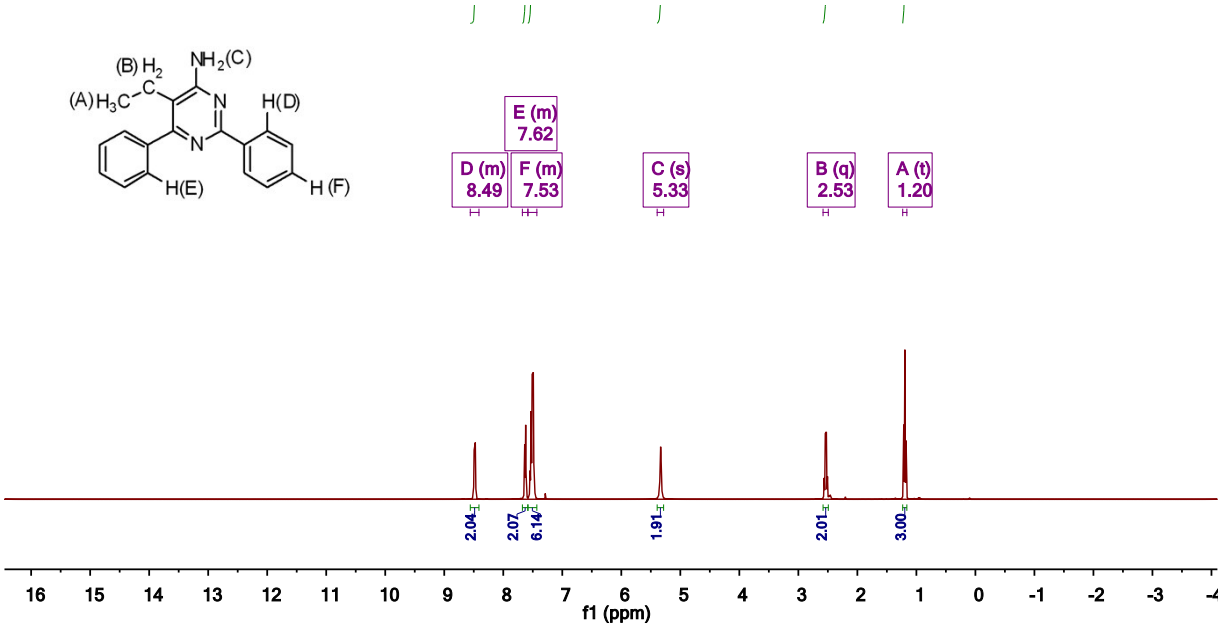
(3b)

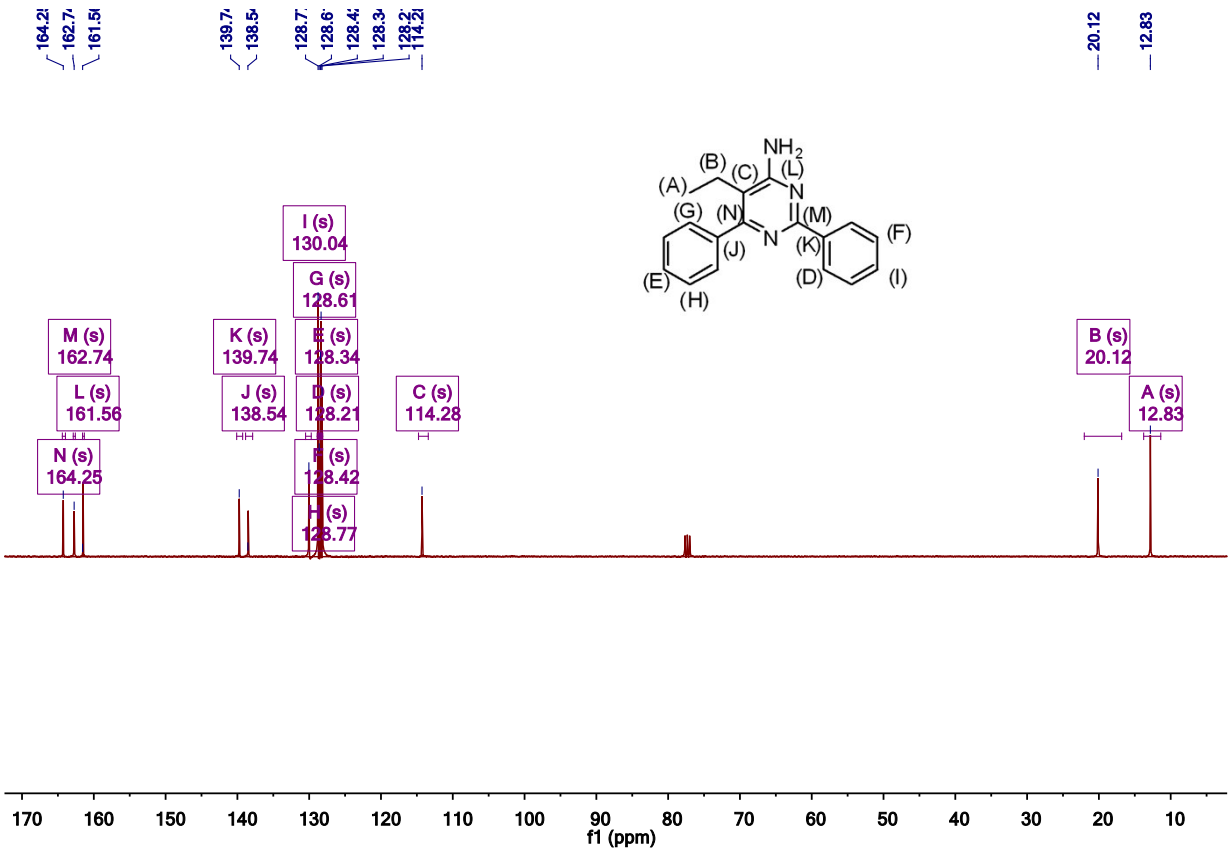

E (dd) 8.54
D (dd) 8.15
C (m) 7.52
B (d) 6.74
A (s) 5.09
2.00
2.00
6.01
1.01
2.00
f1 (ppm)

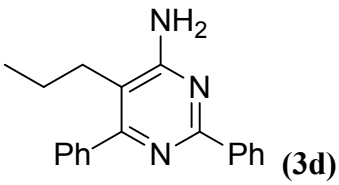

164.53
164.24
163.63
138.44
137.80
130.50
130.38
128.83
128.52
128.38
127.14
98.58
I (s) 164.24
H (s) 163.63
J (s) 164.53
G (s) 138.44
F (s) 137.80
E (d) 130.44
C (d) 128.45
B (s) 127.14
D (s) 128.83
A (s) 98.58
f1 (ppm)



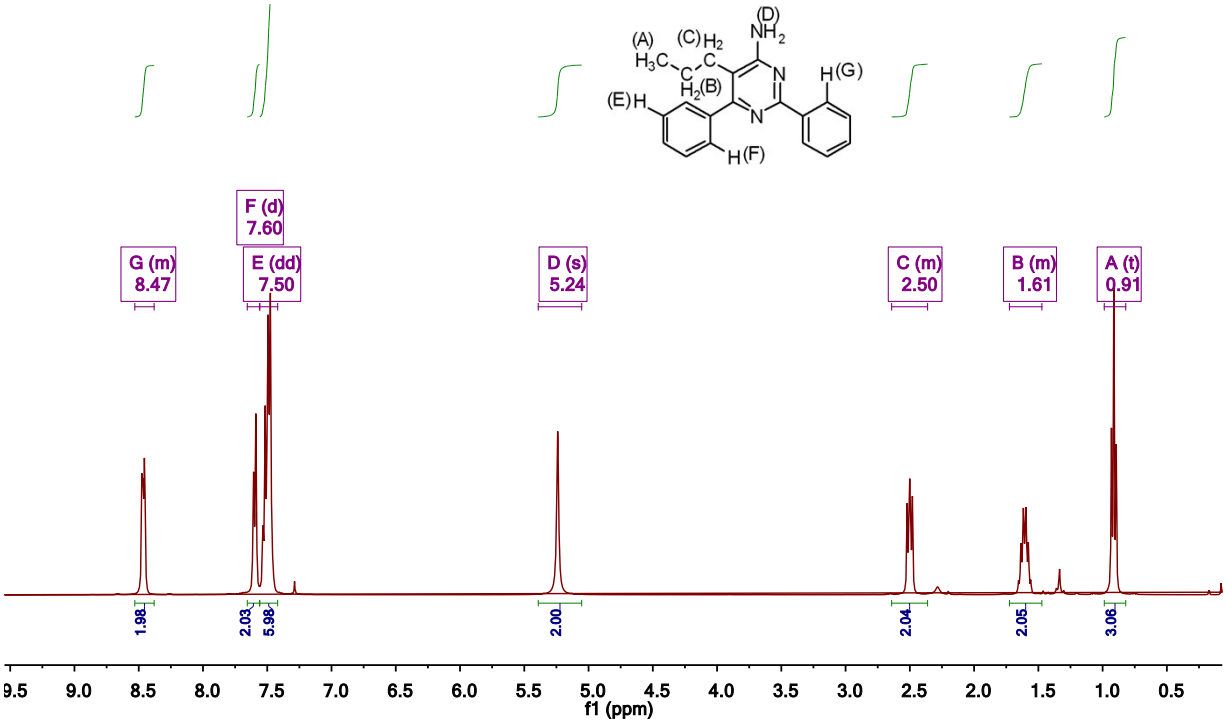
(3c)

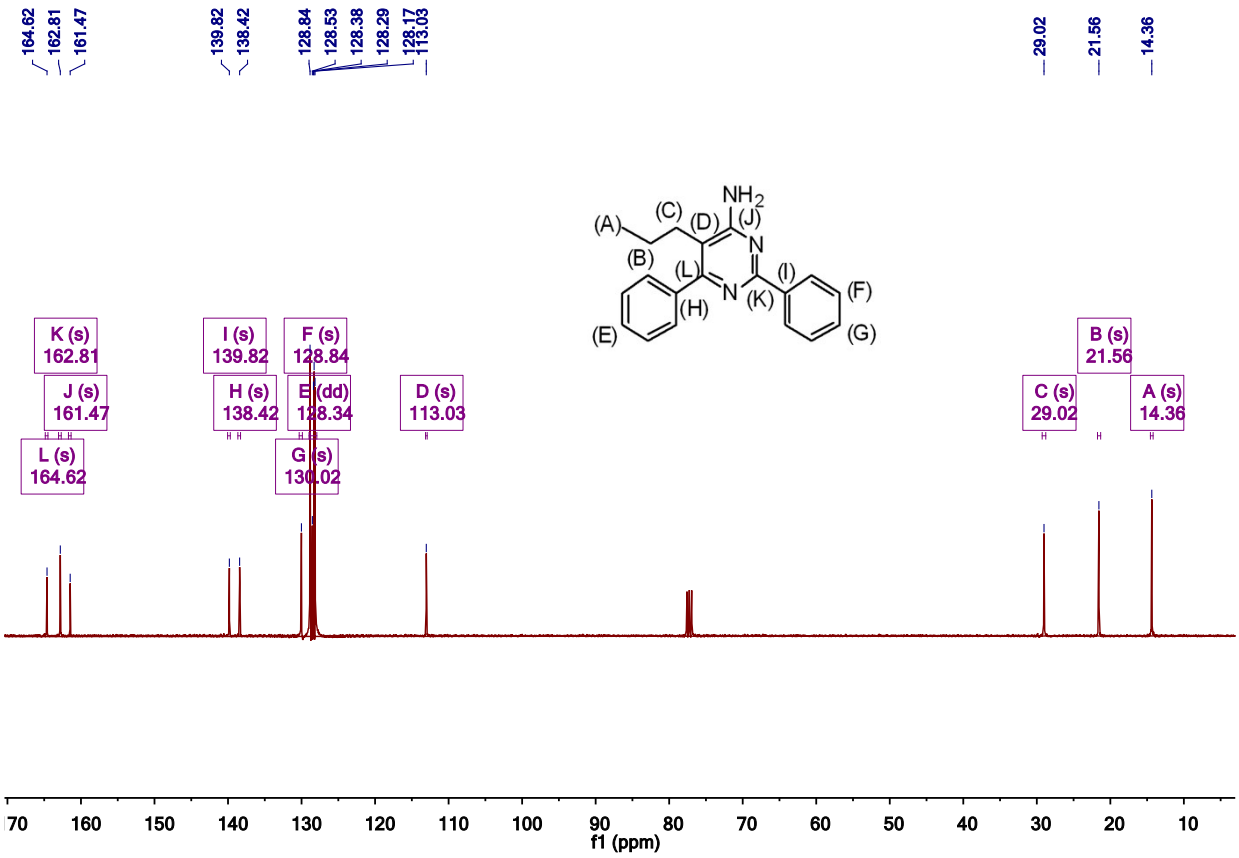

E (m) 7.62
D (m) 8.49
F (m) 7.53
C (s) 5.33
B (q) 2.53
A (t) 1.20
2.04
2.07
6.14
1.91
2.01
3.00
f1 (ppm)

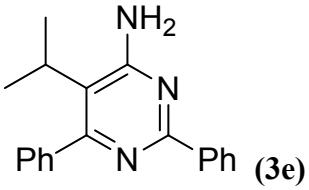

I (s) 130.04
G (s) 128.61
M (s) 162.74
K (s) 139.74
E (s) 128.34
L (s) 161.56
J (s) 138.54
D (s) 128.21
C (s) 114.28
N (s) 164.25
F (s) 128.42
H (s) 128.77
B (s) 20.12
A (s) 12.83
f1 (ppm)



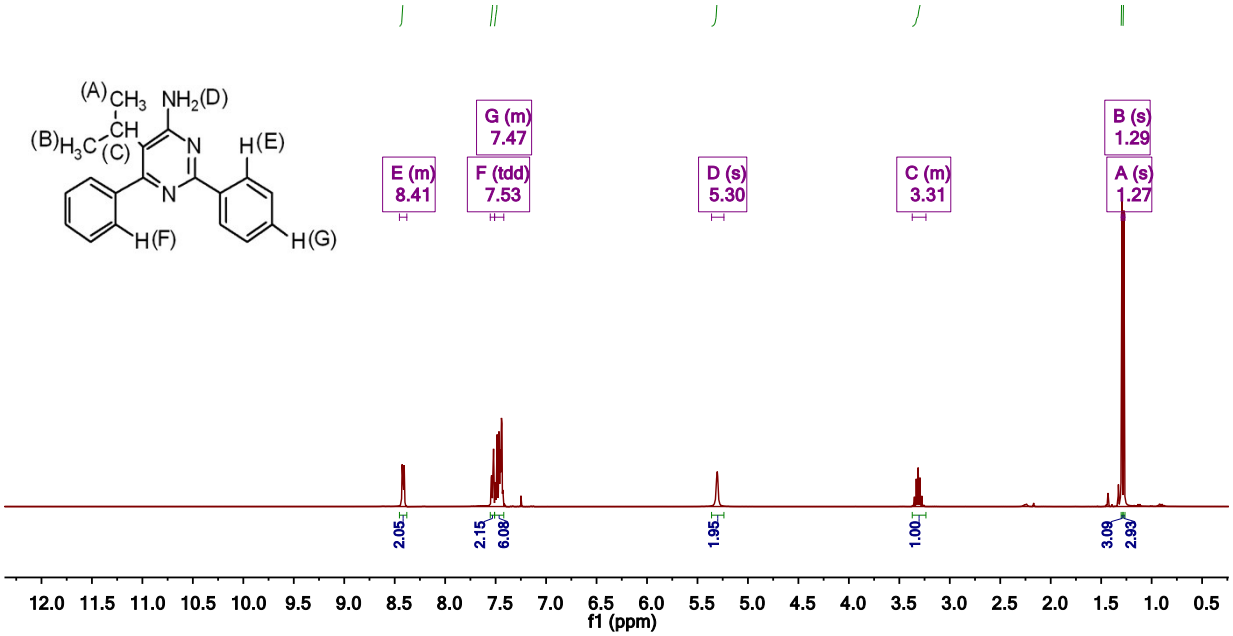
(3d)

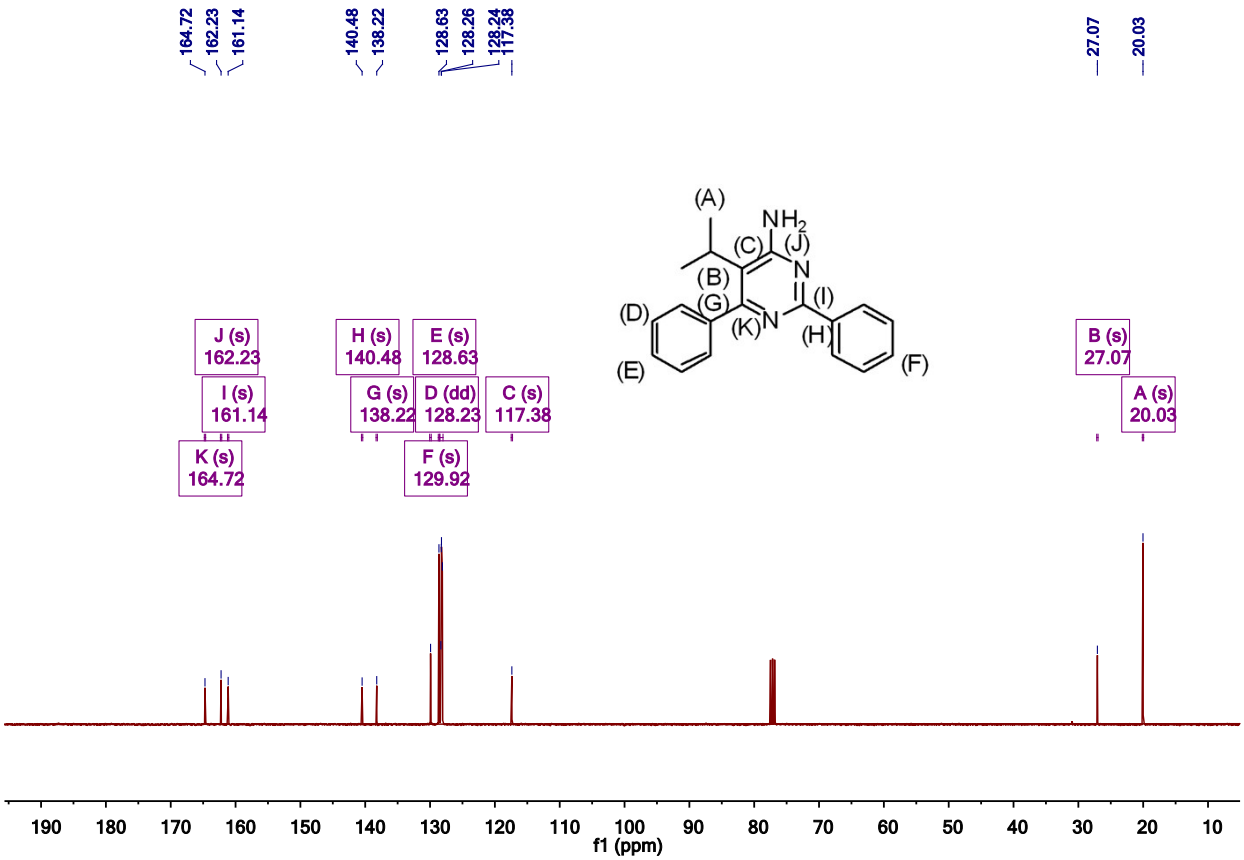

G (m) 8.47
F (d) 7.60
E (dd) 7.50
D (s) 5.24
C (m) 2.50
B (m) 1.61
A (t) 0.91
1.98
2.03
5.98
2.00
2.04
2.05
3.06
f1 (ppm)

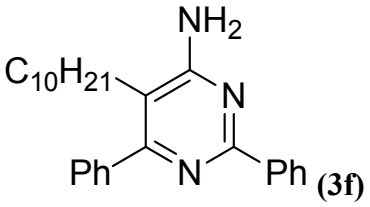

164.62
162.81
161.47
139.82
138.42
128.84
128.53
128.38
128.29
128.17
113.03
29.02
21.56
14.36
K (s) 162.81
J (s) 161.47
L (s) 164.62
I (s) 139.82
H (s) 138.42
F (s) 128.84
E (dd) 128.34
G (s) 130.02
D (s) 113.03
B (s) 21.56
C (s) 29.02
A (s) 14.36
f1 (ppm)



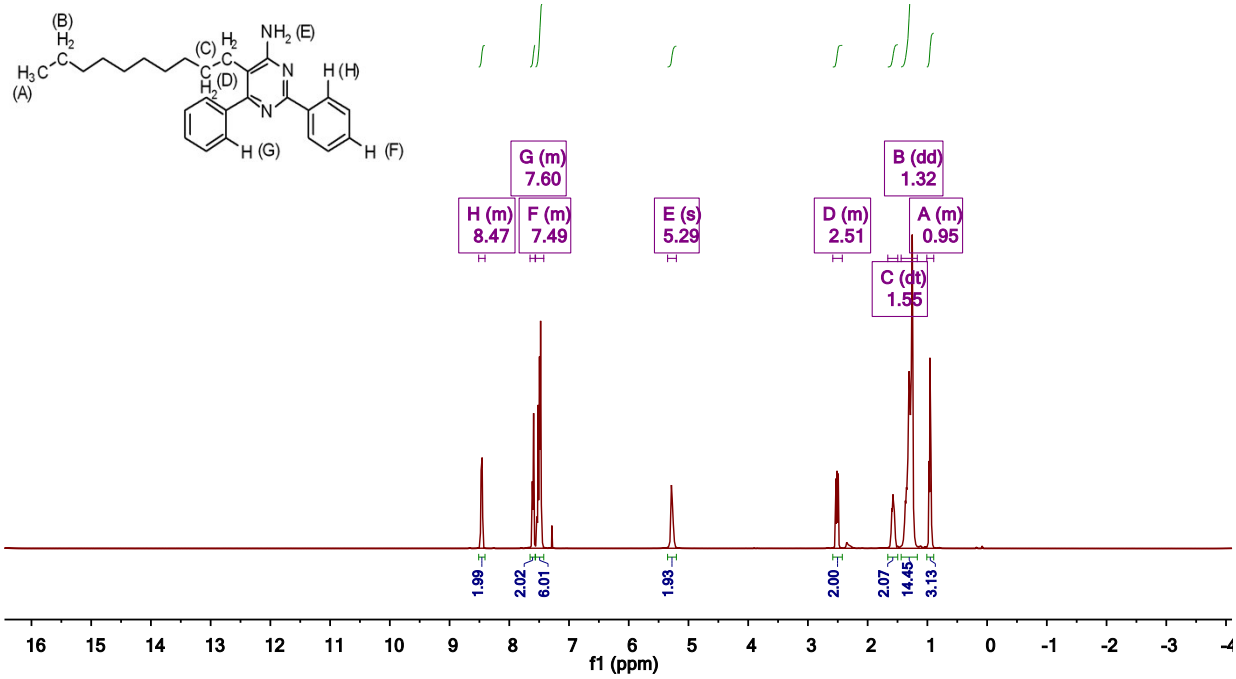
(3e)

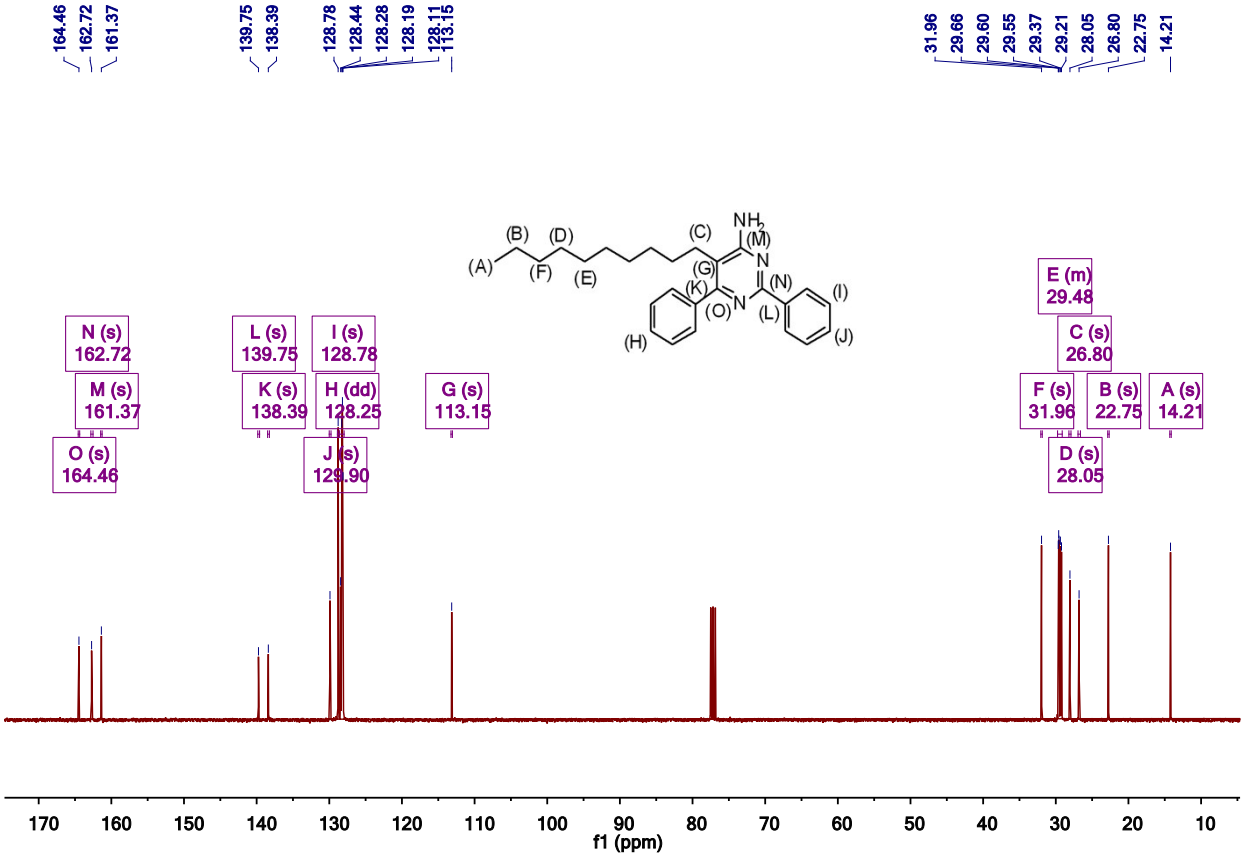

E (m) 8.41
F (tdd) 7.53
G (m) 7.47
D (s) 5.30
C (m) 3.31
B (s) 1.29
A (s) 1.27
2.05
2.15
6.08
1.95
1.00
3.09
2.93
f1 (ppm)

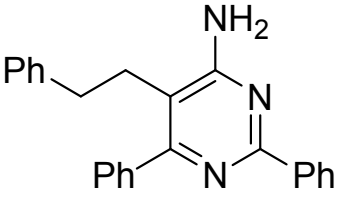

J (s) 162.23
I (s) 161.14
K (s) 164.72
H (s) 140.48
G (s) 138.22
E (s) 128.63
D (dd) 128.23
F (s) 129.92
C (s) 117.38
B (s) 27.07
A (s) 20.03
f1 (ppm)



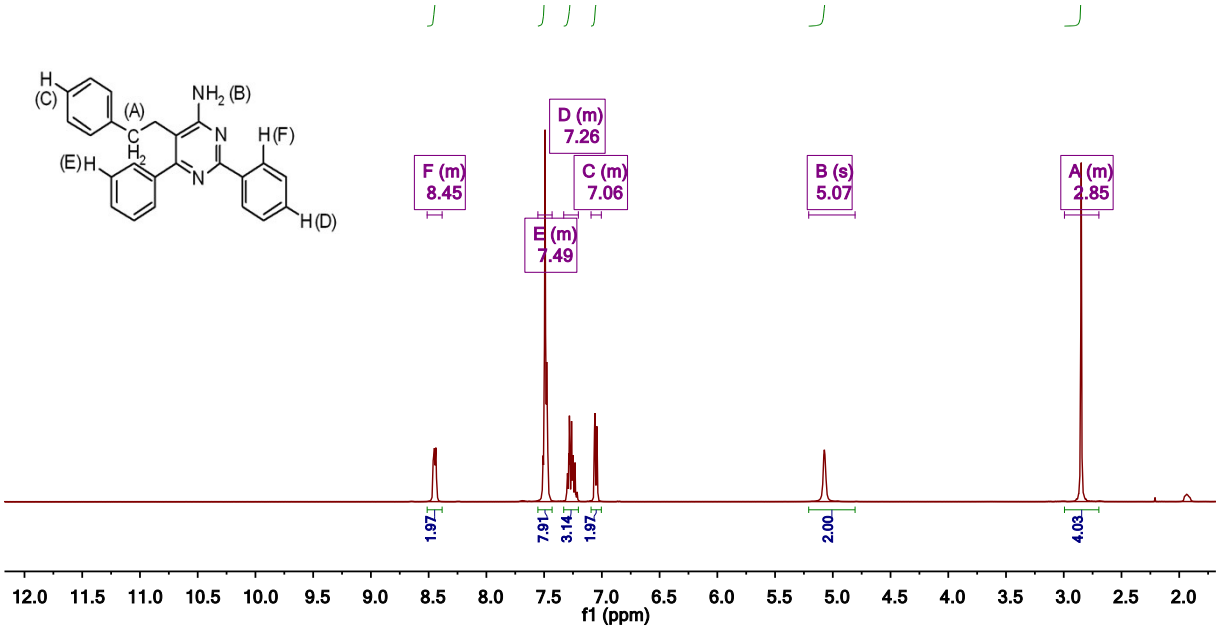
(3f)

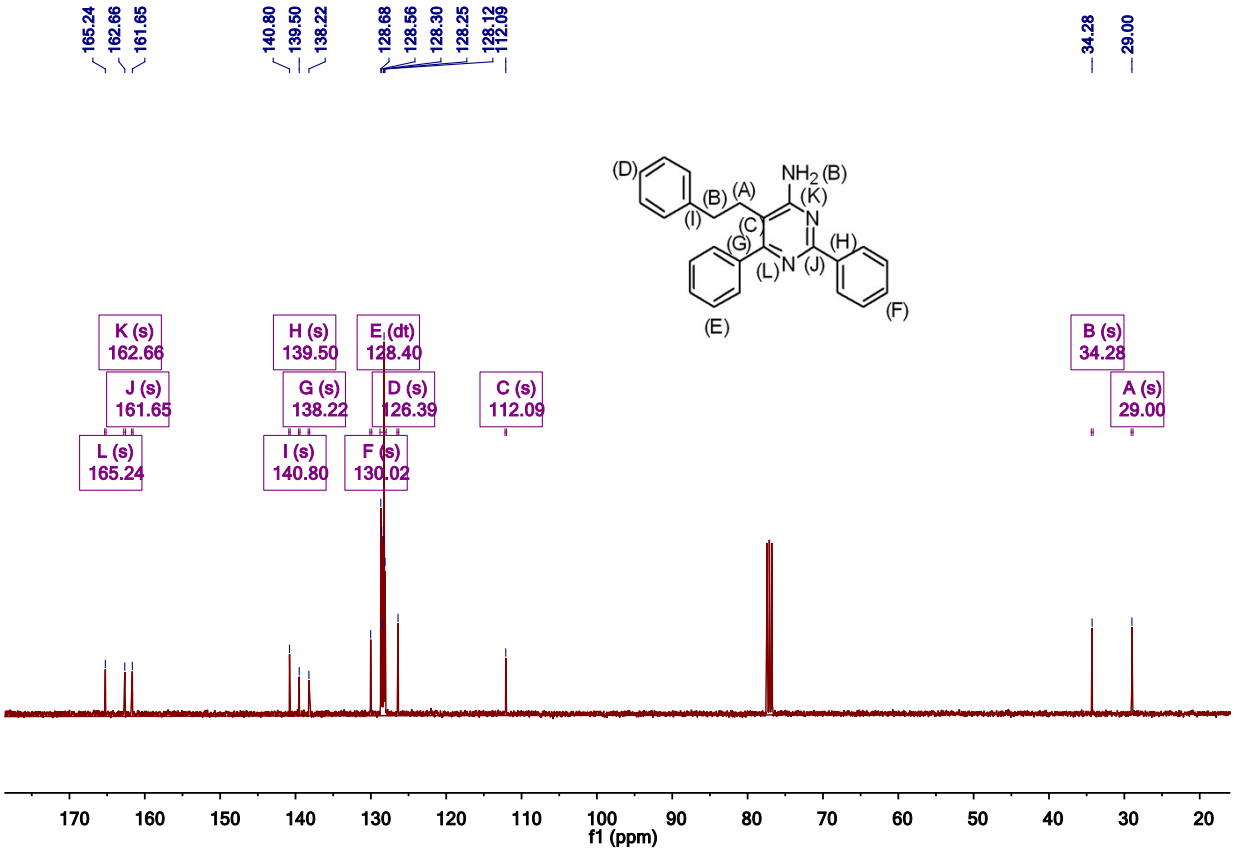

G (m) 7.60
H (m) 8.47
F (m) 7.49
E (s) 5.29
D (m) 2.51
B (dd) 1.32
A (m) 0.95
C (dt) 1.55
f1 (ppm)

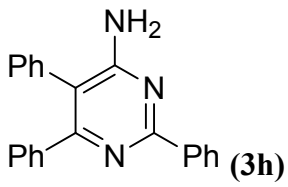

N (s) 162.72
M (s) 161.37
O (s) 164.46
L (s) 139.75
K (s) 138.39
I (s) 128.78
H (dd) 128.25
J (s) 129.90
G (s) 113.15
E (m) 29.48
C (s) 26.80
F (s) 31.96
B (s) 22.75
A (s) 14.21
D (s) 28.05
f1 (ppm)



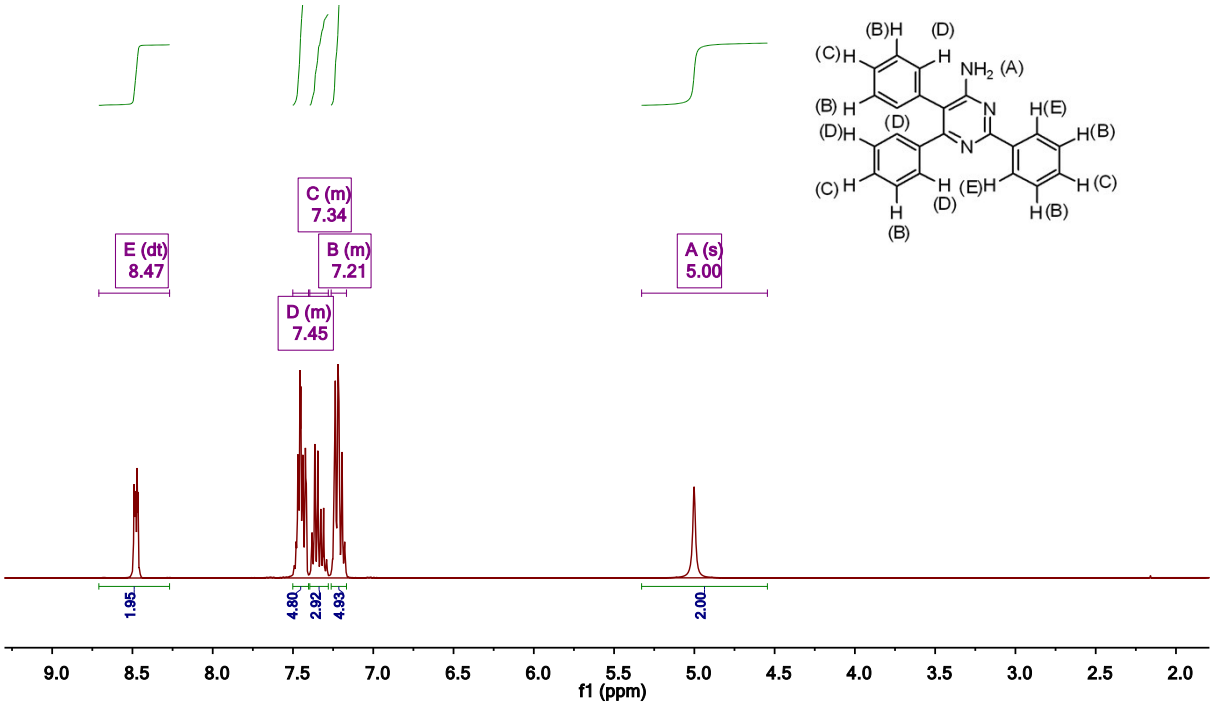
(3g)

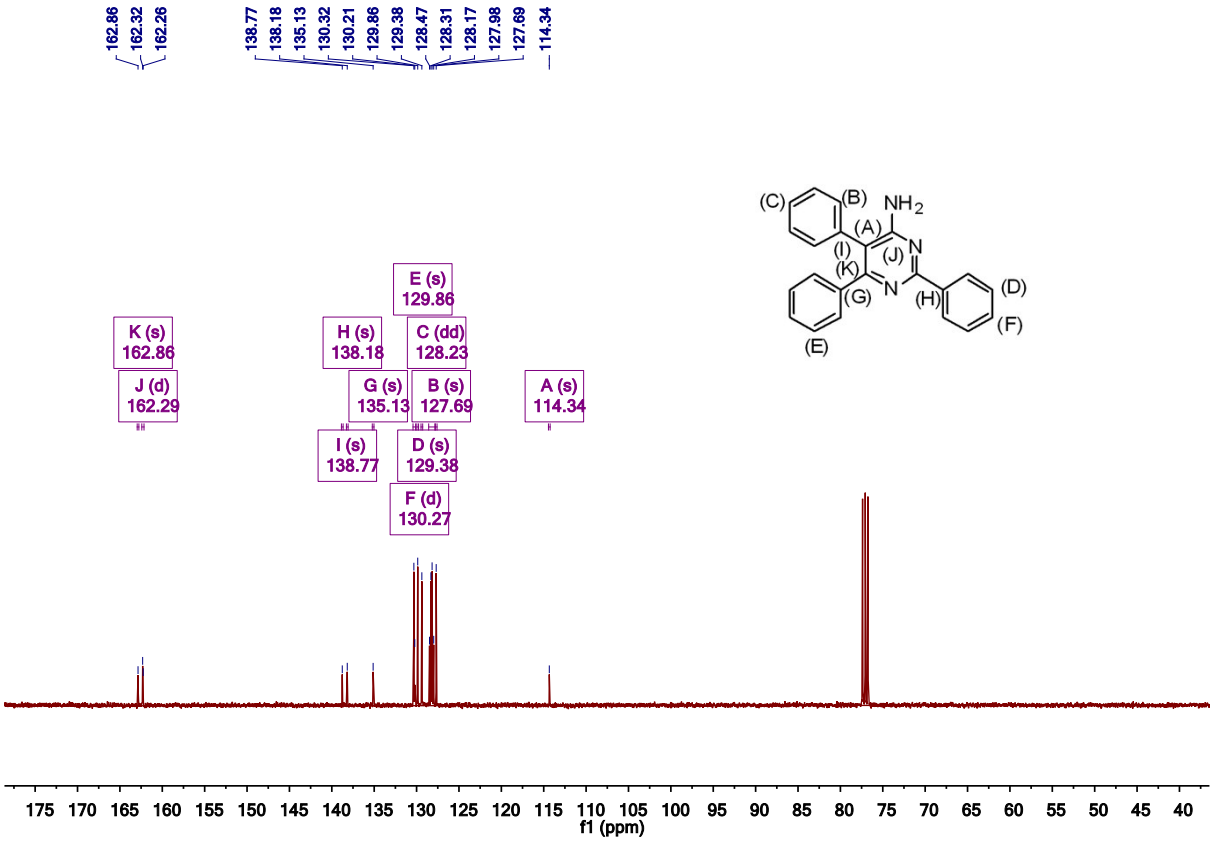

F (m) 8.45
D (m) 7.26
E (m) 7.49
C (m) 7.06
B (s) 5.07
A (m) 2.85
1.97
7.91
3.14
1.97
2.00
4.03
f1 (ppm)

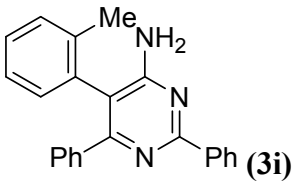

K (s) 162.66
J (s) 161.65
L (s) 165.24
H (s) 139.50
G (s) 138.22
I (s) 140.80
E (dt) 128.40
D (s) 126.39
F (s) 130.02
C (s) 112.09
B (s) 34.28
A (s) 29.00
f1 (ppm)


NH2
Ph
N
Ph
N
Ph

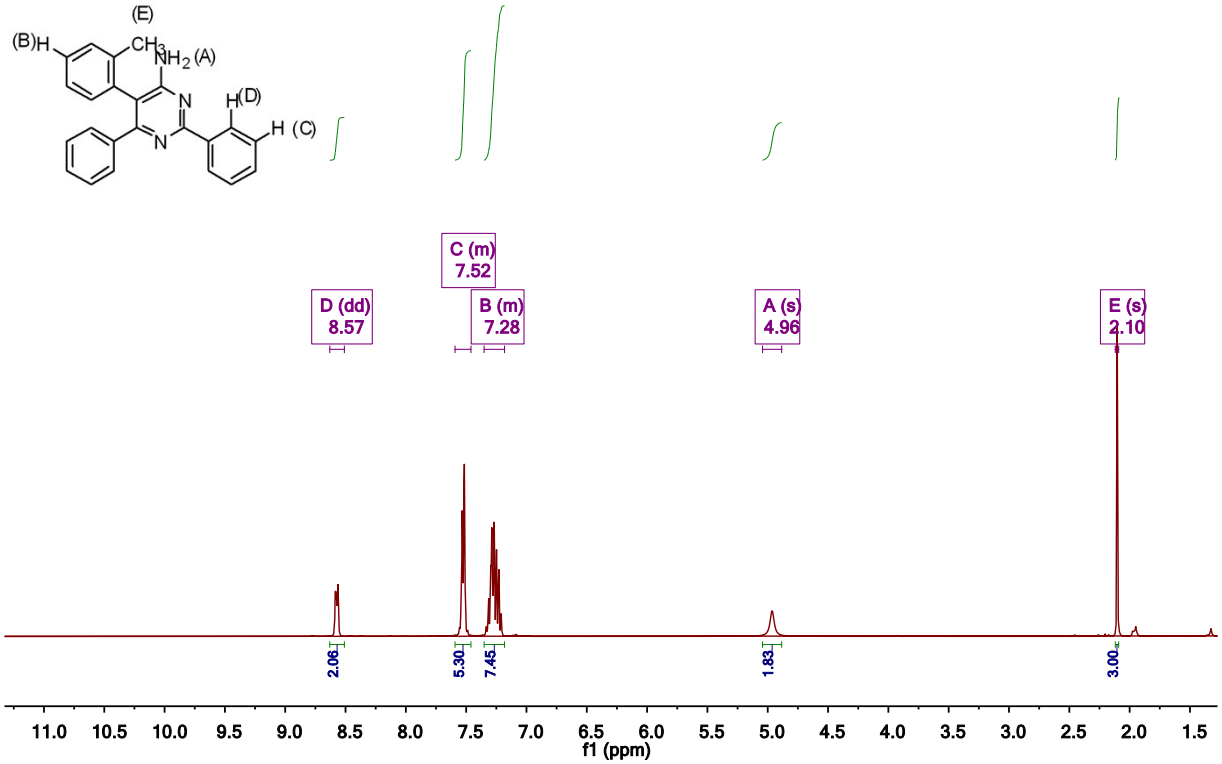
(3h)

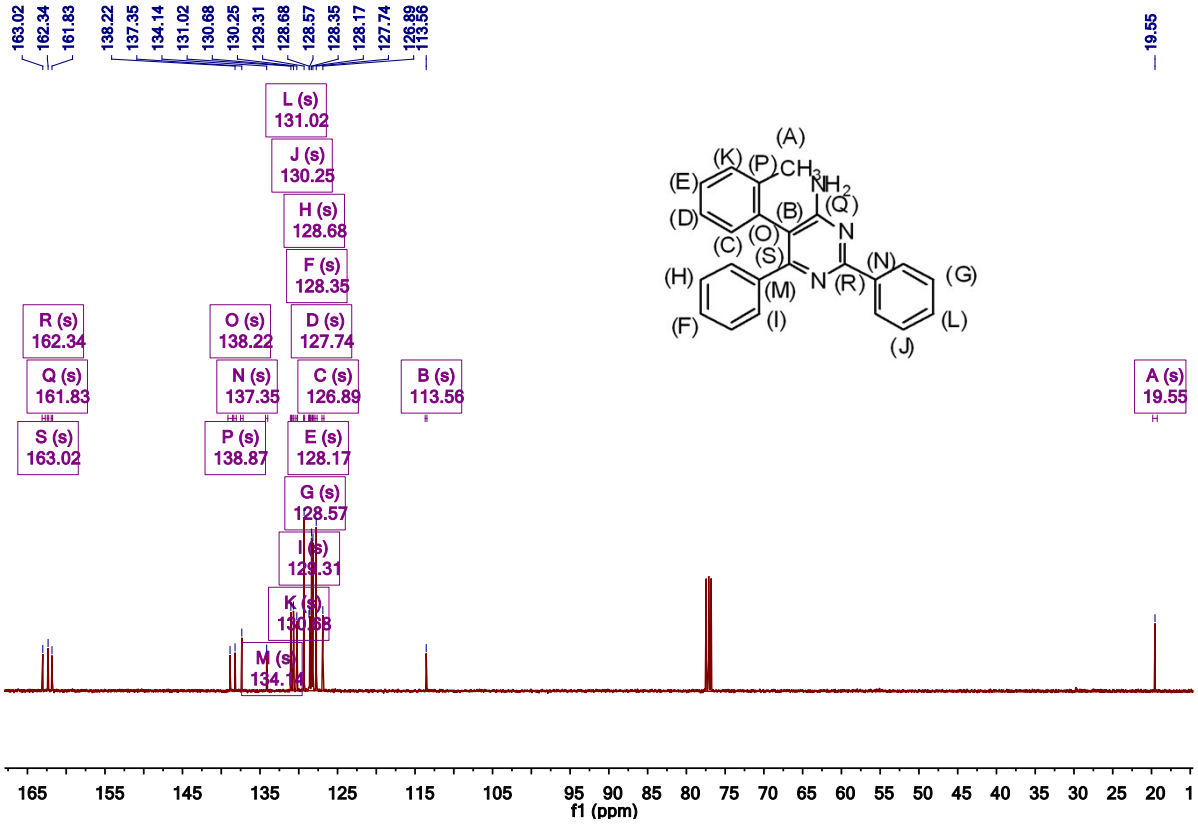

E (dt)
8.47
C (m)
7.34
B (m)
7.21
D (m)
7.45
A (s)
5.00
1.95
4.80
2.92
4.93
2.00
f1 (ppm)

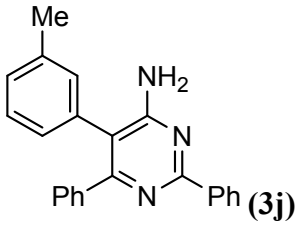

162.86
162.32
162.26
138.77
138.18
135.13
130.32
130.21
129.86
129.38
128.47
128.31
128.17
127.98
127.69
114.34
K (s)
162.86
J (d)
162.29
H (s)
138.18
I (s)
138.77
G (s)
135.13
E (s)
129.86
C (dd)
128.23
B (s)
127.69
D (s)
129.38
F (d)
130.27
A (s)
114.34
f1 (ppm)


Me
NH2
N
Ph
N
Ph

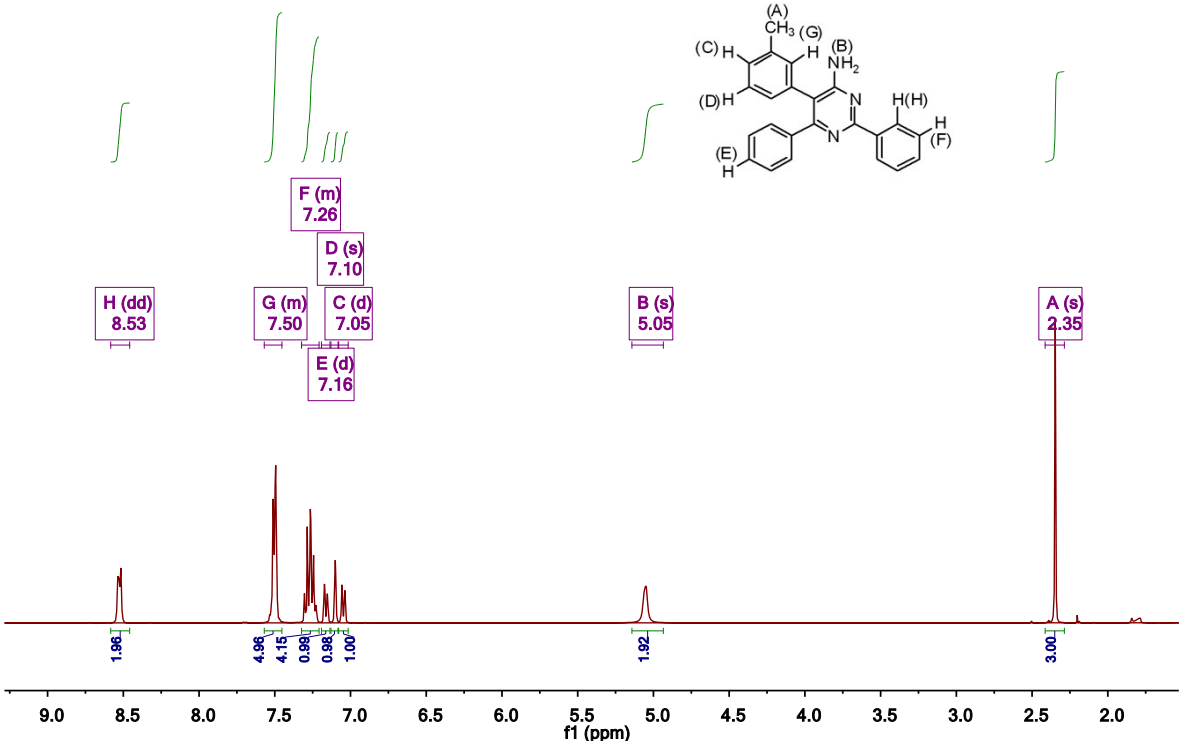
(3i)

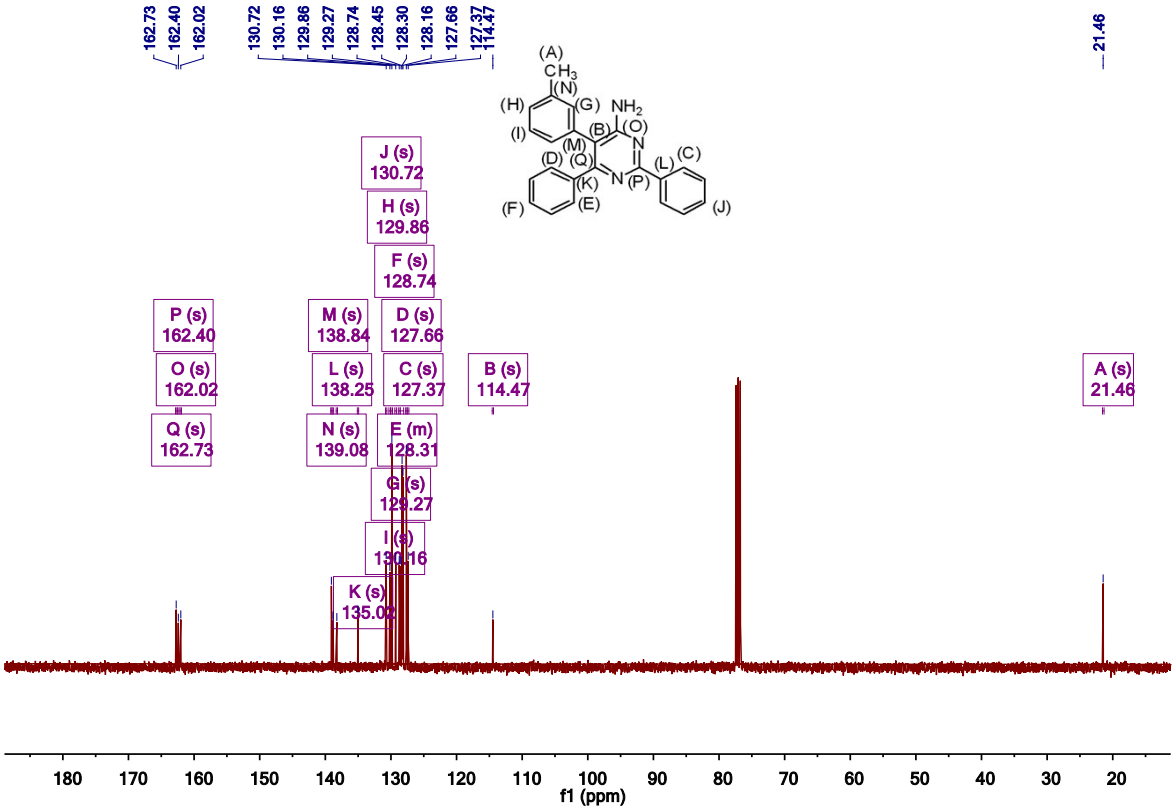

(E)
(B)H
CH3
NH2 (A)
N
H(D)
H (C)
N
D (dd) 8.57
C (m) 7.52
B (m) 7.28
A (s) 4.96
E (s) 2.10
2.06
5.30
7.45
1.83
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)

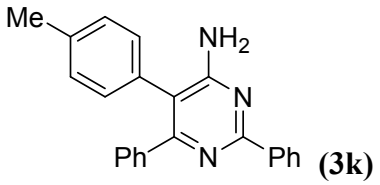

163.02
162.34
161.83
138.22
137.35
134.14
131.02
130.68
130.25
129.31
128.68
128.57
128.35
128.17
127.74
126.89
113.56
19.55
L (s) 131.02
J (s) 130.25
H (s) 128.68
F (s) 128.35
R (s) 162.34
O (s) 138.22
D (s) 127.74
Q (s) 161.83
N (s) 137.35
C (s) 126.89
B (s) 113.56
A (s) 19.55
S (s) 163.02
P (s) 138.87
E (s) 128.17
G (s) 128.57
I (s) 129.31
K (s) 130.68
M (s) 134.14
(A)
(K)
(P)
CH3
NH2
(E)
(Q)
(B)
(D)
N
(O)
(C)
(S)
(N)
(H)
N
(R)
(G)
(M)
(F)
(I)
(L)
(J)
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 1
f1 (ppm)


Me
NH2
N
Ph
N
Ph

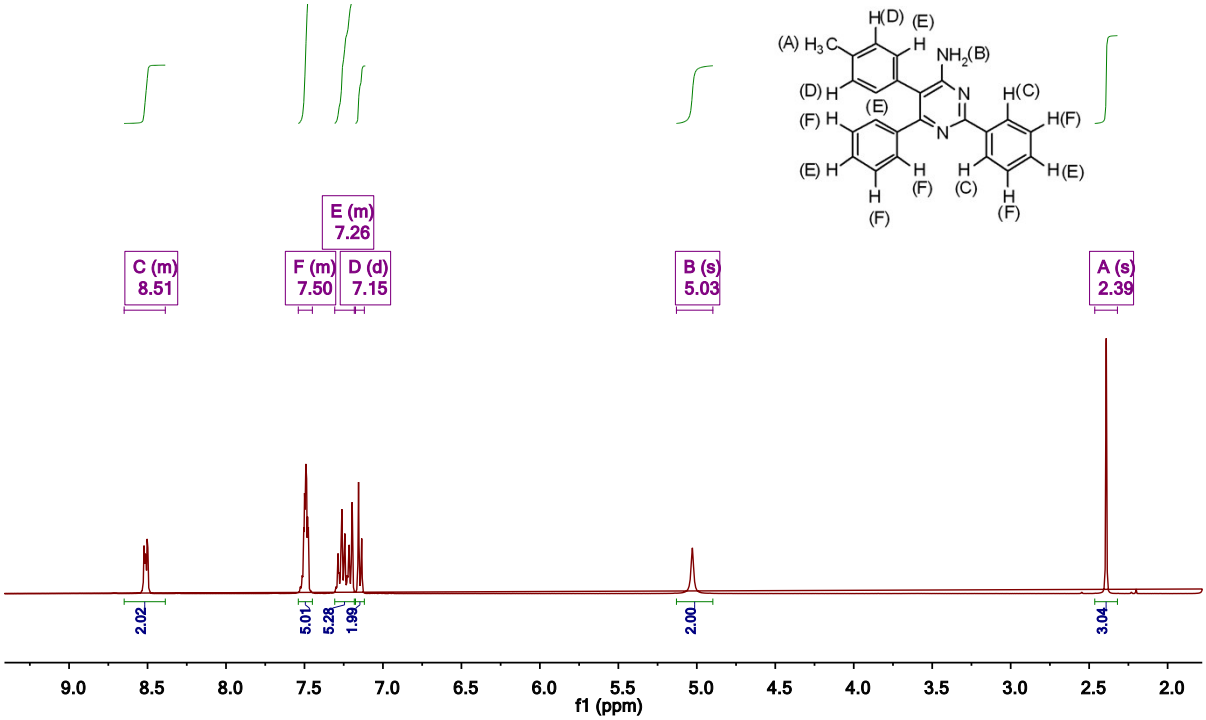
(3j)

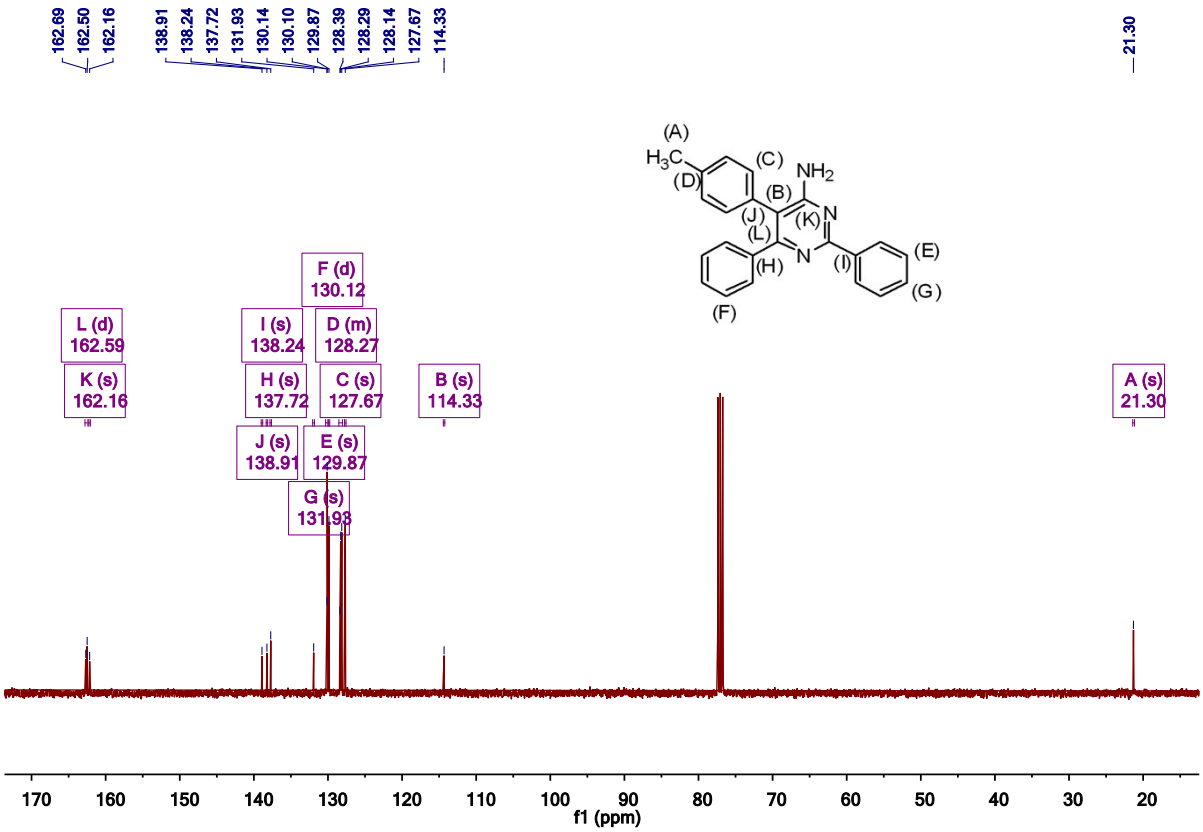

F (m) 7.26
D (s) 7.10
H (dd) 8.53
G (m) 7.50
C (d) 7.05
E (d) 7.16
B (s) 5.05
A (s) 2.35
1.96
4.96
4.15
0.99
0.98
1.00
1.92
3.00
f1 (ppm)

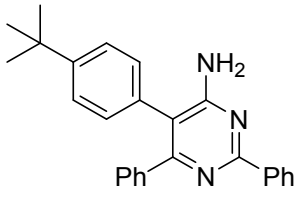

162.73
162.40
162.02
130.72
130.16
129.86
129.27
128.74
128.45
128.30
128.16
127.66
127.37
114.47
21.46
J (s) 130.72
H (s) 129.86
F (s) 128.74
P (s) 162.40
M (s) 138.84
D (s) 127.66
O (s) 162.02
L (s) 138.25
C (s) 127.37
B (s) 114.47
A (s) 21.46
Q (s) 162.73
N (s) 139.08
E (m) 128.31
G (s) 129.27
I (s) 130.16
K (s) 135.02
f1 (ppm)


Me
NH2
N
Ph
N
Ph

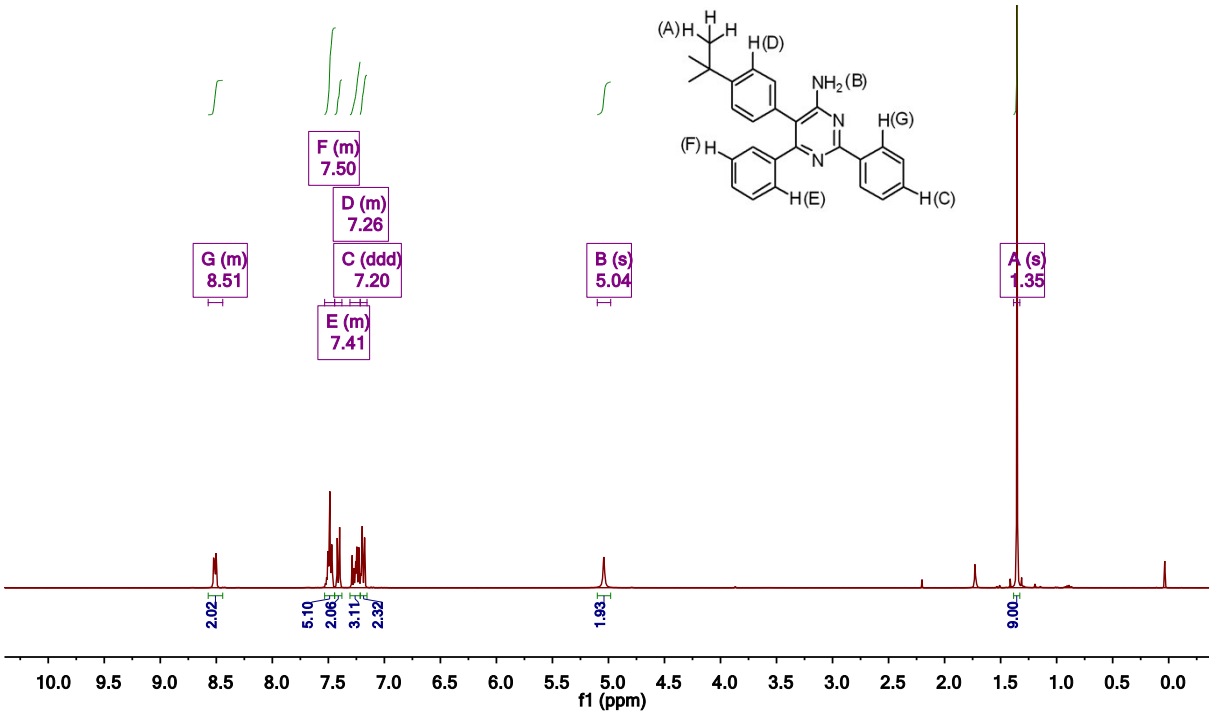
(3k)

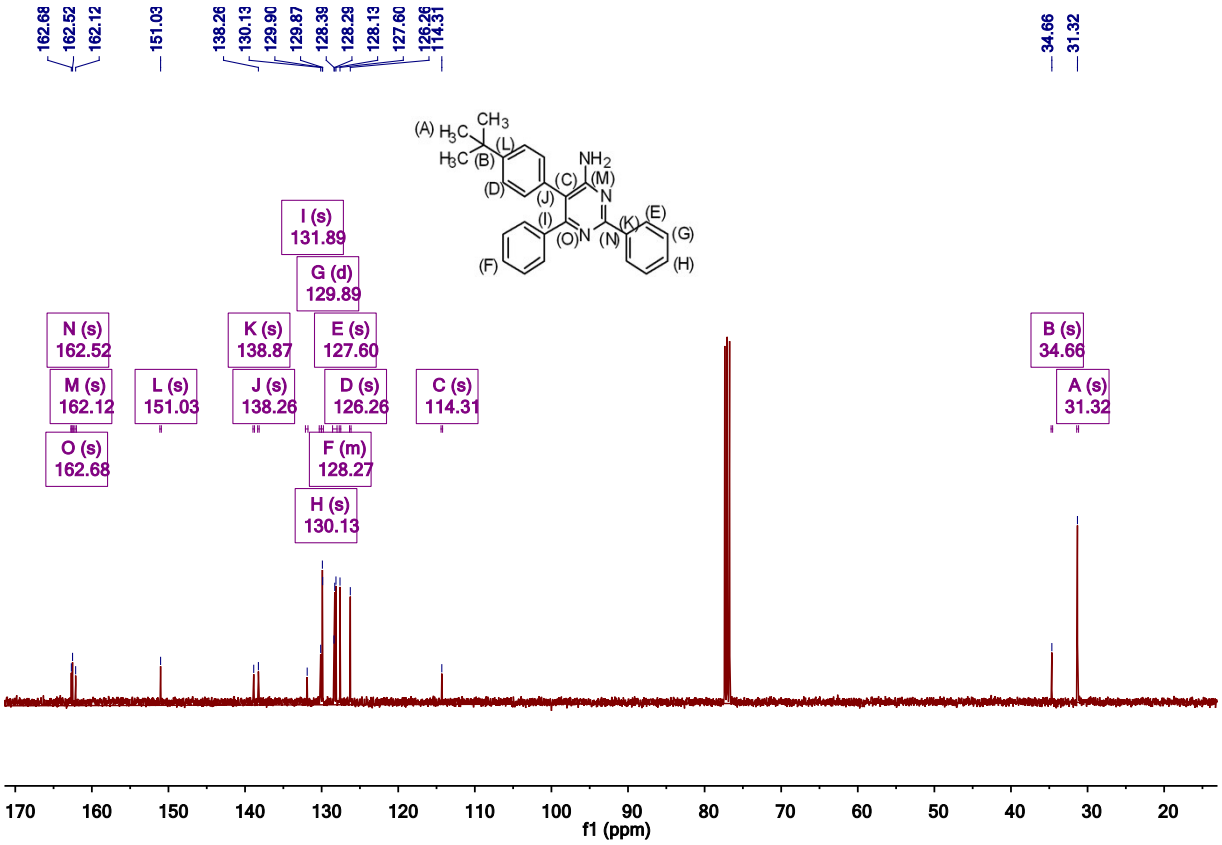

C (m) 8.51
F (m) 7.50
E (m) 7.26
D (d) 7.15
B (s) 5.03
A (s) 2.39
2.02
5.01
5.28
1.99
2.00
3.04
f1 (ppm)

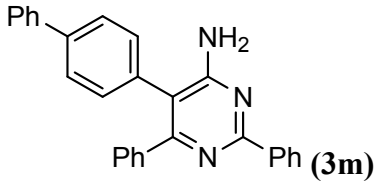

162.69
162.50
162.16
138.91
138.24
137.72
131.93
130.14
130.10
129.87
128.39
128.29
128.14
127.67
114.33
21.30
L (d) 162.59
K (s) 162.16
I (s) 138.24
H (s) 137.72
J (s) 138.91
F (d) 130.12
D (m) 128.27
C (s) 127.67
E (s) 129.87
G (s) 131.93
B (s) 114.33
A (s) 21.30
f1 (ppm)


NH2
N
Ph
N
Ph

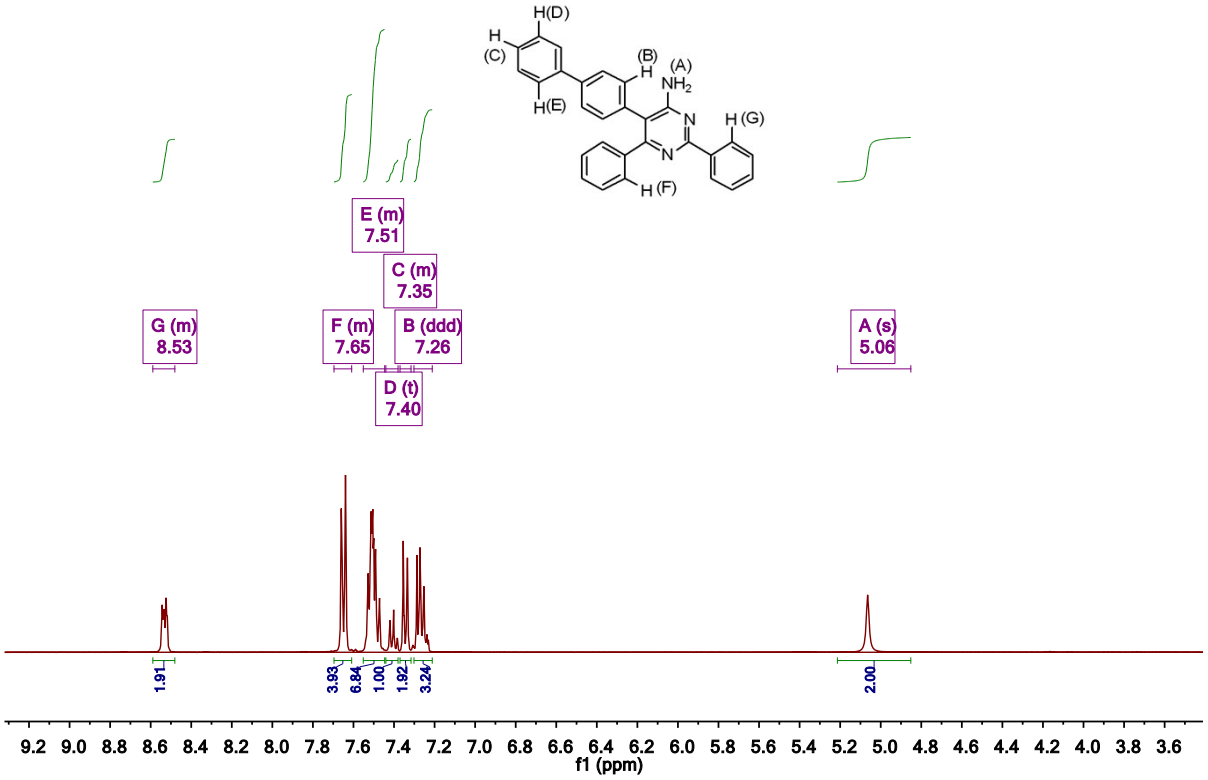
(3l)

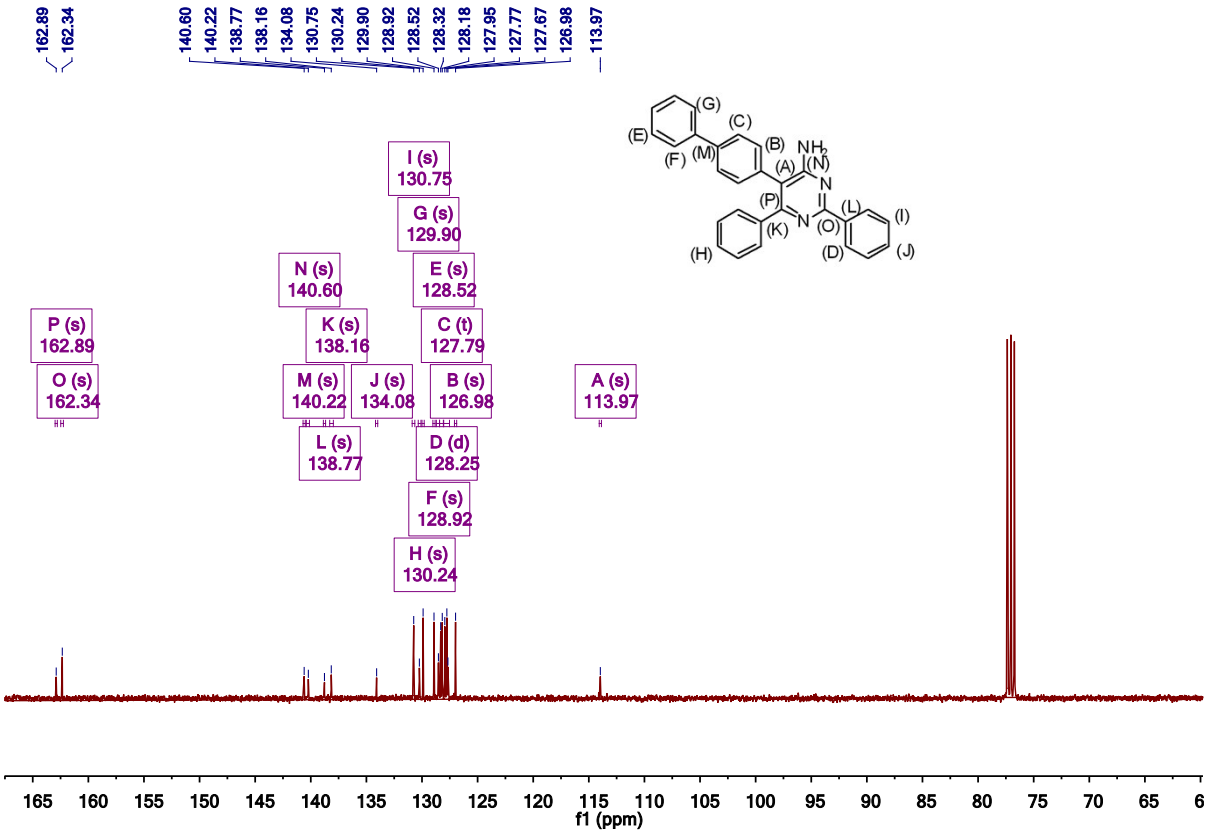

F (m) 7.50
D (m) 7.26
G (m) 8.51
C (ddd) 7.20
E (m) 7.41
B (s) 5.04
A (s) 1.35
2.02
5.10
2.06
3.11
2.32
1.93
9.00
f1 (ppm)

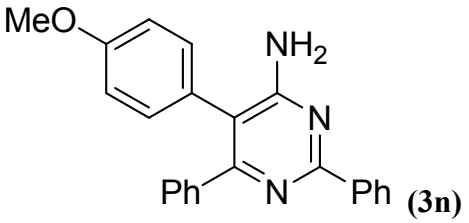

162.68
162.52
162.12
151.03
138.26
130.13
129.90
129.87
128.38
128.29
128.13
127.60
126.26
114.31
34.66
31.32
I (s) 131.89
G (d) 129.89
N (s) 162.52
K (s) 138.87
E (s) 127.60
B (s) 34.66
M (s) 162.12
L (s) 151.03
J (s) 138.26
D (s) 126.26
C (s) 114.31
A (s) 31.32
O (s) 162.68
F (m) 128.27
H (s) 130.13
f1 (ppm)


Ph
NH2
N
Ph
N
Ph

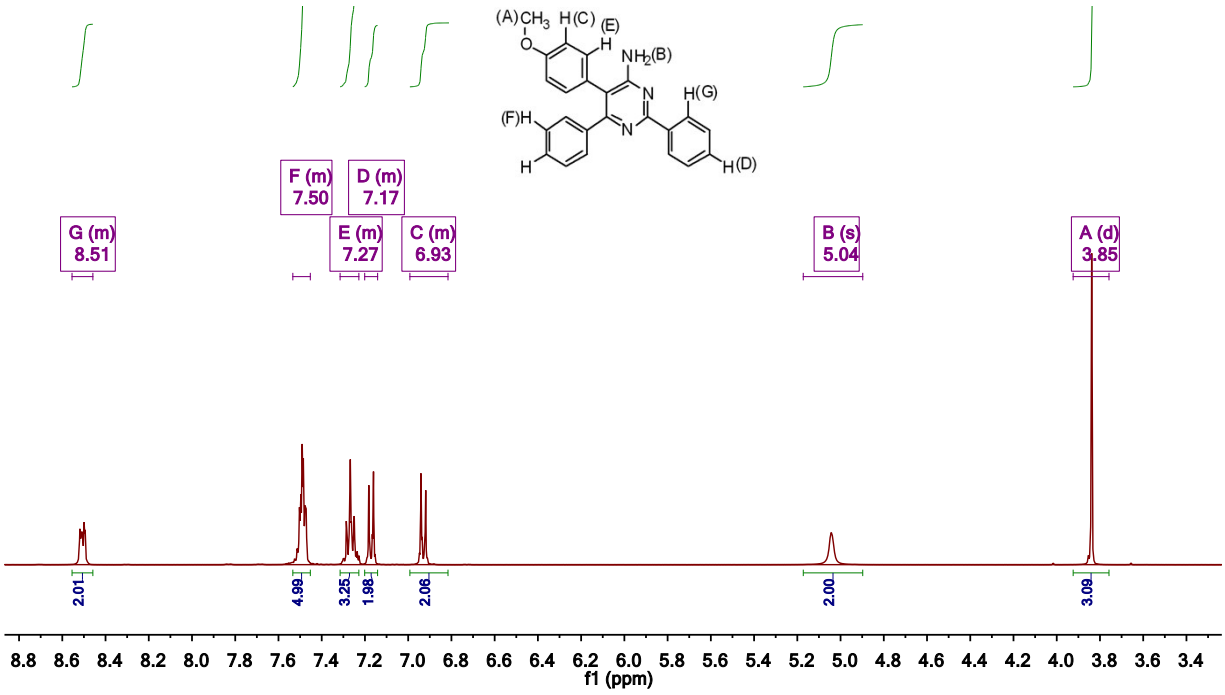
(3m)

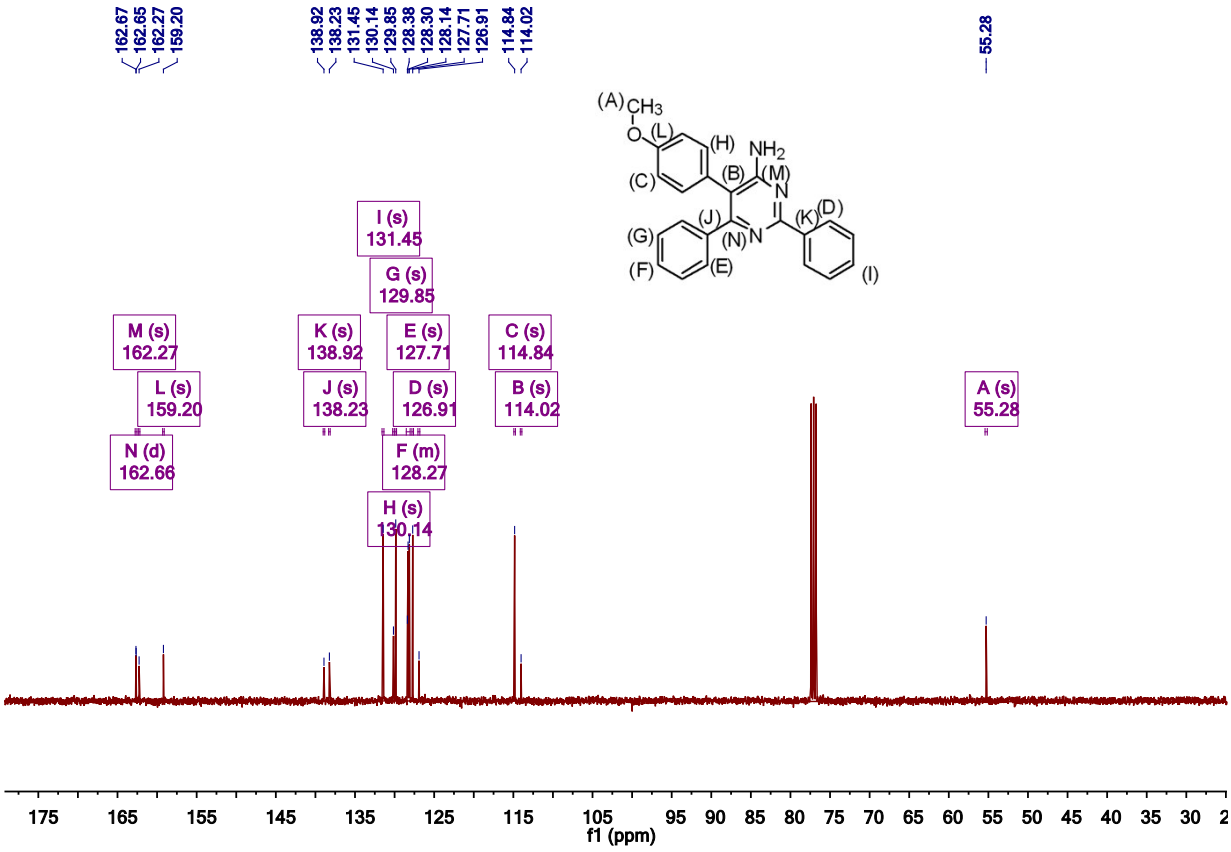

H(D)
H
(C)
H(E)
(B)
H
(A)
NH2
N
N
H (G)
H (F)
E (m)
7.51
C (m)
7.35
G (m)
8.53
F (m)
7.65
B (ddd)
7.26
D (t)
7.40
A (s)
5.06
1.91
3.93
6.84
1.00
1.92
3.24
2.00
9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6
f1 (ppm)

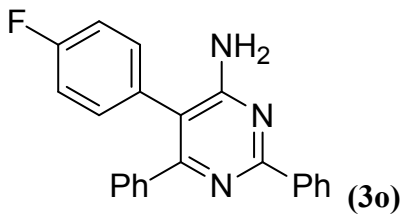

162.89
162.34
140.60
140.22
138.77
138.16
134.08
130.75
130.24
129.90
128.92
128.52
128.32
128.18
127.95
127.77
127.67
126.98
113.97
(G)
(C)
(E)
(B)
NH2
(F)
(M)
(A)
(N)
N
(P)
(L)
(I)
N
(O)
(K)
(H)
(D)
(J)
I (s)
130.75
G (s)
129.90
N (s)
140.60
E (s)
128.52
P (s)
162.89
K (s)
138.16
C (t)
127.79
O (s)
162.34
M (s)
140.22
J (s)
134.08
B (s)
126.98
A (s)
113.97
L (s)
138.77
D (d)
128.25
F (s)
128.92
H (s)
130.24
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 6
f1 (ppm)


MeO
NH2
N
Ph
N
Ph

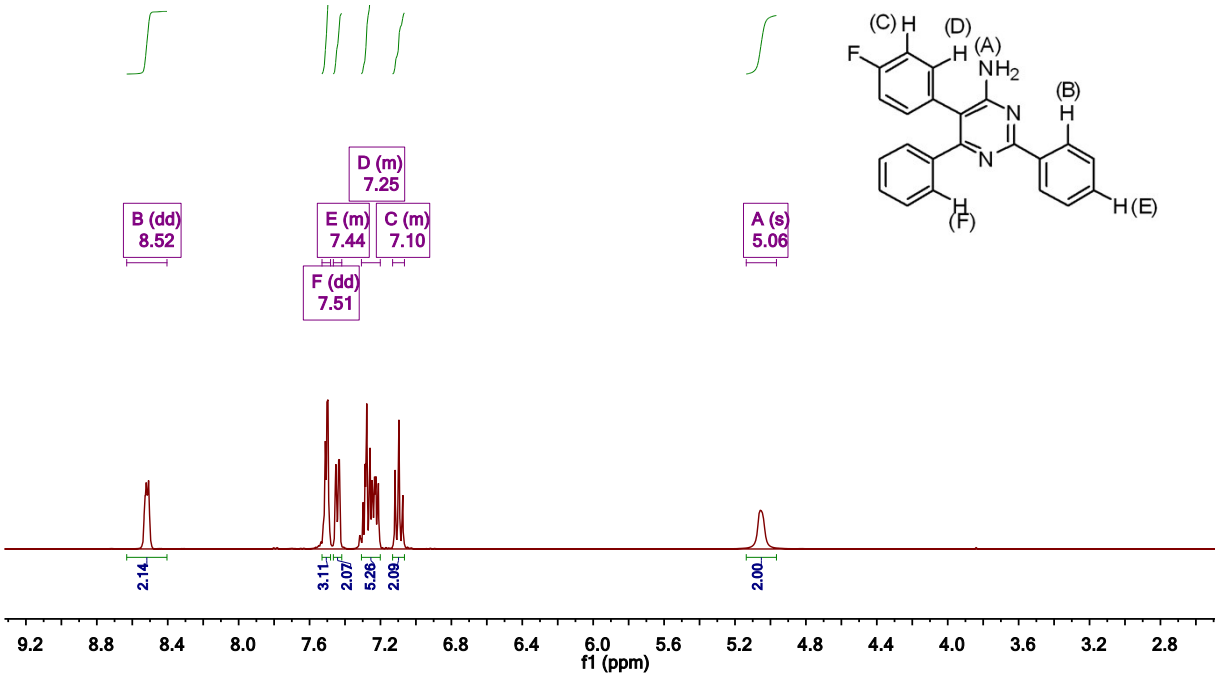
(3n)

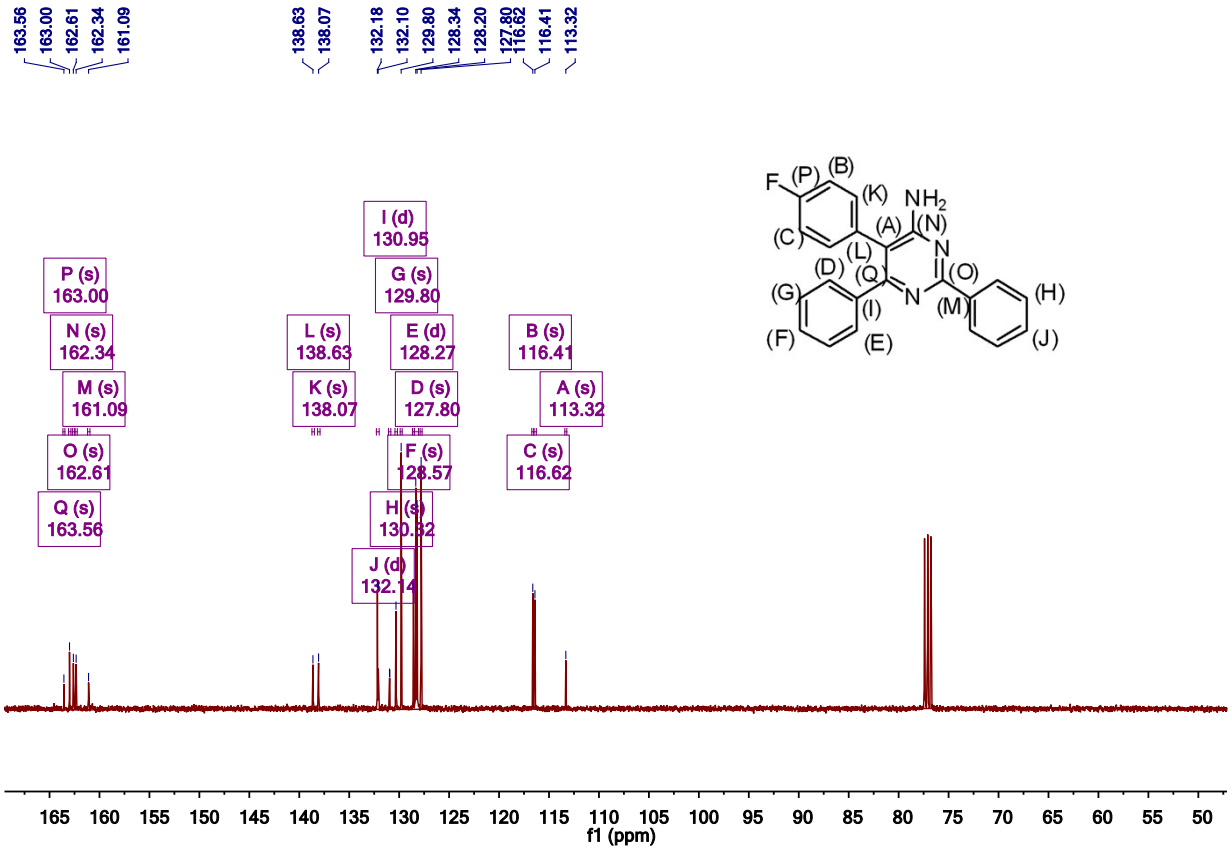

G (m) 8.51
F (m) 7.50
D (m) 7.17
E (m) 7.27
C (m) 6.93
B (s) 5.04
A (d) 3.85
2.01
4.99
3.25
1.98
2.06
2.00
3.09
f1 (ppm)

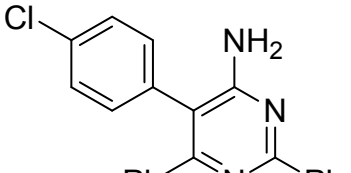

162.67
162.65
162.27
159.20
138.92
138.23
131.45
130.14
129.85
128.38
128.30
128.14
127.71
126.91
114.84
114.02
55.28
I (s) 131.45
G (s) 129.85
M (s) 162.27
L (s) 159.20
N (d) 162.66
K (s) 138.92
J (s) 138.23
E (s) 127.71
D (s) 126.91
F (m) 128.27
H (s) 130.14
C (s) 114.84
B (s) 114.02
A (s) 55.28
f1 (ppm)


F
NH2
N
Ph
N
Ph

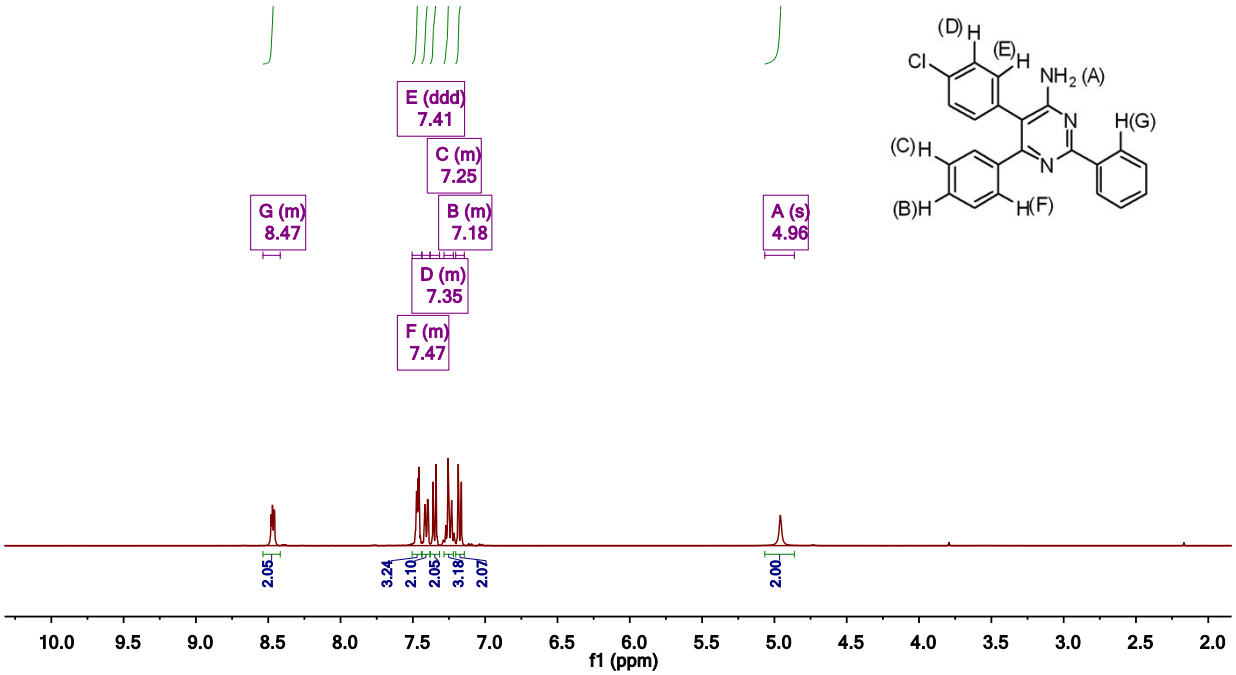
(3o)

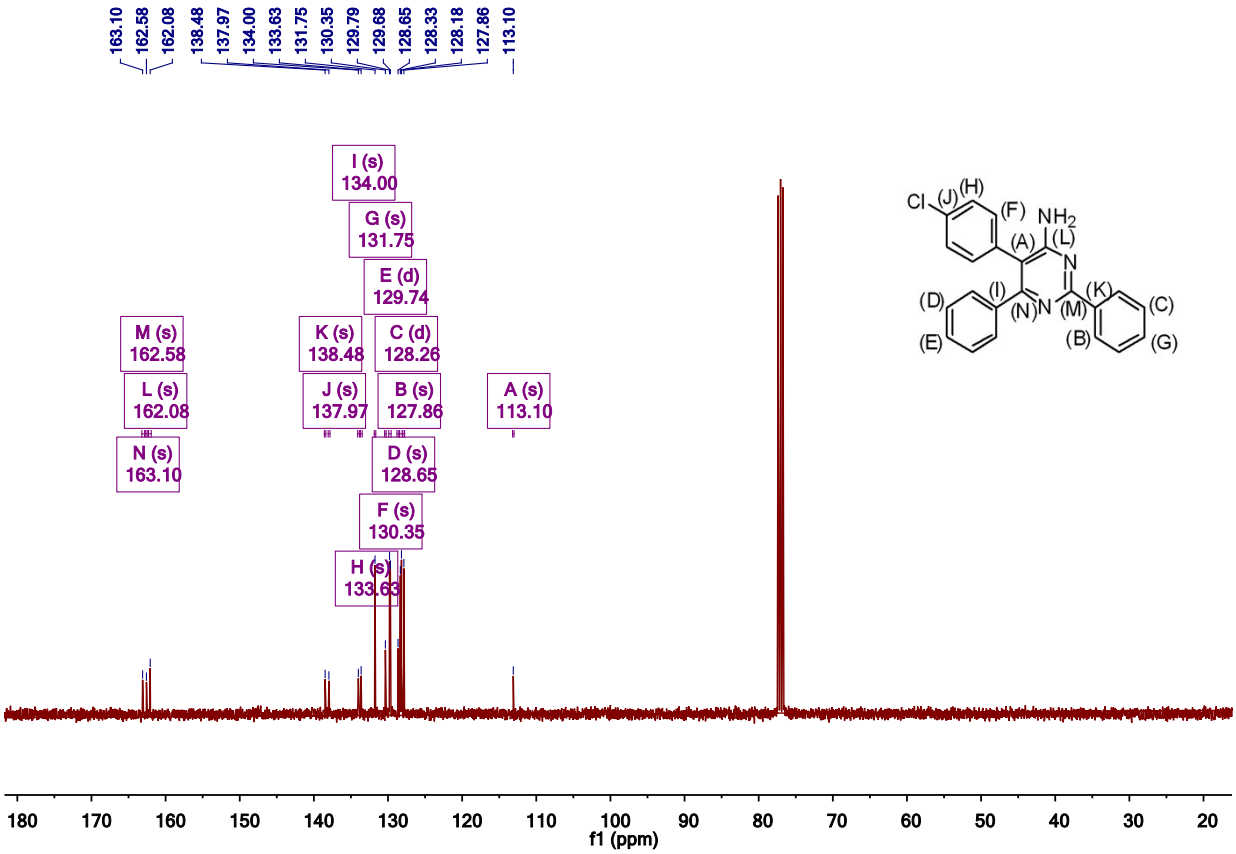

B (dd) 8.52
D (m) 7.25
E (m) 7.44
C (m) 7.10
F (dd) 7.51
A (s) 5.06
2.14
3.11
2.07
5.26
2.09
2.00
f1 (ppm)

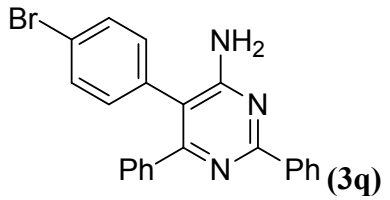

163.56
163.00
162.61
162.34
161.09
138.63
138.07
132.18
132.10
129.80
128.34
128.20
127.80
116.62
116.41
113.32
I (d) 130.95
G (s) 129.80
P (s) 163.00
N (s) 162.34
M (s) 161.09
O (s) 162.61
Q (s) 163.56
L (s) 138.63
K (s) 138.07
E (d) 128.27
D (s) 127.80
F (s) 128.57
H (s) 130.32
J (d) 132.14
B (s) 116.41
A (s) 113.32
C (s) 116.62
f1 (ppm)



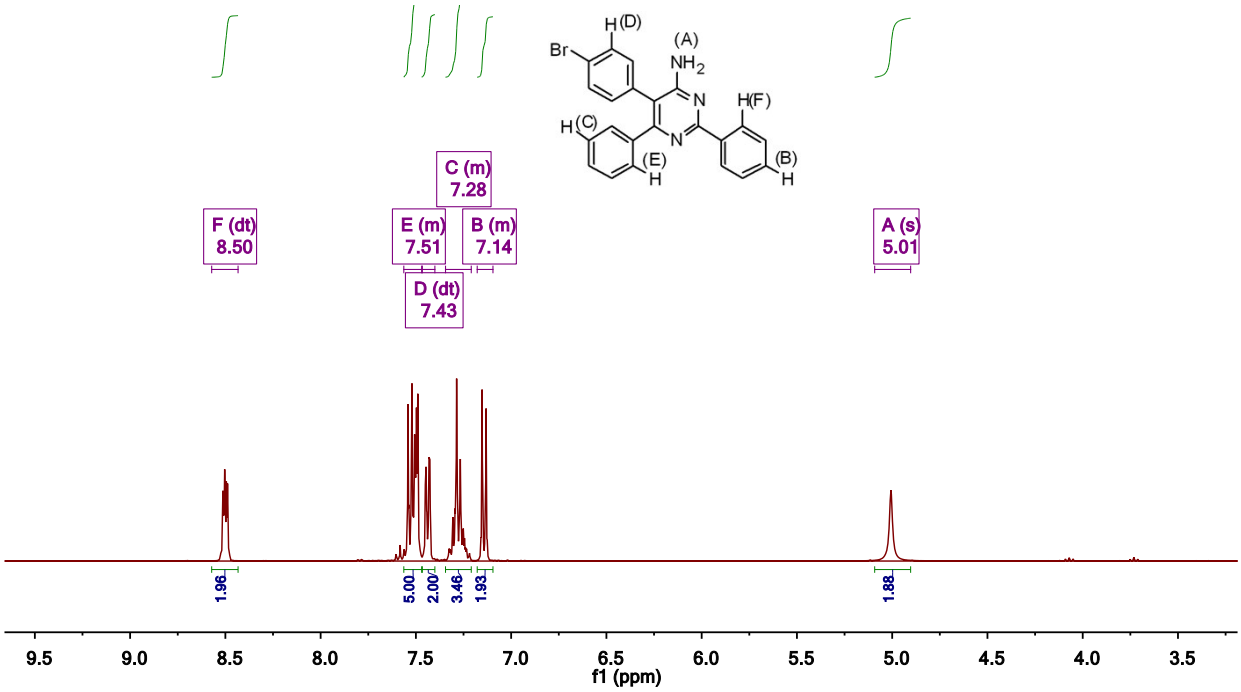
(3p)

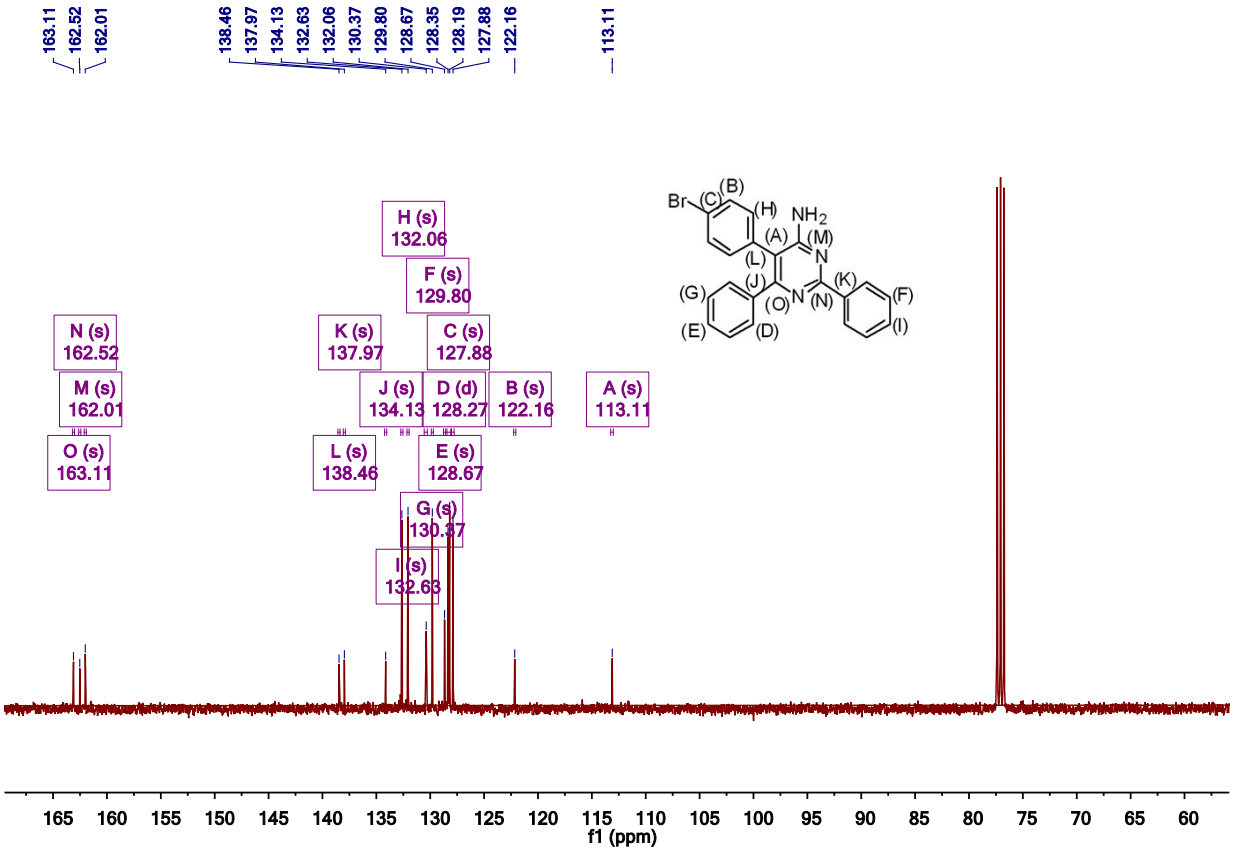

E (ddd) 7.41
C (m) 7.25
G (m) 8.47
B (m) 7.18
A (s) 4.96
D (m) 7.35
F (m) 7.47
2.05
3.24
2.10
2.05
3.18
2.07
2.00
f1 (ppm)

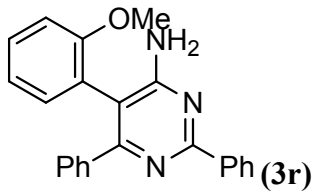

163.10
162.58
162.08
138.48
137.97
134.00
133.63
131.75
130.35
129.79
129.68
128.65
128.33
128.18
127.86
113.10
I (s) 134.00
G (s) 131.75
E (d) 129.74
M (s) 162.58
K (s) 138.48
C (d) 128.26
L (s) 162.08
J (s) 137.97
B (s) 127.86
A (s) 113.10
N (s) 163.10
D (s) 128.65
F (s) 130.35
H (s) 133.63
f1 (ppm)


Br
NH2
N
Ph
N
Ph

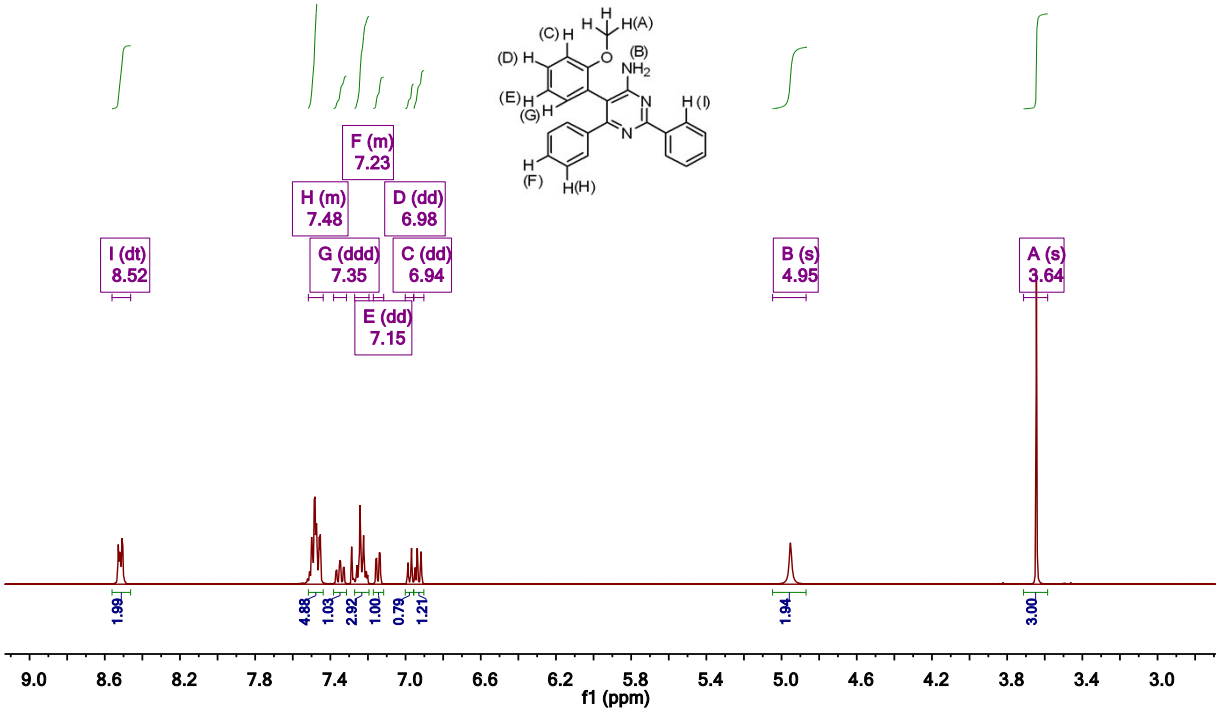
(3q)

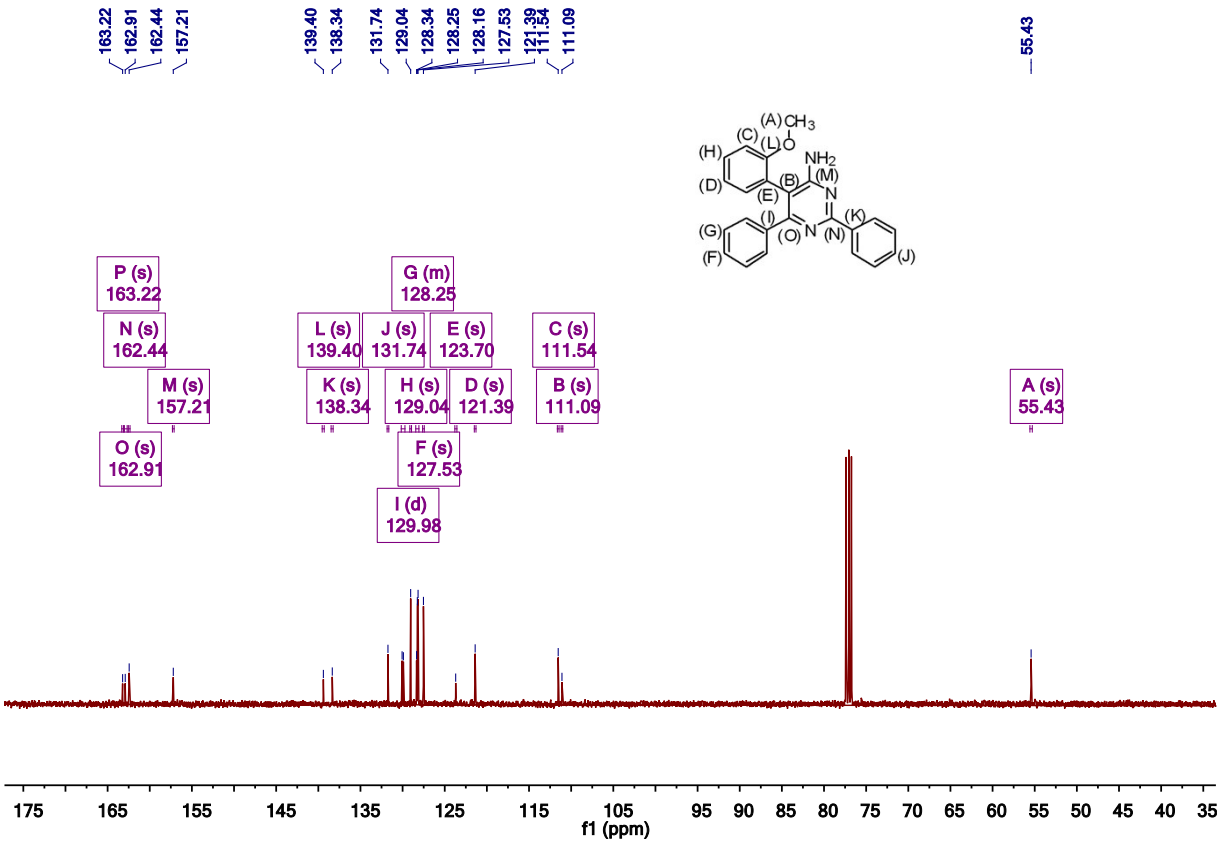

F (dt) 8.50
E (m) 7.51
C (m) 7.28
B (m) 7.14
D (dt) 7.43
A (s) 5.01
1.96
5.00
2.00
3.46
1.93
1.88
f1 (ppm)

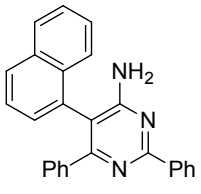

163.11
162.52
162.01
138.46
137.97
134.13
132.63
132.06
130.37
129.80
128.67
128.35
128.19
127.88
122.16
113.11
H (s) 132.06
F (s) 129.80
N (s) 162.52
K (s) 137.97
C (s) 127.88
M (s) 162.01
J (s) 134.13
D (d) 128.27
B (s) 122.16
A (s) 113.11
O (s) 163.11
L (s) 138.46
E (s) 128.67
G (s) 130.37
I (s) 132.63
f1 (ppm)


OMe
NH2
N
Ph
N
Ph

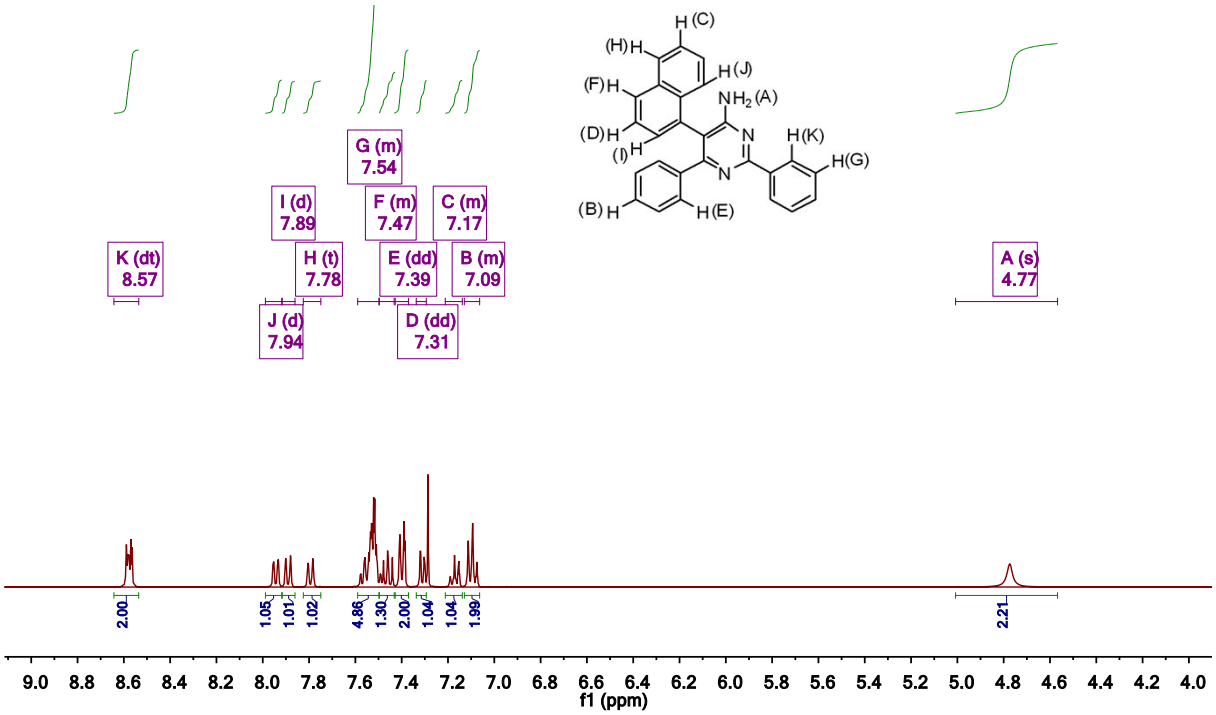
(3r)

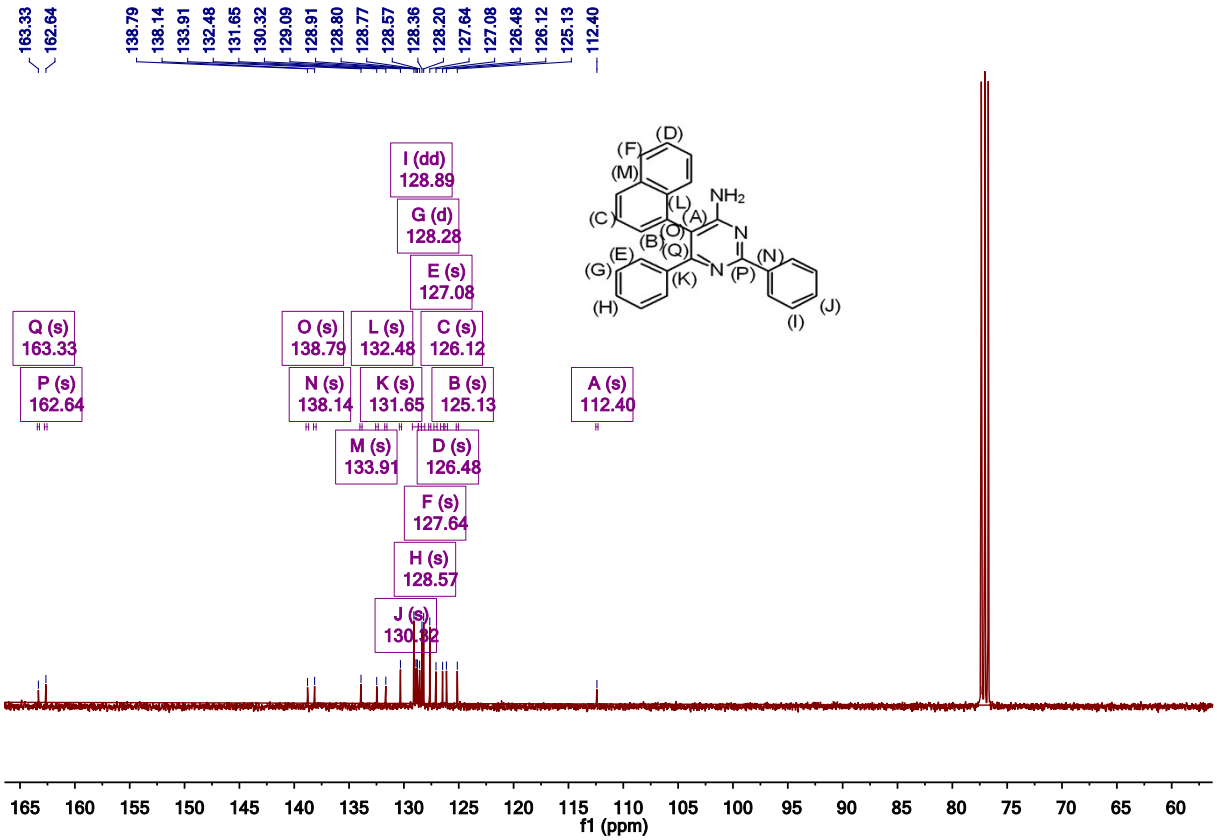

F (m) 7.23
H (m) 7.48
D (dd) 6.98
I (dt) 8.52
G (ddd) 7.35
C (dd) 6.94
E (dd) 7.15
B (s) 4.95
A (s) 3.64
1.98
4.88
1.03
2.92
1.00
0.79
1.21
1.94
3.00
f1 (ppm)

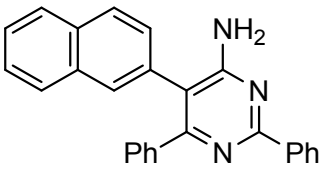

163.22
162.91
162.44
157.21
139.40
138.34
131.74
129.04
128.34
128.25
128.16
127.53
121.39
111.54
111.09
55.43
P (s) 163.22
N (s) 162.44
M (s) 157.21
O (s) 162.91
G (m) 128.25
L (s) 139.40
J (s) 131.74
E (s) 123.70
K (s) 138.34
H (s) 129.04
D (s) 121.39
F (s) 127.53
I (d) 129.98
C (s) 111.54
B (s) 111.09
A (s) 55.43
f1 (ppm)


NH2
N
Ph
N
Ph

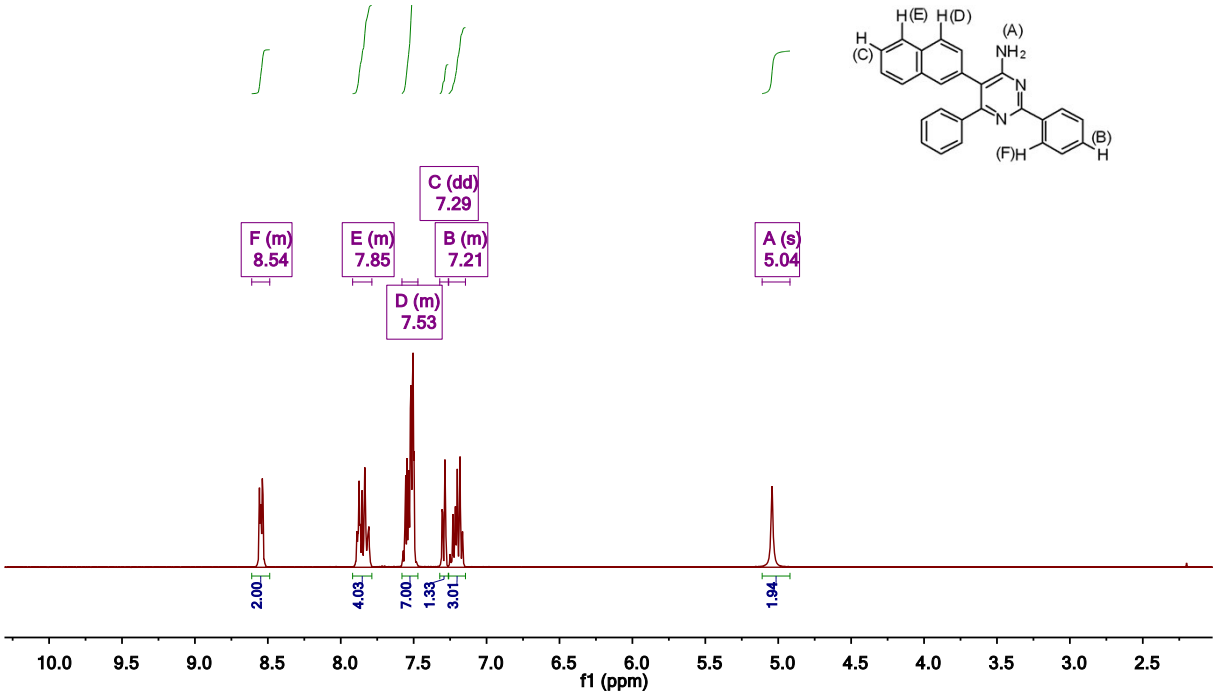
(3s)

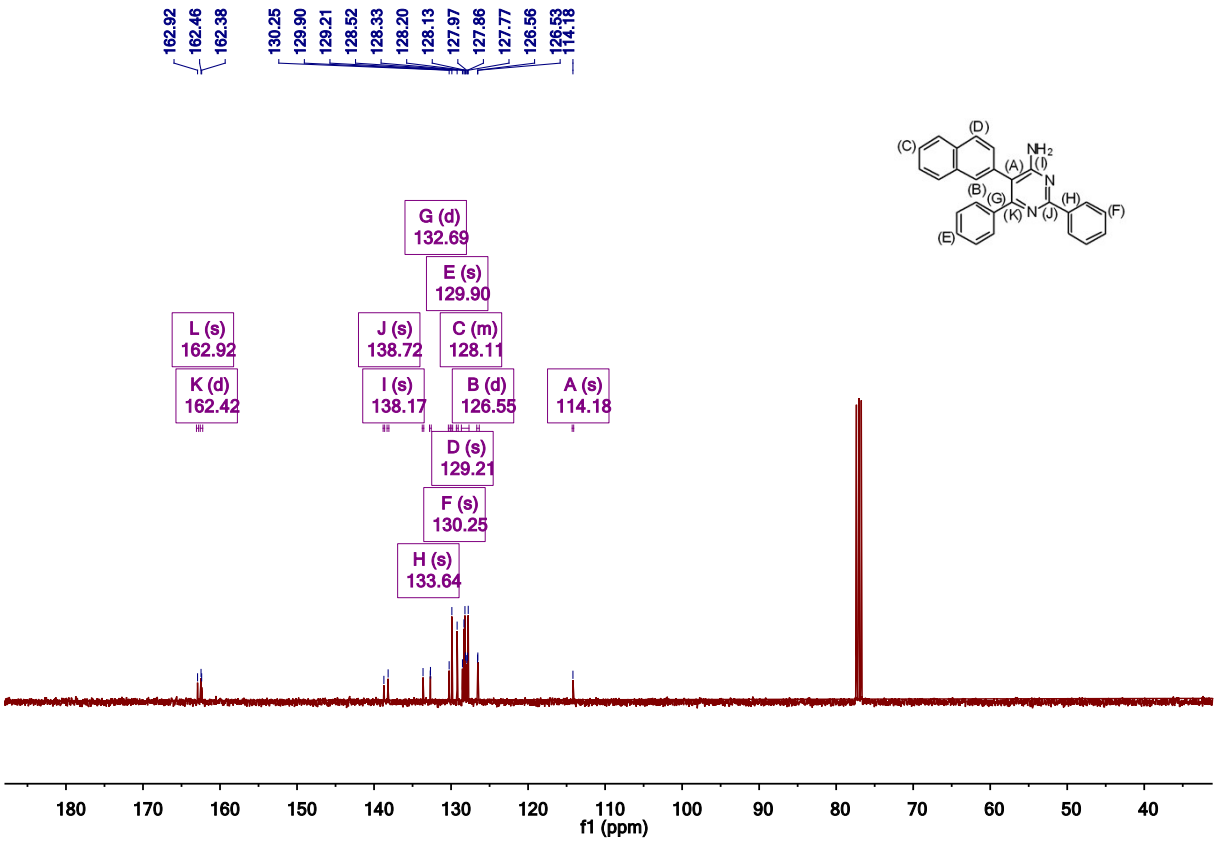

K (dt) 8.57
I (d) 7.89
J (d) 7.94
H (t) 7.78
G (m) 7.54
F (m) 7.47
E (dd) 7.39
D (dd) 7.31
C (m) 7.17
B (m) 7.09
A (s) 4.77
2.00
1.05
1.01
1.02
4.86
1.30
2.00
1.04
1.04
1.99
2.21
f1 (ppm)

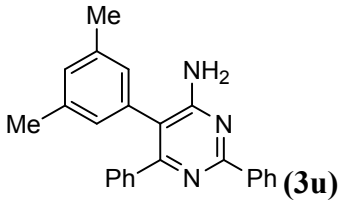

163.33
162.64
138.79
138.14
133.91
132.48
131.65
130.32
129.09
128.91
128.80
128.77
128.57
128.36
128.20
127.64
127.08
126.48
126.12
125.13
112.40
Q (s) 163.33
P (s) 162.64
O (s) 138.79
N (s) 138.14
L (s) 132.48
K (s) 131.65
M (s) 133.91
I (dd) 128.89
G (d) 128.28
E (s) 127.08
C (s) 126.12
B (s) 125.13
D (s) 126.48
F (s) 127.64
H (s) 128.57
J (s) 130.32
A (s) 112.40
f1 (ppm)


NH2
N
Ph
N
Ph

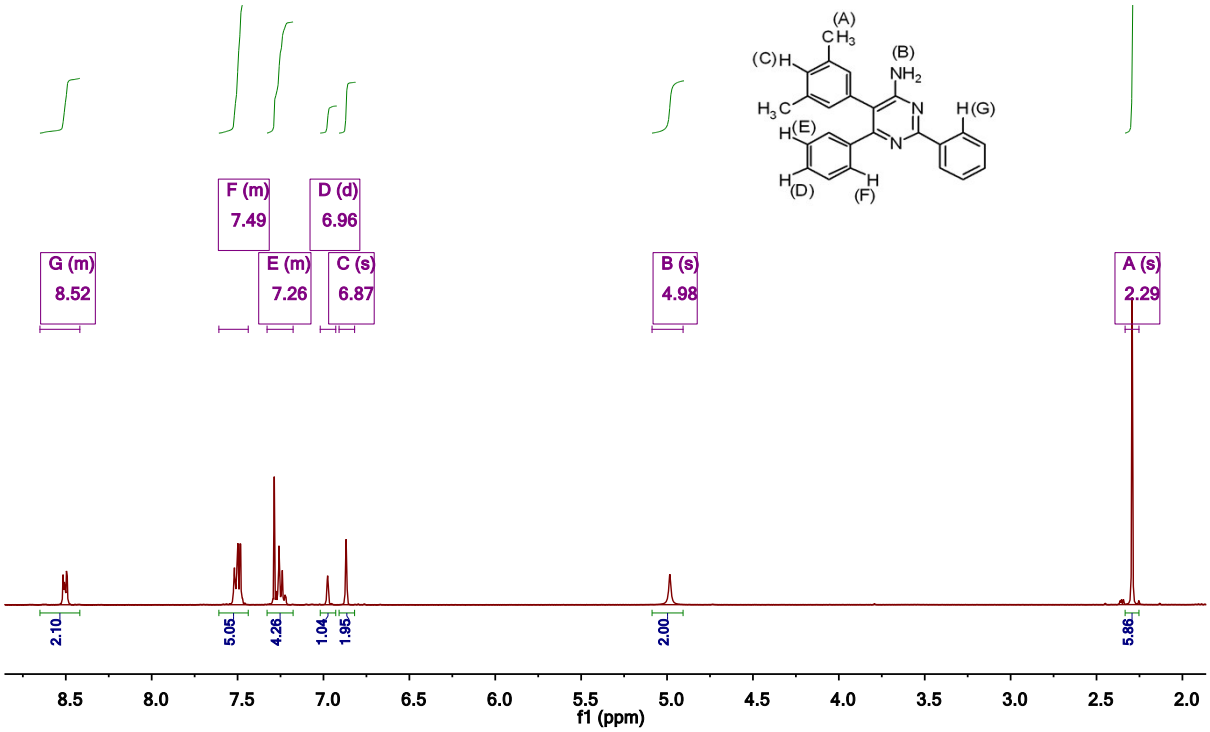
(3t)

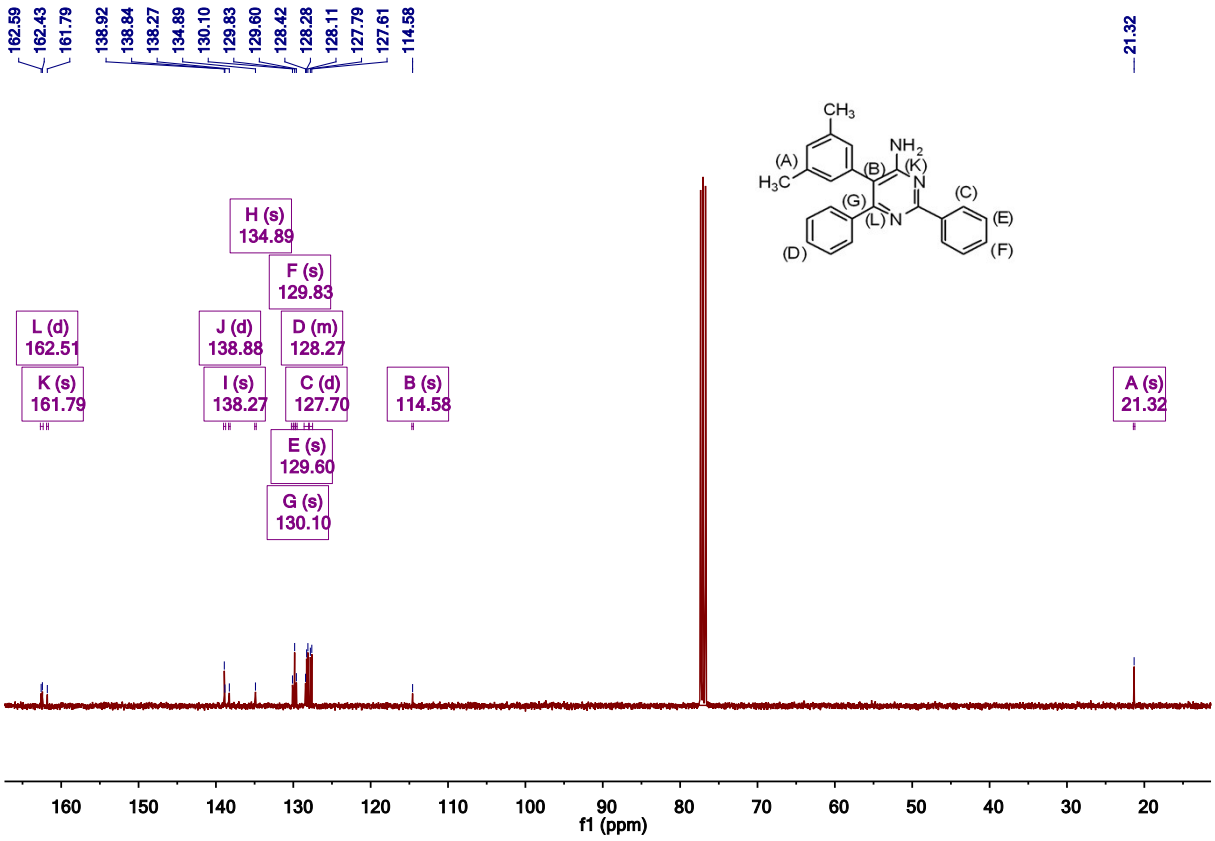

F (m) 8.54
E (m) 7.85
C (dd) 7.29
B (m) 7.21
D (m) 7.53
A (s) 5.04
2.00
4.03
7.00
1.33
3.01
1.94
f1 (ppm)

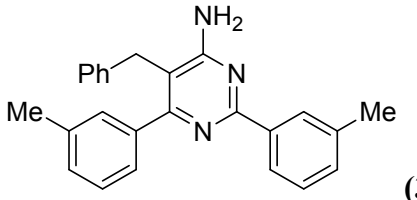

162.92
162.46
162.38
130.25
129.90
129.21
128.52
128.33
128.20
128.13
127.97
127.86
127.77
126.56
126.53
114.18
G (d) 132.69
E (s) 129.90
L (s) 162.92
K (d) 162.42
J (s) 138.72
I (s) 138.17
C (m) 128.11
B (d) 126.55
A (s) 114.18
D (s) 129.21
F (s) 130.25
H (s) 133.64
f1 (ppm)


Me
NH2
Me
N
Ph
N
Ph

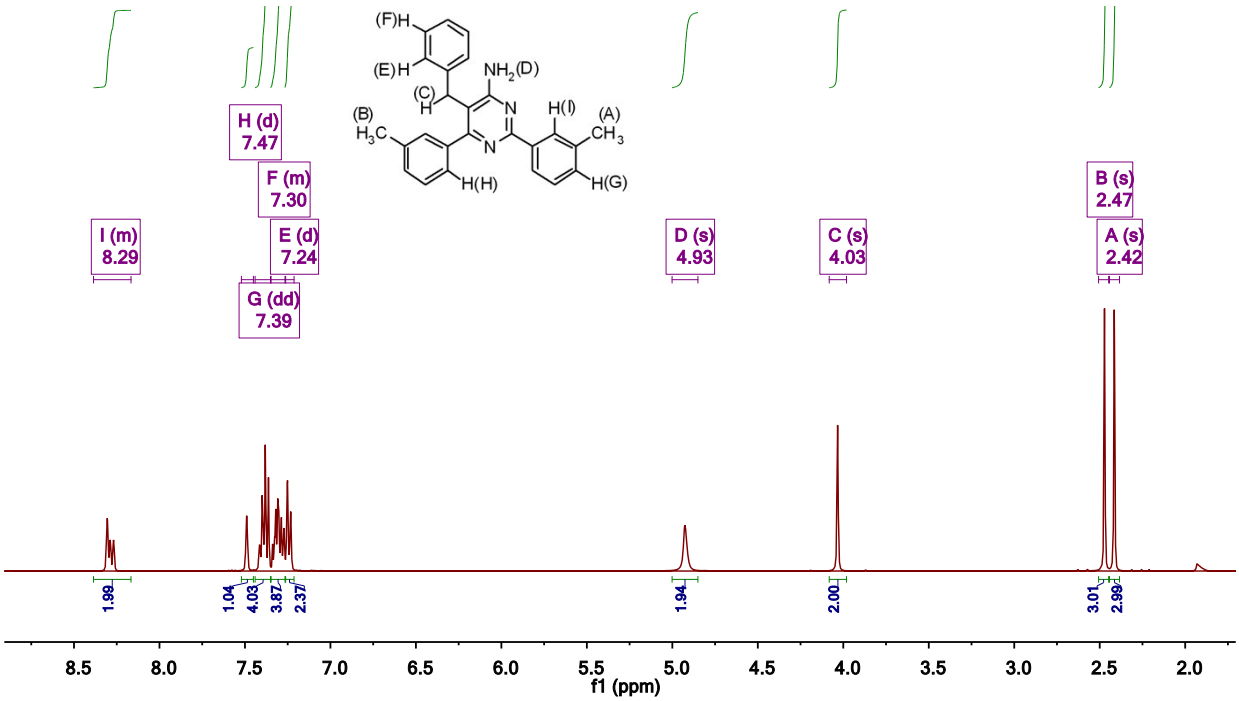
(3u)

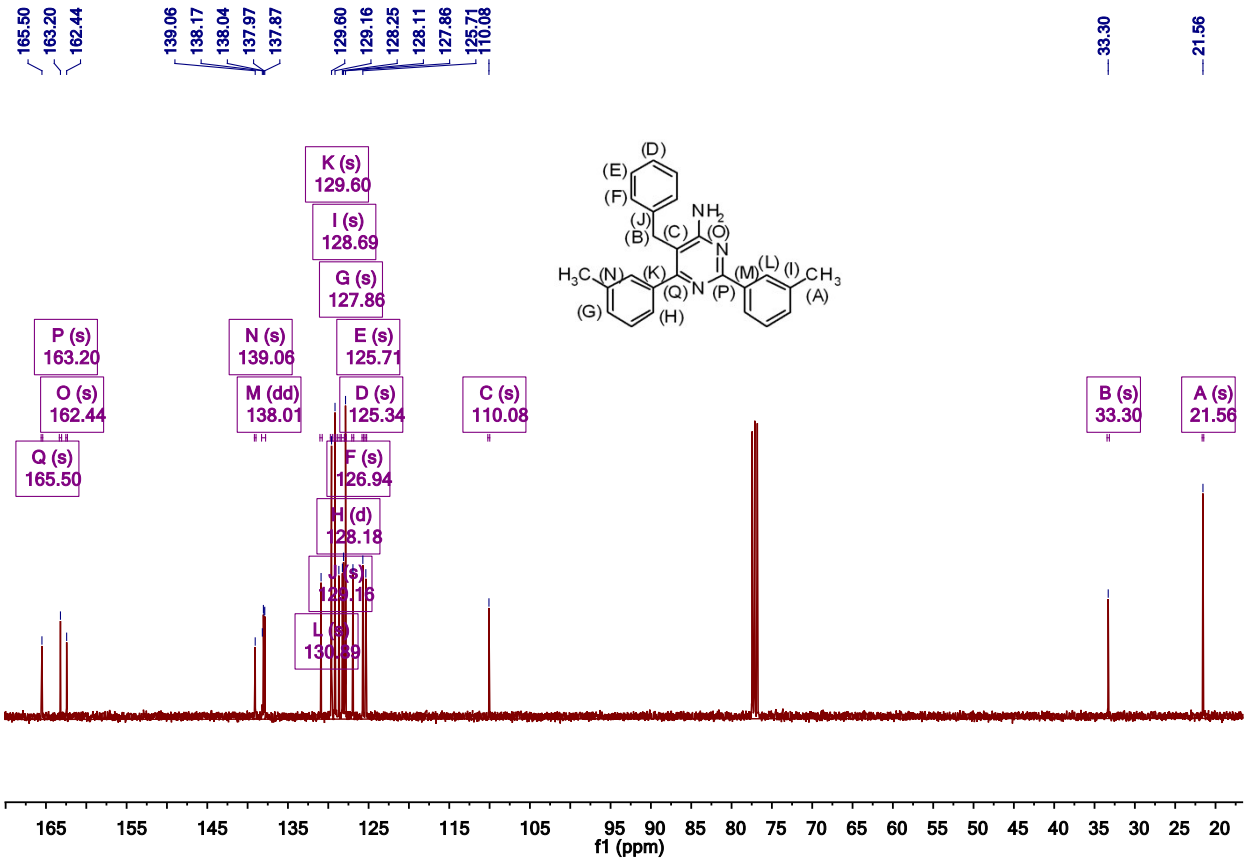

F (m) 7.49
D (d) 6.96
G (m) 8.52
E (m) 7.26
C (s) 6.87
B (s) 4.98
A (s) 2.29
2.10
5.05
4.26
1.04
1.95
2.00
5.86
f1 (ppm)

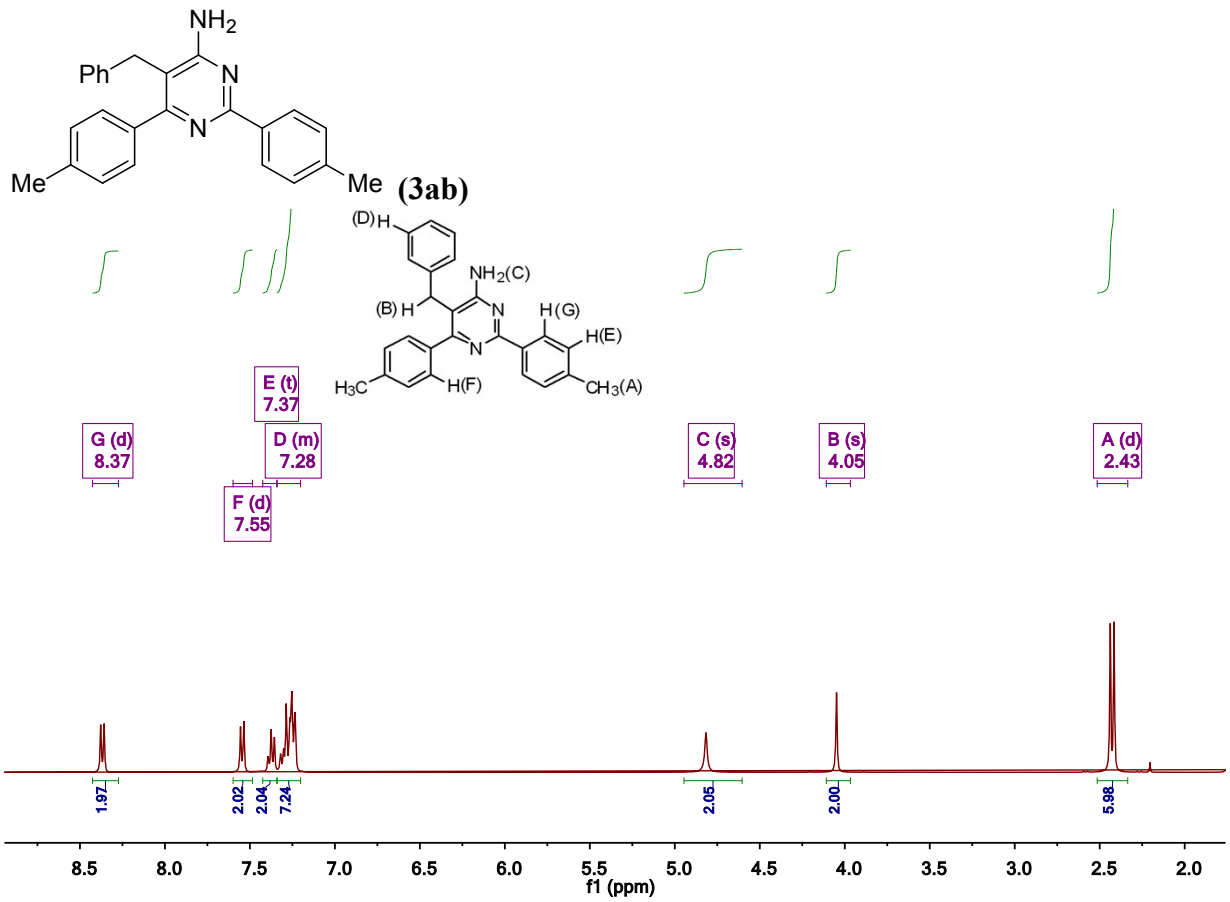

162.59
162.43
161.79
138.92
138.84
138.27
134.89
130.10
129.83
129.60
128.42
128.28
128.11
127.79
127.61
114.58
21.32
H (s) 134.89
F (s) 129.83
L (d) 162.51
J (d) 138.88
D (m) 128.27
K (s) 161.79
I (s) 138.27
C (d) 127.70
B (s) 114.58
A (s) 21.32
E (s) 129.60
G (s) 130.10
f1 (ppm)

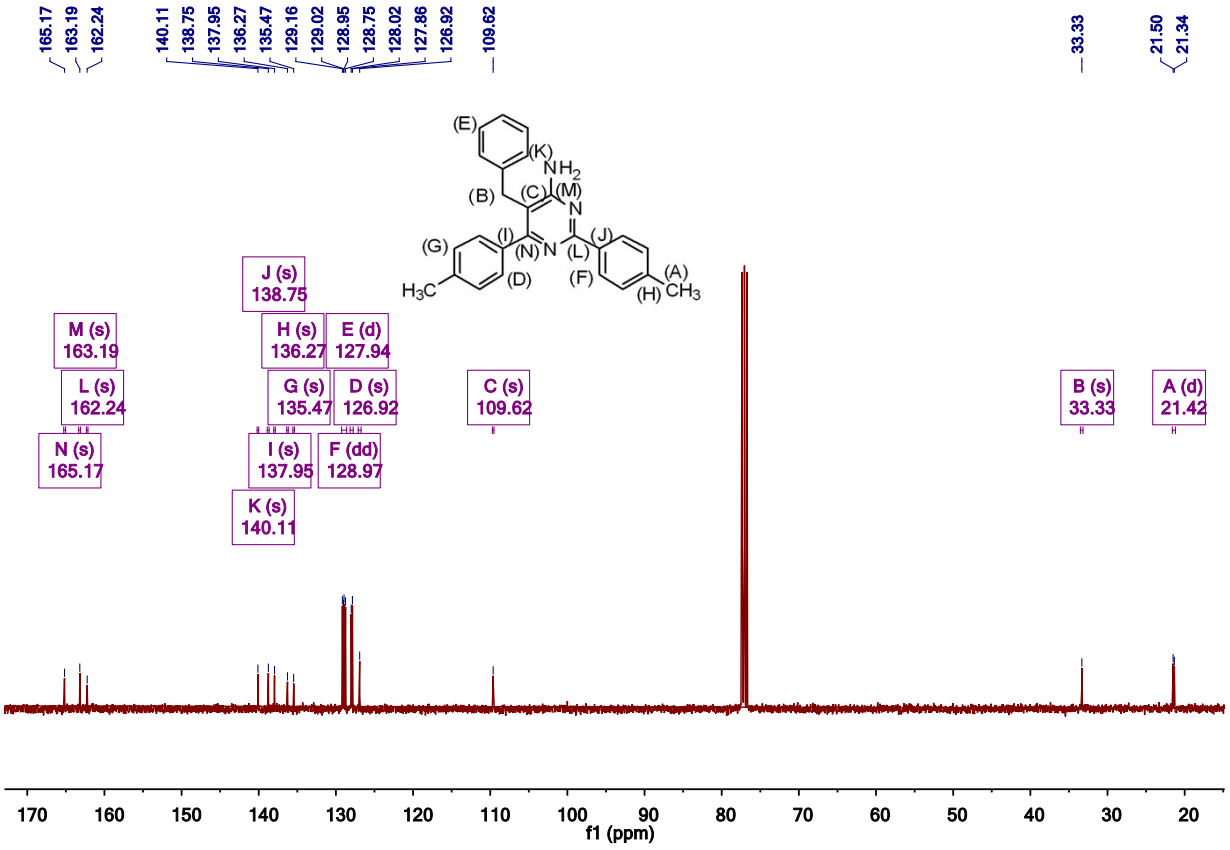

NH2
Ph
N
N
Me
Me

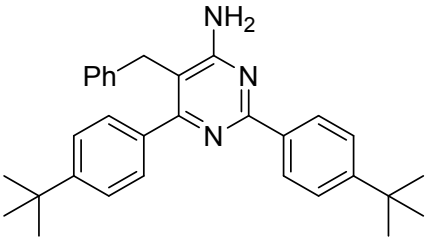
(3aa)


H (d) 7.47
F (m) 7.30
E (d) 7.24
G (dd) 7.39
I (m) 8.29
D (s) 4.93
C (s) 4.03
B (s) 2.47
A (s) 2.42
1.98
1.04
4.03
3.87
2.37
1.94
2.00
3.01
2.99
f1 (ppm)

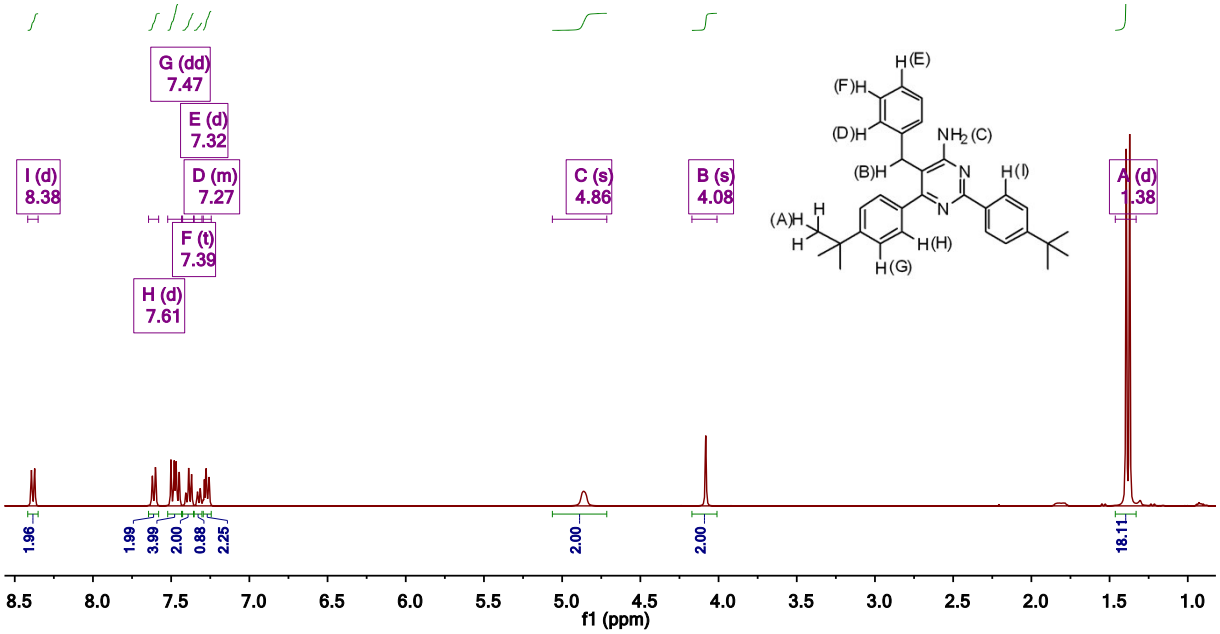

165.50
163.20
162.44
139.06
138.17
138.04
137.97
137.87
129.60
129.16
128.25
128.11
127.86
125.71
110.08
33.30
21.56
K (s) 129.60
I (s) 128.69
G (s) 127.86
P (s) 163.20
O (s) 162.44
Q (s) 165.50
N (s) 139.06
M (dd) 138.01
E (s) 125.71
D (s) 125.34
F (s) 126.94
H (d) 128.18
C (s) 110.08
B (s) 33.30
A (s) 21.56
f1 (ppm)

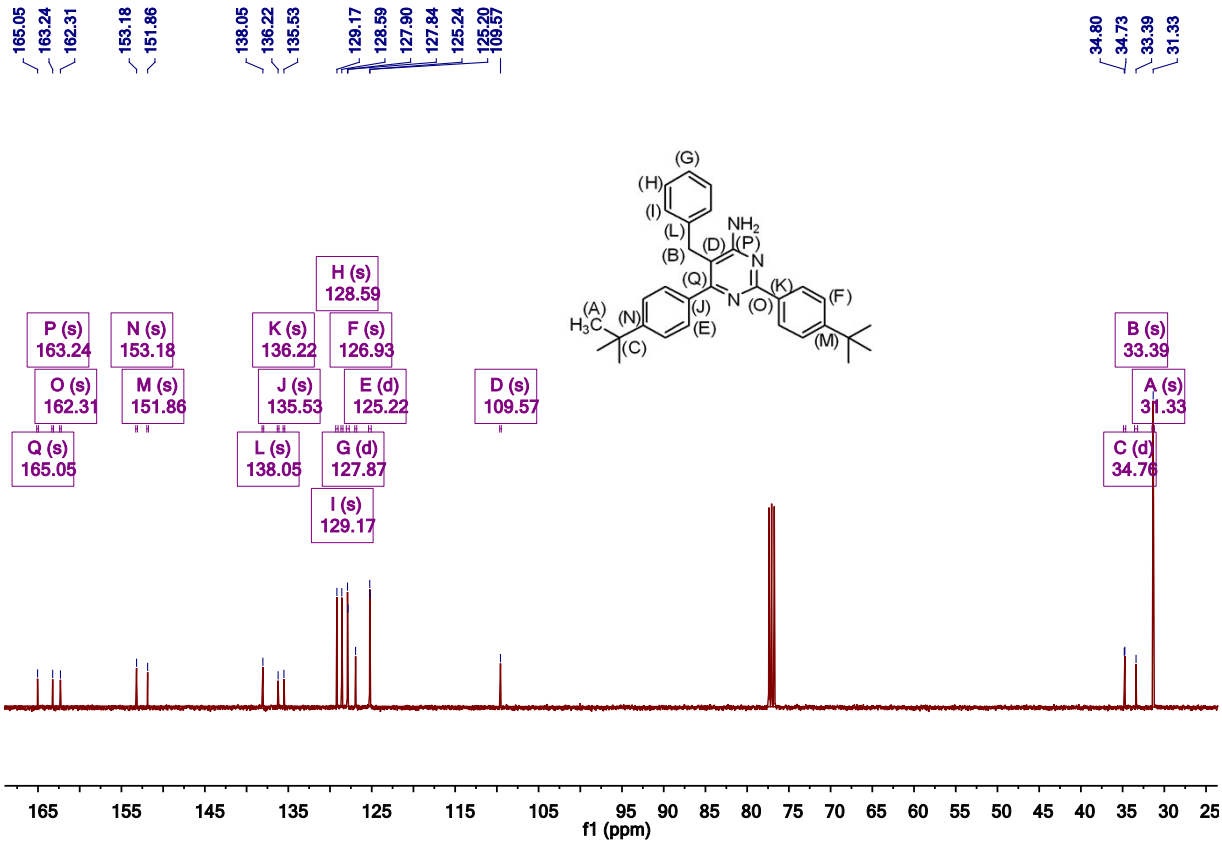

NH2
Ph
N
N
Me
Me
(3ab)
(D)H
NH2(C)
(B)H
N
H(G)
H(E)
N
H3C
H(F)
CH3(A)
E (t) 7.37
G (d) 8.37
D (m) 7.28
F (d) 7.55
C (s) 4.82
B (s) 4.05
A (d) 2.43
1.97
2.02
2.04
7.24
2.05
2.00
5.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)

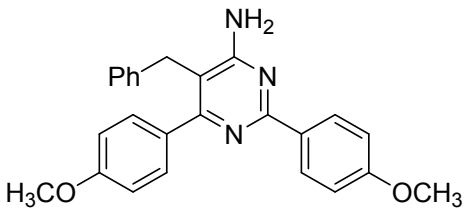

165.17
163.19
162.24
140.11
138.75
137.95
136.27
135.47
129.16
129.02
128.95
128.75
128.02
127.86
126.92
109.62
33.33
21.50
21.34
(E)
(K)
NH2
(B)
(C)
(M)
N
(G)
(I)
(N)
N
(L)
(J)
H3C
(D)
(F)
(A)
(H)
CH3
J (s) 138.75
M (s) 163.19
H (s) 136.27
E (d) 127.94
L (s) 162.24
G (s) 135.47
D (s) 126.92
C (s) 109.62
B (s) 33.33
A (d) 21.42
N (s) 165.17
I (s) 137.95
F (dd) 128.97
K (s) 140.11
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


NH2
Ph
N
N

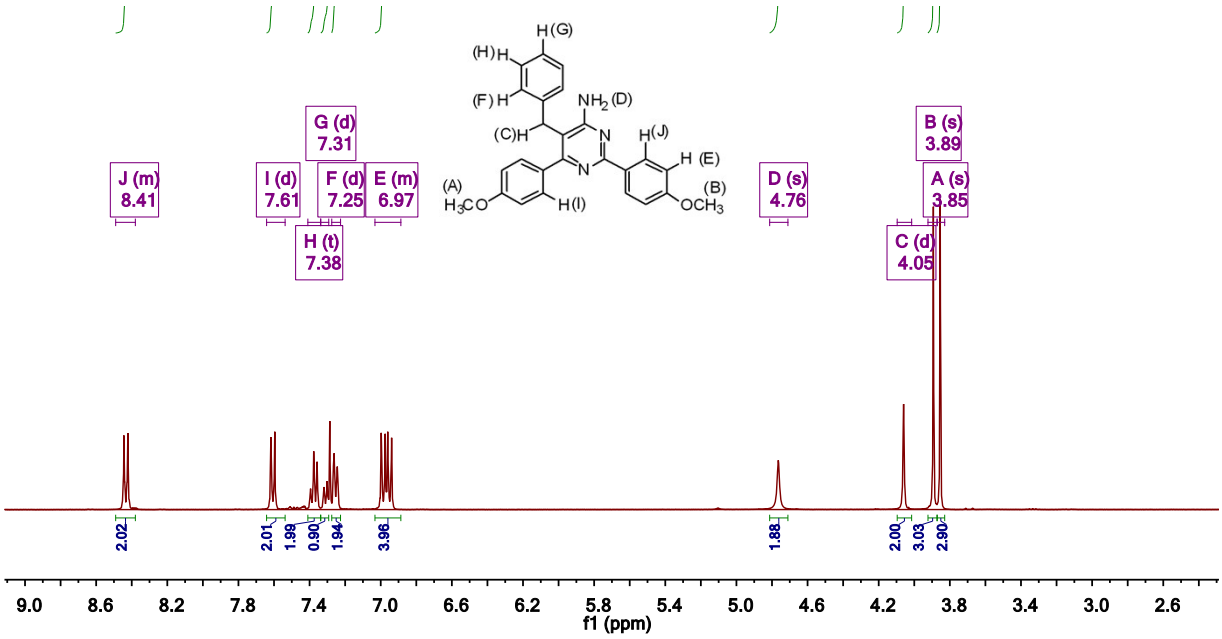
(3ac)

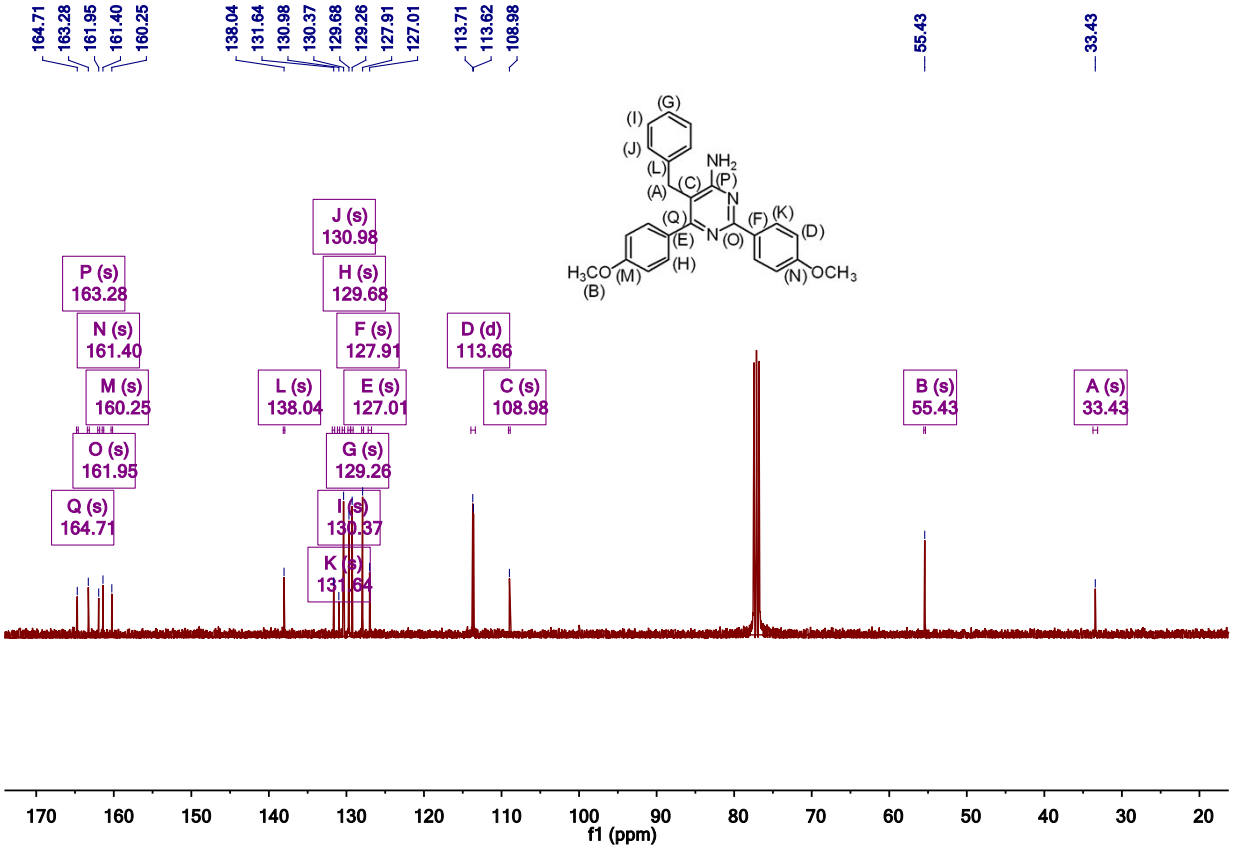

G (dd) 7.47
E (d) 7.32
I (d) 8.38
D (m) 7.27
F (t) 7.39
H (d) 7.61
C (s) 4.86
B (s) 4.08
A (d) 1.38
1.96
1.99
3.99
2.00
0.88
2.25
2.00
2.00
18.11
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

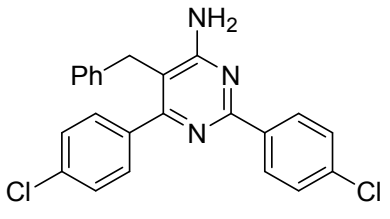

165.05
163.24
162.31
153.18
151.86
138.05
136.22
135.53
129.17
128.59
127.90
127.84
125.24
125.20
109.57
34.80
34.73
33.39
31.33
H (s) 128.59
P (s) 163.24
N (s) 153.18
K (s) 136.22
F (s) 126.93
O (s) 162.31
M (s) 151.86
J (s) 135.53
E (d) 125.22
D (s) 109.57
B (s) 33.39
A (s) 31.33
Q (s) 165.05
L (s) 138.05
G (d) 127.87
C (d) 34.76
I (s) 129.17
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)


NH2
Ph
N
N
H3CO
OCH3

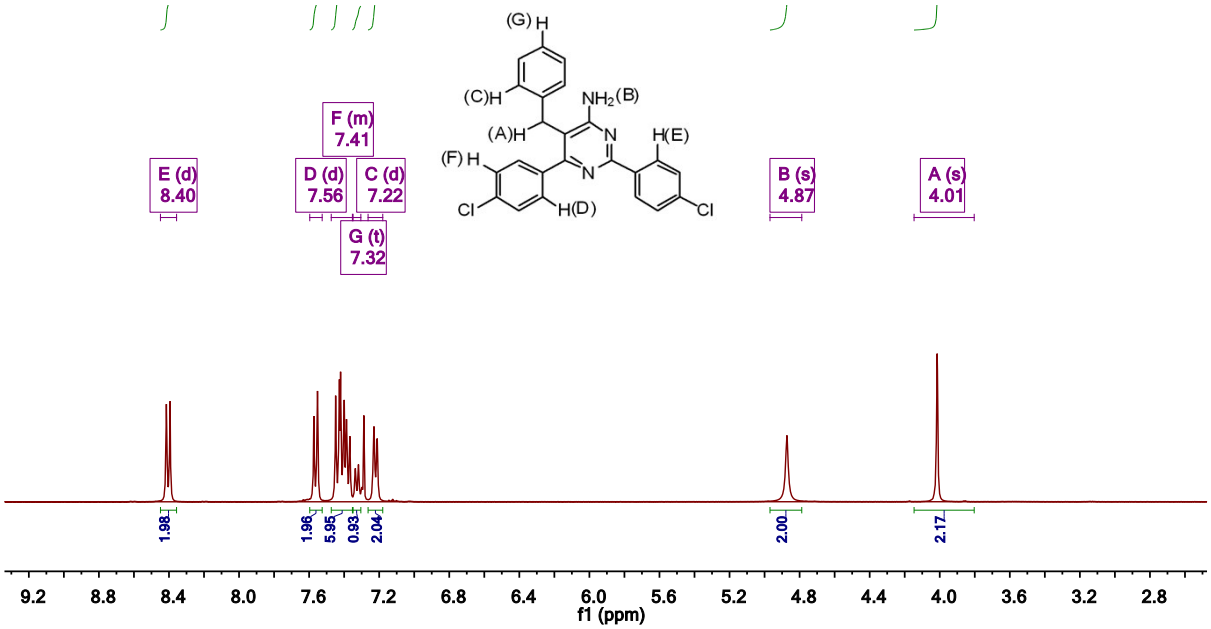
(3ad)

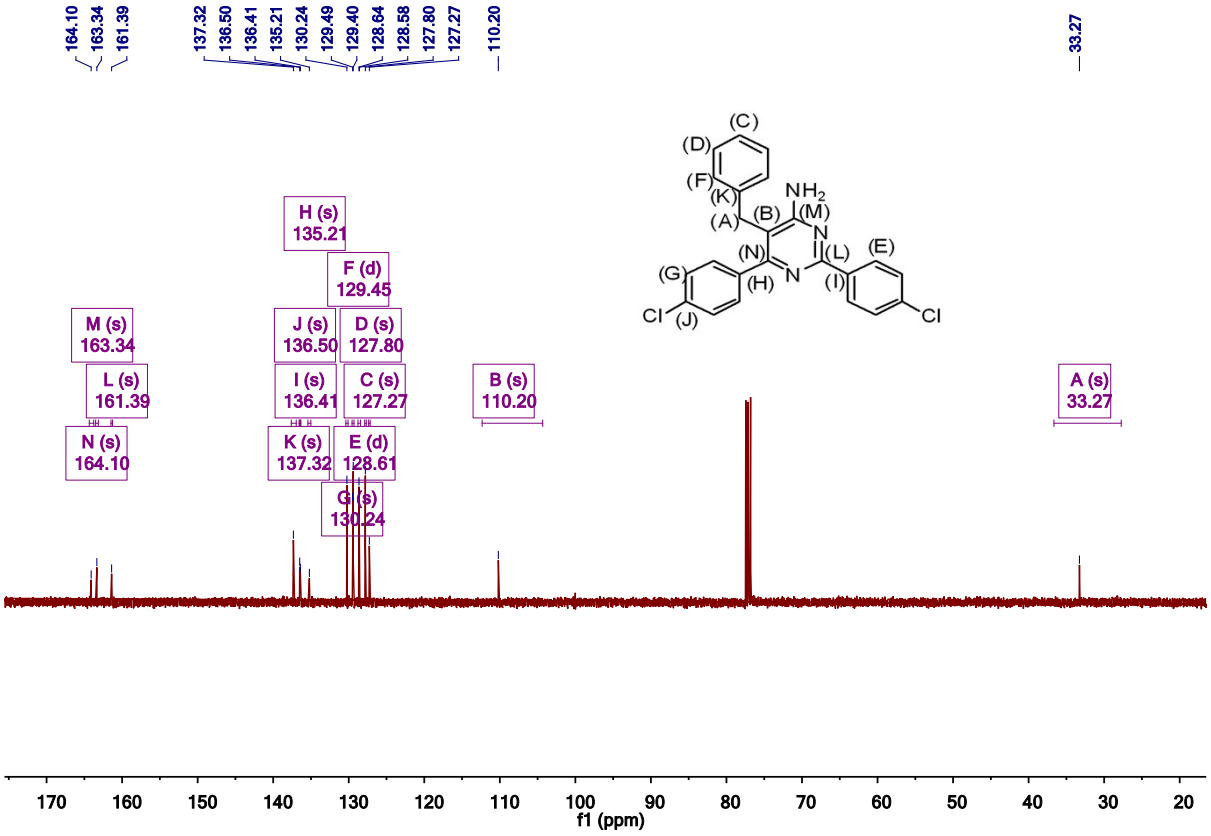

J (m) 8.41
I (d) 7.61
G (d) 7.31
F (d) 7.25
E (m) 6.97
H (t) 7.38
D (s) 4.76
B (s) 3.89
A (s) 3.85
C (d) 4.05
2.02
2.01
1.99
0.90
1.94
3.96
1.88
2.00
3.03
2.90
9.0 8.6 8.2 7.8 7.4 7.0 6.6 6.2 5.8 5.4 5.0 4.6 4.2 3.8 3.4 3.0 2.6
f1 (ppm)

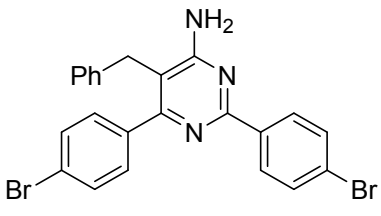

164.71
163.28
161.95
161.40
160.25
138.04
131.64
130.98
130.37
129.68
129.26
127.91
127.01
113.71
113.62
108.98
55.43
33.43
P (s) 163.28
N (s) 161.40
M (s) 160.25
O (s) 161.95
Q (s) 164.71
L (s) 138.04
J (s) 130.98
H (s) 129.68
F (s) 127.91
E (s) 127.01
G (s) 129.26
I (s) 130.37
K (s) 131.64
D (d) 113.66
C (s) 108.98
B (s) 55.43
A (s) 33.43
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


NH2
Ph
N
N
Cl
Cl

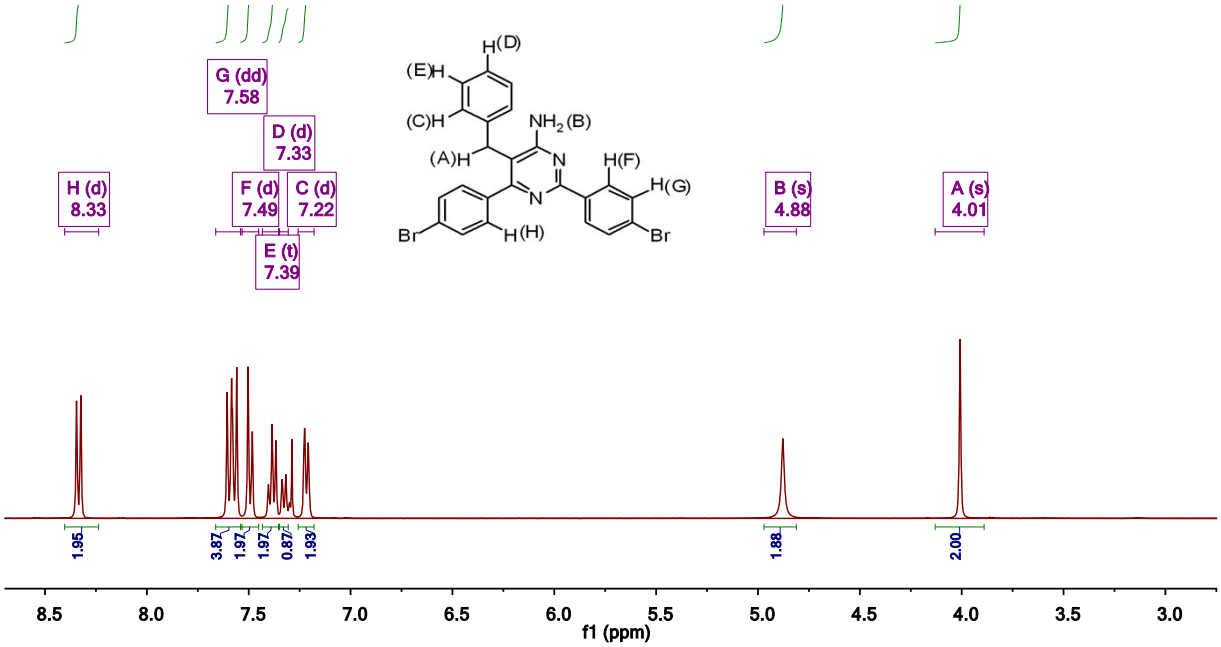
(3ae)

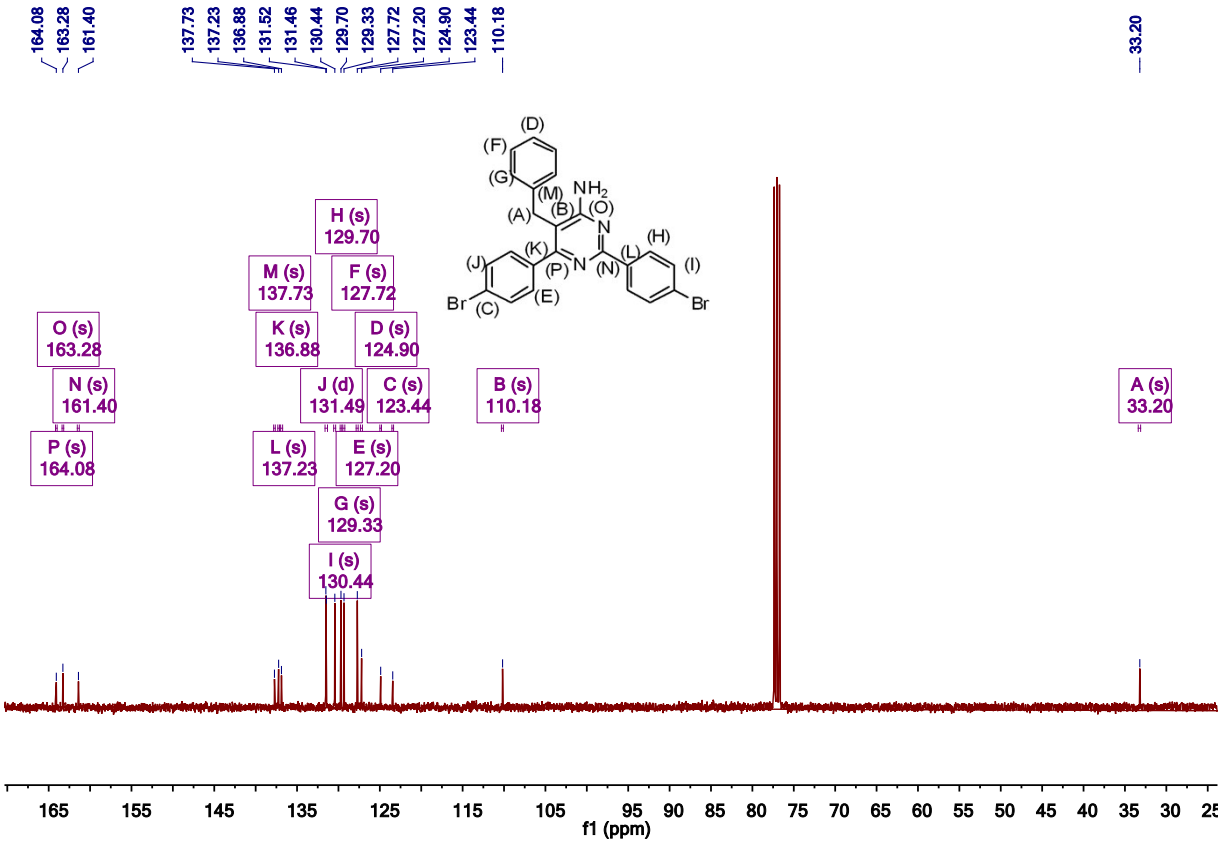

E (d) 8.40
D (d) 7.56
F (m) 7.41
C (d) 7.22
G (t) 7.32
B (s) 4.87
A (s) 4.01
1.98
1.96
5.95
0.93
2.04
2.00
2.17
f1 (ppm)

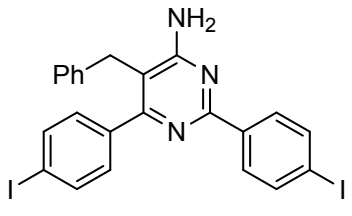

164.10
163.34
161.39
137.32
136.50
136.41
135.21
130.24
129.49
129.40
128.64
128.58
127.80
127.27
110.20
33.27
H (s) 135.21
F (d) 129.45
M (s) 163.34
J (s) 136.50
D (s) 127.80
L (s) 161.39
I (s) 136.41
C (s) 127.27
B (s) 110.20
A (s) 33.27
N (s) 164.10
K (s) 137.32
E (d) 128.61
G (s) 130.24
f1 (ppm)


NH2
Ph
N
N
Br
Br

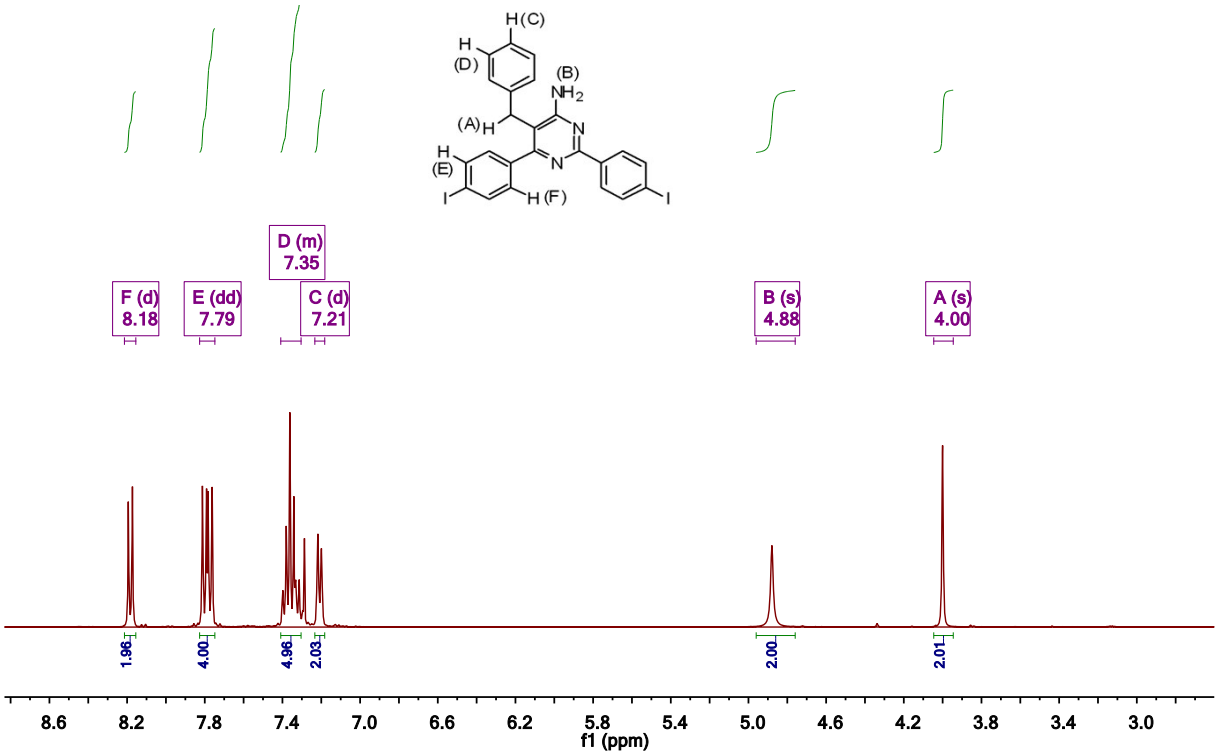
(3af)

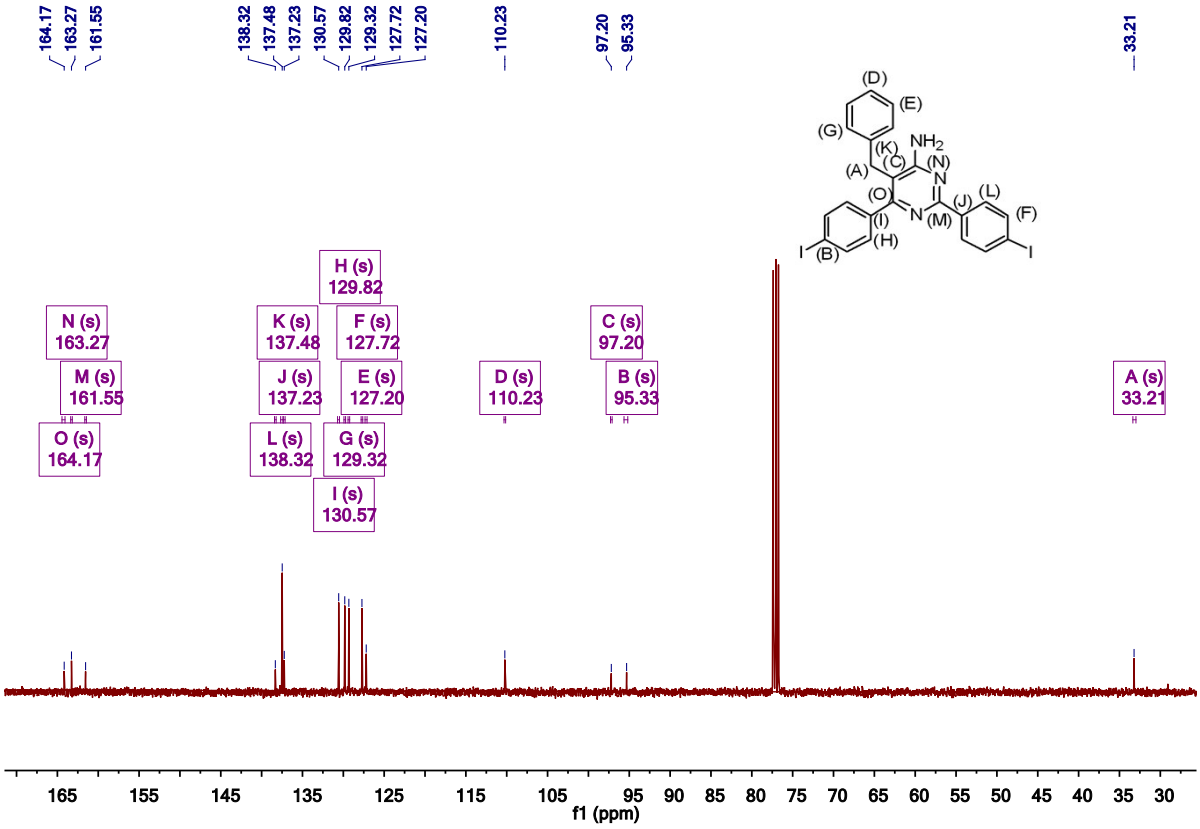

G (dd) 7.58
D (d) 7.33
H (d) 8.33
F (d) 7.49
C (d) 7.22
E (t) 7.39
B (s) 4.88
A (s) 4.01
1.95
3.87
1.97
1.97
0.87
1.93
1.88
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
f1 (ppm)

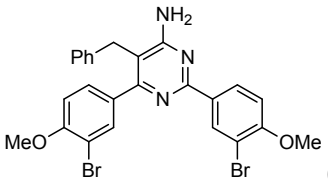

164.08
163.28
161.40
137.73
137.23
136.88
131.52
131.46
130.44
129.70
129.33
127.72
127.20
124.90
123.44
110.18
33.20
H (s) 129.70
M (s) 137.73
F (s) 127.72
O (s) 163.28
K (s) 136.88
D (s) 124.90
N (s) 161.40
J (d) 131.49
C (s) 123.44
B (s) 110.18
A (s) 33.20
P (s) 164.08
L (s) 137.23
E (s) 127.20
G (s) 129.33
I (s) 130.44
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
f1 (ppm)


NH2
Ph
N
N
I
I

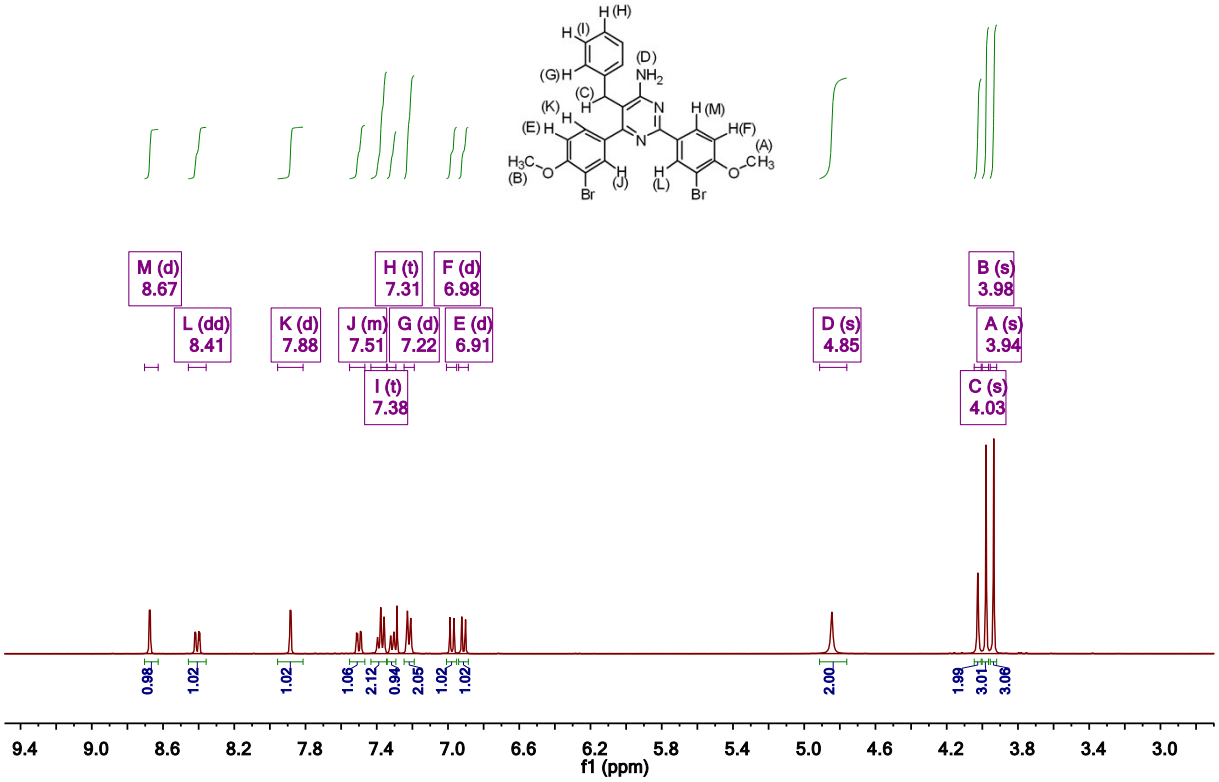
(3ag)

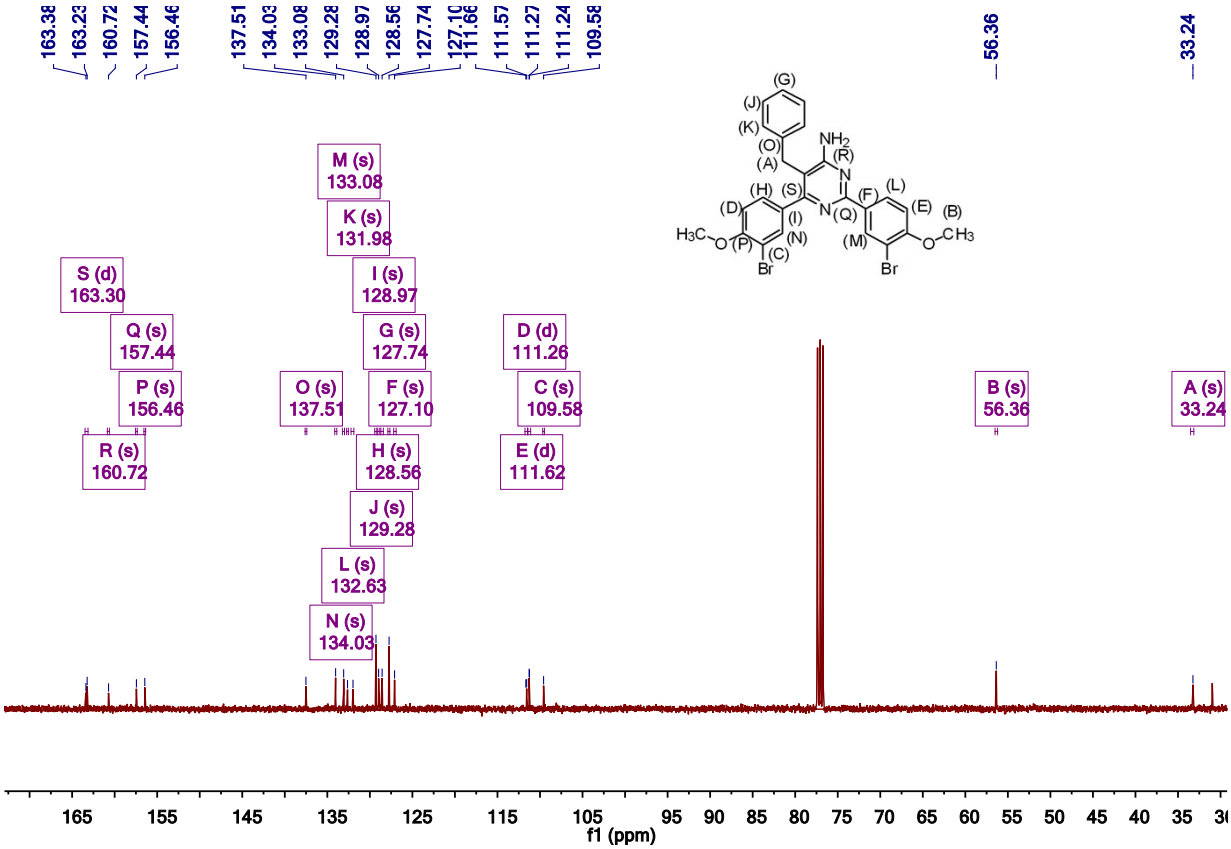

D (m) 7.35
F (d) 8.18
E (dd) 7.79
C (d) 7.21
B (s) 4.88
A (s) 4.00
1.96
4.00
4.98
2.03
2.00
2.01
f1 (ppm)

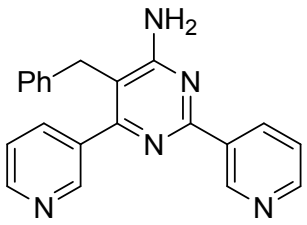

164.17
163.27
161.55
138.32
137.48
137.23
130.57
129.82
129.32
127.72
127.20
110.23
97.20
95.33
33.21
H (s) 129.82
N (s) 163.27
K (s) 137.48
F (s) 127.72
C (s) 97.20
M (s) 161.55
J (s) 137.23
E (s) 127.20
D (s) 110.23
B (s) 95.33
A (s) 33.21
O (s) 164.17
L (s) 138.32
G (s) 129.32
I (s) 130.57
f1 (ppm)


NH2
Ph
N
N
MeO
OMe
Br
Br

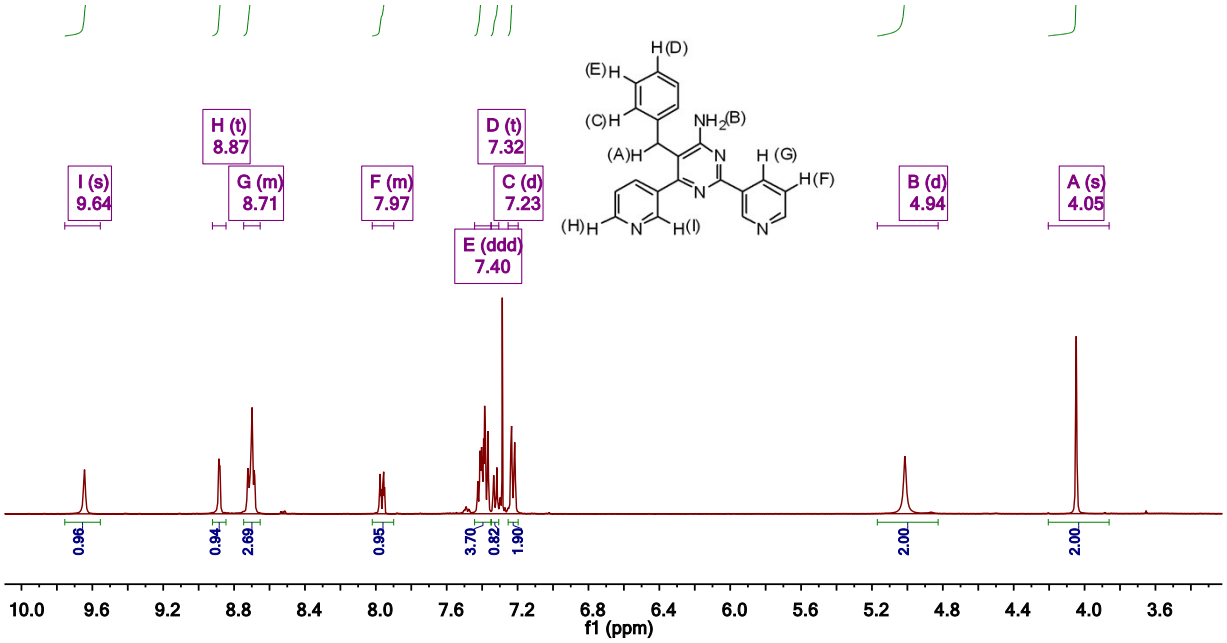
(3ah)

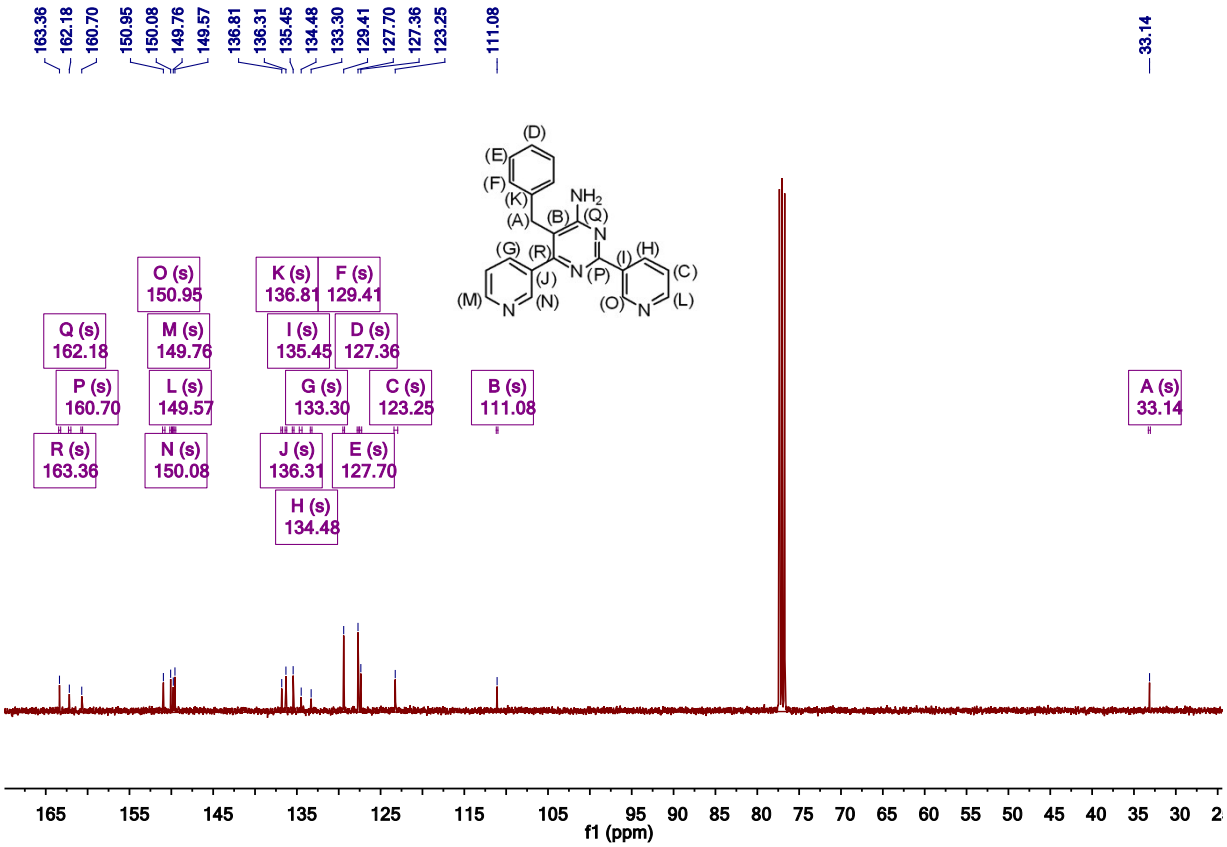

M (d) 8.67
L (dd) 8.41
K (d) 7.88
J (m) 7.51
H (t) 7.31
G (d) 7.22
F (d) 6.98
E (d) 6.91
I (t) 7.38
D (s) 4.85
B (s) 3.98
A (s) 3.94
C (s) 4.03
f1 (ppm)

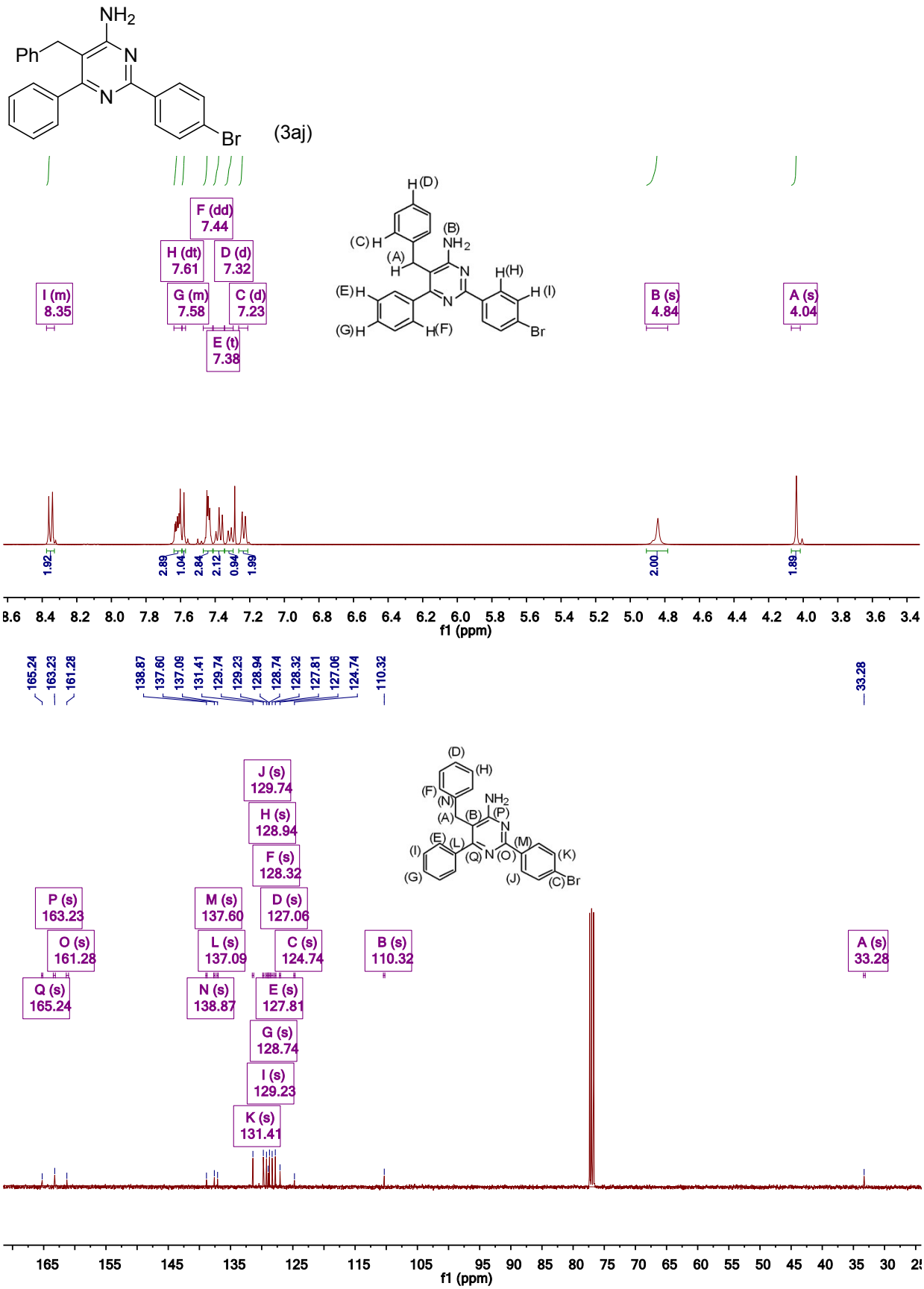

163.38
163.23
160.72
157.44
156.46
137.51
134.03
133.08
129.28
128.97
128.56
127.74
127.10
111.66
111.57
111.27
111.24
109.58
56.36
33.24
M (s) 133.08
K (s) 131.98
I (s) 128.97
S (d) 163.30
Q (s) 157.44
G (s) 127.74
D (d) 111.26
P (s) 156.46
O (s) 137.51
F (s) 127.10
C (s) 109.58
B (s) 56.36
A (s) 33.24
R (s) 160.72
H (s) 128.56
E (d) 111.62
J (s) 129.28
L (s) 132.63
N (s) 134.03
f1 (ppm)

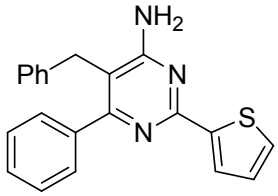

NH2
Ph
N
N
N
N

(3ai)

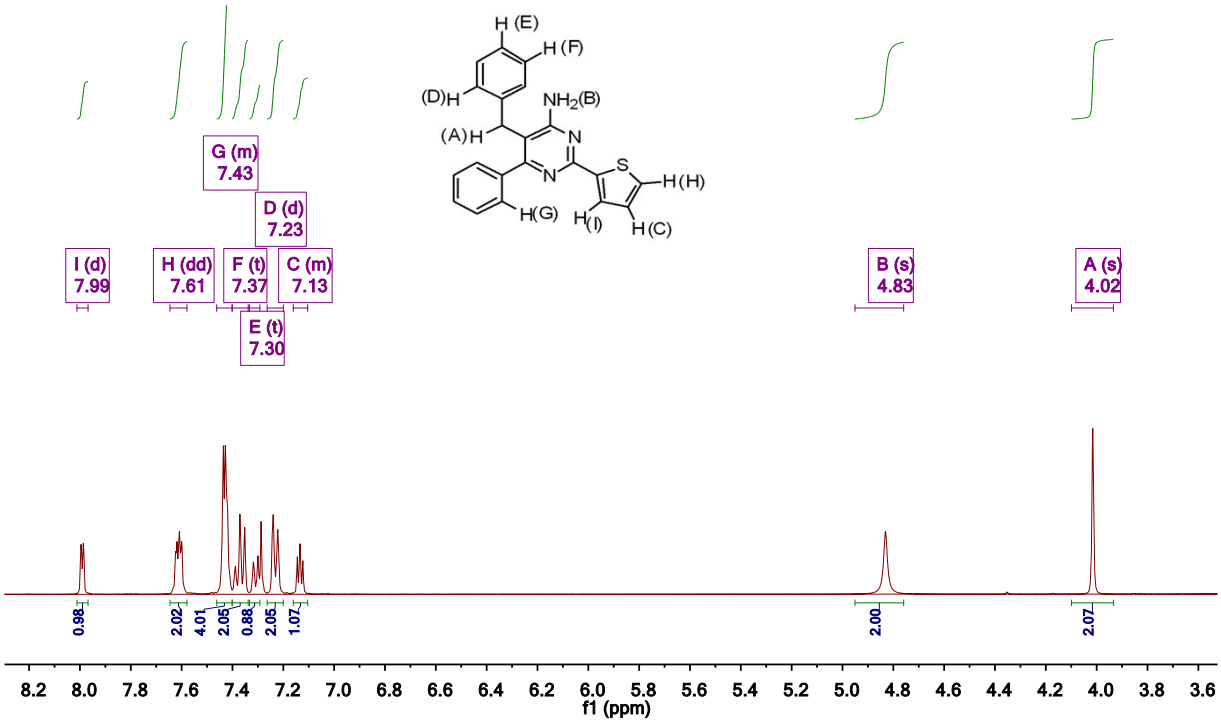

I (s) 9.64
H (t) 8.87
G (m) 8.71
F (m) 7.97
D (t) 7.32
C (d) 7.23
E (ddd) 7.40
B (d) 4.94
A (s) 4.05
0.96
0.94
2.69
0.95
3.70
0.82
1.90
2.00
2.00
f1 (ppm)

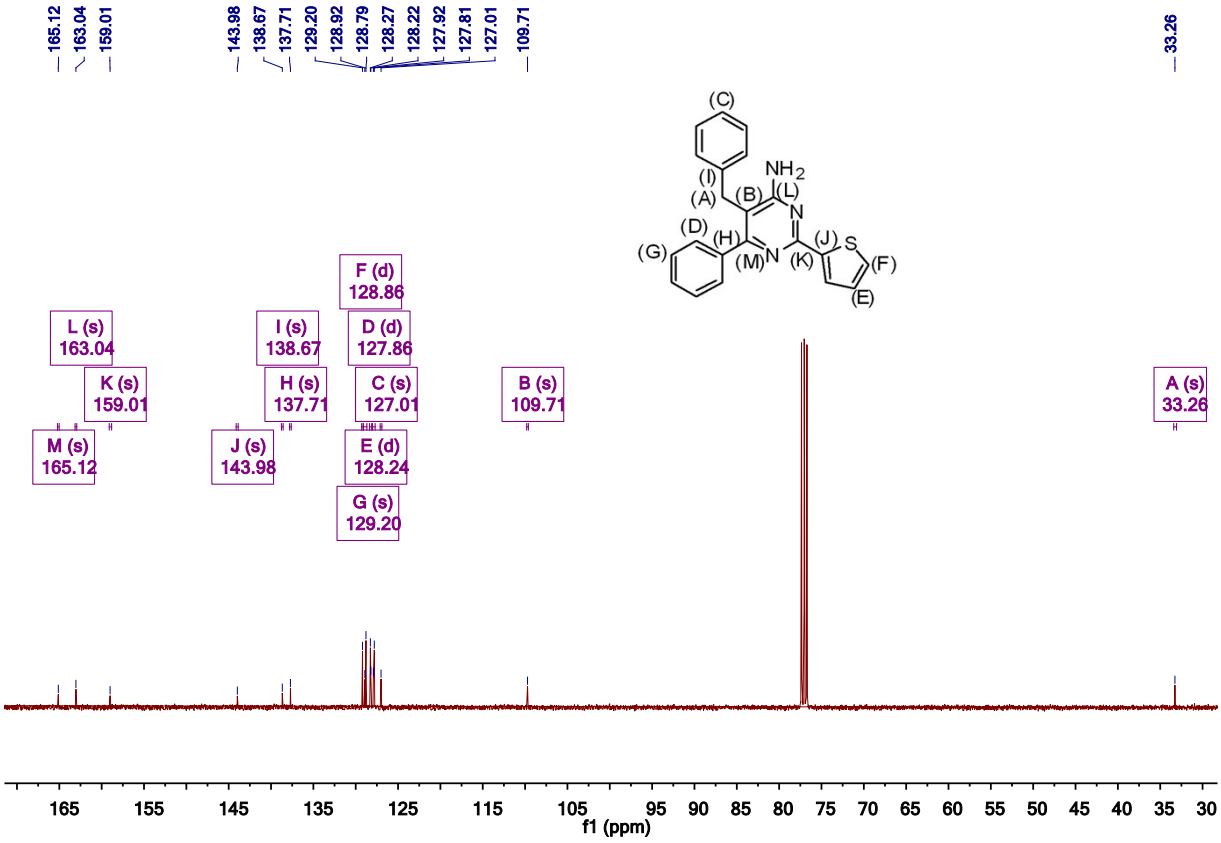

163.36
162.18
160.70
150.95
150.08
149.76
149.57
136.81
136.31
135.45
134.48
133.30
129.41
127.70
127.36
123.25
111.08
33.14
O (s) 150.95
K (s) 136.81
F (s) 129.41
Q (s) 162.18
M (s) 149.76
I (s) 135.45
D (s) 127.36
P (s) 160.70
L (s) 149.57
G (s) 133.30
C (s) 123.25
B (s) 111.08
A (s) 33.14
R (s) 163.36
N (s) 150.08
J (s) 136.31
E (s) 127.70
H (s) 134.48
f1 (ppm)

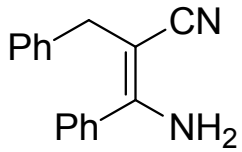

NH2
Ph
N
N
Br
(3aj)
F (dd) 7.44
H (dt) 7.61
D (d) 7.32
I (m) 8.35
G (m) 7.58
C (d) 7.23
E (t) 7.38
B (s) 4.84
A (s) 4.04
1.92
2.89
1.04
2.84
2.12
0.94
1.99
2.00
1.89
f1 (ppm)
165.24
163.23
161.28
138.87
137.60
137.09
131.41
129.74
129.23
128.94
128.74
128.32
127.81
127.06
124.74
110.32
33.28
J (s) 129.74
H (s) 128.94
F (s) 128.32
P (s) 163.23
M (s) 137.60
D (s) 127.06
O (s) 161.28
L (s) 137.09
C (s) 124.74
B (s) 110.32
A (s) 33.28
Q (s) 165.24
N (s) 138.87
E (s) 127.81
G (s) 128.74
I (s) 129.23
K (s) 131.41
f1 (ppm)



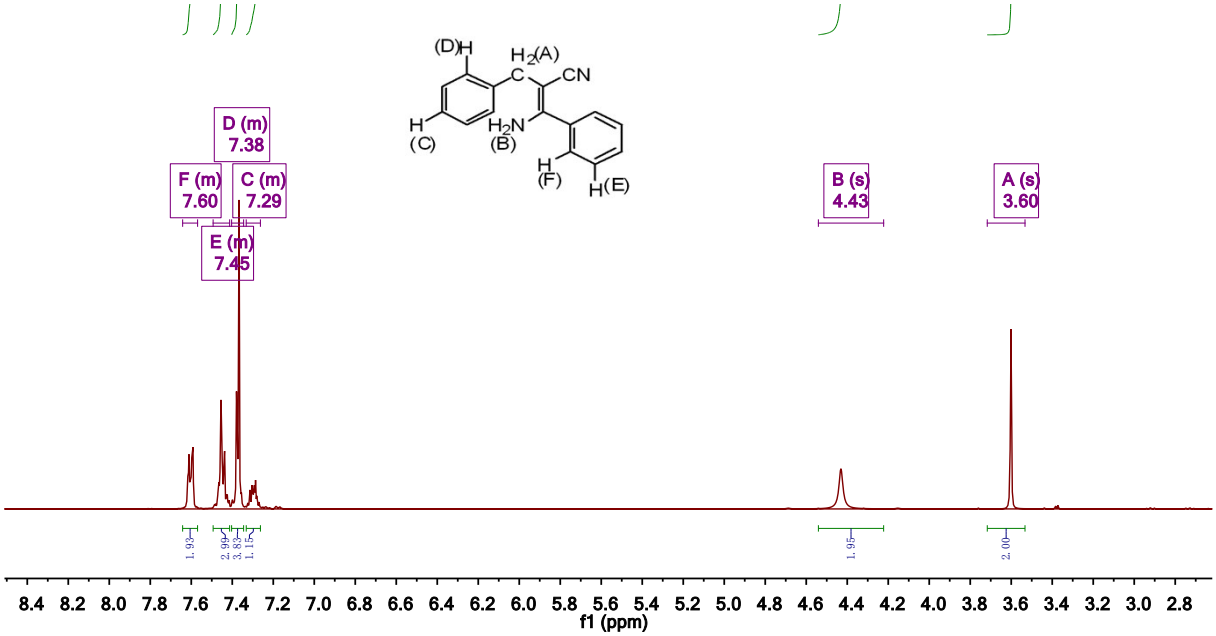
(3ak)

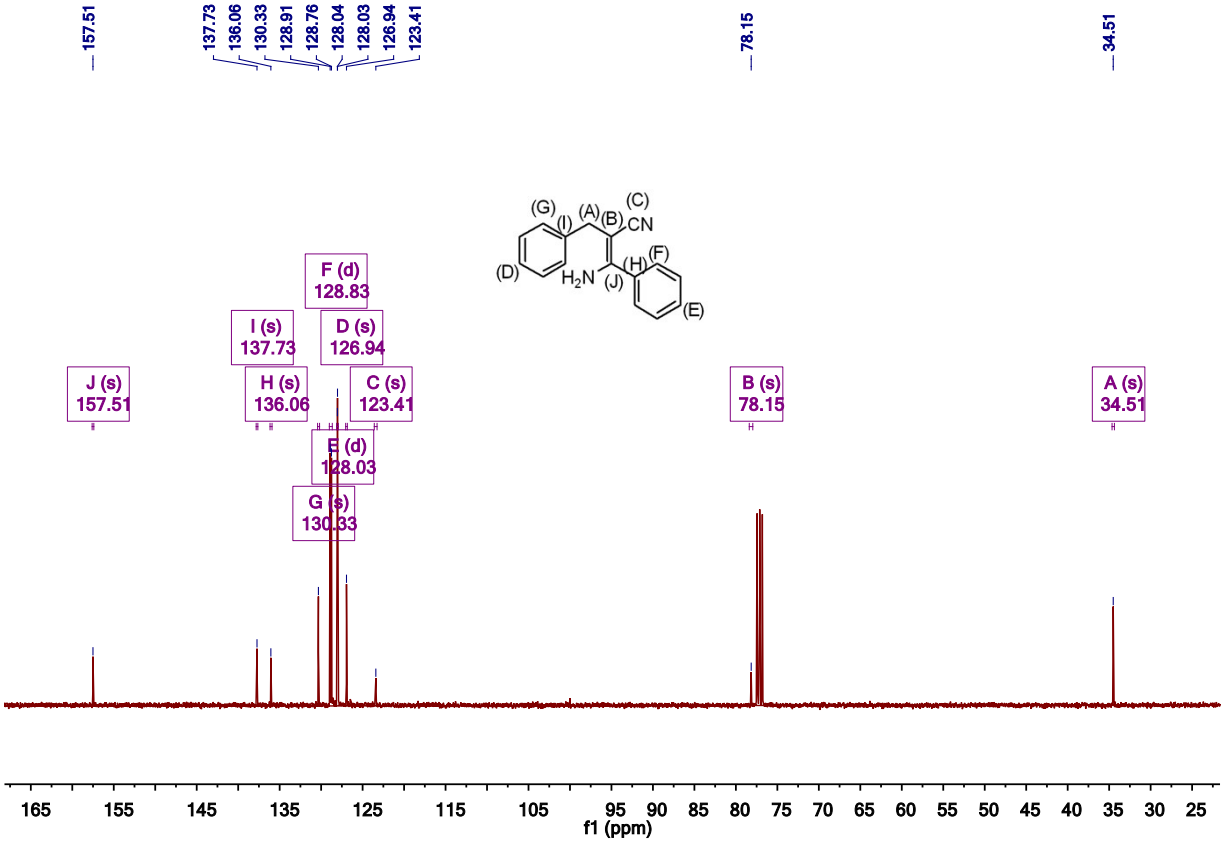

G (m) 7.43
D (d) 7.23
I (d) 7.99
H (dd) 7.61
F (t) 7.37
C (m) 7.13
E (t) 7.30
B (s) 4.83
A (s) 4.02
0.98
2.02
4.01
2.05
0.88
2.05
1.07
2.00
2.07
f1 (ppm)

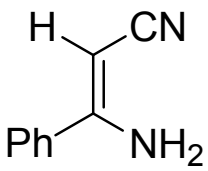

165.12
163.04
159.01
143.98
138.67
137.71
129.20
128.92
128.79
128.27
128.22
127.92
127.81
127.01
109.71
33.26
F (d) 128.86
L (s) 163.04
I (s) 138.67
D (d) 127.86
K (s) 159.01
H (s) 137.71
C (s) 127.01
B (s) 109.71
A (s) 33.26
M (s) 165.12
J (s) 143.98
E (d) 128.24
G (s) 129.20
f1 (ppm)


Ph
CN
Ph
NH2

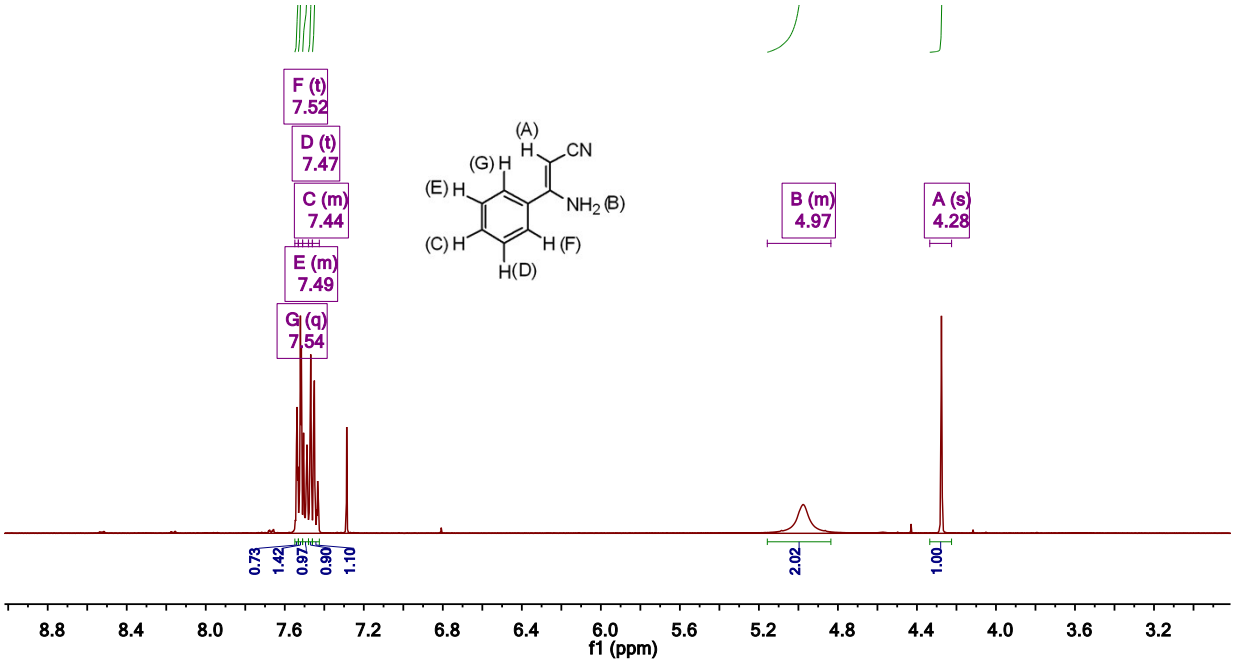
(4a)

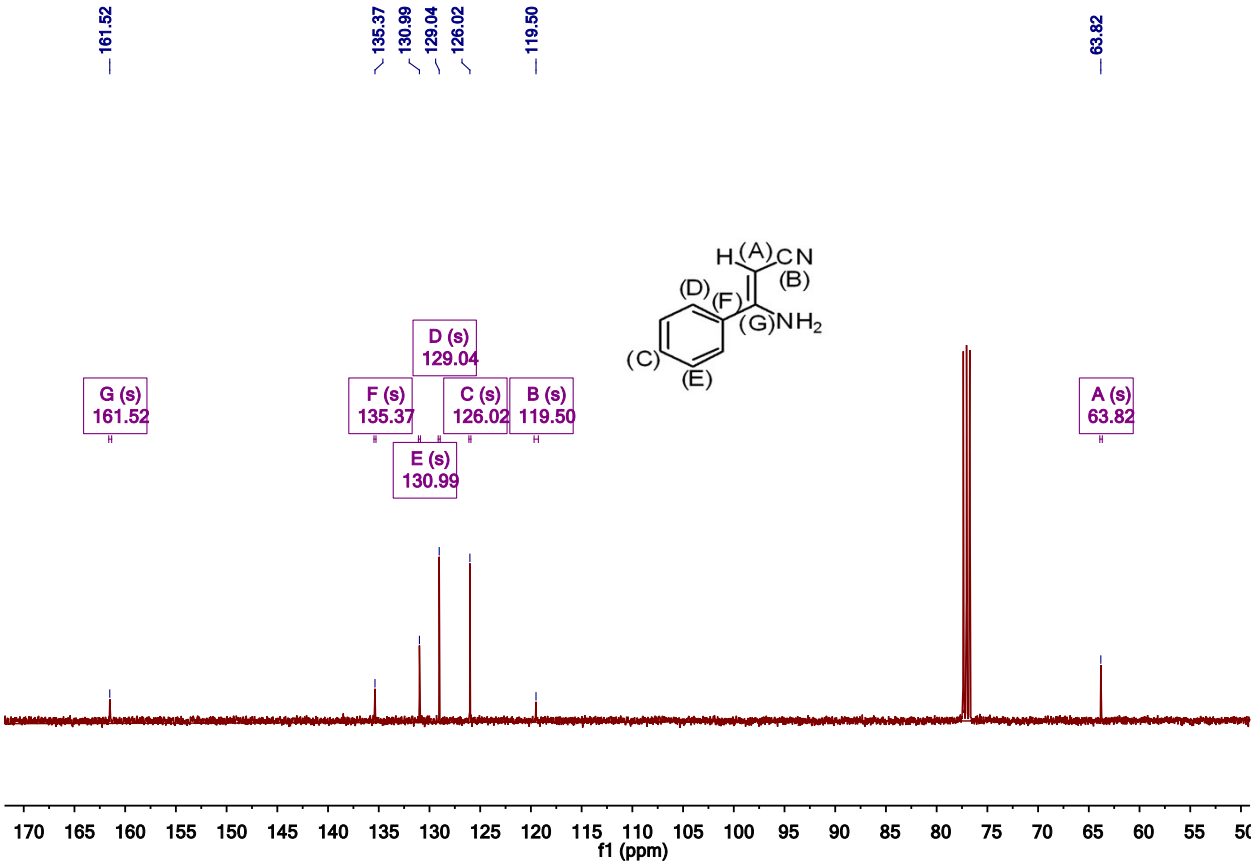

D (m)
7.38
F (m)
7.60
C (m)
7.29
E (m)
7.45
B (s)
4.43
A (s)
3.60
f1 (ppm)

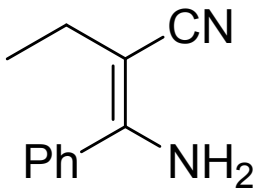

157.51
137.73
136.06
130.33
128.91
128.76
128.04
128.03
126.94
123.41
78.15
34.51
F (d)
128.83
I (s)
137.73
D (s)
126.94
J (s)
157.51
H (s)
136.06
C (s)
123.41
E (d)
128.03
G (s)
130.33
B (s)
78.15
A (s)
34.51
f1 (ppm)



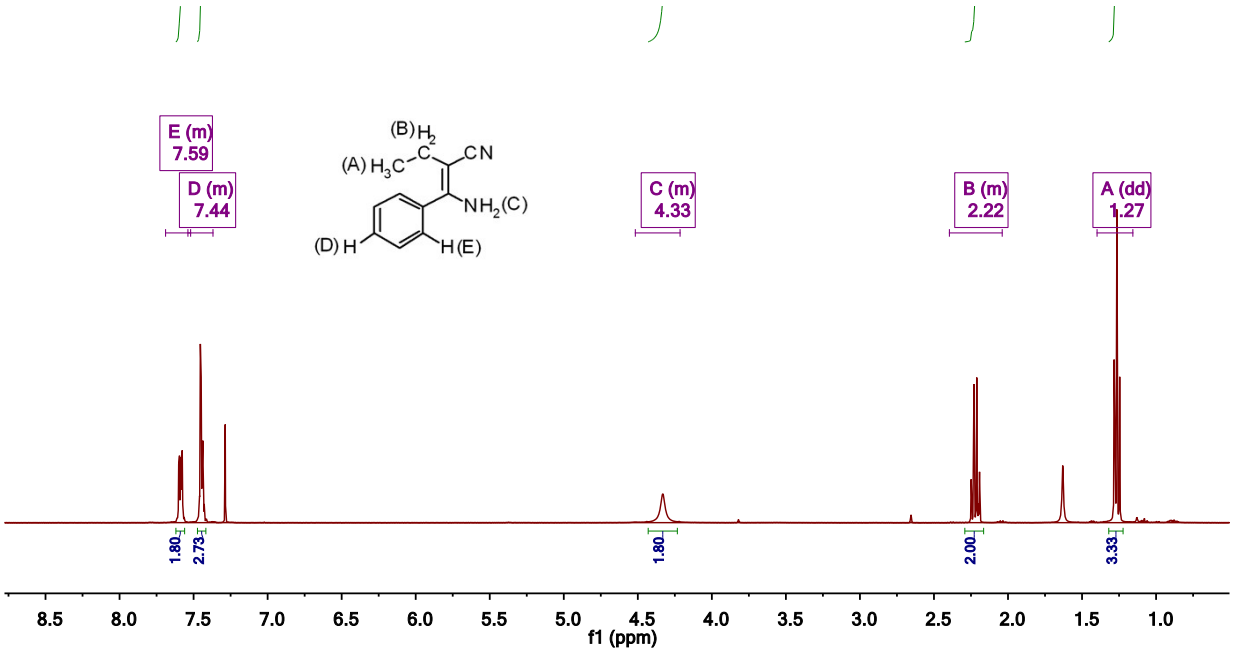
(4b)

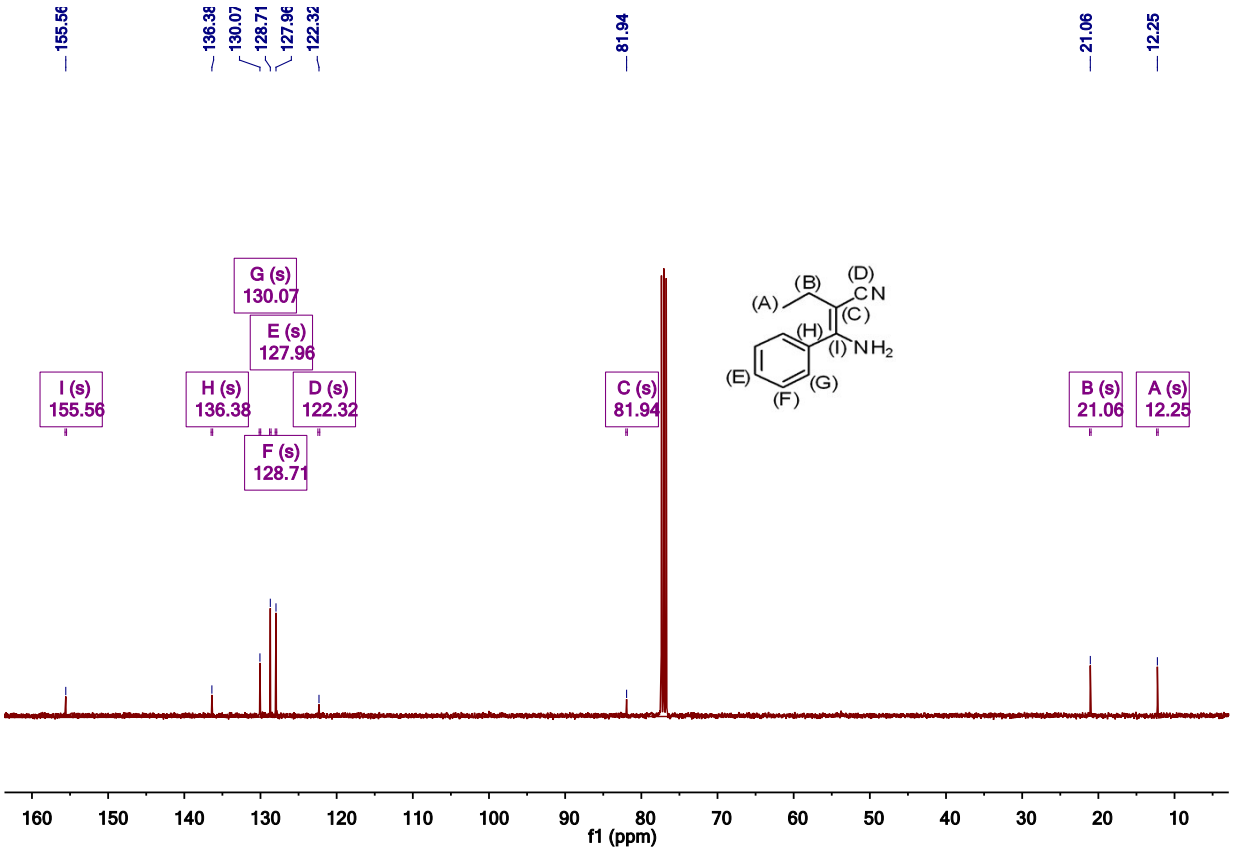

F (t) 7.52
D (t) 7.47
C (m) 7.44
E (m) 7.49
G (q) 7.54
B (m) 4.97
A (s) 4.28
0.73
1.42
0.97
0.90
1.10
2.02
1.00
f1 (ppm)

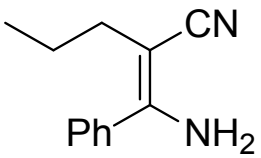

161.52
135.37
130.99
129.04
126.02
119.50
63.82
G (s) 161.52
F (s) 135.37
E (s) 130.99
D (s) 129.04
C (s) 126.02
B (s) 119.50
A (s) 63.82
f1 (ppm)


CN
Ph
NH2

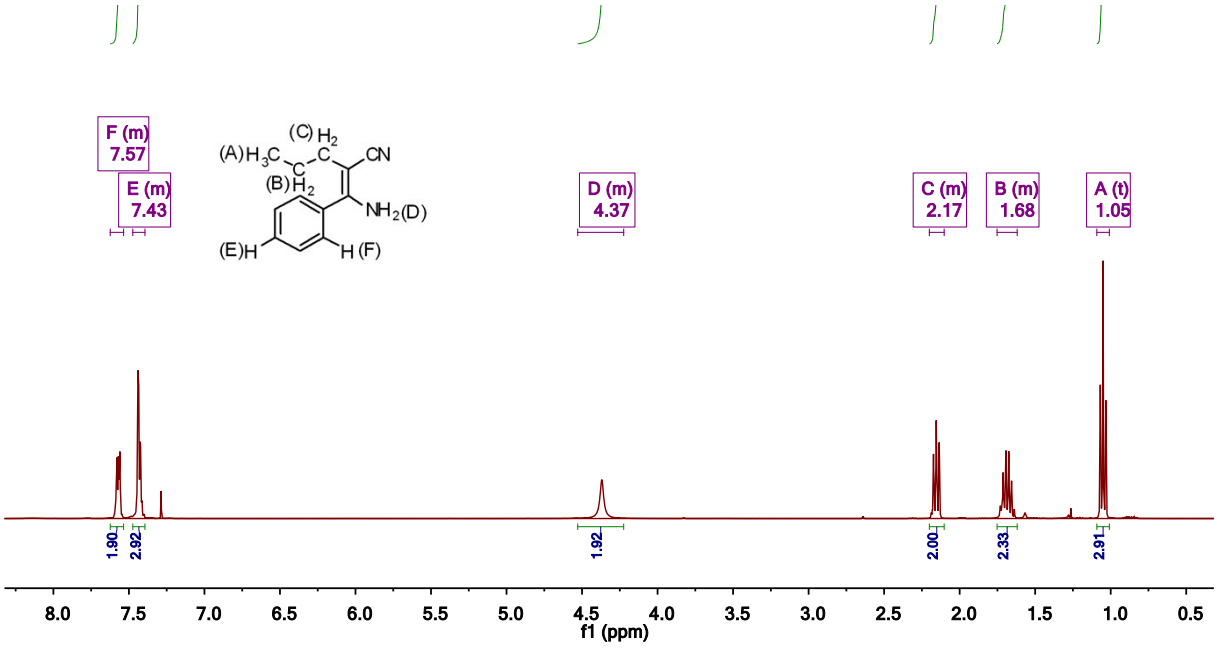
(4c)

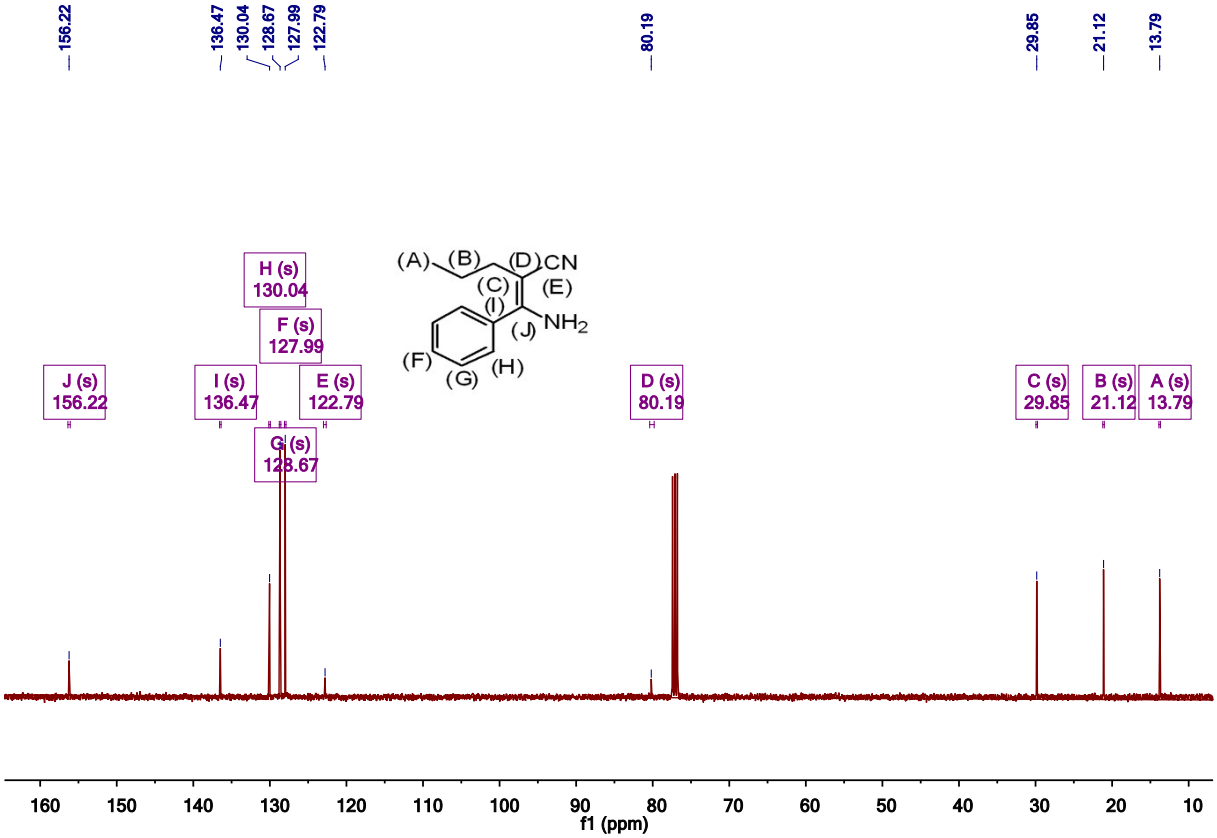

E (m) 7.59
D (m) 7.44
C (m) 4.33
B (m) 2.22
A (dd) 1.27
(B) H2
(A) H3C
CN
NH2(C)
(D) H
H(E)
1.80
2.73
1.80
2.00
3.33
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

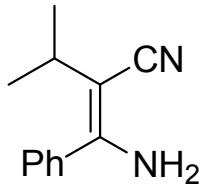

155.56
136.38
130.07
128.71
127.96
122.32
81.94
21.06
12.25
G (s) 130.07
E (s) 127.96
I (s) 155.56
H (s) 136.38
D (s) 122.32
F (s) 128.71
C (s) 81.94
B (s) 21.06
A (s) 12.25
(A)
(B)
(C)
(D)
CN
(H)
(I) NH2
(E)
(F)
(G)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


CN
Ph
NH2

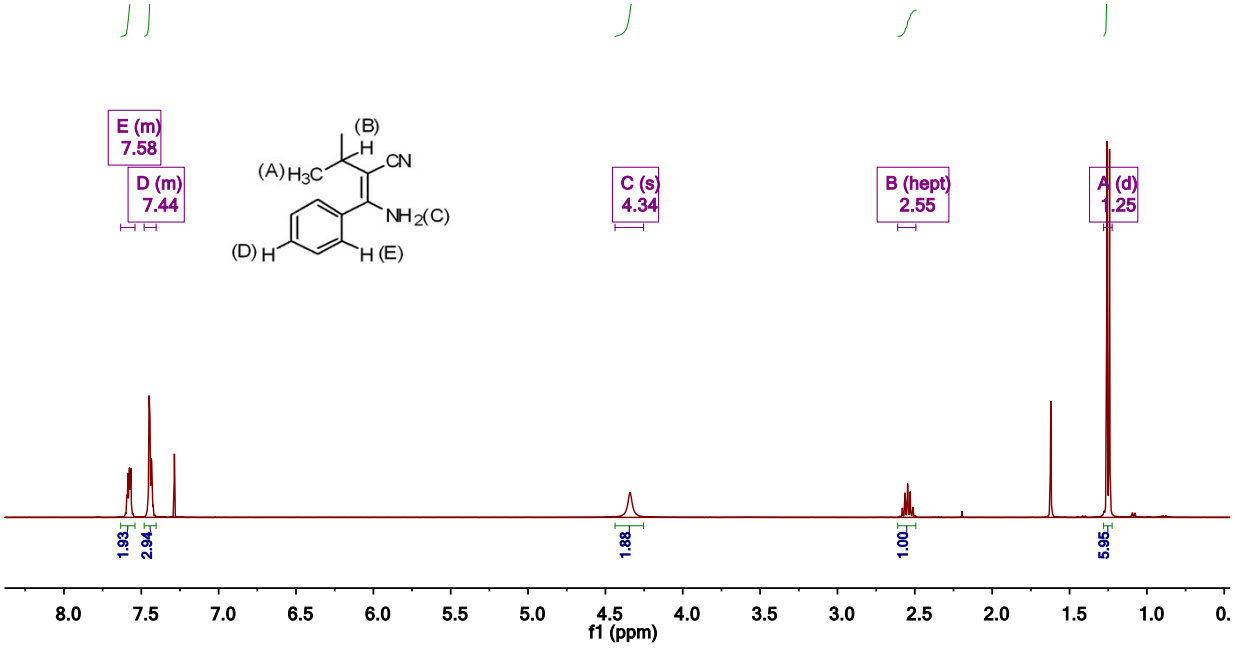
(4d)

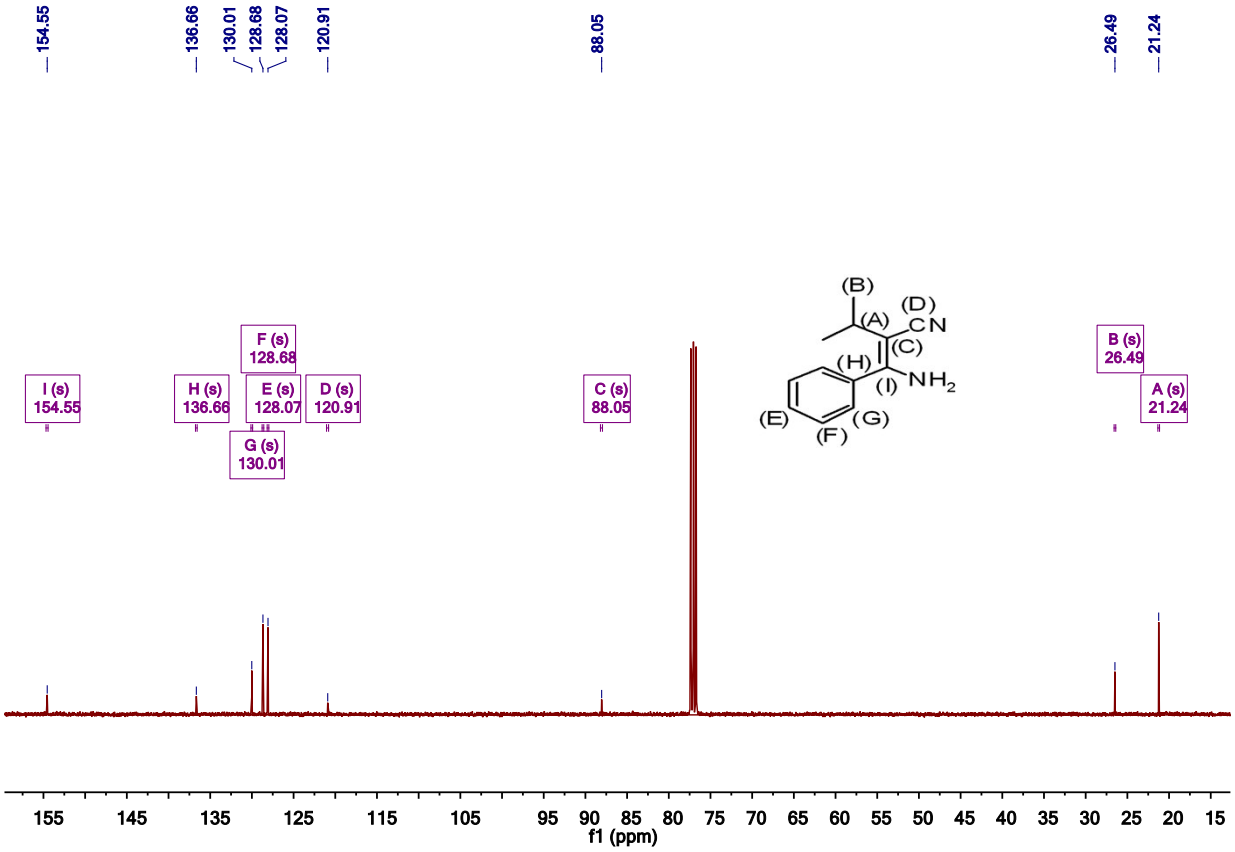

F (m) 7.57
E (m) 7.43
D (m) 4.37
C (m) 2.17
B (m) 1.68
A (t) 1.05
1.90
2.92
1.92
2.00
2.33
2.91
f1 (ppm)

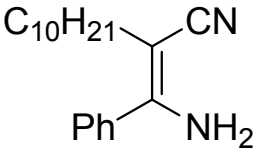

156.22
136.47
130.04
128.67
127.99
122.79
80.19
29.85
21.12
13.79
H (s) 130.04
F (s) 127.99
J (s) 156.22
I (s) 136.47
E (s) 122.79
G (s) 128.67
D (s) 80.19
C (s) 29.85
B (s) 21.12
A (s) 13.79
f1 (ppm)


CN
Ph
NH2

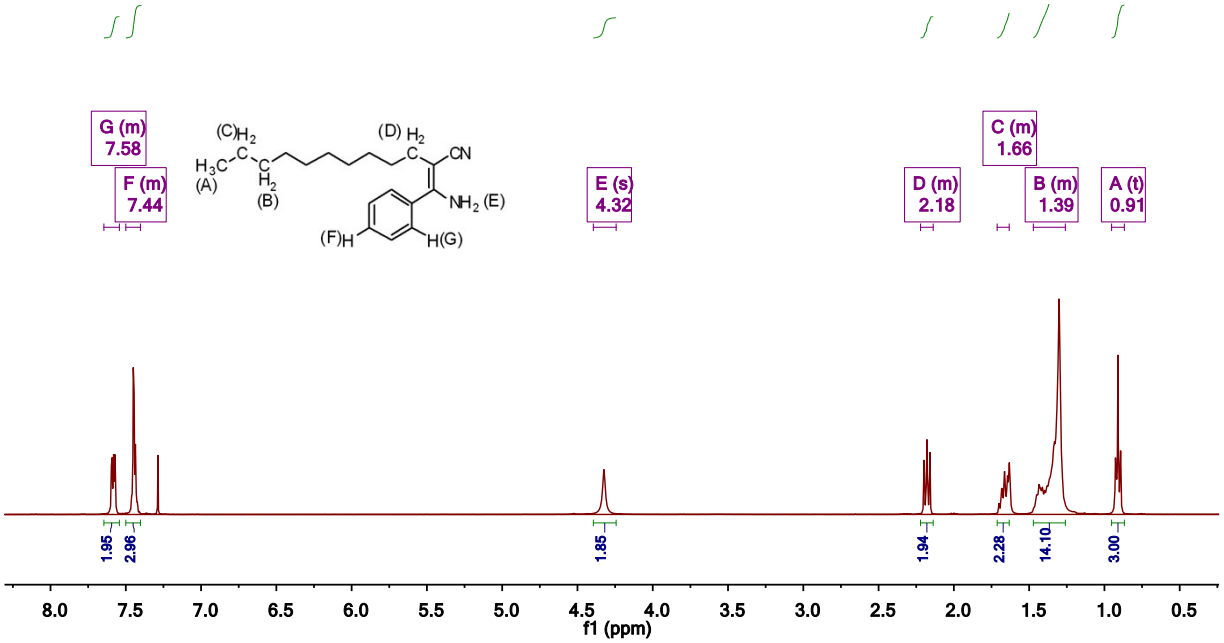
(4e)

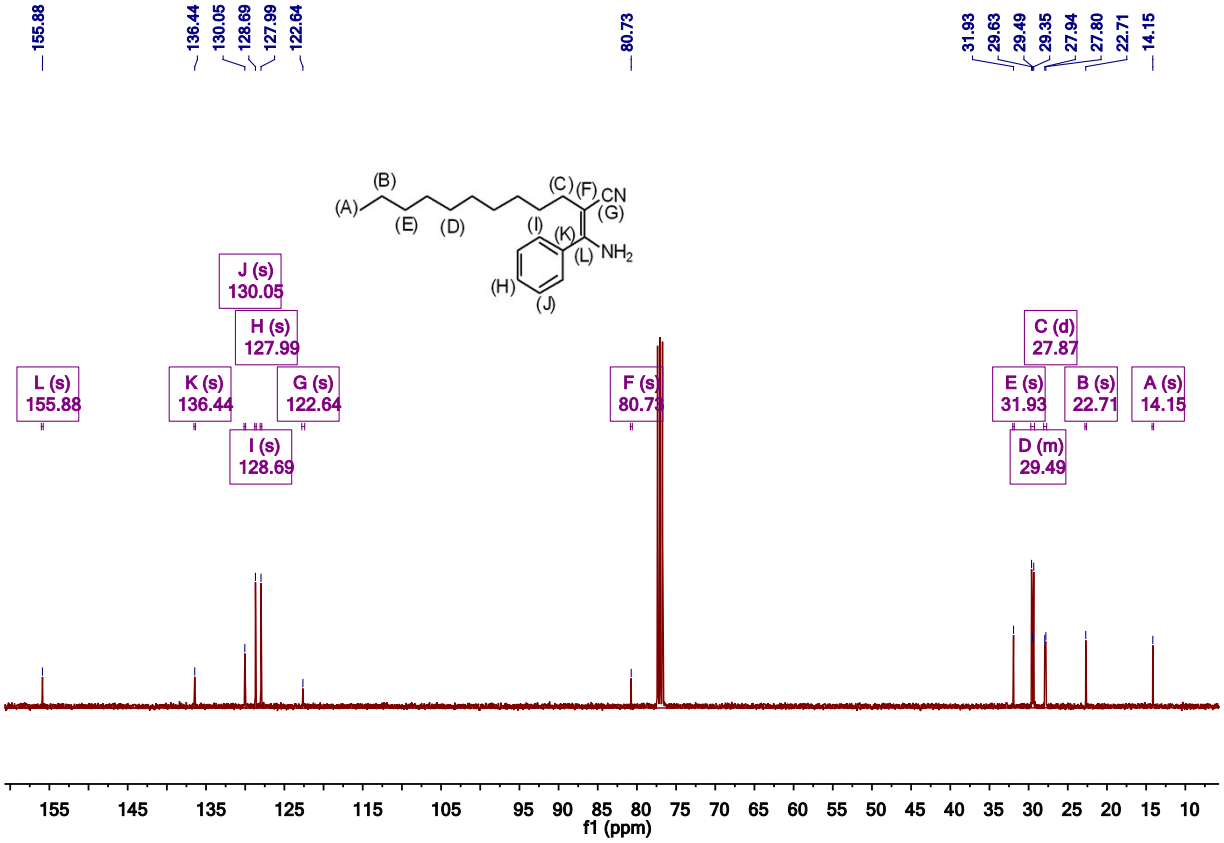

E (m) 7.58
D (m) 7.44
C (s) 4.34
B (hept) 2.55
A (d) 1.25
(A) H3C
(B) H
CN
NH2(C)
(D) H
H (E)
1.93
2.94
1.88
1.00
5.95
f1 (ppm)

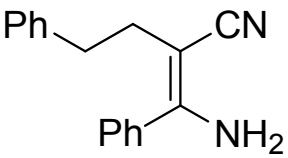

154.55
136.66
130.01
128.68
128.07
120.91
88.05
26.49
21.24
I (s) 154.55
H (s) 136.66
F (s) 128.68
E (s) 128.07
G (s) 130.01
D (s) 120.91
C (s) 88.05
B (s) 26.49
A (s) 21.24
(B)
(A)
(D)
CN
(C)
(H)
(I)
NH2
(E)
(F)
(G)
f1 (ppm)



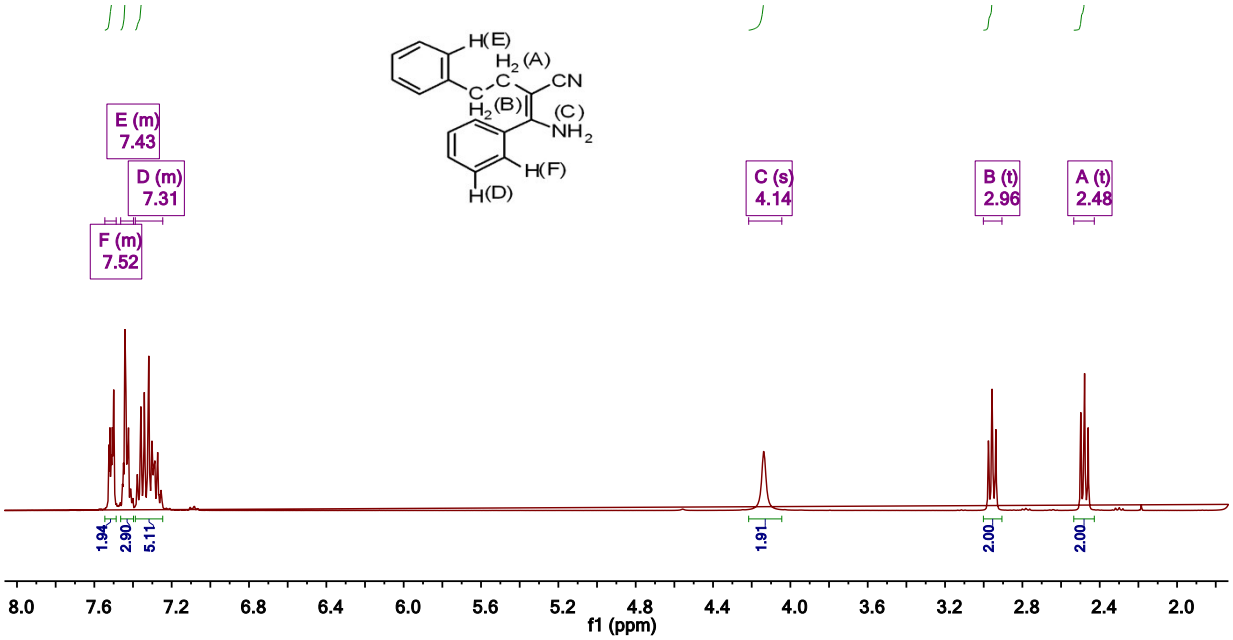
(4f)

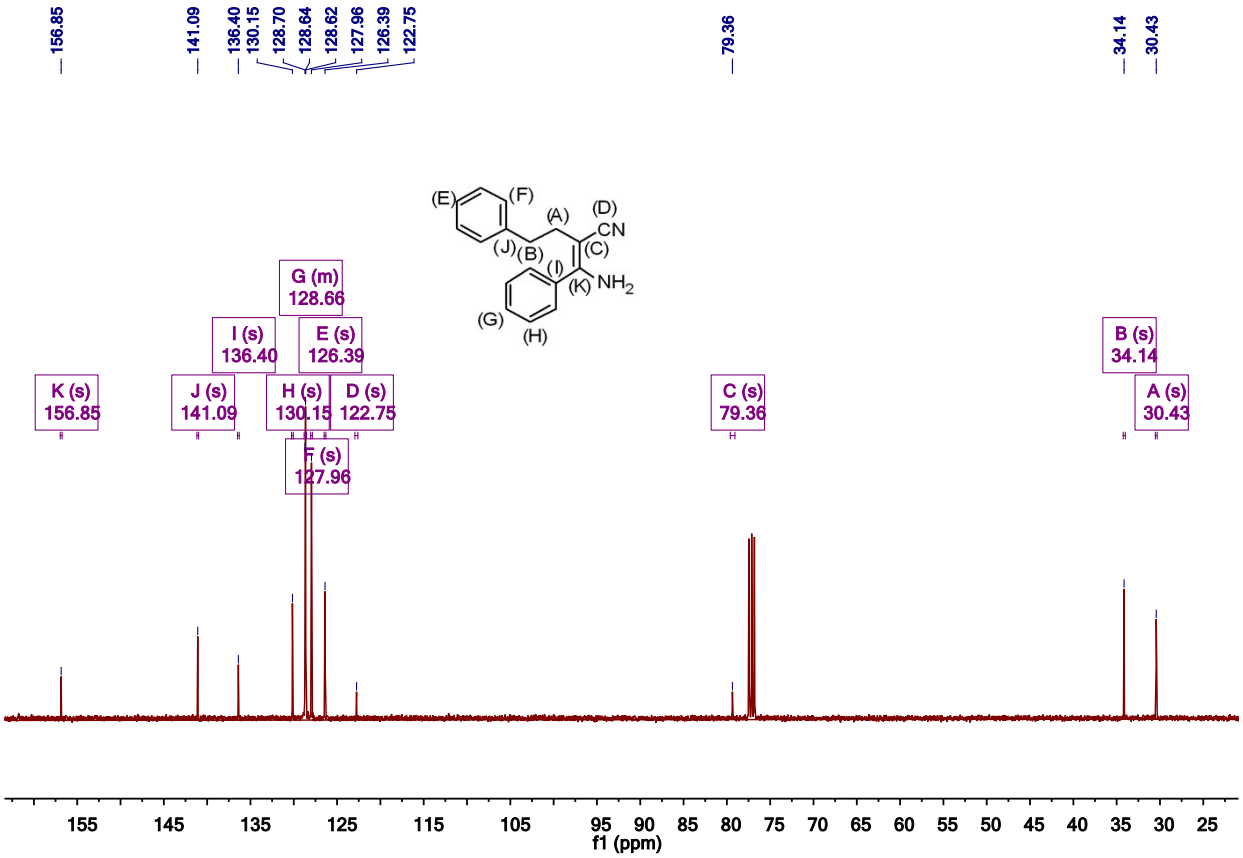

G (m) 7.58
F (m) 7.44
E (s) 4.32
D (m) 2.18
C (m) 1.66
B (m) 1.39
A (t) 0.91
1.95
2.96
1.85
1.94
2.28
14.10
3.00
f1 (ppm)

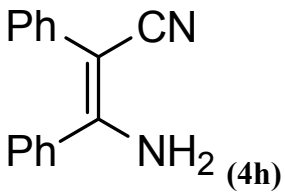

155.88
136.44
130.05
128.69
127.99
122.64
80.73
31.93
29.63
29.49
29.35
27.94
27.80
22.71
14.15
J (s) 130.05
H (s) 127.99
L (s) 155.88
K (s) 136.44
G (s) 122.64
I (s) 128.69
F (s) 80.73
C (d) 27.87
E (s) 31.93
B (s) 22.71
A (s) 14.15
D (m) 29.49
f1 (ppm)



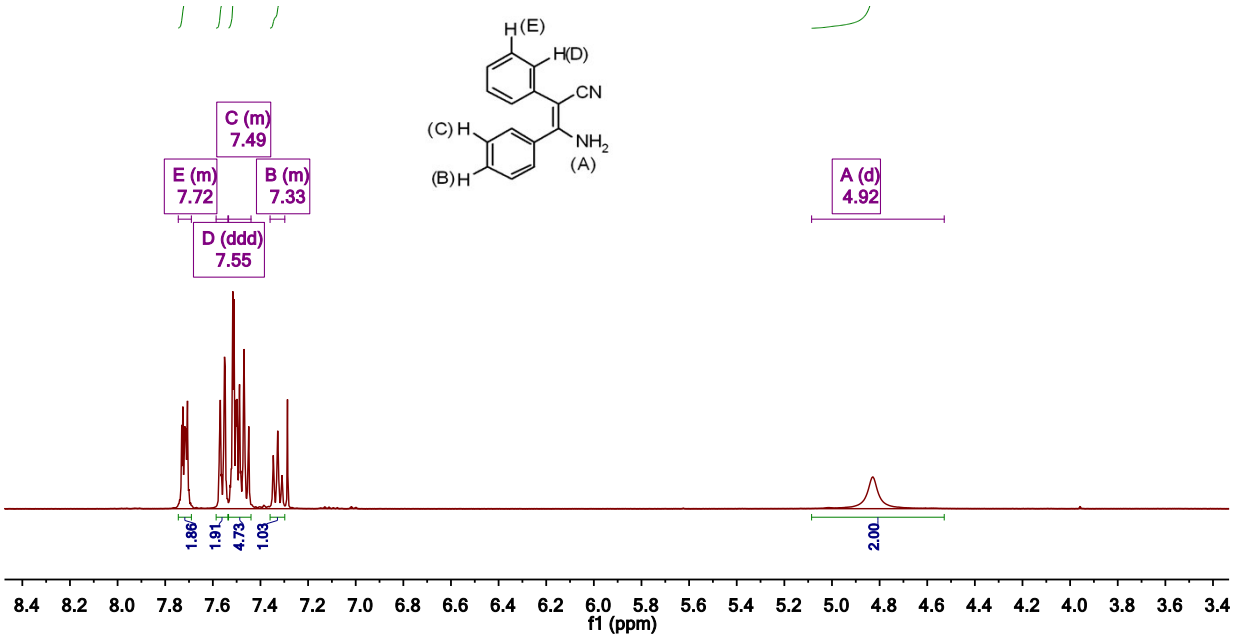
(4g)

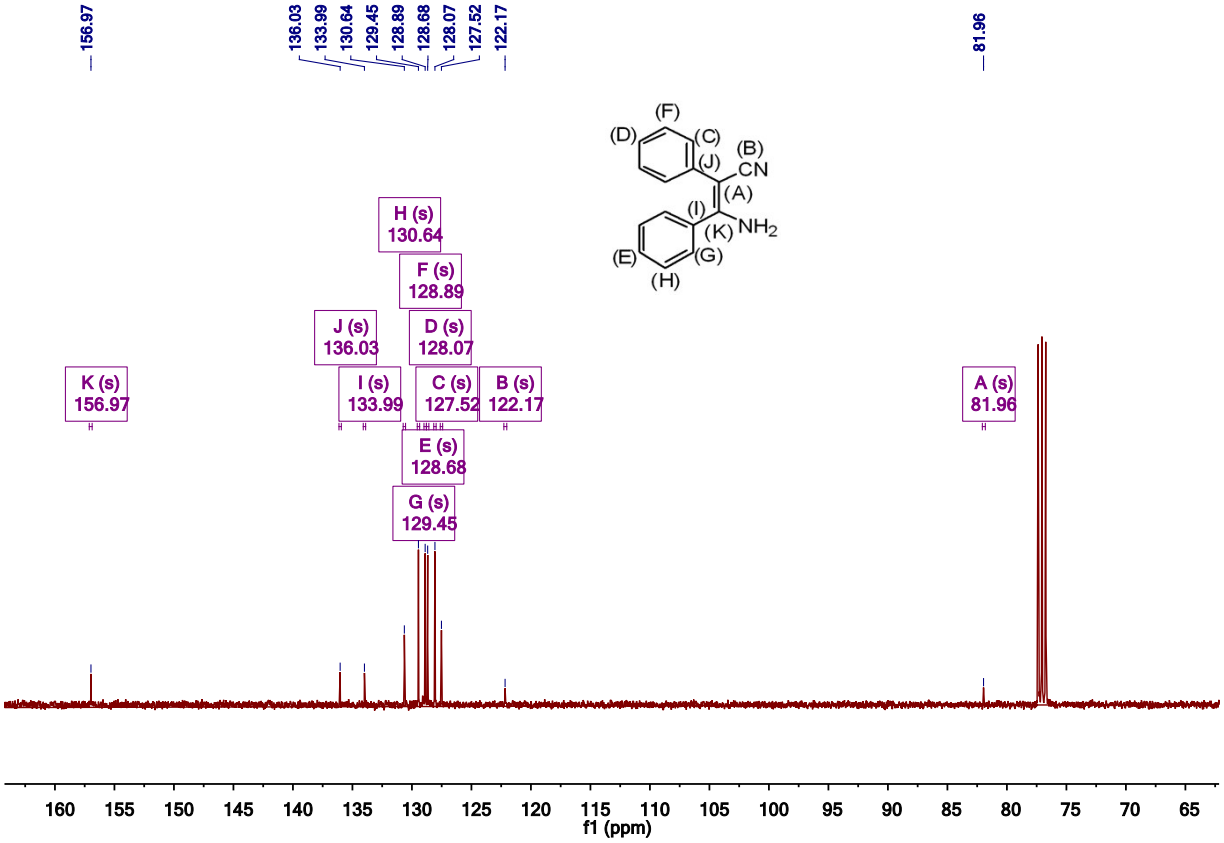

E (m) 7.43
D (m) 7.31
F (m) 7.52
C (s) 4.14
B (t) 2.96
A (t) 2.48
1.94
2.90
5.11
1.91
2.00
2.00
f1 (ppm)

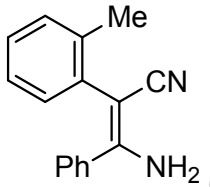

156.85
141.09
136.40
130.15
128.70
128.64
128.62
127.96
126.39
122.75
79.36
34.14
30.43
G (m) 128.66
I (s) 136.40
E (s) 126.39
K (s) 156.85
J (s) 141.09
H (s) 130.15
D (s) 122.75
F (s) 127.96
C (s) 79.36
B (s) 34.14
A (s) 30.43
f1 (ppm)


Ph
CN
Ph
NH2

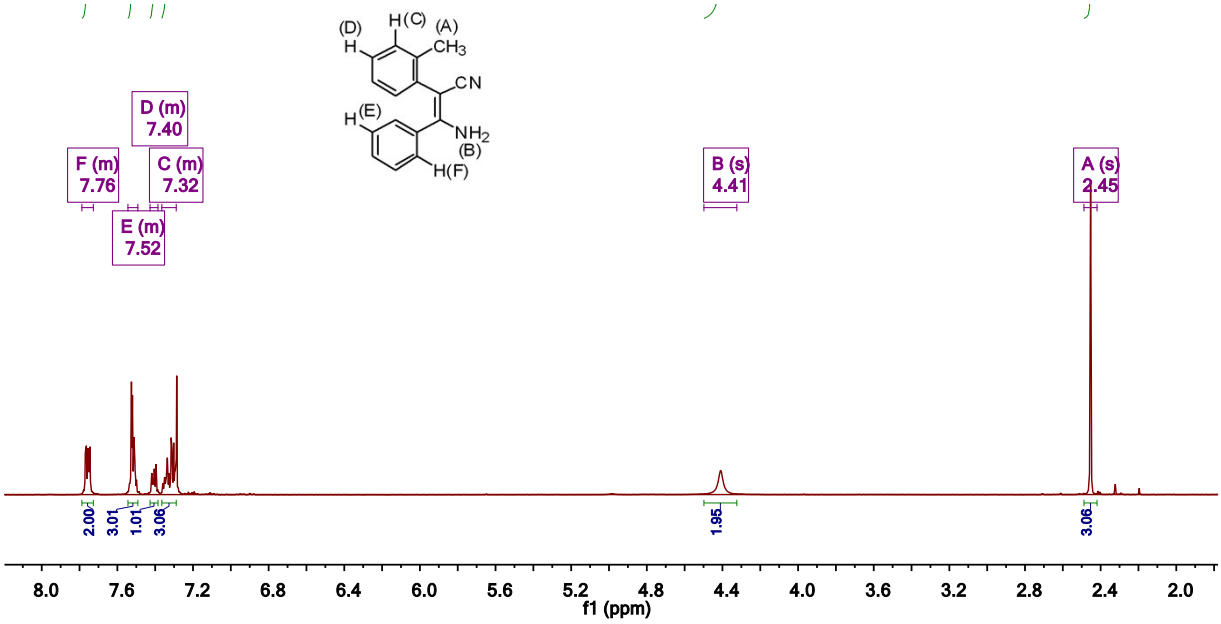
(4h)

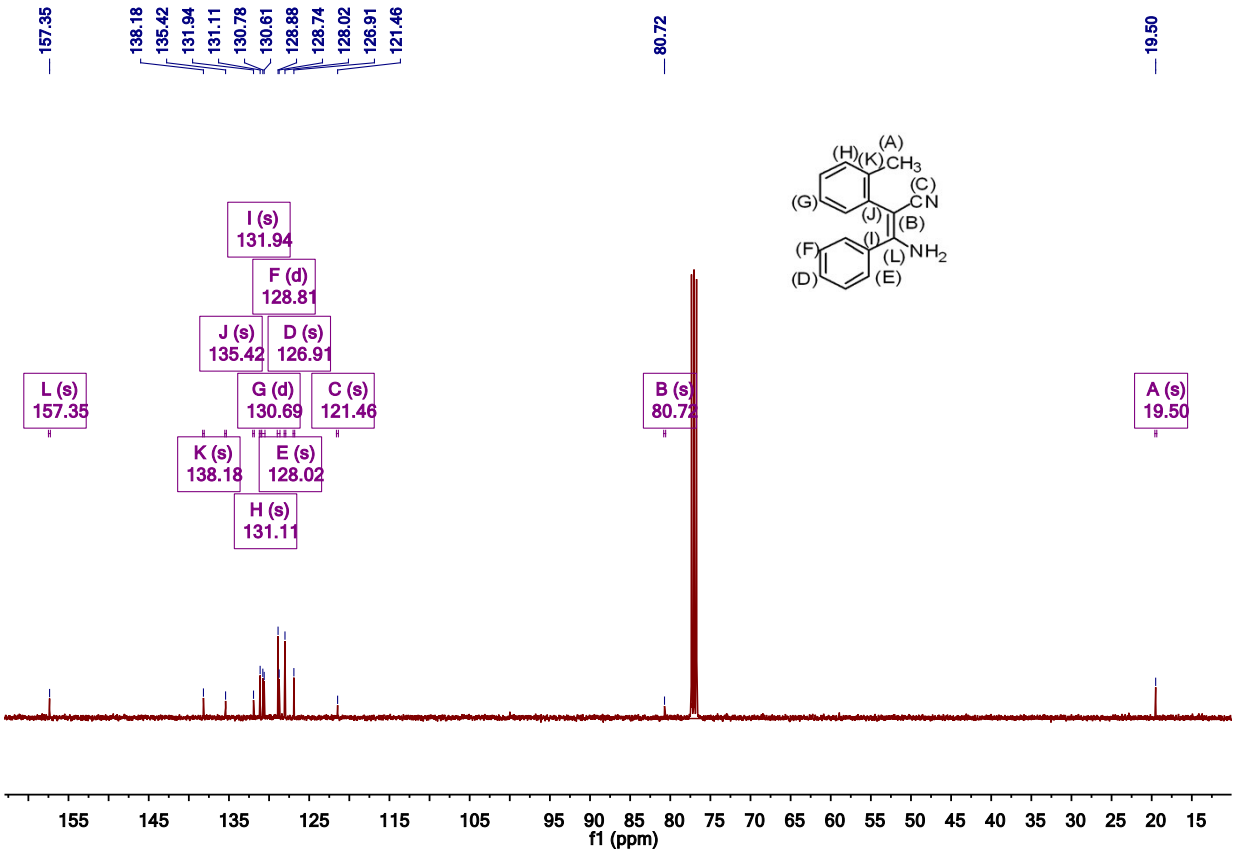

C (m) 7.49
E (m) 7.72
B (m) 7.33
D (ddd) 7.55
A (d) 4.92
1.86
1.91
4.73
1.03
2.00
f1 (ppm)

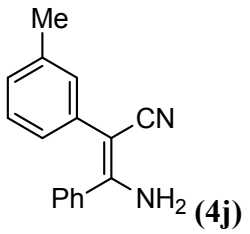

156.97
136.03
133.99
130.64
129.45
128.89
128.68
128.07
127.52
122.17
81.96
H (s) 130.64
F (s) 128.89
J (s) 136.03
D (s) 128.07
K (s) 156.97
I (s) 133.99
C (s) 127.52
B (s) 122.17
E (s) 128.68
G (s) 129.45
A (s) 81.96
f1 (ppm)


Me
CN
Ph
NH2

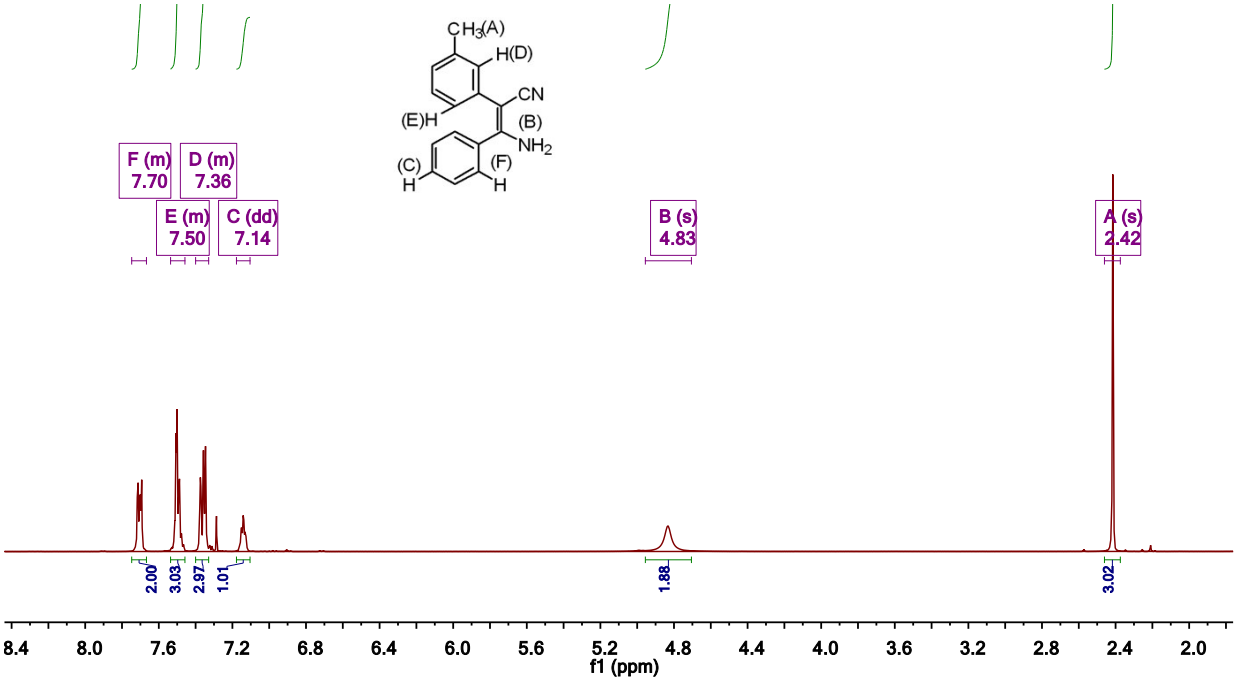
(4i)

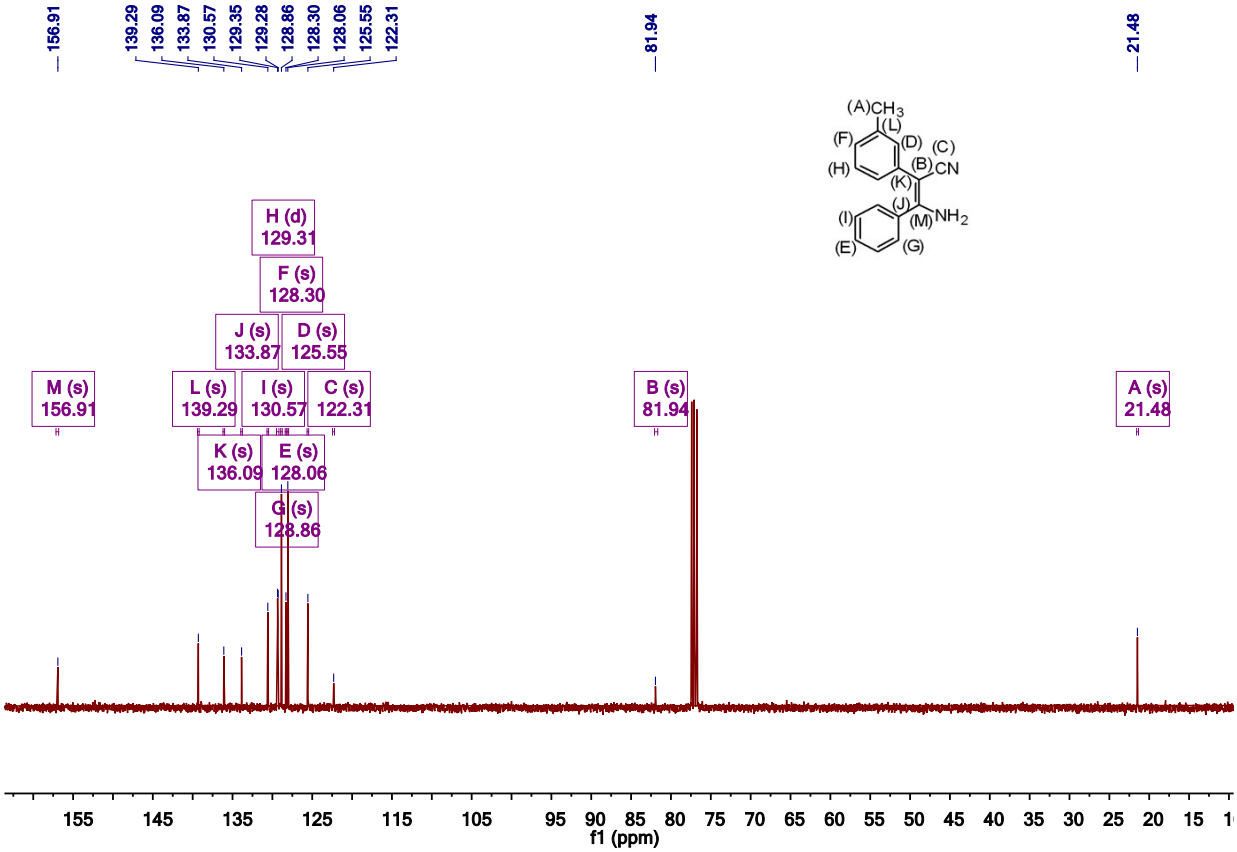

D (m) 7.40
F (m) 7.76
C (m) 7.32
E (m) 7.52
B (s) 4.41
A (s) 2.45
2.00
3.01
1.01
3.06
1.95
3.06
f1 (ppm)

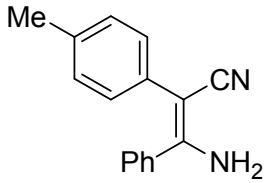

157.35
138.18
135.42
131.94
131.11
130.78
130.61
128.88
128.74
128.02
126.91
121.46
80.72
19.50
I (s) 131.94
F (d) 128.81
J (s) 135.42
D (s) 126.91
L (s) 157.35
G (d) 130.69
C (s) 121.46
K (s) 138.18
E (s) 128.02
H (s) 131.11
B (s) 80.72
A (s) 19.50
f1 (ppm)


Me
CN
Ph
NH2

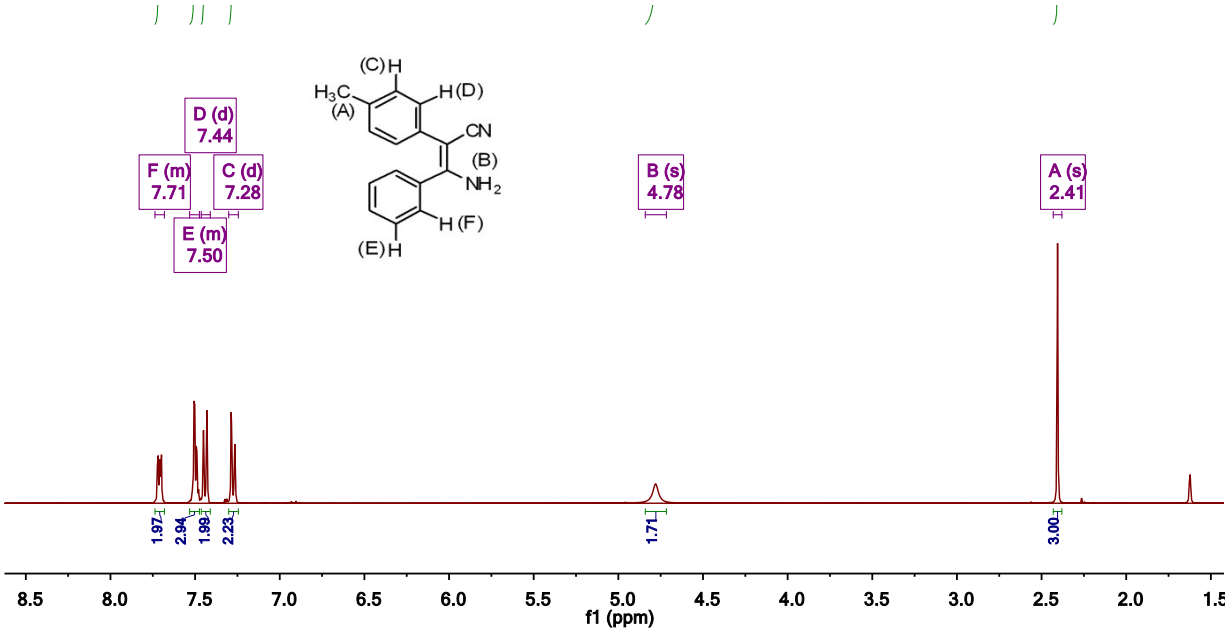
(4j)

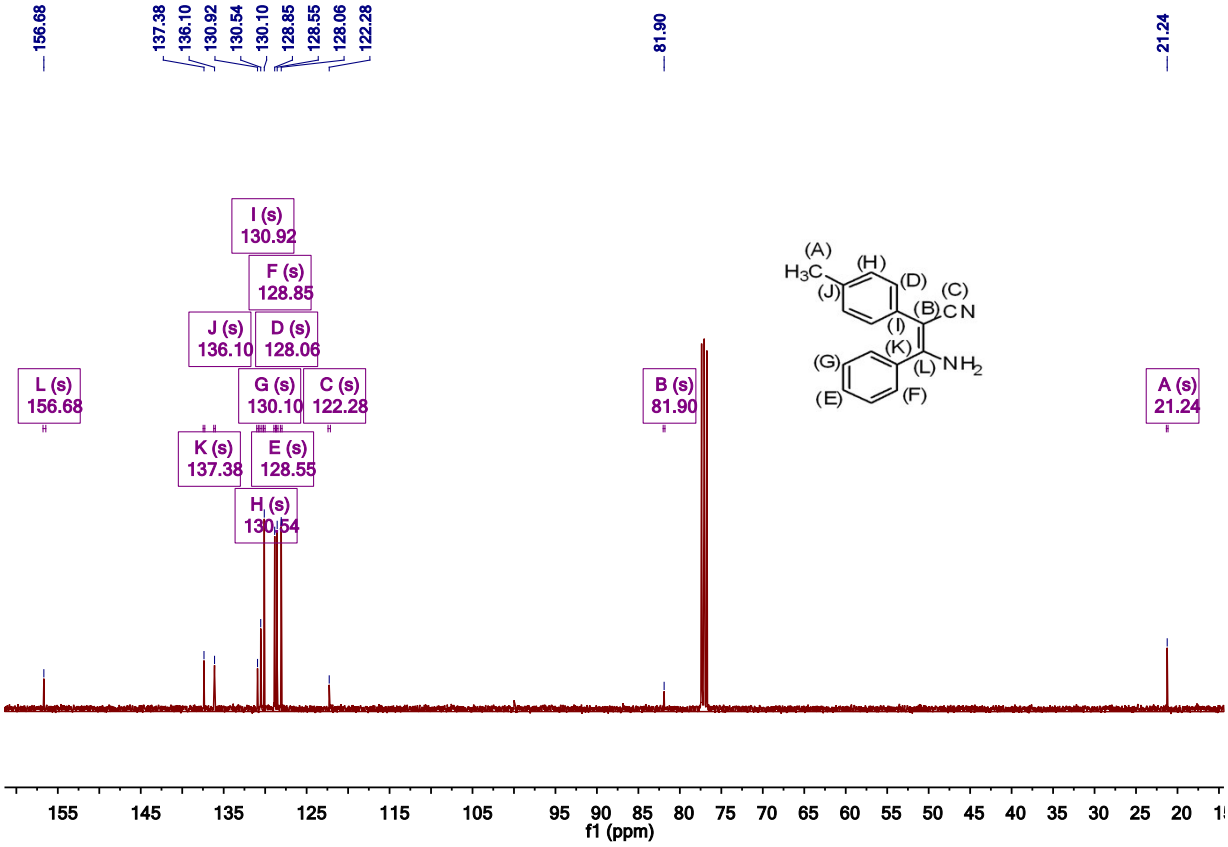

F (m) 7.70
D (m) 7.36
E (m) 7.50
C (dd) 7.14
B (s) 4.83
A (s) 2.42
2.00
3.03
2.97
1.01
1.88
3.02
f1 (ppm)

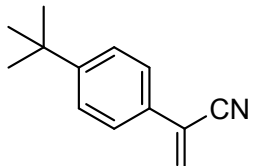

156.91
139.29
136.09
133.87
130.57
129.35
129.28
128.86
128.30
128.06
125.55
122.31
81.94
21.48
H (d) 129.31
F (s) 128.30
J (s) 133.87
D (s) 125.55
M (s) 156.91
L (s) 139.29
I (s) 130.57
C (s) 122.31
K (s) 136.09
E (s) 128.06
G (s) 128.86
B (s) 81.94
A (s) 21.48
f1 (ppm)


Me
CN
Ph
NH2

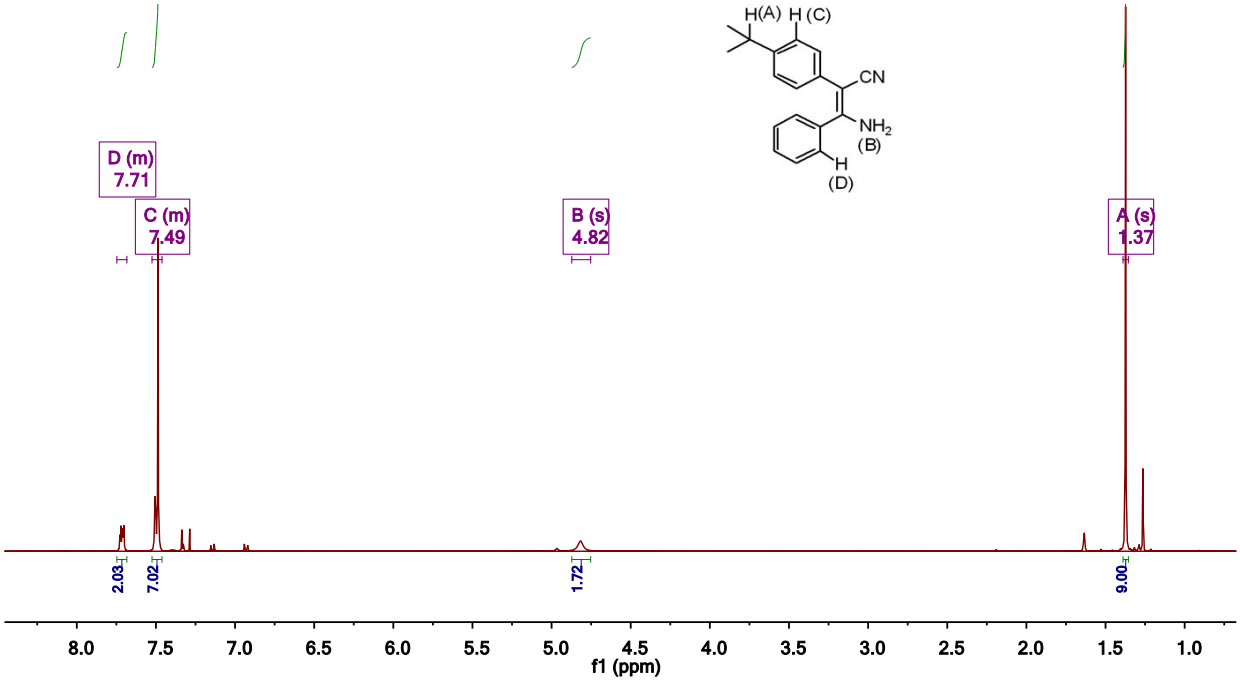
(4k)

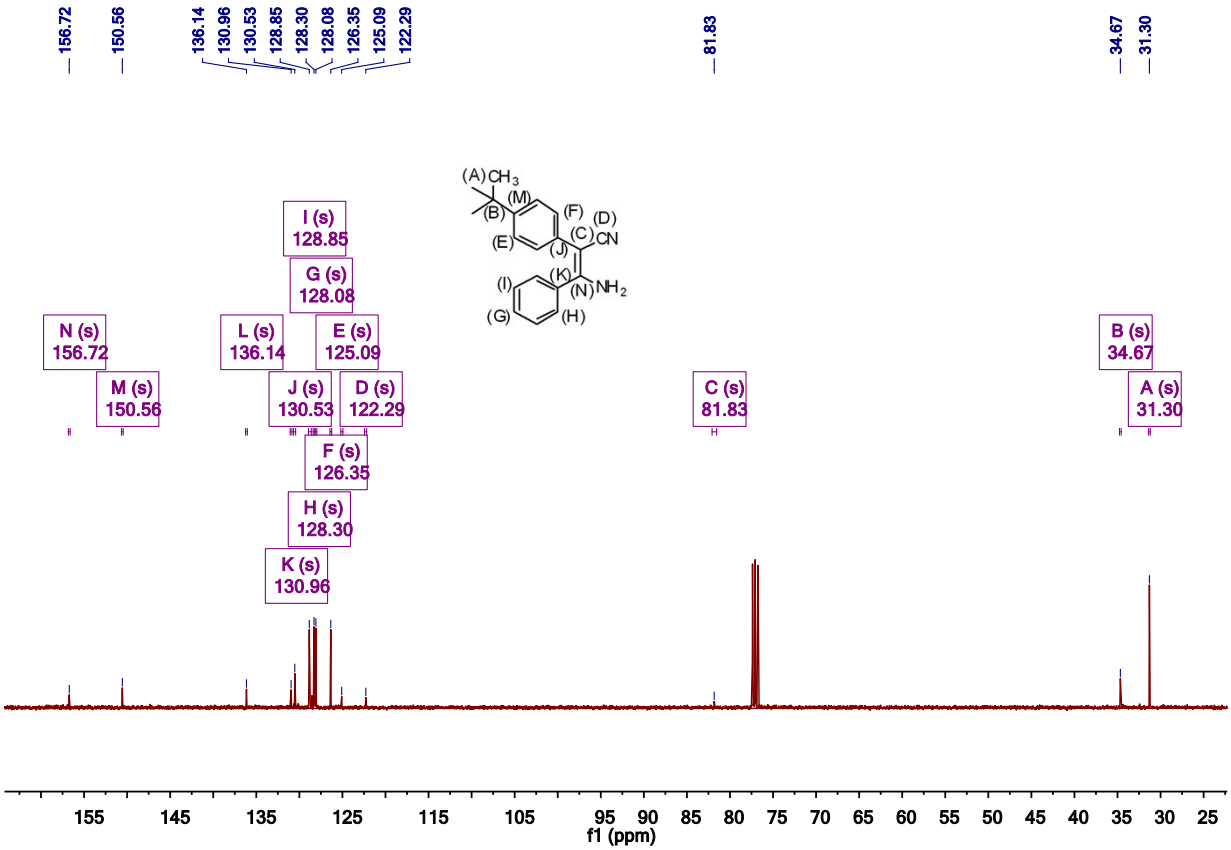

D (d) 7.44
F (m) 7.71
C (d) 7.28
E (m) 7.50
B (s) 4.78
A (s) 2.41
1.97
2.94
1.98
2.23
1.71
3.00
f1 (ppm)

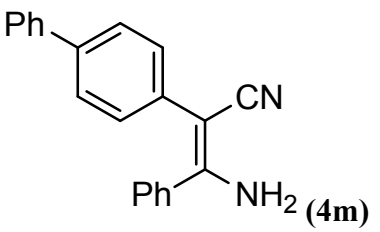

156.68
137.38
136.10
130.92
130.54
130.10
128.85
128.55
128.06
122.28
81.90
21.24
I (s) 130.92
F (s) 128.85
J (s) 136.10
D (s) 128.06
L (s) 156.68
G (s) 130.10
C (s) 122.28
K (s) 137.38
E (s) 128.55
H (s) 130.54
B (s) 81.90
A (s) 21.24
f1 (ppm)


CN
Ph
NH2

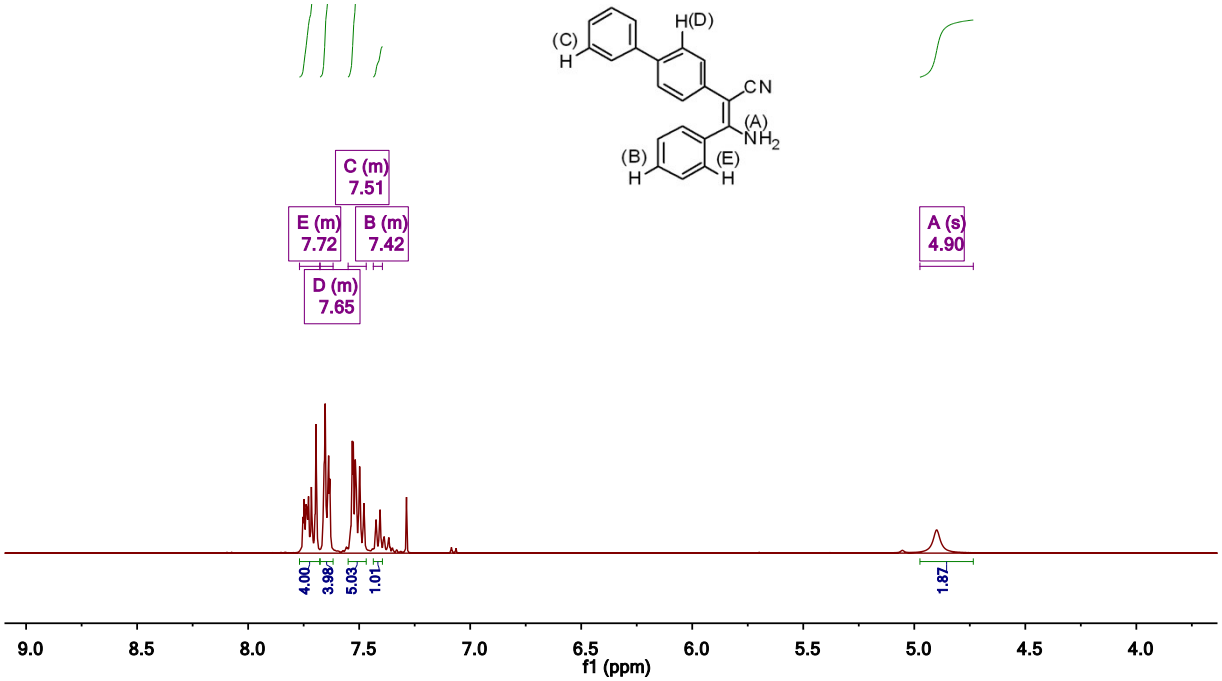
(4l)

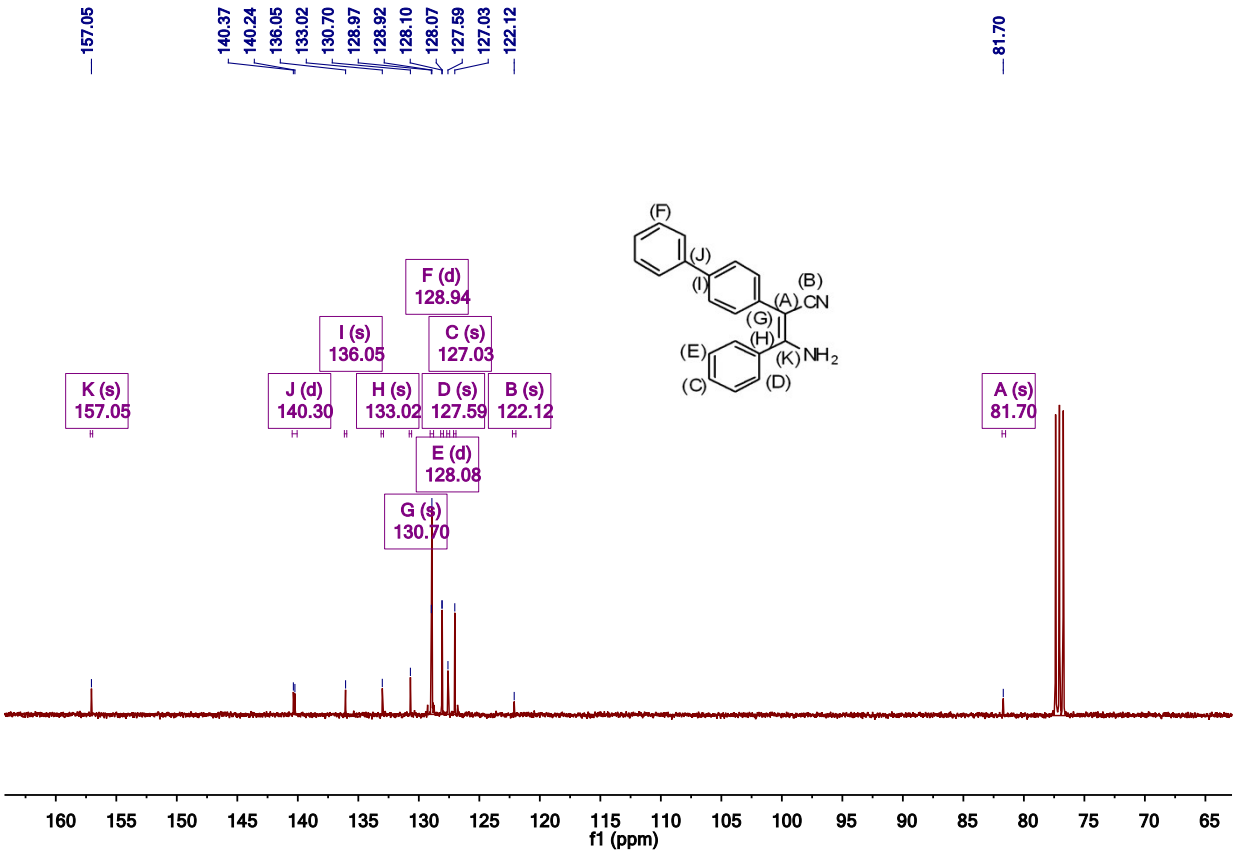

H(A) H (C)
CN
NH2
(B)
H
(D)
D (m)
7.71
C (m)
7.49
B (s)
4.82
A (s)
1.37
2.03
7.02
1.72
9.00
f1 (ppm)

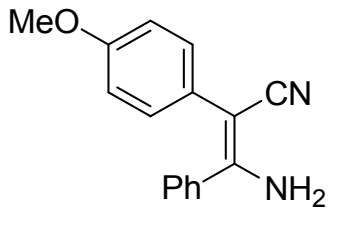

156.72
150.56
136.14
130.96
130.53
128.85
128.30
128.08
126.35
125.09
122.29
81.83
34.67
31.30
(A) CH3
(B)
(M)
(F)
(D)
(E)
(C)
CN
(J)
(K)
(I)
(N)
NH2
(G)
(H)
I (s)
128.85
G (s)
128.08
N (s)
156.72
L (s)
136.14
E (s)
125.09
M (s)
150.56
J (s)
130.53
D (s)
122.29
F (s)
126.35
H (s)
128.30
K (s)
130.96
C (s)
81.83
B (s)
34.67
A (s)
31.30
f1 (ppm)


Ph
CN
Ph
NH2

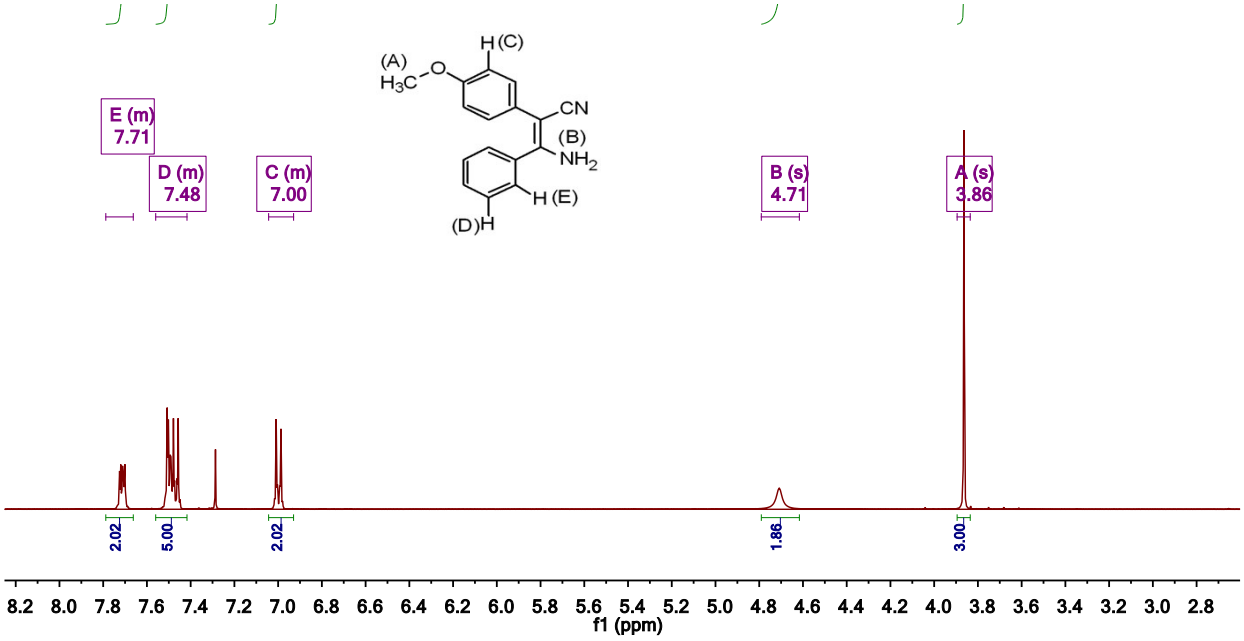
(4m)

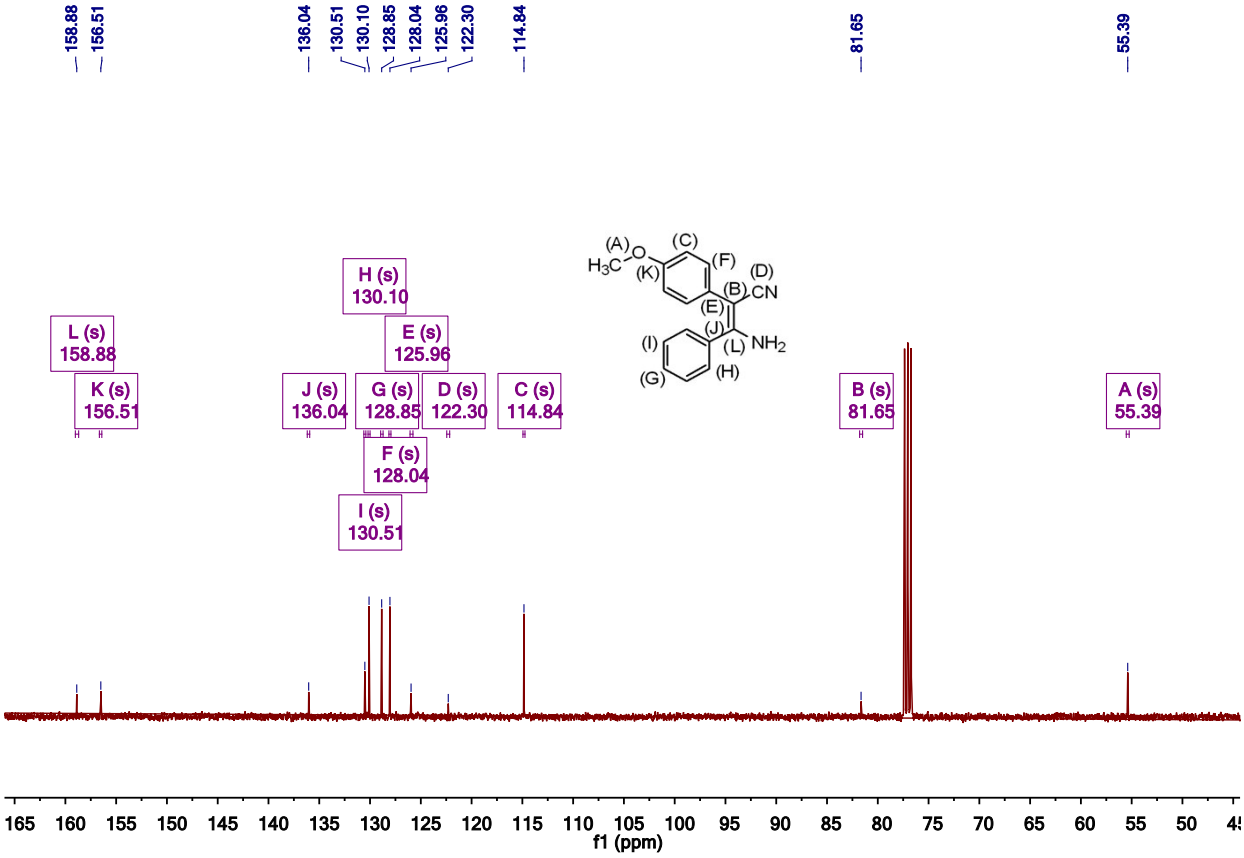

C (m) 7.51
E (m) 7.72
B (m) 7.42
D (m) 7.65
A (s) 4.90
4.00
3.98
5.03
1.01
1.87
f1 (ppm)

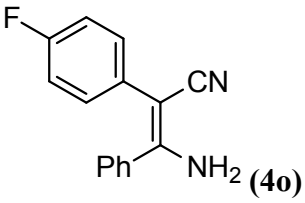

157.05
140.37
140.24
136.05
133.02
130.70
128.97
128.92
128.10
128.07
127.59
127.03
122.12
81.70
F (d) 128.94
I (s) 136.05
C (s) 127.03
K (s) 157.05
J (d) 140.30
H (s) 133.02
D (s) 127.59
B (s) 122.12
E (d) 128.08
G (s) 130.70
A (s) 81.70
f1 (ppm)


MeO
CN
Ph
NH2

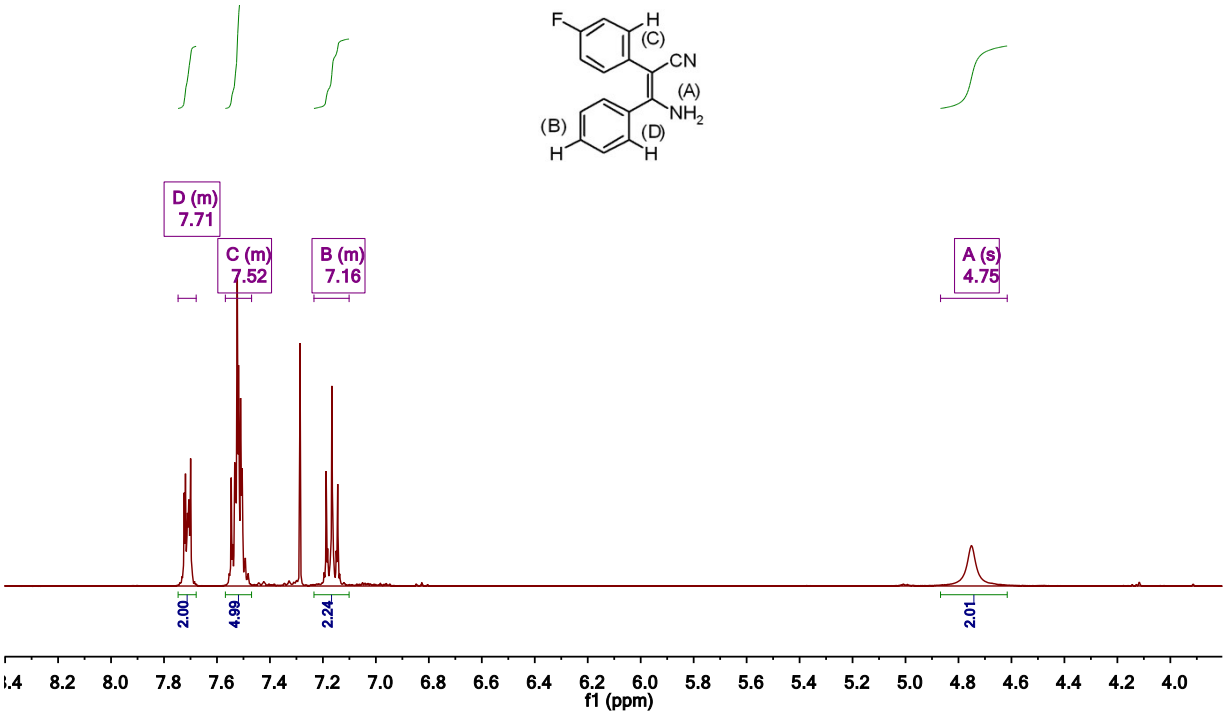
(4n)

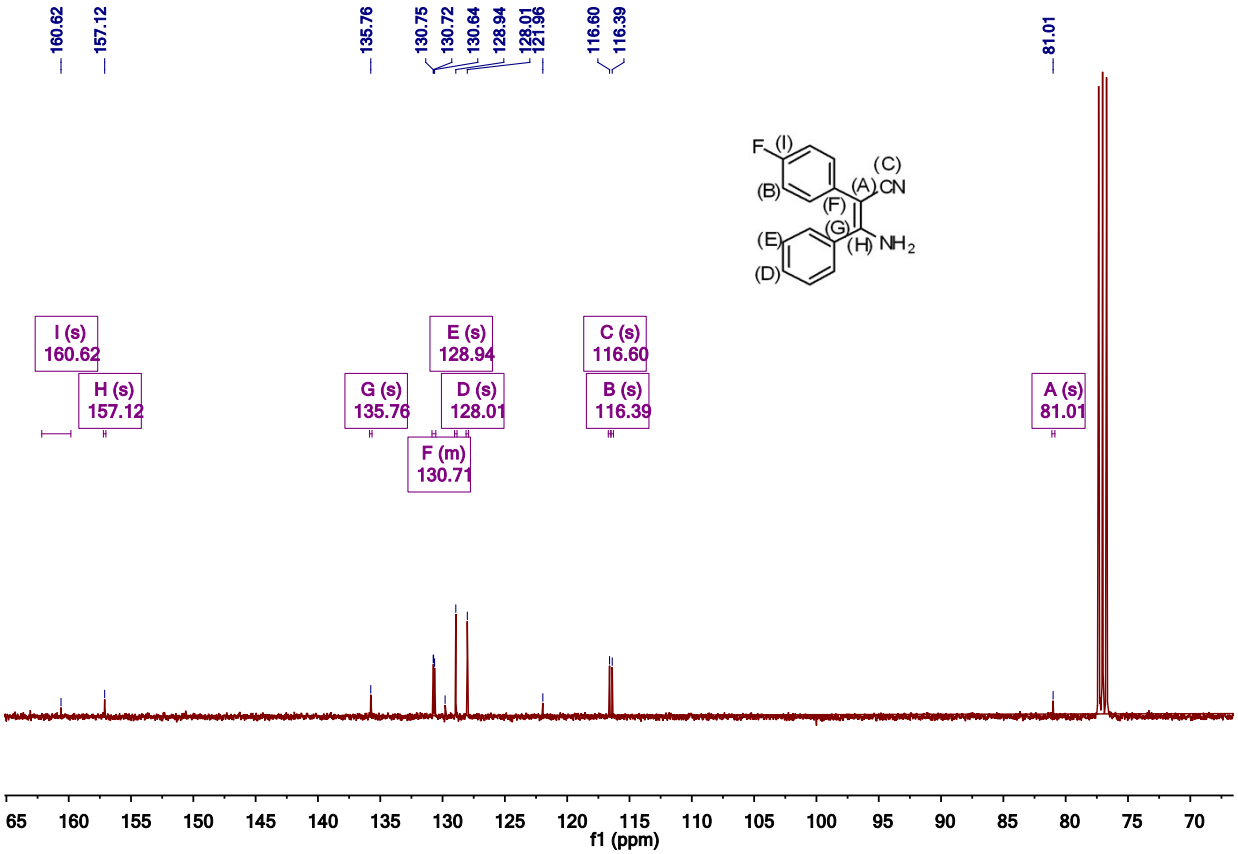

E (m) 7.71
D (m) 7.48
C (m) 7.00
B (s) 4.71
A (s) 3.86
2.02
5.00
2.02
1.86
3.00
f1 (ppm)

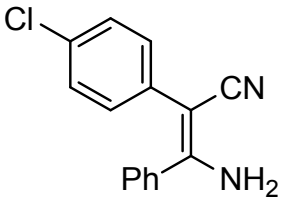

158.88
156.51
136.04
130.51
130.10
128.85
128.04
125.96
122.30
114.84
81.65
55.39
L (s) 158.88
K (s) 156.51
J (s) 136.04
H (s) 130.10
G (s) 128.85
D (s) 122.30
E (s) 125.96
C (s) 114.84
F (s) 128.04
I (s) 130.51
B (s) 81.65
A (s) 55.39
f1 (ppm)


F
CN
Ph
NH2

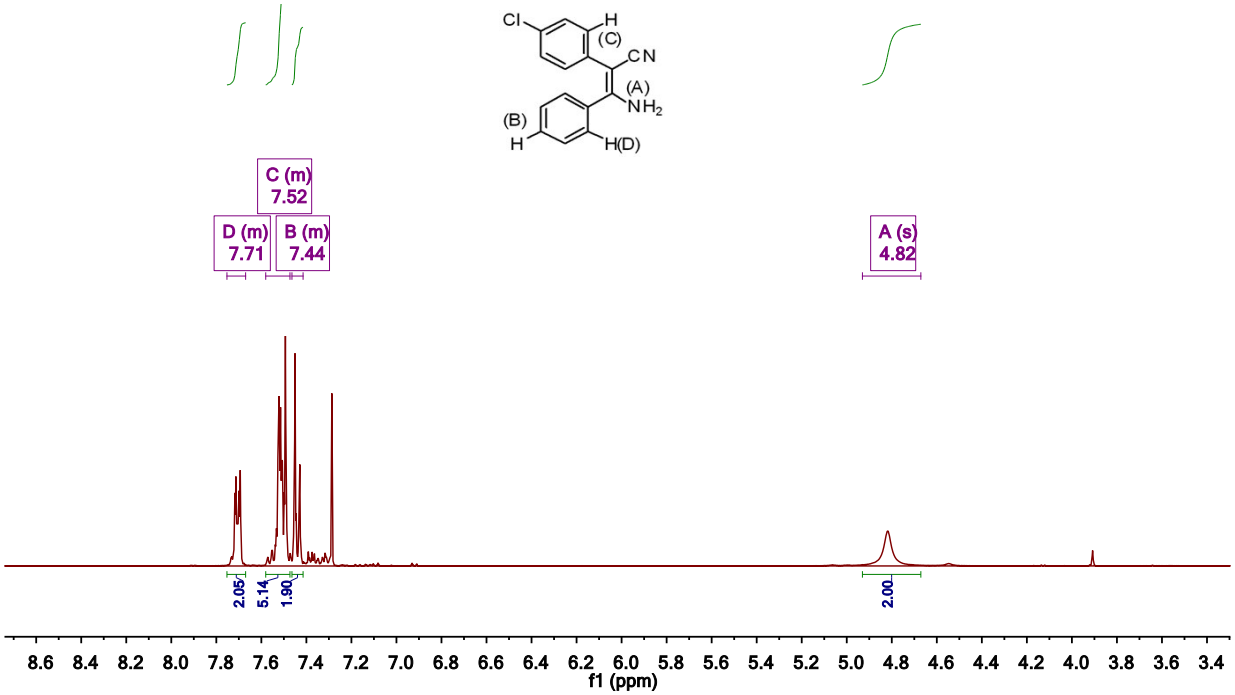
(4o)

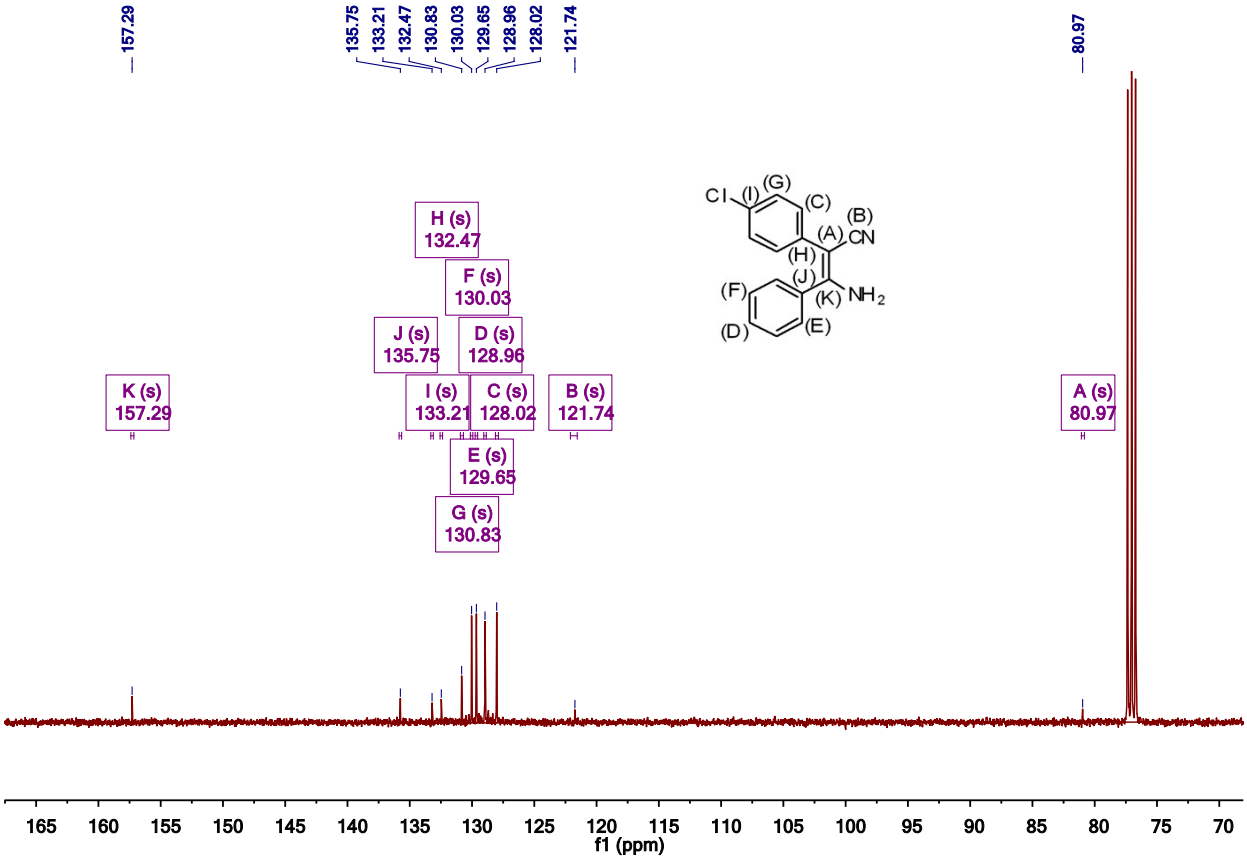

D (m) 7.71
C (m) 7.52
B (m) 7.16
A (s) 4.75
2.00
4.99
2.24
2.01
f1 (ppm)

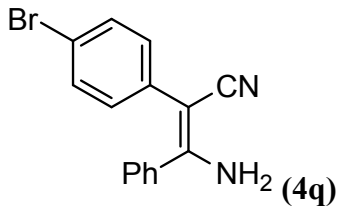

160.62
157.12
135.76
130.75
130.72
130.64
128.94
128.01
121.96
116.60
116.39
81.01
I (s) 160.62
H (s) 157.12
G (s) 135.76
E (s) 128.94
D (s) 128.01
F (m) 130.71
C (s) 116.60
B (s) 116.39
A (s) 81.01
f1 (ppm)


Cl
CN
Ph
NH2

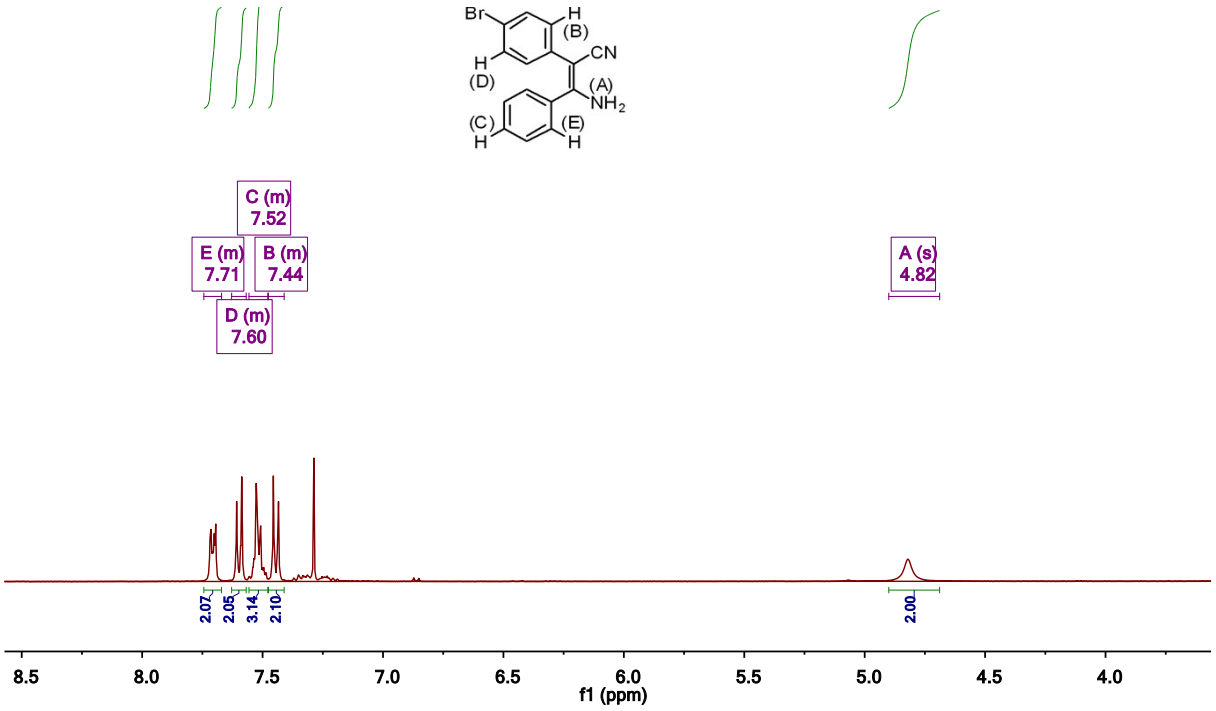
(4p)

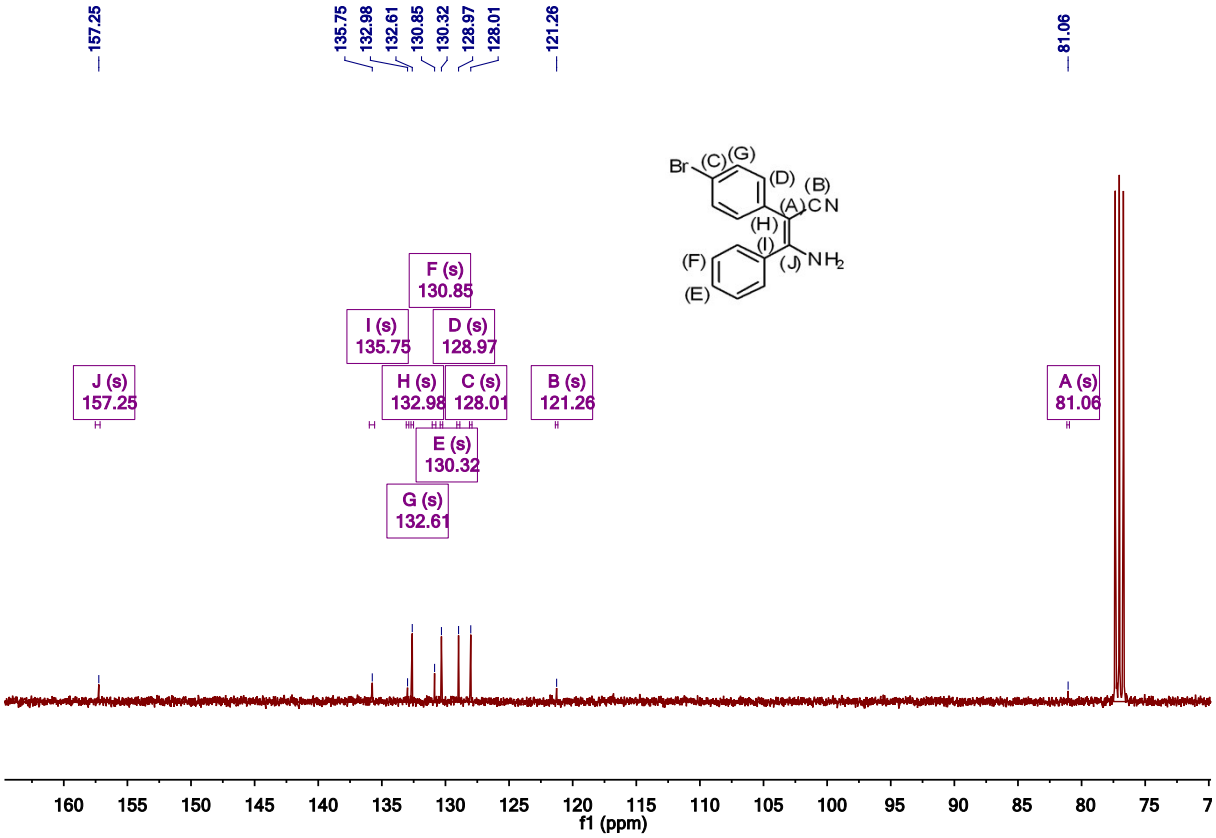

C (m) 7.52
D (m) 7.71
B (m) 7.44
A (s) 4.82
2.05
5.14
1.90
2.00
f1 (ppm)

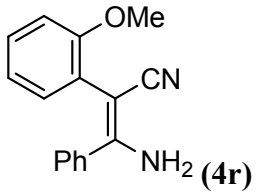

157.29
135.75
133.21
132.47
130.83
130.03
129.65
128.96
128.02
121.74
80.97
H (s) 132.47
F (s) 130.03
J (s) 135.75
D (s) 128.96
K (s) 157.29
I (s) 133.21
C (s) 128.02
B (s) 121.74
E (s) 129.65
G (s) 130.83
A (s) 80.97
f1 (ppm)


Br
CN
Ph
NH2

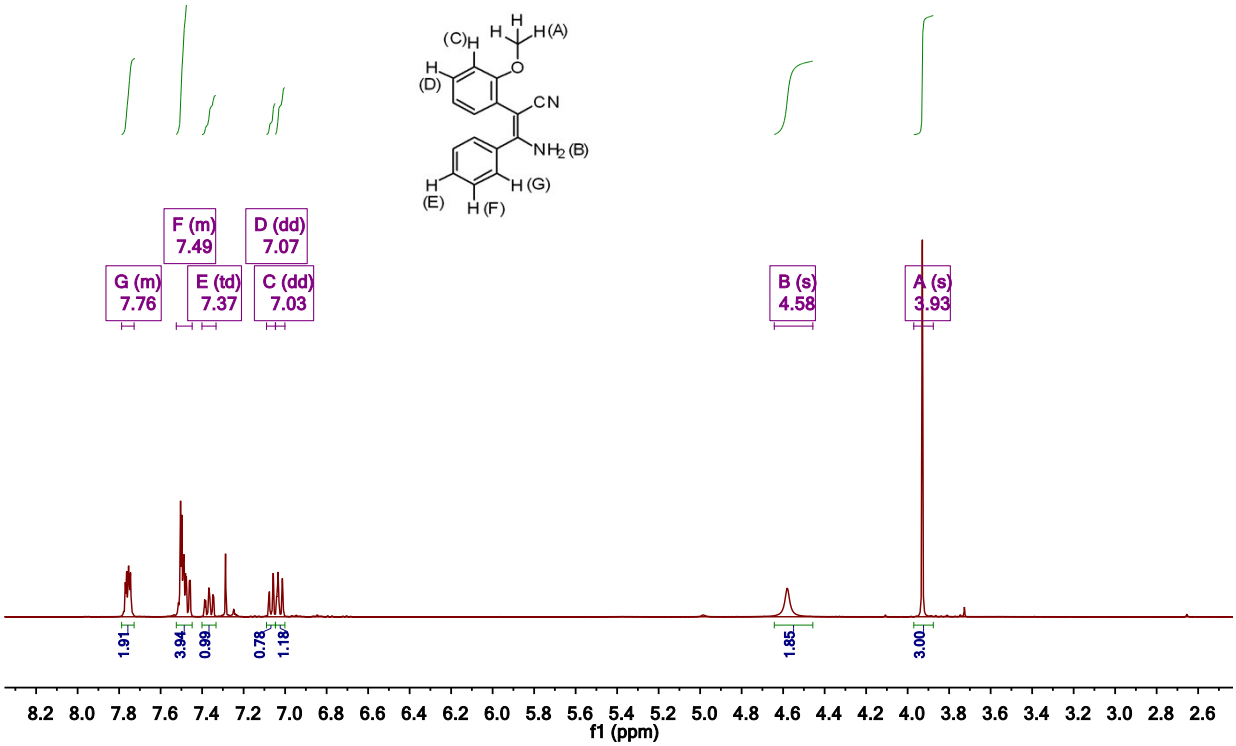
(4q)

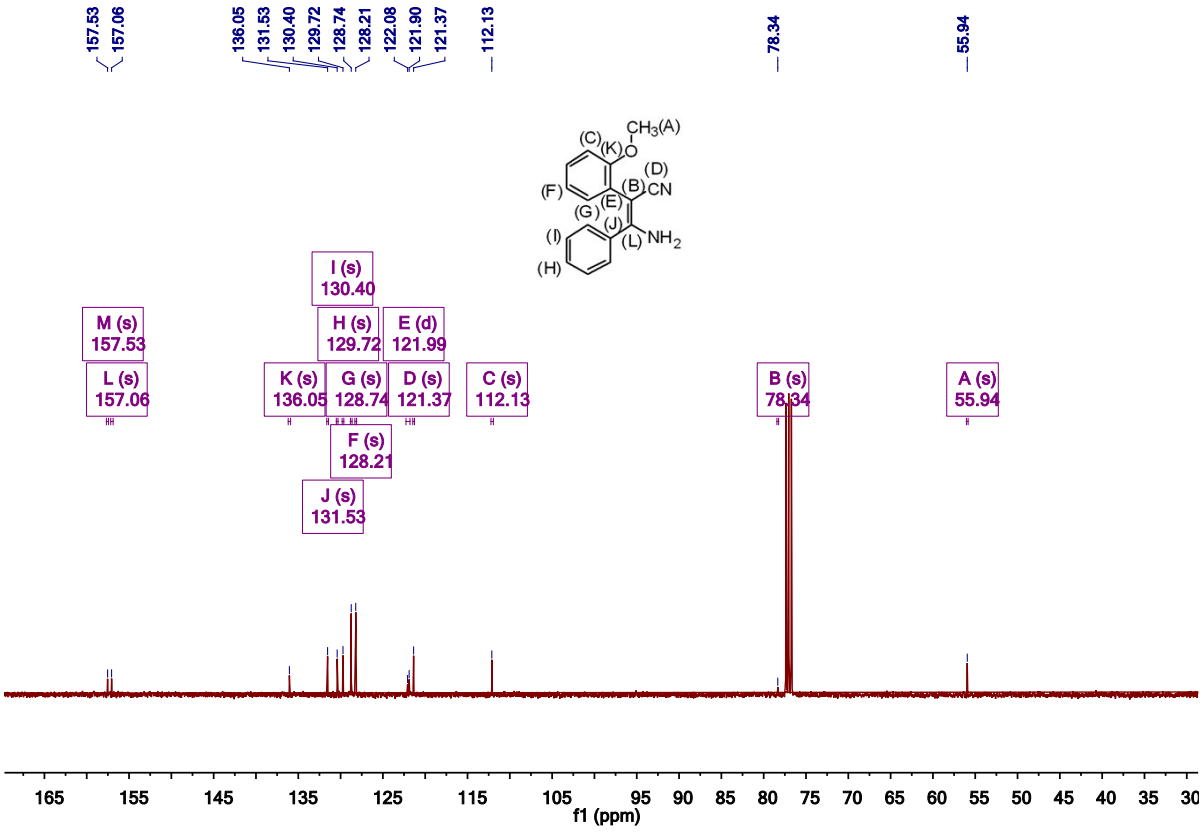

C (m) 7.52
E (m) 7.71
B (m) 7.44
D (m) 7.60
A (s) 4.82
2.07
2.05
3.14
2.10
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
f1 (ppm)

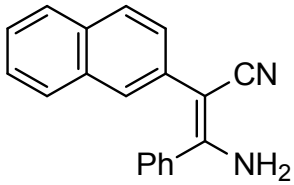

157.25
135.75
132.98
132.61
130.85
130.32
128.97
128.01
121.26
81.06
F (s) 130.85
I (s) 135.75
D (s) 128.97
J (s) 157.25
H (s) 132.98
C (s) 128.01
B (s) 121.26
A (s) 81.06
E (s) 130.32
G (s) 132.61
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
f1 (ppm)


OMe
CN
Ph
NH2

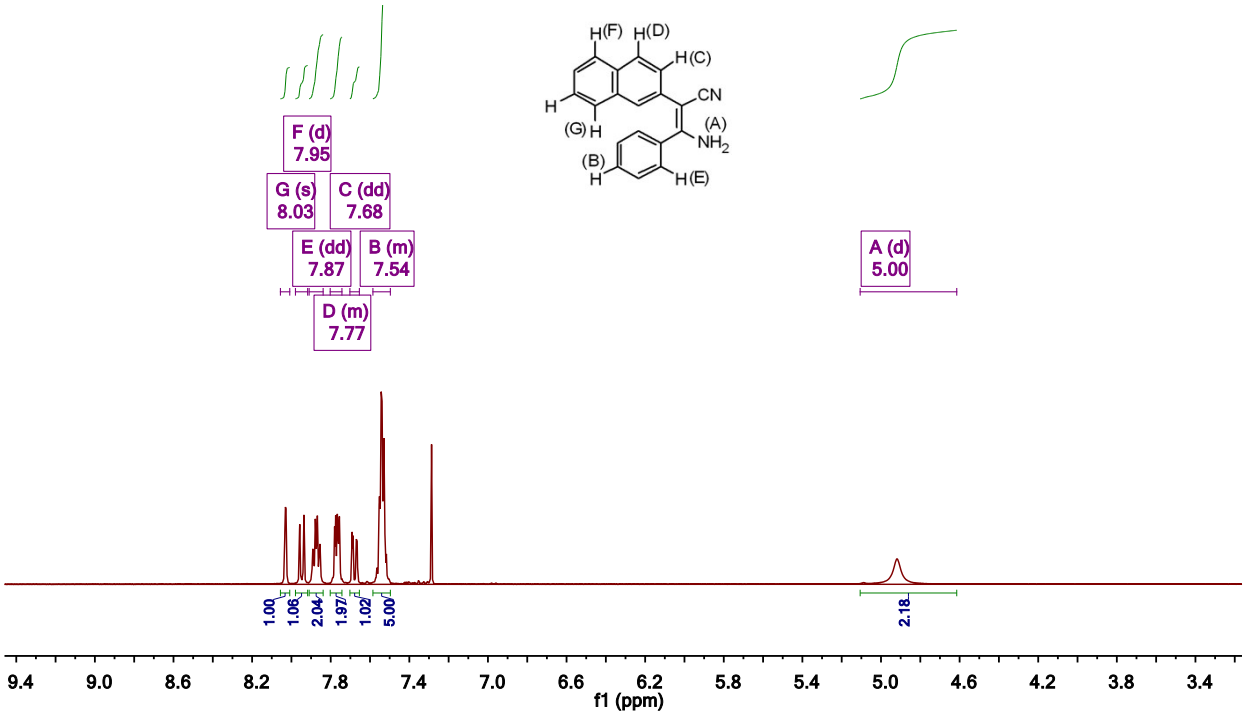
(4r)

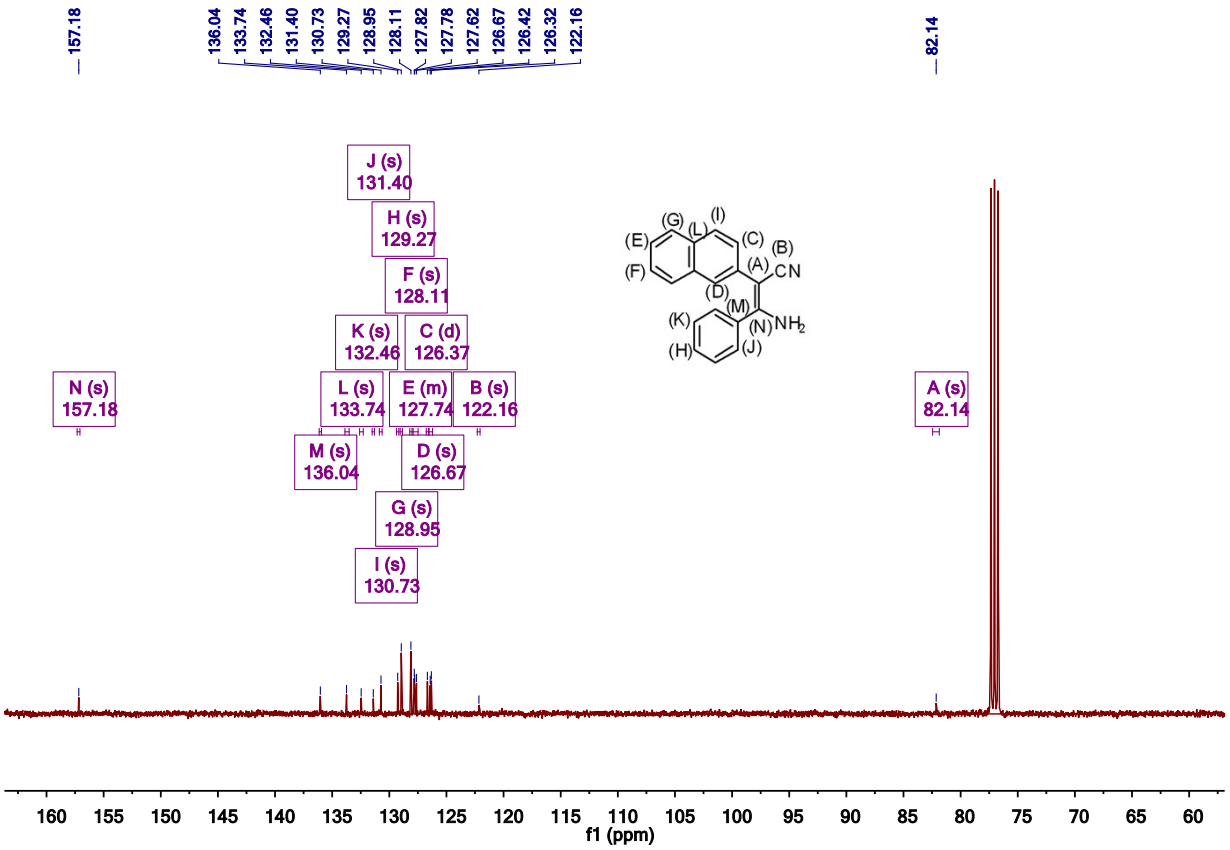

F (m) 7.49
D (dd) 7.07
G (m) 7.76
E (td) 7.37
C (dd) 7.03
B (s) 4.58
A (s) 3.93
1.91
3.94
0.99
0.78
1.18
1.85
3.00
f1 (ppm)

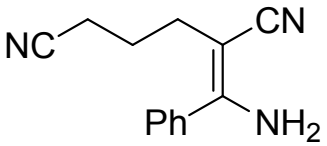

157.53
157.06
136.05
131.53
130.40
129.72
128.74
128.21
122.08
121.90
121.37
112.13
78.34
55.94
I (s) 130.40
M (s) 157.53
H (s) 129.72
E (d) 121.99
L (s) 157.06
K (s) 136.05
G (s) 128.74
D (s) 121.37
C (s) 112.13
B (s) 78.34
A (s) 55.94
F (s) 128.21
J (s) 131.53
f1 (ppm)


CN
Ph
NH2

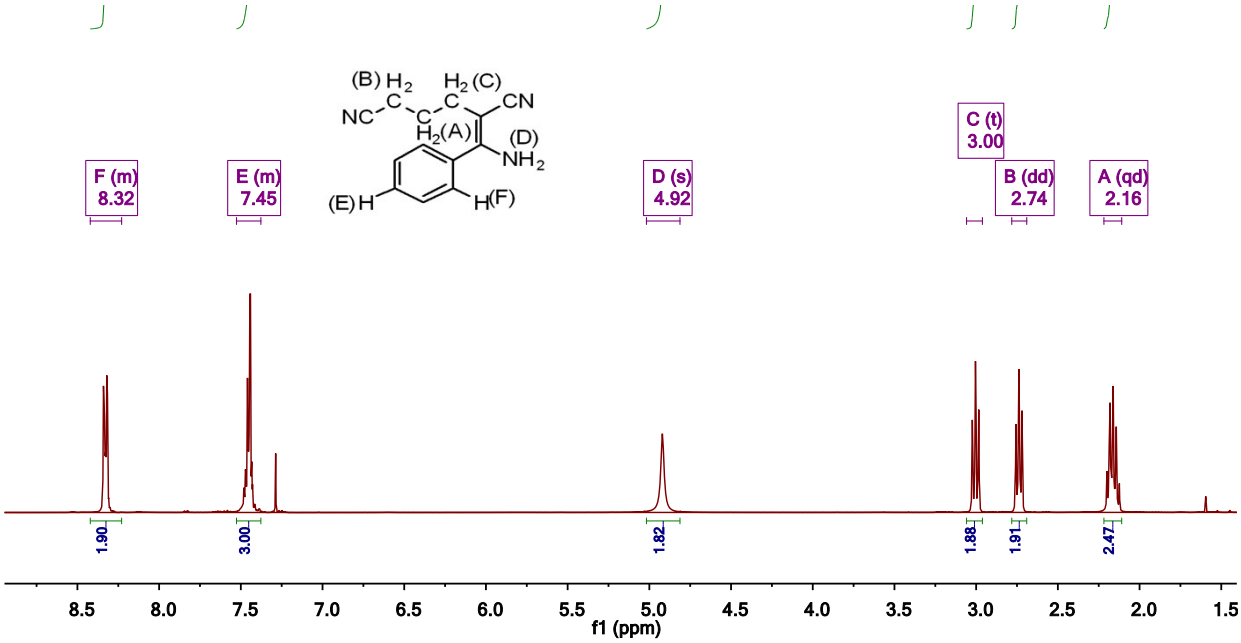
(4s)

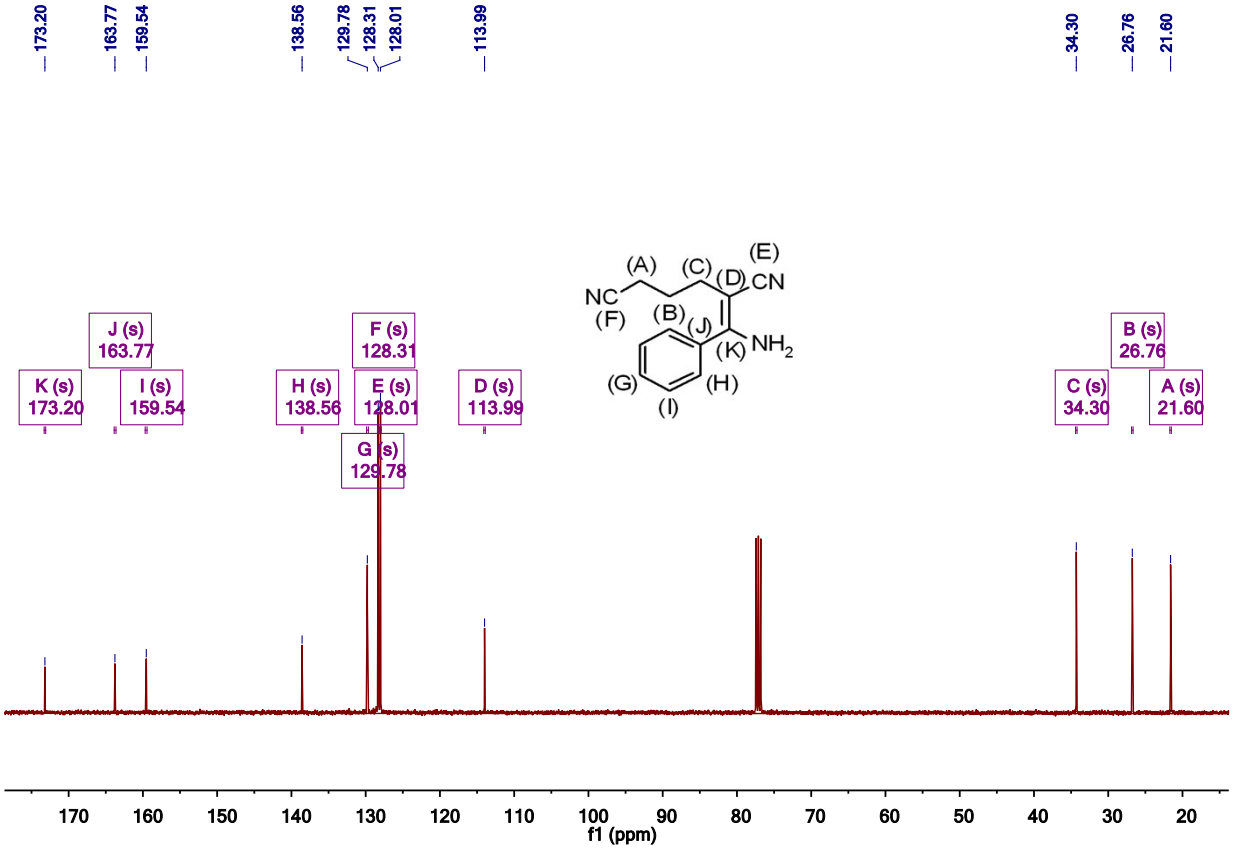

F (d) 7.95
G (s) 8.03
C (dd) 7.68
E (dd) 7.87
B (m) 7.54
D (m) 7.77
A (d) 5.00
1.00
1.06
2.04
1.97
1.02
5.00
2.18
9.4 9.0 8.6 8.2 7.8 7.4 7.0 6.6 6.2 5.8 5.4 5.0 4.6 4.2 3.8 3.4
f1 (ppm)

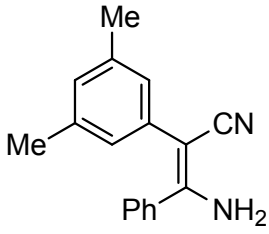

157.18
136.04
133.74
132.46
131.40
130.73
129.27
128.95
128.11
127.82
127.78
127.62
126.67
126.42
126.32
122.16
82.14
J (s) 131.40
H (s) 129.27
F (s) 128.11
K (s) 132.46
C (d) 126.37
N (s) 157.18
L (s) 133.74
E (m) 127.74
B (s) 122.16
M (s) 136.04
D (s) 126.67
G (s) 128.95
I (s) 130.73
A (s) 82.14
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60
f1 (ppm)



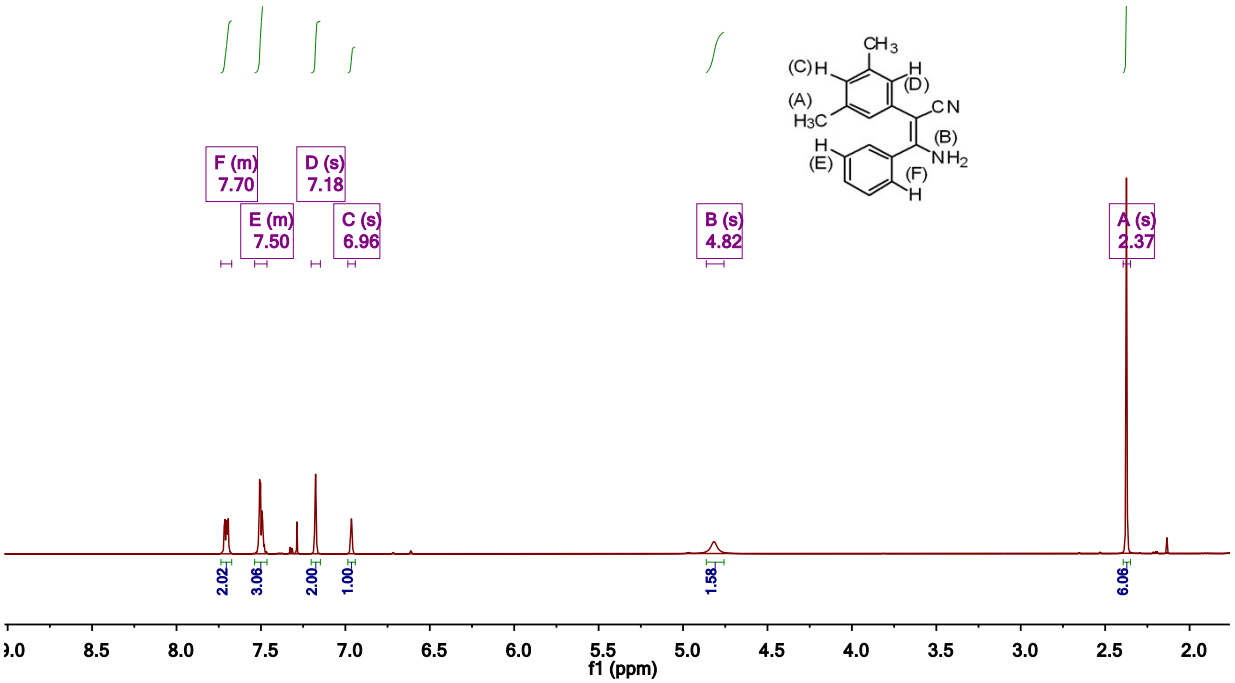
(4t)

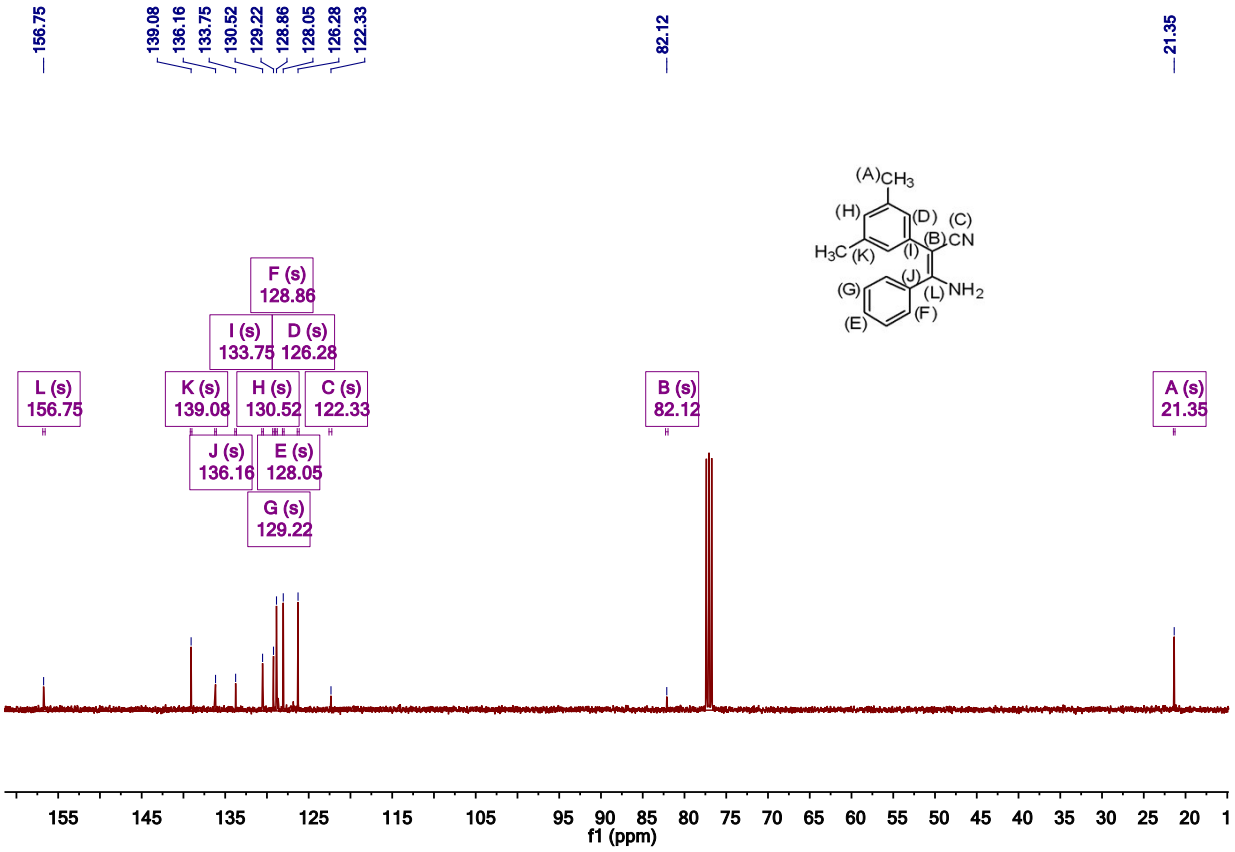

F (m) 8.32
E (m) 7.45
D (s) 4.92
C (t) 3.00
B (dd) 2.74
A (qd) 2.16
1.90
3.00
1.82
1.88
1.91
2.47
f1 (ppm)

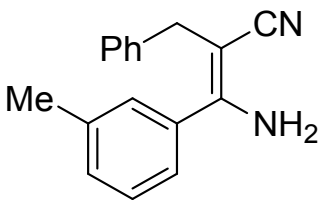

173.20
163.77
159.54
138.56
129.78
128.31
128.01
113.99
34.30
26.76
21.60
J (s) 163.77
K (s) 173.20
I (s) 159.54
H (s) 138.56
F (s) 128.31
E (s) 128.01
G (s) 129.78
D (s) 113.99
B (s) 26.76
C (s) 34.30
A (s) 21.60
f1 (ppm)


Me
Me
CN
Ph
NH2

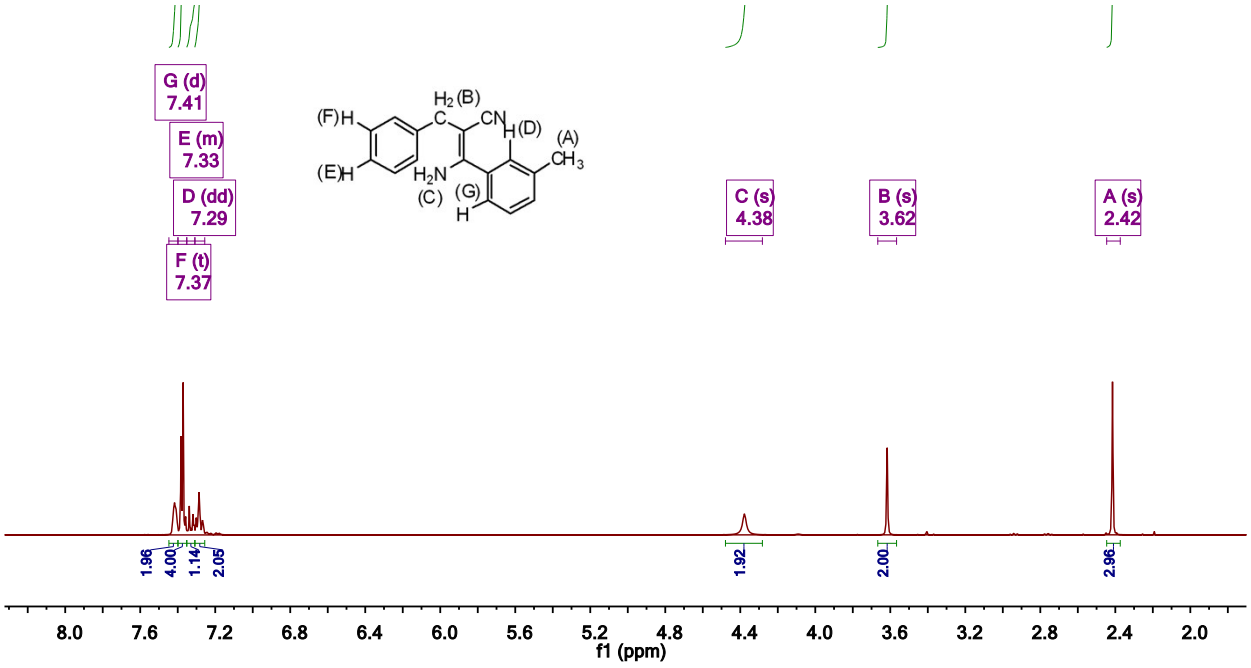
(4u)

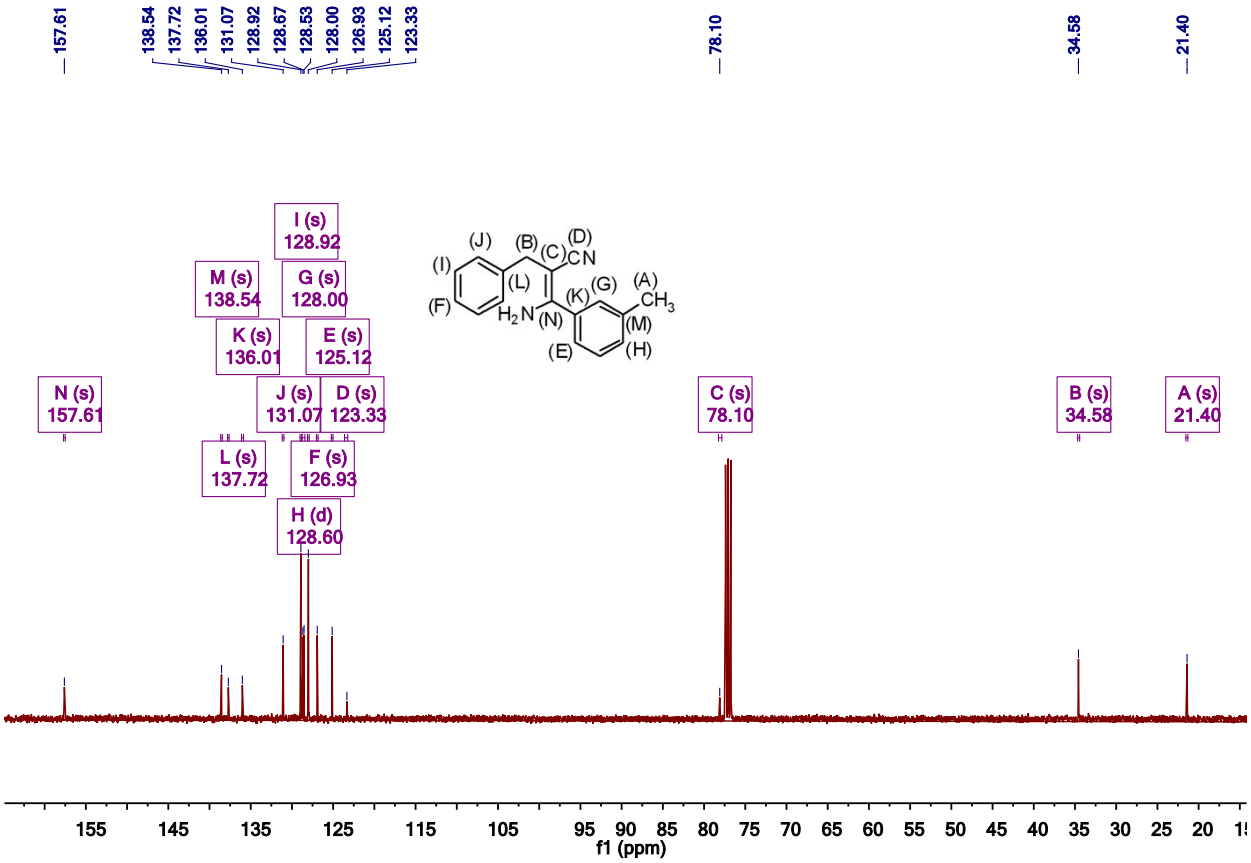

F (m) 7.70
D (s) 7.18
E (m) 7.50
C (s) 6.96
B (s) 4.82
A (s) 2.37
2.02
3.06
2.00
1.00
1.58
6.06
f1 (ppm)

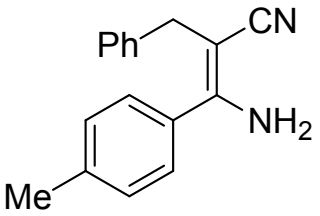

156.75
139.08
136.16
133.75
130.52
129.22
128.86
128.05
126.28
122.33
82.12
21.35
F (s) 128.86
I (s) 133.75
D (s) 126.28
L (s) 156.75
K (s) 139.08
H (s) 130.52
C (s) 122.33
J (s) 136.16
E (s) 128.05
G (s) 129.22
B (s) 82.12
A (s) 21.35
f1 (ppm)


Ph
CN
Me
NH2

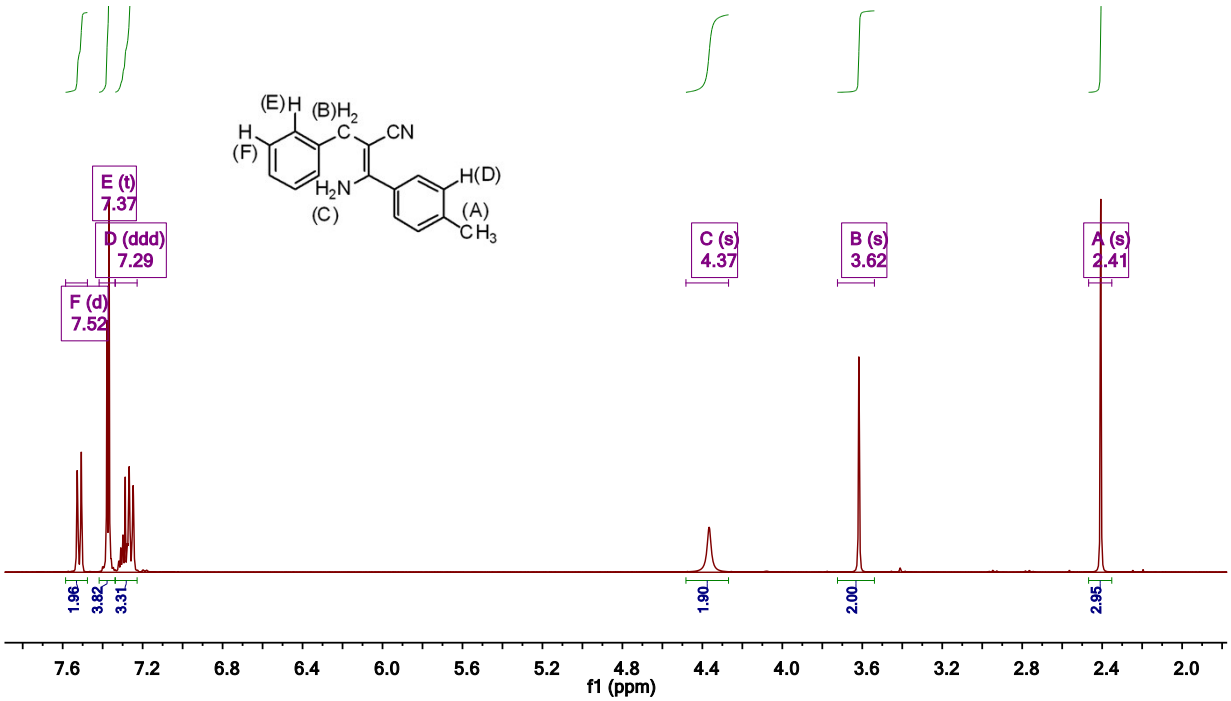
(4aa)

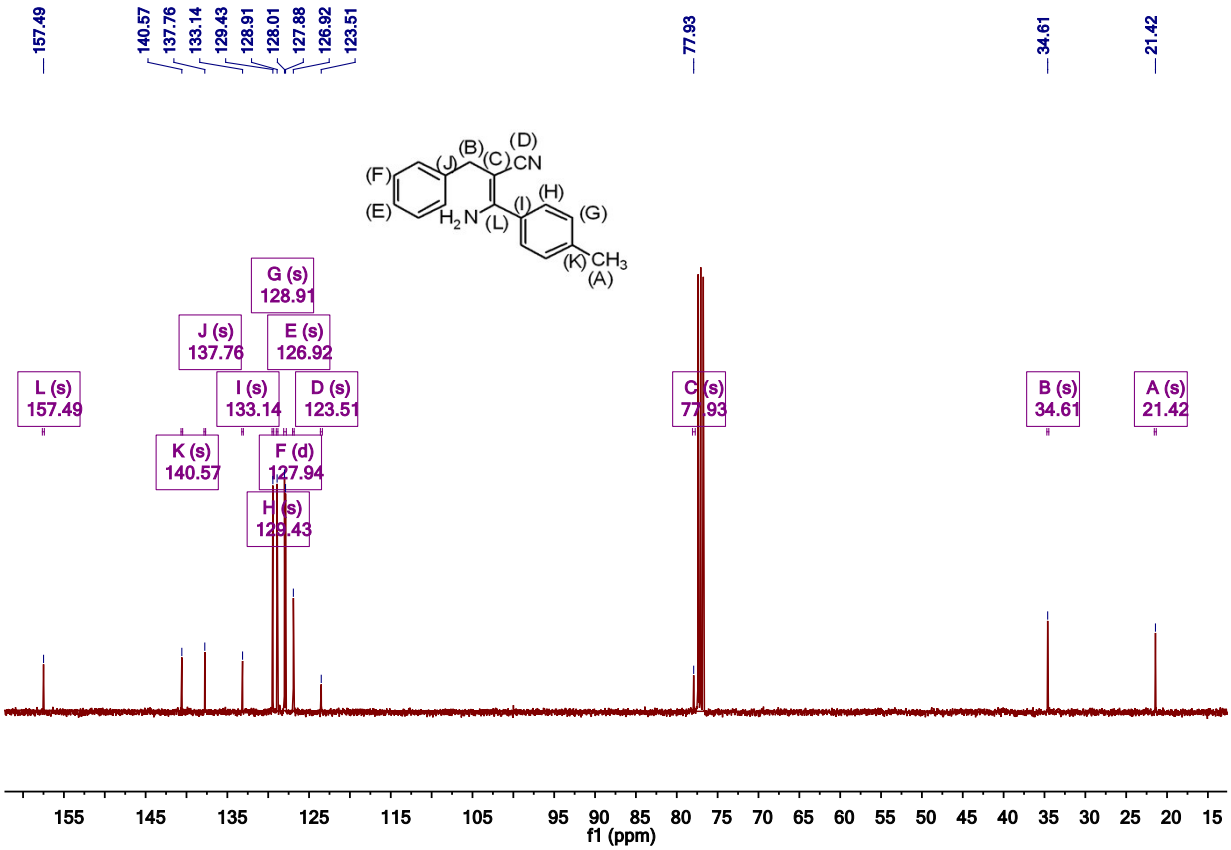

G (d) 7.41
E (m) 7.33
D (dd) 7.29
F (t) 7.37
C (s) 4.38
B (s) 3.62
A (s) 2.42
1.96
4.00
1.14
2.05
1.92
2.00
2.96
f1 (ppm)

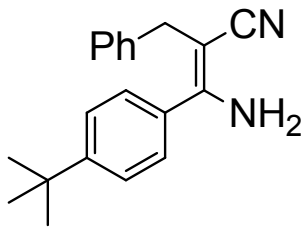

157.61
138.54
137.72
136.01
131.07
128.92
128.67
128.53
128.00
126.93
125.12
123.33
78.10
34.58
21.40
I (s) 128.92
M (s) 138.54
G (s) 128.00
K (s) 136.01
E (s) 125.12
N (s) 157.61
J (s) 131.07
D (s) 123.33
L (s) 137.72
F (s) 126.93
H (d) 128.60
C (s) 78.10
B (s) 34.58
A (s) 21.40
f1 (ppm)


Ph
CN
NH2
Me

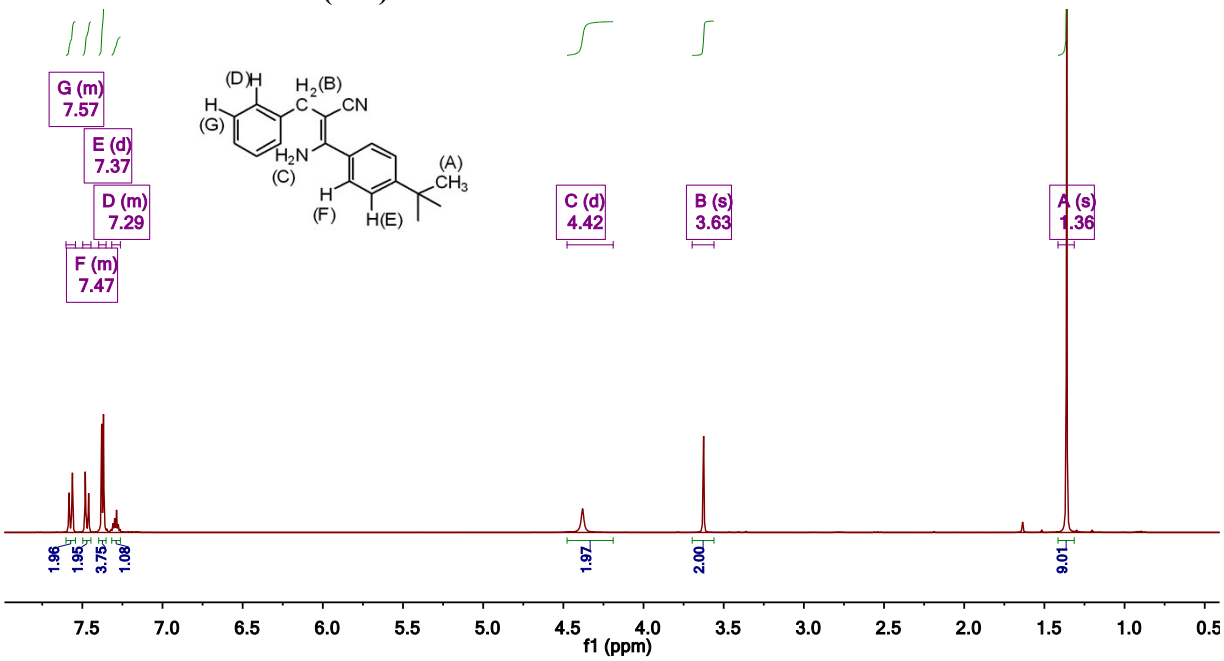
(4ab)

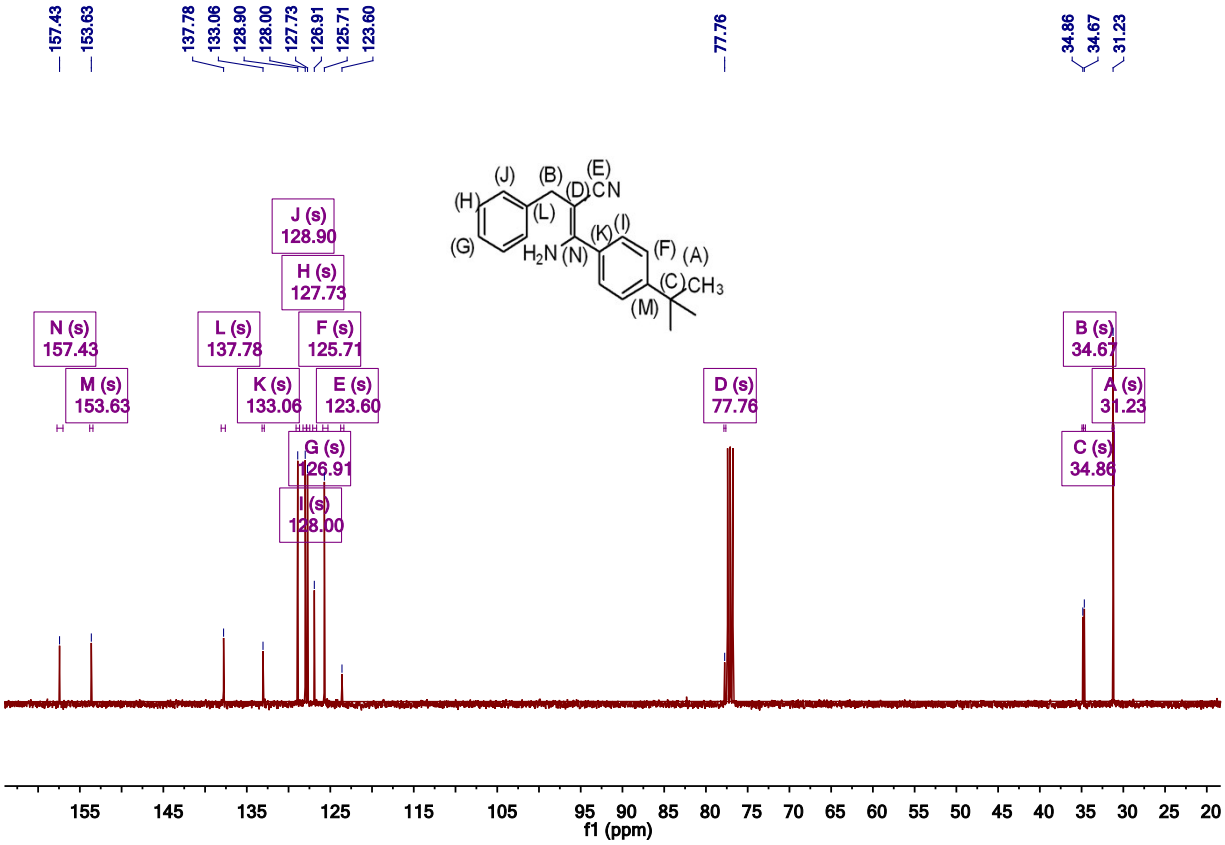

E (t) 7.37
D (ddd) 7.29
F (d) 7.52
C (s) 4.37
B (s) 3.62
A (s) 2.41
1.96
3.82
3.31
1.90
2.00
2.95
f1 (ppm)

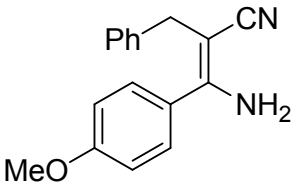

157.49
140.57
137.76
133.14
129.43
128.91
128.01
127.88
126.92
123.51
77.93
34.61
21.42
G (s) 128.91
J (s) 137.76
E (s) 126.92
L (s) 157.49
I (s) 133.14
D (s) 123.51
C (s) 77.93
B (s) 34.61
A (s) 21.42
K (s) 140.57
F (d) 127.94
H (s) 129.43
f1 (ppm)


Ph
CN
NH2

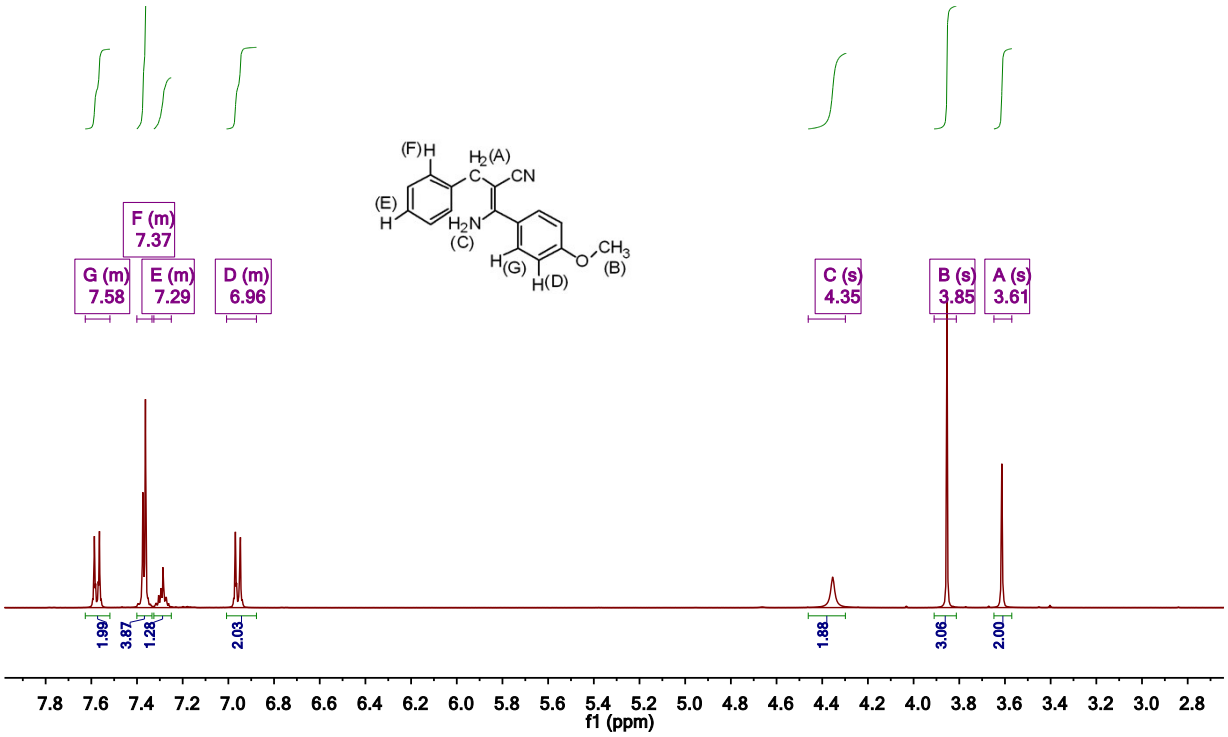
(4ac)

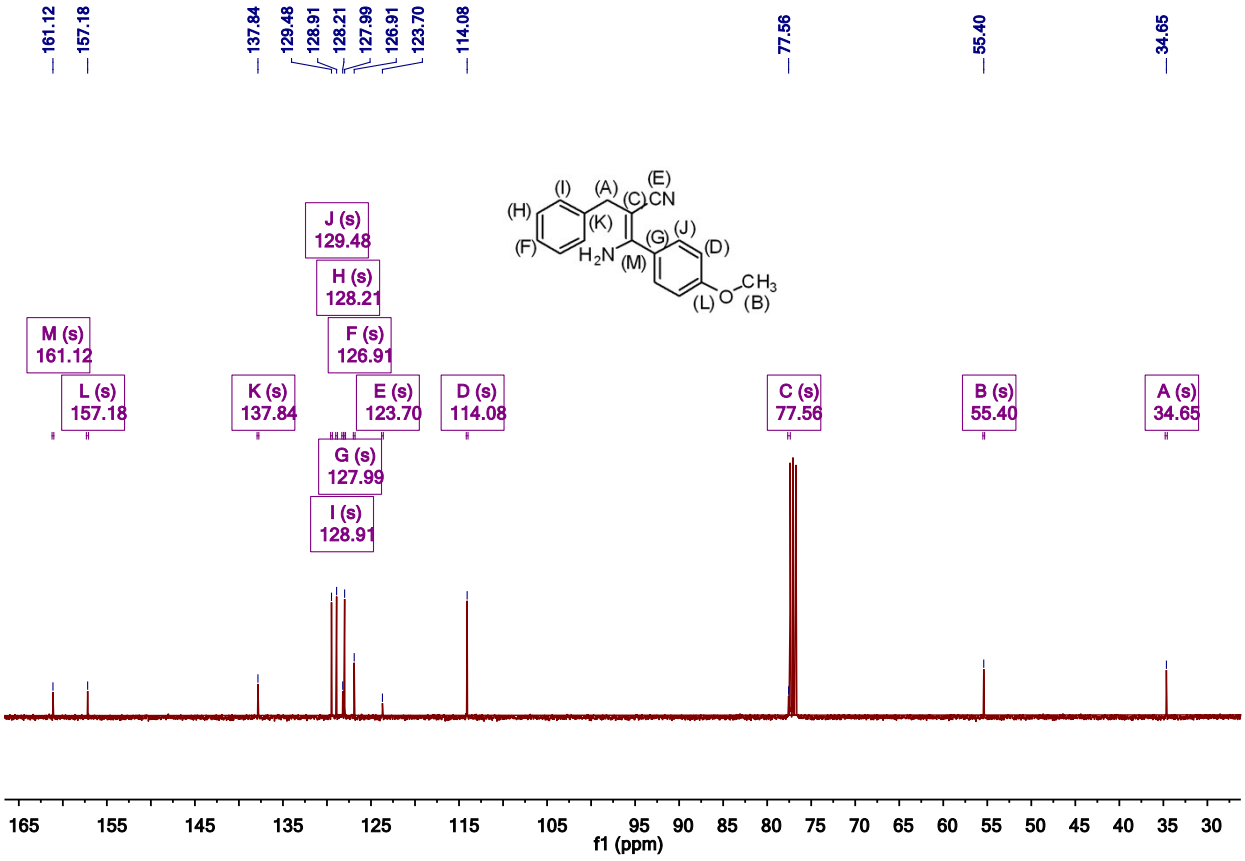

G (m) 7.57
E (d) 7.37
D (m) 7.29
F (m) 7.47
C (d) 4.42
B (s) 3.63
A (s) 1.36
1.96
1.95
3.75
1.08
1.97
2.00
9.01
f1 (ppm)

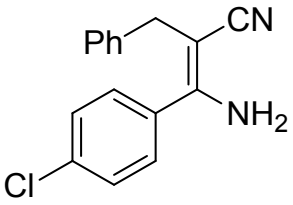

157.43
153.63
137.78
133.06
128.90
128.00
127.73
126.91
125.71
123.60
77.76
34.86
34.67
31.23
J (s) 128.90
H (s) 127.73
N (s) 157.43
L (s) 137.78
F (s) 125.71
M (s) 153.63
K (s) 133.06
E (s) 123.60
G (s) 126.91
I (s) 128.00
D (s) 77.76
B (s) 34.67
A (s) 31.23
C (s) 34.86
f1 (ppm)


Ph
CN
NH2
MeO

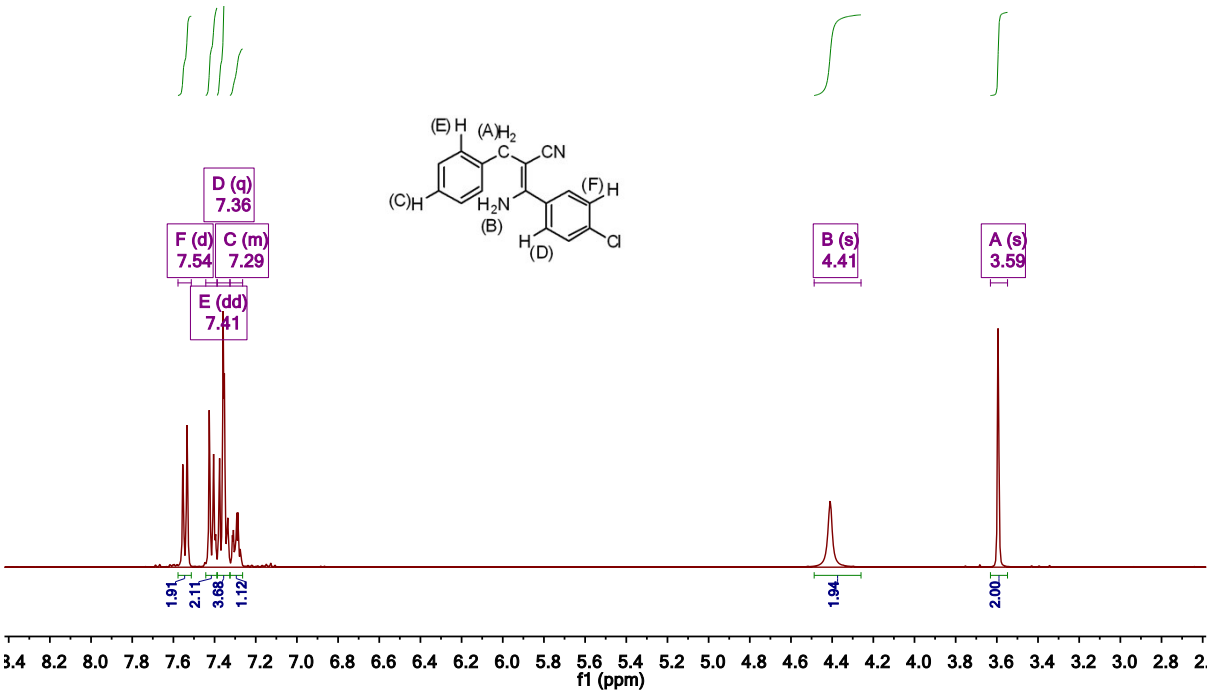
(4ad)

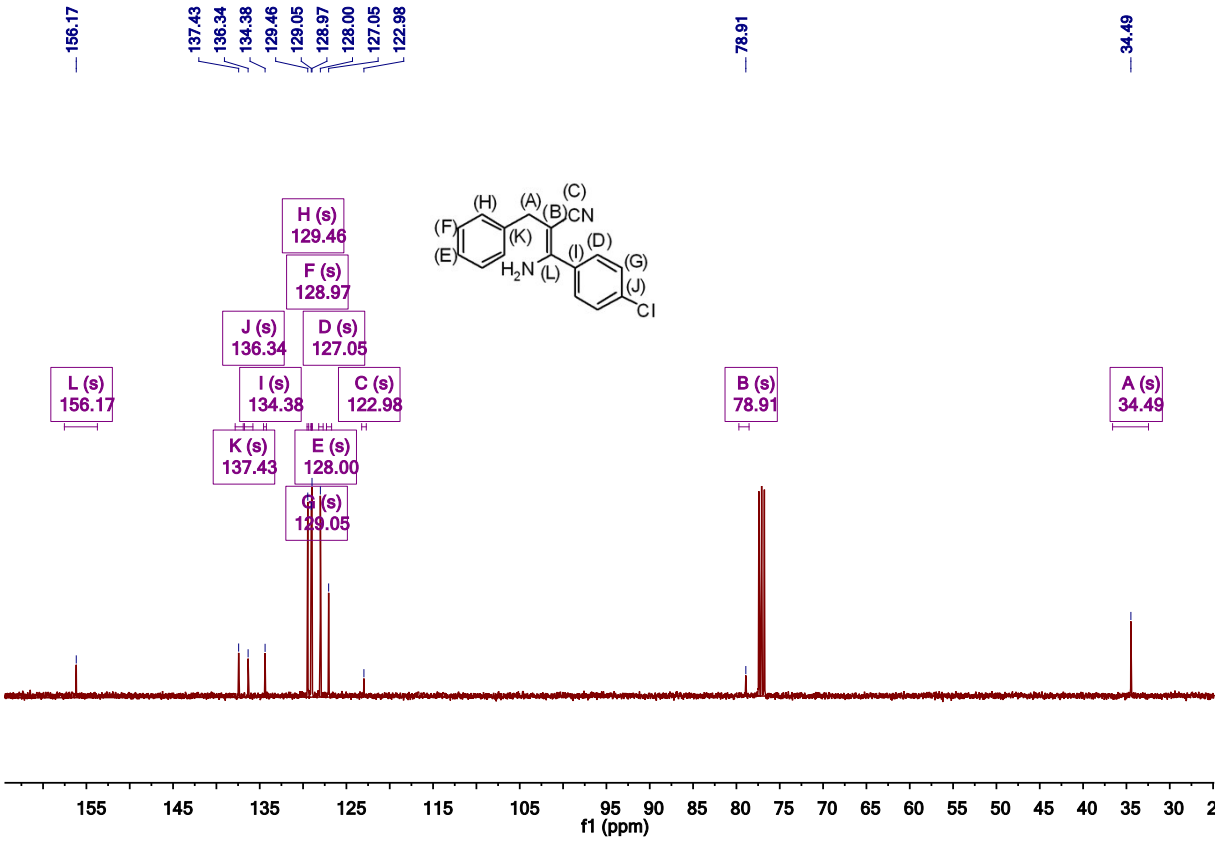

F (m) 7.37
G (m) 7.58
E (m) 7.29
D (m) 6.96
C (s) 4.35
B (s) 3.85
A (s) 3.61
1.99
3.87
1.28
2.03
1.88
3.06
2.00
f1 (ppm)

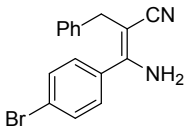

161.12
157.18
137.84
129.48
128.91
128.21
127.99
126.91
123.70
114.08
77.56
55.40
34.65
J (s) 129.48
H (s) 128.21
F (s) 126.91
M (s) 161.12
L (s) 157.18
K (s) 137.84
E (s) 123.70
D (s) 114.08
C (s) 77.56
B (s) 55.40
A (s) 34.65
G (s) 127.99
I (s) 128.91
f1 (ppm)


Ph
CN
NH2
Cl

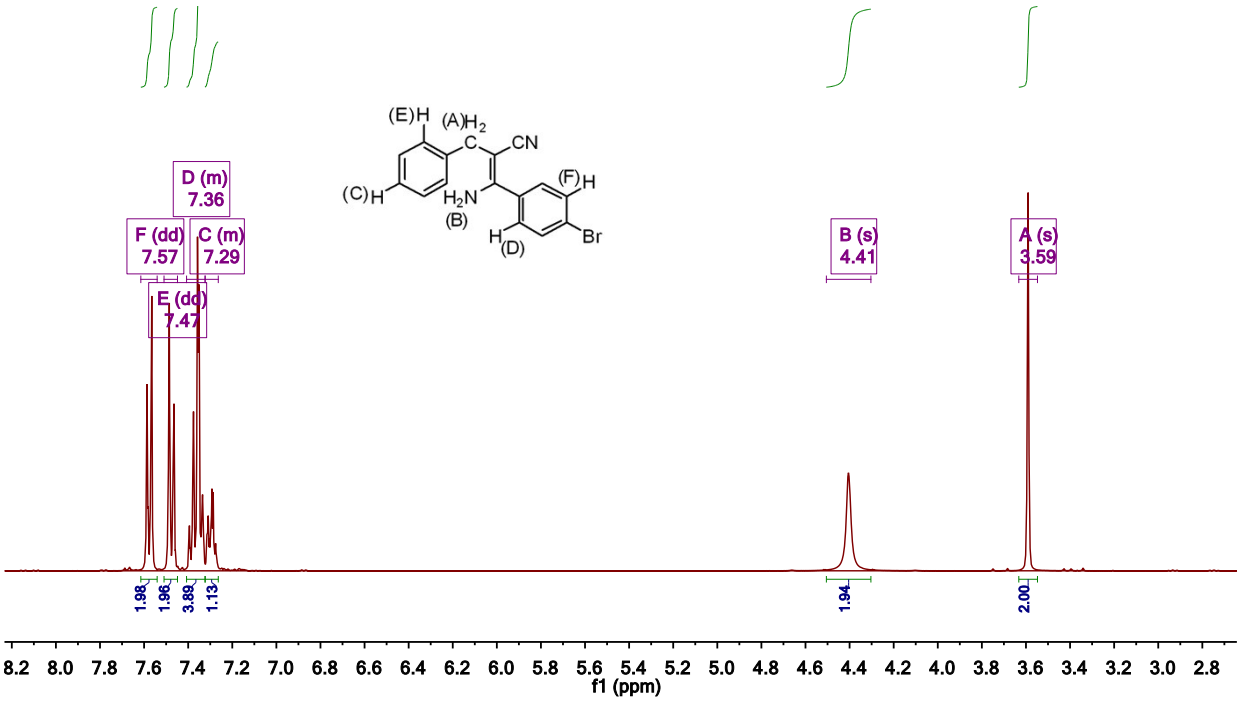
(4ae)

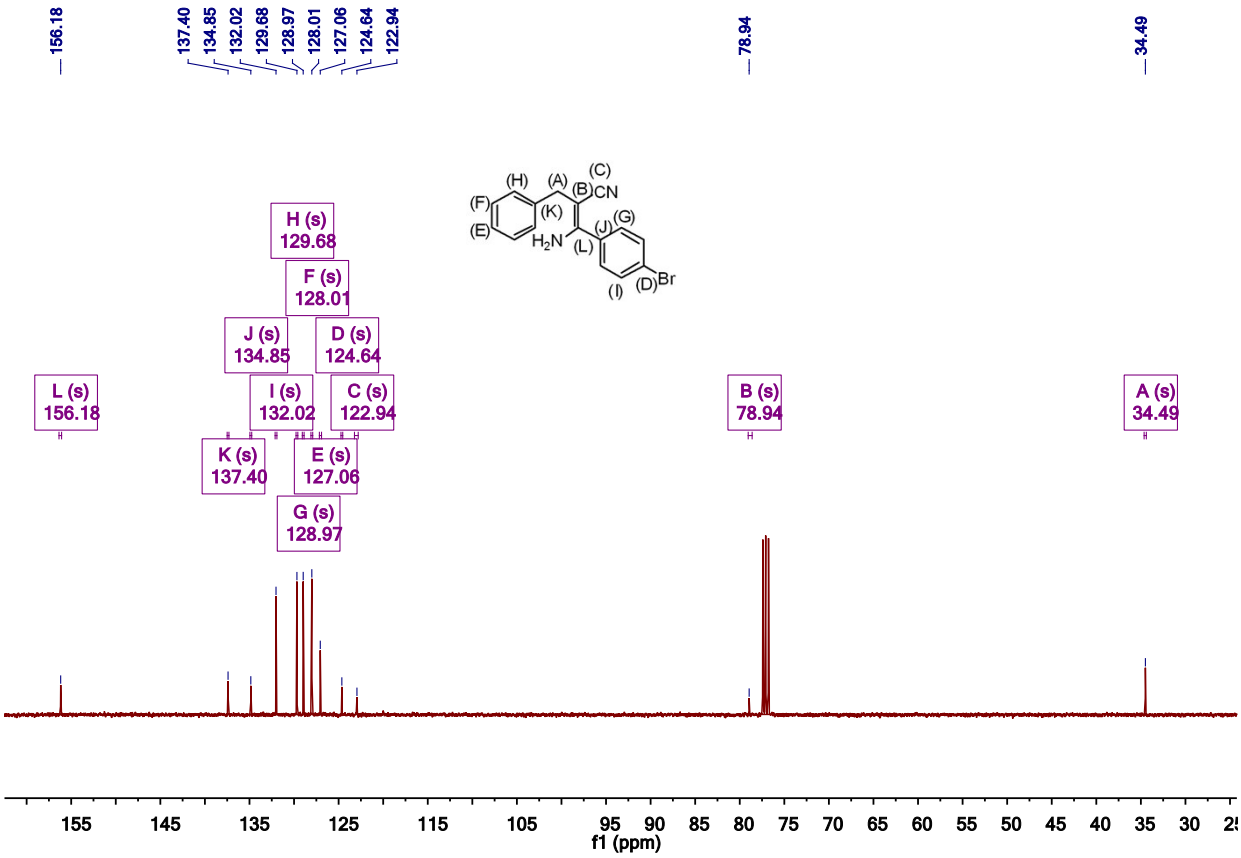

D (q) 7.36
F (d) 7.54
C (m) 7.29
E (dd) 7.41
B (s) 4.41
A (s) 3.59
1.91
2.11
3.68
1.12
1.94
2.00
f1 (ppm)

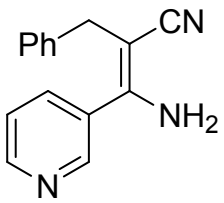

156.17
137.43
136.34
134.38
129.46
129.05
128.97
128.00
127.05
122.98
78.91
34.49
H (s) 129.46
F (s) 128.97
J (s) 136.34
D (s) 127.05
L (s) 156.17
I (s) 134.38
C (s) 122.98
K (s) 137.43
E (s) 128.00
G (s) 129.05
B (s) 78.91
A (s) 34.49
f1 (ppm)


Ph
CN
NH2
Br

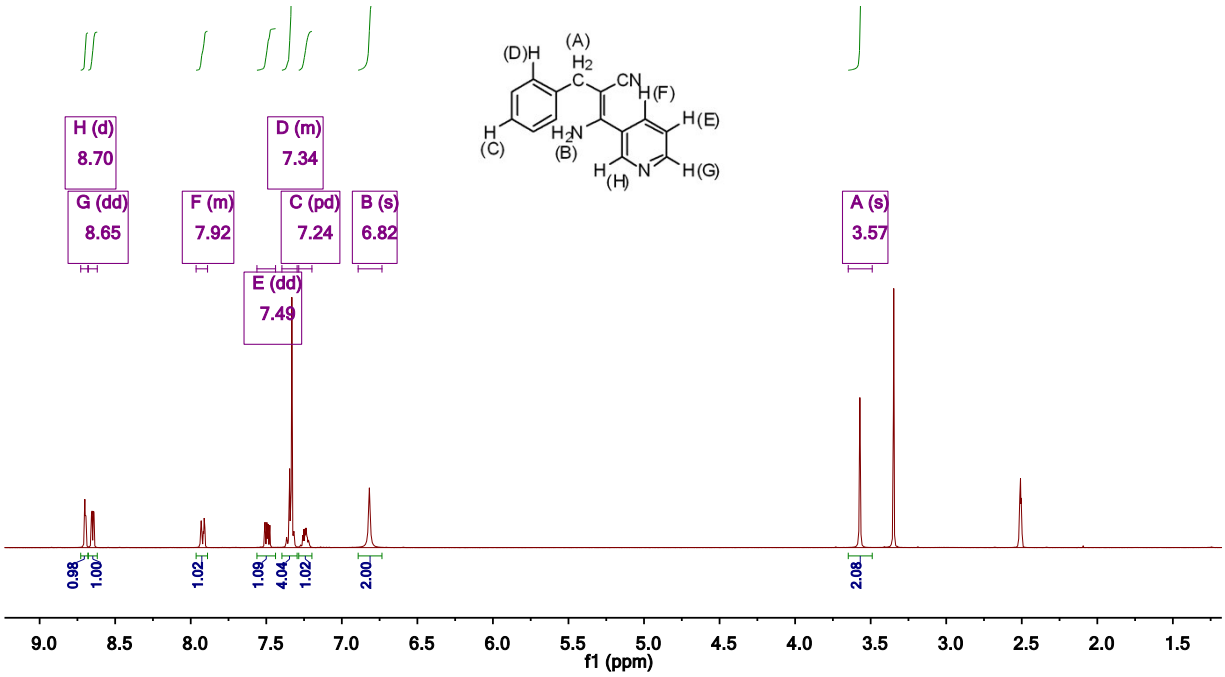
(4af)

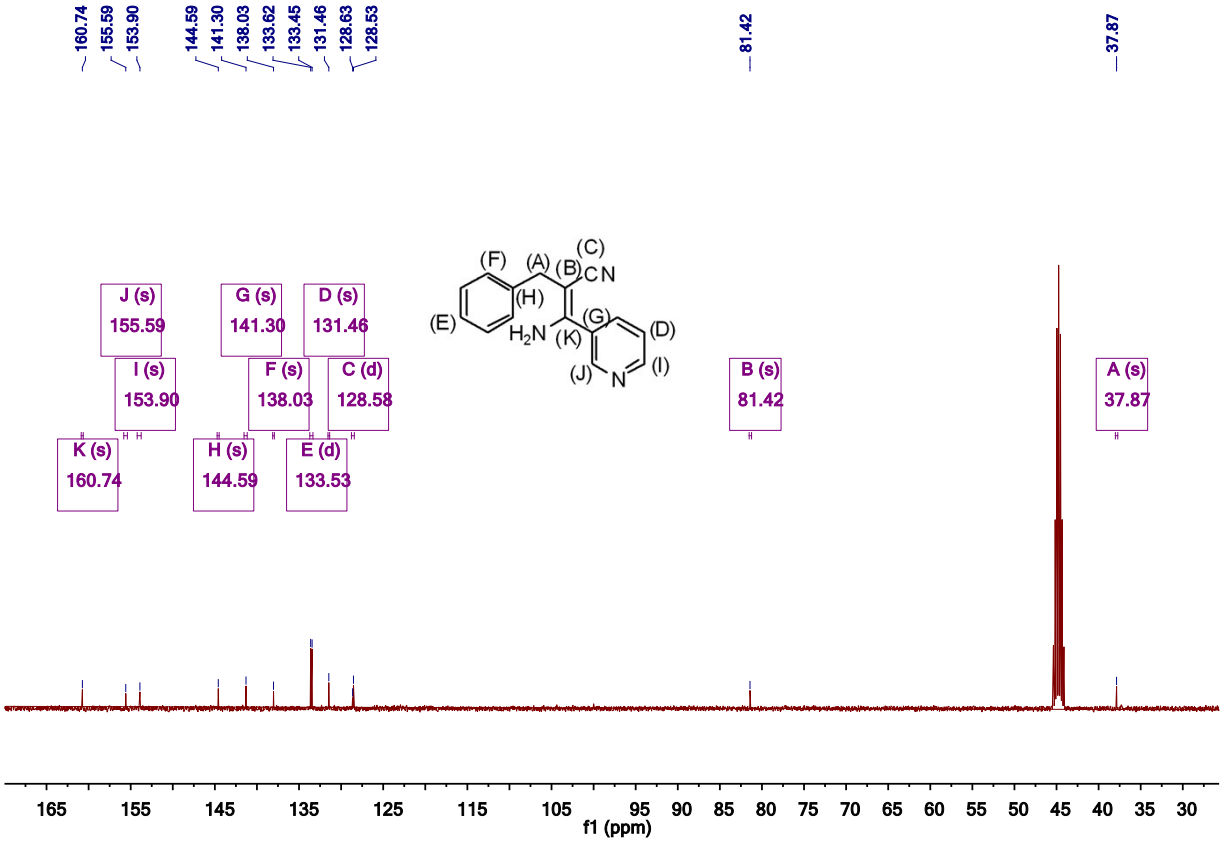

D (m)
7.36
F (dd)
7.57
C (m)
7.29
E (dd)
7.47
B (s)
4.41
A (s)
3.59
1.98
1.96
3.88
1.13
1.94
2.00
f1 (ppm)


156.18
137.40
134.85
132.02
129.68
128.97
128.01
127.06
124.64
122.94
78.94
34.49
H (s)
129.68
F (s)
128.01
J (s)
134.85
D (s)
124.64
L (s)
156.18
I (s)
132.02
C (s)
122.94
B (s)
78.94
A (s)
34.49
K (s)
137.40
E (s)
127.06
G (s)
128.97
f1 (ppm)


Ph
CN
NH2
N

(4ag)


H (d) 8.70
G (dd) 8.65
F (m) 7.92
D (m) 7.34
C (pd) 7.24
E (dd) 7.49
B (s) 6.82
A (s) 3.57
0.98
1.00
1.02
1.09
4.04
1.02
2.00
2.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
f1 (ppm)


160.74
155.59
153.90
144.59
141.30
138.03
133.62
133.45
131.46
128.63
128.53
81.42
37.87
J (s) 155.59
I (s) 153.90
K (s) 160.74
G (s) 141.30
F (s) 138.03
H (s) 144.59
D (s) 131.46
C (d) 128.58
E (d) 133.53
B (s) 81.42
A (s) 37.87
165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)