Supporting information for

Addition of Allyl Grignard to Nitriles Under Air and Room Temperature. Experimental and Computational Mechanistic Insights in pH-Switchable Synthesis

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1.- General Methods and Materials

All reagents were obtained from commercial suppliers and used without further purification. Allylmagnesium bromide (1M in diethyl ether) was purchased from Sigma Aldrich and its concentration was established by titration with *L*-menthol.[1]

Infrared spectra were recorded on a Bruker Tensor 27 spectrometer, using an ATR accessory.

NMR spectra were recorded on a Bruker Avance Neo 400 spectrometer operating at 400.13 MHz for ^{1}H, 100.62 MHz for ^{13}C and 376 MHz for ^{19}F. All ^{13}C and ^{19}F spectra were proton decoupled. ^{1}H and ^{13}C NMR spectra were referenced against the appropriate solvent signal. ^{19}F NMR spectra were referenced against $CFCl_3$. Characterisation details, including ^{1}H, ^{19}F and $^{13}C\{^{1}H\}$ NMR spectra, for compounds **2a-j**, **3a,d,e,f**, **4a** and **5a-c,g,i,j** are included in the following sections of this Supporting Information.

HRMS were measured in ESI mode, with a TOF mass analyser (Bruker model Impact II).

2.- Experimental procedure and characterisation details

2.1.- General procedure for the synthesis of tetrahydropyridines 2a-j, in the presence of air and without additional solvent added

Syntheses were performed under air and at room temperature. A glass tube was charged with the appropriate nitrile (**1a-j**, 0.5 mmol) and allylmagnesium bromide (0.5 mmol) was added with a vigorous stirring. After 5 seconds of stirring, the reaction was quenched with 2 mL of a saturated solution of NH_4Cl and then heated to 100 ºC for 20 minutes. After reaching room temperature, 5 mL of distillated water were added, and the mixture was extracted with 2-MeTHF (3 x 5 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and the solvent was concentrated in vacuo. Yields of the reaction crudes were determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard (0.5 mmol). All reactions were done in triplicate to ensure good reproducibility of obtained yields. Separation and purification of every compound were carried out using TLC glass plate silica (employing hexane:ethyl acetate mixtures). Isolated yields: **2a**, 94%, 67.1 mg; **2b**, 92%, 71.3 mg; **2c**, 93%, 80 mg; **2d**, 60%, 45.8 mg; **2e**, 89%, 88.4 mg; **2f**, 84%, 72.3 mg; **2g**, 86%, 61.1 mg; **2h**, 95%, 82.6 mg; **2i**, 93%, 69.9 mg; **2j**, 61%, 31.9 mg.

2.2.- Procedure for the synthesis of enamines *Z/E*-3a,d,e,f in the presence of air and without additional solvent added.

Synthesis was performed under air and at room temperature. A glass tube was charged with the desired nitrile (**3a,d,e,f**, 0.5 mmol) and allylmagnesium bromide (0.5 mmol) was added with a vigorous stirring. After 3 seconds of stirring, the reaction was quenched with 2 mL of a commercial solution of NH_3. After addition of NaCl, the reaction was extracted with 2-MeTHF (3 x 5 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and the solvent was concentrated in vacuo to obtain mixtures of *Z/E*-**3a,d,e,f**. The yields of these mixtures were determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard (0.5 mmol). The reaction was done in triplicate to ensure good reproducibility of obtained yield.

2.3.- Procedure for the synthesis of 4a, in the presence of air and without additional solvent added.

Synthesis was performed under air and at room temperature. A glass tube was charged with the benzonitrile (**1a**, 0.5 mmol) and allylmagnesium bromide (1 mmol) was added with a vigorous stirring. After 5 seconds of stirring, the reaction was quenched with 2 mL of a saturated solution of NH_4Cl and then 5 mL of distillated water were added, and the reaction was extracted with 2-MeTHF (3 x 5 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and the solvent was concentrated in vacuo. A 97% yield in the reaction crude was determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard (0.5 mmol). The reaction was done in triplicate to ensure good reproducibility of obtained yield. Separation and purification of **4a** were carried out using TLC glass plate silica (employing hexane:ethyl acetate mixtures). Isolated yield: 93%, 84.5 mg.

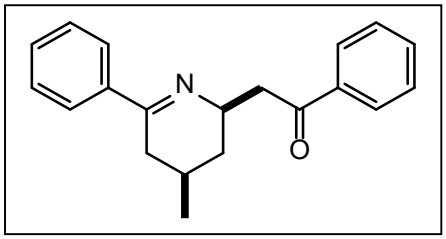
2.4.- Procedure for the synthesis of 5a-c,g,i,j, in the presence of air and without additional solvent added

Syntheses were performed under air and at room temperature. A glass tube was charged with the desired nitrile (**1a-c,g,i,j**, 0.5 mmol) and allylmagnesium bromide (0.5 mmol) was added with a vigorous stirring. After 5 seconds of stirring, the reaction was quenched with 2 mL of a saturated solution of NH_3 and then heated to 100 °C for 20 minutes. After reaching room temperature, 5 mL of distilled water and NaCl were added,

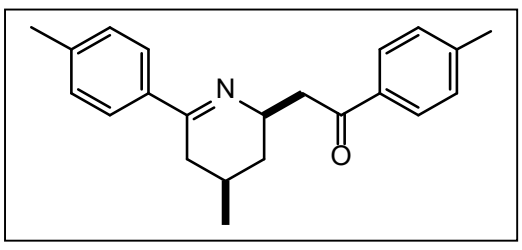
and the reaction was extracted with 2-MeTHF (3 x 5 mL). The combined organic phases were dried over anhydrous $MgSO_4$ and the solvent was concentrated in vacuo. Yields were determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard (0.5 mmol). The reaction was done in triplicate to ensure good reproducibility of obtained yield. Isolated yields: **5a**, 99%, 80 mg; **5b**, 96%, 81.7 mg; **5c**, 98%, 92.8 mg; **5g**, 86%, 65.5 mg; **5i**, 99%, 82.9 mg; **5j**, 59%, 29.8 mg.

2.5.- Procedure for the synthesis of intermediated I.

Synthesis was performed under inert atmosphere and at room temperature inside de glovebox. A glass tube was charged with allylmagnesium bromide (0.5 mmol), and the solvent was removed under vacuum. Then, the white solid was dissolved in deuterated THF and transferred into a young NMR tube, and the benzonitrile (**1a**, 0.5 mmol) was added.

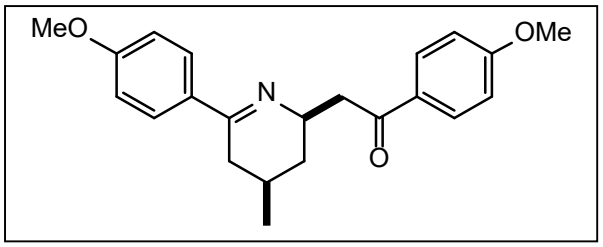


2-((2R,4R)-4-methyl-6-phenyl-2,3,4,5-tetrahydropyridin-2-yl)-1-phenylethanone (2a): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.91 (q, 1H, *J* = 11.9 Hz), 1.06 (d, 3H, *J* = 6.4 Hz), 1.91-2.11 (m, 3H), 2.80-2.88 (m, 1H), 3.08 (dd, 1H, *J* = 16.0, 8.4 Hz), 3.62 (dd, 1H, *J* = 16.0, 5.5 Hz), 4.25 (bs, 1H), 7.34-7.37 (m, 3Harom), 7.45-7.50 (m, 2Harom), 7.54-7.59 (m, 1Harom), 7.75-7.78 (m, 2Harom), 8.03-8.06 (m, 2Harom). ^{13}C{^{1}H} NMR ($CDCl_3$) δ (ppm) = 22.4, 26.7, 35.8, 36.9, 42.3, 57.5, 126.3, 128.3, 128.5, 128.7, 129.8, 133.0, 137.7, 139.9, 165.4, 199.9. FT-IR (cm^{-1}) = 2925, 2358, 1718, 1684, 1599, 1560, 1491, 1450, 1420, 1373, 1316, 1266, 1215, 1181, 1103, 1073, 1027, 1003. HRMS: m/z 292.16 ($M + H^+$).

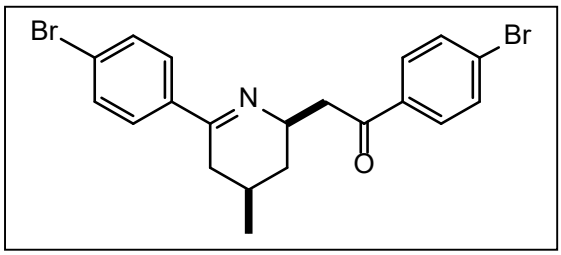


2-((2R,4R)-4-methyl-6-(p-tolyl)-2,3,4,5-tetrahydropyridin-2-yl)-1-(p-tolyl)ethanone (2b): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.88 (q, 1H, *J* = 11.9 Hz), 1.04 (d, 3H, *J* = 6.3 Hz), 1.90-2.08 (m, 3H), 2.35 (s, 3H), 2.42 (s, 3H), 2.78-2.86 (m, 1H), 3.03 (dd, 1H, *J* = 15.9, 8.6 Hz), 3.59 (dd, 1H, *J* = 15.9, 5.3 Hz), 4.21 (bs, 1H), 7.15 (d, 2Harom, *J* = 8.0 Hz), 7.26 (d, 2Harom, *J* = 8.0 Hz), 7.66 (d, 2Harom, *J* = 8.0 Hz), 7.94 (d, 2Harom, *J* = 8.0 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$) δ (ppm) = 21.4, 21.8, 22.4, 26.7, 35.8, 36.9, 47.2, 57.4, 126.3, 128.6, 129.0, 129.3, 135.3, 137.2,

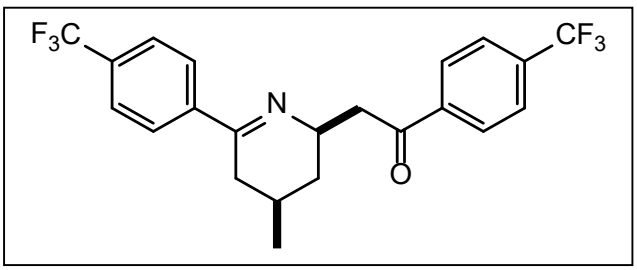
139.8, 143.8, 165.3, 199.5. FT-IR (cm^{-1}) = 2923, 2360, 1718, 1684, 1608, 1576, 1543, 1458, 1409, 1375, 1267, 12125, 1208, 1181, 1111, 1038, 1003. HRMS: m/z 320.20 ($M + H^+$).



1-(4-methoxyphenyl)-2-((2R,4R)-6-(4-methoxyphenyl)-4-methyl-2,3,4,5-tetrahydropyridin-2-yl)ethanone (2c): ^1H NMR ($CDCl_3$) δ (ppm) = 0.87 (q, 1H, *J* = 11.9 Hz), 1.04 (d, 3H, *J* = 6.5 Hz), 1.86-2.05 (m, 3H), 2.78-2.84 (m, 1H), 3.00 (dd, 1H, *J* = 15.6, 8.5 Hz), 3.59 (dd, 1H, *J* = 15.6, 5.4 Hz), 3.82 (s, 3H), 3.87 (s, 3H), 4.19 (bs, 1H), 6.86 (d, 2Harom, *J* = 8.9 Hz), 6.94 (d, 2Harom, *J* = 8.9 Hz), 7.74 (d, 2Harom, *J* = 8.9 Hz), 8.03 (d, 2Harom, *J* = 8.9 Hz). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 22.4, 26.8, 35.6, 37.0, 47.1, 55.4, 55.6, 57.5, 113.5, 113.8, 127.8, 130.8, 130.9, 132.6, 160.9, 163.5, 164.4, 198.4. FT-IR (cm^{-1}) = 2924, 2839, 2365, 2034, 1671, 1598, 1575, 1509, 1457, 1418, 1370, 1308, 1251, 1160, 1111, 1029. HRMS: m/z 352.19 ($M + H^+$).

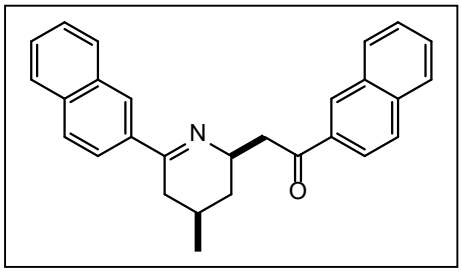


1-(4-bromophenyl)-2-((2R,4R)-6-(4-bromophenyl)-4-methyl-2,3,4,5-tetrahydropyridin-2-yl)ethanone (2d): ^1H NMR ($CDCl_3$) δ (ppm) = 0.90 (q, 1H, *J* = 11.9 Hz), 1.05 (d, 3H, *J* = 6.5 Hz), 1.86-2.03 (m, 3H), 2.74-2.79 (m, 1H), 3.02 (dd, 1H, *J* = 15.8, 7.7 Hz), 3.48 (dd, 1H, *J* = 15.8, 6.1 Hz), 4.19 (bs, 1H), 7.45 (d, 2Harom, *J* = 8.6 Hz), 7.58-7.61 (m, 4Harom), 7.87 (d, 2Harom, *J* = 8.6 Hz). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 22.3, 26.6, 35.4, 36.7, 46.8, 57.6, 124.2, 127.9, 128.2, 130.0, 131.3, 131.9, 136.4, 138.4, 164.2, 198.7. FT-IR (cm^{-1}) = 2921, 2852, 2232, 1919, 1684, 1635, 1586, 1485, 1458, 1397, 1372, 1320, 1266, 1204, 1178, 1071, 1010. HRMS: m/z 447.99 ($M + H^+$).

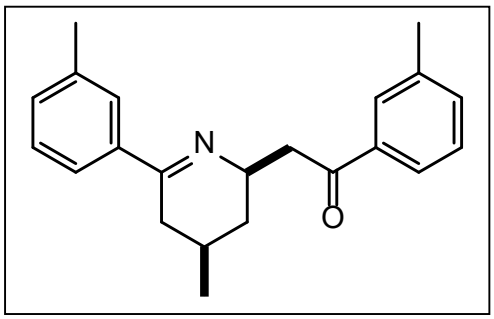


2-((2R,4R)-4-methyl-6-(4-(trifluoromethyl)phenyl)-2,3,4,5-tetrahydropyridin-2-yl)-1-(4-(trifluoromethyl)phenyl)ethanone (2e): ^1H NMR ($CDCl_3$) δ (ppm) =

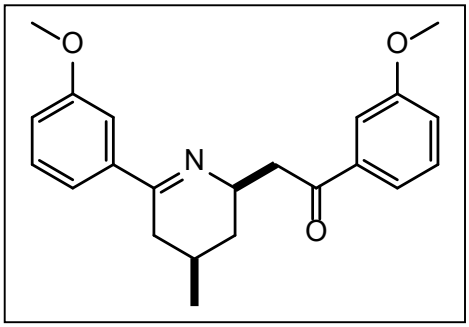
0.93-1.00 (m, 1H), 1.09 (d, 3H, *J* = 6.5 Hz), 1.25-1.28 (m, 1H), 2.03-2.11 (m, 2H), 2.80-2.85 (m, 1H), 3.12 (dd, 1H, *J* = 15.9, 7.5 Hz), 3.56 (dd, 1H, *J* = 15.9, 6.3 Hz), 4.27 (bs, 1H), 7.58 (d, 2Harom. *J* = 8.2 Hz), 7.74 (d, 2Harom. *J* = 8.2 Hz), 7.82 (d, 2Harom. *J* = 8.2 Hz), 8.12 (d, 2Harom. *J* = 8.1 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) =22.3, 26.7, 35.7, 36.7, 47.1, 57.8, 125.3, 125.8, 126.6, 128.8, 131.5, 131.7, 134.4, 134.6, 140.0, 142.7, 164.5, 198.9. ^{19}F NMR ($CDCl_3$) δ (ppm) = -63.1, -62.7. FT-IR (cm^{-1}) = 2960, 2853, 1688, 1410, 1322, 1262, 1164, 1121, 1109, 1064, 1015, 831, 773, 704. HRMS: m/z 428.14 ($M + H^+$).



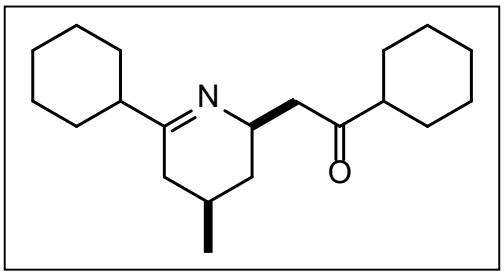
2-((2R,4R)-4-methyl-6-(naphthalen-2-yl)-2,3,4,5-tetrahydropyridin-2-yl)-1-(naphthalen-2-yl)ethanone (2f): ^{1}H NMR ($CDCl_3$) δ (ppm) = 1.02 (q, 1H, *J* = 11.7 Hz), 1.12 (d, 3H, *J* = 6.5 Hz), 1.98, (bs, 1H), 2.10-2.23 (m, 2H), 2.98-3.03 (m, 1H), 3.25 (dd, 1H, *J* = 15.6, 8.2 Hz), 3.80 (dd, 1H, *J* = 15.6, 5.8 Hz), 4.38 (bs, 1H), 7.47-7.63 (m, 4Harom), 7.75-8.16 (m, 9Harom), 8.63 (s, 1Harom. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 22.4, 26.8, 35.7, 37.0, 47.3, 58.0, 124.0, 124.3, 126.1, 126.2, 126.7, 126.8, 127.7, 127.9, 128.5, 128.8, 129.8, 130.4, 132.7, 133.1, 134.2, 134.3, 135.1, 135.7, 137.1 (2C), 165.1, 199.9. FT-IR (cm^{-1}) = 2939, 2921, 2866, 2226, 1671, 1624, 1596, 1541, 1506, 1468, 1361, 1318, 1274, 1208, 1182, 1123, 1100, 1043, 1013. HRMS: m/z 392.20 ($M + H^+$).



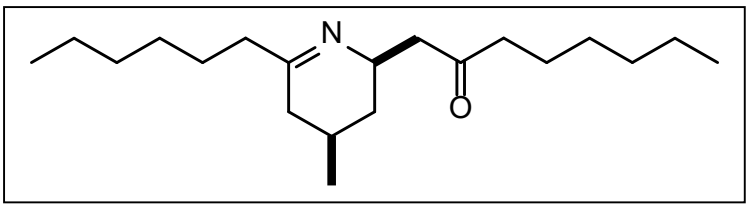
2-((2R,4R)-4-methyl-6-(*m*-tolyl)-2,3,4,5-tetrahydropyridin-2-yl)-1-(*m*-tolyl)ethanone (2g): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.90 (m, 1H), 1.06 (d, 3H, *J* = 6.5 Hz), 2.03-2.07 (m, 3H), 2.37 (s, 3H), 2.43 (s, 3H), 2.83-2.87 (m, 1H), 3.08 (dd, 1H, *J* = 15.9, 8.6 Hz), 3.64 (dd, 1H, *J* = 15.9, 5.2 Hz), 4.24 (bs, 1H), 7.19-7.21 (m, 1Harom), 7.25-7.28 (m, 1Harom), 7.36-7.40 (m, 2Harom), 7.55-7.60 (m, 2Harom), 7.85-7.88 (m, 2Harom). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 21.5, 22.4, 26.7, 29.9, 35.9, 36.9, 47.4, 57.6, 123.5, 125.6, 125.7, 127.0, 128.2, 128.5, 129.1, 130.5, 133.8, 137.8, 137.9, 138.4, 165.7, 200.1. FT-IR (cm^{-1}) = 2924, 2854, 1680, 1603, 1585, 1456, 1364, 1271, 1184, 1081, 968, 893, 785, 747, 690. HRMS: m/z 320.20 ($M + H^+$).



1-(3-methoxyphenyl)-2-((2R,4R)-6-(3-methoxyphenyl)-4-methyl-2,3,4,5-tetrahydropyridin-2-yl)ethanone (2h): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.86-0.93 (m, 1H), 1.04 (d, 3H, *J* = 6.5 Hz), 1.25-1.28 (m, 1H), 2.00-2.04 (m, 2H), 2.78-2.83 (m, 2H), 3.04 (dd, 1H, *J* = 15.8, 8.3 Hz), 3.58 (dd, 1H, *J* = 15.8, 5.7 Hz), 3.76 (s, 3H), 3.84 (s. 3H), 4.23 (bs, 1H), 6.90-6.92 (m, 1Harom), 7.09-7.11 (m, 1Harom), 7.23-7.25 (m, 1Harom), 7.30-7.32 (m, 1Harom), 7.34-7.38 (m, 2Harom), 7.55-7.56 (m, 1Harom), 7.61-7.63 (m, 1Harom). ^{13}C{^{1}H} NMR ($CDCl_3$) δ (ppm) = 22.4, 26.8, 35.9, 36.9, 47.3, 55.4, 55.6, 57.8, 111.2, 112.6, 116.0, 118.9, 119.6, 121.2, 129.3, 129.6, 139.2, 141.3, 159.7, 160.0, 165.2, 199.8. FT-IR (cm^{-1}) = 2927, 2855, 1682, 1583, 1487, 1455, 1431, 1259, 1040, 877, 785, 759, 687. HRMS: m/z 352.19 ($M + H^+$).

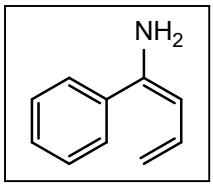


1-cyclohexyl-2-(6-cyclohexyl-4-methyl-2,3,4,5-tetrahydropyridin-2-yl)ethanone (2i): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.57-0.64 (m, 1H), 0.88 (d, 3H, *J* = 6.5 Hz), 1.15-1.33 (m, 11H), 1.50-1.54 (m, 1H), 1.62-1.83 (m, 11H), 1.99-2.03 (m, 1H), 2.18-2.23 (m, 1H), 2.34-2.39 (m, 1H), 2.45 (dd, 1H, *J* = 15.9, 8.6 Hz), 2.84 (dd, 1H, *J* = 15.9, 5.2 Hz), 3.75 (bs, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$) δ (ppm) = 22.2, 25.7, 25.8, 26.0, 26.2, 26.3 (2C), 26.4, 28.3, 28.4, 30.3, 30.6, 35.6, 37.1, 48.9, 49.2, 51.6, 56.3, 174.4, 213.7. FT-IR (cm^{-1}) = 2926, 2853, 1703, 1449, 1373, 1144, 1000, 950, 893. HRMS: m/z 304.26 ($M + H^+$).

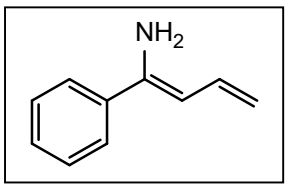


1-(6-hexyl-4-methyl-2,3,4,5-tetrahydropyridin-2-yl)octan-2-one (2j): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.66-0.73 (m, 1H), 0.88 (t, 6H, *J* = 6.9 Hz), 0.92 (d, 3H, *J* = 6.4 Hz), 1.15-1.20 (m, 1H), 1.24-1.31 (m, 12H), 1.54-1.60 (m, 4H), 1.80-1.83 (m, 1H), 2.12-2.16 (m, 2H), 2.22-2.26 (m, 1H), 2.38-2.50 (m, 4H), 2.83 (dd, 1H, J = 15.8, 5.5 Hz), 3.78 (bs, 1H). ^{13}C{^{1}H} NMR ($CDCl_3$) δ (ppm) = 14.0, 14.1, 22.1, 22.6, 22.7, 23.5, 26.4, 26.5, 29.8, 31.5, 31.6, 31.8, 36.8, 37.9, 40.7, 44.1,

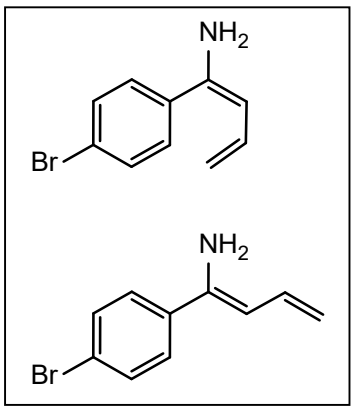
50.8, 56.2, 171.9, 210.9. FT-IR (cm^{-1}) = 2955, 2928, 2871, 1711, 1652, 1458, 1375, 728. HRMS: m/z 308.29 ($M + H^+$).



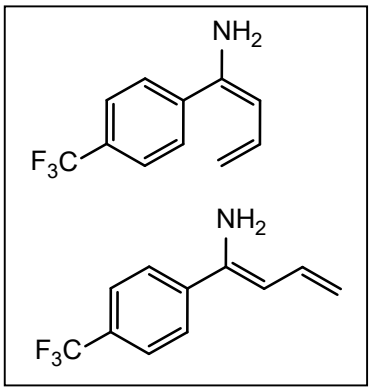
(*E*)-1-phenylbuta-1,3-dien-1-amine (*E*-3a): ^{1}H NMR ($CDCl_3$) δ (ppm) =3.76 (bs, 2H), 4.94 (ddd, 1H, *J* = 10.3, 1.9, 0.8 Hz), 5.14 (ddd, 1H, *J* = 16.6, 1.9, 0.8 Hz), 5.47 (d, 1H, *J* = 11.2 Hz), 6.56 (ddd, 1H, *J* = 16.6, 11.2, 10.3 Hz), 7.32-7.35 (m, 3Harom), 7.53-7.55 (m, 2Harom) . $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 102.9, 112.1, 125.8, 128.4, 128.5, 128.6, 131.2, 139.4, 142.7.



(*Z*)-1-phenylbuta-1,3-dien-1-amine (*Z*-3a): ^{1}H NMR ($CDCl_3$) δ (ppm) =3.51 (bs, 2H), 4.63 (ddd, 1H, *J* = 10.2, 2.2, 0.8 Hz), 5.14 (ddd, 1H, *J* = 16.7, 2.2, 0.8 Hz), 5.54 (d, 1H, *J* = 11.0 Hz), 6.33 (ddd, 1H, *J* = 16.7, 11.0, 10.2 Hz), 7.29-7.46 (m, 5Harom). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 104.1, 108.9, 126.4, 128.3, 128.4, 128.9, 138.5, 141.1.

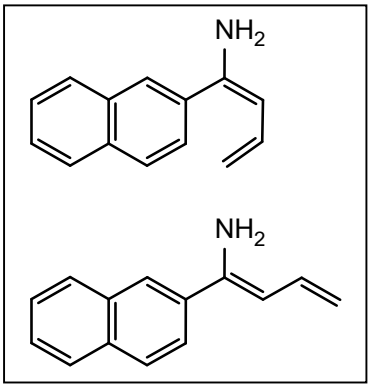


(*E*)-1-(4-bromophenyl)buta-1,3-dien-1-amine (*E*-3d); (*Z*)-1-(4-bromophenyl)buta-1,3-dien-1-amine (*Z*-3d): ^{1}H NMR ($CDCl_3$) δ (ppm) major isomer (*E*) = 3.63 (bs, 2H), 4.87-4.89 (ddd, 1H, *J* = 10.3, 1.9, 0.8 Hz), 5.05-5.09 (ddd, 1H, *J* = 16.6, 1.9, 0.8 Hz), 5.35 (d, 1H, *J* = 11.2 Hz), 6.40-6.48 (m, 1H), 7.30-7.32 (m, 2H), 7.36-7.38 (m, 2H). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) mix of isomers (*E* and Z) = 103.4, 112.7, 119.1, 127.7, 127.8, 127.9, 128.2, 129.9, 131.2, 131.3, 131.5, 131.6, 131.9, 133.5. FT-IR (cm^{-1}) = 3067, 2923, 1912, 1681, 1633, 1584, 1484, 1395, 1205, 1176, 1070, 1007, 909, 816, 731. HRMS: m/z 224.01 ($M + H^+$).

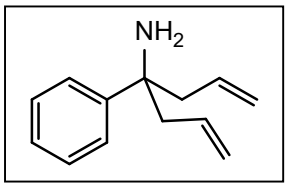


(*E*)-1-(4-(trifluoromethyl)phenyl)buta-1,3-dien-1-amine (*E*-3e); (*Z*)-1-(4-(trifluoromethyl)phenyl)buta-1,3-dien-1-amine (*Z*-3e): ^{1}H NMR ($CDCl_3$) δ (ppm) major isomer (*E*) = 3.67 (bs, 2H), 4.91-4.94 (ddd, 1H, *J* = 10.3, 1.8, 0.8 Hz), 5.09-5.13 (ddd, 1H, *J* = 16.6, 1.8, 0.8 Hz), 5.43 (d, 1H, *J* = 11.2 Hz), 6.43-6.50 (m, 1H), 7.49-7.51 (m, 2H), 7.54-7.59 (m, 2H). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) mix of isomers (*E* and Z) = 119.4, 125.2, 125.2,

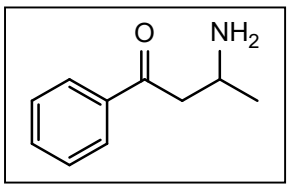
125.3, 125.3, 125.4, 125.7, 125.8, 126.5, 126.6, 128.8, 133.3, 140.4, 142.7, 164.5, 198.9. ^{19}F NMR ($CDCl_3$) δ (ppm) mix of isomers (*E* and Z) = -62.6 (*E*), -62.9 (*Z*). FT-IR (cm^{-1}) = 2928, 1687, 1409, 1321, 1163, 1119, 1065, 1015, 834. HRMS: m/z 214.08 ($M + H^+$).



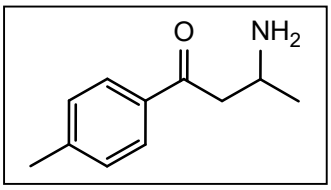
(*E*)-1-(naphthalen-2-yl)buta-1,3-dien-1-amine (*E*-3f); (*Z*)-1-(naphthalen-2-yl)buta-1,3-dien-1-amine (*Z*-3f): ^1H NMR ($CDCl_3$) δ (ppm) major isomer (*E*)= 3.68 (bs, 2H), 4.81-4.83 (ddd, 1H, *J* = 10.3, 1.9, 0.8 Hz), 5.02-5.06 (ddd, 1H, *J* = 16.6, 1.9, 0.8 Hz), 5.47 (d, 1H, *J* = 11.2 Hz), 6.40-6.48 (m, 1H), 7.26-7.29 (m, 2H), 7.46-7.48 (dd, 1H, *J* = 8.6, 1.9 Hz), 7.58-7.63 (m, 3H), 7.79 (m, 1H). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm)) mix of isomers (*E* and Z) = 109.4, 118.8, 119.3, 124.0, 124.2, 124.4, 125.7, 126.0, 126.2, 126.7, 126.8, 127.5, 127.6, 127.7, 127.8, 128.2, 128.4, 128.5, 128.8, 129.7, 130.3, 132.6, 133.9, 135.1, 135.6. FT-IR (cm^{-1}) = 3296, 3057, 2923, 2226, 1924, 1675, 1626, 1597, 1504, 1468, 1370, 1275, 1184, 1124, 907, 858, 818, 745, 730. HRMS: m/z 196.11 ($M + H^+$).



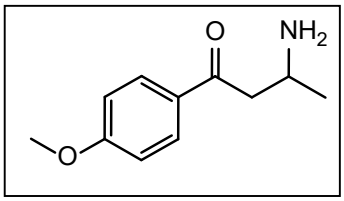
4-phenylhepta-1,6-dien-4-amine (4a): ^1H NMR ($CDCl_3$) δ (ppm) = 1.56 (bs, 2H), 2.42 (dd, 2H, *J* = 13.6, 8.5 Hz), 2.65 (dd, 2H, *J* = 13.6, 6.1), 5.02-5.10 (m. 4H), 5.47-5.57 (m, 2H), 7.20-7.24 (m, 1Harom), 7.32-7.36 (m, 2Harom), 7.42-7.44 (m, 2Harom). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 48.2, 57.0, 118.7, 125.9, 126.3, 128.2, 134.0, 146.8. FT-IR (cm^{-1}) = 3370, 3075, 3025, 2977, 2910, 1664, 1638, 1600, 1494, 1445, 1415, 1260, 1075, 1001. HRMS: m/z 188.14 ($M + H^+$).



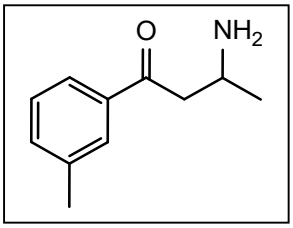
4-phenylhepta-1,6-dien-4-amine (5a): ^1H NMR ($CDCl_3$) δ (ppm) = 1.18 (d, 3H, *J* = 6.4 Hz), 1.76 (bs, 1H), 2.95-3.07 (m, 2H), 3.58-3.62 (m, 1H), 7.44-7.47 (m, 2Harom), 7.54-7.56 (m, 1Harom), 7.94-7.96 (m, 2Harom). $^{13}C\{^1H\}$ NMR ($CDCl_3$) δ (ppm) = 23.9, 43.5, 48.3, 128.1, 128.7, 133.3, 137.2, 199.83. FT-IR (cm^{-1}) = 3445, 3061, 2965, 2925, 2336, 2228, 2683, 1597, 1558, 1491, 1447, 1359, 1266, 1214, 1181, 1154, 1068, 1025, 1003. HRMS: m/z 164.10 ($M + H^+$).



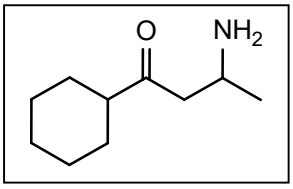
3-amino-1-(*p*-tolyl)butan-1-one (5b): ^{1}H NMR ($CDCl_3$) δ (ppm) = 1.09 (d, 3H, *J* = 6.4 Hz), 1.50 (bs, 2H), 2.32 (s, 3H), 2.83-2.96 (m, 2H), 3.48-3.52 (m, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 21.7, 23.9, 43.6, 48.2, 128.3 (2C), 128.9, 129.4 (2C), 129.9, 199.4. FT-IR (cm^{-1}) = 3425, 2922, 2227, 1679, 1645, 1605, 1571, 1509, 1373, 1225, 1204, 1181, 915, 813, 721. HRMS: m/z 178.12 ($M + H^+$).



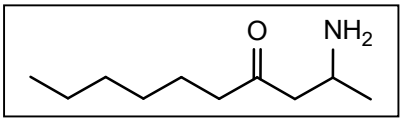
3-amino-1-(4-methoxyphenyl)butan-1-one (5c): ^{1}H NMR ($CDCl_3$) δ (ppm) = 1.06 (d, 3H, *J* = 6.5 Hz), 1.45 (bs, 2H), 2.77-2.90 (m, 2H), 3.44-3.48 (m, 1H), 3.73 (s, 3H), 6.81 (d, 2H, *J* = 8.9 Hz), 7.82 (d, 2H, *J* = 9.0 Hz). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 23.7, 43.4, 47.8, 55.3, 113.6 (2C), 127,4. 130.2 (2C), 163.4, 198.0. FT-IR (cm^{-1}) = 3413, 2961, 2838, 2048, 1672, 1598, 1509, 1458, 1418, 1358, 1305, 1251, 1170, 1076, 1028, 830. HRMS: m/z 194.11 ($M + H^+$).



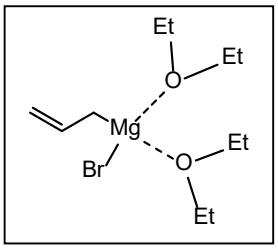
3-amino-1-(*m*-tolyl)butan-1-one (5g): ^{1}H NMR ($CDCl_3$) δ (ppm) = 1.18 (d, 3H, *J* = 6.4 Hz), 1.60 (bs, 2H), 2.41 (s, 3H), 2.93-3.06 (m, 2H), 3.56-3.61 (m, 1H), 7.35 (s, 1H), 7.74-7.77 (m, 3H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 21.5, 29.9, 43.6, 48.4, 125.4, 128.6, 128.7, 134.1, 137.3, 138.6, 200.1. FT-IR (cm^{-1}) = 3446, 2959, 2923, 2854, 1680, 1650, 1602, 1584, 1454, 1374, 1285, 1244, 1163, 1081, 891, 785, 704. HRMS: m/z 178.12 ($M + H^+$).



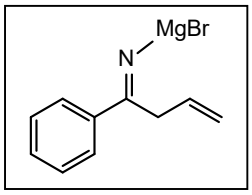
3-amino-1-cyclohexylbutan-1-one (5i): ^{1}H NMR ($CDCl_3$) δ (ppm) = 1.05 (d, 3H, *J* = 6.4 Hz), 1.23-1.28 (m, 6H), 1.45 (bs, 2H), 1.63-1.66 (m, 1H), 1.74-1.83 (m, 4H), 2.39-2.52 (m, 2H), 3.35-3.42 (m, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) =23.8, 25.8 (2C), 25.9, 28.4, 28.5, 43.0, 50.2, 51.3, 214.0. FT-IR (cm^{-1}) = 2927, 2853, 1703, 1448, 1373, 1145, 1003, 893. HRMS: m/z 170.15 ($M + H^+$).



2-aminodecan-4-one (5j): ^{1}H NMR ($CDCl_3$) δ (ppm) = 0.86-0.90 (m, 6H), 1.04-1.05 (m, 2H), 1.25-1.32 (m, 8H), 1.52-1.57 (m, 2H), 2.35-2.39 (m, 2H), 3.14-3.22 (m, 1H). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) δ (ppm) = 14.1, 14.2, 20.5, 21.6, 22.6, 23.5, 26.7, 29.8, 31.5, 210.9. FT-IR (cm^{-1}) = 3276, 2956, 2929, 2859, 1696, 1458, 1376, 1157, 1055, 728. HRMS: m/z 171.18 ($M + H^+$).



Allylmagnesium bormide bisetherate: ^{1}H NMR (THF-d_8) δ (ppm) = 1.10 (t, 12H, *J* = 7.0 Hz), 2.36 (d, 4H, *J* = 11.3Hz), 3.37 (q, 8H, *J* = 7.0 Hz), 6.25 (p, 1H, *J* = 11.3Hz). ^{13}C{^{1}H} NMR (THF-d_8) δ (ppm) = 26.4, 57.3, 68.4, 149.7.



Magnesium (1-phenylbut-3-en-1-ylidene)amide bromide (I): ^{1}H NMR (THF-d_8) δ (ppm) = 3.58 (d, 2H, J = 7.2 Hz), 4.95-4.98 (m, 1H), 5.88-5.96 (m, 1H), 7.28-7.34 (m, 3Harom), 7.73-7.75 (m, 2Harom).^{13}C{^{1}H} NMR (THF-d_8) δ (ppm) = 50.1, 117.4, 127.5, 129.0, 130.2, 133.0, 173.6.

3.- ^{1}H and $^{13}C\{^{1}H\}$ spectra

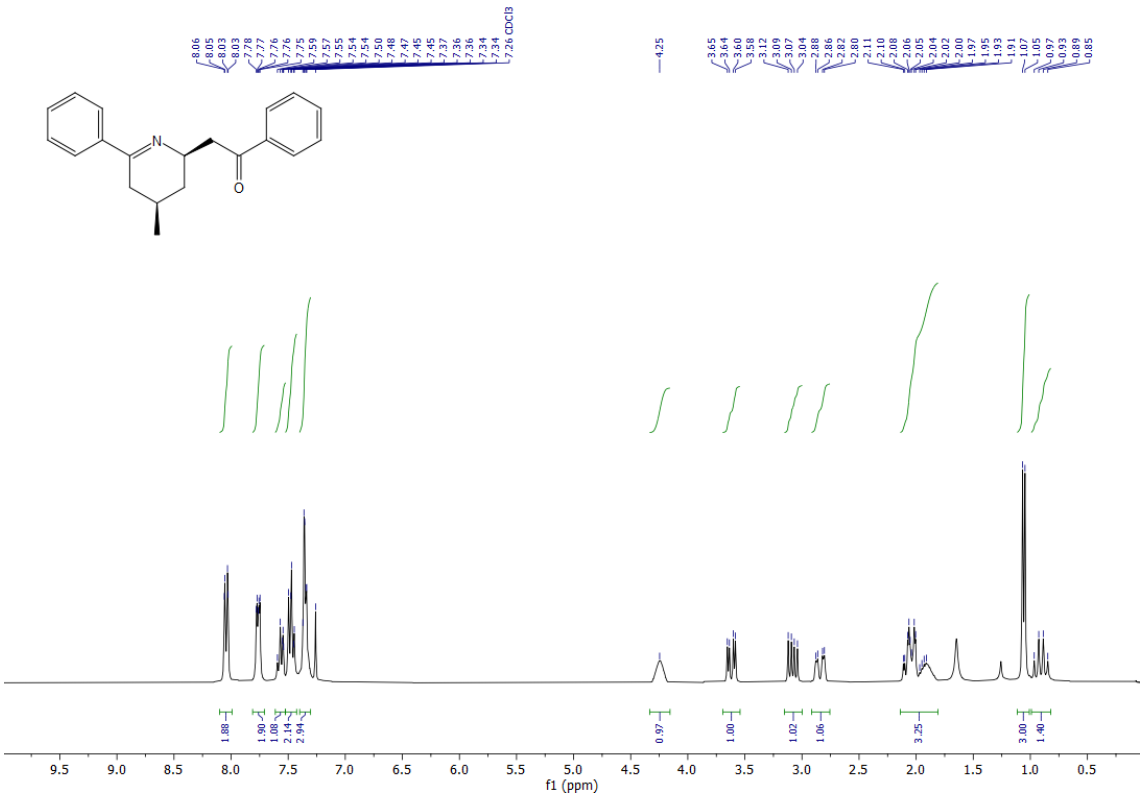


Figure 1. ^{1}H-NMR full chart for **2a** in $CDCl_3$.

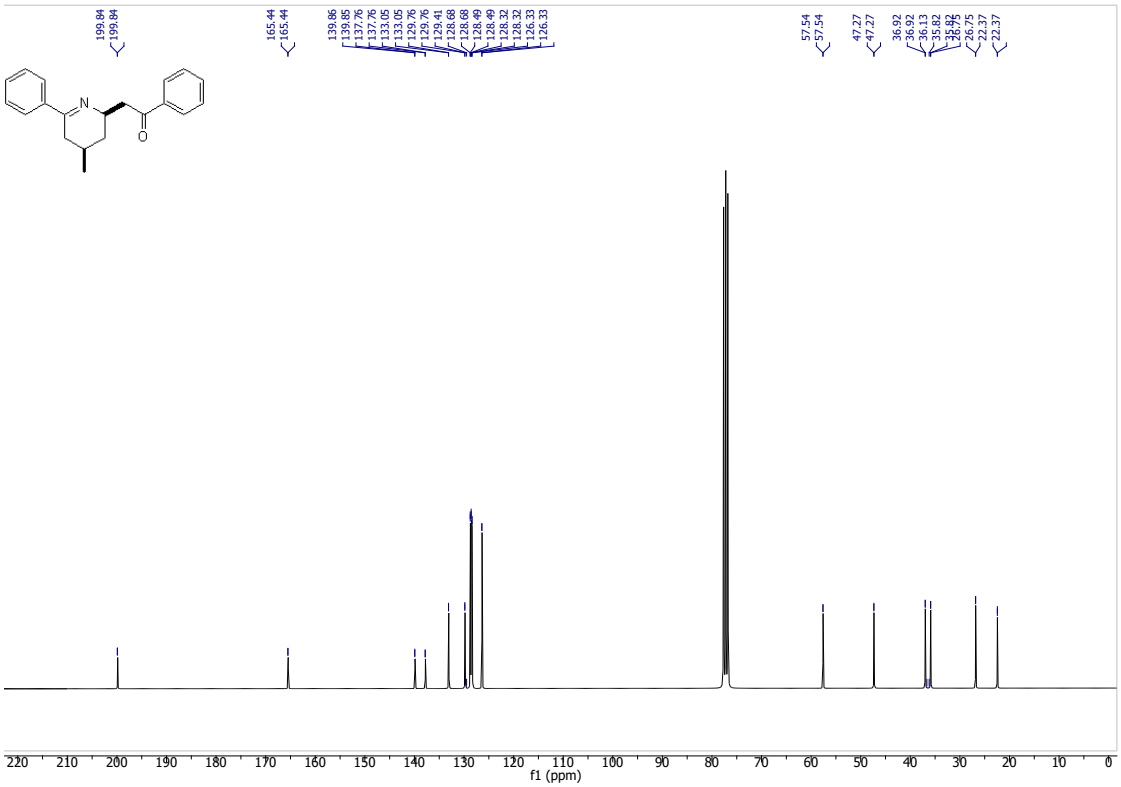


Figure 2. ^{13}C-NMR full chart for **2a** in $CDCl_3$.

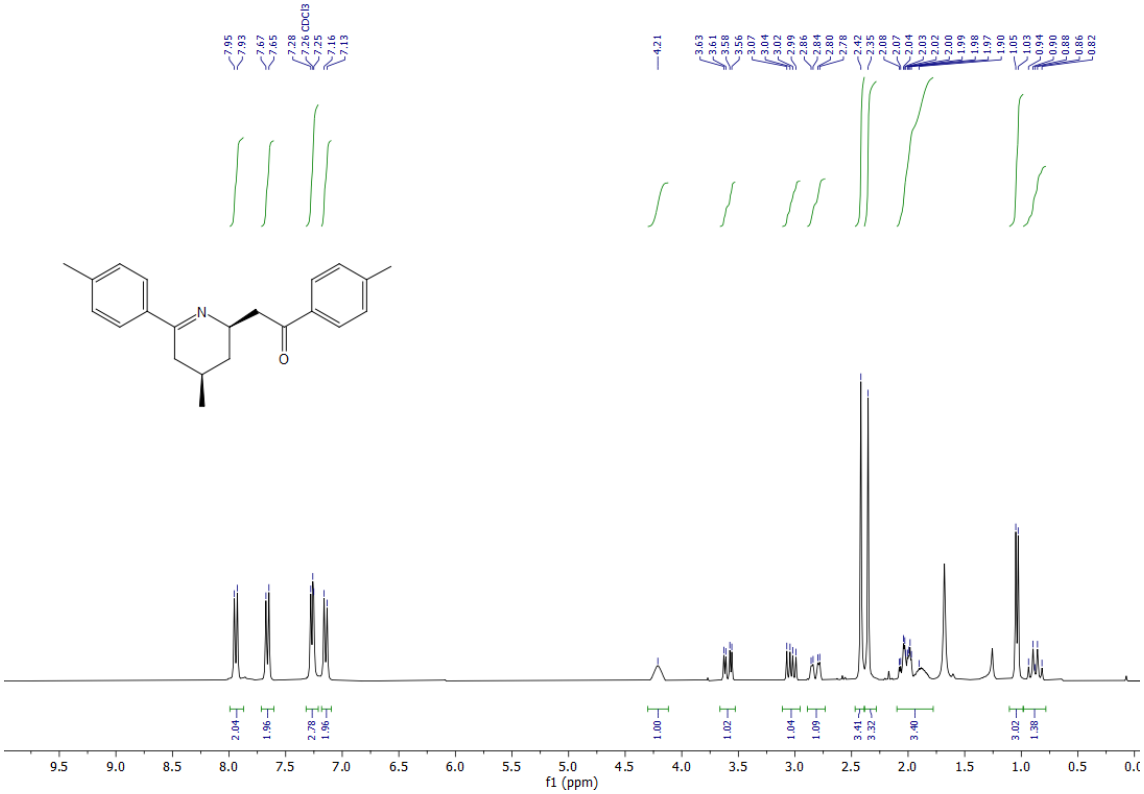


Figure 3. ^{1}H-NMR full chart for **2b** in $CDCl_3$.

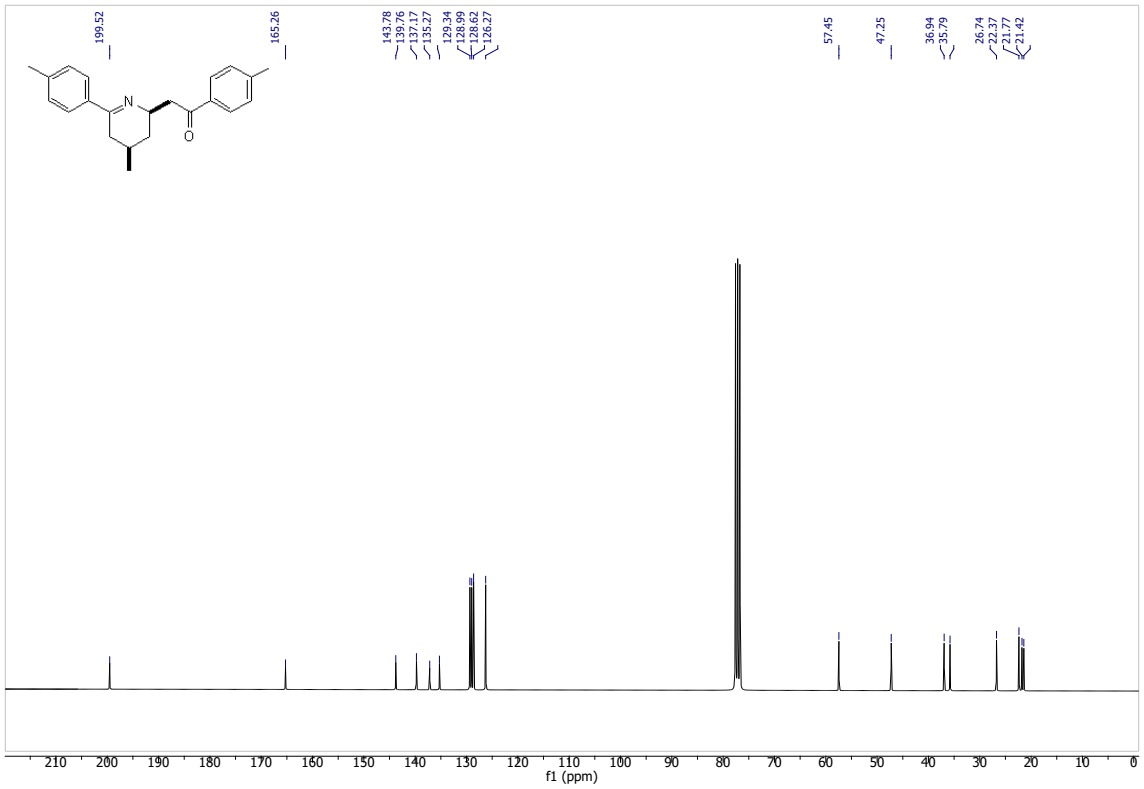


Figure 4. ^{13}C-NMR full chart for **2b** in $CDCl_3$.

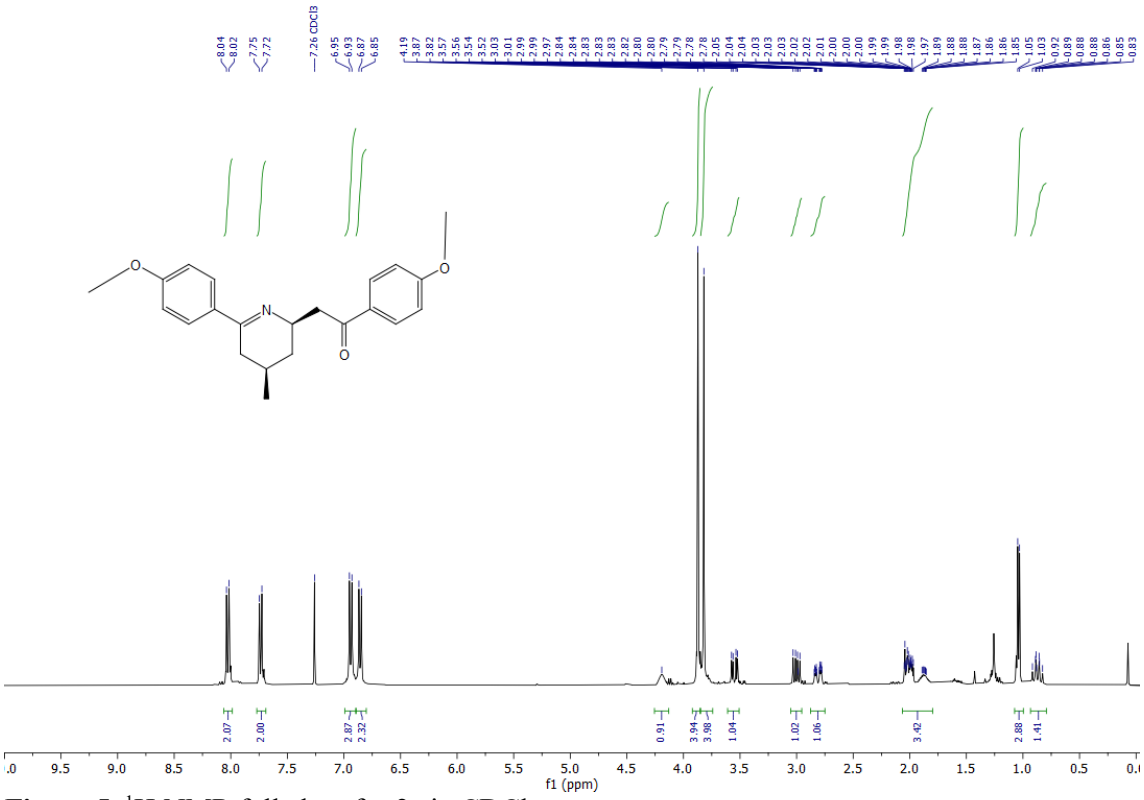


Figure 5. ^{1}H-NMR full chart for **2c** in $CDCl_3$.

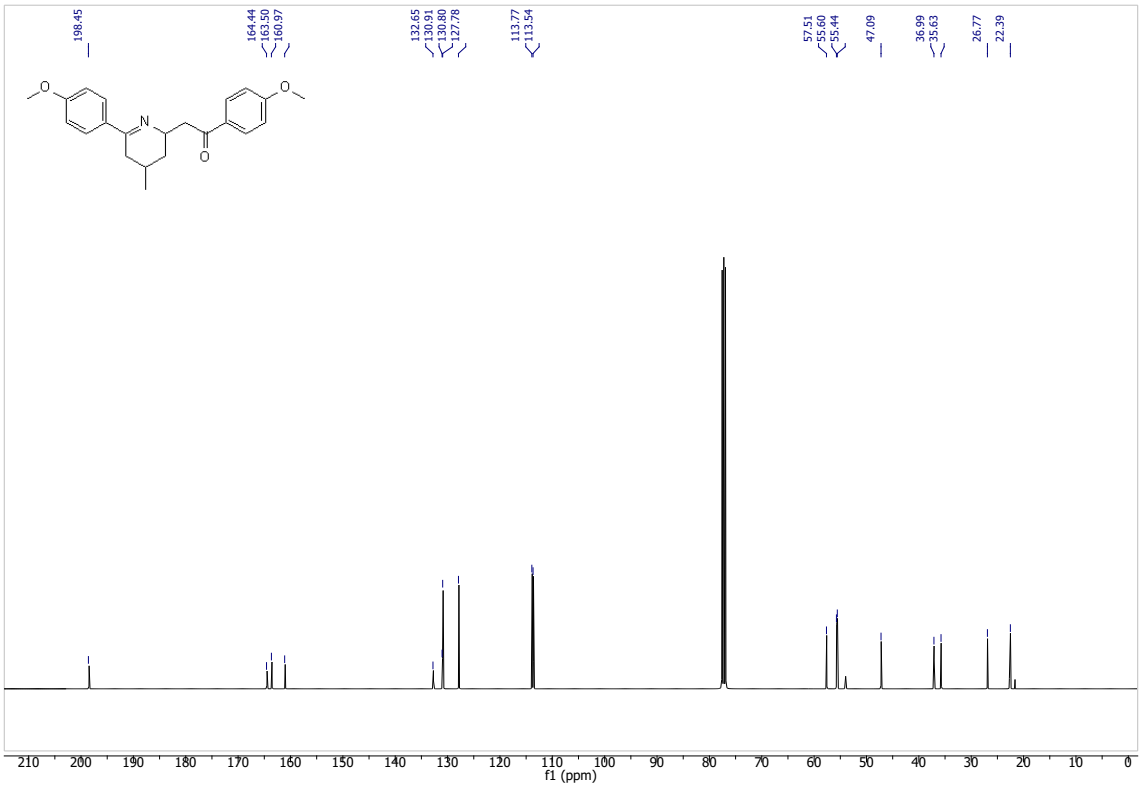


Figure 6. ^{13}C-NMR full chart for **2c** in $CDCl_3$.

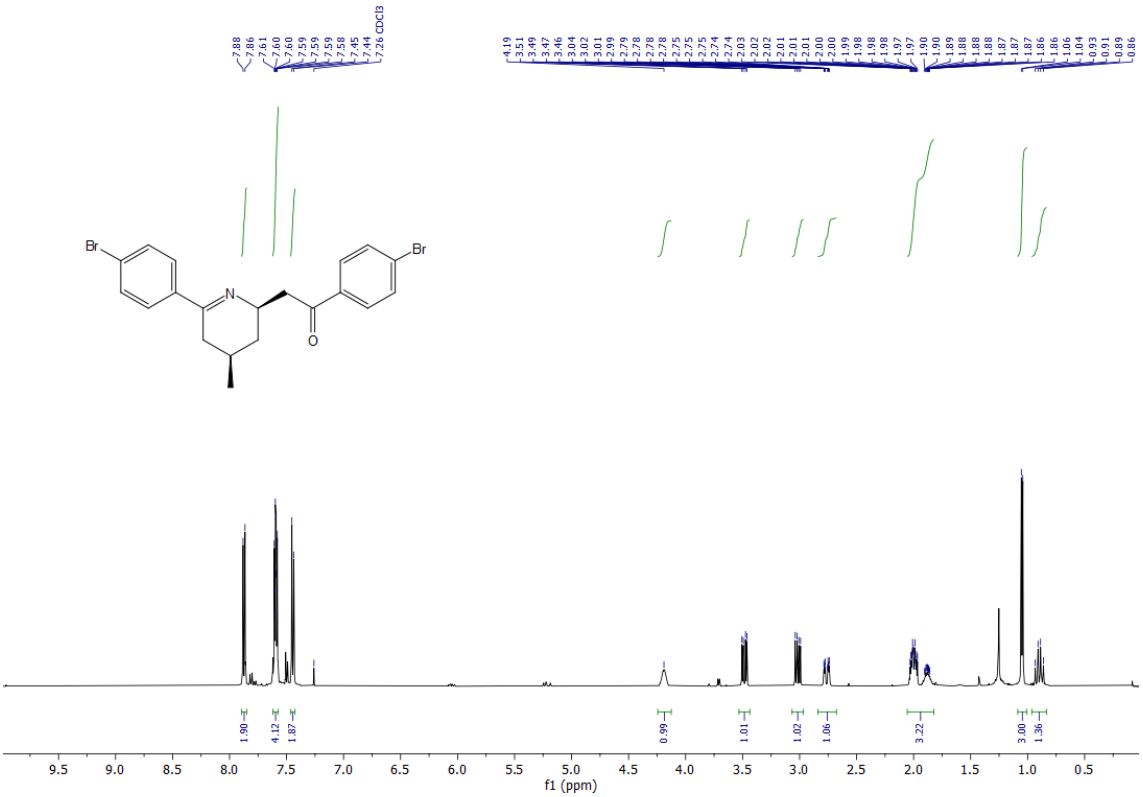


Figure 7. ^{1}H-NMR full chart for **2d** in $CDCl_3$.

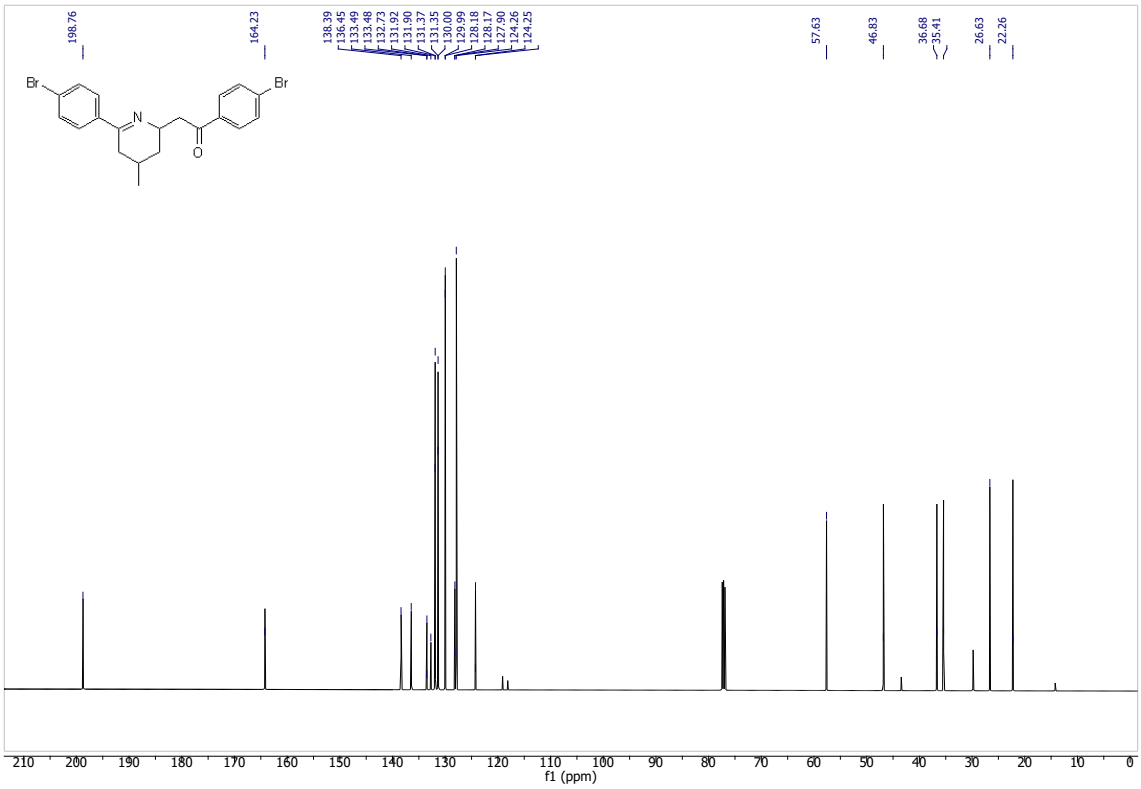


Figure 8. ^{13}C-NMR full chart for **2d** in $CDCl_3$.

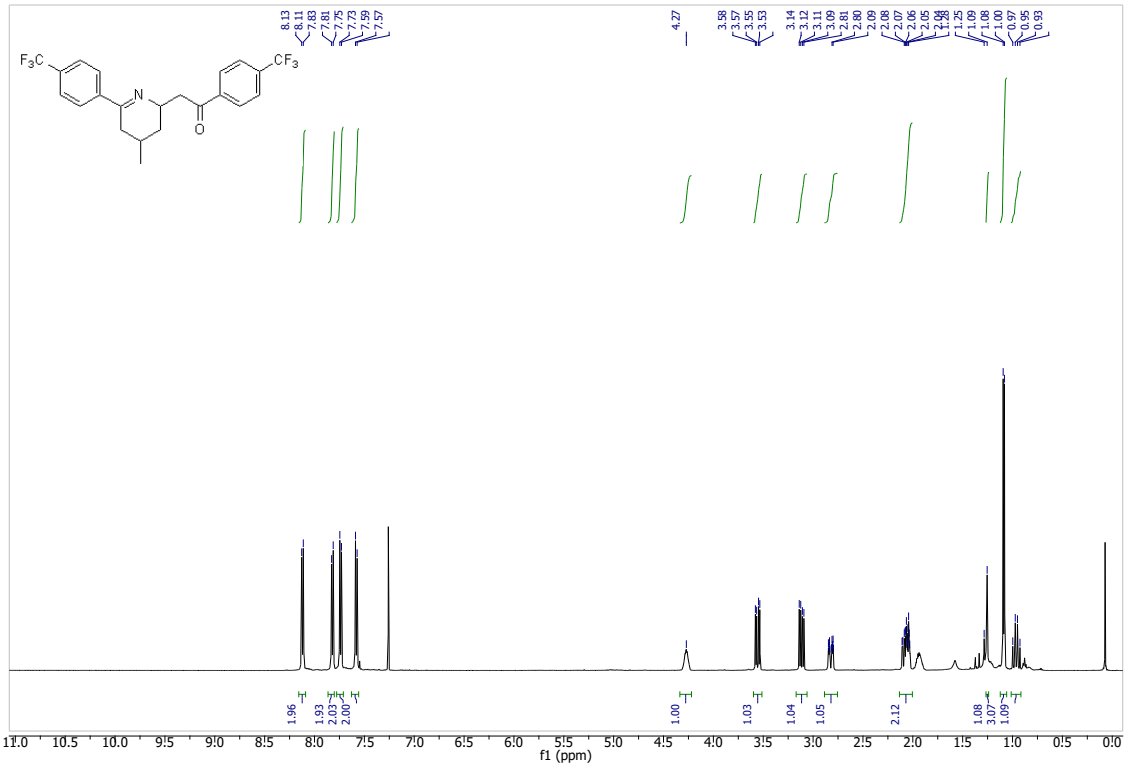


Figure 9. ^{1}H-NMR full chart for **2e** in $CDCl_3$.

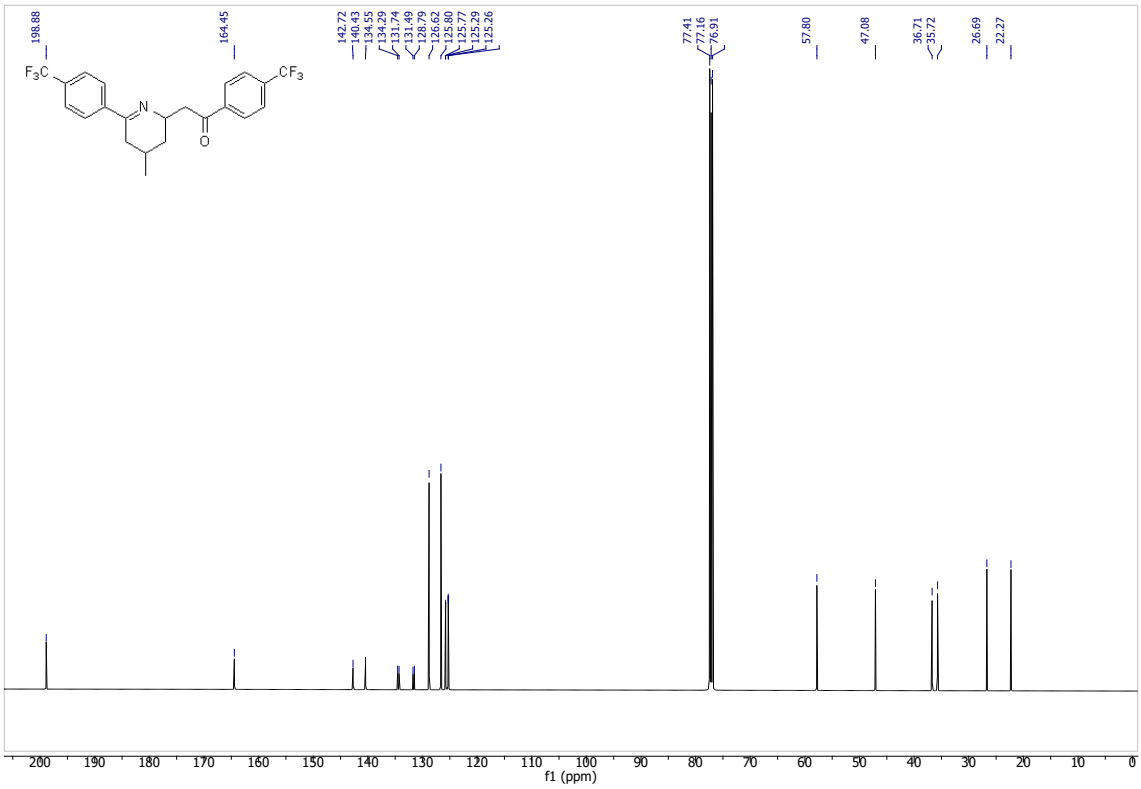


Figure 10. ^{13}C-NMR full chart for **2e** in $CDCl_3$.

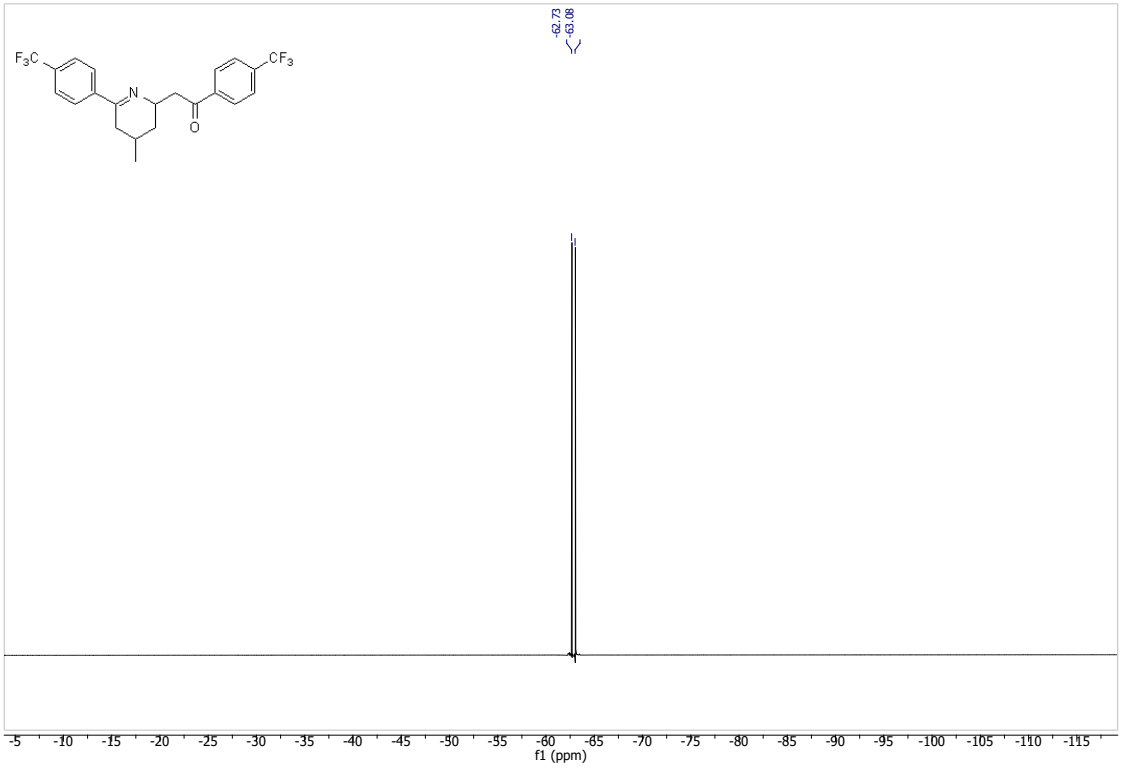


Figure 11. ^{19}F-NMR full chart for **2e** in $CDCl_3$.

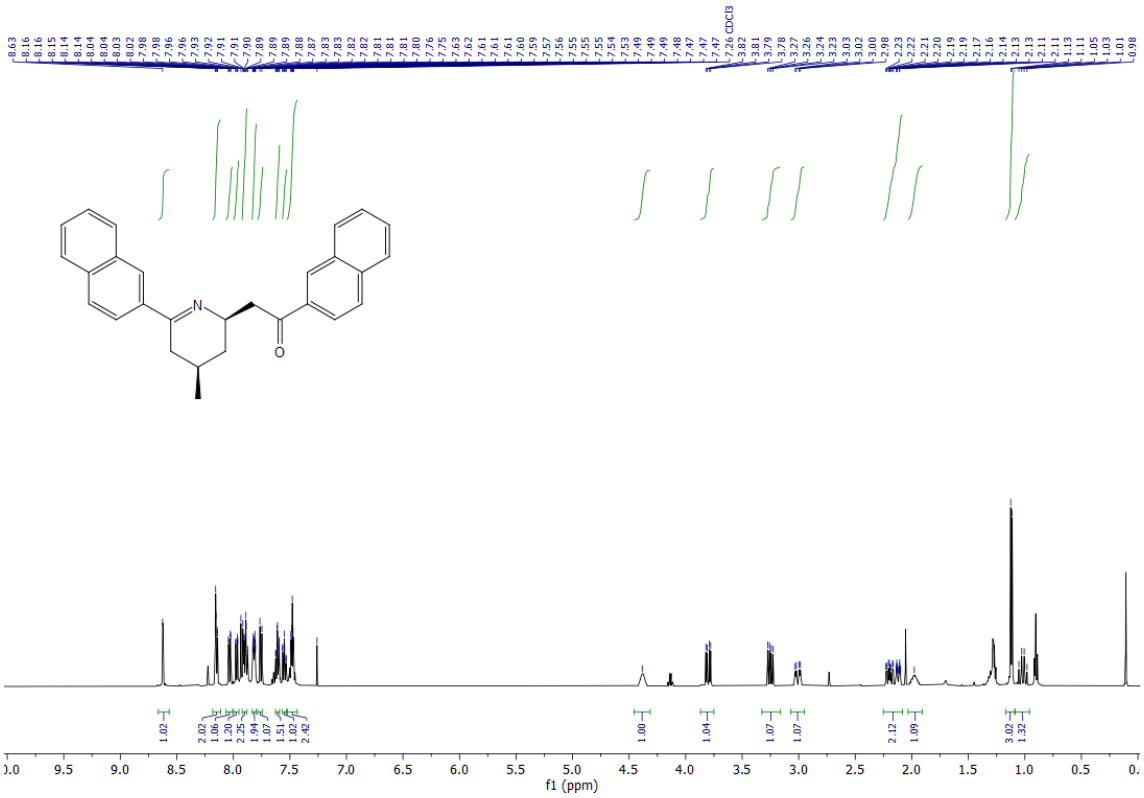


Figure 12. ^{1}H-NMR full chart for **2f** in $CDCl_3$.

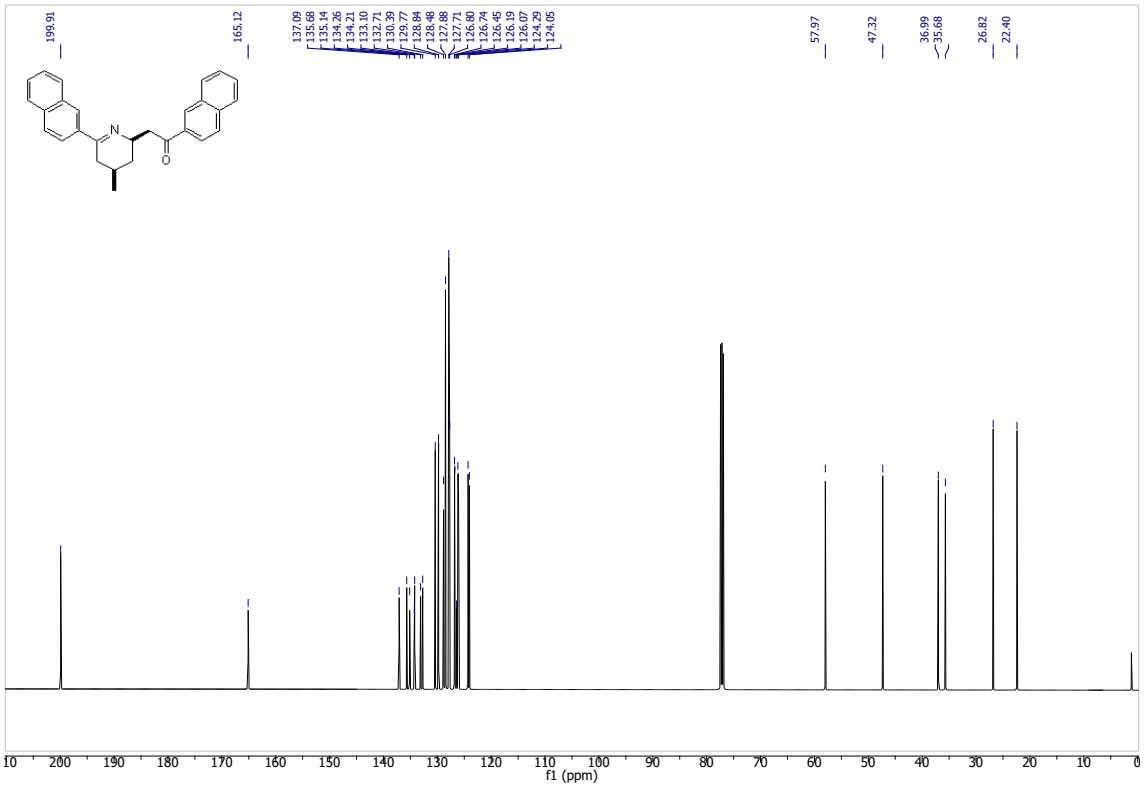


Figure 13. ^{13}C-NMR full chart for **2f** in $CDCl_3$.

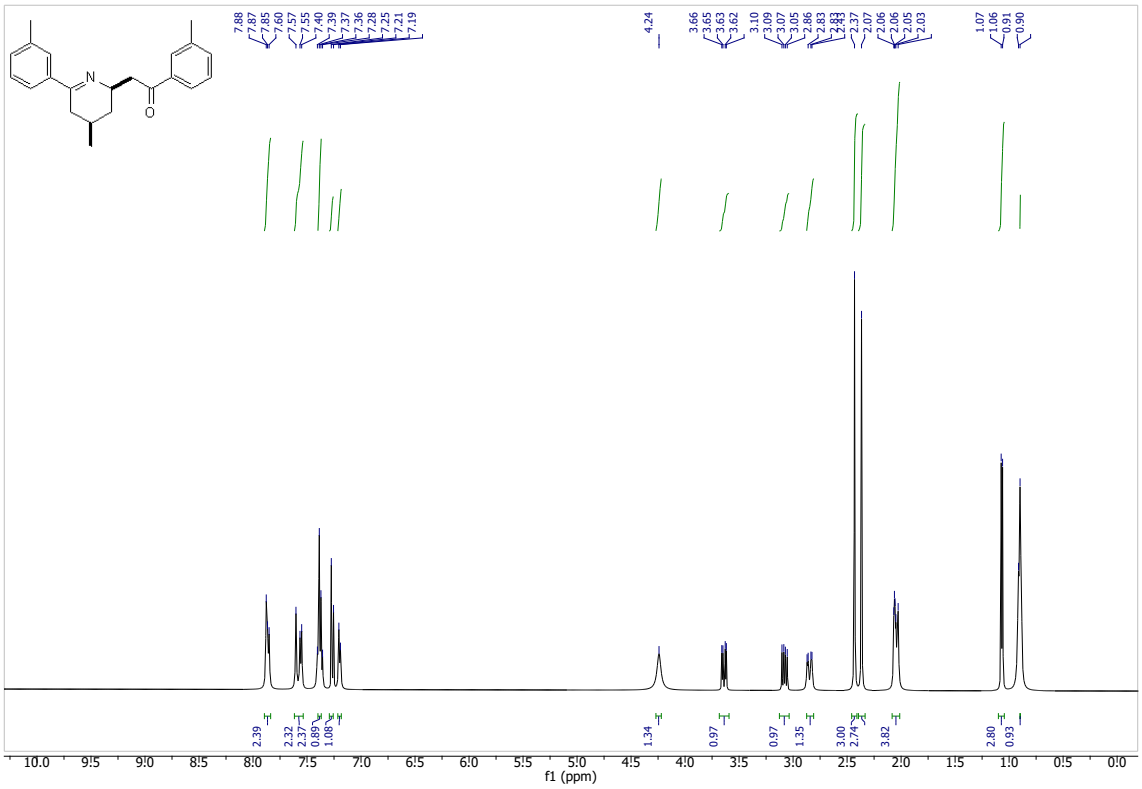


Figure 14. ^{1}H-NMR full chart for **2g** in $CDCl_3$.

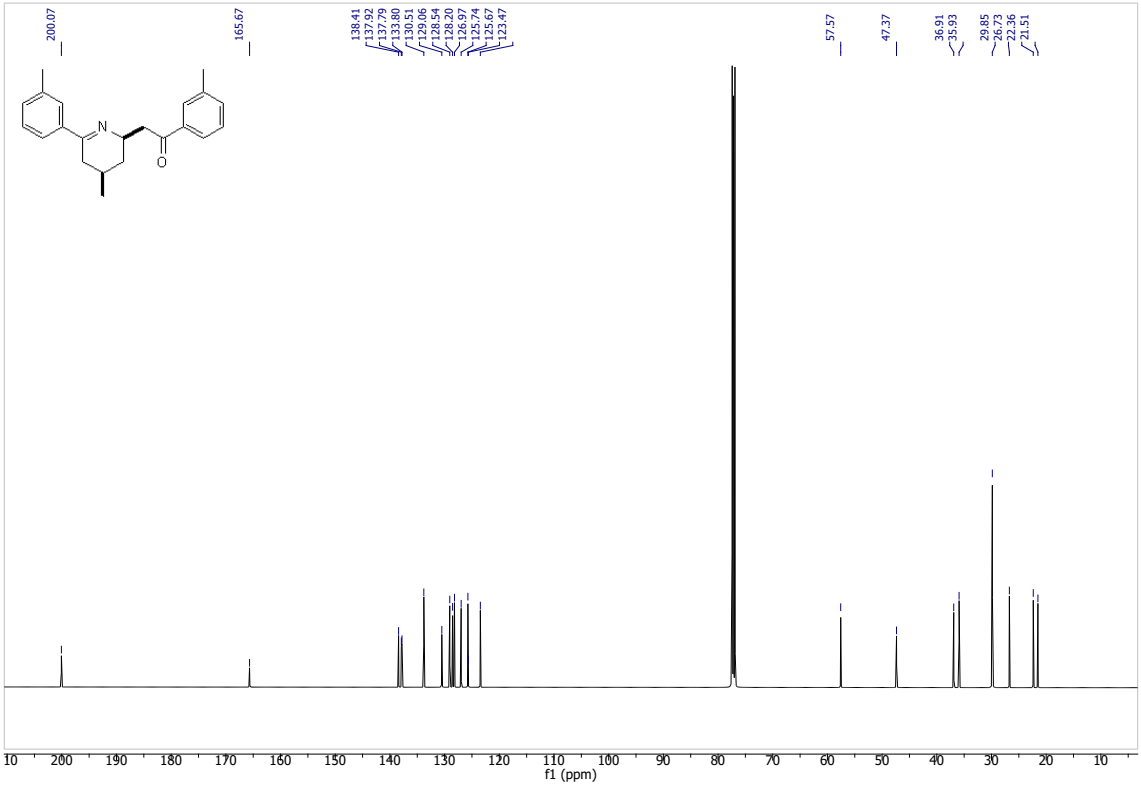


Figure 15. ^{13}C-NMR full chart for **2g** in $CDCl_3$.

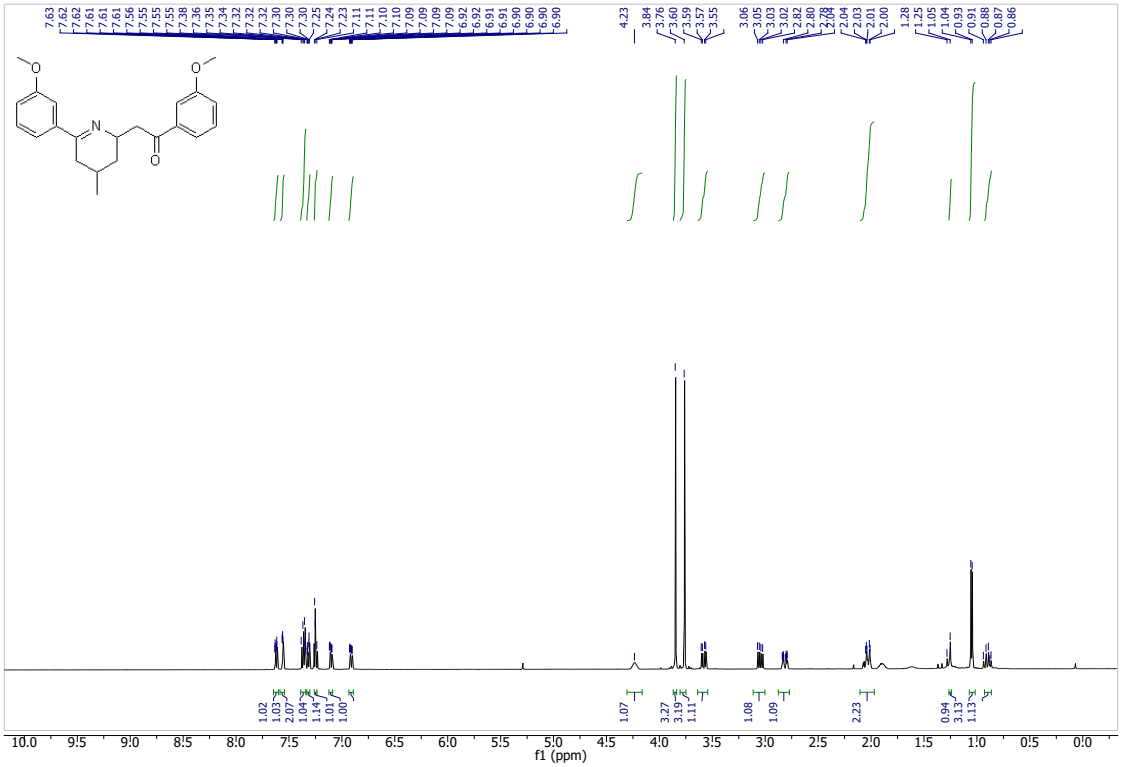


Figure 16. ^{1}H-NMR full chart for **2h** in $CDCl_3$.

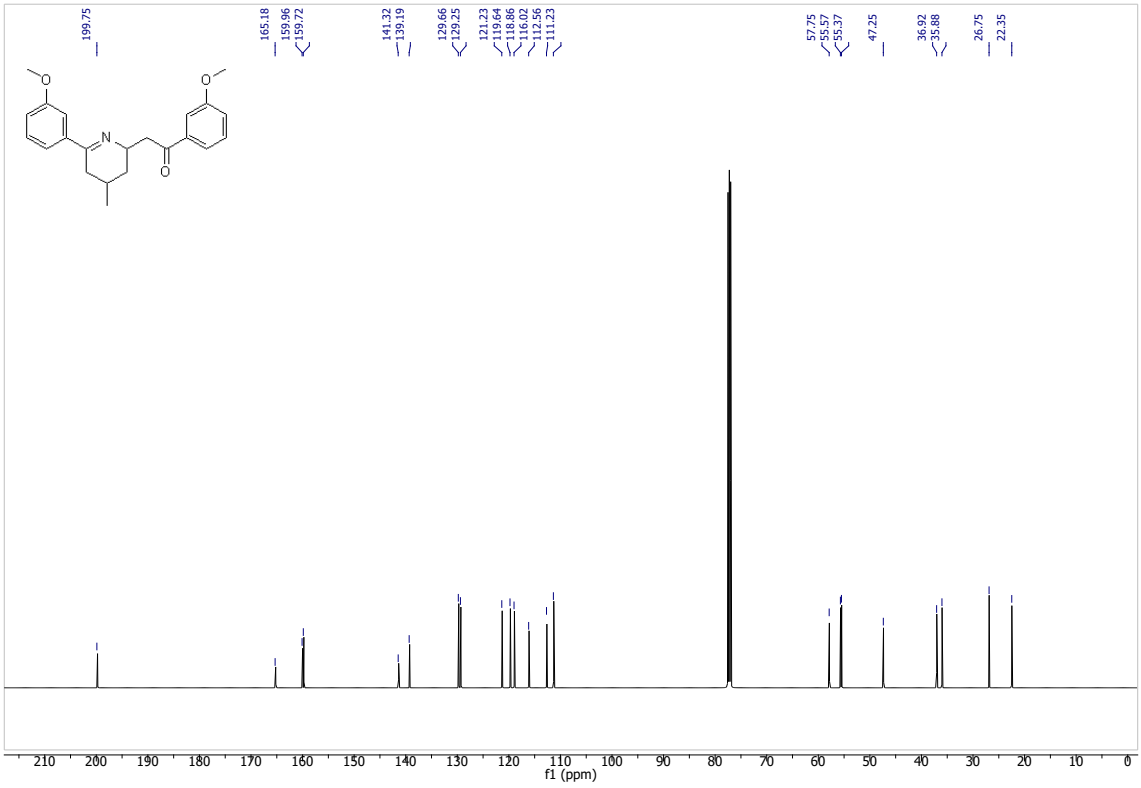


Figure 17. ^{13}C-NMR full chart for **2h** in $CDCl_3$.

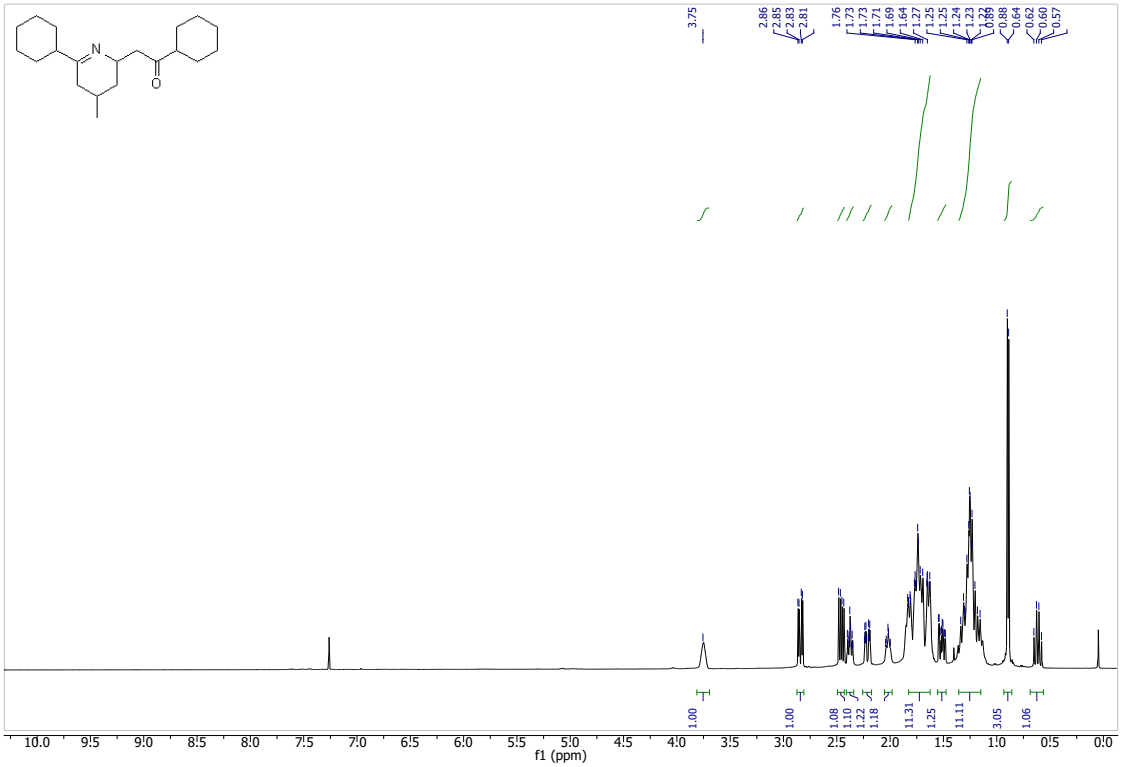


Figure 18. ^{1}H-NMR full chart for **2i** in $CDCl_3$.

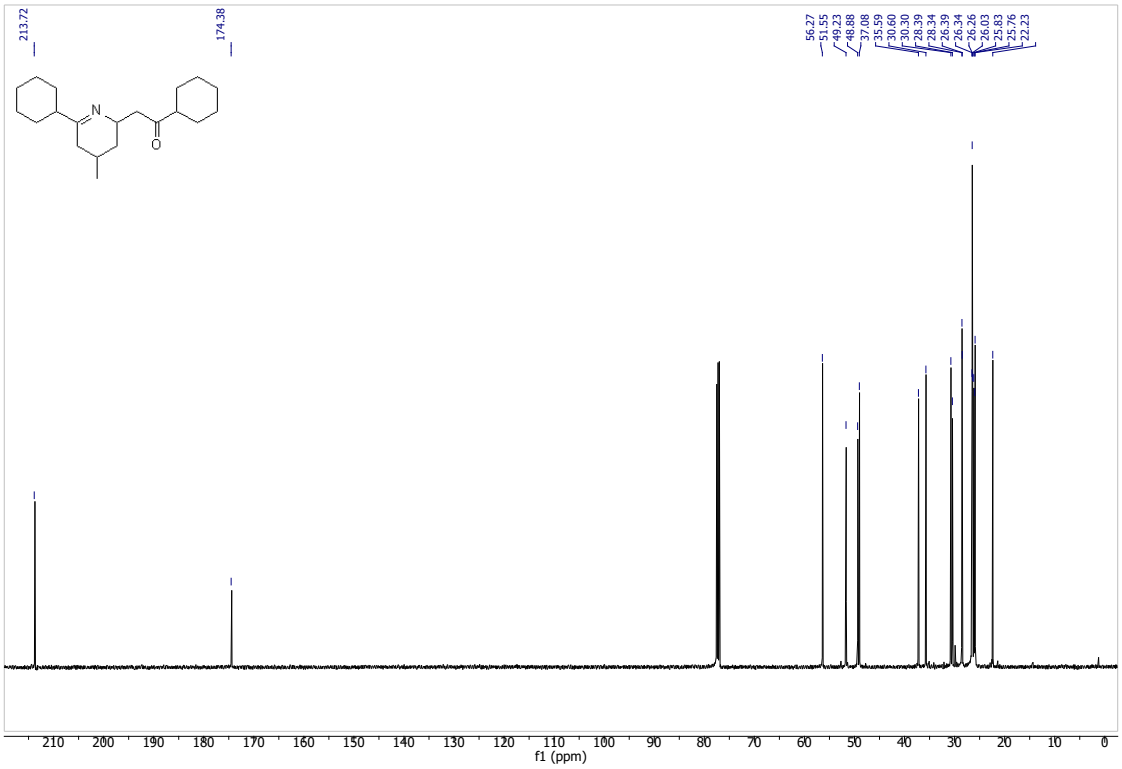


Figure 19. ^{13}C-NMR full chart for **2i** in $CDCl_3$.

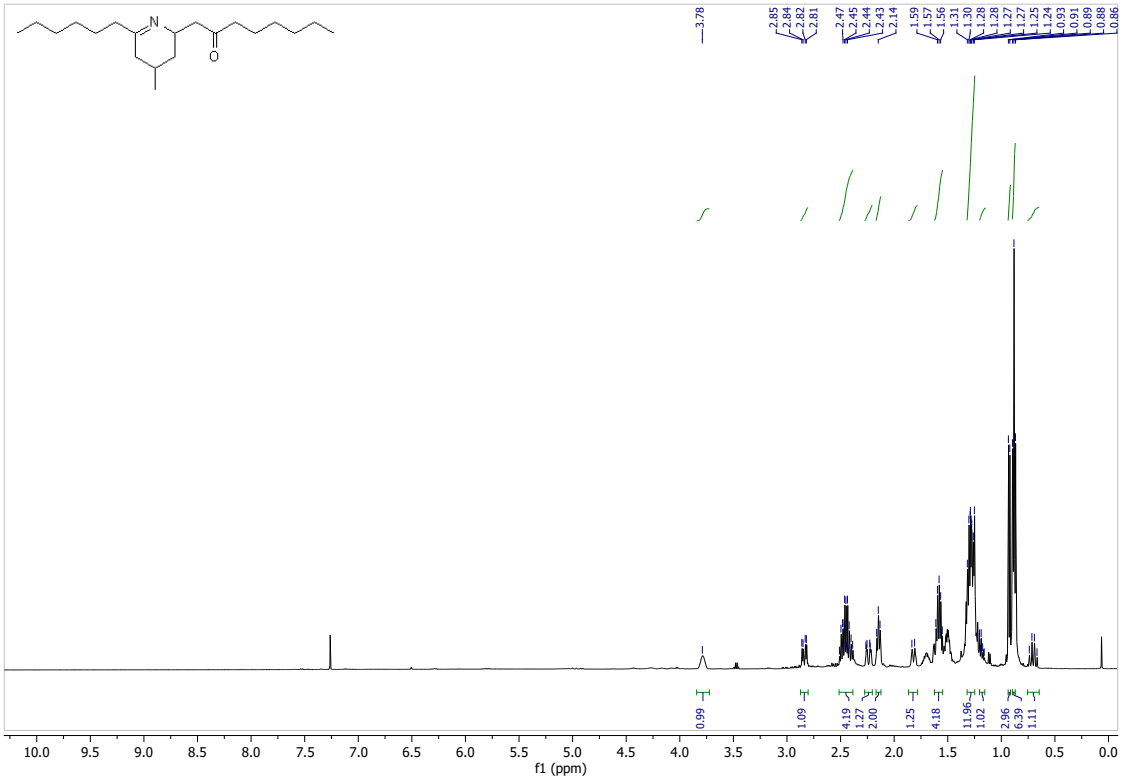


Figure 20. ^{1}H-NMR full chart for **2j** in $CDCl_3$.

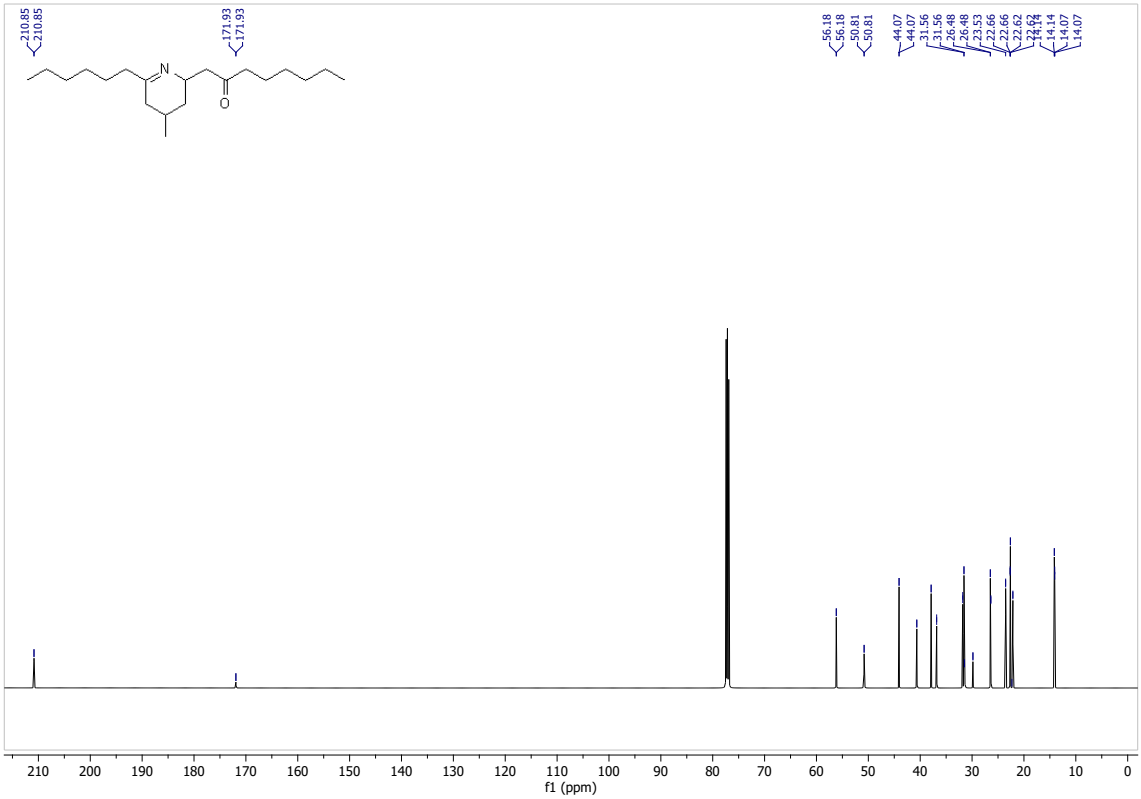


Figure 21. ^{13}C-NMR full chart for **2j** in $CDCl_3$.

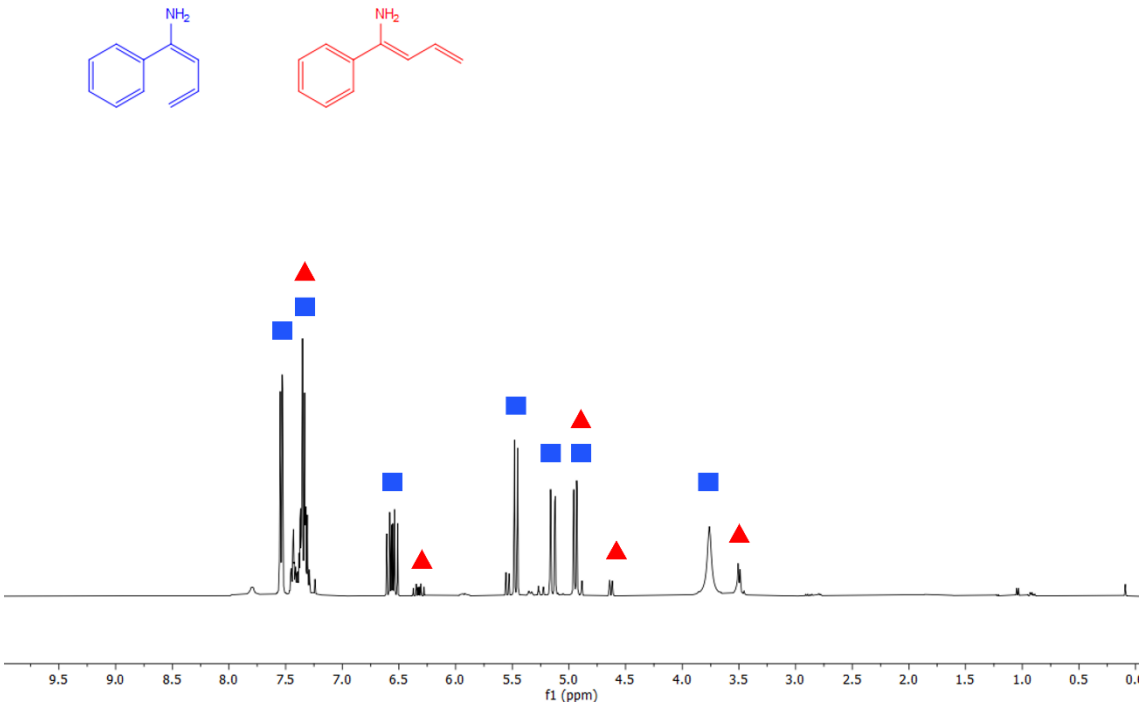


Figure 22. ^{1}H-NMR full chart for ***E*-3a** and ***Z*-3a** in $CDCl_3$.

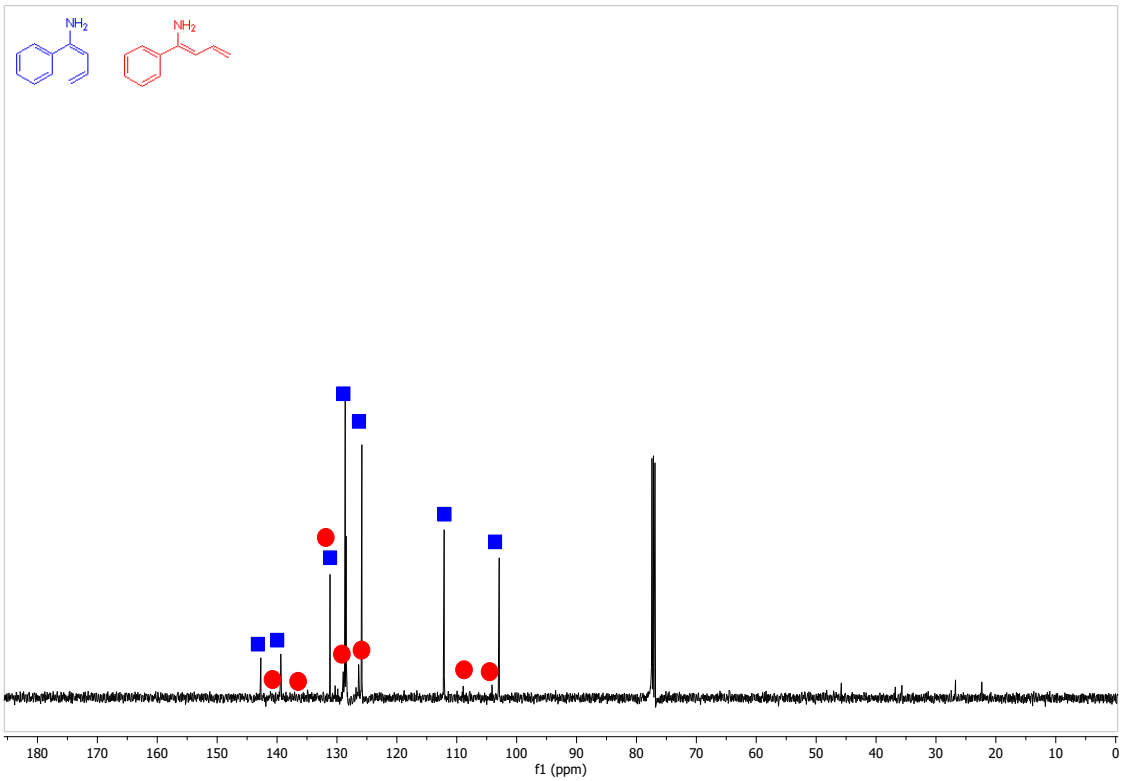


Figure 23. ^{13}C-NMR full chart for ***E*-3a** and ***Z*-3a** in $CDCl_3$.

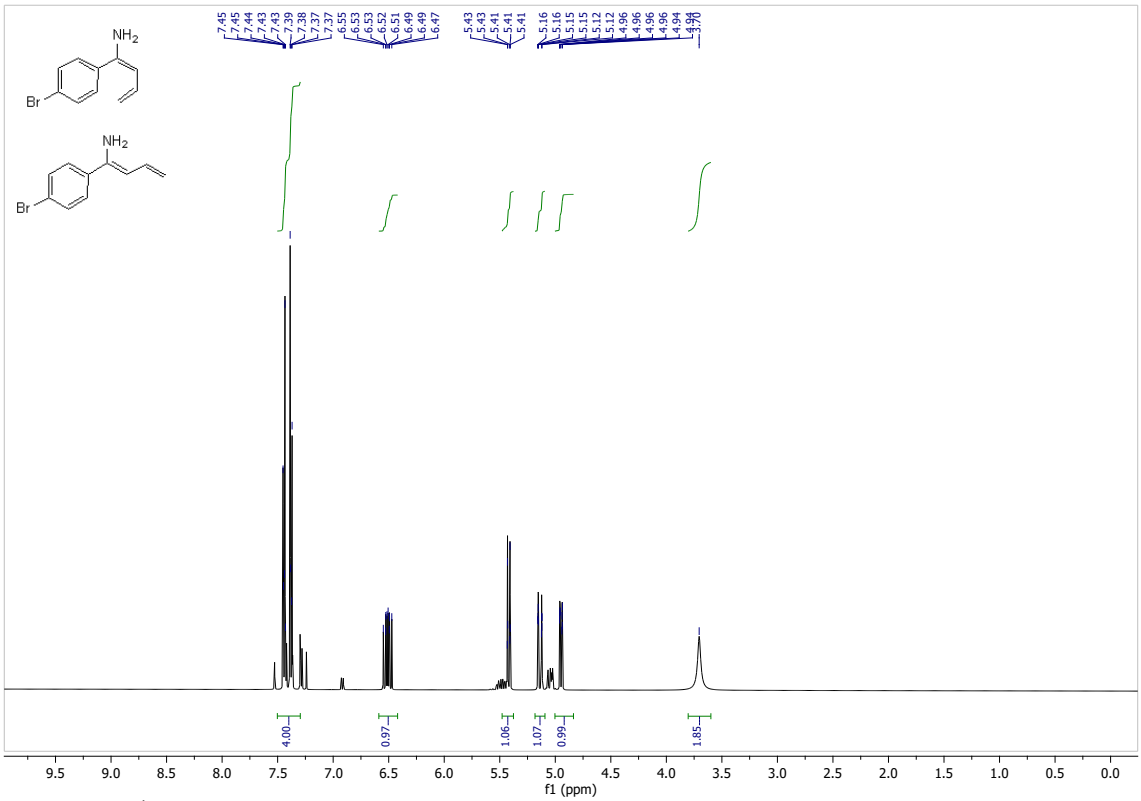


Figure 24. ^{1}H-NMR full chart for ***E*-3d** and ***Z*-3d** in $CDCl_3$.

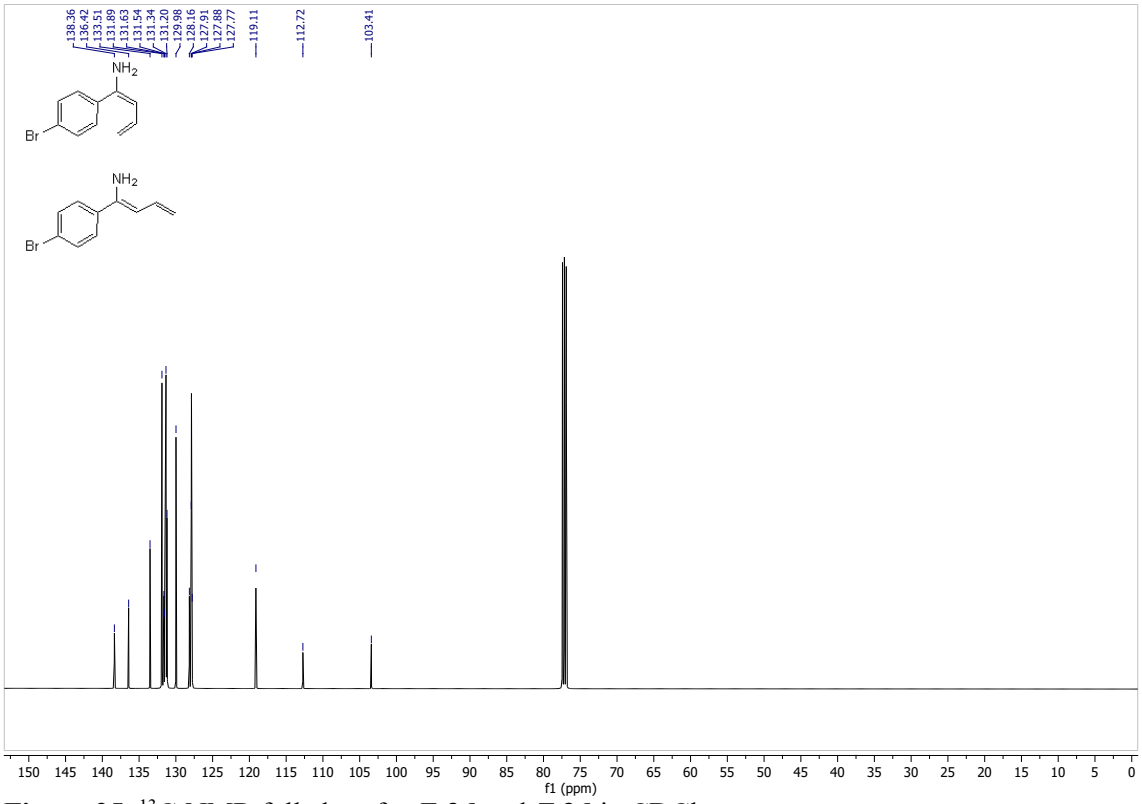


Figure 25. ^{13}C-NMR full chart for ***E*-3d** and ***Z*-3d** in $CDCl_3$.

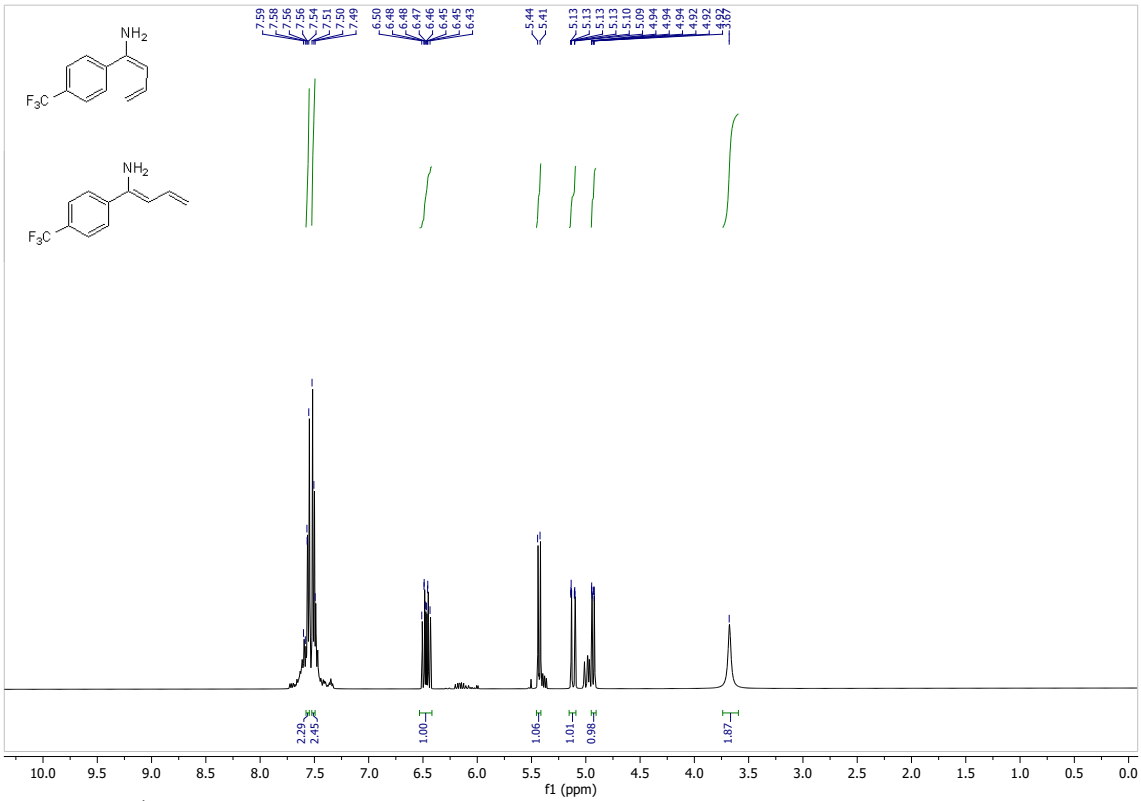


Figure 26. ^{1}H-NMR full chart ***E*-3e** and ***Z*-3e** in $CDCl_3$.

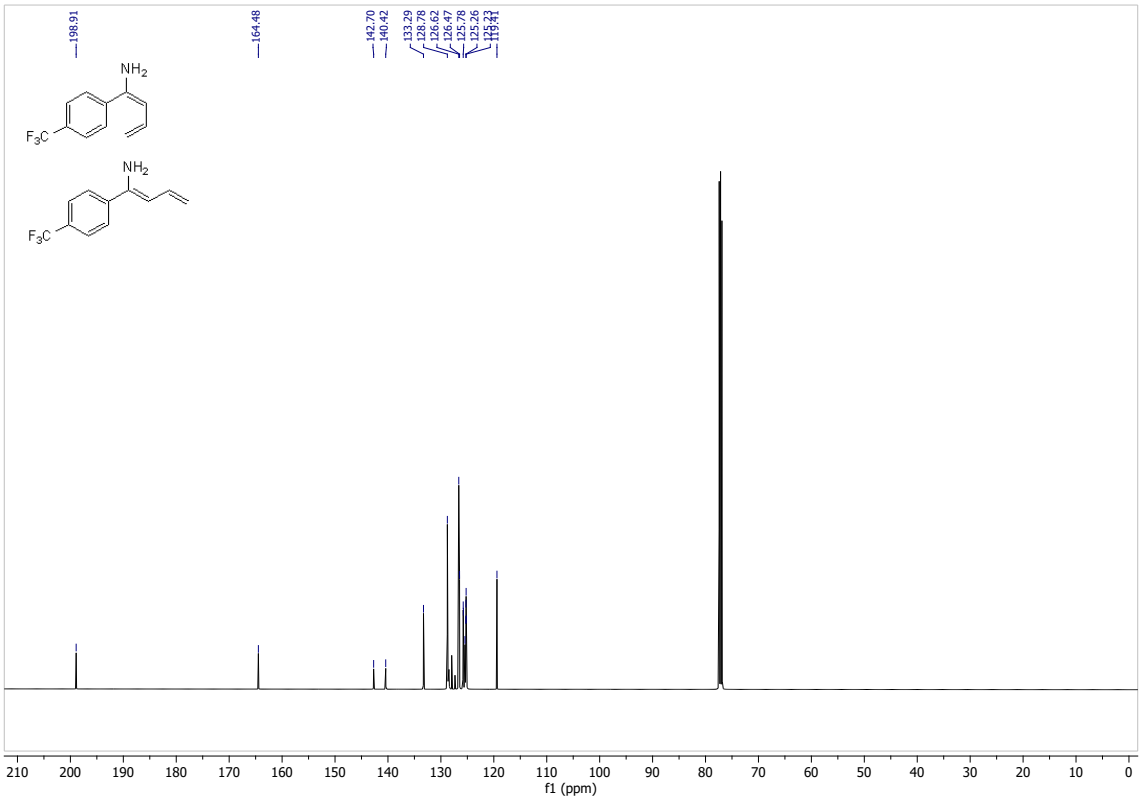


Figure 27. ^{13}C-NMR full chart for ***E*-3e** and ***Z*-3e** in $CDCl_3$.

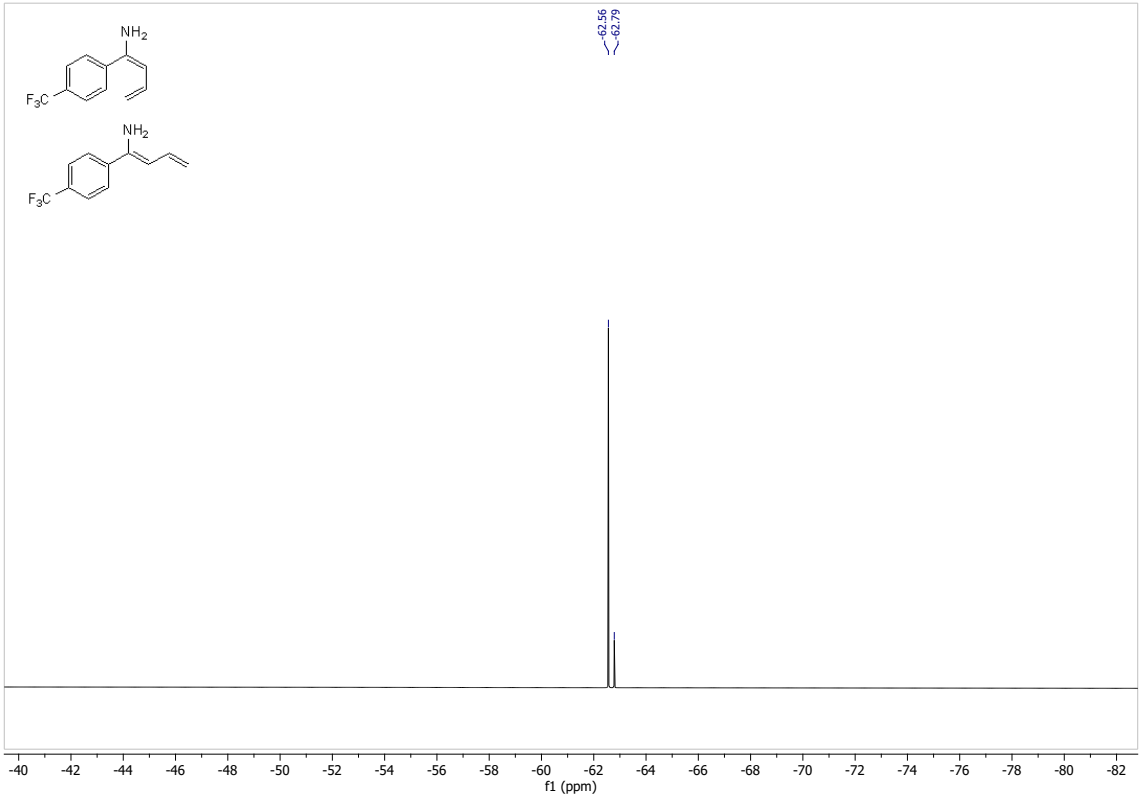


Figure 28. ^{19}F-NMR full chart for ***E*-3e** and ***Z*-3e** in $CDCl_3$.

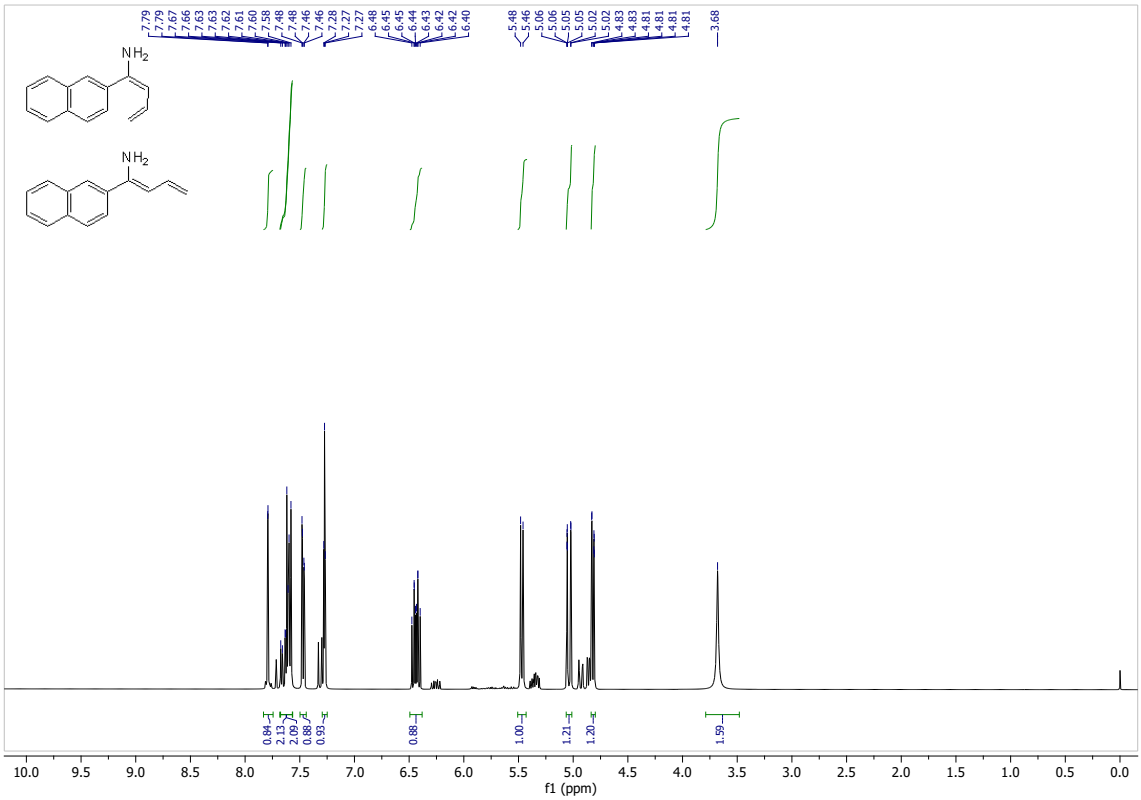


Figure 29. ^{1}H-NMR full chart for ***E*-3f** in $CDCl_3$.

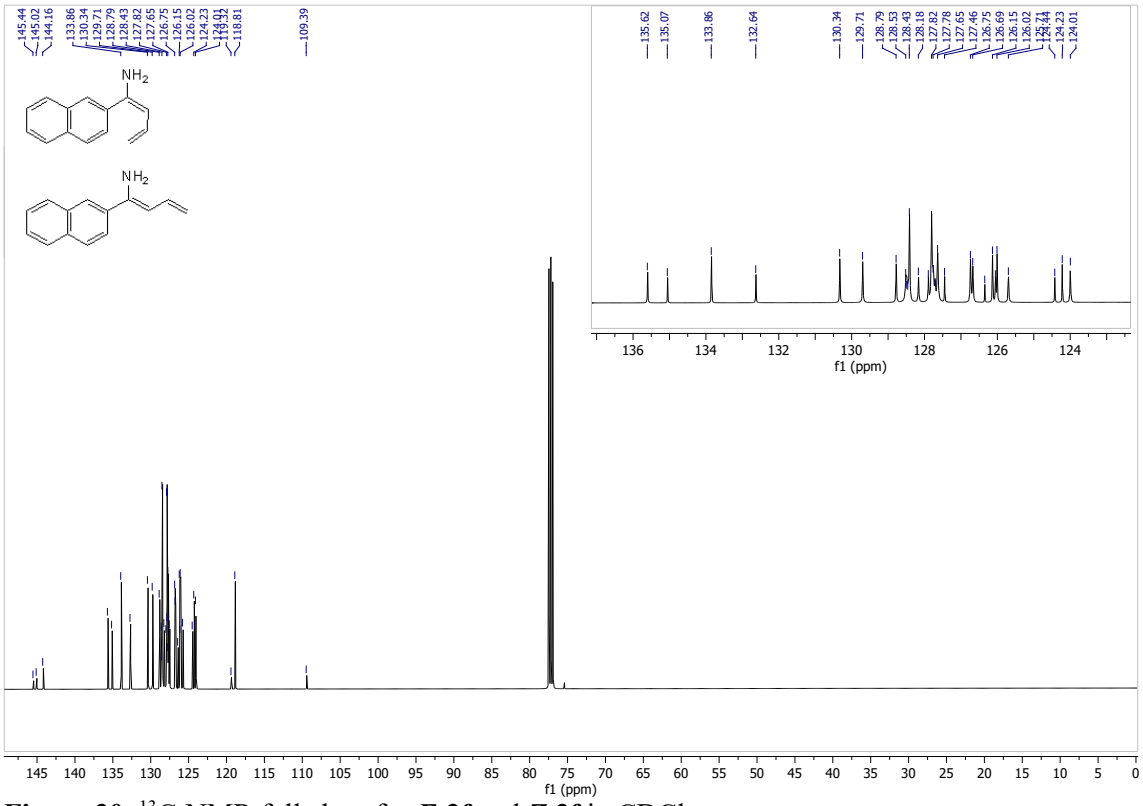


Figure 30. ^{13}C-NMR full chart for ***E*-3f** and ***Z*-3f** in $CDCl_3$.

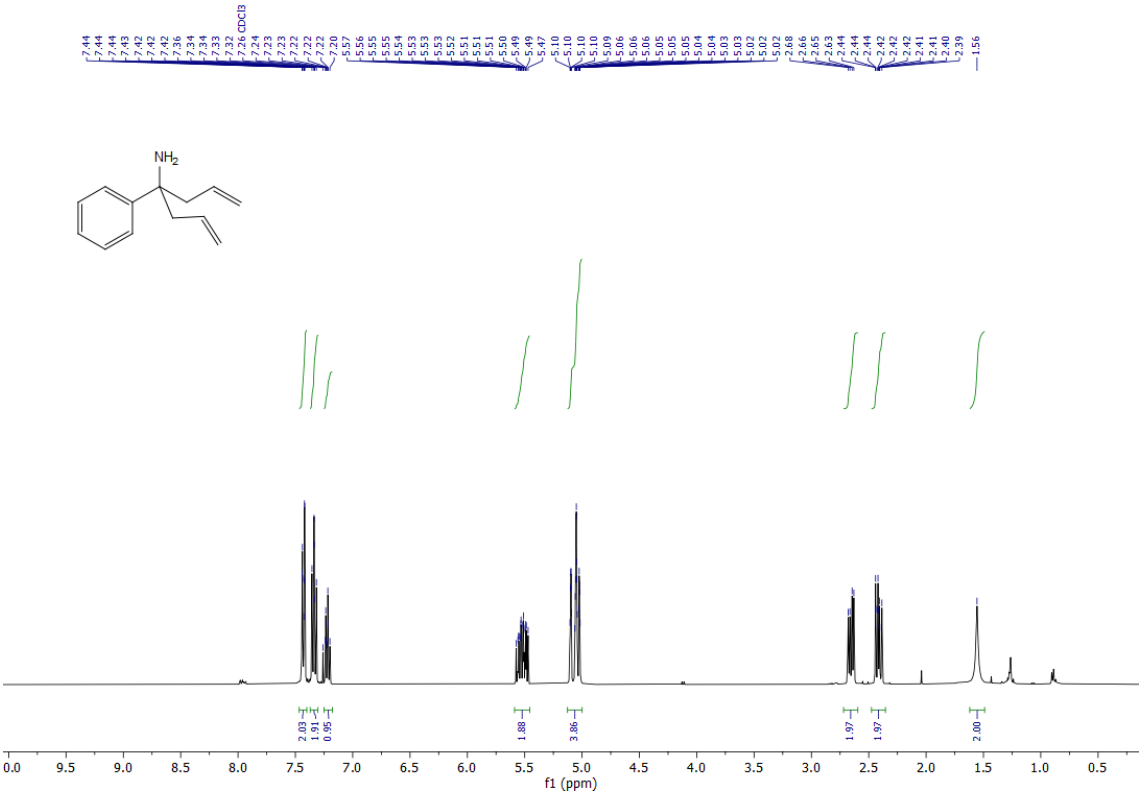


Figure 31. ^{1}H-NMR full chart for **4a** in $CDCl_3$.

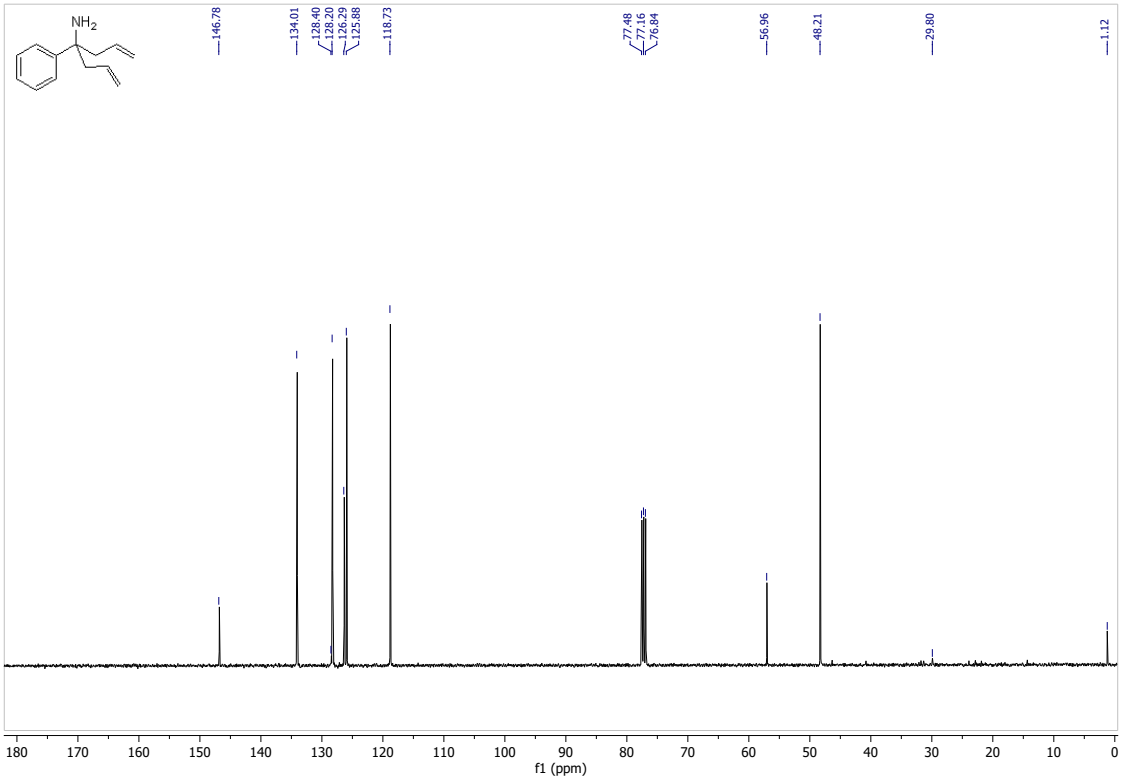


Figure 32. ^{13}C-NMR full chart for **4a** in $CDCl_3$.

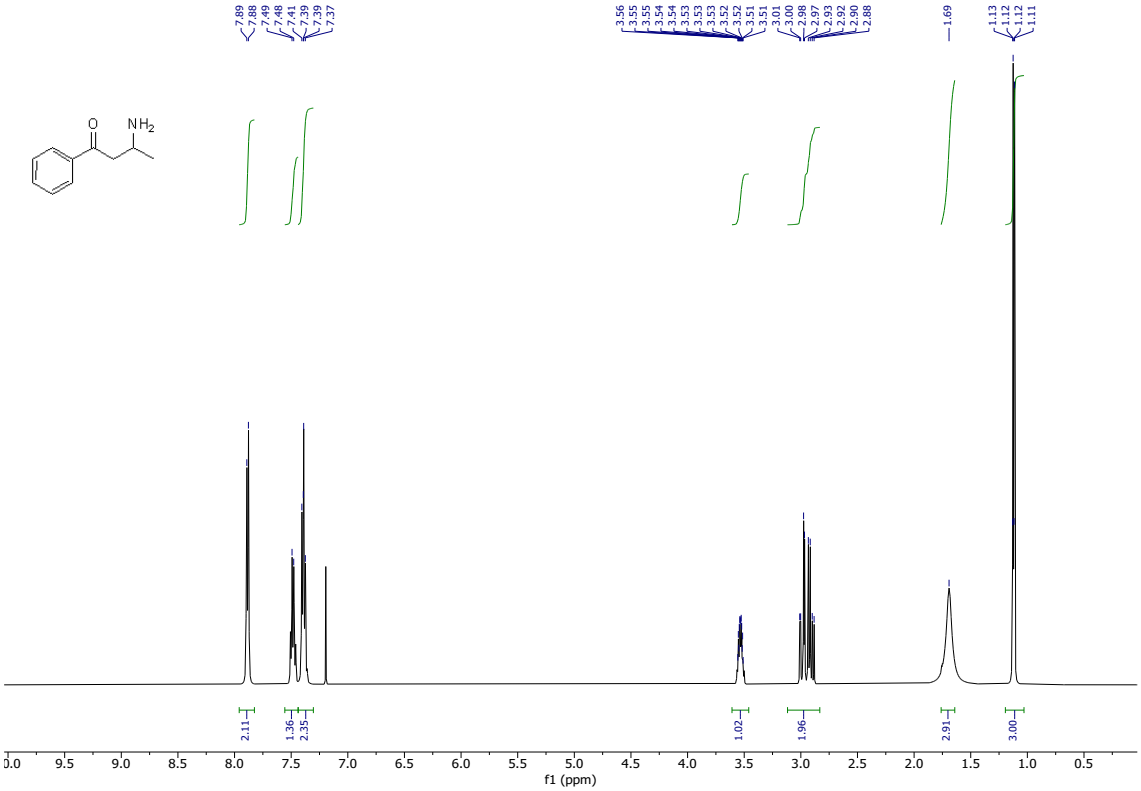


Figure 33. ^{1}H-NMR full chart for **5a** in $CDCl_3$.

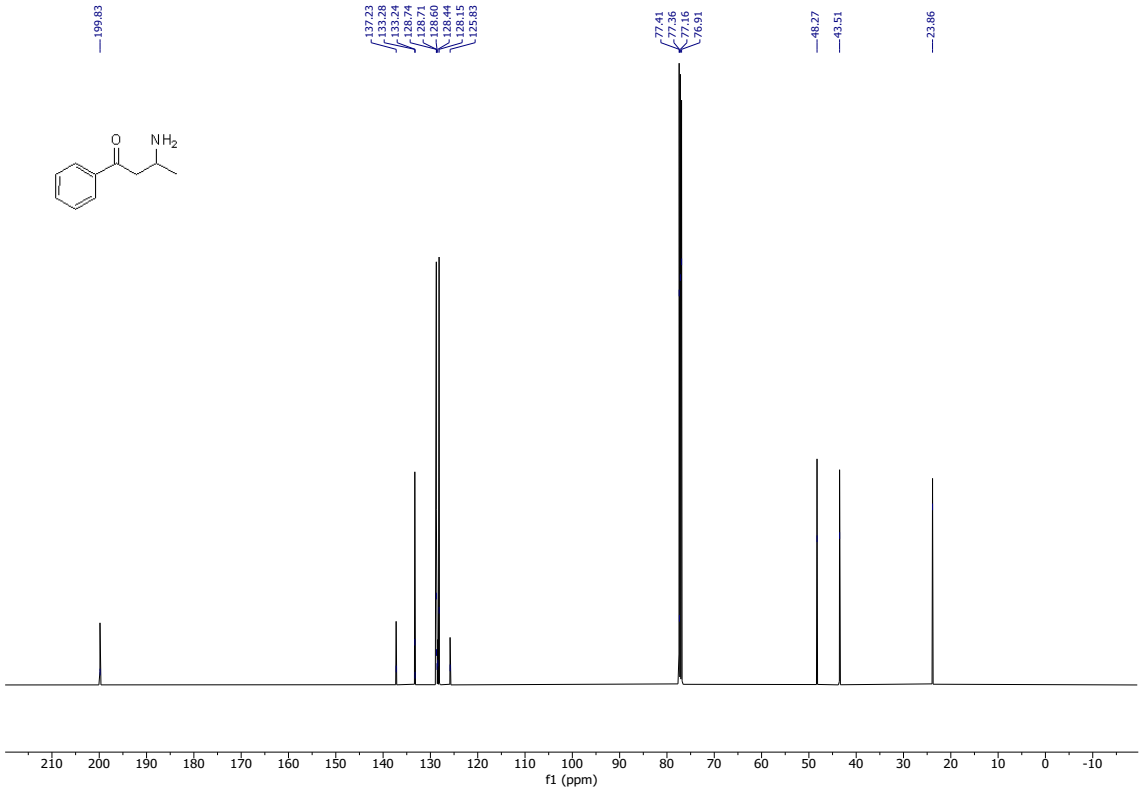


Figure 34. ^{13}C-NMR full chart for **5a** in $CDCl_3$.

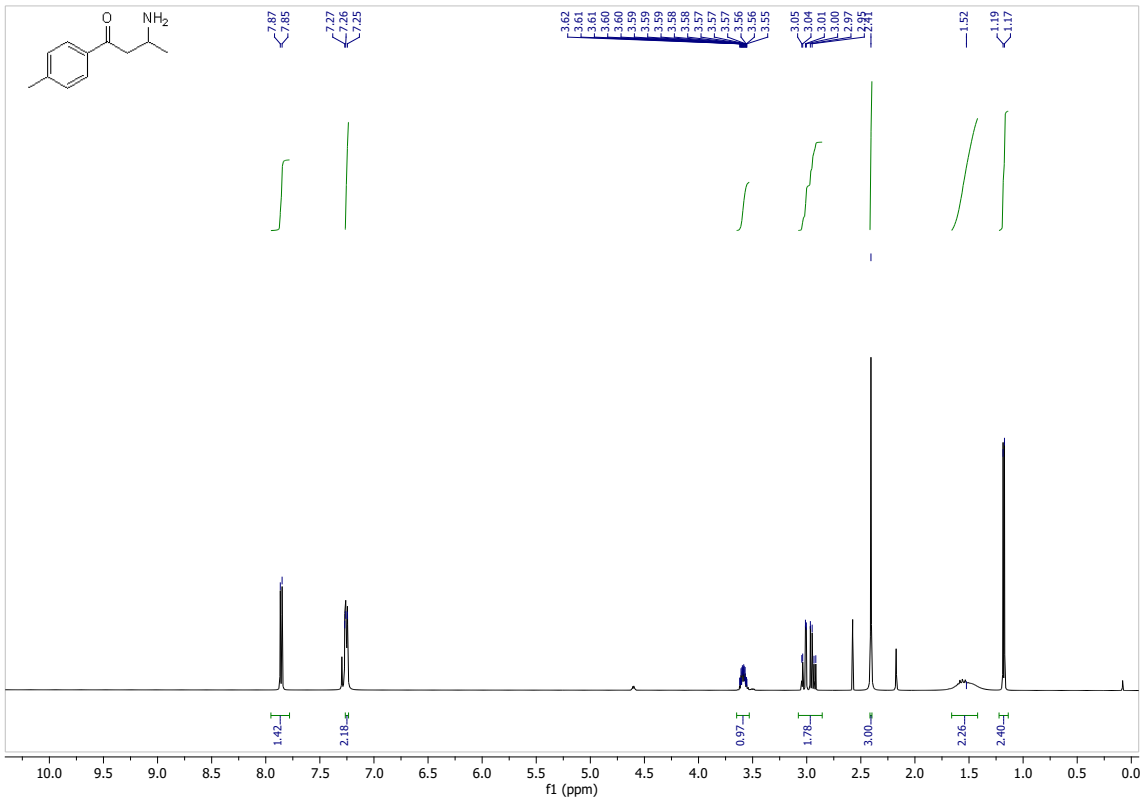


Figure 35. ^{1}H-NMR full chart for **5b** in $CDCl_3$.

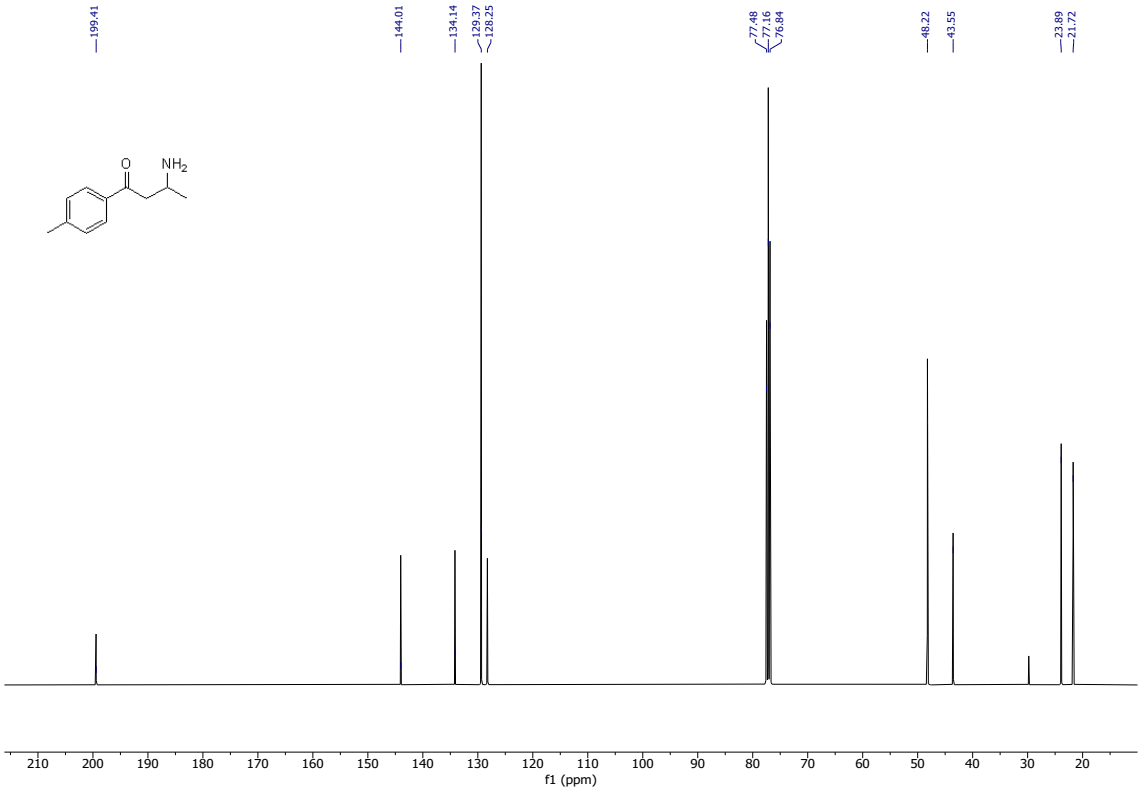


Figure 36. ^{13}C-NMR full chart for **5b** in $CDCl_3$.

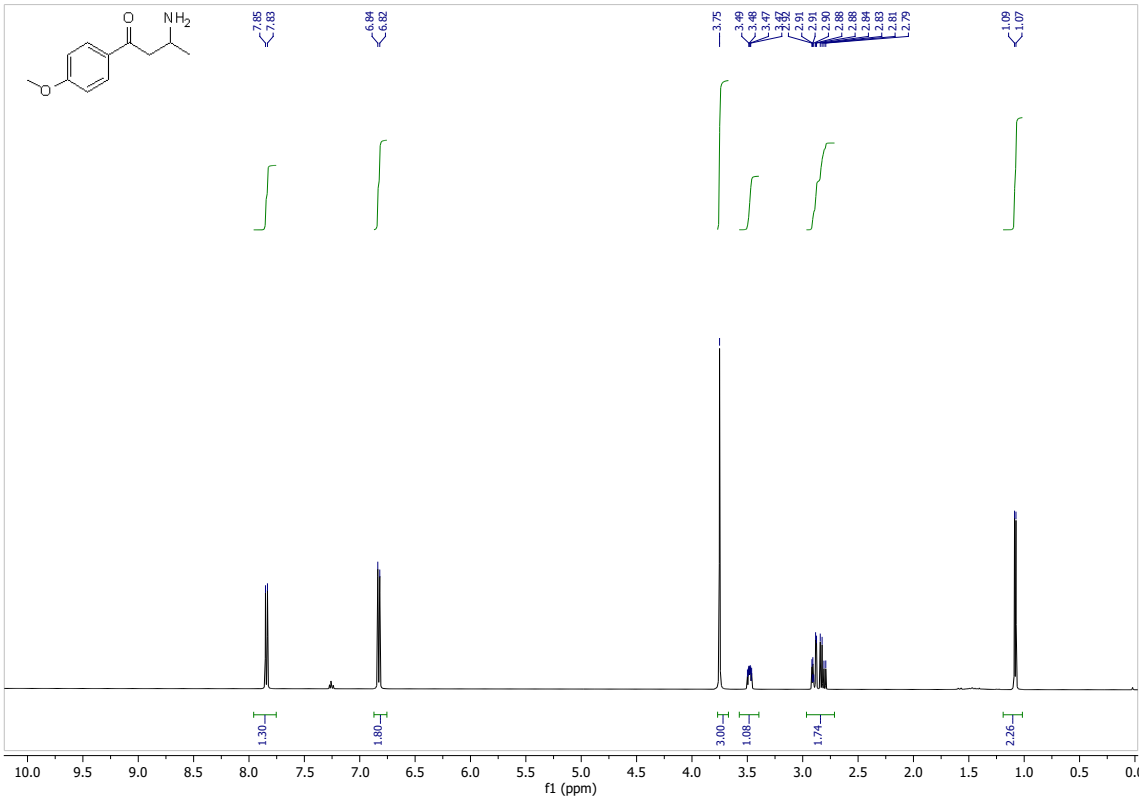


Figure 37. ^{13}H-NMR full chart for **5c** in $CDCl_3$.

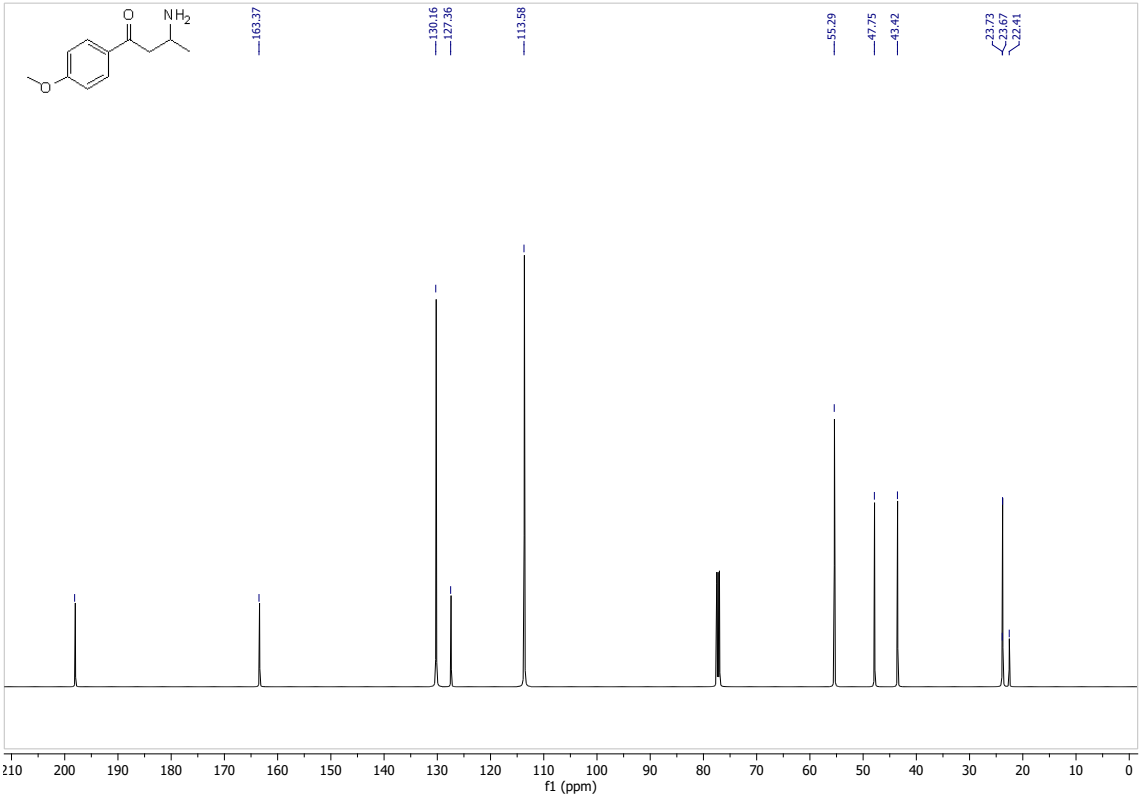


Figure 38. ^{13}C-NMR full chart for **5c** in $CDCl_3$.

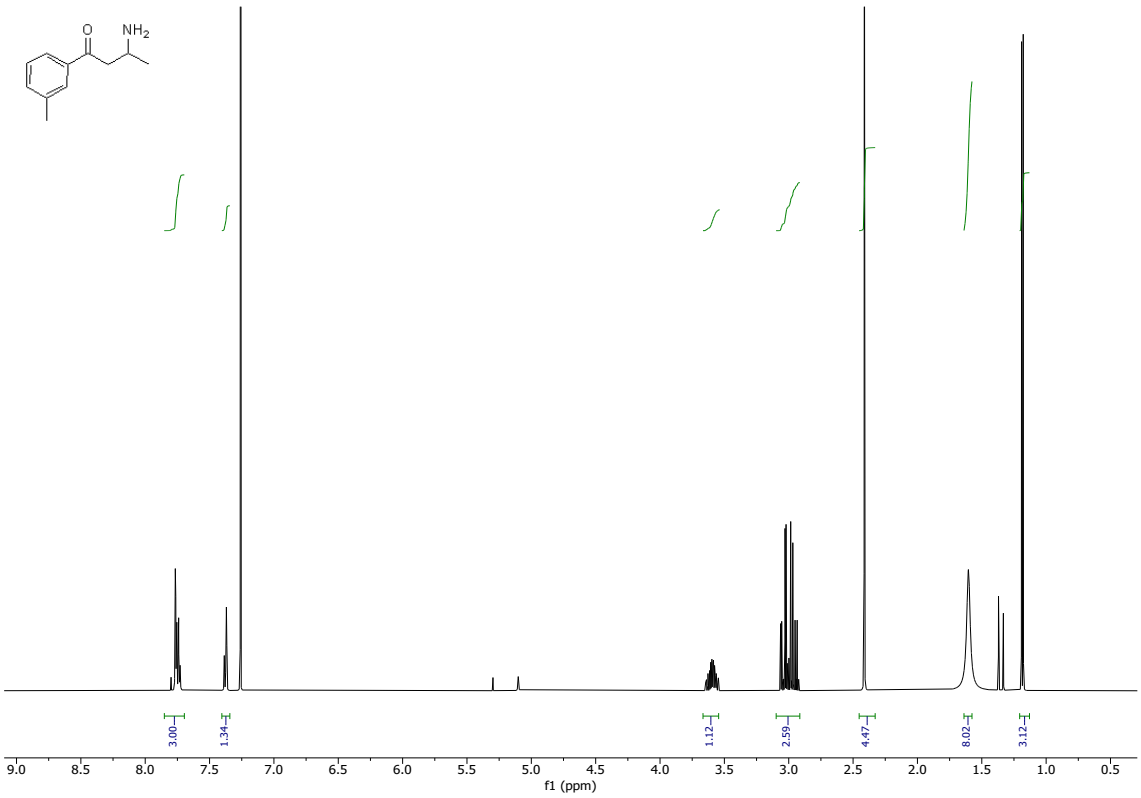


Figure 39. ^{1}H-NMR full chart for **5g** in $CDCl_3$.

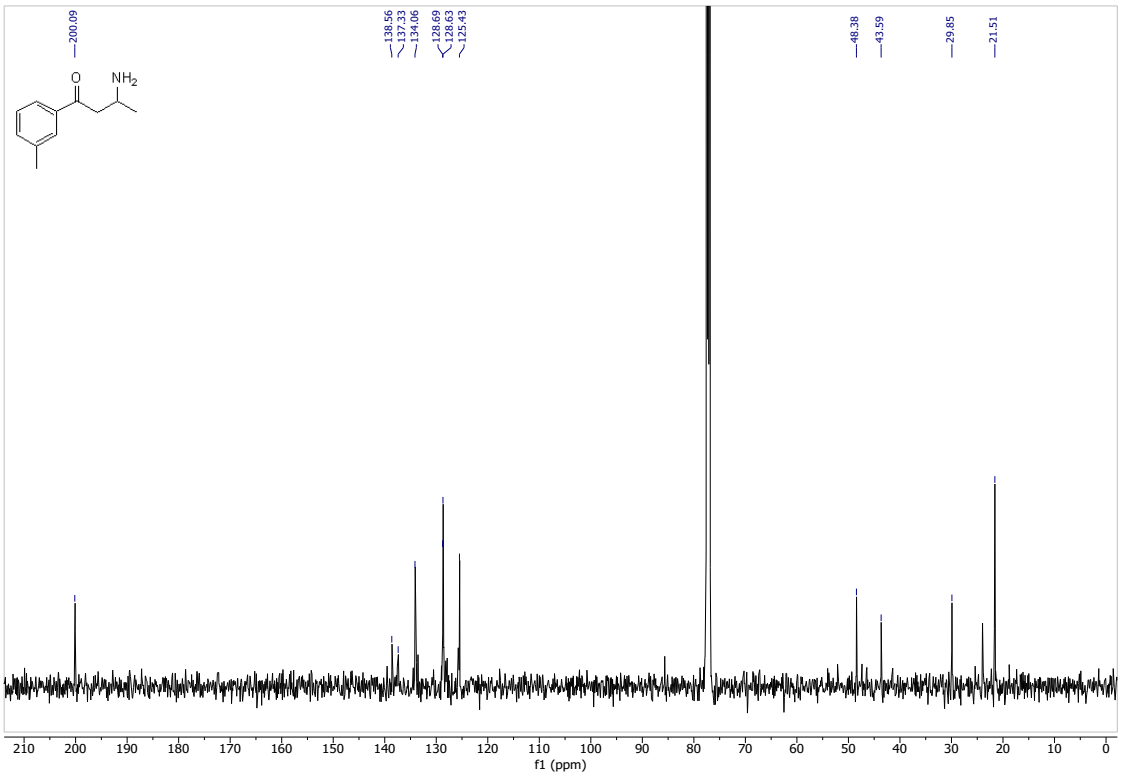


Figure 40. ^{13}C-NMR full chart for **5g** in $CDCl_3$.

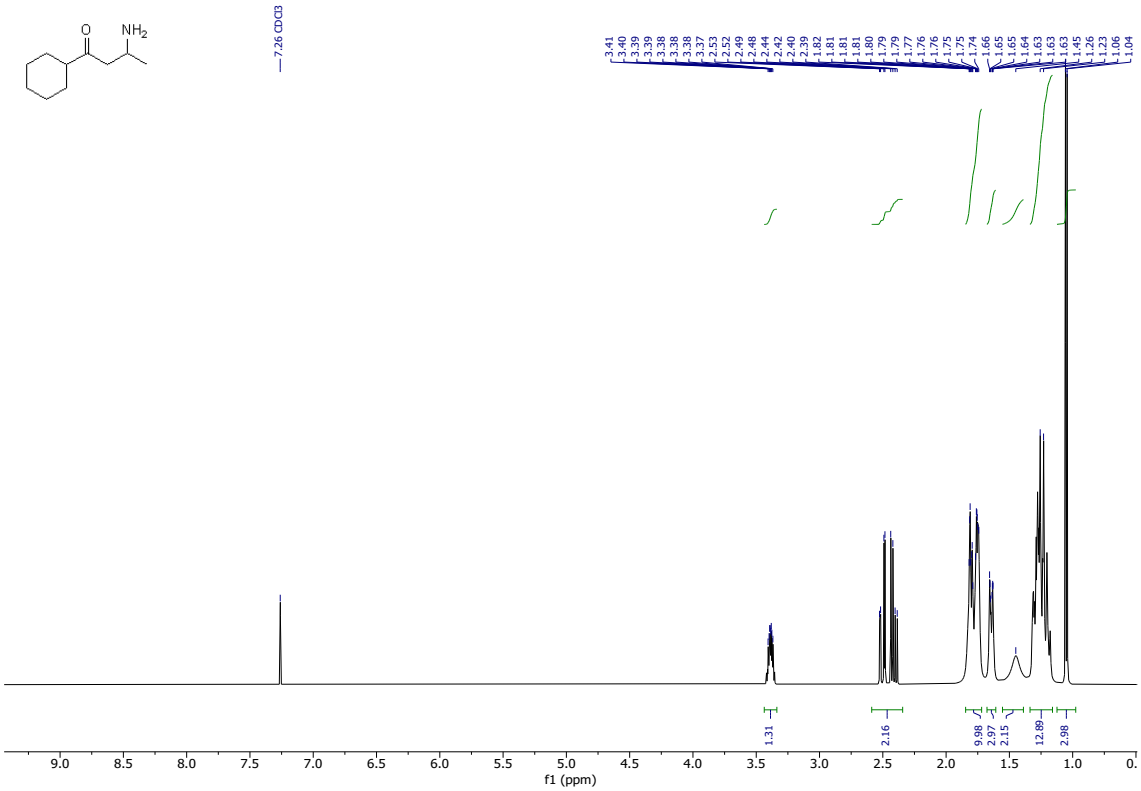


Figure 41. ^{1}H-NMR full chart for **5i** in $CDCl_3$.

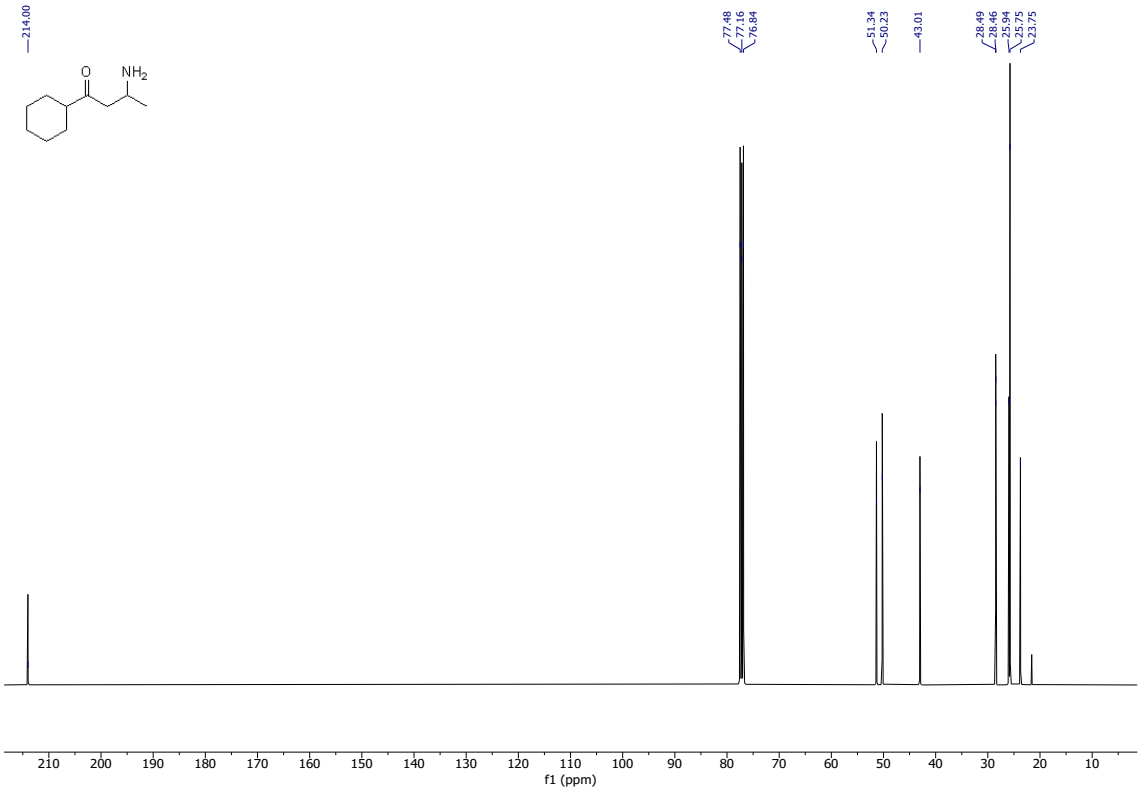


Figure 42. ^{13}C-NMR full chart for **5i** in $CDCl_3$.

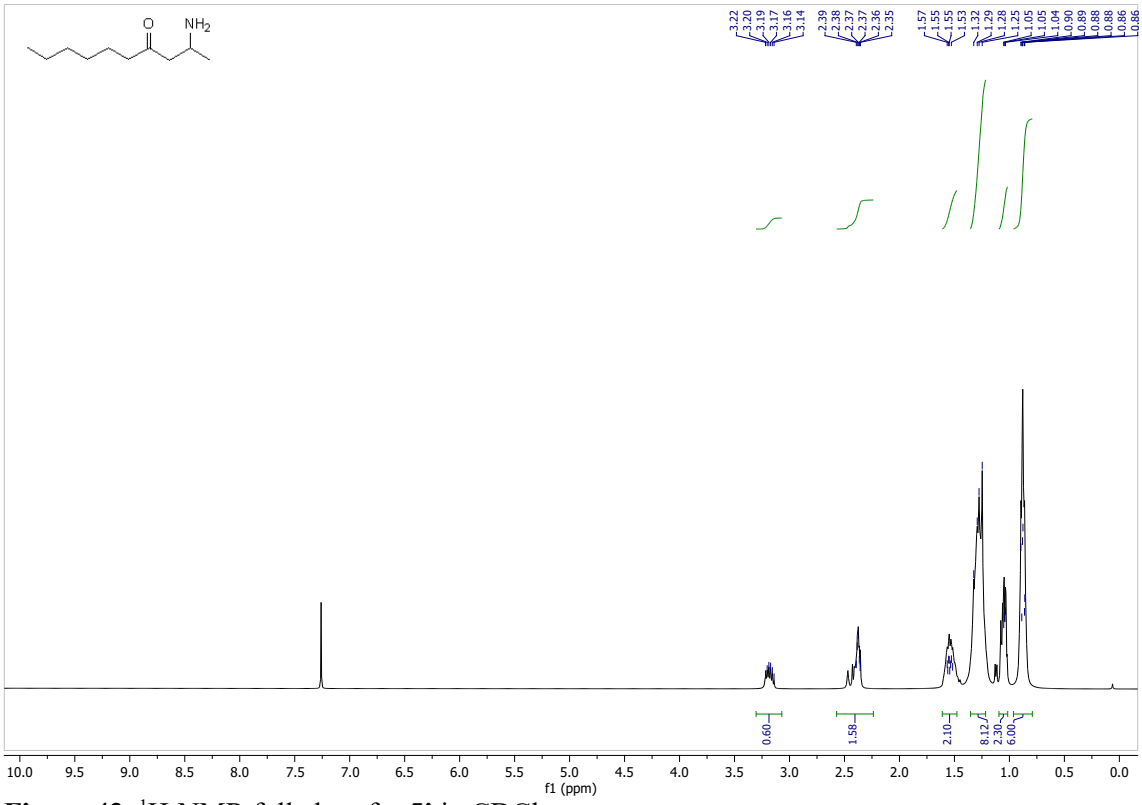


Figure 43. ^{1}H-NMR full chart for **5j** in $CDCl_3$.

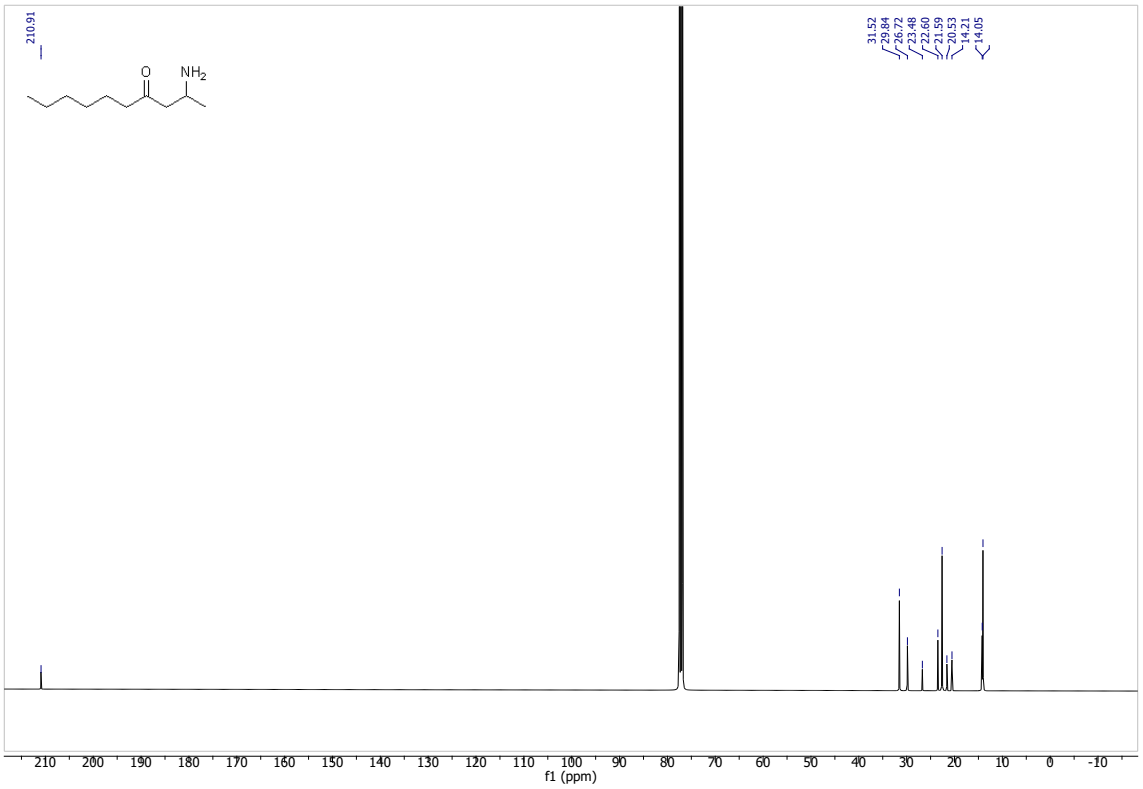


Figure 44. ^{13}C-NMR full chart for **5j** in $CDCl_3$.

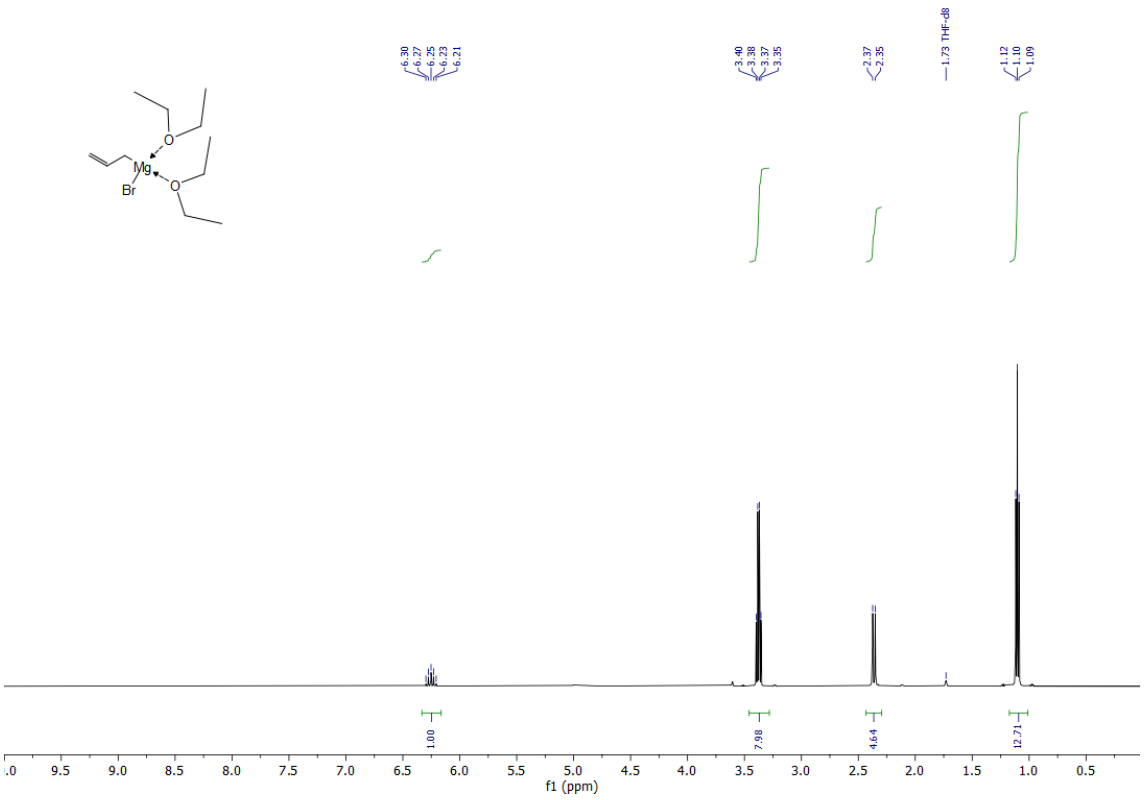


Figure 45. ^{1}H-NMR full chart for **allylmagnesium bromide** in THF-d_8.

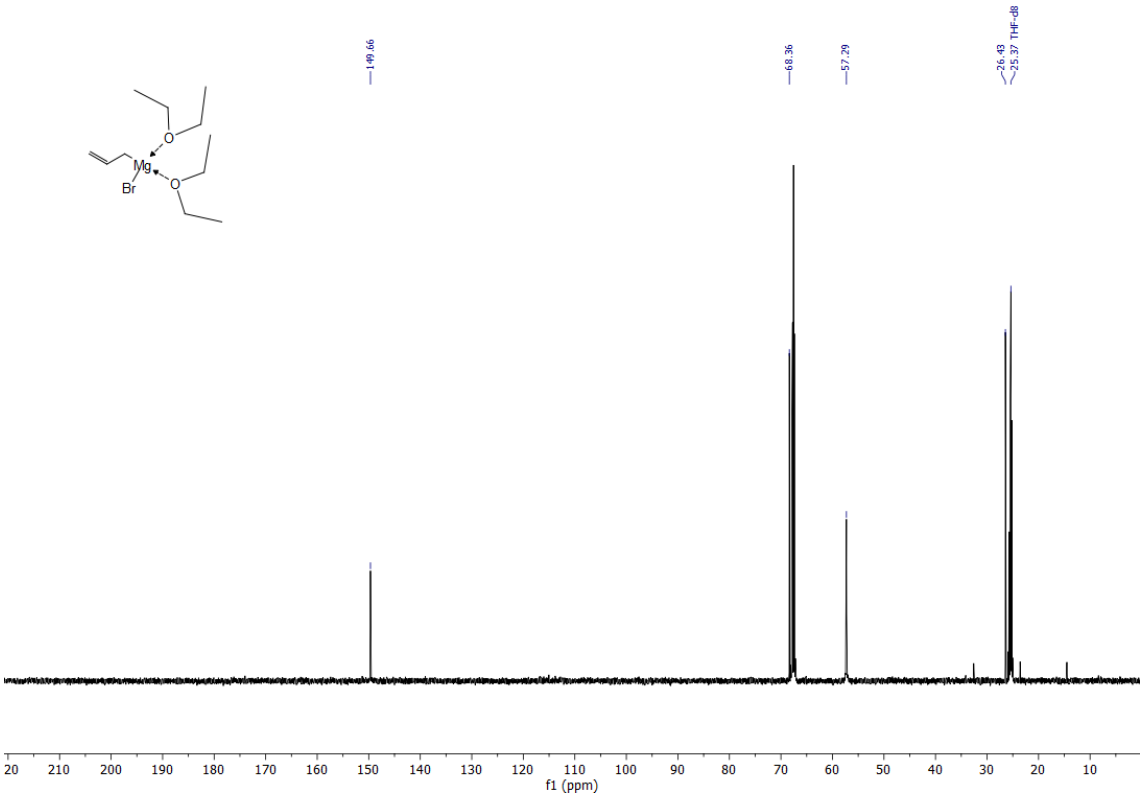


Figure 46. ^{13}C-NMR full chart for **allylmagnesium bromide** in THF-d_8.

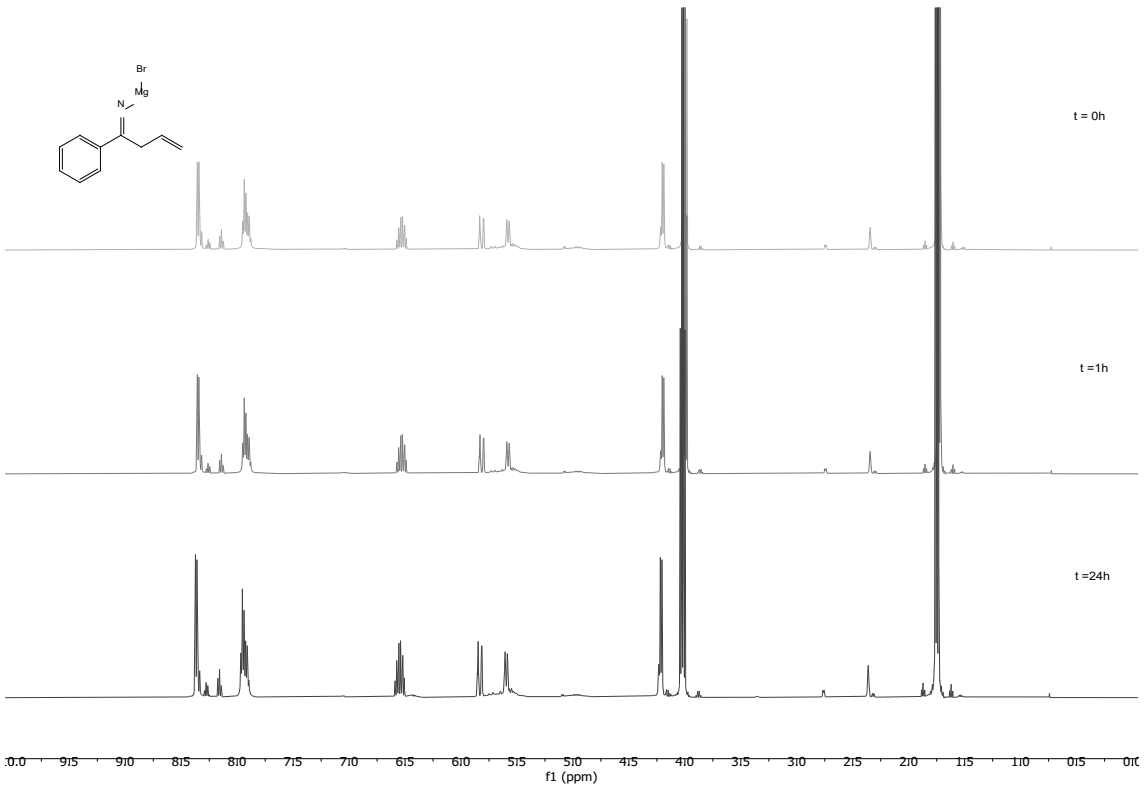


Figure 47. ^{1}H-NMR full chart of the reaction between allylmagnesium bromide (in Et_2O) and benzonitrile in THF-d_8 at different times, under inert atmosphere at room temperature in a Young-valve NMR tube.

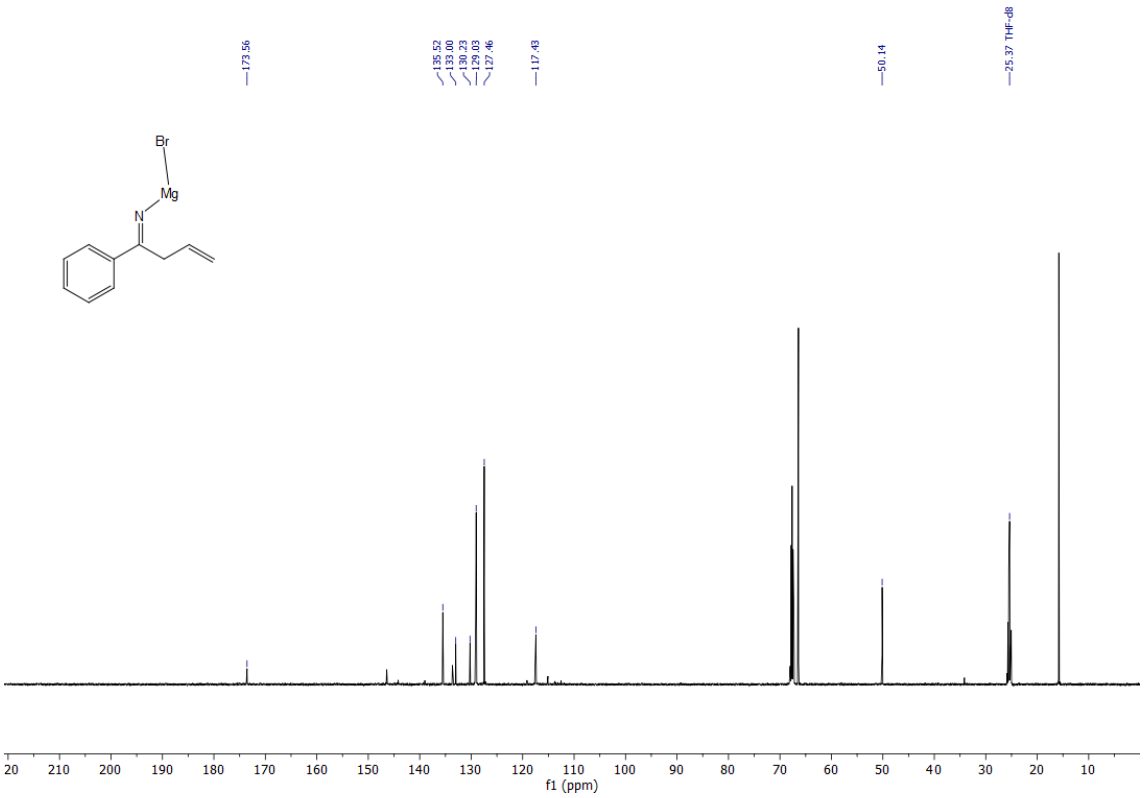


Figure 48. ^{13}C-NMR full chart for **I** in THF-d_8.

4.- Computational methods

Computational Details.

All the calculations reported in this paper were obtained with the Gaussian 09 suite of programs.[2] All species were optimized using the B3LYP functional[3] in conjunction with the D3 dispersion correction suggested by Grimme et al.[4] using the standard double-ζ quality def2-SVP[5] basis sets for all atoms. Solvents effects were taken into account during the geometry optimizations using the polarizable continuum model (PCM).[6] This level is denoted PCM(solvent)-B3LYP-D3/def2-SVP. All stationary points were characterized by frequency calculations.[7] Reactants and products have positive definite Hessian matrices, whereas transition structures show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the intrinsic reaction coordinate (IRC) method.[8] Single-point calculations were carried out at the same DFT level using the much larger triple-ζ quality def2-TZVPP basis set.[5]

Cartesian coordinates (in Å) and free energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the PCM(solvent)-B3LYP-D3/def2-SVP.

IV: G= -1082.832819

C	1.985195000	2.414619000	-0.807358000
C	3.072546000	1.584977000	-0.349842000
C	3.066867000	0.202160000	-0.334569000
H	1.213459000	1.917292000	-1.415088000
C	1.858116000	3.751301000	-0.630494000
C	-2.961356000	0.031294000	0.431508000
C	-3.014981000	1.163393000	1.421674000
C	-2.473943000	2.382965000	1.256512000
H	2.591281000	4.320209000	-0.048772000
H	1.033617000	4.310513000	-1.078928000
H	-3.560195000	0.961423000	2.352577000
Mg	0.038319000	-0.189121000	-0.154006000
N	-1.883812000	-0.390901000	-0.092185000
N	1.941021000	-0.556319000	-0.539836000
H	-2.568005000	3.095005000	2.086369000
C	-4.299618000	-0.602175000	0.109992000
C	-5.516420000	0.039008000	0.403258000
C	-4.342117000	-1.855555000	-0.526865000
C	-6.738944000	-0.553166000	0.066865000
C	-5.558717000	-2.452453000	-0.856180000
C	-6.764707000	-1.801786000	-0.561101000
H	-5.510368000	1.020181000	0.883344000
H	-3.393216000	-2.344284000	-0.757948000
H	-7.674358000	-0.034972000	0.294635000
H	-5.571888000	-3.430013000	-1.346227000
H	-7.719107000	-2.267147000	-0.821431000
C	4.342820000	-0.523732000	-0.043527000
C	5.585325000	-0.034524000	-0.492381000
C	4.330759000	-1.734804000	0.676512000
C	6.769569000	-0.724099000	-0.223362000
C	5.514590000	-2.426248000	0.945699000
C	6.740560000	-1.923897000	0.497008000
H	5.615226000	0.884894000	-1.080842000
H	3.380068000	-2.126803000	1.045680000
H	7.720808000	-0.328620000	-0.589448000
H	5.479989000	-3.359397000	1.514372000
H	7.667258000	-2.465660000	0.703083000
C	-1.764490000	2.898708000	0.038699000
H	-2.132191000	3.904266000	-0.226787000
H	-0.679757000	3.009344000	0.217805000
H	-1.897335000	2.236639000	-0.829268000
H	3.967118000	2.097154000	0.013317000
H	2.190986000	-1.515952000	-0.776510000

TS: G= -1082.788618

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C	-1.907791000	0.942352000	0.494775000
C	-2.533787000	-0.319961000	0.465961000
H	-0.094277000	0.428845000	1.546145000
C	0.097897000	2.418106000	0.762551000

C	2.568011000	0.306603000	-0.490318000
C	2.416994000	1.729427000	-0.611556000
C	1.200041000	2.422408000	-0.856631000
H	-0.529688000	3.279088000	0.500207000
H	0.872409000	2.656788000	1.494803000
H	3.252664000	2.347657000	-0.270818000
Mg	0.040100000	-1.471154000	-0.179784000
N	1.609993000	-0.556819000	-0.630683000
N	-1.820231000	-1.469819000	0.561472000
H	1.351401000	3.510931000	-0.867645000
C	3.956559000	-0.191173000	-0.112926000
C	4.795054000	0.484389000	0.792860000
C	4.418336000	-1.405344000	-0.653031000
C	6.043833000	-0.037207000	1.149945000
C	5.671634000	-1.920428000	-0.315600000
C	6.491471000	-1.239231000	0.593138000
H	4.459918000	1.420106000	1.246098000
H	3.766834000	-1.940261000	-1.348127000
H	6.668781000	0.498656000	1.870130000
H	6.013317000	-2.858742000	-0.762356000
H	7.470030000	-1.643690000	0.865697000
C	-4.007891000	-0.391425000	0.267230000
C	-4.864055000	0.604073000	0.780310000
C	-4.587594000	-1.467237000	-0.436141000
C	-6.245325000	0.528040000	0.592802000
C	-5.968956000	-1.542702000	-0.624523000
C	-6.804875000	-0.545205000	-0.110391000
H	-4.440104000	1.431234000	1.353295000
H	-3.943268000	-2.239350000	-0.863514000
H	-6.890871000	1.306961000	1.006773000
H	-6.394827000	-2.380274000	-1.183108000
H	-7.886510000	-0.604573000	-0.255241000
C	0.229919000	1.997688000	-1.944280000
H	-0.712364000	2.565584000	-1.894203000
H	0.688541000	2.186831000	-2.929931000
H	0.006109000	0.927884000	-1.877486000
H	-2.482504000	1.792944000	0.118800000
H	-2.410478000	-2.282340000	0.725508000

adduct: G= -1082.849246

C	0.012882000	1.365031000	-1.189739000
C	1.301131000	0.951999000	-0.498122000
C	1.952369000	-0.224285000	-0.762681000
H	0.234115000	1.307204000	-2.278740000
C	-0.400859000	2.827797000	-0.931447000
C	-2.076857000	0.787219000	-0.043742000
C	-2.163448000	1.986651000	0.603109000
C	-1.130663000	3.066075000	0.405890000
H	0.488359000	3.475619000	-1.014282000
H	-1.087220000	3.123630000	-1.742447000
H	-2.955009000	2.137144000	1.341621000
Mg	-0.537361000	-1.293931000	-1.706208000
N	-1.118523000	0.423721000	-0.958156000
N	1.421789000	-1.230309000	-1.566594000
H	-1.646967000	4.042356000	0.314564000

C	-3.089115000	-0.273898000	0.250258000
C	-4.459344000	-0.060418000	0.021579000
C	-2.686865000	-1.523447000	0.762595000
C	-5.396177000	-1.066110000	0.282289000
C	-3.621797000	-2.532290000	1.021407000
C	-4.981435000	-2.307881000	0.776681000
H	-4.781793000	0.906724000	-0.371480000
H	-1.632799000	-1.683446000	1.011250000
H	-6.457040000	-0.881056000	0.092346000
H	-3.290069000	-3.488835000	1.434693000
H	-5.714244000	-3.093431000	0.978404000
C	3.284811000	-0.487309000	-0.130476000
C	4.230132000	0.540785000	0.054003000
C	3.637063000	-1.785273000	0.289582000
C	5.467454000	0.285930000	0.649930000
C	4.875146000	-2.043247000	0.884658000
C	5.797544000	-1.008123000	1.069621000
H	3.992374000	1.547848000	-0.295347000
H	2.918058000	-2.598104000	0.161993000
H	6.184874000	1.101447000	0.776528000
H	5.118376000	-3.058194000	1.211413000
H	6.767890000	-1.208555000	1.531403000
C	-0.190152000	3.189766000	1.621021000
H	0.574028000	3.972052000	1.465625000
H	-0.763893000	3.452345000	2.525432000
H	0.324503000	2.238490000	1.823456000
H	1.746310000	1.638486000	0.222237000
H	2.134697000	-1.892269000	-1.859405000

IV-S: G= -1392.592260

C	1.379820000	2.661758000	-0.289731000
C	2.637721000	1.972118000	-0.425983000
C	2.799152000	0.611929000	-0.645952000
H	0.471614000	2.102073000	-0.555132000
C	1.207023000	3.949453000	0.093222000
C	-2.876486000	0.586311000	-0.435629000
C	-2.782727000	2.088994000	-0.429084000
C	-2.265117000	2.853734000	0.547909000
H	2.057486000	4.581628000	0.372102000
H	0.213921000	4.403433000	0.118918000
H	-3.197034000	2.596898000	-1.309811000
Mg	-0.020893000	-0.453444000	0.284725000
N	-1.921253000	-0.192042000	-0.139827000
N	1.799942000	-0.314267000	-0.576985000
H	-2.246862000	3.938614000	0.383996000
C	-4.233094000	0.051575000	-0.864771000
C	-4.333361000	-1.240337000	-1.410514000
C	-5.412393000	0.800856000	-0.709263000
C	-5.568360000	-1.768279000	-1.788708000
C	-6.655480000	0.270248000	-1.073725000
C	-6.737976000	-1.014921000	-1.617826000
H	-3.413866000	-1.816570000	-1.535698000
H	-5.359892000	1.805680000	-0.282536000
H	-5.623832000	-2.770850000	-2.222530000
H	-7.562726000	0.864269000	-0.932351000

H	-7.707030000	-1.427997000	-1.910556000
C	4.185836000	0.109457000	-0.918954000
C	5.081840000	0.824466000	-1.736687000
C	4.626488000	-1.109248000	-0.367021000
C	6.369713000	0.343531000	-1.986035000
C	5.915404000	-1.590203000	-0.611069000
C	6.794227000	-0.865647000	-1.423477000
H	4.750747000	1.757828000	-2.197044000
H	3.952493000	-1.674638000	0.280017000
H	7.043745000	0.911977000	-2.632625000
H	6.237184000	-2.533002000	-0.160184000
H	7.801312000	-1.242347000	-1.620397000
C	-1.708045000	2.385782000	1.858911000
H	-0.606065000	2.439844000	1.845471000
H	-2.049943000	3.033691000	2.683396000
H	-1.989634000	1.347196000	2.073688000
H	3.542754000	2.579658000	-0.340006000
H	2.108201000	-1.187622000	-1.004479000
O	-0.017682000	-2.513344000	0.650224000
C	1.115384000	-3.152338000	1.226572000
H	1.423985000	-4.019443000	0.618267000
H	1.925492000	-2.412582000	1.250207000
H	0.890049000	-3.488368000	2.253664000
O	0.376531000	-0.147701000	2.302497000
C	1.546014000	0.505328000	2.797834000
H	2.171685000	-0.209199000	3.359812000
H	2.100227000	0.887519000	1.931596000
H	1.262200000	1.344058000	3.455230000
C	-1.177622000	-3.340239000	0.541405000
H	-0.985042000	-4.181314000	-0.146404000
H	-1.457355000	-3.735420000	1.533668000
H	-1.975429000	-2.692489000	0.155468000
C	-0.479139000	-0.679509000	3.307787000
H	-1.350775000	-1.115291000	2.802240000
H	0.044179000	-1.460842000	3.885703000
H	-0.815618000	0.118558000	3.990244000

TS-S: G= -1392.549185

C	-0.612256000	-2.045785000	-0.967308000
C	-1.925449000	-1.709435000	-0.577810000
C	-2.546134000	-0.467758000	-0.824171000
H	-0.106015000	-1.383592000	-1.676497000
C	0.073197000	-3.216484000	-0.559572000
C	2.579872000	-0.950248000	0.136888000
C	2.434993000	-2.313345000	0.600066000
C	1.215679000	-2.921114000	1.001038000
H	-0.561410000	-4.005499000	-0.135281000
H	0.834976000	-3.600078000	-1.242355000
H	3.237931000	-3.002561000	0.311908000
Mg	-0.019772000	0.858860000	-0.166121000
N	1.626287000	-0.096467000	0.002283000
N	-1.811350000	0.633250000	-1.106422000
H	1.348605000	-3.987564000	1.231024000
C	3.991763000	-0.561334000	-0.291177000
C	4.184896000	0.287235000	-1.394719000

C	5.125959000	-0.988486000	0.420103000
C	5.465151000	0.688248000	-1.783308000
C	6.410752000	-0.576288000	0.046327000
C	6.586989000	0.261329000	-1.059860000
H	3.301287000	0.623324000	-1.943185000
H	4.993315000	-1.638838000	1.289131000
H	5.592882000	1.335984000	-2.655865000
H	7.278293000	-0.908860000	0.624025000
H	7.589817000	0.580941000	-1.356404000
C	-4.027807000	-0.358754000	-0.701994000
C	-4.871358000	-1.461603000	-0.952112000
C	-4.634347000	0.862921000	-0.340104000
C	-6.257462000	-1.349900000	-0.833945000
C	-6.021364000	0.976015000	-0.223436000
C	-6.841276000	-0.130649000	-0.468573000
H	-4.431404000	-2.409506000	-1.267966000
H	-4.008203000	1.732435000	-0.126928000
H	-6.888877000	-2.218304000	-1.039717000
H	-6.464311000	1.932500000	0.066705000
H	-7.927133000	-0.043474000	-0.380223000
C	0.281902000	-2.255690000	1.996887000
H	-0.657357000	-2.819273000	2.114308000
H	0.773072000	-2.201849000	2.983662000
H	0.039897000	-1.235485000	1.684050000
H	-2.507174000	-2.472667000	-0.053205000
H	-2.379467000	1.389767000	-1.482246000
O	0.476074000	2.851666000	-0.410465000
C	-0.480949000	3.890550000	-0.239523000
H	-0.371117000	4.652859000	-1.029061000
H	-1.477188000	3.434293000	-0.308163000
H	-0.364707000	4.365624000	0.749896000
O	-0.595666000	1.237554000	1.818045000
C	-1.852524000	0.917484000	2.407246000
H	-2.203879000	1.751113000	3.039059000
H	-2.560749000	0.745912000	1.589438000
H	-1.770457000	0.001782000	3.016834000
C	1.840317000	3.281135000	-0.382965000
H	2.046464000	3.947230000	-1.237696000
H	2.051851000	3.815338000	0.559472000
H	2.450567000	2.370060000	-0.442145000
C	0.453244000	1.462547000	2.759731000
H	1.375890000	1.623988000	2.188402000
H	0.224782000	2.345506000	3.380611000
H	0.586537000	0.577802000	3.403925000

adduct-S: G= -1392.613686

C	-0.493107000	1.250134000	1.577159000
C	-1.795572000	1.004197000	0.831126000
C	-2.278127000	-0.251723000	0.563494000
H	-0.577053000	0.656167000	2.514113000
C	-0.316555000	2.719863000	2.001999000
C	1.493497000	1.618317000	0.208355000
C	1.302322000	2.975095000	0.140911000
C	0.171228000	3.651289000	0.872040000
H	-1.259220000	3.091216000	2.439421000

H	0.440938000	2.747853000	2.803819000
H	2.022472000	3.593805000	-0.399803000
Mg	0.430816000	-1.237047000	0.589894000
N	0.715460000	0.721258000	0.893043000
N	-1.547157000	-1.401851000	0.798998000
H	0.566606000	4.561439000	1.365585000
C	2.689036000	1.034707000	-0.480763000
C	3.478762000	0.051275000	0.146962000
C	3.069098000	1.449254000	-1.772257000
C	4.610904000	-0.480209000	-0.477309000
C	4.200599000	0.919340000	-2.400113000
C	4.980823000	-0.048053000	-1.755719000
H	3.208914000	-0.277634000	1.151023000
H	2.457237000	2.193376000	-2.286905000
H	5.212016000	-1.232662000	0.041035000
H	4.470075000	1.258806000	-3.404117000
H	5.864276000	-0.463507000	-2.247261000
C	-3.623204000	-0.395229000	-0.081882000
C	-4.701065000	0.449123000	0.249383000
C	-3.848355000	-1.396457000	-1.047595000
C	-5.945442000	0.309558000	-0.369859000
C	-5.092174000	-1.538233000	-1.669335000
C	-6.148803000	-0.684903000	-1.334283000
H	-4.557140000	1.211743000	1.018036000
H	-3.025122000	-2.059743000	-1.324331000
H	-6.766945000	0.974821000	-0.089415000
H	-5.235840000	-2.317116000	-2.423724000
H	-7.124096000	-0.797048000	-1.815323000
C	-0.938162000	4.137950000	-0.082105000
H	-1.776657000	4.600179000	0.469488000
H	-0.536610000	4.891626000	-0.780199000
H	-1.336130000	3.309433000	-0.686068000
H	-2.391514000	1.863863000	0.525697000
H	-2.132667000	-2.231532000	0.751196000
O	1.523909000	-2.293474000	1.976810000
C	1.620397000	-3.715264000	2.049226000
H	0.931904000	-4.111167000	2.814307000
H	1.343320000	-4.117357000	1.064993000
H	2.653633000	-4.016116000	2.289526000
O	0.786041000	-1.642694000	-1.415431000
C	0.041339000	-0.764553000	-2.272450000
H	-0.304419000	-1.316392000	-3.161746000
H	-0.822029000	-0.397338000	-1.702781000
H	0.672444000	0.086369000	-2.573408000
C	1.861285000	-1.612382000	3.192945000
H	1.193445000	-1.937962000	4.007213000
H	2.910047000	-1.820204000	3.460765000
H	1.725236000	-0.539316000	2.999921000
C	1.936032000	-2.215942000	-2.036685000
H	2.432412000	-2.852591000	-1.293192000
H	1.631107000	-2.829712000	-2.900927000
H	2.633309000	-1.428157000	-2.360476000

A: G= -441.956270

C	0.875985000	0.295787000	0.268975000

C	1.738037000	-0.896435000	-0.107260000
C	3.223005000	-0.764223000	-0.334792000
H	1.297203000	-1.365224000	-1.005950000
N	1.393940000	1.378617000	0.711788000
H	3.679649000	-1.722362000	-0.617813000
C	-0.606591000	0.104434000	0.103784000
C	-1.222647000	-1.143004000	0.316411000
C	-1.414856000	1.195570000	-0.267406000
C	-2.607192000	-1.285977000	0.187962000
C	-2.796400000	1.049901000	-0.408471000
C	-3.398647000	-0.191707000	-0.176038000
H	-0.626437000	-2.010565000	0.604352000
H	-0.954845000	2.166203000	-0.470006000
H	-3.069111000	-2.259017000	0.372779000
H	-3.403976000	1.907453000	-0.708067000
H	-4.480016000	-0.307033000	-0.283738000
C	4.016286000	0.309830000	-0.258877000
H	5.084092000	0.217919000	-0.480992000
H	3.625445000	1.285427000	0.029787000
H	0.662270000	2.056006000	0.954192000
H	1.586279000	-1.664170000	0.677210000

B: G= -441.966263

C	-0.881893000	-0.196253000	0.137938000
C	-1.710764000	0.826277000	-0.247856000
C	-3.164112000	0.862340000	-0.228149000
H	-1.223268000	1.738234000	-0.597787000
N	-1.329119000	-1.429792000	0.575755000
H	-3.581398000	1.878451000	-0.239995000
C	0.598772000	-0.054266000	0.053875000
C	1.236956000	1.172945000	0.320174000
C	1.399688000	-1.161151000	-0.292469000
C	2.625298000	1.291864000	0.230022000
C	2.789177000	-1.040629000	-0.381769000
C	3.408537000	0.186160000	-0.122225000
H	0.640418000	2.035683000	0.623472000
H	0.926663000	-2.119896000	-0.515994000
H	3.099958000	2.252066000	0.447790000
H	3.389684000	-1.910051000	-0.661545000
H	4.495295000	0.280087000	-0.189213000
C	-4.057791000	-0.153933000	-0.218208000
H	-5.131069000	0.053077000	-0.191171000
H	-3.772137000	-1.205493000	-0.299961000
H	-0.705166000	-1.922342000	1.208499000
H	-2.298347000	-1.471393000	0.877617000

TS1: G= -441.928633

C	-0.899201000	-0.229007000	-0.103478000
C	-1.720243000	0.855417000	-0.534304000
C	-3.069713000	0.885609000	-0.203519000
H	-1.232266000	1.764058000	-0.888399000
N	-1.472778000	-1.344535000	0.341354000
H	-3.541495000	1.876919000	-0.148860000
C	0.582969000	-0.068550000	-0.047631000
C	1.188997000	1.172639000	0.226660000

C	1.411884000	-1.186071000	-0.269172000
C	2.579686000	1.289085000	0.285341000
C	2.802759000	-1.067873000	-0.213671000
C	3.391270000	0.170272000	0.064682000
H	0.567976000	2.048946000	0.421440000
H	0.962104000	-2.151870000	-0.511788000
H	3.032060000	2.257851000	0.511533000
H	3.428849000	-1.944633000	-0.396847000
H	4.479234000	0.264018000	0.108204000
C	-3.799663000	-0.262326000	0.235343000
H	-4.756432000	-0.070173000	0.737918000
H	-3.875623000	-1.094133000	-0.481946000
H	-2.716867000	-0.994601000	0.681811000
H	-0.850556000	-1.899816000	0.935954000

TS1': G= -594.651864

C	-0.005131000	-0.083979000	-0.121257000
C	0.595834000	-1.371388000	-0.291704000
C	1.858234000	-1.693621000	-0.742130000
H	-0.083314000	-2.209732000	-0.132318000
N	0.646416000	1.060471000	-0.070381000
H	2.043080000	-2.774312000	-0.796411000
C	-1.491681000	-0.018609000	-0.012534000
C	-2.202768000	-0.942909000	0.775116000
C	-2.203610000	0.984234000	-0.698232000
C	-3.592027000	-0.855033000	0.883895000
C	-3.594356000	1.057995000	-0.599331000
C	-4.291907000	0.141482000	0.194713000
H	-1.667604000	-1.716248000	1.329181000
H	-1.671801000	1.693409000	-1.337151000
H	-4.129909000	-1.568555000	1.512420000
H	-4.134754000	1.831673000	-1.149644000
H	-5.379871000	0.202436000	0.274903000
C	2.970665000	-0.857687000	-1.120861000
H	3.657816000	-1.359516000	-1.816906000
H	2.701909000	0.148639000	-1.470367000
H	3.627651000	-0.618241000	-0.123572000
H	0.090833000	1.897120000	0.091946000
O	4.354235000	-0.081661000	1.092387000
H	3.767553000	-0.476233000	1.756101000
H	3.687411000	1.092455000	0.779361000
H	1.696304000	1.247940000	0.041207000
O	3.080990000	1.929777000	0.443255000
H	3.528467000	2.238037000	-0.357271000

C: G= -441.965819

C	-0.851219000	-0.467477000	-0.102758000
C	-1.719726000	0.596778000	-0.662710000
C	-3.028407000	0.806062000	-0.411529000
H	-1.219590000	1.298835000	-1.336823000
N	-1.352203000	-1.584758000	0.295944000
H	-3.489436000	1.655352000	-0.931977000
C	0.618784000	-0.162588000	-0.048552000
C	1.079865000	1.133494000	0.245811000
C	1.564997000	-1.180440000	-0.269286000

C	2.449092000	1.398633000	0.339463000
C	2.933276000	-0.912925000	-0.189288000
C	3.379664000	0.377351000	0.119715000
H	0.361575000	1.937206000	0.423408000
H	1.226687000	-2.187515000	-0.526920000
H	2.790214000	2.407657000	0.584292000
H	3.654325000	-1.712734000	-0.375712000
H	4.450328000	0.586995000	0.183850000
C	-3.941591000	0.040705000	0.493690000
H	-4.585807000	0.730900000	1.063287000
H	-4.619810000	-0.594457000	-0.105652000
H	-3.394157000	-0.623270000	1.173464000
H	-0.617311000	-2.183219000	0.689847000

TS2: G= -883.881967

C	0.313121000	-0.987962000	1.218994000
C	1.538922000	-0.313222000	1.007340000
C	2.728018000	-0.740565000	0.420083000
H	-0.416572000	-0.403453000	1.783884000
C	-0.139378000	-2.262187000	0.793767000
C	-2.402334000	-0.120447000	-0.485712000
C	-2.257048000	-1.504342000	-0.784415000
C	-1.005527000	-2.160774000	-0.948570000
H	0.592204000	-3.035663000	0.544548000
H	-0.970961000	-2.675425000	1.368506000
H	-3.135869000	-2.138390000	-0.641897000
N	-1.361981000	0.688447000	-0.448500000
N	2.972241000	-2.009833000	0.012198000
H	-1.124328000	-3.244428000	-1.088131000
C	-3.779978000	0.383158000	-0.144476000
C	-4.650788000	-0.335144000	0.695597000
C	-4.213674000	1.625318000	-0.645306000
C	-5.910171000	0.173754000	1.027889000
C	-5.475628000	2.131562000	-0.322450000
C	-6.329267000	1.407702000	0.517983000
H	-4.329675000	-1.293563000	1.109975000
H	-3.554497000	2.192705000	-1.307729000
H	-6.565936000	-0.394691000	1.692892000
H	-5.795763000	3.093327000	-0.732134000
H	-7.315390000	1.803385000	0.774480000
C	3.845582000	0.221482000	0.234675000
C	3.593119000	1.558227000	-0.133328000
C	5.183890000	-0.184722000	0.411876000
C	4.644582000	2.459322000	-0.310367000
C	6.233662000	0.719426000	0.236210000
C	5.968982000	2.044830000	-0.125820000
H	2.565321000	1.883379000	-0.306633000
H	5.405239000	-1.209757000	0.718760000
H	4.429008000	3.489546000	-0.604525000
H	7.263562000	0.388026000	0.390565000
H	6.790929000	2.751110000	-0.266297000
C	0.081640000	-1.597620000	-1.849463000
H	0.995788000	-2.207903000	-1.809130000
H	-0.284524000	-1.597061000	-2.890732000
H	0.321711000	-0.565311000	-1.571019000

H	1.562240000	0.713470000	1.375274000
H	-1.648073000	1.596641000	-0.068406000
H	2.336489000	-2.766156000	0.216082000
H	3.800921000	-2.236868000	-0.521265000

TS2': G= -883.867438

C	-0.102073000	-1.591277000	-1.280885000
C	-1.390948000	-0.963851000	-1.775535000
C	-2.616273000	-1.023550000	-0.873171000
H	0.738034000	-1.408840000	-1.955461000
C	-0.011335000	-2.682259000	-0.421198000
C	1.811496000	-0.232270000	0.474584000
C	1.699200000	-1.343236000	1.343041000
C	0.495807000	-2.029252000	1.566736000
H	-0.938077000	-3.160303000	-0.100340000
H	0.861505000	-3.330602000	-0.508007000
H	2.626342000	-1.844903000	1.632282000
N	0.730483000	0.191264000	-0.168190000
N	-3.118566000	-2.173529000	-0.611857000
H	0.622678000	-3.015296000	2.033133000
C	3.163538000	0.336061000	0.164720000
C	4.304498000	-0.475385000	0.018883000
C	3.307627000	1.725937000	-0.011270000
C	5.545885000	0.084446000	-0.296518000
C	4.549244000	2.287118000	-0.321125000
C	5.674108000	1.467647000	-0.465891000
H	4.217659000	-1.558263000	0.129662000
H	2.437461000	2.375662000	0.114067000
H	6.416799000	-0.564994000	-0.417622000
H	4.639635000	3.369548000	-0.443773000
H	6.645861000	1.904524000	-0.709521000
C	-3.206523000	0.265501000	-0.386431000
C	-2.394691000	1.360841000	-0.036569000
C	-4.603076000	0.392300000	-0.260213000
C	-2.967010000	2.539443000	0.449961000
C	-5.173675000	1.576946000	0.210657000
C	-4.356266000	2.654260000	0.571446000
H	-1.308902000	1.266480000	-0.108744000
H	-5.252588000	-0.435828000	-0.555828000
H	-2.322083000	3.374439000	0.735916000
H	-6.260465000	1.661735000	0.289236000
H	-4.801600000	3.581278000	0.941486000
C	-0.801282000	-1.362556000	1.962998000
H	-1.658813000	-2.041424000	1.860998000
H	-0.726391000	-1.075410000	3.027386000
H	-0.991393000	-0.458268000	1.379533000
H	-1.194607000	0.068745000	-2.092426000
H	0.990131000	0.841067000	-0.916925000
H	-3.925756000	-2.082686000	0.015596000
H	-1.668364000	-1.511997000	-2.695637000

D: G= -883.962652

C	-0.035565000	-1.235790000	-0.914980000
C	-1.473392000	-0.773527000	-0.888043000
C	-2.044800000	-0.005893000	0.079109000

H	0.198712000	-1.548884000	-1.953103000
C	0.217327000	-2.457096000	-0.012655000
C	2.219448000	-0.487939000	-0.243433000
C	2.615059000	-1.767412000	-0.034219000
C	1.671655000	-2.946131000	-0.104112000
H	-0.013672000	-2.174979000	1.029341000
H	-0.480272000	-3.261771000	-0.291587000
H	3.649740000	-1.956380000	0.260842000
N	0.883446000	-0.161593000	-0.515176000
N	-1.366570000	0.413613000	1.223667000
H	1.799721000	-3.446495000	-1.085203000
C	3.143003000	0.671796000	-0.117213000
C	4.501868000	0.564265000	-0.472044000
C	2.677718000	1.911873000	0.364471000
C	5.367826000	1.650819000	-0.332689000
C	3.544821000	2.999882000	0.500884000
C	4.894242000	2.874779000	0.155418000
H	4.877044000	-0.376504000	-0.880463000
H	1.630144000	2.020217000	0.653741000
H	6.417559000	1.544821000	-0.618714000
H	3.162796000	3.949609000	0.884409000
H	5.571621000	3.726126000	0.259414000
C	-3.488921000	0.359769000	0.023379000
C	-4.139576000	0.601652000	-1.201985000
C	-4.240368000	0.473968000	1.209736000
C	-5.497389000	0.926398000	-1.240957000
C	-5.598664000	0.801663000	1.170225000
C	-6.234659000	1.027341000	-0.054969000
H	-3.567790000	0.554644000	-2.131189000
H	-3.756757000	0.283817000	2.170198000
H	-5.980405000	1.114304000	-2.203473000
H	-6.163810000	0.876069000	2.103073000
H	-7.295993000	1.286468000	-0.086170000
C	1.983977000	-3.986137000	0.979432000
H	1.303383000	-4.850251000	0.907887000
H	3.017079000	-4.359374000	0.887357000
H	1.873239000	-3.546721000	1.985249000
H	-2.117533000	-1.172696000	-1.673109000
H	0.769855000	0.676915000	-1.079164000
H	-0.352790000	0.354246000	1.123358000
H	-1.661657000	1.316988000	1.585745000

E: G= -883.958895

C	-0.008682000	1.182918000	-1.028990000
C	1.432322000	0.657501000	-1.051696000
C	2.073566000	0.164240000	0.233942000
H	-0.219120000	1.501729000	-2.072696000
C	-0.233133000	2.413697000	-0.143918000
C	-2.241839000	0.454181000	-0.294594000
C	-2.630087000	1.738358000	-0.081330000
C	-1.685577000	2.910399000	-0.236170000
H	-0.002479000	2.145167000	0.896987000
H	0.467228000	3.208488000	-0.448718000
H	-3.639237000	1.929442000	0.290787000
N	-0.938922000	0.126276000	-0.652894000

N	1.447284000	0.195348000	1.348838000
H	-1.830674000	3.362977000	-1.238351000
C	-3.150109000	-0.704120000	-0.075224000
C	-4.524688000	-0.624454000	-0.369333000
C	-2.647719000	-1.914537000	0.442680000
C	-5.370334000	-1.712340000	-0.139815000
C	-3.494082000	-3.003562000	0.669159000
C	-4.859610000	-2.907761000	0.380523000
H	-4.927706000	0.294724000	-0.800166000
H	-1.586176000	-1.989522000	0.688639000
H	-6.433730000	-1.630294000	-0.379802000
H	-3.084320000	-3.930413000	1.079431000
H	-5.521307000	-3.760039000	0.554815000
C	3.491983000	-0.318854000	0.108709000
C	3.924717000	-1.090751000	-0.984982000
C	4.423059000	-0.002213000	1.116311000
C	5.242594000	-1.551928000	-1.055425000
C	5.742933000	-0.451555000	1.039474000
C	6.156375000	-1.232452000	-0.045864000
H	3.226514000	-1.356199000	-1.780866000
H	4.114062000	0.620789000	1.959665000
H	5.556090000	-2.164365000	-1.904566000
H	6.453038000	-0.185345000	1.826403000
H	7.188409000	-1.586805000	-0.106407000
C	-1.968309000	4.004710000	0.800002000
H	-1.287611000	4.862037000	0.669787000
H	-3.002508000	4.376835000	0.714376000
H	-1.834830000	3.615727000	1.823729000
H	2.086528000	1.443613000	-1.468274000
H	-0.841331000	-0.732631000	-1.184921000
H	2.035289000	-0.185275000	2.099411000
H	1.485055000	-0.160854000	-1.791616000

B-H: G= -442.385147

C	0.840815000	0.098428000	0.115733000
C	1.718659000	-0.891620000	-0.143071000
C	3.178707000	-0.865581000	-0.020672000
H	1.283784000	-1.852500000	-0.431515000
N	1.368958000	1.404916000	0.572543000
H	3.612489000	-1.768584000	0.425739000
C	-0.630745000	0.017294000	0.040077000
C	-1.285639000	-1.221036000	0.204391000
C	-1.413813000	1.164388000	-0.199499000
C	-2.673724000	-1.308186000	0.112998000
C	-2.805378000	1.072746000	-0.285047000
C	-3.440379000	-0.162286000	-0.132470000
H	-0.707838000	-2.119036000	0.430015000
H	-0.954289000	2.144003000	-0.346998000
H	-3.162016000	-2.275894000	0.248902000
H	-3.391943000	1.973840000	-0.477486000
H	-4.528603000	-0.232537000	-0.197528000
C	4.008405000	0.107294000	-0.437567000
H	5.087700000	0.016760000	-0.292381000
H	3.662428000	0.992557000	-0.979986000
H	0.823536000	1.777593000	1.363756000

H	2.350389000	1.314717000	0.883607000
H	1.360215000	2.126019000	-0.163168000

TS1-H: G= -518.730298

C	-0.465741000	-0.168213000	-0.406926000
C	-1.218420000	0.932760000	-0.790683000
C	-2.631752000	1.074491000	-0.819014000
H	-0.652305000	1.842310000	-0.990355000
N	-1.023701000	-1.394388000	-0.119530000
H	-2.956978000	2.119736000	-0.892680000
C	0.992796000	-0.040375000	-0.179611000
C	1.535931000	1.127809000	0.391276000
C	1.861928000	-1.092917000	-0.532227000
C	2.910753000	1.238436000	0.601269000
C	3.237436000	-0.974332000	-0.328094000
C	3.765088000	0.189827000	0.240917000
H	0.874161000	1.939006000	0.700181000
H	1.469443000	-1.997563000	-1.003021000
H	3.316450000	2.144261000	1.057538000
H	3.899815000	-1.792193000	-0.620533000
H	4.841466000	0.279088000	0.405855000
C	-3.652994000	0.146854000	-0.635294000
H	-4.684215000	0.502522000	-0.713875000
H	-3.524944000	-0.914777000	-0.868737000
H	-3.339739000	-0.070632000	0.795172000
H	-0.380096000	-2.142446000	0.127088000
O	-2.903144000	-0.526436000	1.804118000
H	-2.604104000	0.179812000	2.407714000
H	-2.097254000	-1.000557000	1.465034000
H	-1.780789000	-1.722414000	-0.715288000

TS1'-H: G= -595.106017

C	-0.054645000	-0.516066000	0.424340000
C	-0.778197000	-1.392869000	-0.387711000
C	-2.141862000	-1.746623000	-0.335755000
H	-0.200090000	-1.870309000	-1.178424000
N	-0.585812000	0.148028000	1.481255000
H	-2.431737000	-2.442555000	-1.132992000
C	1.370473000	-0.234288000	0.122403000
C	1.803669000	-0.078708000	-1.208550000
C	2.311002000	-0.118440000	1.165083000
C	3.144215000	0.190804000	-1.486777000
C	3.652933000	0.139634000	0.880845000
C	4.072225000	0.297940000	-0.444507000
H	1.082102000	-0.140251000	-2.025286000
H	2.005171000	-0.267289000	2.203654000
H	3.464835000	0.323655000	-2.522558000
H	4.374471000	0.210517000	1.697857000
H	5.122093000	0.504784000	-0.665333000
C	-3.209874000	-1.301018000	0.455585000
H	-4.132967000	-1.888735000	0.406300000
H	-3.056318000	-0.810683000	1.422283000
H	-3.579400000	-0.170182000	-0.302227000
H	0.033301000	0.680252000	2.086059000
O	-3.905814000	0.895304000	-0.836565000

H	-3.793673000	0.784855000	-1.796410000
H	-3.189820000	1.558234000	-0.529252000
H	-1.416153000	-0.212524000	1.940361000
H	-1.449786000	1.810681000	0.572052000
O	-2.022015000	2.401742000	0.045579000
H	-2.328331000	3.074787000	0.673294000

C-H: G= -442.413769

C	-0.806291000	0.427070000	0.219688000
C	-1.701572000	-0.598037000	0.738487000
C	-2.984408000	-0.822822000	0.365455000
H	-1.248127000	-1.277440000	1.462980000
N	-1.269974000	1.608981000	-0.113573000
H	-3.480689000	-1.653070000	0.881260000
C	0.629726000	0.151689000	0.094374000
C	1.068076000	-1.169855000	-0.134615000
C	1.581588000	1.190062000	0.191364000
C	2.426698000	-1.439561000	-0.287010000
C	2.938574000	0.910187000	0.051454000
C	3.362234000	-0.402444000	-0.192917000
H	0.341677000	-1.979490000	-0.222782000
H	1.269288000	2.211506000	0.419305000
H	2.757721000	-2.462016000	-0.479687000
H	3.670185000	1.715379000	0.143657000
H	4.427457000	-0.618435000	-0.303342000
C	-3.808921000	-0.151663000	-0.679924000
H	-4.359752000	-0.911502000	-1.256166000
H	-4.577722000	0.480247000	-0.198875000
H	-3.232878000	0.471808000	-1.377099000
H	-0.683008000	2.310916000	-0.559090000
H	-2.228565000	1.881468000	0.086719000

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