*Supporting Information for*

# Ir-Catalyzed Cross-Coupling of Styrene Derivatives with Allylic Carbonates: Free Amine Assisted Vinyl C-H Bond Activation

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**General Methods**. Unless stated otherwise, all reactions were carried out in flame-dried glassware under a dry argon atmosphere. All solvents were purified and dried according to standard methods prior to use.

$^{1}H$ and $^{13}C$ NMR spectra were recorded on a Varian instrument (300 MHz and 75 MHz, respectively) and internally referenced to tetramethylsilane signal or residual protio solvent signals. Data for $^{1}H$ NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration). Data for $^{13}C$ NMR are reported in terms of chemical shift (δ, ppm).

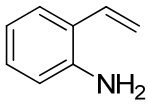
The phosphoramidite ligands[1], the substituted allylic carbonates[2] and styrene derivatives[3] were prepared according to the reported procedures.


(1) Alexakis, K. Tissot-Croset, D. Polet, *Angew. Chem. Int. Ed.* **2004**, *43*, 426-2428.

(2) Wuts, P. G. M.; Ashford, S. W.; Anderson, A. M.; Atkins, J. R. *Org. Lett.* **2003**, *5*, 1483-1485.

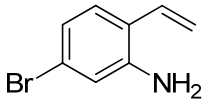
(3) (a) Theeraladanon, C.; Arisawa, M.; Nakagawa, M.; Nishida, A. *Tetrahedron: Asymmetry* **2005**, *16*, 827. (b) Lee, B. S.; Lee, J. K.; Chi, D. Y. *J. Org. Chem.* **2002**, *67*, 7884. (c) Izumi, T.; Sugano, M.; Konno, T.; *J. Heterocycl. Chem.* **1992**, *29*, 899. (d) Cooper, M. K.; Yaniuk, D. W. *J. Organomet. Chem.* **1981**, *221*, 231.

(4) (a) Sato, T.; Ishida, S.; Ishibashi, H.; Ikeda, M. *J. Chem. Soc. Perkin Trans. 1* **1991**, 353. (b) Denmark, S. E.; Butler, C. R. *Org. Lett.* **2006**, *8*, 63. (c) A, Mitsuhiro.; T, Yukiyoshi.; T, Kazuyuki.; N, Masako.; N, Atsushi. *J. Org. Chem.* **2006**, *71*, 4255. (d) Yus, M.; Foubelo, F.; Ferrandez, J. V. *Eur. J. Org. Chem.* **2001**, 2809.



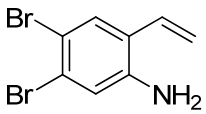
**1a**

Colorless oil.[3a] $^1$H NMR (300 MHz, $CDCl_3$) δ 3.75 (br, 2 H), 5.32 (d, *J* = 11.1 Hz, 1 H), 5.63 (d, *J* = 17.7 Hz, 1 H), 6.68 (d, *J* = 7.8 Hz, 1 H), 6.73-6.82 (m, 2 H), 7.09 (t, *J* = 7.8 Hz, 1 H), 7.29 (d, *J* = 7.5 Hz, 1 H).



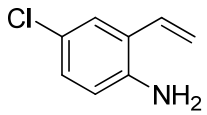
**1b**

Yellow oil. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.75 (br, 2 H), 5.35 (d, *J* = 10.8 Hz, 1 H), 5.63 (d, *J* = 17.4 Hz, 1 H), 6.56 (d, *J* = 8.4 Hz, 1 H), 6.67 (dd, *J* = 17.7, 11.1 Hz, 1 H), 7.16 (d, *J* = 8.7 Hz, 1 H), 7.38 (s, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 116.2, 118.3, 121.5, 121.9, 122.7, 128.5, 131.5, 144.8. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3386, 1627, 1588, 1560, 1485, 1415, 1301, 1256, 990, 887, 806; MS (EI, *m/z*, rel. intsity) 196 ($M^+$, 7), 117 (100); HRMS (EI) calcd for $C_8H_8BrN$ ($M^+$): 196.9840 Found: 196.9839.



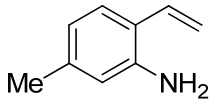
**1c**

White solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.79 (br, 2 H), 5.37 (dd, *J* = 10.8, 0.9 Hz, 1 H), 5.62 (dd, *J* = 17.4, 0.9 Hz, 1 H), 6.58 (dd, *J* = 17.4, 11.1 Hz, 1 H), 6.93 (s, 1 H), 7.44 (s, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 112.5, 117.5, 120.1, 123.8, 125.0, 130.6, 131.4, 143.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3450, 3369, 2924, 2854, 1626, 1467, 1377, 1267, 995, 991, 884; MS (EI, *m/z*, rel. intensity) 275 ($M^+$, 2), 43 (100); HRMS (EI) calcd for $C_8H_7Br_2N$ ($M^+$): 274.8945 Found: 274.8949; m.p. 77-79 $^oC$.



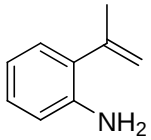

**1d**

Brown liquid.[3b] $^1$H NMR (400 MHz, $CDCl_3$) δ 3.73 (br, 2 H), 5.36 (dd, *J* = 10.8, 1.2 Hz, 1 H), 5.63 (dd, *J* = 18.4, 1.2 Hz, 1 H), 6.60 (d, *J* = 8.4 Hz, 1 H), 6.68 (dd, *J* = 17.2, 10.8 Hz, 1 H), 7.03 (dd, *J* = 8.4, 2.4 Hz, 1 H), 7.24 (d, *J* = 2.4 Hz, 1 H).




**1e**

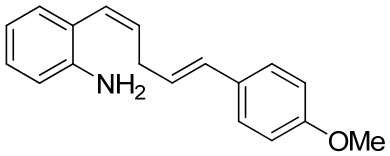
Yellow oil.[3c] $^1$H NMR (300 MHz, $CDCl_3$) δ 2.25 (s, 3 H), 3.69 (br, 2 H), 5.25 (dd, *J* = 11.1, 1.5 Hz, 1 H), 5.58 (dd, *J* = 17.4, 1.5 Hz, 1 H), 6.49 (s, 1 H), 6.58 (d, *J* = 7.8 Hz, 1 H), 6.73 (dd, *J* = 17.4, 11.1 Hz, 1 H), 7.18 (d, *J* = 8.1 Hz, 1 H).




**5**

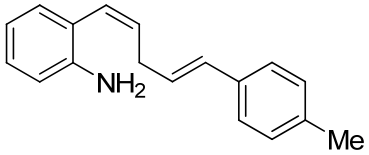
Yellow oil.[3d] $^1$H NMR (300 MHz, $CDCl_3$) δ 2.07 (s, 3 H), 3.83 (br, 2 H), 5.06 (s, 1 H), 5.29 (s, 1 H), 6.69-6.76 (m, 2 H), 7.03-7.08 (m, 2 H).

**General Procedure for the Iridium-Catalyzed Cross-Coupling of Styrene Derivatives with Allylic Carbonates:** A flame dried Schlenk tube was cooled to room temperature and filled with argon. To this flask were added $[Ir(COD)Cl]_2$ (2.7 mg, 0.004 mmol, 2 mol%), phosphoramidite ligand $\mathbf{L_1}$ (4.3 mg, 0.008 mmol, 4 mol%), THF (0.5 mL) and propylamine (0.5 mL). The reaction mixture was heated at 50 $^oC$ for 0.5 h, and the color of the solution was changed from orange to light yellow. Then the reaction mixture was cooled to room temperature, and the solvent was removed *in vacuo*. To the same flask, styrene derivative **1** or **5** (0.20 mmol), allylic carbonate **2** (0.22 mmol), $K_3PO_4$ (0.22 mmol) and degassed THF (2 mL) were added. The reaction mixture was stirred at 60 $^oC$ for 2-6 h. After the reaction was complete (monitored by TLC), the crude reaction mixture was filtrated with celite and washed with EtOAc. The solvents were removed under reduced pressure. The ratio of **3**/**4** was determined by $^1H$ NMR of the crude reaction mixture. Then the residue was purified by silica gel column chromatography to afford the product.



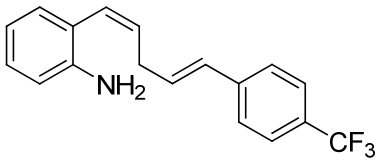

**3aa**

Red oil, yield 87%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.03 (dd, *J* = 6.3, 7.8 Hz, 2 H), 3.67 (br, 2 H), 3.78 (s, 3 H), 5.86 (dt, *J* = 11.4, 7.5 Hz, 1 H), 6.08 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.36 (d, *J* = 15.6 Hz, 1 H), 6.39 (d, *J* = 11.1 Hz, 1 H), 6.76-6.68 (m, 2 H), 6.83 (d, *J* = 8.7 Hz, 2 H), 7.11-7.06 (m, 2 H), 7.27 (d, *J* = 6.0 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 55.2, 113.9, 115.1, 118.0, 122.7, 125.9, 126.3, 127.0, 128.1, 129.6, 129.7, 130.4, 131.7, 144.0, 158.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3464, 3376, 3005, 1607, 1511, 1249, 1176, 1033, 753; MS (EI, *m/z*, rel. intensity) 265 ($M^+$, 72), 130 (100); HRMS (EI) calcd for $C_{18}H_{19}NO$ ($M^+$): 265.1467 Found: 265.1472.




**3ab**

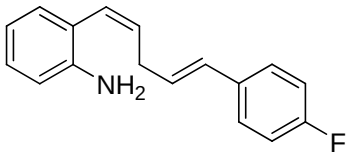
Red oil, yield 93%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 2.32 (s, 3 H), 3.05 (dd, *J* = 6.3, 7.5 Hz, 2 H), 3.67 (br, 2 H), 5.87 (dt, *J* = 11.1, 7.8 Hz, 1 H), 6.18 (dt, *J* = 15.9, 6.6 Hz, 1 H), 6.42-6.36 (m, 2 H), 6.77-6.68 (m, 2 H), 7.11-7.06 (m, 4 H), 7.25-7.22 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 21.1, 32.1, 115.2, 118.1, 122.7, 125.9, 126.1, 127.5, 128.2, 129.2, 129.6, 130.2, 131.6, 134.8, 136.7, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 3381, 3023, 2920, 1616, 1574, 1512, 1492, 1455, 1307, 967, 752; MS (EI, *m/z*, rel. intensity) 249 ($M^+$, 85), 130 (100); HRMS (EI) calcd for $C_{18}H_{19}N$ ($M^+$): 249.1517 Found: 249.1519.




**3ac**

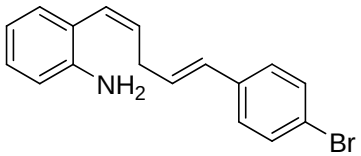
Red oil, yield 95%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.10 (dd, *J* = 6.3, 7.2 Hz, 2 H), 3.69 (br, 2 H), 5.88 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.34 (dt, *J* = 15.9, 6.0 Hz, 1 H),

6.47-6.43 (m, 2 H), 6.78-6.71 (m, 2 H), 7.13-7.06 (m, 2 H), 7.42 (d, $J$ = 8.1 Hz, 2 H), 7.54 (d, $J$ = 8.1 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 115.2, 118.1, 122.5, 125.3 (q, $J$ = 3.45 Hz), 126.1, 126.7, 128.3, 128.5, 129.0, 129.2, 129.5, 130.7, 131.4, 141.0, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 3382, 3021, 1616, 1492, 1456, 1328, 1165, 1122, 1068, 1016, 753; MS (EI, *m/*z, rel. intensity) 303 ($M^+$, 81), 118 (100); HRMS (EI) calcd for $C_{18}H_{16}F_3N$ ($M^+$): 303.1235 Found: 303.1233. Anal. calcd for $C_{18}H_{16}F_3N$: C, 71.28; H, 5.32; N, 4.62; Found: C, 71.33; H, 5.29; N, 4.33.




**3ad**

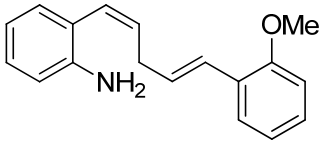
Red oil, yield 93%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.10 (dd, $J$ = 6.3, 7.5 Hz, 2 H), 3.69 (br, 2 H), 5.87 (dt, $J$ = 11.1, 7.5 Hz, 1 H), 6.14 (dt, $J$ = 15.9, 6.0 Hz, 1 H), 6.44-6.35 (m, 2 H), 6.77-6.70 (m, 2 H), 7.38-6.95 (m, 6 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 115.2, 115.5, 118.1, 122.6, 126.3, 127.4 (d, $J$ = 7.43 Hz), 128.2, 129.4 (d, $J$ = 24.6 Hz), 131.3, 133.7, 144.0, 162.0 (d, $J$ = 244.4 Hz). IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 3382, 3026, 1749, 1616, 1602, 1508, 1228, 1158, 752; MS (EI, *m/*z, rel. intensity) 253 ($M^+$, 98), 130 (100); HRMS (EI) calcd for $C_{17}H_{16}FN$ ($M^+$): 253.1267 Found: 253.1268.




**3ae**

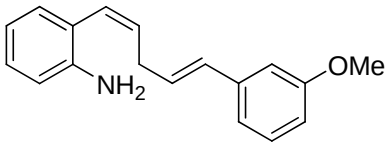
Red oil, yield 99%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.05 (dd, $J$ = 6.0, 7.5 Hz, 2 H), 3.69 (br, 2 H), 5.86 (dt, $J$ = 11.4, 7.5 Hz, 1 H), 6.22 (dt, $J$ = 15.9, 6.0 Hz, 1 H), 6.36 (d, $J$ = 15.9 Hz, 1 H), 6.43 (d, $J$ = 11.4 Hz, 1 H), 6.77-6.70 (m, 2 H), 7.10-7.06 (m, 2 H), 7.10 (d, $J$ = 8.4 Hz, 2 H), 7.40 (d, $J$ = 8.7 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 115.2, 118.0, 120.6, 122.5, 126.4, 127.5, 128.2, 129.2, 129.4, 129.5, 131.0, 131.5, 136.5, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3381, 3024, 2925, 1616, 1488, 1455,

1072, 1008, 752; MS (EI, *m/z*, rel. intensity) 313 ($M^+$, 44), 118 (100); HRMS (EI) calcd for $C_{17}H_{16}BrN$ ($M^+$): 313.0466 Found: 313.0474. Anal. calcd for $C_{17}H_{16}BrN$: C, 64.98; H, 5.13; N, 4.46; Found: C, 65.27; H, 4.86; N, 4.34.



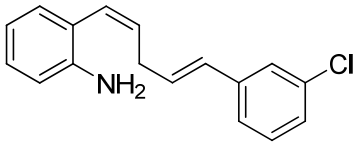

**3af**

Red oil, yield 86%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.08 (dd, *J* = 6.3, 7.2 Hz, 2 H), 3.69 (br, 2 H), 3.83 (s, 3 H), 5.90 (dt, *J* = 11.1, 7.2 Hz, 1 H), 6.22 (dt, *J* = 16.2, 6.3 Hz, 1 H), 6.40 (d, *J* = 11.4 Hz, 1 H), 6.69-6.93 (m, 5 H), 7.06-7.24 (m, 3 H), 7.41 (d, *J* = 7.8 Hz, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.5, 55.4, 110.7, 115.1, 118.0, 120.6, 122.8, 125.1, 126.0, 126.5, 126.6, 128.0, 128.1, 129.2, 129.7, 131.8, 144.0, 156.3. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3379, 3006, 2835, 1616, 1579, 1491, 1455, 1267, 1156, 1045, 968, 753, 689; MS (EI, *m/z*, rel. intensity) 265 ($M^+$, 77), 107 (100); HRMS (EI) calcd for $C_{18}H_{19}NO$ ($M^+$): 265.1467 Found: 265.1465.



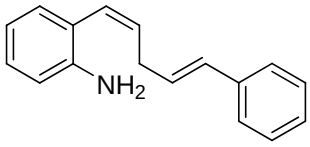

**3ag**

Red oil, yield 92%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.06 (dd, *J* = 6.3, 7.5 Hz, 2 H), 3.69 (br, 2 H), 3.80 (s, 3 H), 5.87 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.23 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.37-6.44 (m, 2 H), 6.69-6.78 (m, 3 H), 6.88-6.95 (m, 2 H), 7.01-7.12 (m, 2 H), 7.18-7.24 (m, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 55.1, 111.3, 112.6, 115.1, 118.0, 118.6, 122.6, 126.2, 128.2, 128.9, 129.4, 129.6, 130.2, 131.3, 139.0, 144.0, 159.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3381, 3006, 2936, 2837, 1748, 1616, 1598, 1489, 1245, 1028, 749; MS (EI, *m/z*, rel. intensity) 265 ($M^+$, 63), 130 (100); HRMS (EI) calcd for $C_{18}H_{19}NO$ ($M^+$): 265.1467 Found: 265.1464.



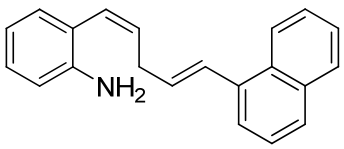

**3ah**

Red oil, yield 99%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.06 (dd, *J* = 6.3, 7.2 Hz, 2 H), 3.68 (br, 2 H), 5.85 (dt, *J* = 11.1, 7.2 Hz, 1 H), 6.24 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.35 (d, *J* = 16.2 Hz, 1 H), 6.42 (d, *J* = 11.1 Hz, 1 H), 6.69-6.778 (m, 2 H), 7.05-7.23 (m, 5 H), 7.32 (s, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 115.2, 118.1, 122.5, 124.2, 125.9, 126.5, 126.9, 128.2, 129.1, 129.5, 129.7, 130.2, 130.9, 134.4, 139.4, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3464, 3379, 3023, 1617, 1593, 1492, 1456, 991, 751, 682; MS (EI, *m/*z, rel. intensity) 269 ($M^+$, 76), 118 (100); HRMS (EI) calcd for $C_{17}H_{16}NCl$ ($M^+$): 269.0971 Found: 269.0973.




**3ai**

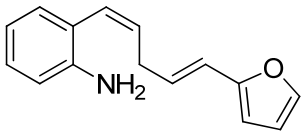
Red oil, yield 94%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.06 (dd, *J* = 6.3, 7.5 Hz, 2 H), 3.68 (br, 2 H), 5.87 (dt, *J* = 11.1, 7.8 Hz, 1 H), 6.23 (dt, *J* = 15.9, 7.2 Hz, 1 H), 6.40-6.45 (m, 2 H), 6.69-6.77 (m, 2 H), 7.07-7.35 (m, 7 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 115.1, 118.1, 122.7, 126.0, 126.2, 127.0, 127.5, 128.2, 128.5, 129.6, 130.4, 131.4, 137.6, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3380, 3025, 1616, 1575, 1494, 1454, 1306, 1157, 965, 749, 693; MS (EI, *m/*z, rel. intensity) 235 ($M^+$, 100), 130 (96); HRMS (EI) calcd for $C_{17}H_{17}N$ ($M^+$): 235.1361 Found: 235.1363.




**3aj**

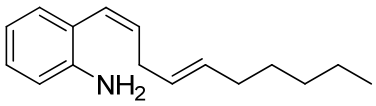
Red oil, yield 98%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.17 (dd, *J* = 6.0, 7.8 Hz, 2 H), 3.69 (br, 2 H), 5.96 (dt, *J* = 11.1, 7.8 Hz, 1 H), 6.24 (dt, *J* = 15.3, 6.3 Hz, 1 H), 6.45 (d,

*J* = 11.1 Hz, 1 H), 6.70-6.79 (m, 2 H), 7.08-8.10 (m, 10 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.5, 115.2, 118.1, 122.7, 123.5, 123.8, 125.5, 125.6, 125.8, 126.4, 127.4, 127.6, 128.2, 128.4, 129.6, 131.0, 131.4, 131.8, 133.5, 135.4, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 3381, 3059, 3007, 1616, 1491, 1455, 966, 778, 751; MS (EI, *m/z*, rel. intensity) 285 ($M^+$, 13), 157 (100); HRMS (EI) calcd for $C_{21}H_{19}N$ ($M^+$): 285.1517 Found: 285.1518.



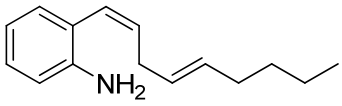

**3ak**

Red oil, yield 92%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.03 (dd, *J* = 6.3, 6.9 Hz, 2 H), 3.67 (br, 2 H), 5.85 (dt, *J* = 11.1, 7.2 Hz, 1 H), 6.14-6.43 (m, 5 H), 6.69-7.31 (m, 5 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 31.7, 106.5, 111.1, 115.1, 118.1, 119.0, 122.6, 126.4, 127.5, 128.2, 129.5, 131.1, 141.4, 144.0, 153.1. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3377, 3022, 2930, 1619, 1492, 1456, 1013, 961, 749; MS (EI, *m/z*, rel. intensity) 225 ($M^+$, 38), 130 (100); HRMS (EI) calcd for $C_{15}H_{15}N$ ($M^+$): 225.1154 Found: 225.1159.



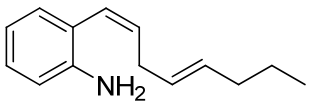

**3al**

Red oil, yield 95%. $^1$H NMR (300 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.9 Hz, 3 H), 1.24-1.37 (m, 6 H), 1.96-2.02 (m, 2 H), 2.82-2.86 (m, 2 H), 3.66 (br, 2 H), 5.43-5.47 (m, 2 H), 5.79 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.32 (d, *J* = 11.1 Hz, 1 H), 6.68-6.76 (m, 2 H) 7.04-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 14.1, 22.5, 29.1, 31.4, 31.7, 32.6, 115.1, 118.0, 122.9, 125.2, 127.8, 128.0, 129.6, 131.4, 132.5, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3470, 3383, 2958, 2926, 2856, 1617, 1492, 1456, 1304, 970, 749; MS (EI, *m/z*, rel. intensity) 229 ($M^+$, 51), 106 (100); Anal. calcd for $C_{16}H_{23}N$: C, 83.79; H, 10.11; N, 6.11; Found: C, 83.49; H, 10.18; N, 6.18.



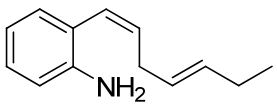
**3am**

Red oil, yield 92%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.2 Hz, 3 H), 1.28-1.35 (m, 4 H), 1.97-2.03 (m, 2 H), 2.81-2.86 (m, 2 H), 3.66 (br, 2 H), 5.37-5.52 (m, 2 H), 5.78 (dt, *J* = 11.1, 7.2 Hz, 1 H), 6.32 (d, *J* = 11.1 Hz, 1 H), 6.69 (d, *J* = 7.5 Hz, 1 H), 6.74 (d, *J* = 7.2 Hz, 1 H), 7.04-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.9, 22.2, 31.6, 31.8, 32.3, 115.1, 118.0, 122.9, 125.2, 127.8, 128.0, 129.6, 131.4, 132.6, 143.9. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3473, 3382, 2961, 2928, 1617, 1492, 1456, 1262, 1028, 969, 798, 749, 697; MS (EI, *m/z*, rel. intensity) 215 ($M^+$, 54), 106 (100); HRMS (EI) calcd for $C_{15}H_{21}N$ ($M^+$): 215.1674 Found: 215.1669. Anal. calcd for $C_{15}H_{21}N$: C, 83.67; H, 9.83; N, 6.50; Found: C, 83.49; H, 9.67; N, 6.25.



**3an**

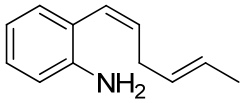
Red oil, yield 93%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.5 Hz, 3 H), 1.37 (m, 2 H), 1.94-2.01 (m, 2 H), 2.82-2.86 (m, 2 H), 3.66 (br, 2 H), 5.43-5.74 (m, 2 H), 5.79 (dt, *J* = 11.1, 7.8 Hz, 1 H), 6.32 (d, *J* = 11.1 Hz, 1 H), 6.67-6.75 (m, 2 H), 7.04-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.6, 31.7, 34.7, 115.1, 118.0, 122.9, 125.3, 128.0, 128.1, 129.6, 131.2, 132.6, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 3383, 2960, 2927, 1616, 1492, 1455, 1304, 1265, 1075, 968, 750; MS (EI, *m/z*, rel. intensity) 201 ($M^+$, 74), 144 (100); HRMS (EI) calcd for $C_{14}H_{19}N$ ($M^+$): 201.1517 Found: 201.1523.



**3ao**

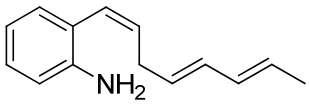
Red oil, yield 94%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.97 (t, *J* = 7.8 Hz, 3 H), 2.01 (quint, *J* = 7.5 Hz, 2 H), 2.84 (dd, *J* = 4.2, 6.0 Hz, 2 H), 3.67 (br, 2 H), 5.37-5.56 (m, 2

H), 5.79 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.33 (d, *J* = 11.1 Hz, 1 H), 6.68-6.76 (m, 2 H), 7.05-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.8, 25.6, 31.7, 115.1, 118.0, 122.9, 125.3, 126.9, 128.0, 129.6, 132.6, 132.9, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3468, 3381, 2964, 1616, 1492, 1456, 1262, 1077, 967, 796, 749; MS (EI, *m/*z, rel. intensity) 187 ($M^+$, 67), 118 (100); HRMS (EI) calcd for $C_{13}H_{17}N$ ($M^+$): 187.1362 Found: 187.1361.



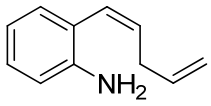

**3ap**

Red oil, yield 94%. $^1$H NMR (300 MHz, $CDCl_3$) δ 1.66 (d, *J* = 3.9 Hz, 3 H), 2.82 (d, J = 6.9 Hz, 2 H), 3.67 (br, 2 H), 5.45-5.50 (m, 2 H), 5.78 (dt, *J* = 11.4, 7.5 Hz, 1 H), 6.32 (d, *J* = 11.4 Hz, 1 H), 6.68-6.76 (m, 2 H), 7.04-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 18.0, 31.7, 115.1, 118.0, 122.9, 125.3, 125.7, 128.0, 129.1, 129.6, 132.5, 143.9. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3474, 2964, 2920, 1616, 1492, 1455, 1263, 796; MS (EI, *m/*z, rel. intensity) 173 ($M^+$, 66), 118 (100); HRMS (EI) calcd for $C_{12}H_{15}N$ ($M^+$): 173.1204 Found: 173.1207.



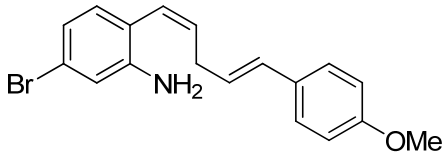

**3aq**

Red oil, yield 90%. $^1$H NMR (300 MHz, $CDCl_3$) δ 1.73 (d, *J* = 6.3 Hz, 3 H), 2.91 (t, *J* = 6.9 Hz, 2 H), 3.66 (br, 2 H), 5.54-5.64 (m, 2 H), 5.79 (dt, *J* = 11.1, 7.5 Hz, 1 H), 5.99-6.09 (m, 2 H), 6.35 (d, *J* = 11.1 Hz, 1 H), 6.67-6.75 (m, 2 H) 7.03-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 18.0, 31.6, 115.1, 119.0, 122.7, 125.7, 127.6, 128.1, 129.3, 129.6, 130.9, 131.4, 131.7, 143.9. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3464, 3377, 3015, 1618, 1577, 1492, 1455, 1305, 1158, 989, 750; MS (EI, *m/*z, rel. intensity) 199 ($M^+$, 31), 130 (100); HRMS (EI) calcd for $C_{14}H_{17}N$ ($M^+$): 199.1361 Found: 199.1362.



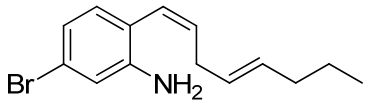
**3ar**

Red oil, yield 75% (Note: in some cases, the allylic amination product can be observed). $^{1}$H NMR (300 MHz, $CDCl_3$) δ 2.91 (dd, *J* = 6.0, 7.8 Hz, 2 H), 3.67 (br, 2 H), 5.01-5.12 (m, 2 H), 5.57-5.91 (m, 2 H), 6.38 (d, J = 11.4 Hz, 1 H), 6.69-6.76 (m, 2 H), 7.04-7.11 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.8, 115.1, 118.0, 122.8, 126.1, 128.1, 129.6, 131.4, 136.7, 144.0. MS (EI, *m/z*, rel. intensity) 159 ($M^+$, 69), 144 (100); HRMS (EI) calcd for $C_{11}H_{13}N$ ($M^+$): 159.1048 Found: 159.1051.



**3ba**

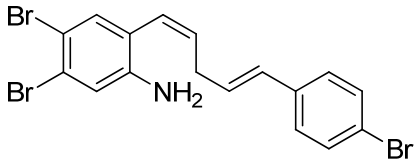
Red oil, yield 91%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.01 (dd, *J* = 6.9, 7.5 Hz, 2 H), 3.70 (br, 2 H), 3.80 (s, 3 H), 5.90 (dt, *J* = 10.8, 7.5 Hz, 1 H), 6.06 (dt, *J* = 15.9, 6.6 Hz, 1 H), 6.30 (d, *J* = 11.4 Hz, 1 H), 6.36 (d, *J* = 16.2 Hz, 1 H), 6.58 (d, *J* = 8.1 Hz, 1 H), 6.83 (d, *J* = 8.7 Hz, 2 H), 7.11-7.06 (m, 2 H), 7.27 (d, *J* = 6.0 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.1, 55.2, 109.6, 113.9, 116.6, 124.6, 124.8, 125.7, 127.1, 130.1, 130.3, 130.7, 131.9, 133.0, 143.1, 158.8. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3380, 2922, 1608, 1511, 1484, 1249, 1176, 1033, 967, 838, 813; MS (EI, *m/z*, rel. intensity) 343 ($M^+$, 47), 121 (100); HRMS (EI) calcd for $C_{18}H_{18}BrNO$ ($M^+$): 343.0572 Found: 343.0578.



**3bn**

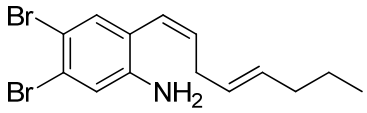
Red oil, yield 93%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.5 Hz, 3 H), 1.37 (m, 2 H), 1.95-2.02 (m, 2 H), 2.82 (m, 2 H), 3.68 (br, 2 H), 5.37-5.52 (m, 2 H), 5.83 (dt, *J* = 11.1, 7.8 Hz, 1 H), 6.24 (d, *J* = 11.4 Hz, 1 H), 6.57 (d, *J* = 9.0 Hz, 1 H), 7.13-7.16 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.6, 31.8, 34.7, 109.6, 116.5, 124.1,

124.8, 127.6, 130.6, 131.5, 132.0, 133.7, 143.1. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3479, 3388, 3008, 2958, 1616, 1485, 1412, 1286, 1145, 968, 812; MS (EI, *m/z*, rel. intensity) 279 ($M^+$, 18), 43 (100); HRMS (EI) calcd for $C_{14}H_{18}BrN$ ($M^+$): 279.0623 Found: 279.0624.



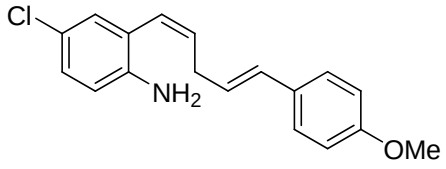

**3ce**

Red solid, yield 73%. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.05 (dd, *J* = 6.3, 6.6 Hz, 2 H), 3.75 (br, 2 H), 5.93 (dt, *J* = 11.1, 7.2 Hz, 1 H), 6.19 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.26 (d, *J* = 11.1 Hz, 1 H), 6.35 (d, *J* = 15.9 Hz, 1 H), 6.98 (s, 1 H), 7.20 (d, *J* = 8.4 Hz, 2 H), 7.26 (s, 1 H), 7.42 (d, *J* = 8.4 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.1, 111.5, 119.4, 120.9, 123.4, 124.4, 127.6, 128.5, 129.7, 131.6, 132.9, 133.6, 136.3, 144.3. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3481, 3388, 2924, 1616, 1487, 1475, 1290, 1116, 1072, 1009, 967, 846; MS (EI, *m/z*, rel. intensity) 468 ($M^+$, 6), 115 (100); HRMS (EI) calcd for $C_{17}H_{14}Br_3N$ ($M^+$): 468.8676 Found: 468.8669.



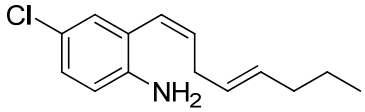

**3cn**

Red oil, yield 83%. $^1$H NMR (300 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.5 Hz, 3 H), 1.39 (m, 2 H), 1.98 (q, *J* = 7.5 Hz, 2 H), 2.79 (dd, *J* = 5.7, 6.3 Hz, 2 H), 3.73 (br, 2 H), 5.36-5.52 (m, 2 H), 5.85 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.16 (d, *J* = 11.1 Hz, 1 H), 6.05 (s, 1 H), 7.24 (s, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.5, 31.8, 34.7, 111.4, 119.2, 123.1, 123.2, 123.8, 127.3, 131.7, 133.6, 134.3, 144.3. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3483, 3391, 2959, 2926, 1614, 1475, 1376, 1288, 1261, 1116, 968, 910; MS (EI, *m/z*, rel. intensity) 357 ($M^+$, 17), 41 (100); HRMS (EI) calcd for $C_{14}H_{17}NBr_2$ ($M^+$): 356.9728 Found: 356.9731.



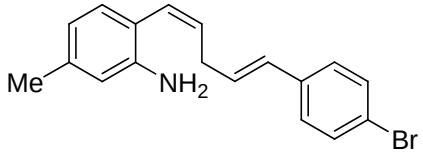

**3da**

Yellow oil, yield 82%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.01 (dd, *J* = 6.3, 7.5 Hz, 2 H), 3.68 (br, 2 H), 3.78 (s, 3 H), 5.90 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.06 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.31 (d, *J* = 14.1 Hz, 1 H), 6.36 (d, *J* = 16.2 Hz, 1 H), 6.61 (d, *J* = 7.8 Hz, 1 H), 6.84 (d, *J* = 8.4 Hz, 2 H), 7.01-7.05 (m, 2 H), 7.27 (d, *J* = 8.7 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 32.0, 55.2, 113.9, 116.2, 122.5, 124.0, 124.8, 125.7, 127.1, 127.8, 129.1, 130.0, 130.3, 132.9, 142.6, 158.9. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3475, 3383, 3006, 2836, 1608, 1511, 1487, 1248, 1176, 1035, 967, 815; MS (EI, *m/*z, rel. intensity) 299 ($M^+$, 66), 121 (100); HRMS (EI) calcd for $C_{18}H_{18}ClNO$ ($M^+$): 299.1077 Found: 299.1076.



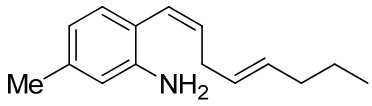

**3dn**

Light yellow oil, yield 78%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.5 Hz, 3 H), 1.38 (m, 2 H), 1.98 (q, *J* = 7.5 Hz, 2 H), 2.82 (dd, *J* = 5.7, 6.6 Hz, 2 H), 3.67 (br, 2 H), 5.37-5.51 (m, 2 H), 5.83 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.24 (d, *J* = 11.1 Hz, 1 H), 6.60-6.63 (m, 1 H), 7.01-7.03 (m, 2H) $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.6, 22.6, 31.8, 34.7, 116.1, 122.5, 124.2, 127.6, 127.7, 129.1, 131.5, 133.6, 142.6. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3480, 3390, 2960, 2929, 1618, 1488, 1415, 1285, 967, 814; MS (EI, *m/*z, rel. intensity) 235 ($M^+$, 89), 140 (100); HRMS (EI) calcd for $C_{14}H_{18}NCl$ ($M^+$): 235.1128 Found: 235.1131.



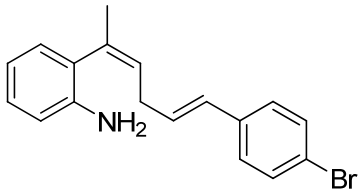

**3ee**

Yellow oil, yield 86%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 2.26 (s, 3 H), 3.05 (t, *J* = 6.6 Hz, 2 H), 3.63 (br, 2 H), 5.81 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.22 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.35 (d, *J* = 15.6 Hz, 1 H), 6.39 (d, *J* = 10.8 Hz, 1 H), 6.53 (s, 1 H), 6.57 (d, *J* = 7.8 Hz, 1 H), 6.96 (d, *J* = 7.5 Hz, 1 H), 7.21 (d, *J* = 7.8 Hz, 2 H), 7.40 (d, *J* = 8.7 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 21.2, 32.0, 115.9, 118.9, 119.7, 120.6, 126.3, 127.5, 129.1, 129.4, 129.5, 130.5, 131.5, 136.5, 138.1, 143.8. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3463, 3381, 3007, 2919, 1622, 1487, 1073, 1008, 966, 817; MS (EI, *m/*z, rel. intensity) 327 ($M^+$, 59), 158 (100); HRMS (EI) calcd for $C_{18}H_{18}NBr$ ($M^+$): 327.0623 Found: 327.0617.




**3en**

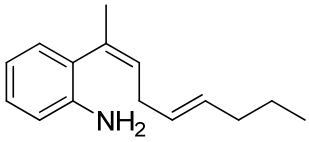
Light yellow oil, yield 83%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.5 Hz, 3 H), 1.37 (m, 2 H), 1.98 (q, *J* = 6.3 Hz, 2 H), 2.26 (s, 3H), 2.83 (m, 2 H), 3.61 (br, 2 H), 5.44-5.47 (m, 2 H), 5.78 (dt, *J* = 11.1, 7.5 Hz, 1 H), 6.29 (d, *J* = 11.1 Hz, 1 H), 6.52 (s, 1 H), 6.56 (d, *J* = 7.8 Hz, 1 H), 6.95 (d, *J* = 7.5 Hz, 1 H) $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.6, 21.2, 22.6, 31.8, 34.7, 115.8, 118.9, 120.1, 125.1, 128.1, 129.5, 131.1, 132.1, 137.8, 143.8. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3462, 3007, 2960, 2928, 1622, 1508, 1458, 1297, 968, 817; MS (EI, *m/*z, rel. intensity) 215 ($M^+$, 100), 120 (82); HRMS (EI) calcd for $C_{15}H_{21}N$ ($M^+$): 215.1674 Found: 215.1677.




**6e**

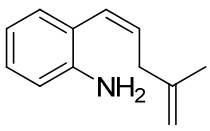
Yellow oil, yield 80%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 2.00 (s, 3 H), 2.72 (dd, *J* = 6.6, 6.3 Hz, 2 H), 3.67 (br, 2 H), 5.65 (t, *J* = 7.2 Hz, 1 H), 6.13 (dt, *J* = 15.9, 6.3 Hz, 1 H), 6.25 (d, *J* = 15.6 Hz, 1 H), 6.71-6.78 (m, 2 H), 6.94 (d, *J* = 7.2 Hz, 1 H), 7.09 (t, *J* =

7.5 Hz, 1 H), 7.17 (d, *J* = 8.1 Hz, 2 H), 7.39 (d, *J* = 8.4 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 24.5, 32.7, 115.0, 118.3, 120.5, 126.1, 127.1, 127.5, 127.9, 128.6, 128.7, 129.8, 131.5, 135.4, 136.6, 142.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3471, 3379, 3024, 2965, 1613, 1488, 1297, 1073, 1008, 966, 751; MS (EI, *m/*z, rel. intensity) 327 ($M^+$, 19), 132 (100); HRMS (EI) calcd for $C_{18}H_{18}NBr$ ($M^+$): 327.0623 Found: 327.0624.



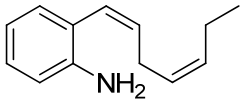

**6n**

Light yellow oil, yield 51%. $^1$H NMR (300 MHz, $CDCl_3$) δ 0.87 (t, *J* = 7.5 Hz, 3 H), 1.37 (m, 2 H), 1.90-1.94 (m, 2 H), 1.97 (s, 3H), 2.49-2.51 (m, 2 H), 3.65 (br, 2 H), 5.34-5.37 (m, 2 H), 5.58 (t, *J* = 7.5 Hz, 1 H), 6.69-6.76 (m, 2 H), 6.92 (d, *J* = 7.2 Hz, 1 H), 7.06 (t, *J* = 7.5 Hz, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 13.7, 22.6, 24.5, 32.4, 34.7, 115.0, 118.2, 127.5, 127.7, 128.4, 128.7, 130.6, 134.0, 142.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3385, 2962, 2927, 1613, 1495, 1454, 1295, 1262, 1095, 968, 746; MS (EI, *m/*z, rel. intensity) 215 ($M^+$, 29), 43 (100); HRMS (EI) calcd for $C_{15}H_{21}N$ ($M^+$): 215.1674 Found: 215.1672.



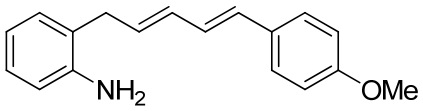

**3au**

Red oil, yield 96%. $^1$H NMR (300 MHz, $CDCl_3$) δ 1.72 (s, 3 H), 2.83 (d, *J* = 7.5 Hz, 2 H), 3.54 (br, 2 H), 4.77 (s, 2 H), 5.86 (dt, *J* = 11.4, 7.5 Hz, 1 H), 6.40 (d, *J* = 11.4 Hz, 1 H), 6.68-6.76 (m, 2 H), 7.04-7.10 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 22.9, 36.6, 110.3, 115.1, 118.0, 122.8, 126.3, 128.0, 129.6, 131.6, 143.9, 144.7. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3378, 2977, 1712, 1615, 1454, 1302, 1155, 887, 750; MS (EI, *m/*z, rel. intensity) 173 ($M^+$, 22), 117 (100); HRMS (EI) calcd for $C_{12}H_{15}N$ ($M^+$): 173.1204 Found: 173.1203.



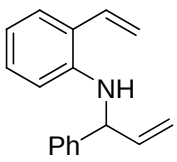

**10**

Yellow oil, yield 86%. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 0.973 (t, *J* = 7.8 Hz, 3 H), 1.99 (quint, *J* = 6.9 Hz, 2 H), 2.89 (t, *J* = 6.9 Hz, 2 H), 3.67 (br, 2 H), 5.30-5.43 (m, 2 H), 5.76 (dt, *J* = 10.8, 7.5 Hz, 1 H), 6.31 (d, *J* = 11.1 Hz, 1 H), 6.70-6.77 (m, 2 H), 7.04-7.11 (m, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 14.2, 20.5, 26.9, 115.1, 118.0, 122.9, 125.1, 126.6, 128.0, 129.7, 132.5, 132.8, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3472, 3381, 2963, 2874, 1617, 1492, 1456, 1303, 1277, 1157, 1070, 793, 750; MS (EI, *m/*z, rel. intensity) 187 ($M^+$, 80), 144 (100); HRMS (EI) calcd for $C_{13}H_{17}N$ ($M^+$): 187.1362 Found: 187.1361.



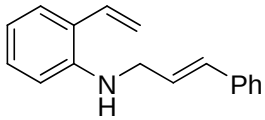

**4aa**

Red oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.36 (d, *J* = 6.6 Hz, 2 H), 3.63 (br, 2 H), 3.77 (s, 3 H), 5.85 (dt, *J* = 15.3, 6.3 Hz, 1 H), 6.21 (dd, *J* = 15.3, 15.0 Hz, 1 H), 6.39 (d, *J* = 15.6 Hz, 1 H), 6.59-6.67 (m, 2 H), 6.75 (t, *J* = 7.5 Hz, 1 H), 6.82 (d, *J* = 8.1 Hz, 2 H), 7.05 (d, *J* = 7.2 Hz, 2 H), 7.28 (d, *J* = 8.4 Hz, 2 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 35.3, 55.2, 114.0, 115.7, 118.8, 124.2, 126.6, 127.3, 127.5, 130.1, 130.7, 130.7, 131.9, 144.7, 159.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3383, 1599, 1509, 1458, 1248, 1178, 1025, 992, 829, 755; MS (EI, *m/*z, rel. intensity) 265 ($M^+$, 99), 130 (100); HRMS (EI) calcd for $C_{18}H_{19}NO$ ($M^+$): 265.1467 Found: 265.1469.



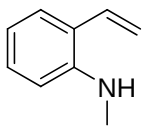

**7**

Yellow oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 4.18 (br, 1 H), 4.96 (d, *J* = 5.4 Hz, 1 H), 5.20-5.33 (m, 3 H), 5.62 (d, *J* = 17.4 Hz, 1 H), 6.04 (ddd, *J* = 16.8, 9.9, 5.7 Hz, 1 H), 6.54 (d, *J* = 7.8 Hz, 1 H), 6.70 (t, *J* = 7.5 Hz, 1 H), 6.80 (dd, *J* = 10.8, 10.8 Hz, 1 H), 7.06 (t, *J* = 7.2 Hz, 1 H), 7.21-7.39 (m, 6 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 60.7, 112.2, 116.1, 116.5, 117.6, 124.4, 126.0, 127.0, 127.3, 127.4, 128.7, 132.9, 139.1, 141.7, 144.0. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3423, 2962, 2920, 1735, 1602, 1506, 1458, 1262, 1313, 1262, 1093, 1024, 802, 748, 701; MS (EI, *m/z*, rel. intensity) 235 ($M^+$, 25), 117 (100); HRMS (EI) calcd for $C_{17}H_{17}N$ ($M^+$): 235.1361 Found: 235.1363.



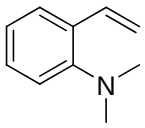

**8**

Yellow oil. $^{1}$H NMR (300 MHz, $CDCl_3$) δ 3.97 (br, 1 H), 3.98 (br, 2H), 5.33 (dd, *J* = 11.1, 1.5 Hz, 1 H), 5.63 (dd, *J* = 17.1, 1.5 Hz, 1 H), 6.36 (dt, *J* = 15.9, 5.7 Hz, 1 H), 6.63 (d, *J* = 16.2 Hz, 1 H), 6.69-6.84 (m, 3 H),7.16-7.40 (m, 7 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 46.2, 111.0, 116.5, 117.5, 124.4, 126.3, 126.8, 127.4, 127.6, 128.6, 129.0, 131.6, 132.8, 136.7, 144.9. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3732, 3433, 3028, 2922, 2850, 1600, 1505, 1454, 1313, 1256, 967, 909, 745; MS (EI, *m/z*, rel. intensity) 235 ($M^+$, 19), 117 (100); HRMS (EI) calcd for $C_{17}H_{17}N$ ($M^+$): 235.1361 Found: 235.1362.



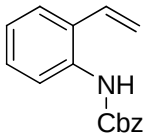

**9a**

Yellow oil.[4a] $^{1}$H NMR (300 MHz, $CDCl_3$) δ 2.86 (s, 3 H), 3.85 (br, 1 H), 5.30 (dd, *J* = 11.1, 1.8 Hz, 1 H), 5.59 (dd, *J* = 17.4, 1.8 Hz, 1 H), 6.63 (d, *J* = 8.4 Hz, 1 H), 6.69-6.78 (m, 2 H), 7.18-7.24 (m, 2 H).



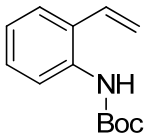
**9b**

Yellow oil.[4b] $^1$H NMR (400 MHz, $CDCl_3$) δ 2.71 (s, 6 H), 5.23 (dd, *J* = 11.2, 1.6 Hz, 1 H), 5.66 (dd, *J* = 17.6, 1.6 Hz, 1 H), 6.97-7.01 (m, 2 H), 7.07 (dd, *J* = 10.8, 10.8 Hz, 1 H), 7.19-7.23 (m, 1 H), 7.47 (dd, *J* = 7.6, 1.6 Hz, 1 H).



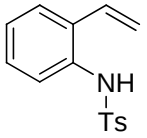
**9c**

Colorless needles.[4c] $^1$H NMR (300 MHz, $CDCl_3$) δ 5.20 (s, 2 H), 5.39 (dd, *J* = 11.1, 1.2 Hz, 1 H), 5.65 (dd, *J* = 17.1, 1.2 Hz, 1 H), 6.65 (br, 1 H), 6.78 (dd, *J* = 17.1, 11.1 Hz, 1 H), 7.10 (t, *J* = 7.5 Hz, 1 H), 7.25-7.40 (m, 7 H), 7.81 (br, 1 H).



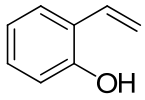
**9d**

Colorless oil.[4c] $^1$H NMR (300 MHz, $CDCl_3$) δ 1.52 (s, 9 H), 5.41 (dd, *J* = 11.1, 1.2 Hz, 1 H), 5.66 (dd, *J* = 17.7, 1.2 Hz, 1 H), 6.42 (br, 1 H), 6.82 (dd, *J* = 17.4, 11.4 Hz, 1 H), 7.08 (t, *J* = 7.5 Hz, 1 H), 7.24-7.29 (m, 1 H), 7.38 (d, *J* = 7.5 Hz, 1 H), 7.80 (d, *J* = 7.2 Hz, 1 H).



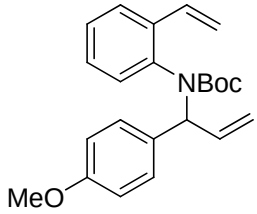
**9e**

White solid.[3a] $^1$H NMR (300 MHz, $CDCl_3$) δ 2.38 (s, 3 H), 5.25 (dd, *J* = 11.1, 1.2 Hz, 1 H), 5.51 (dd, *J* = 17.7, 1.2 Hz, 1 H), 6.50-6.56 (m, 1 H), 6.59 (br, 1 H), 7.13-7.36 (m, 6 H), 7.61 (d, *J* = 8.1 Hz, 2 H).

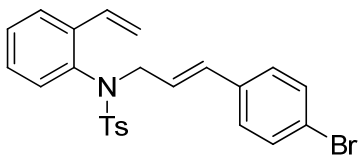



**9f**

Yellow oil.[4d] $^1$H NMR (300 MHz, $CDCl_3$) δ 5.03 (br, 1 H), 5.36 (dd, *J* = 11.1, 1.2 Hz, 1 H), 5.74 (dd, *J* = 18.0, 0.9 Hz, 1 H), 6.79 (d, *J* = 7.8 Hz, 1 H), 6.89-6.99 (m, 2 H), 7.14 (t, *J* = 7.5 Hz, 1 H), 7.39 (d, *J* = 7.5 Hz, 1 H).

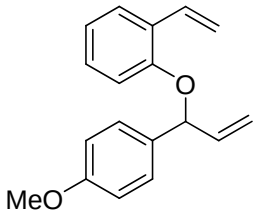



Colorless oil. $^1$H NMR (300 MHz, $CDCl_3$) [conformational isomers (1.3/1 ratio) were observed in solution] δ 1.32 (s, 9 H), 3.81 (s, 3 H), 5.14 (d, *J* = 10.5 Hz, 1 H), 5.20-5.50 (m, 2 Hz), 5.68-5.83 (m, 2 H), 6.36 (ddd, *J* = 17.4, 10.5, 7.2 Hz, 1 H), 6.70-6.80 (m, 2 H), 6.86 (d, *J* = 8.4 Hz, 1 H), 7.03-7.28 (m, 5 H), 7.42-7.60 (m, 1 H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 28.2, 55.1, 55.2, 80.1, 113.3, 113.5, 114.5, 115.0, 117.1, 118.5, 125.3, 127.3, 127.4, 127.8, 128.9, 129.3, 130.0, 132.9, 133.5, 135.0, 136.9, 137.5, 154.4, 154.7, 158.7, 158.8. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 1695, 1610, 1512, 1454, 1367, 1315, 1249, 1171, 1036, 770. MS (ESI, *m/z*, rel. intensity) 388 ($MNa^+$, 100); HRMS (EI) calcd for $C_{23}H_{27}NO_3$ ($M^+$): 365.1991 Found: 365.1993.

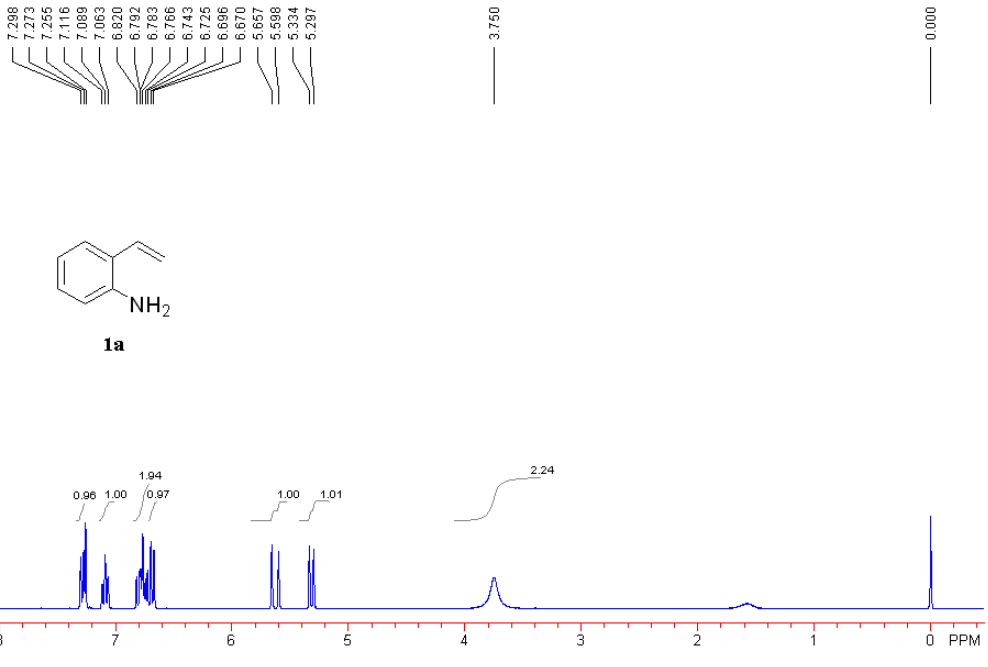



White solid. $^1$H NMR (300 MHz, $CDCl_3$) δ 2.45 (s, 3 H), 4.13 (br, 1 H), 4.38 (br, 1 H), 5.31 (dd, *J* = 11.1, 0.9 Hz, 1 H), 5.69 (dd, *J* = 17.4, 0.9 Hz, 1 H), 6.08 (dt, *J* = 15.3,

6.9 Hz, 1 H), 6.21 (d, *J* = 15.9 Hz, 1 H), 6.73 (dd, *J* = 7.8, 0.9 Hz, 1 H), 6.99-7.11 (m, 3 H), 7.13 (t, *J* = 7.8 Hz, 1 H), 7.28-7.30 (m, 3 H), 7.37 (d, *J* = 8.4 Hz, 2 H), 7.60-7.63 (m, 3 H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 21.6, 54.3, 116.0, 121.6, 124.6, 126.2, 127.9, 128.0, 128.1, 128.7, 129.2, 129.6, 131.6, 132.8, 132.9, 135.3, 136.4, 136.7, 138.7, 143.6. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 3063, 2920, 1486, 1346, 1158, 1095, 1070, 888, 820, 790, 715; MS (EI, *m/z*, rel. intensity) 467 ($M^+$, 1), 116 (100); HRMS (EI) calcd for $C_{24}H_{22}BrNO_2S$ ($M^+$): 467.0555 Found: 467.0559; m.p. 115-117 °C.




Colorless oil. $^1$H NMR (300 MHz, $CDCl_3$) δ 3.80 (s, 3 H), 5.25 (dd, *J* = 10.8, 9.0 Hz, 2 H), 5.33 (d, *J* = 18.6 Hz, 1 H), 5.61 (d, *J* = 5.4 Hz, 1 H), 5.75 (d, *J* = 18.0 Hz, 1 H), 6.10 (ddd, *J* = 15.9, 10.2, 5.4 Hz, 1 H), 6.82-6.93 (m, 4 H), 7.09-7.21 (m, 2 H), 7.33 (d, *J* = 7.5 Hz, 2 H), 7.49 (d, *J* = 7.8 Hz, 1 H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 55.2, 80.8, 114.0, 114.2, 114.6, 116.0, 120.9, 126.3, 127.8, 127.9, 128.5, 131.7, 132.1, 138.1, 154.9, 159.3. IR (thin film): $\nu_{max}$ ($cm^{-1}$) = 2919, 2851, 1608, 1512, 1454, 1248, 1176, 1033, 969, 837; MS (EI, *m/z*, rel. intensity) 266 ($M^+$, 18), 147 (100); HRMS (EI) calcd for $C_{18}H_{18}O_2$ ($M^+$): 266.1307 Found: 266.1304.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6.670
5.657
5.598
5.334
5.297
3.750
0.000
NH2
1a
0.96
1.00
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1.00
1.01
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8
7
6
5
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3
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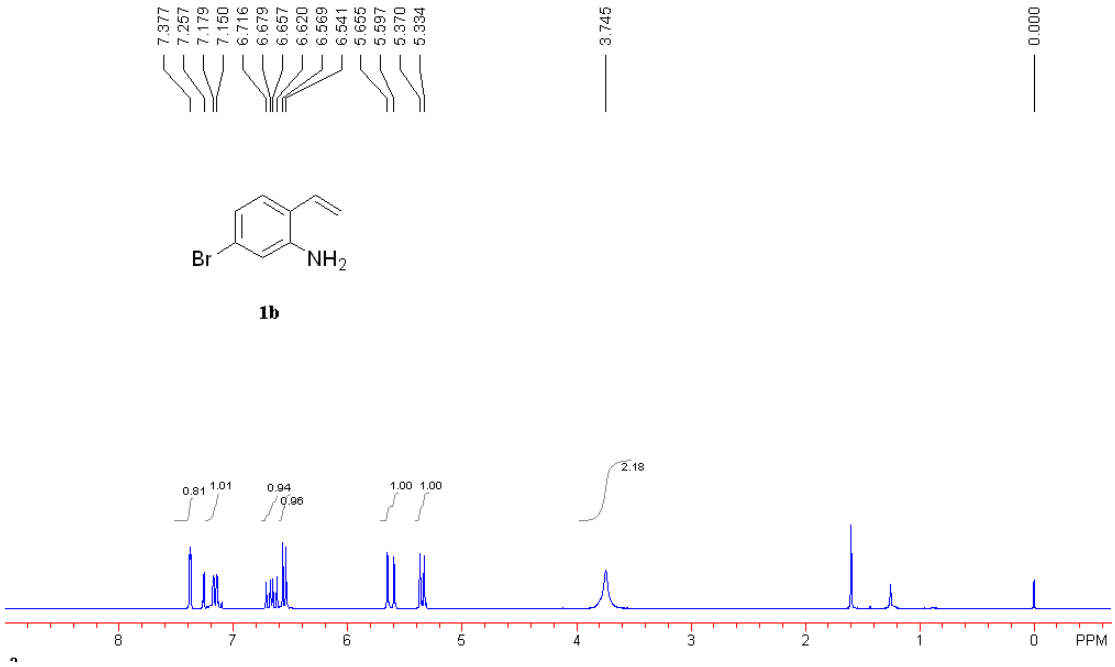
PPM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6.541
5.655
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5.370
5.334
3.745
0.000
Br
NH2
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1.01
0.94
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1.00
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8
7
6
5
4
3
2
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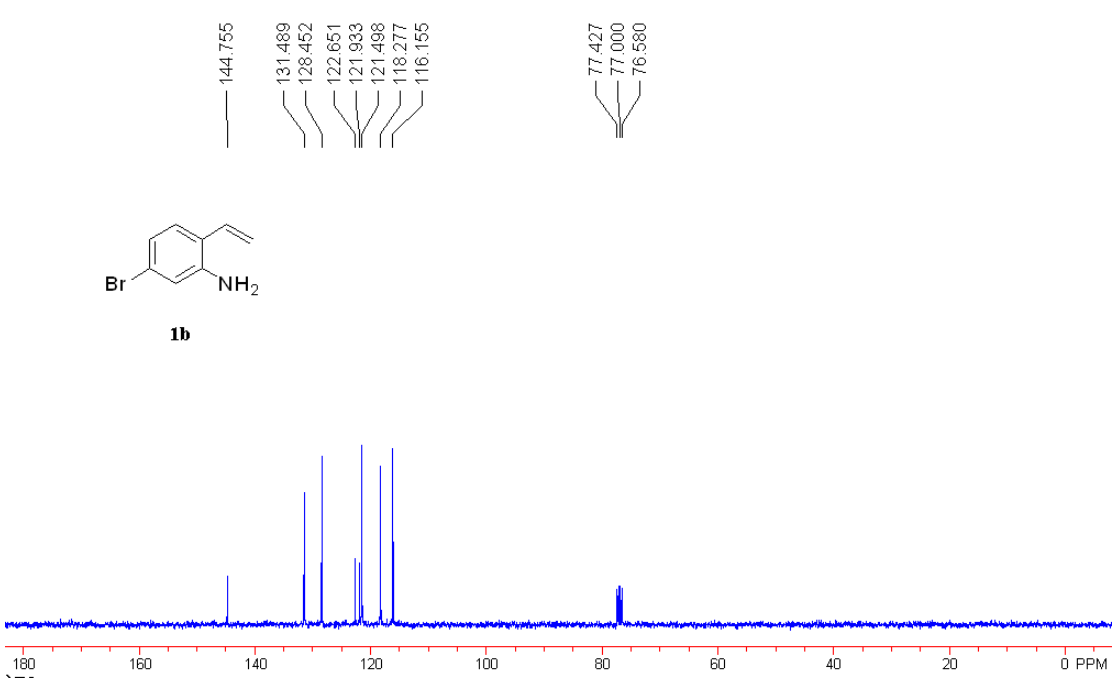
0
PPM

**1b**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160
140
120
100
80
60
40
20
0 PPM

**1b**


7.444
7.257
6.932
6.627
6.590
6.569
6.532
5.651
5.648
5.593
5.590
5.386
5.383
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5.346
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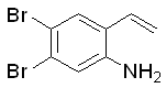
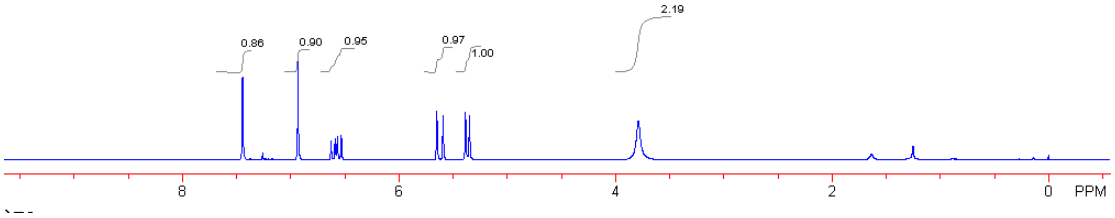
0.000


Br
Br
NH2

**1c**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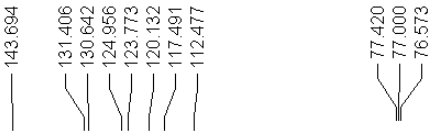
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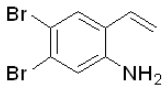
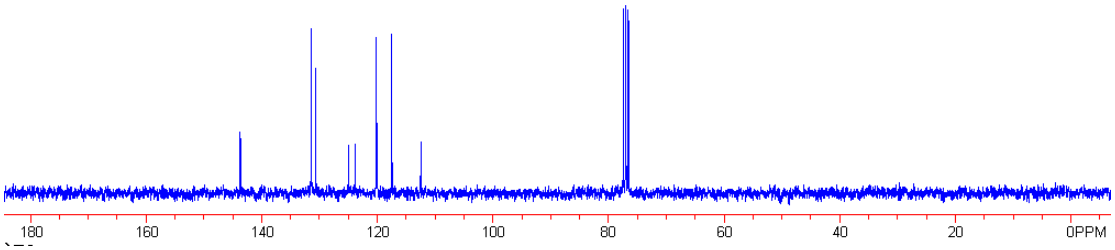
117.491
112.477
77.420
77.000
76.573


Br
Br
NH2

**1c**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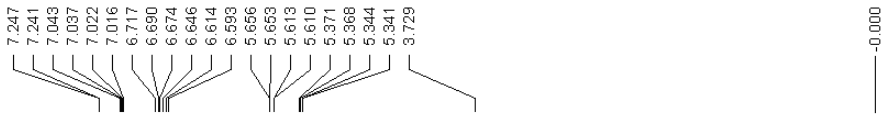
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7.241
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7.037
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7.016
6.717
6.690
6.674
6.646
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6.593
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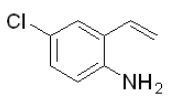
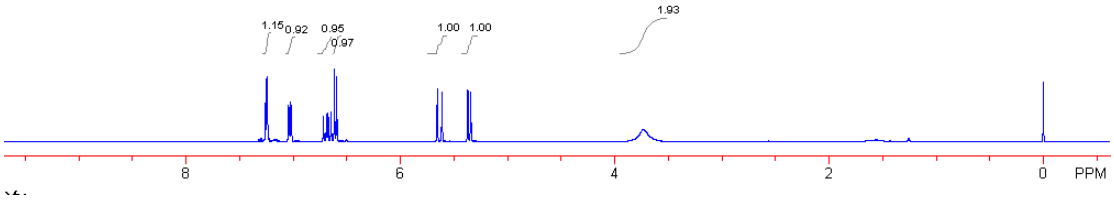
5.653
5.613
5.610
5.371
5.368
5.344
5.341
3.729
-0.000


Cl
NH2

**1d**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0.97
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1.00
1.93
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6
4
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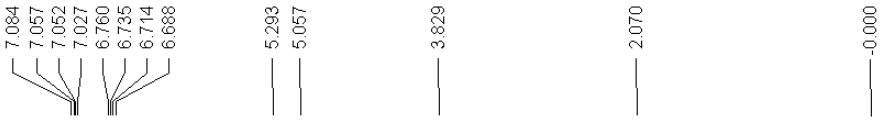
PPM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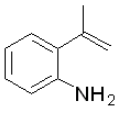
7.057
7.052
7.027
6.760
6.735
6.714
6.688
5.293
5.057
3.829
2.070
-0.000


NH2

**5**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3.00
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6
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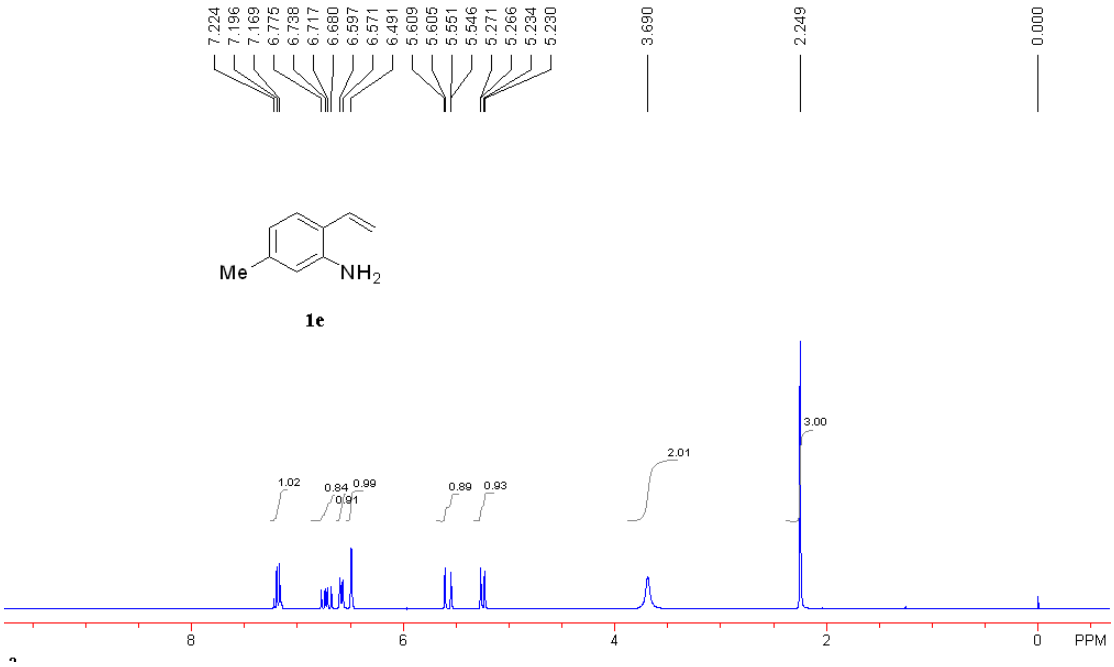
2
1
0 PPM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6.717
6.680
6.597
6.571
6.491
5.609
5.605
5.551
5.546
5.271
5.266
5.234
5.230
3.690
2.249
0.000
Me
NH2
1e
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0.91
0.99
0.89
0.93
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3.00
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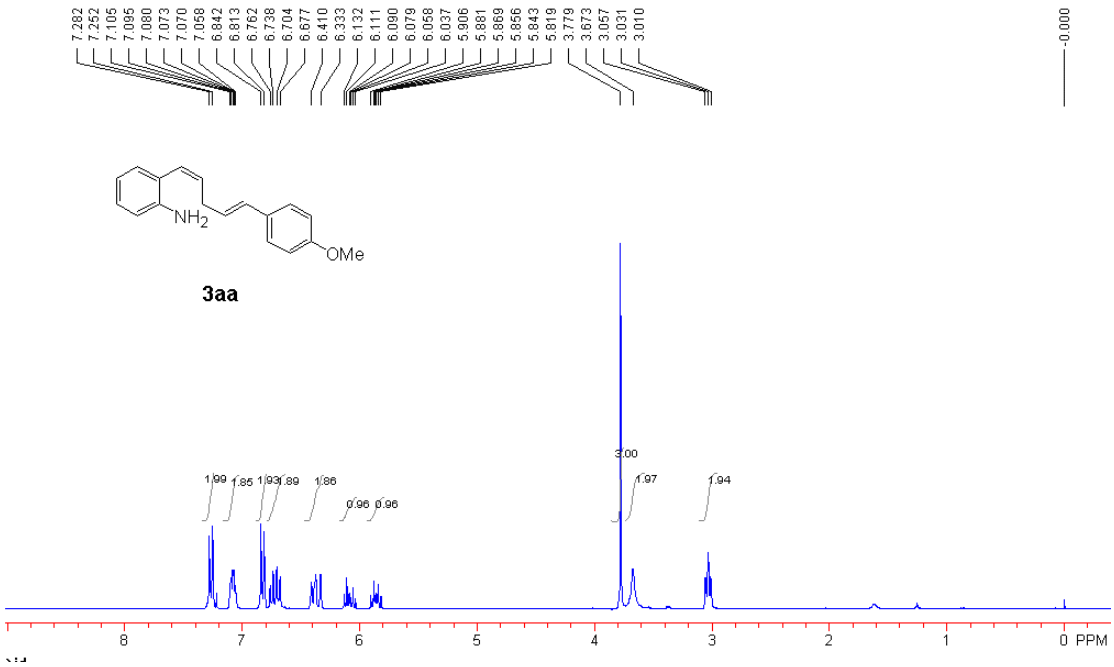
0
PPM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7.080
7.073
7.070
7.058
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6.813
6.762
6.738
6.704
6.677
6.410
6.333
6.132
6.111
6.090
6.079
6.058
6.037
5.906
5.881
5.869
5.856
5.843
5.819
3.779
3.673
3.057
3.031
3.010
-0.000
NH2
OMe
3aa
1.99
1.85
1.93
1.89
1.86
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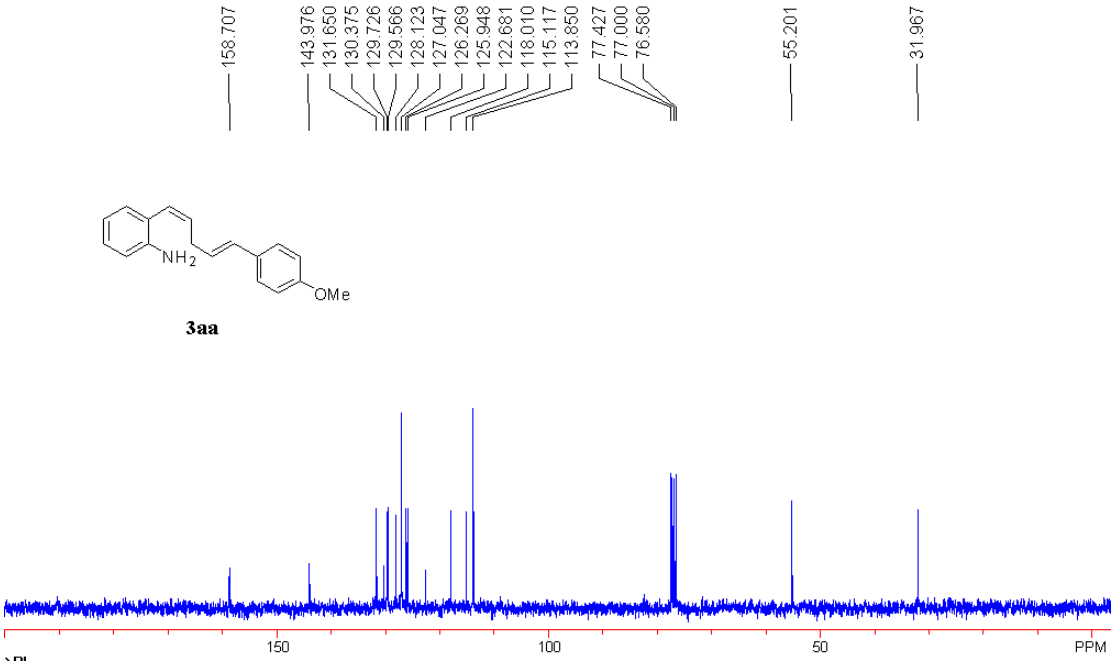
0.96
3.00
1.97
1.94
8
7
6
5
4
3
2
1
0 PPM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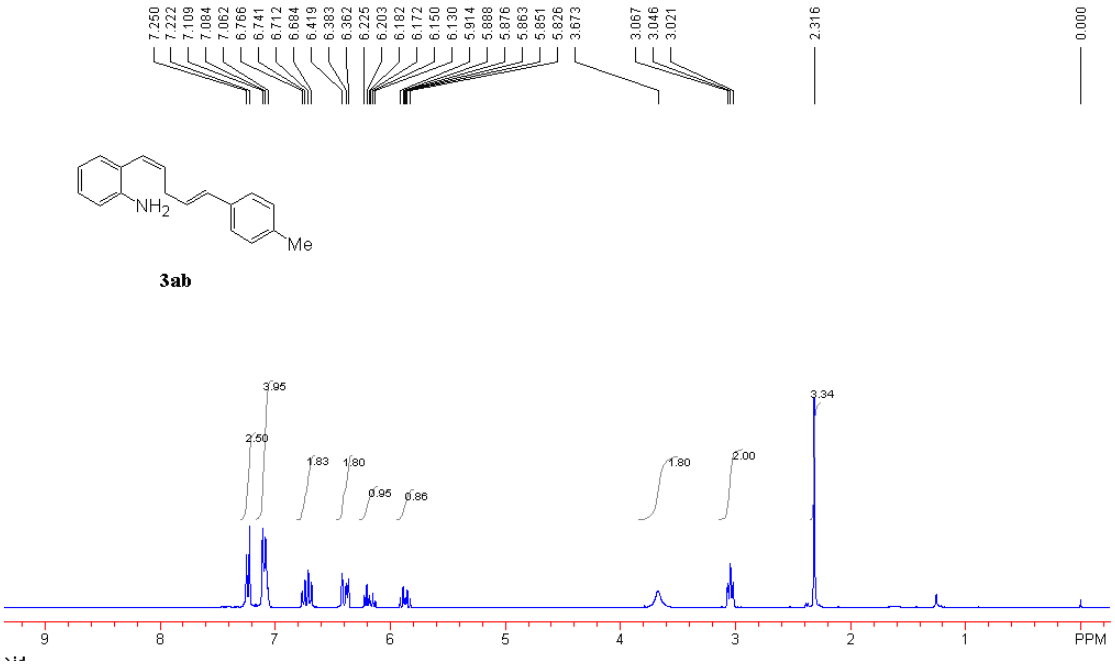
143.976
131.650
130.375
129.726
129.566
128.123
127.047
126.269
125.948
122.681
118.010
115.117
113.850
77.427
77.000
76.580
55.201
31.967
NH2
OMe
3aa
150
100
50
PPM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7.062
6.766
6.741
6.712
6.684
6.419
6.383
6.362
6.225
6.203
6.182
6.172
6.150
6.130
5.914
5.888
5.876
5.863
5.851
5.826
3.673
3.067
3.046
3.021
2.316
0.000
NH2
Me
3.95
2.50
1.83
1.80
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2.00
3.34
9
8
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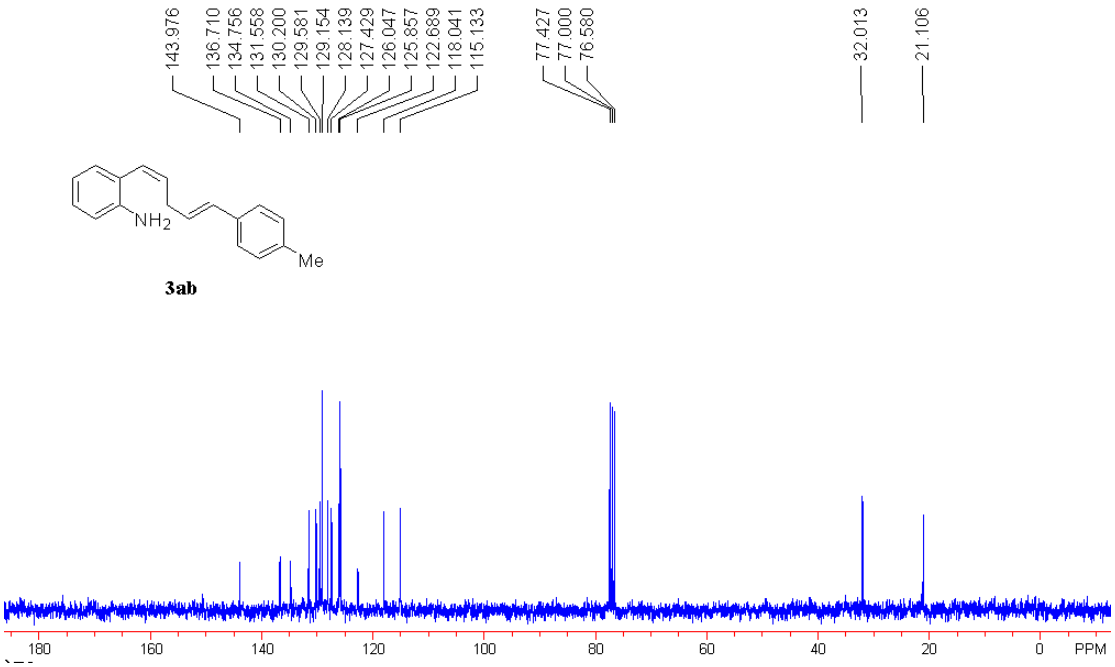
6
5
4
3
2
1
PPM

**3ab**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131.558
130.200
129.581
129.154
128.139
127.429
126.047
125.857
122.689
118.041
115.133
77.427
77.000
76.580
32.013
21.106
NH2
Me
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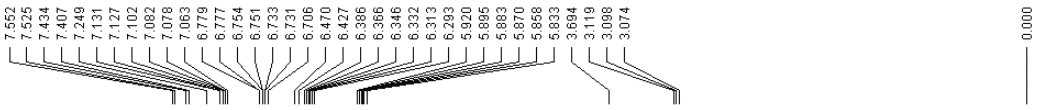
160
140
120
100
80
60
40
20
0
PPM

**3ab**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7.407
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7.131
7.127
7.102
7.082
7.078
7.063
6.779
6.777
6.754
6.751
6.733
6.731
6.706
6.470
6.427
6.386
6.366
6.346
6.332
6.313
6.293
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5.895
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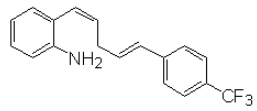
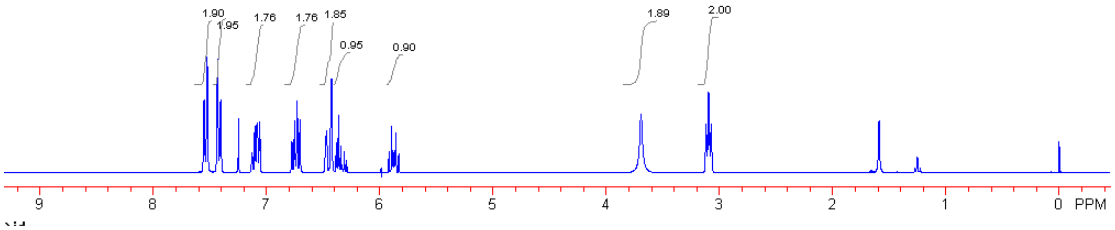
3.098
3.074
0.000


NH2
CF3

**3ac**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1.76
1.85
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0.90
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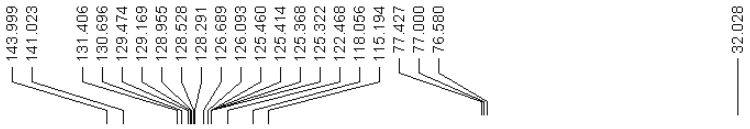
9
8
7
6
5
4
3
2
1
0
PPM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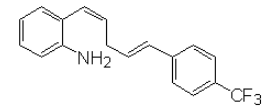
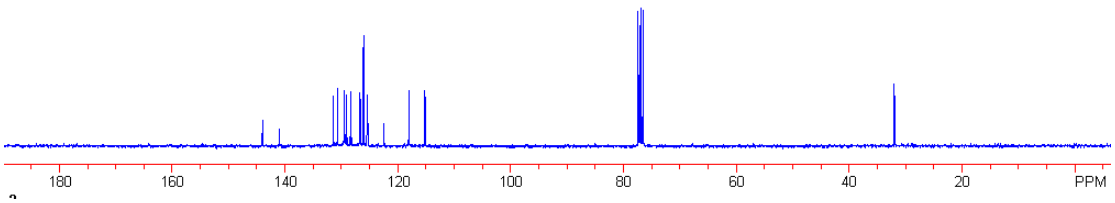
128.955
128.528
128.291
126.689
126.093
125.460
125.414
125.368
125.322
122.468
118.056
115.194
77.427
77.000
76.580
32.028


NH2
CF3

**3ac**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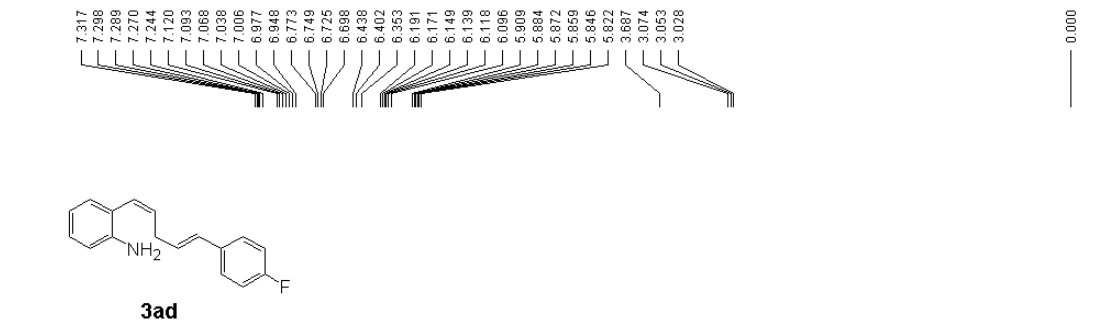
160
140
120
100
80
60
40
20
PPM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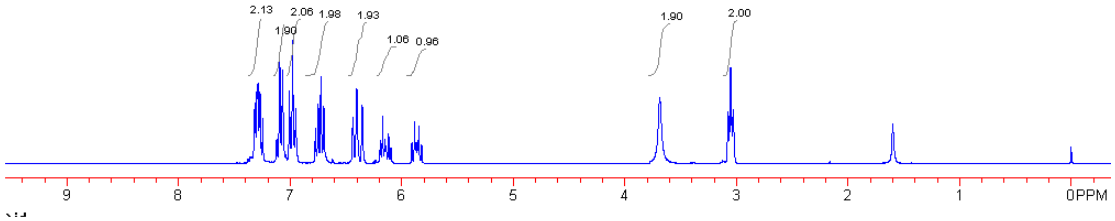
7.068
7.038
7.006
6.977
6.948
6.773
6.749
6.725
6.698
6.438
6.402
6.353
6.191
6.171
6.149
6.139
6.118
6.096
5.909
5.884
5.872
5.859
5.846
5.822
3.687
3.074
3.053
3.028
0.000
NH2
F

**3ad**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2.06
1.98
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1.06
0.96
1.90
2.00
9
8
7
6
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3
2
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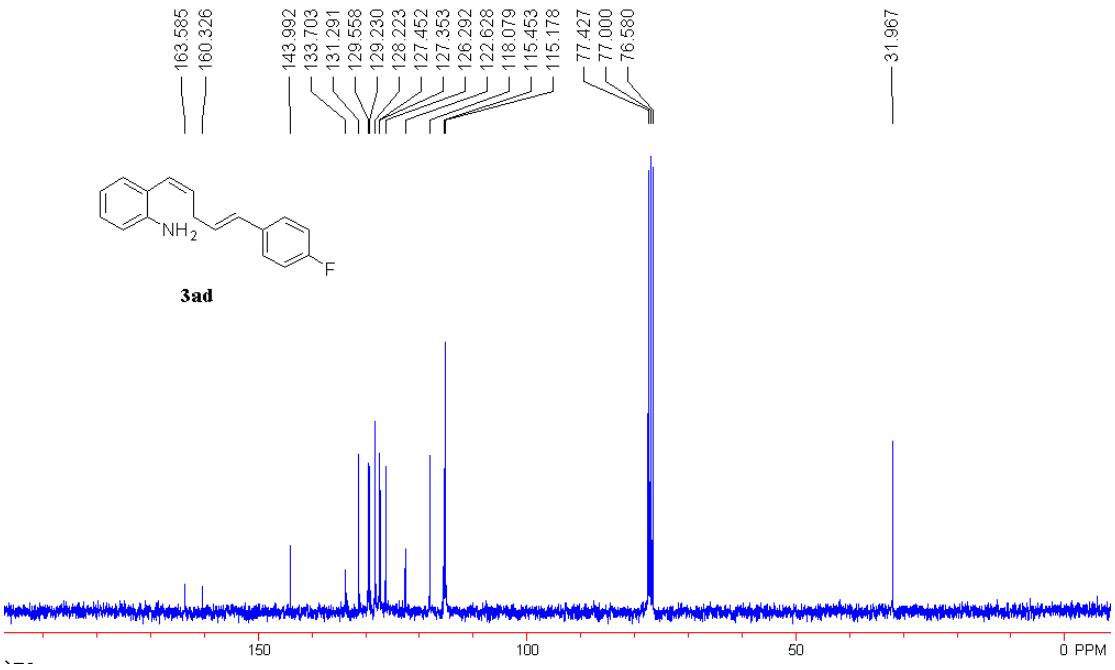
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129.558
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128.223
127.452
127.353
126.292
122.628
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77.427
77.000
76.580
31.967
NH2
F
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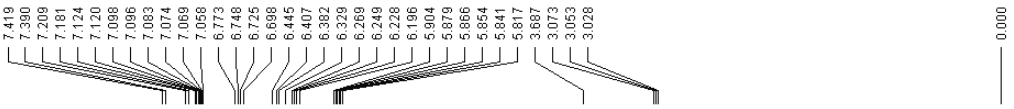
100
50
0 PPM

**3ad**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7.096
7.083
7.074
7.069
7.058
6.773
6.748
6.725
6.698
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6.407
6.382
6.329
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6.249
6.228
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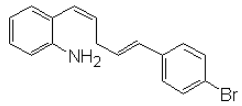
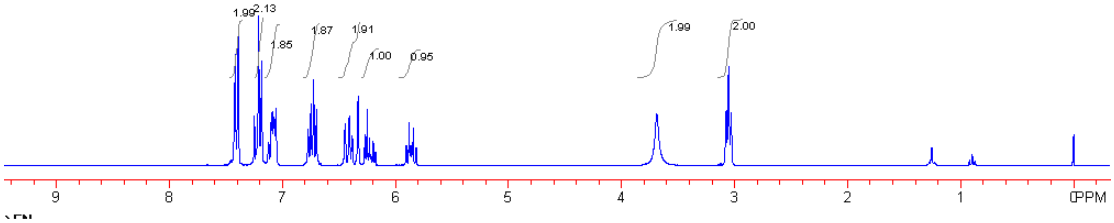
5.817
3.687
3.073
3.053
3.028
0.000


NH2
Br

**3ae**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2.13
1.85
1.87
1.91
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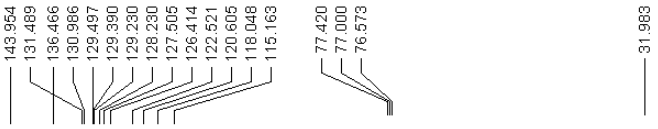
0.95
1.99
2.00
9
8
7
6
5
4
3
2
1
PPM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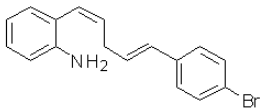
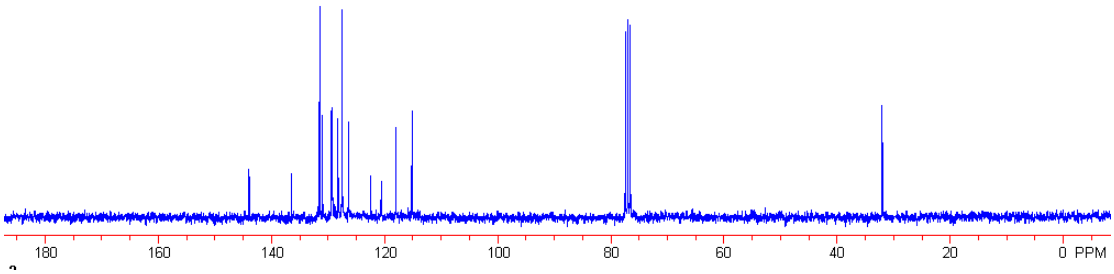
126.414
122.521
120.605
118.048
115.163
77.420
77.000
76.573
31.983


NH2
Br

**3ae**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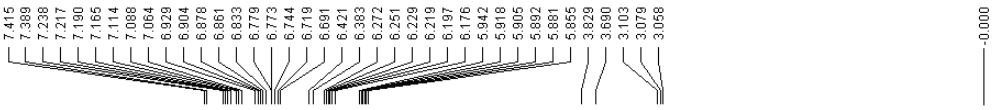
160
140
120
100
80
60
40
20
0 PPM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7.088
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6.904
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6.861
6.833
6.779
6.773
6.744
6.719
6.691
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6.272
6.251
6.229
6.219
6.197
6.176
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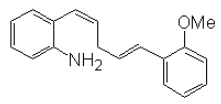
OMe
NH2

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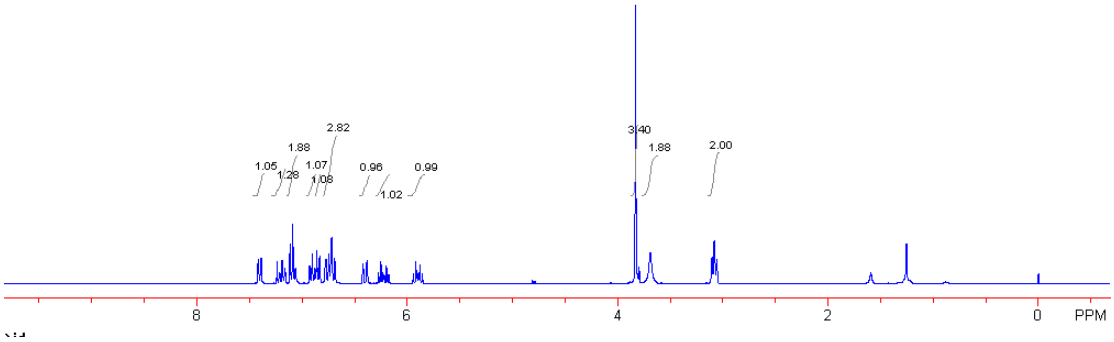
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1.08
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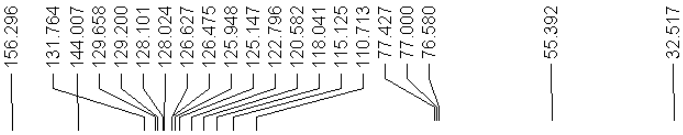
1.02
0.99
3.40
1.88
2.00
8
6
4
2
0
PPM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128.024
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120.582
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110.713
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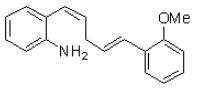
77.000
76.580
55.392
32.517


OMe
NH2

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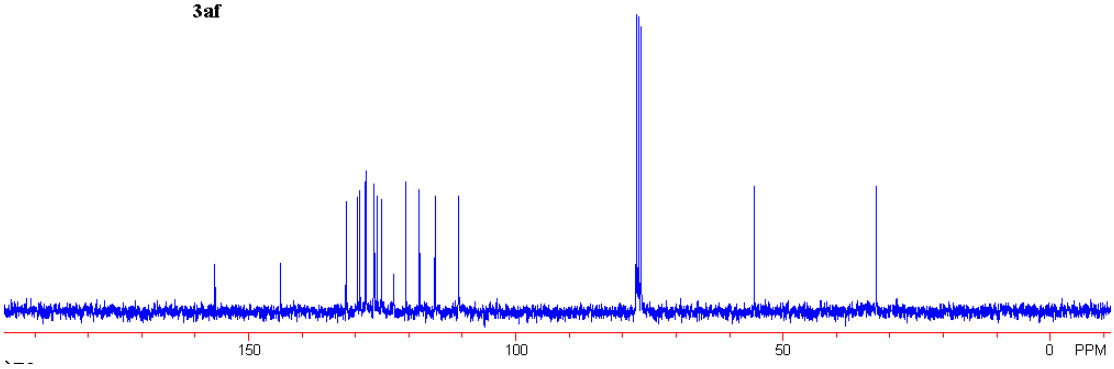
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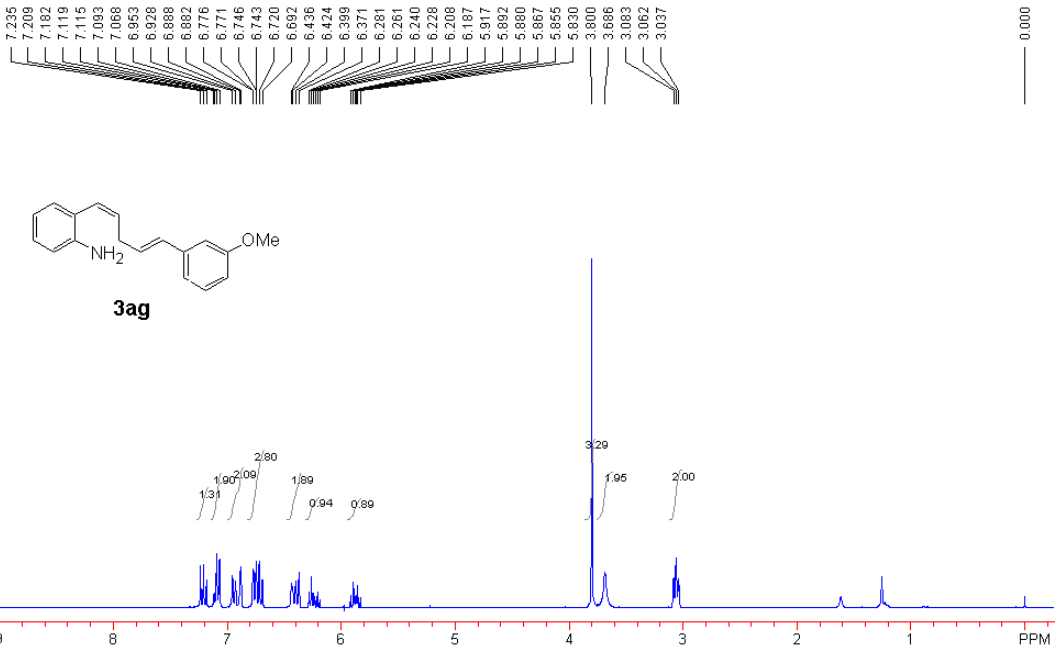
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5.830
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3.686
3.083
3.062
3.037
0.000
NH2
OMe
3ag
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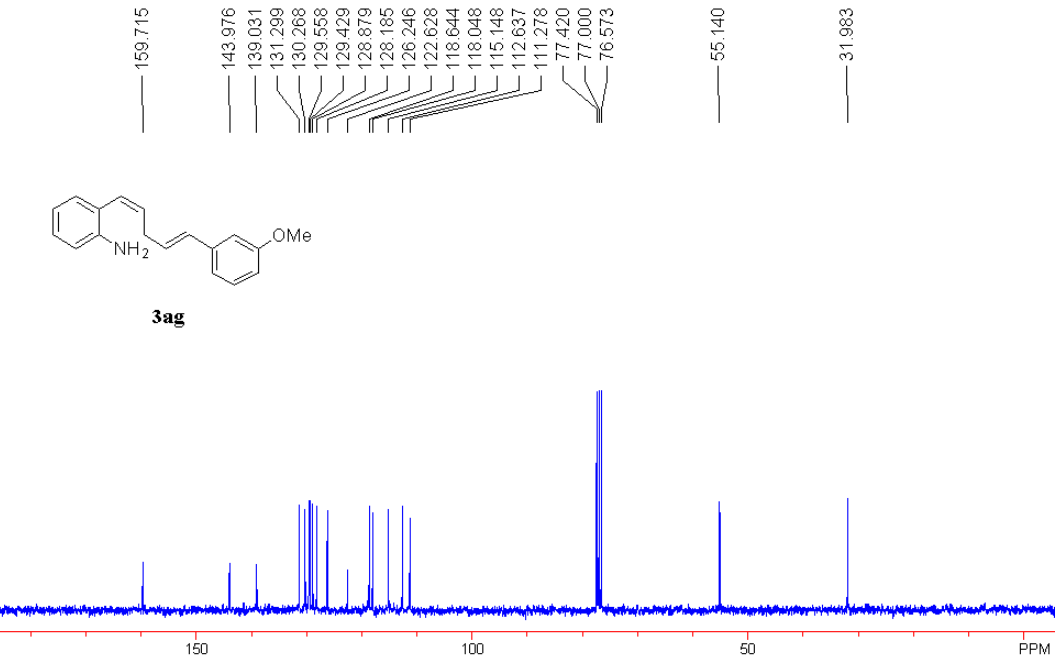
1.90
2.09
2.80
1.89
0.94
0.89
3.29
1.95
2.00
9
8
7
6
5
4
3
2
1
PPM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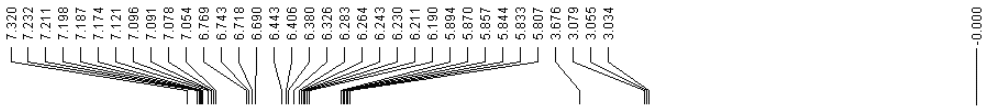
128.879
128.185
126.246
122.628
118.644
118.048
115.148
112.637
111.278
77.420
77.000
76.573
55.140
31.983
NH2
OMe
3ag
150
100
50
PPM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7.211
7.198
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7.174
7.121
7.096
7.091
7.078
7.054
6.769
6.743
6.718
6.690
6.443
6.406
6.380
6.326
6.283
6.264
6.243
6.230
6.211
6.190
5.894
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5.857
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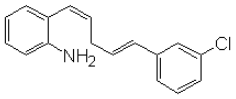
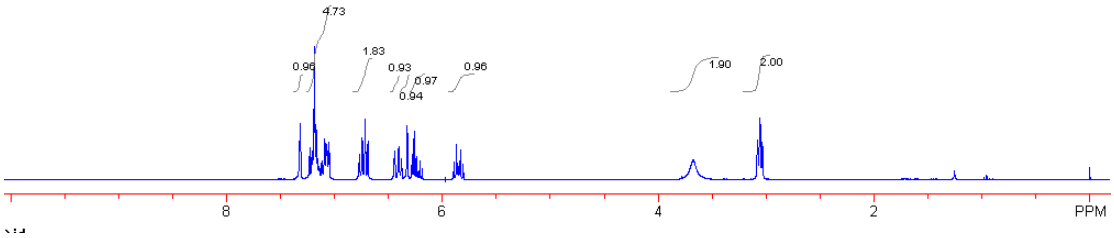
5.833
5.807
3.676
3.079
3.055
3.034
-0.000


NH2
Cl

**3ah**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0.93
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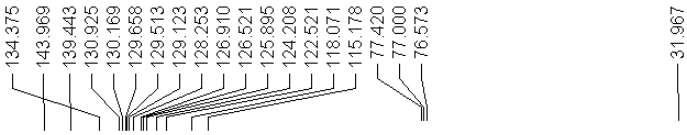
0.94
0.96
1.90
2.00
8
6
4
2
PPM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139.443
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129.123
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125.895
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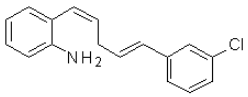
115.178
77.420
77.000
76.573
31.967


NH2
Cl

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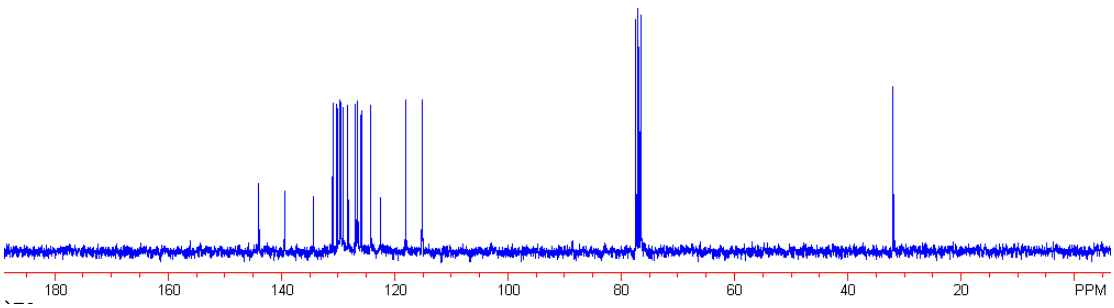
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80
60
40
20
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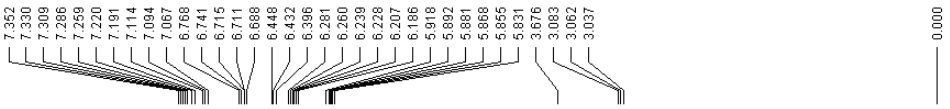
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7.114
7.094
7.067
6.768
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6.715
6.711
6.688
6.448
6.432
6.396
6.281
6.260
6.239
6.228
6.207
6.186
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3.037
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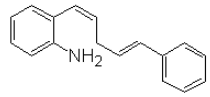
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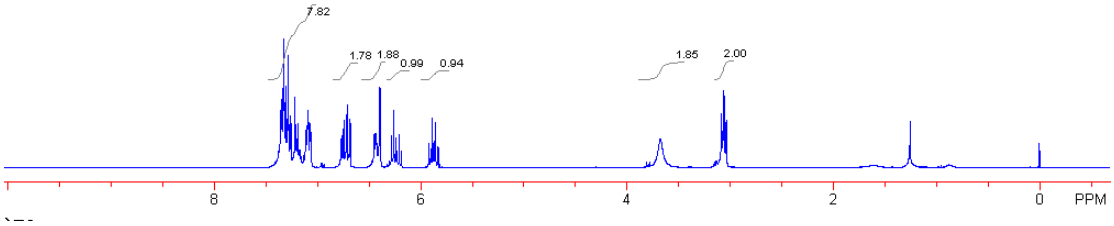
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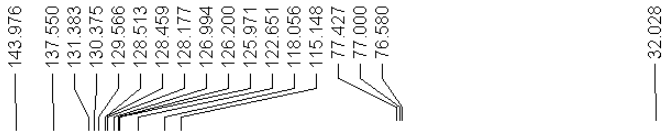
0.94
1.85
2.00
8
6
4
2
0
PPM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130.375
129.566
128.513
128.459
128.177
126.994
126.200
125.971
122.651
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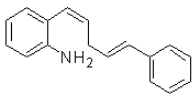
115.148
77.427
77.000
76.580
32.028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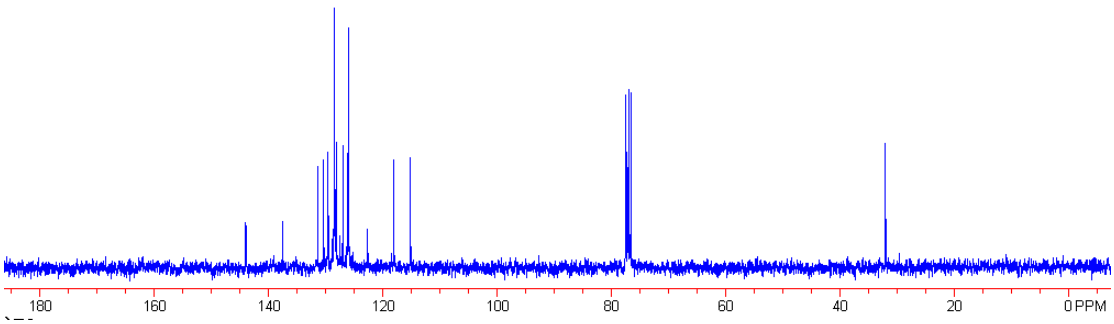
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120
100
80
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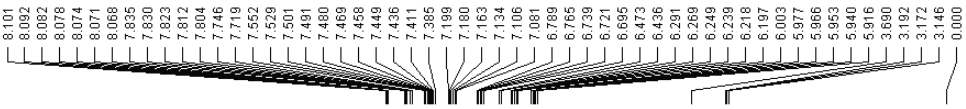
40
20
0 PPM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8.082
8.078
8.074
8.071
8.068
7.835
7.830
7.823
7.812
7.804
7.746
7.719
7.552
7.529
7.501
7.491
7.480
7.469
7.458
7.449
7.436
7.411
7.385
7.199
7.180
7.163
7.134
7.106
7.081
6.789
6.765
6.739
6.721
6.695
6.473
6.436
6.291
6.269
6.249
6.239
6.218
6.197
6.003
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5.940
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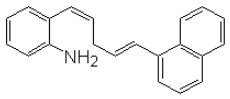
3.172
3.146
0.000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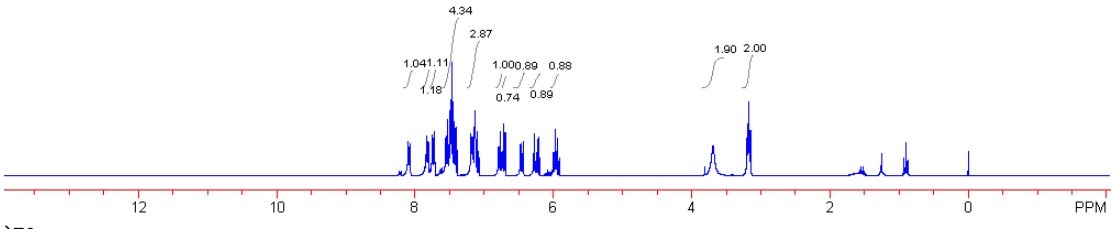
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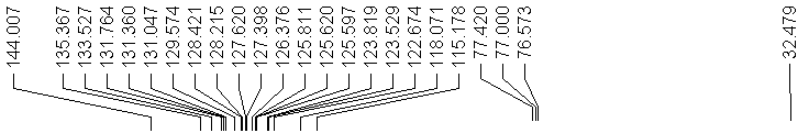
1.11
1.18
1.00
0.89
0.88
0.74
0.89
1.90
2.00
12
10
8
6
4
2
0
PPM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131.764
131.360
131.047
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128.421
128.215
127.620
127.398
126.376
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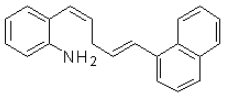
115.178
77.420
77.000
76.573
32.479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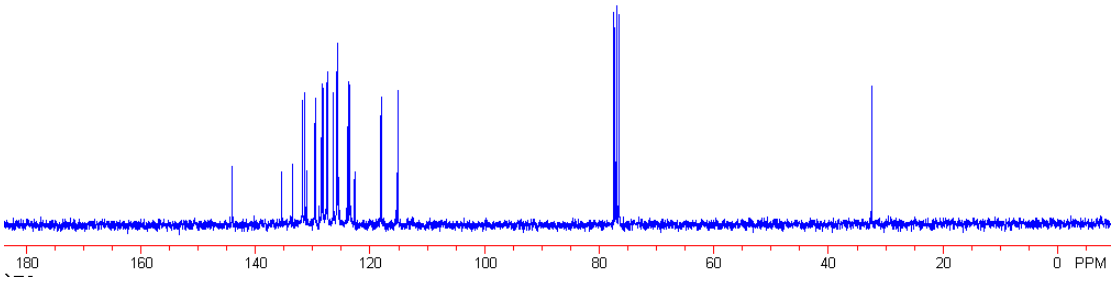
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80
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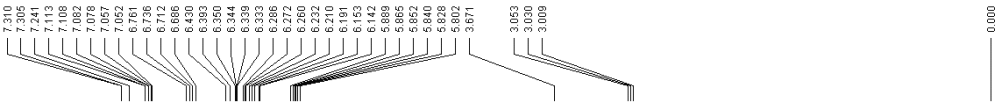
PPM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7.108
7.082
7.078
7.057
7.052
6.761
6.736
6.712
6.686
6.430
6.393
6.350
6.344
6.339
6.333
6.286
6.272
6.260
6.232
6.210
6.191
6.153
6.142
5.889
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5.852
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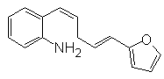
5.828
5.802
3.671
3.053
3.030
3.009
0.000


NH2
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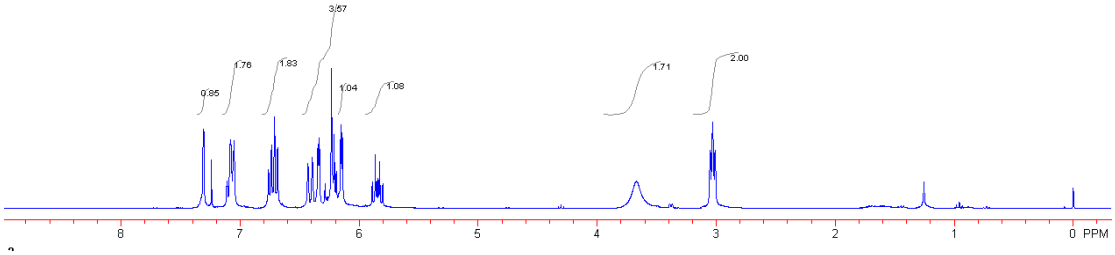
**3ak**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1.08
1.71
2.00
8
7
6
5
4
3
2
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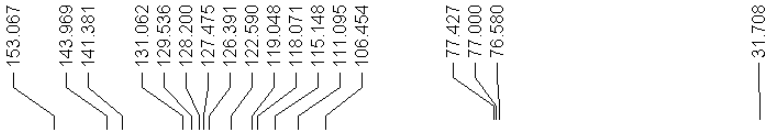
0 PPM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141.381
131.062
129.536
128.200
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106.454
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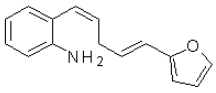
31.708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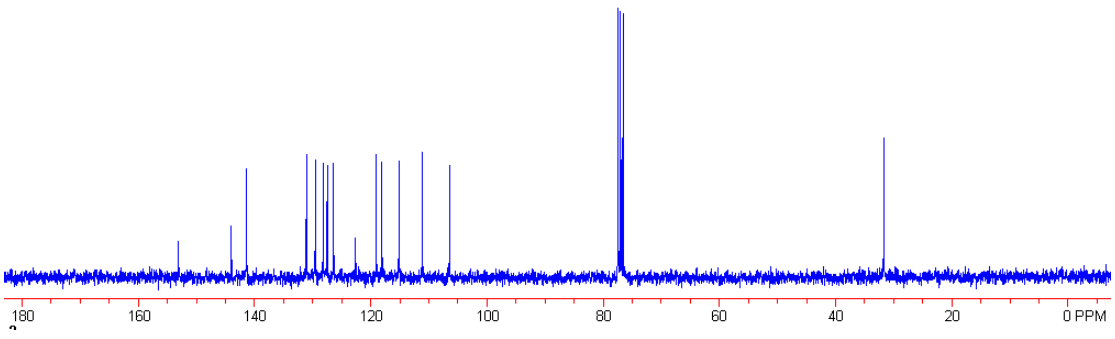
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120
100
80
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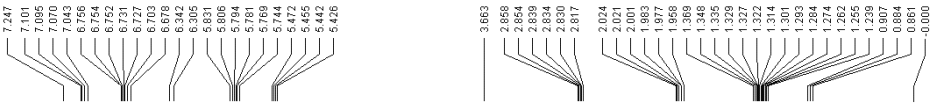
40
20
0 PPM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6.305
5.831
5.806
5.794
5.781
5.769
5.744
5.472
5.455
5.442
5.426
3.663
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2.854
2.839
2.834
2.830
2.817
2.024
2.021
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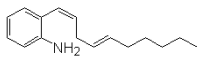
0.000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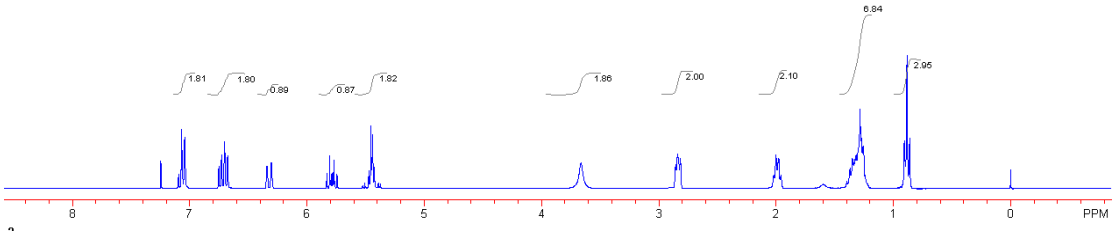
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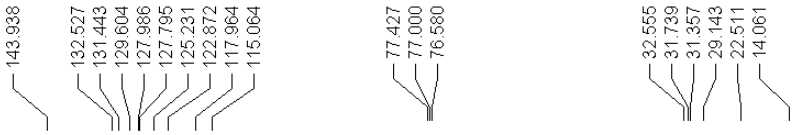
8
7
6
5
4
3
2
1
0
PPM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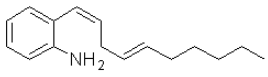
22.511
14.061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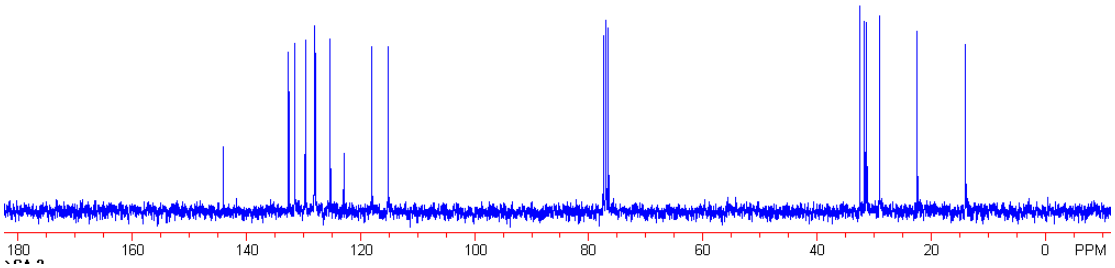
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160
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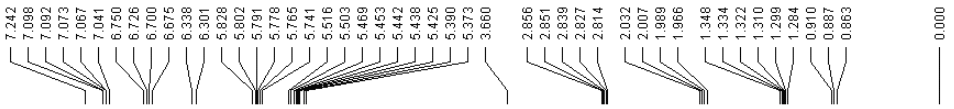
120
100
80
60
40
20
0
PPM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6.726
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6.675
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5.828
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5.516
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5.425
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5.373
3.660
2.856
2.851
2.839
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2.814
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2.007
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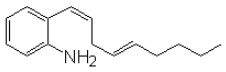
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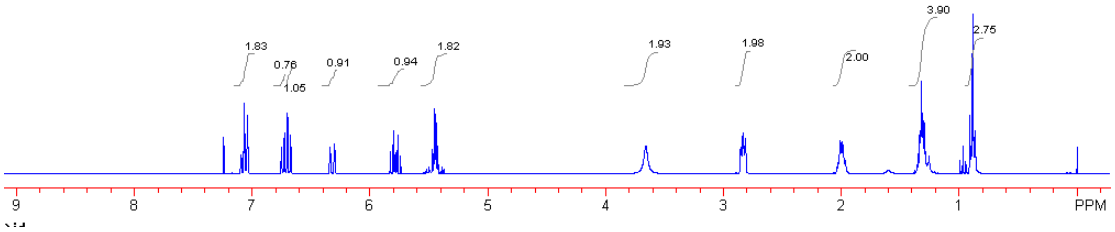
**3am**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2.75
9
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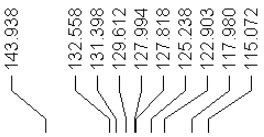
7
6
5
4
3
2
1
PPM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131.398
129.612
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127.818
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115.072
77.420
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32.257
31.746
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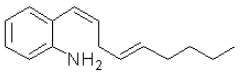
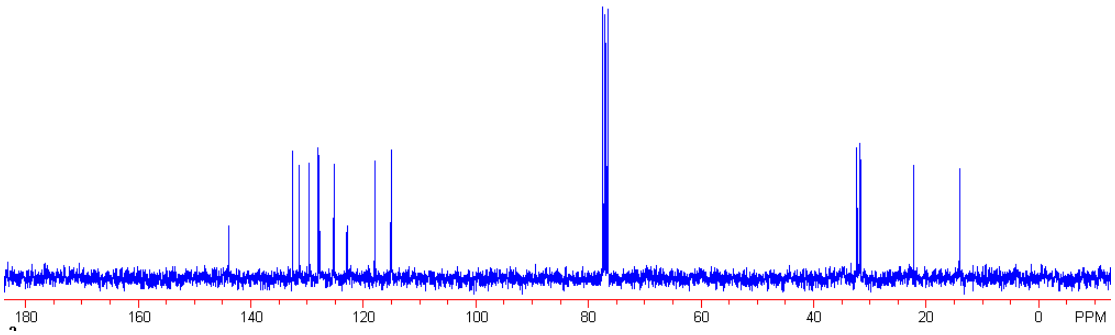
22.167
13.931


NH2

**3am**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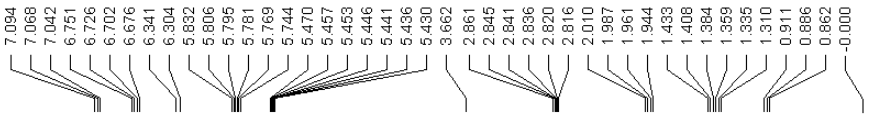
80
60
40
20
0
PPM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5.441
5.436
5.430
3.662
2.861
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2.836
2.820
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2.010
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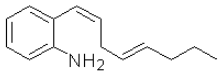
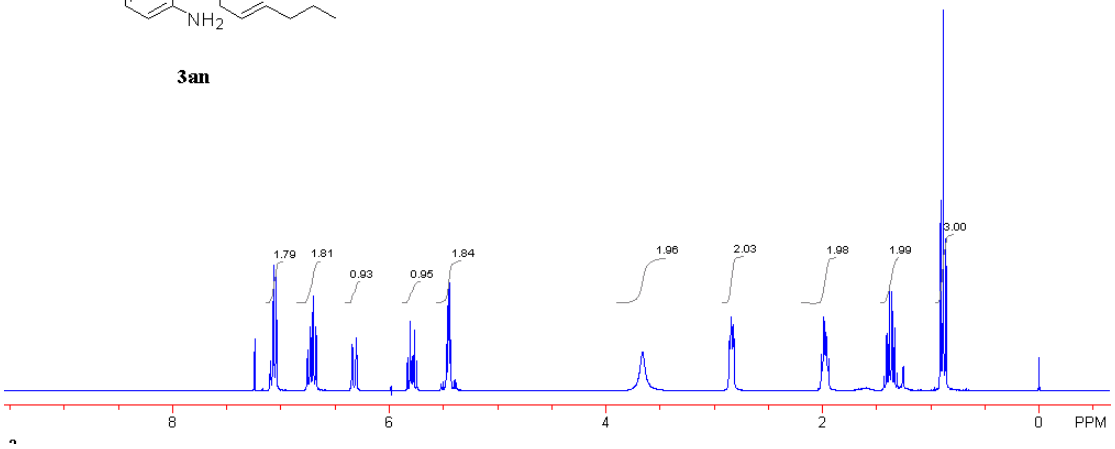

NH2

**3an**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3.00
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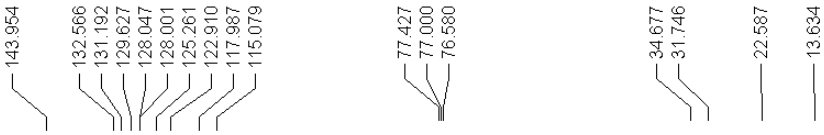
PPM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129.627
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77.427
77.000
76.580
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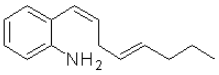
13.634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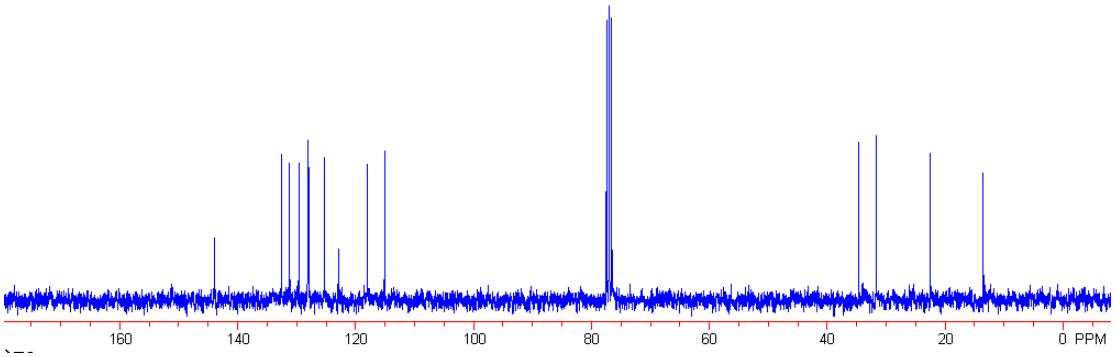
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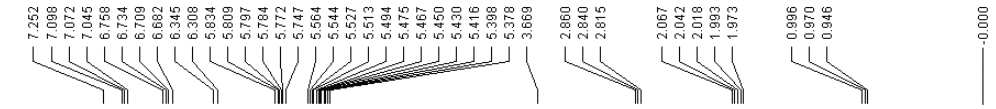
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5.513
5.494
5.475
5.467
5.450
5.430
5.416
5.398
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3.669
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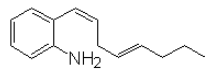
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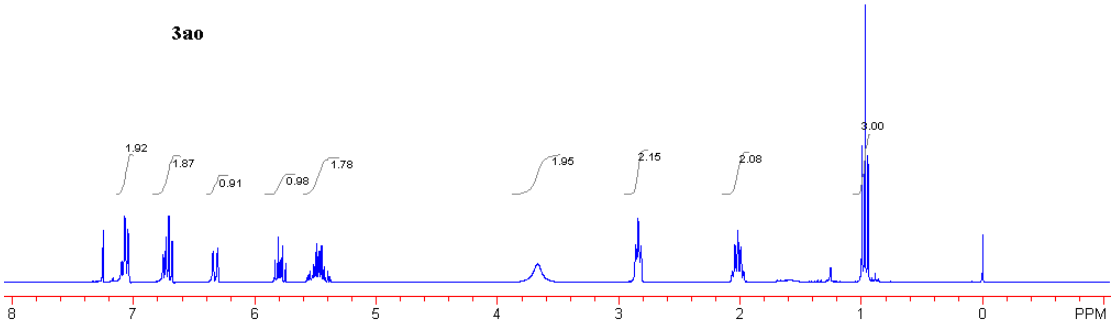
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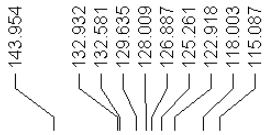
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129.635
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122.918
118.003
115.087
77.420
77.000
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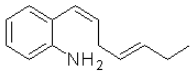
13.794


NH2

**3ao**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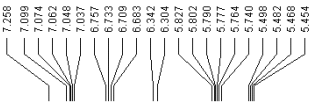
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5.827
5.802
5.790
5.777
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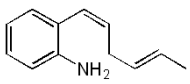
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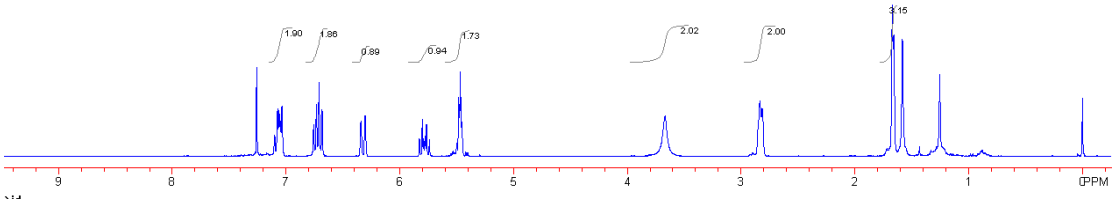
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3.15
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2
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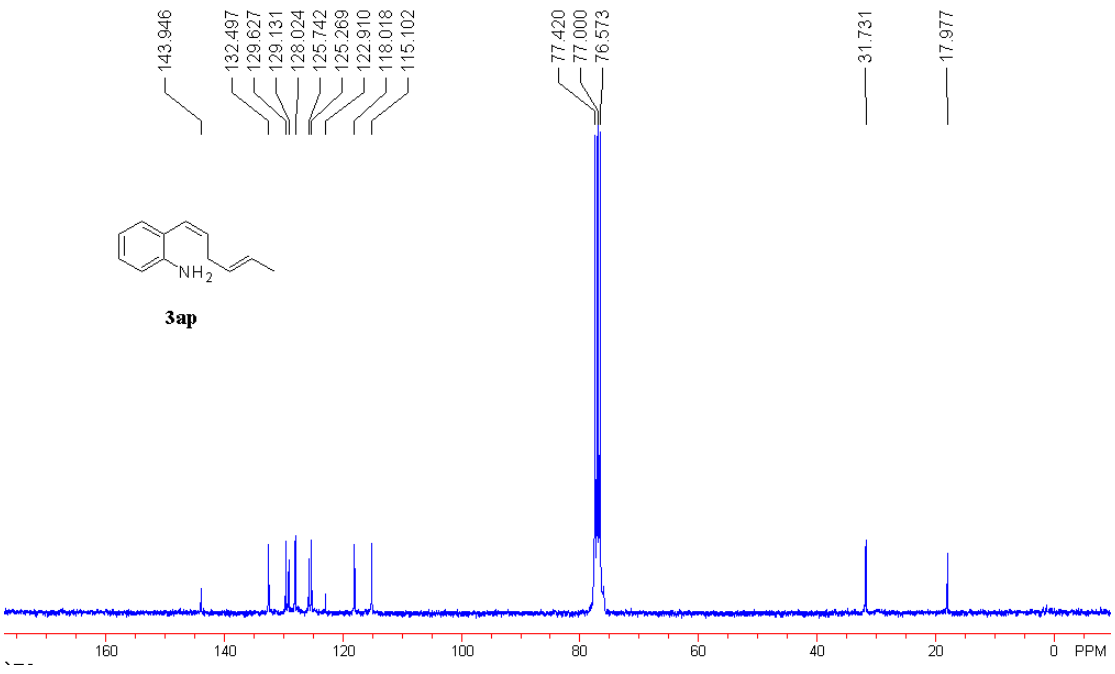
0PPM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122.910
118.018
115.102
77.420
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17.977
NH2
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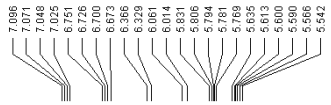
120
100
80
60
40
20
0 PPM

**3ap**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6.673
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6.061
6.014
5.831
5.806
5.794
5.781
5.769
5.635
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1.720
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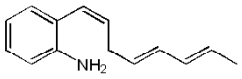
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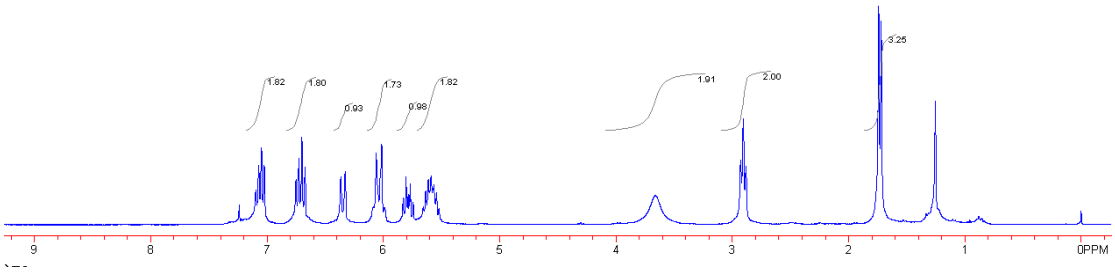
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2.00
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3
2
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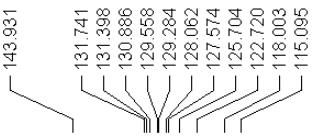
0PPM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130.886
129.558
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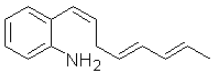
127.574
125.704
122.720
118.003
115.095
77.420
77.000
76.573
31.586
18.000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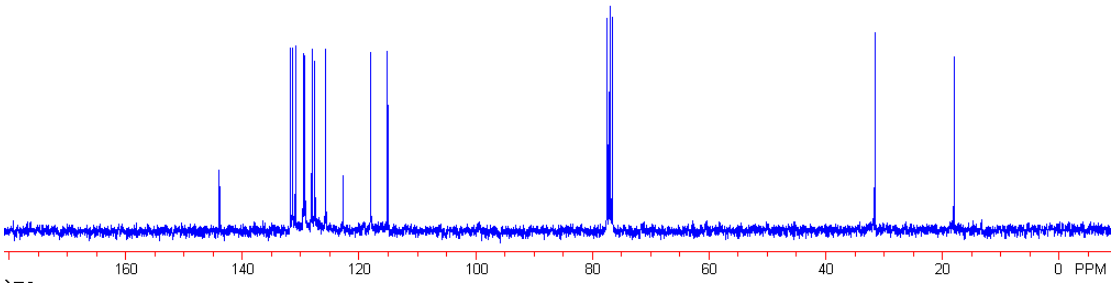
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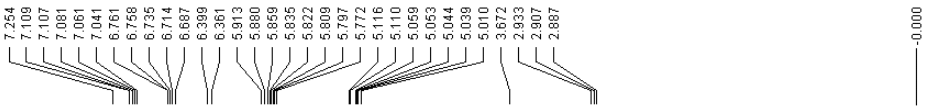
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6.361
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5.880
5.859
5.835
5.822
5.809
5.797
5.772
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5.044
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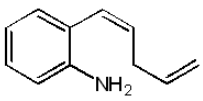
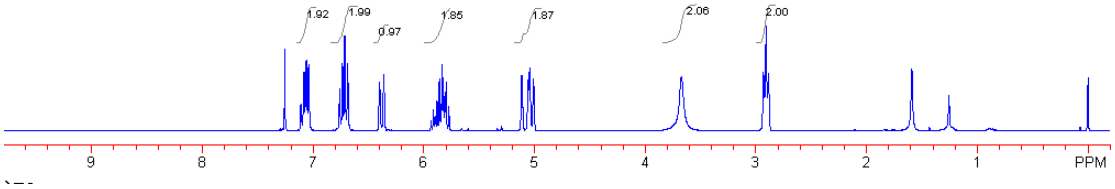
2.887
-0.000


NH2

**3ar**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1.87
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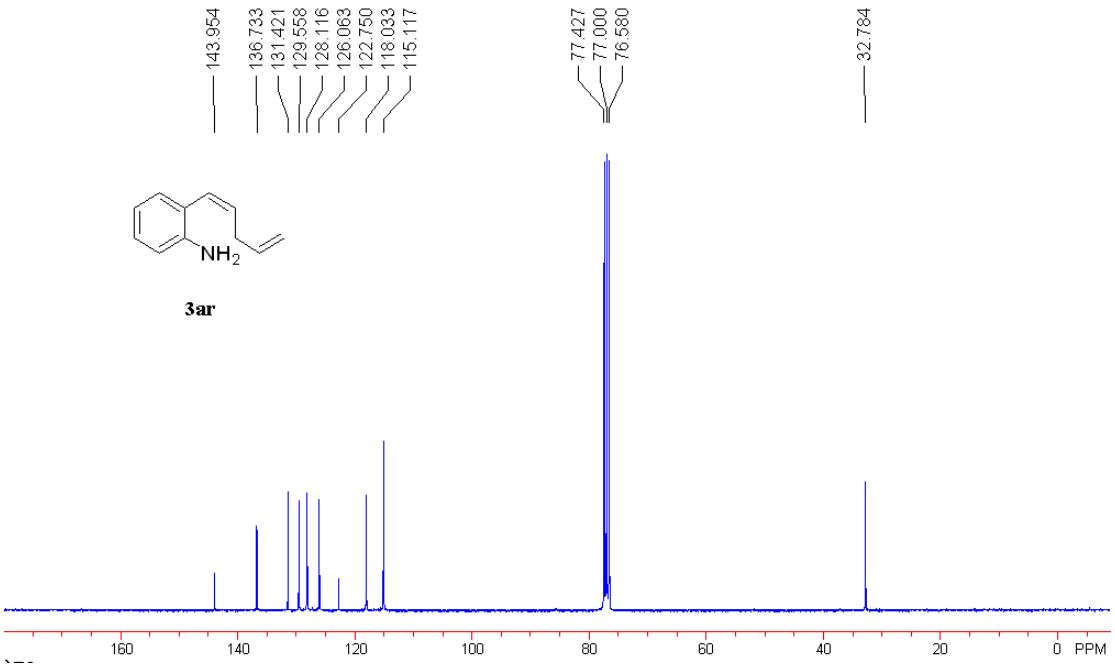
2.00
9
8
7
6
5
4
3
2
1
PPM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131.421
129.558
128.116
126.063
122.750
118.033
115.117
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77.000
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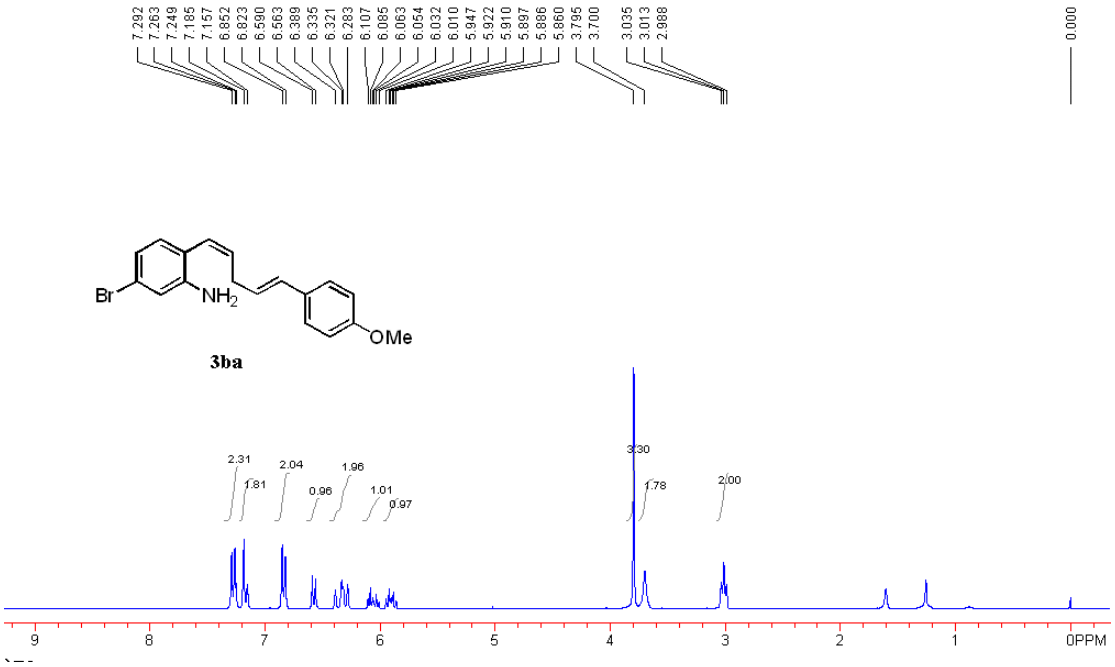
32.784
160
140
120
100
80
60
40
20
0
PPM


NH2

**3ar**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6.283
6.107
6.085
6.063
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6.032
6.010
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5.922
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5.886
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3.700
3.035
3.013
2.988
0.000
Br
NH2
OMe
3ba
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1.81
2.04
0.96
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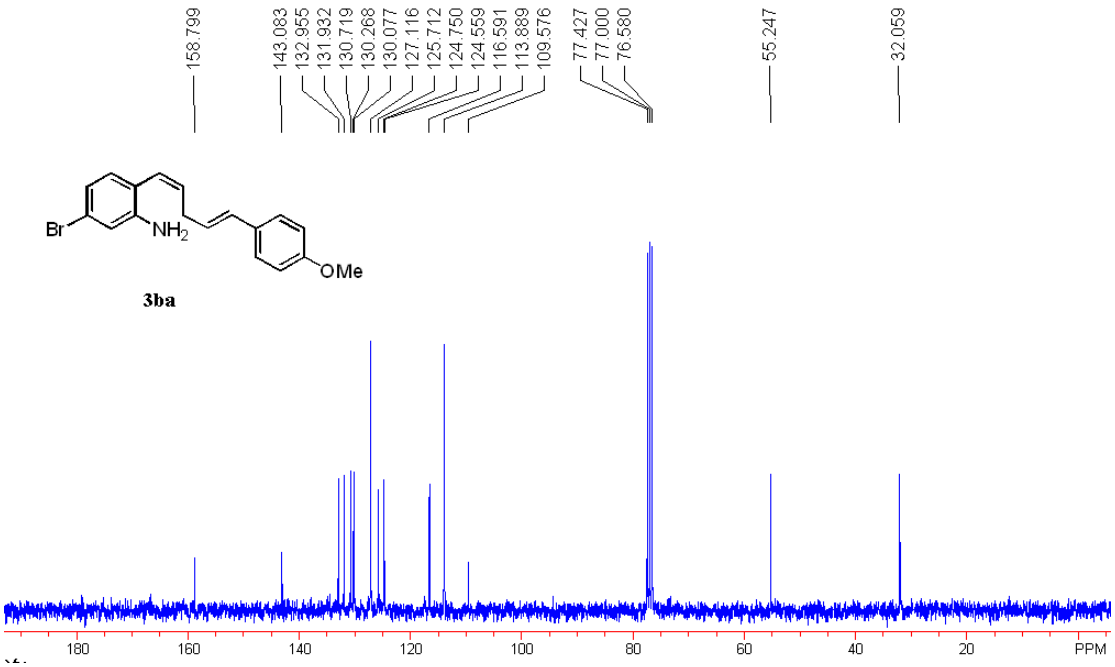
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77.427
77.000
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Br
NH2
OMe
3ba
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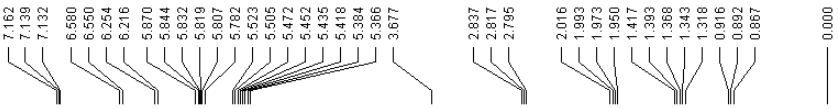
40
20
PPM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5.782
5.523
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5.472
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5.418
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2.016
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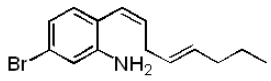
Br
NH2

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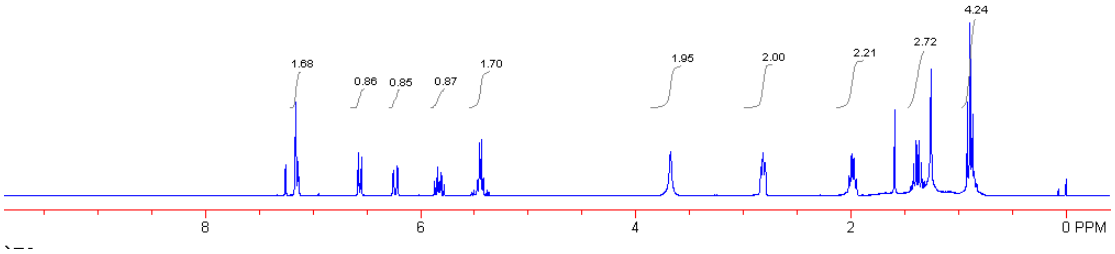
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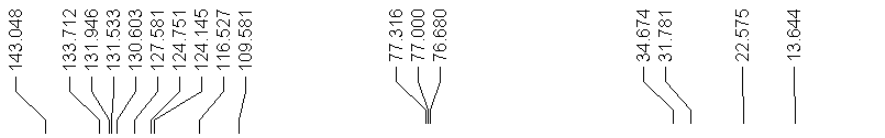
4.24
8
6
4
2
0 PPM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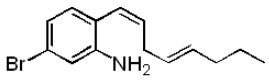
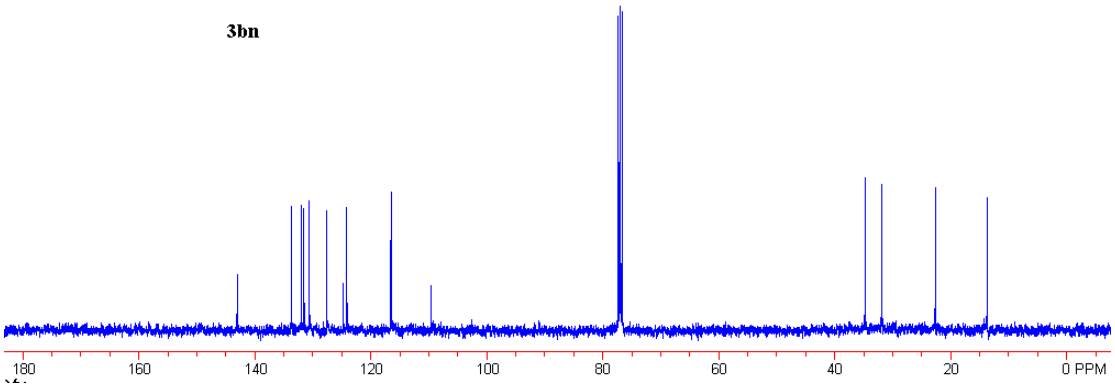
13.644


Br
NH2

**3bn**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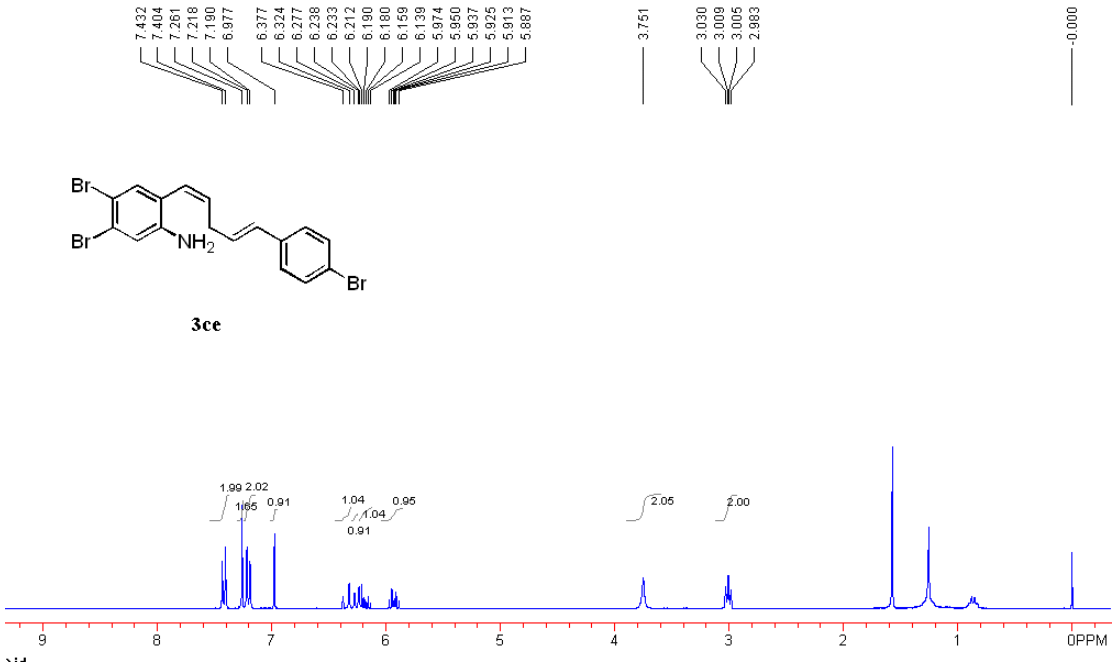
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6.238
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6.190
6.180
6.159
6.139
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5.950
5.937
5.925
5.913
5.887
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3.030
3.009
3.005
2.983
0.000
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Br
NH2
Br
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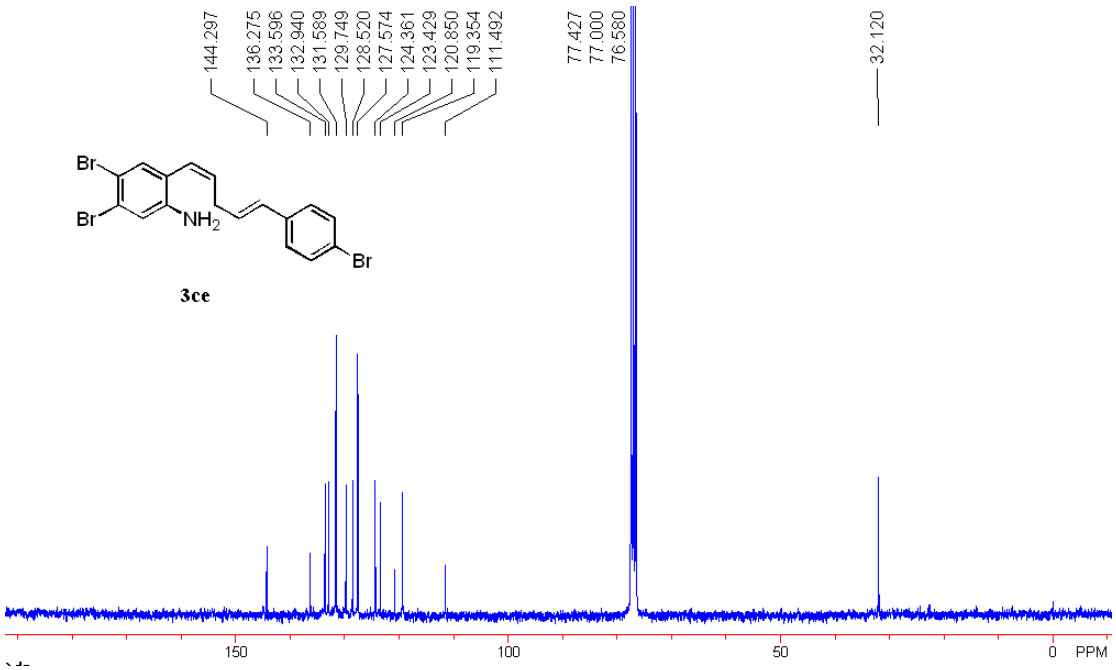
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123.429
120.850
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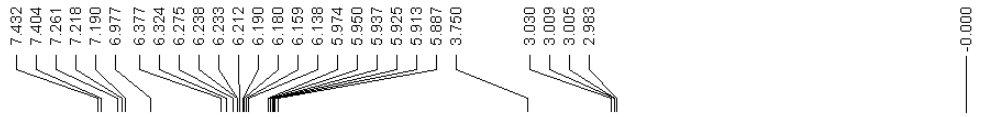
77.000
76.580
32.120
Br
Br
NH2
Br
3ce
150
100
50
0
PPM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5.913
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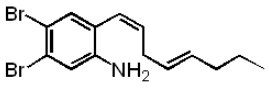
Br
Br
NH2

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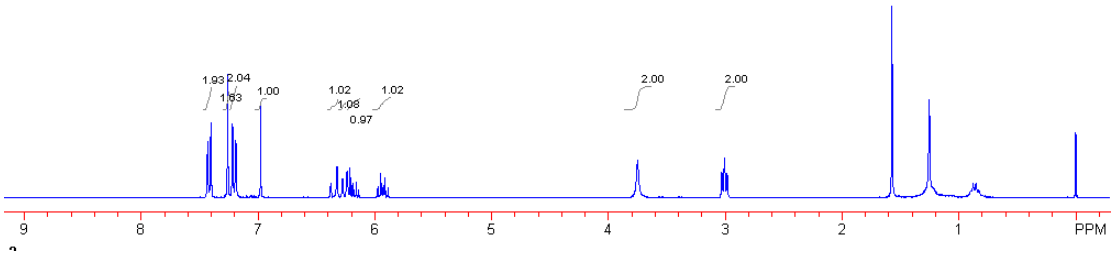
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1.02
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2.00
9
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7
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2
1
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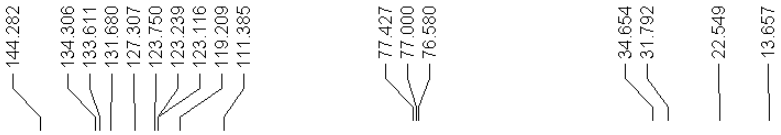
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131.680
127.307
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76.580
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22.549
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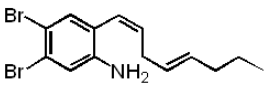
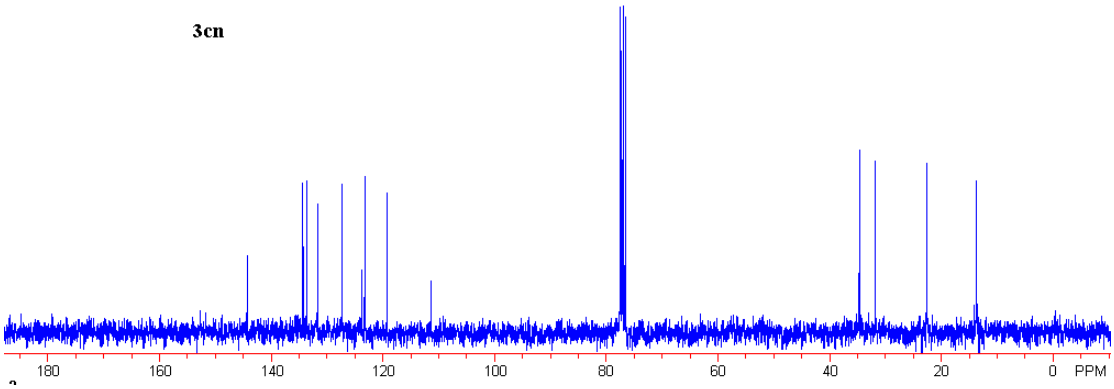

Br
Br
NH2

**3cn**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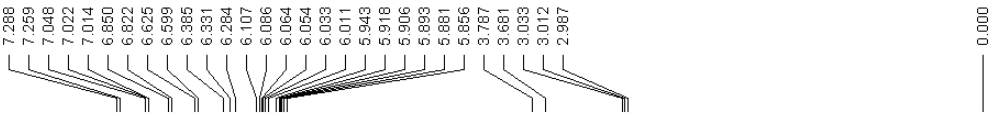
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7.022
7.014
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6.625
6.599
6.385
6.331
6.284
6.107
6.086
6.064
6.054
6.033
6.011
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5.856
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3.681
3.033
3.012
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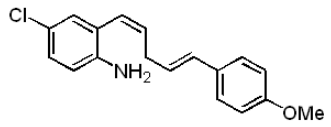
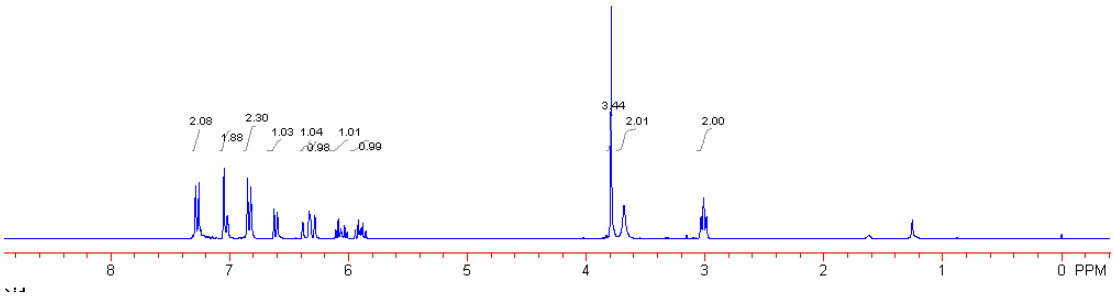
0.000


Cl
NH2
OMe

**3da**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1.04
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0.99
3.44
2.01
2.00
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7
6
5
4
3
2
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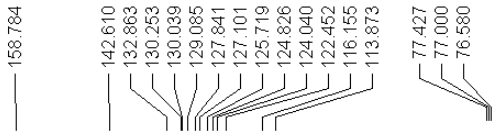
0 PPM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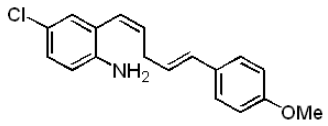
55.224
32.021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NH2
OMe

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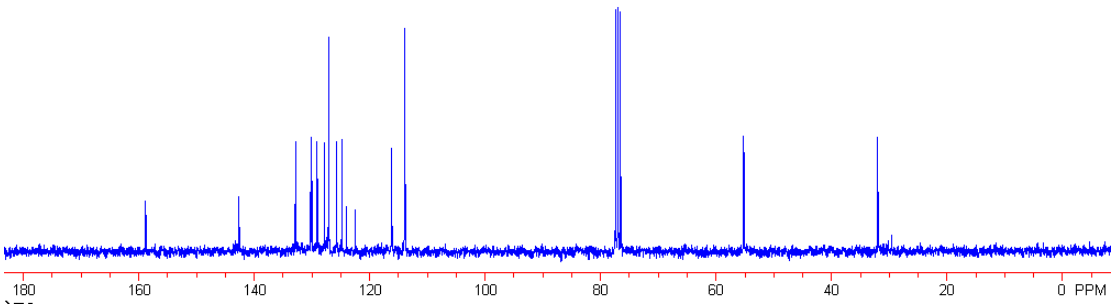
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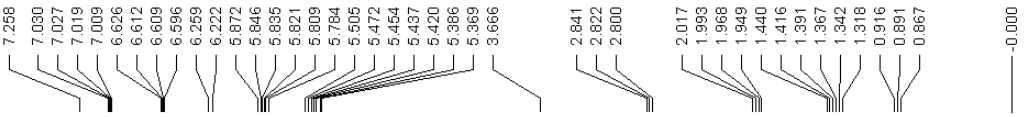
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6.609
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6.259
6.222
5.872
5.846
5.835
5.821
5.809
5.784
5.505
5.472
5.454
5.437
5.420
5.386
5.369
3.666
2.841
2.822
2.800
2.017
1.993
1.968
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1.391
1.367
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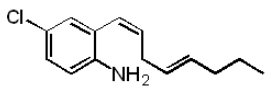
0.867
-0.000


Cl
NH2

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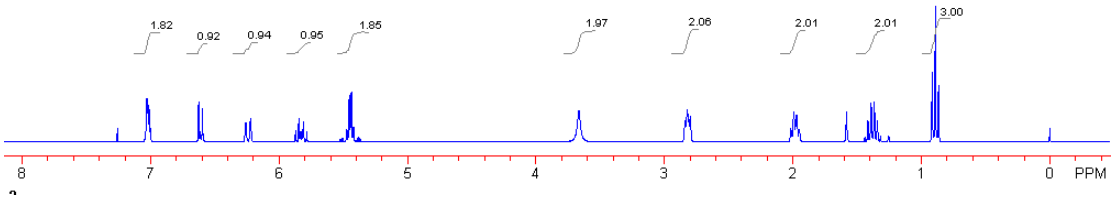
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0.94
0.95
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1.97
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2.01
2.01
3.00
8
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5
4
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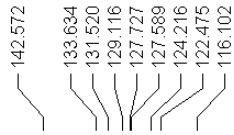
0
PPM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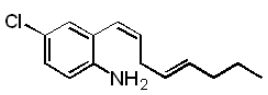
131.520
129.116
127.727
127.589
124.216
122.475
116.102
77.420
77.000
76.573
34.677
31.761
22.572
13.649


Cl
NH2

**3dn**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100
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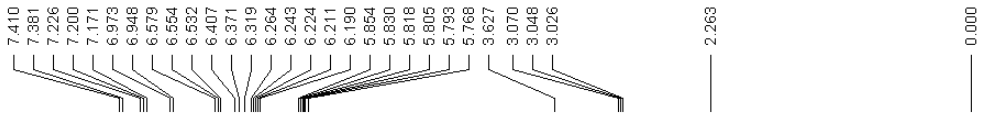
40
20
PPM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7.381
7.226
7.200
7.171
6.973
6.948
6.579
6.554
6.532
6.407
6.371
6.319
6.264
6.243
6.224
6.211
6.190
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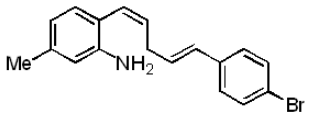
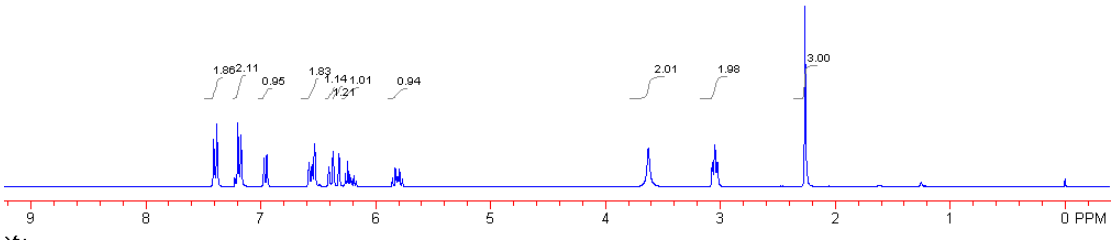
5.830
5.818
5.805
5.793
5.768
3.627
3.070
3.048
3.026
2.263
0.000


Me
NH2
Br

**3ee**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1.14
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1.21
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2.01
1.98
3.00
9
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7
6
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2
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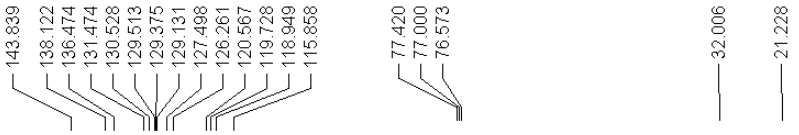
0 PPM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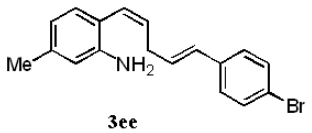
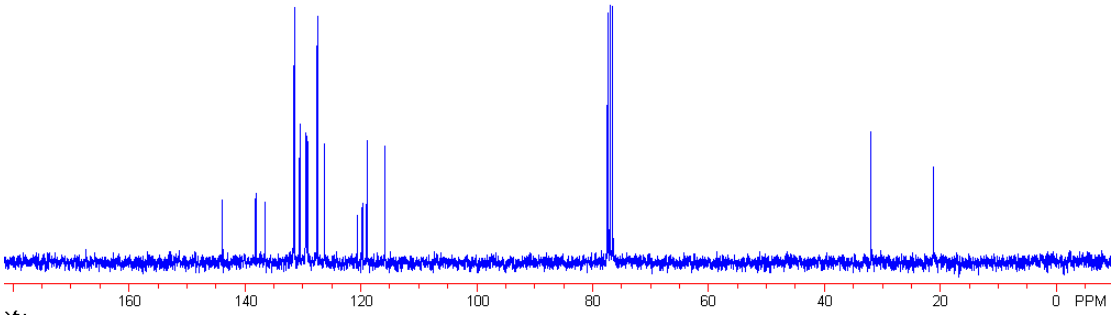
136.474
131.474
130.528
129.513
129.375
129.131
127.498
126.261
120.567
119.728
118.949
115.858
77.420
77.000
76.573
32.006
21.228


Me
NH2
Br

**3ee**


160
140
120
100
80
60
40
20
0 PPM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6.939
6.571
6.545
6.523
6.311
6.274
5.791
5.765
5.753
5.740
5.728
5.703
5.466
5.454
5.449
5.444
3.615
2.862
2.847
2.833
2.828
2.259
2.007
1.984
1.966
1.946
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1.405
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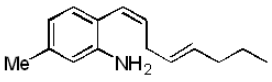
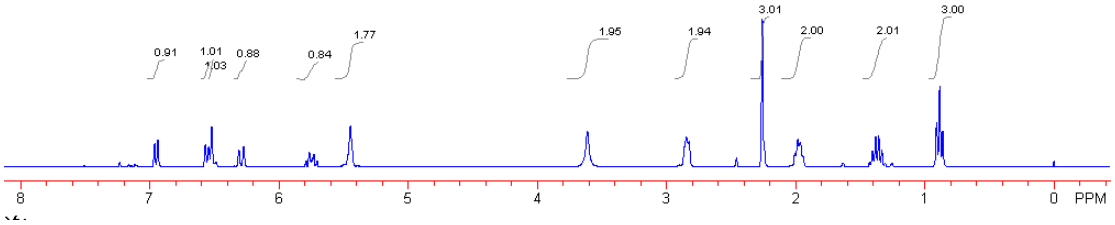
1.358
1.335
1.307
0.908
0.883
0.859
-0.000


Me
NH2

**3en**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1.77
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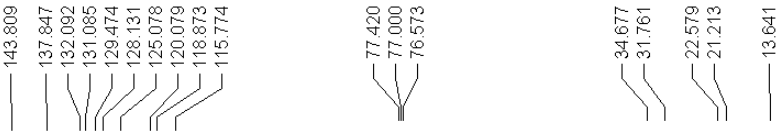
1.94
3.01
2.00
2.01
3.00
8
7
6
5
4
3
2
1
0
PPM


143.809
137.847
132.092
131.085
129.474
128.131
125.078
120.079
118.873
115.774
77.420
77.000
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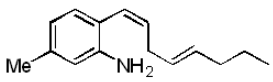
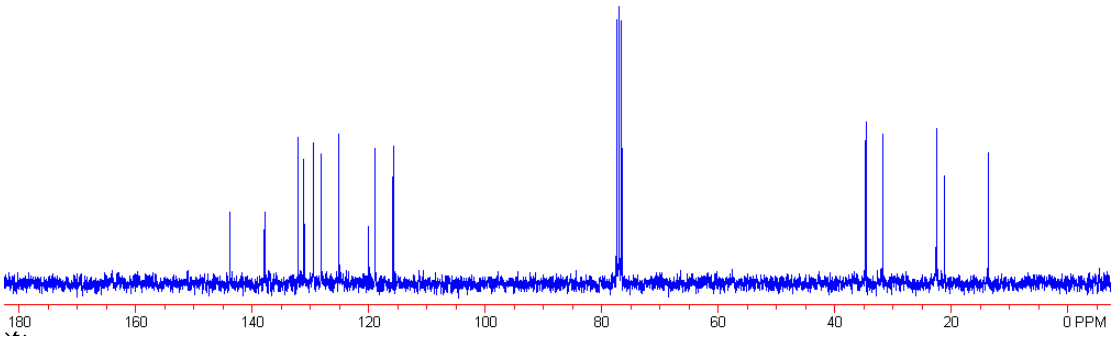
34.677
31.761
22.579
21.213
13.641


Me
NH2

**3en**


180
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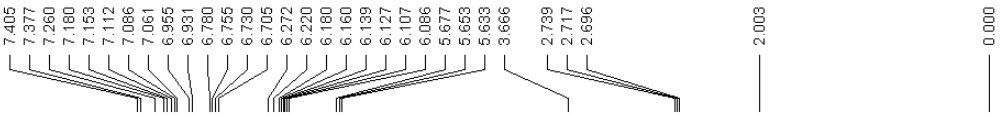
120
100
80
60
40
20
0 PPM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7.112
7.086
7.061
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6.931
6.780
6.755
6.730
6.705
6.272
6.220
6.180
6.160
6.139
6.127
6.107
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5.677
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5.633
3.666
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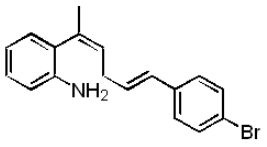
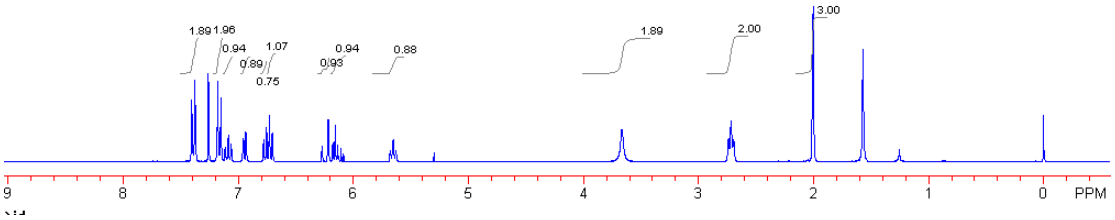
2.717
2.696
2.003
0.000


NH2
Br

**6e**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0.89
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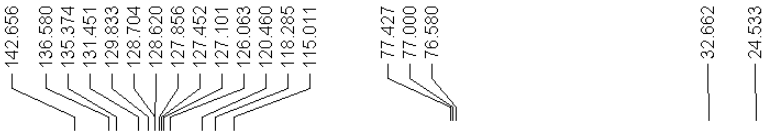
0.75
0.94
0.93
0.88
1.89
2.00
3.00
9
8
7
6
5
4
3
2
1
0
PPM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135.374
131.451
129.833
128.704
128.620
127.856
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126.063
120.460
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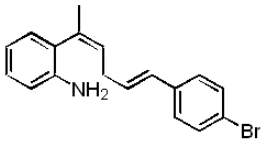
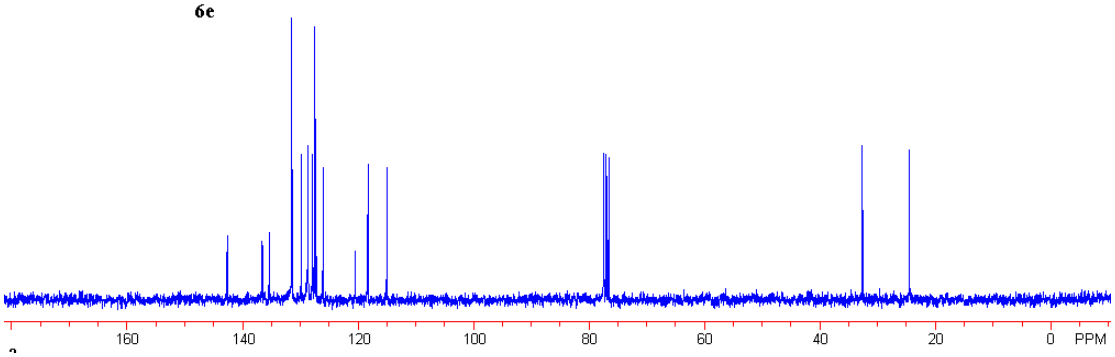
115.011
77.427
77.000
76.580
32.662
24.533


NH2
Br

**6e**


160
140
120
100
80
60
40
20
0
PPM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7.090
7.065
7.039
6.934
6.910
6.762
6.738
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5.601
5.576
5.553
5.370
5.361
5.354
5.346
5.337
3.653
2.504
2.486
1.967
1.943
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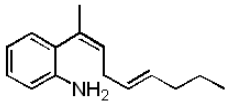
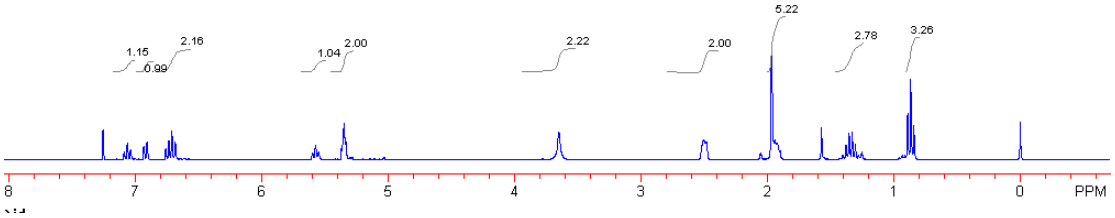
-0.000


NH2

**6n**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1.04
2.00
2.22
2.00
5.22
2.78
3.26
8
7
6
5
4
3
2
1
0
PPM


142.748
134.046
130.627
128.719
128.398
127.666
127.482
118.232
114.950
77.427
77.000
76.580
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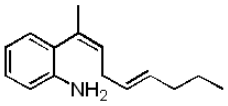
22.640
13.664


NH2

**6n**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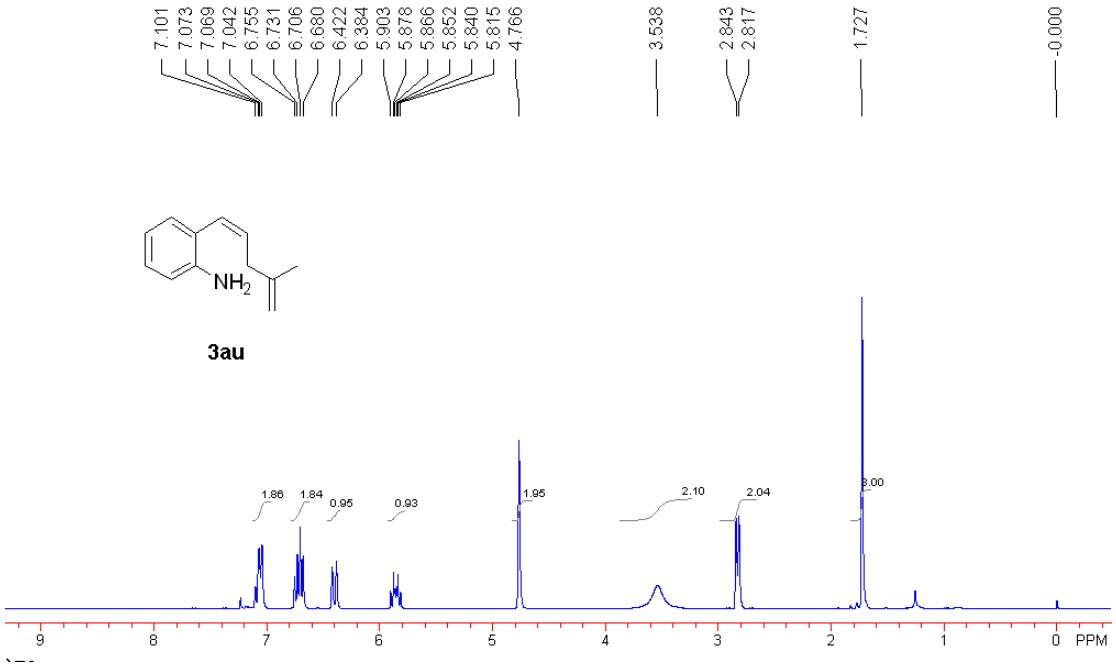
100
80
60
40
20
0
PPM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7.069
7.042
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6.731
6.706
6.680
6.422
6.384
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5.852
5.840
5.815
4.766
3.538
2.843
2.817
1.727
-0.000
NH2
3au
1.86
1.84
0.95
0.93
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2.10
2.04
3.00
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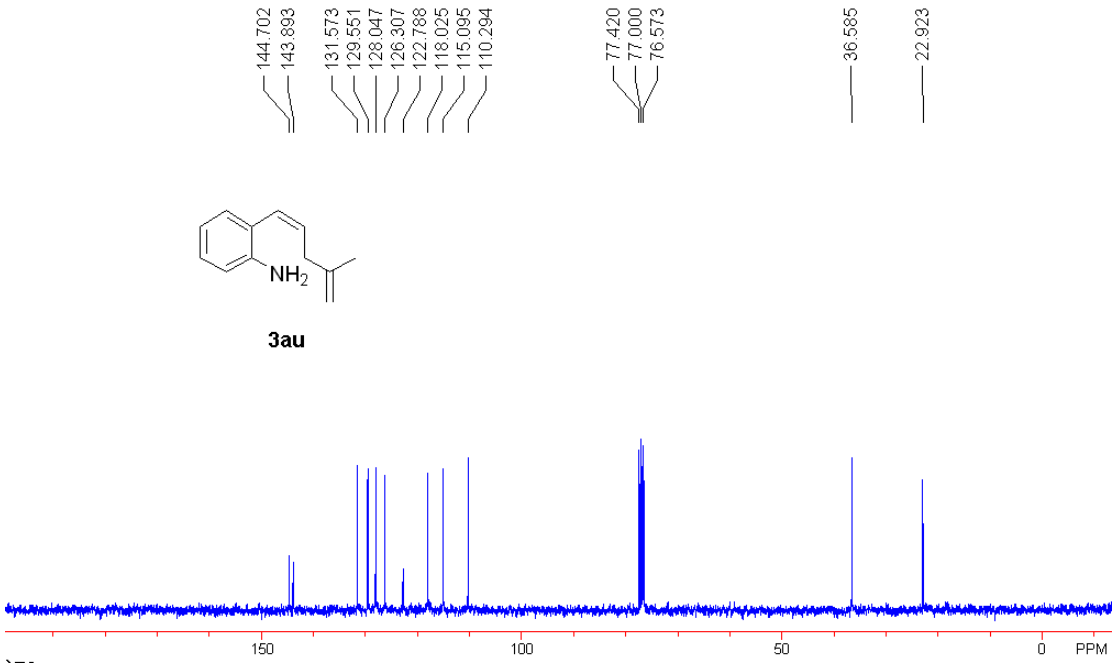
PPM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126.307
122.788
118.025
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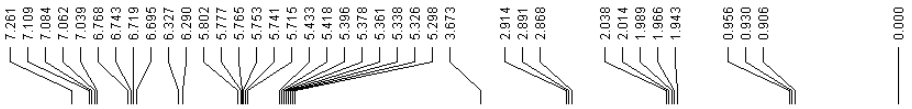
110.294
77.420
77.000
76.573
36.585
22.923
NH2
3au
150
100
50
0
PPM


7.261
7.109
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6.768
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5.753
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5.715
5.433
5.418
5.396
5.378
5.361
5.338
5.326
5.298
3.673
2.914
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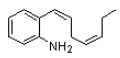
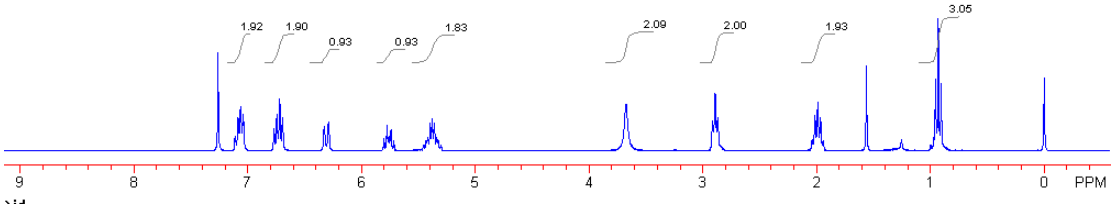
0.000


NH2

**10**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0.93
1.83
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2.00
1.93
3.05
9
8
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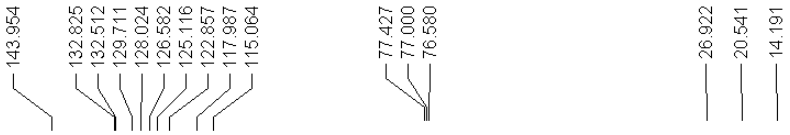
6
5
4
3
2
1
0
PPM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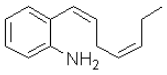
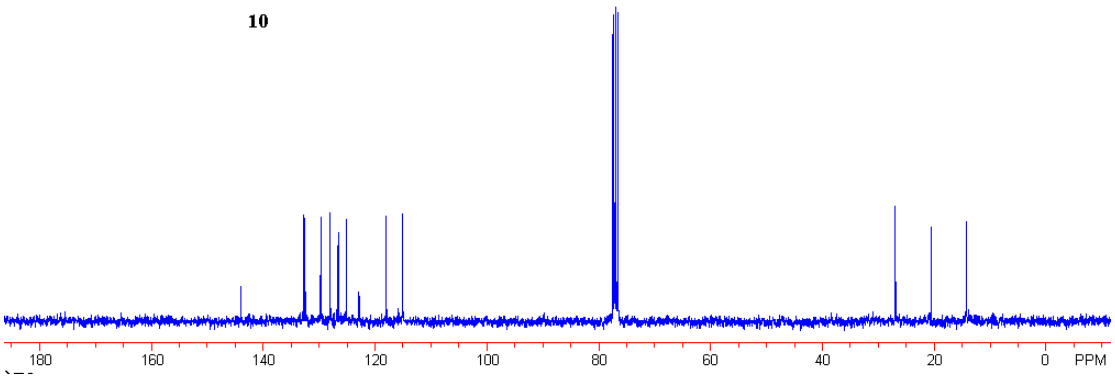
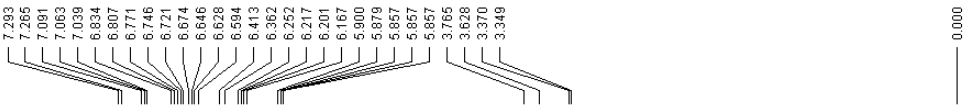
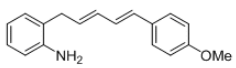
132.512
129.711
128.024
126.582
125.116
122.857
117.987
115.064
77.427
77.000
76.580
26.922
20.541
14.191


NH2

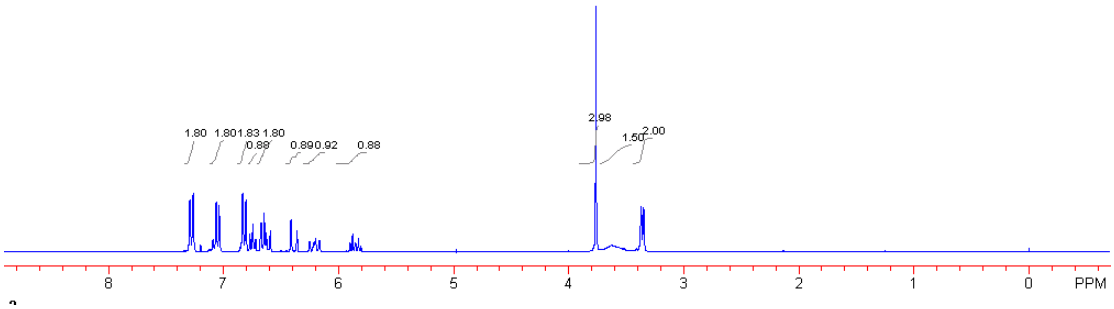
**10**

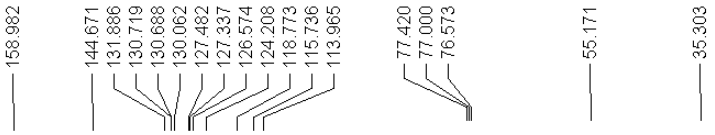

180
160
140
120
100
80
60
40
20
0
PPM

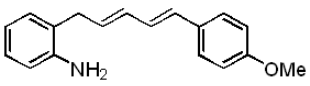

7.293
7.265
7.091
7.063
7.039
6.834
6.807
6.771
6.746
6.721
6.674
6.646
6.628
6.594
6.413
6.362
6.252
6.217
6.201
6.167
5.900
5.879
5.857
5.857
5.857
3.765
3.628
3.370
3.349
0.000


NH2
OMe

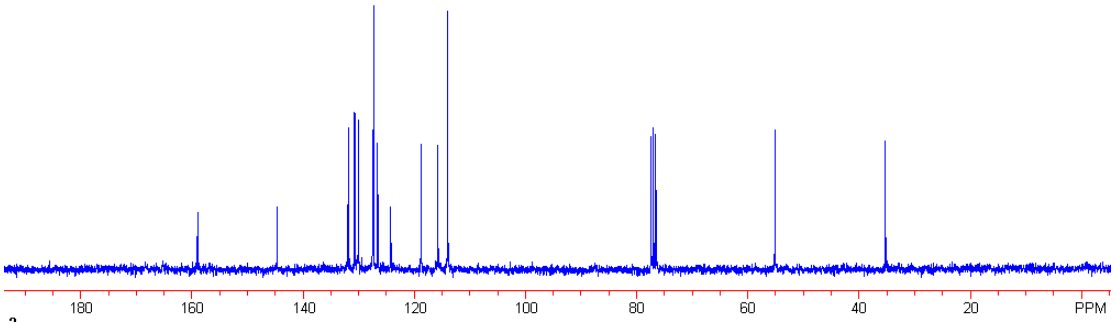
**4aa**

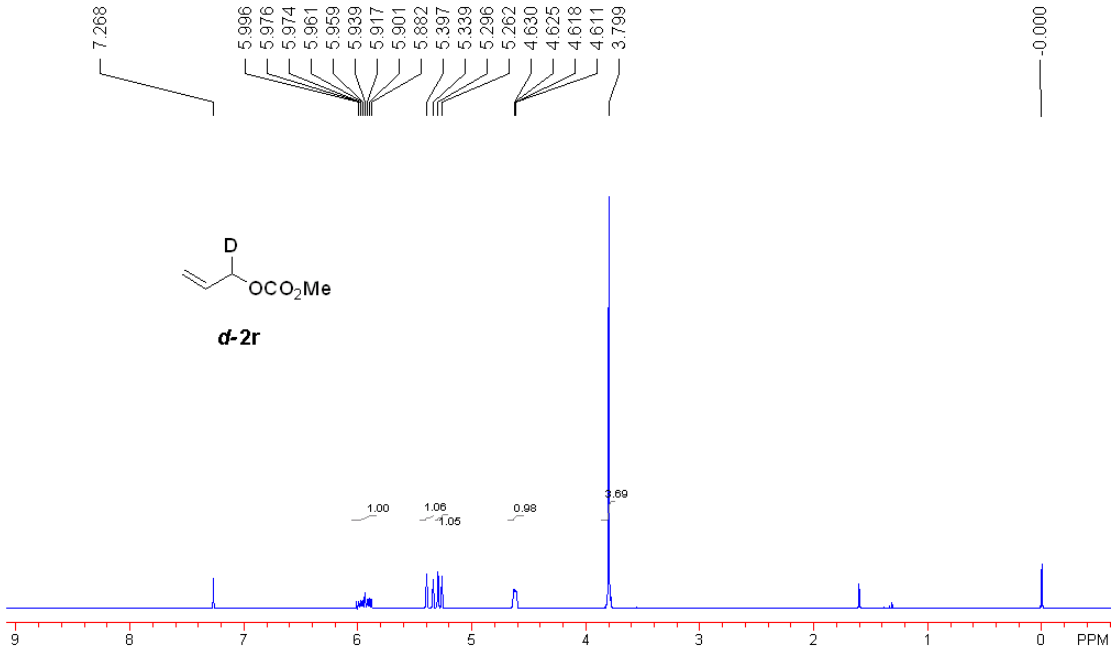

1.80
1.80
1.83
0.88
1.80
0.89
0.90
0.92
0.88
2.98
1.50
2.00
8
7
6
5
4
3
2
1
0
PPM

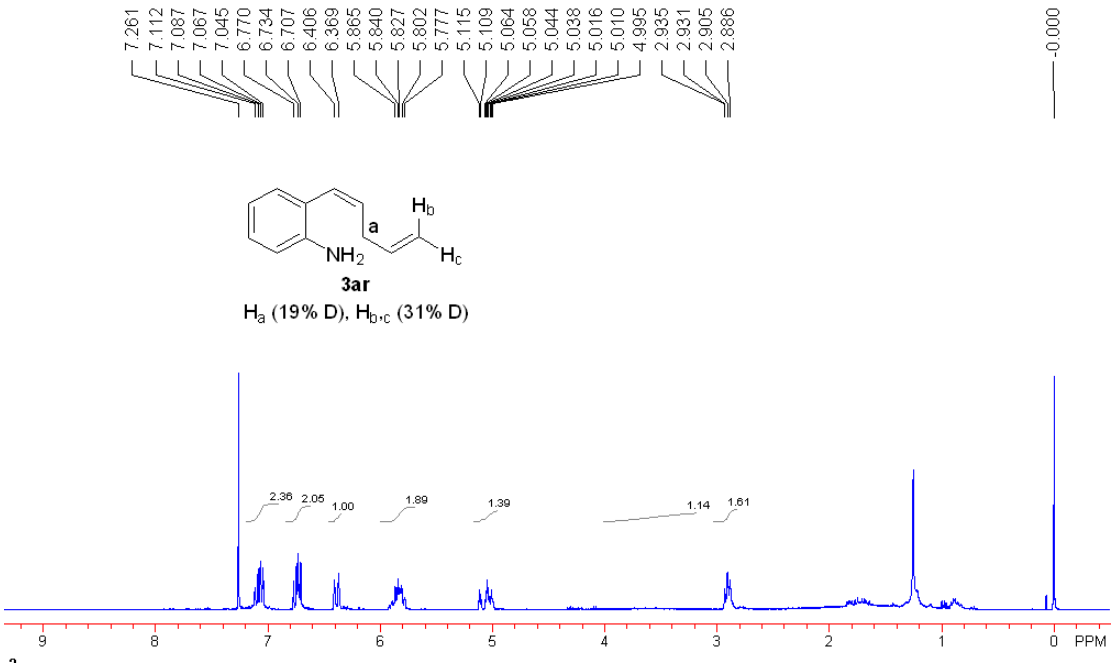

158.982
144.671
131.886
130.719
130.688
130.062
127.482
127.337
126.574
124.208
118.773
115.736
113.965
77.420
77.000
76.573
55.171
35.303

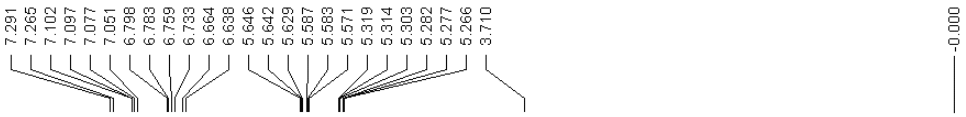

NH2
OMe

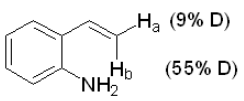
**4aa**


180
160
140
120
100
80
60
40
20
PPM

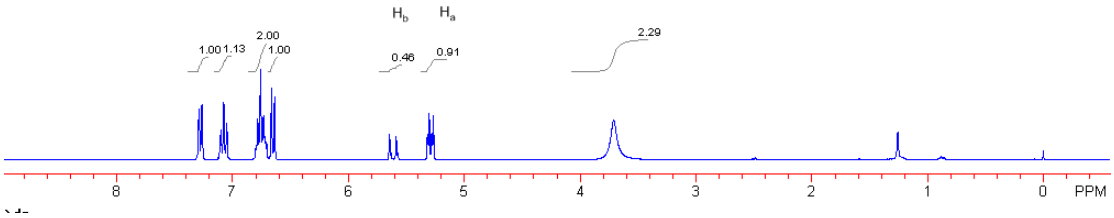

7.268
5.996
5.976
5.974
5.961
5.959
5.939
5.917
5.901
5.882
5.397
5.339
5.296
5.262
4.630
4.625
4.618
4.611
3.799
-0.000
D
OCO2Me
d-2r
1.00
1.06
1.05
0.98
3.69
9
8
7
6
5
4
3
2
1
0
PPM

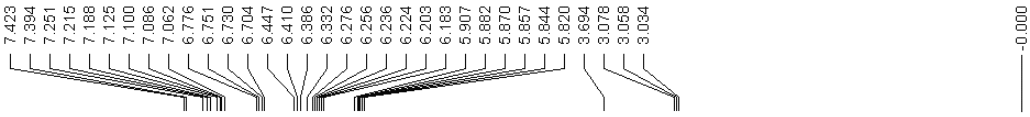

7.261
7.112
7.087
7.067
7.045
6.770
6.734
6.707
6.406
6.369
5.865
5.840
5.827
5.802
5.777
5.115
5.109
5.064
5.058
5.044
5.038
5.016
5.010
4.995
2.935
2.931
2.905
2.886
-0.000
Hb
a
NH2
Hc
3ar
Ha (19% D), Hb,c (31% D)
2.36
2.05
1.00
1.89
1.39
1.14
1.61
9
8
7
6
5
4
3
2
1
0
PPM

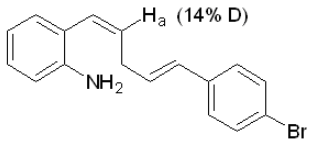

7.291
7.265
7.102
7.097
7.077
7.051
6.798
6.783
6.759
6.733
6.664
6.638
5.646
5.642
5.629
5.587
5.583
5.571
5.319
5.314
5.303
5.282
5.277
5.266
3.710
-0.000


Ha (9% D)
Hb (55% D)
NH2

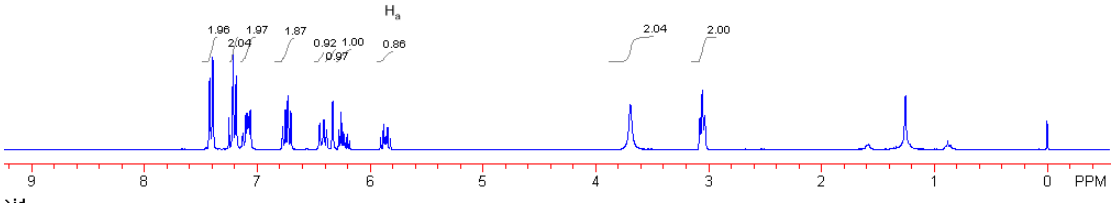
**d-1a**

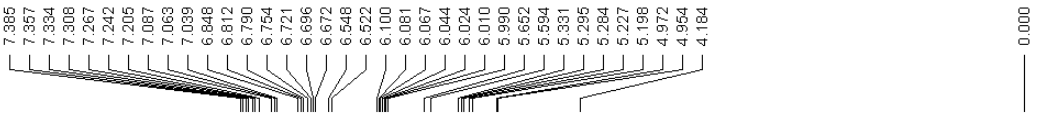

Hb
Ha
1.00
1.13
2.00
1.00
0.46
0.91
2.29
8
7
6
5
4
3
2
1
0
PPM

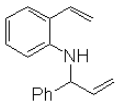

7.423
7.394
7.251
7.215
7.188
7.125
7.100
7.086
7.062
6.776
6.751
6.730
6.704
6.447
6.410
6.386
6.332
6.276
6.256
6.236
6.224
6.203
6.183
5.907
5.882
5.870
5.857
5.844
5.820
3.694
3.078
3.058
3.034
-0.000


Ha (14% D)
NH2
Br

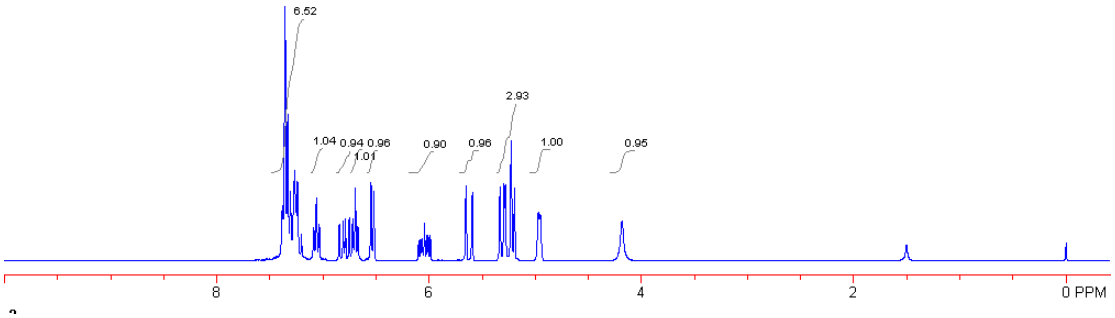
**d-3ae**

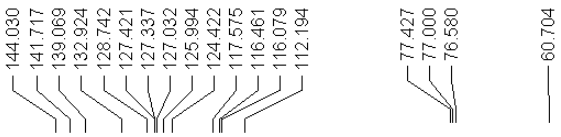

Ha
1.96
1.97
2.04
1.87
0.92
1.00
0.97
0.86
2.04
2.00
9
8
7
6
5
4
3
2
1
0
PPM

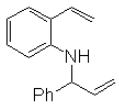

7.385
7.357
7.334
7.308
7.267
7.242
7.205
7.087
7.063
7.039
6.848
6.812
6.790
6.754
6.721
6.696
6.672
6.548
6.522
6.100
6.081
6.067
6.044
6.024
6.010
5.990
5.652
5.594
5.331
5.295
5.284
5.227
5.198
4.972
4.954
4.184
0.000


NH
Ph

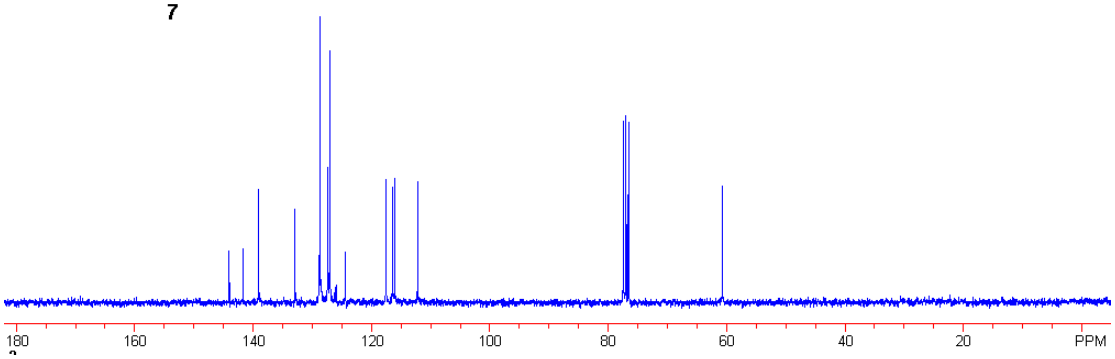
**7**

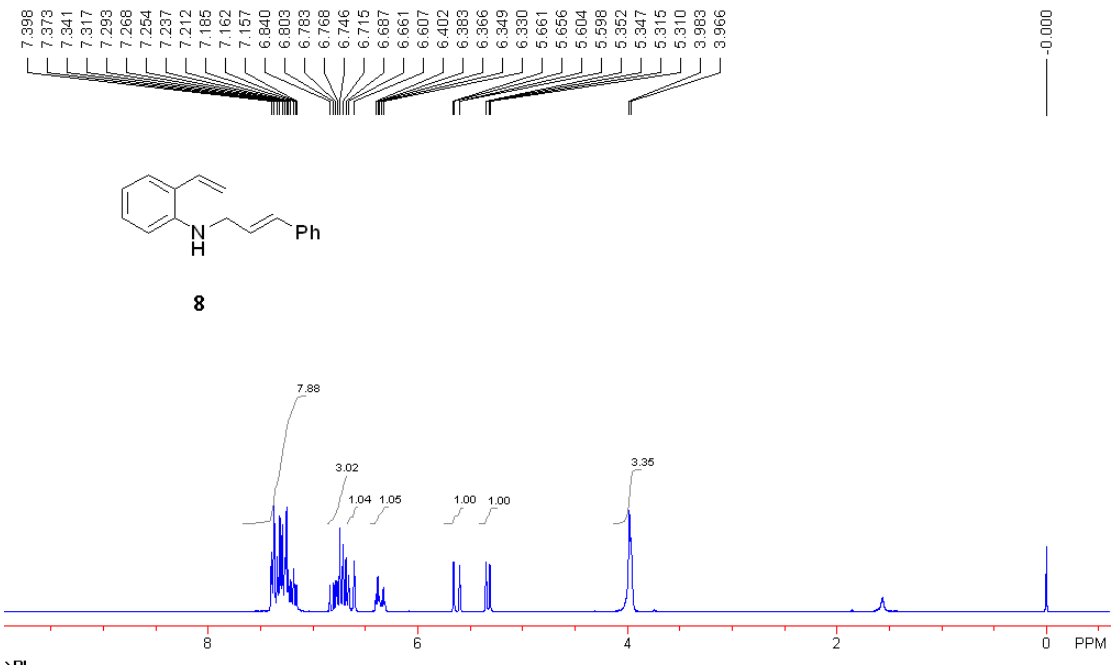

6.52
1.04
0.94
0.96
1.01
0.90
0.96
2.93
1.00
0.95
8
6
4
2
0 PPM


144.030
141.717
139.069
132.924
128.742
127.421
127.337
127.032
125.994
124.422
117.575
116.461
116.079
112.194
77.427
77.000
76.580
60.704


NH
Ph

**7**


180
160
140
120
100
80
60
40
20
PPM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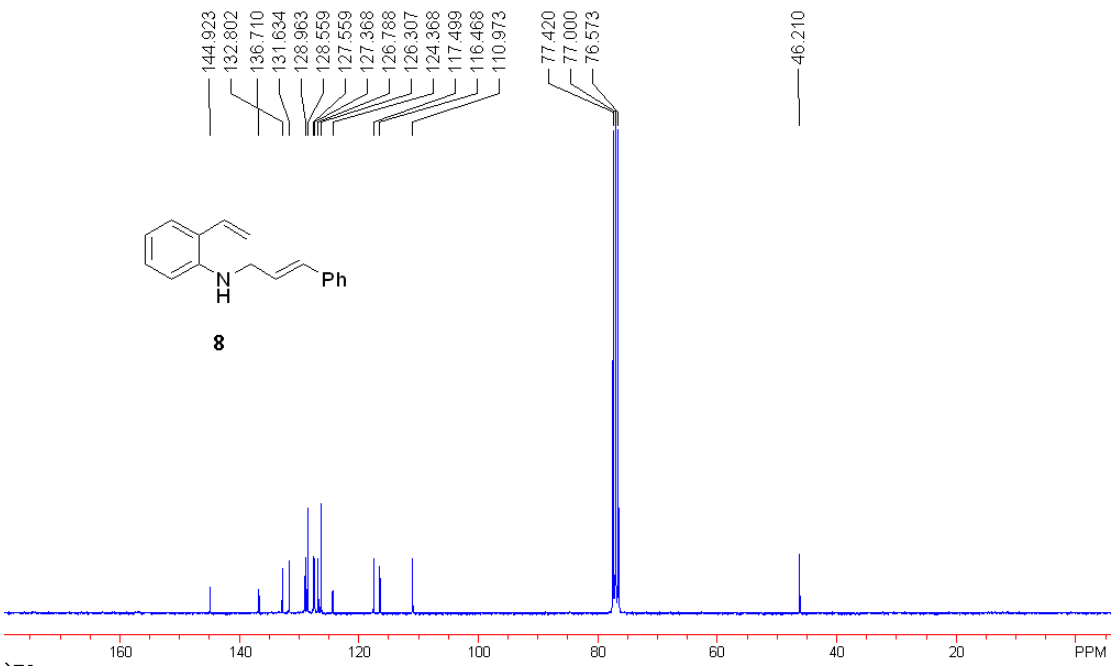
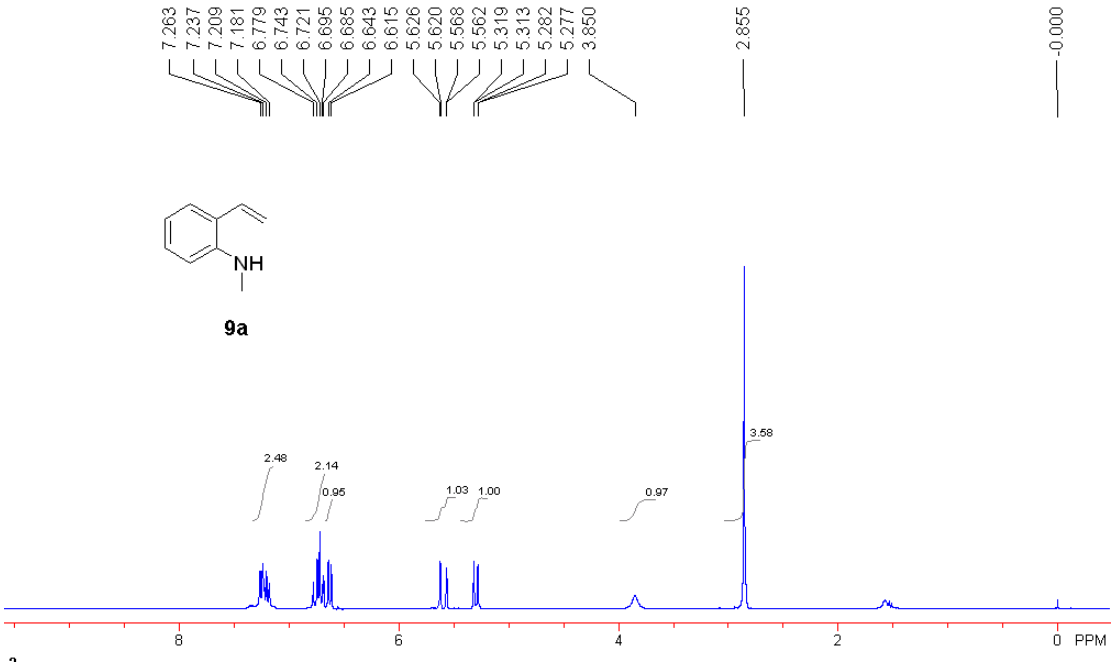
7.373
7.341
7.317
7.293
7.268
7.254
7.237
7.212
7.185
7.162
7.157
6.840
6.803
6.783
6.768
6.746
6.715
6.687
6.661
6.607
6.402
6.383
6.366
6.349
6.330
5.661
5.656
5.604
5.598
5.352
5.347
5.315
5.310
3.983
3.966
-0.000
N
H
Ph

**8**

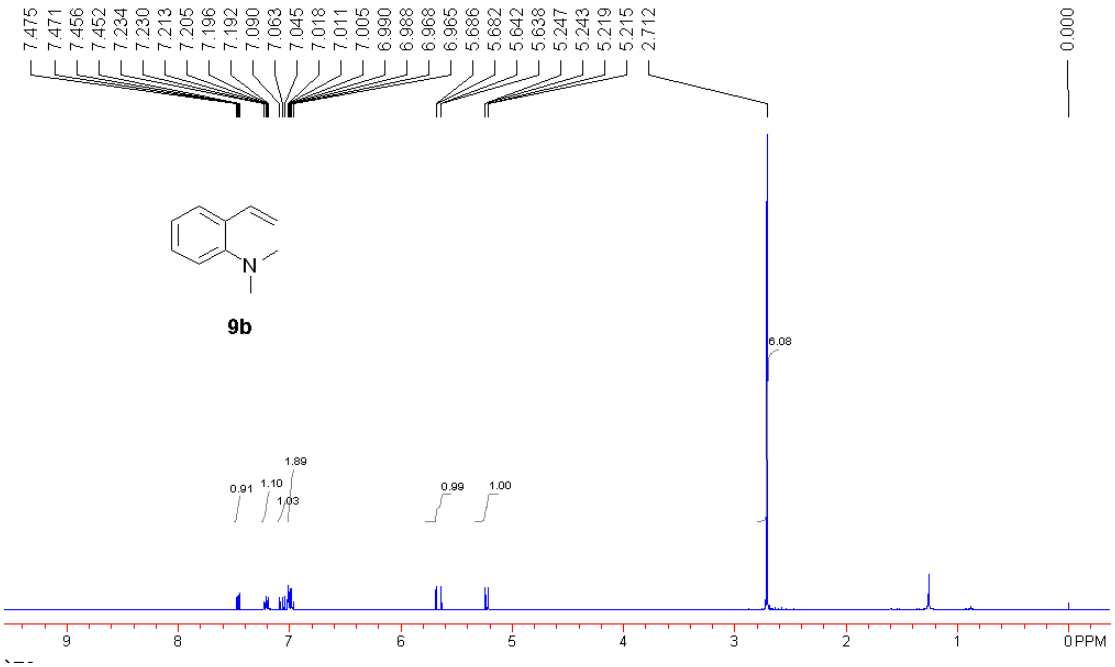

7.88
3.02
1.04
1.05
1.00
1.00
3.35
8
6
4
2
0
PPM


144.923
132.802
136.710
131.634
128.963
128.559
127.559
127.368
126.788
126.307
124.368
117.499
116.468
110.973
77.420
77.000
76.573
46.210
N
H
Ph
160
140
120
100
80
60
40
20
PPM

**8**


7.263
7.237
7.209
7.181
6.779
6.743
6.721
6.695
6.685
6.643
6.615
5.626
5.620
5.568
5.562
5.319
5.313
5.282
5.277
3.850
2.855
-0.000
NH
2.48
2.14
0.95
1.03
1.00
0.97
3.58
8
6
4
2
0 PPM

**9a**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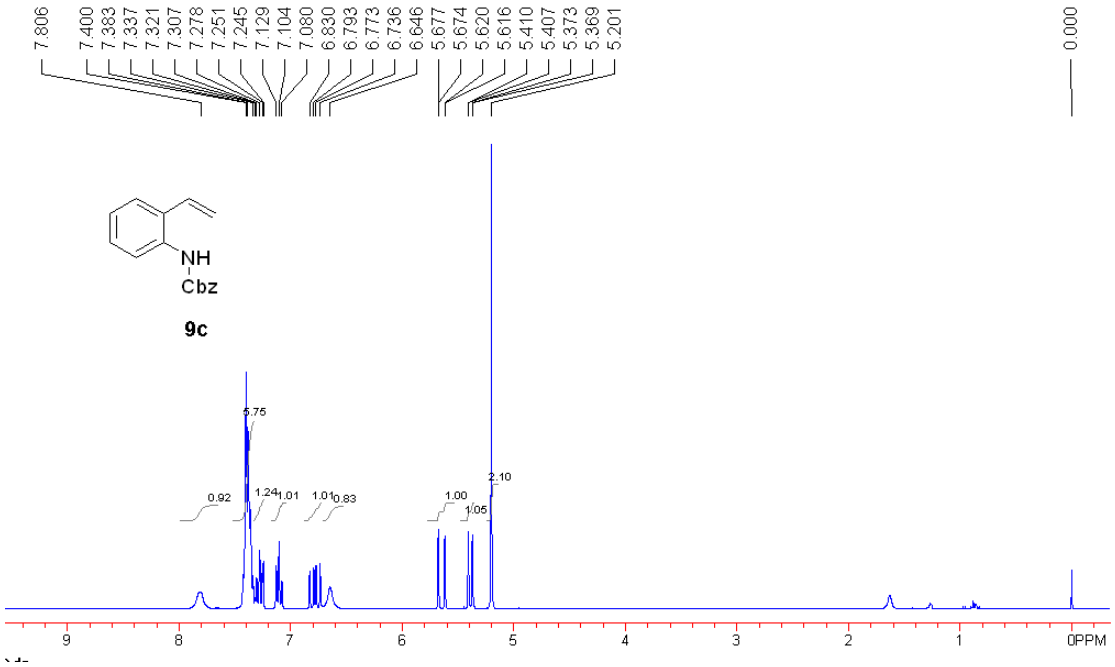
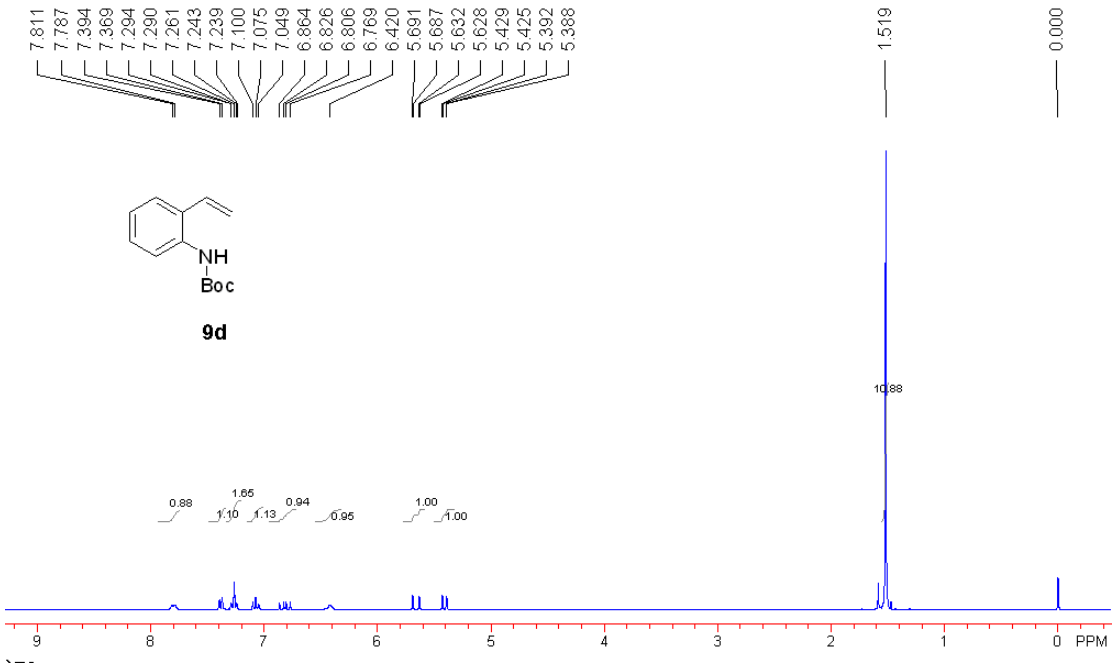
7.471
7.456
7.452
7.234
7.230
7.213
7.205
7.196
7.192
7.090
7.063
7.045
7.018
7.011
7.005
6.990
6.988
6.968
6.965
5.686
5.682
5.642
5.638
5.247
5.243
5.219
5.215
2.712
0.000
N
6.08
1.89
1.10
1.03
0.91
0.99
1.00
9
8
7
6
5
4
3
2
1
0 PPM

**9b**


7.806
7.400
7.383
7.337
7.321
7.307
7.278
7.251
7.245
7.129
7.104
7.080
6.830
6.793
6.773
6.736
6.646
5.677
5.674
5.620
5.616
5.410
5.407
5.373
5.369
5.201
0.000
NH
Cbz
9c
5.75
0.92
1.24
1.01
1.01
0.83
1.00
1.05
2.10
9
8
7
6
5
4
3
2
1
0PPM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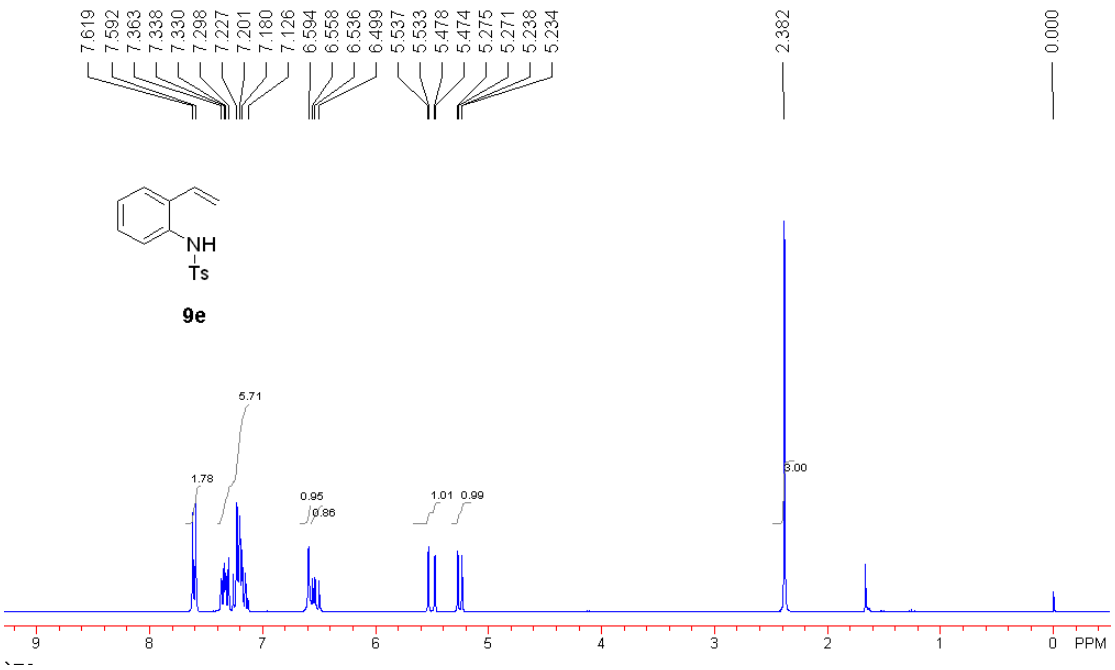
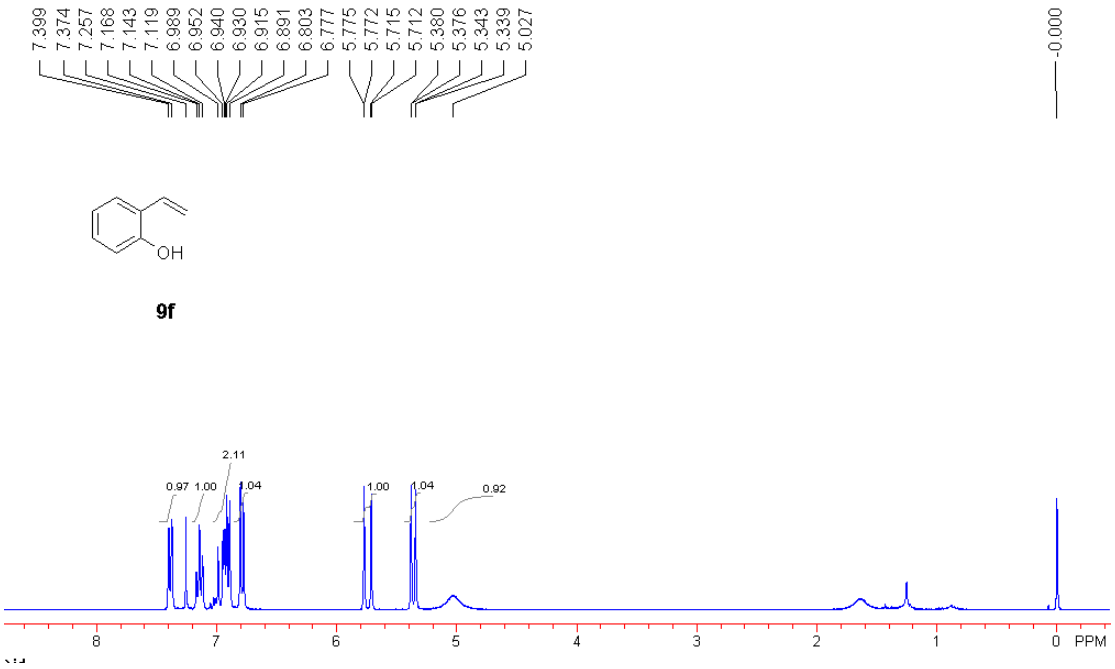
7.787
7.394
7.369
7.294
7.290
7.261
7.243
7.239
7.100
7.075
7.049
6.864
6.826
6.806
6.769
6.420
5.691
5.687
5.632
5.628
5.429
5.425
5.392
5.388
1.519
0.000
NH
Boc
9d
10.88
0.88
1.65
1.10
1.13
0.94
0.95
1.00
1.00
9
8
7
6
5
4
3
2
1
0 PPM


7.619
7.592
7.363
7.338
7.330
7.298
7.227
7.201
7.180
7.126
6.594
6.558
6.536
6.499
5.537
5.533
5.478
5.474
5.275
5.271
5.238
5.234
2.382
0.000
NH
Ts
5.71
1.78
0.95
0.86
1.01
0.99
3.00
9
8
7
6
5
4
3
2
1
0
PPM

**9e**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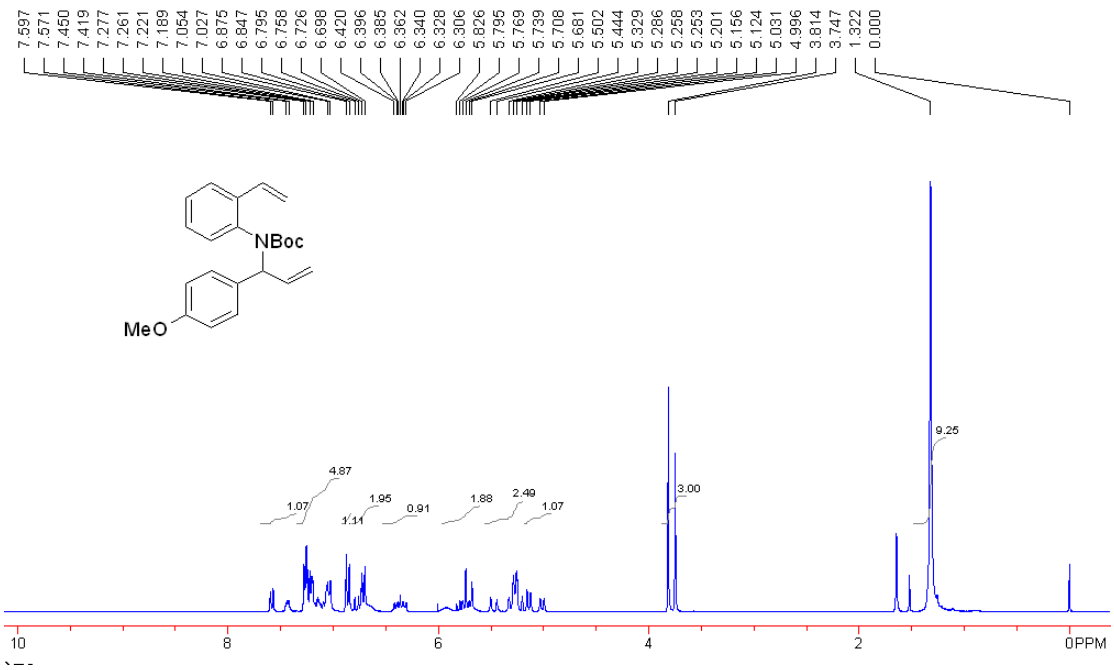
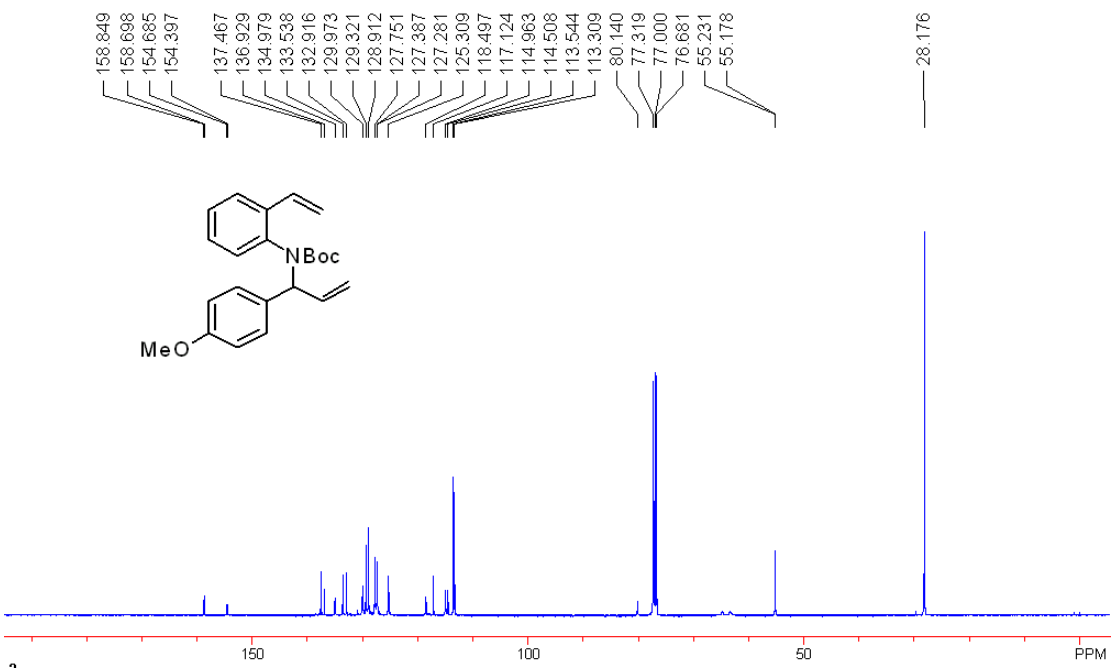
7.168
7.143
7.119
6.989
6.952
6.940
6.930
6.915
6.891
6.803
6.777
5.775
5.772
5.715
5.712
5.380
5.376
5.343
5.339
5.027
-0.000
OH
2.11
0.97
1.00
1.04
1.00
1.04
0.92
8
7
6
5
4
3
2
1
0
PPM

**9f**


7.597
7.571
7.450
7.419
7.277
7.261
7.221
7.189
7.054
7.027
6.875
6.847
6.795
6.758
6.726
6.698
6.420
6.396
6.385
6.362
6.340
6.328
6.306
5.826
5.795
5.769
5.739
5.708
5.681
5.502
5.444
5.329
5.286
5.258
5.253
5.201
5.156
5.124
5.031
4.996
3.814
3.747
1.322
0.000
NBoc
MeO
4.87
1.07
1.95
1.11
0.91
1.88
2.49
1.07
3.00
9.25
10
8
6
4
2
0PPM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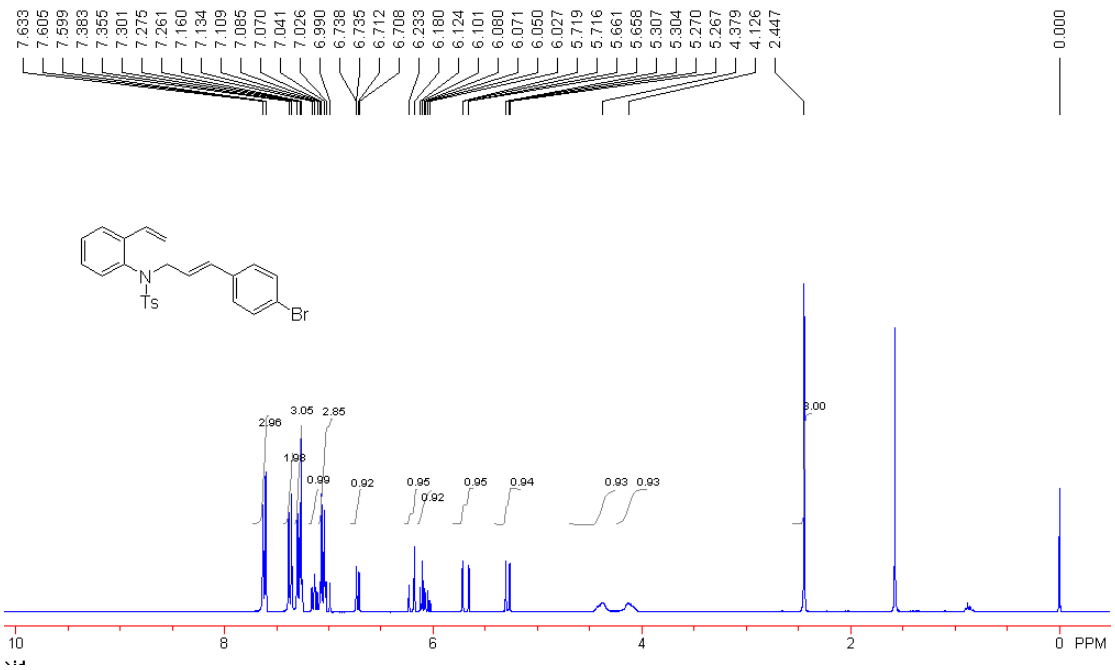
158.698
154.685
154.397
137.467
136.929
134.979
133.538
132.916
129.973
129.321
128.912
127.751
127.387
127.281
125.309
118.497
117.124
114.963
114.508
113.544
113.309
80.140
77.319
77.000
76.681
55.231
55.178
28.176
NBoc
MeO
150
100
50
PPM


7.633
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7.070
7.041
7.026
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6.735
6.712
6.708
6.233
6.180
6.124
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6.080
6.071
6.050
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5.719
5.716
5.661
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5.307
5.304
5.270
5.267
4.379
4.126
2.447
0.000
Ts
Br
2.96
3.05
2.85
1.98
0.99
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0.93
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10
8
6
4
2
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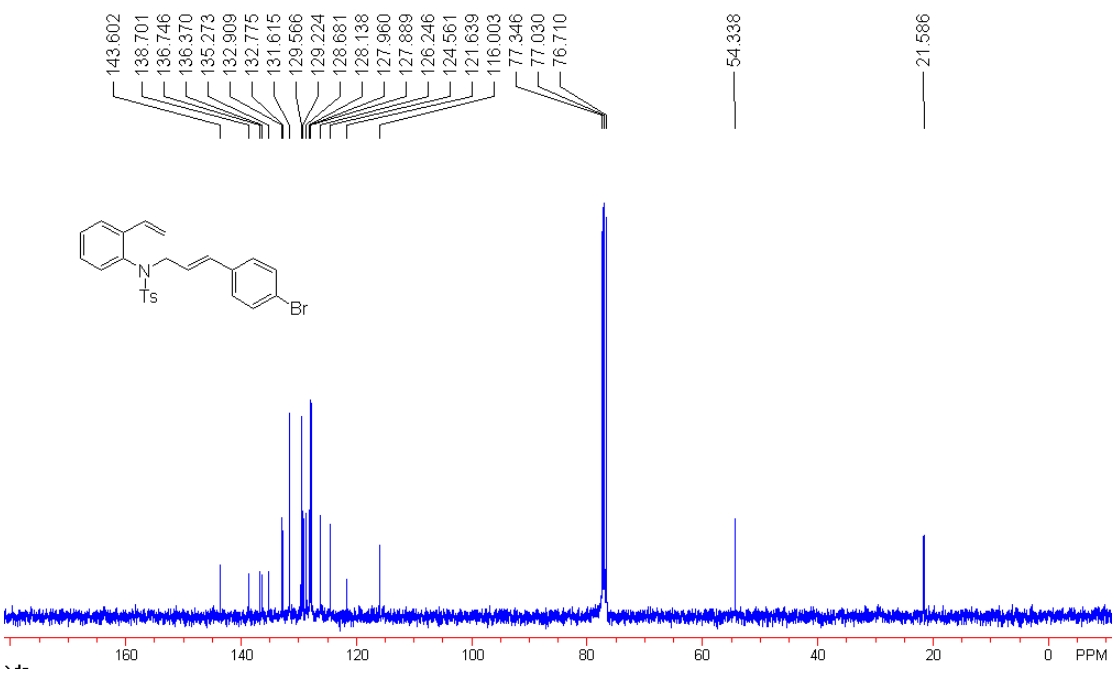
PPM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135.273
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131.615
129.566
129.224
128.681
128.138
127.960
127.889
126.246
124.561
121.639
116.003
77.346
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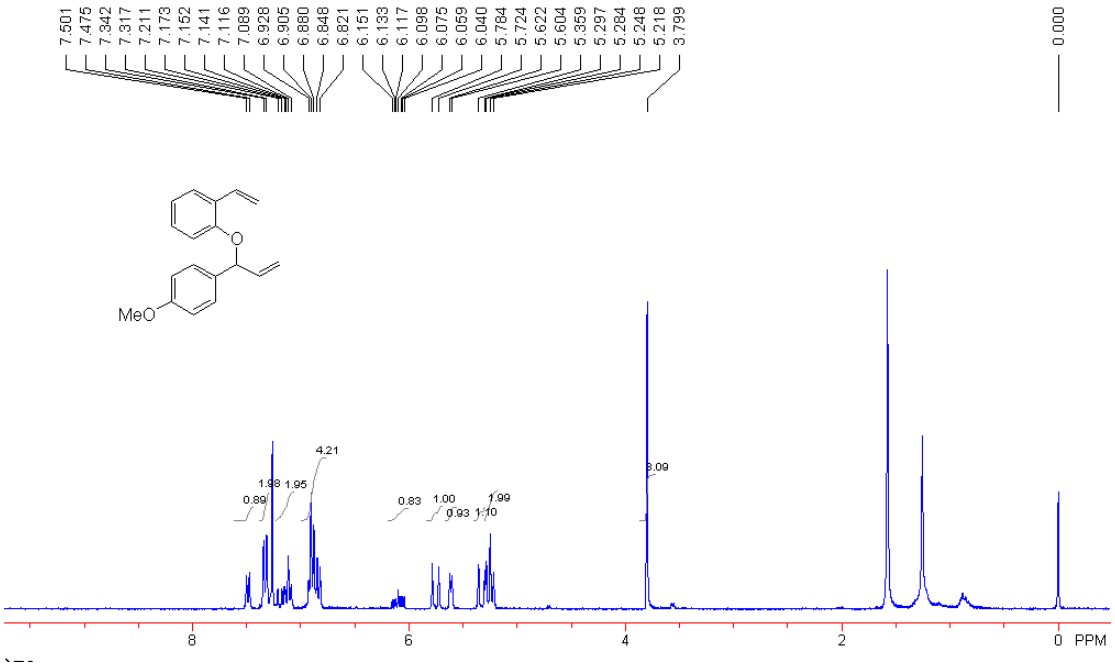
54.338
21.586
Ts
Br
160
140
120
100
80
60
40
20
0
PPM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7.141
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7.089
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6.905
6.880
6.848
6.821
6.151
6.133
6.117
6.098
6.075
6.059
6.040
5.784
5.724
5.622
5.604
5.359
5.297
5.284
5.248
5.218
3.799
0.000
MeO
4.21
1.98
1.95
0.89
0.83
1.00
0.93
1.99
1.10
3.09
8
6
4
2
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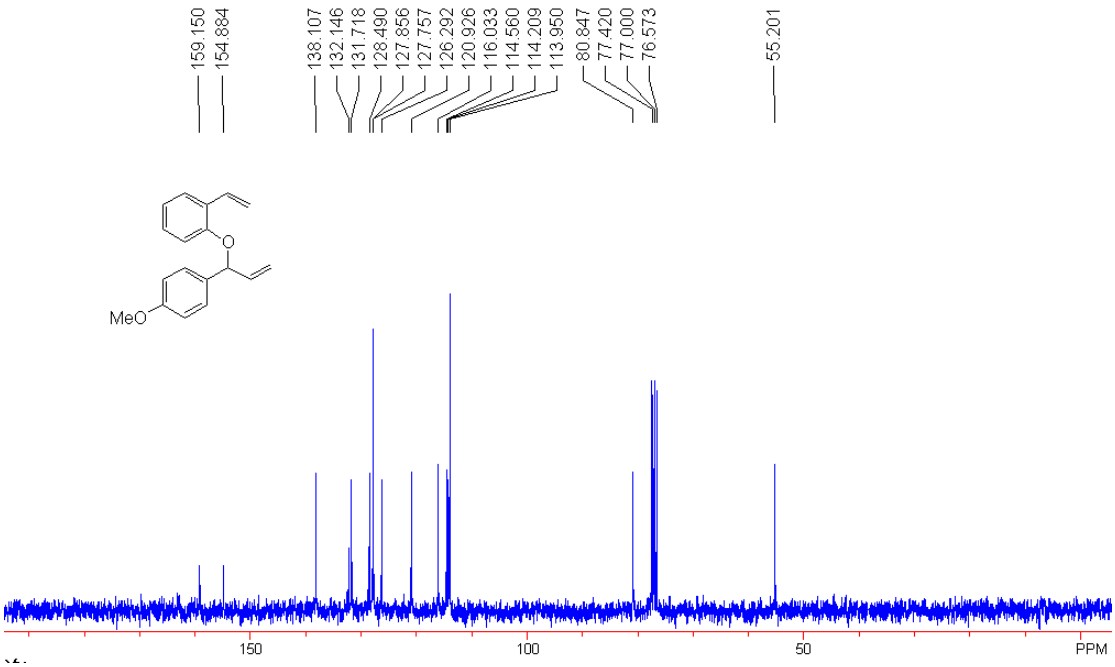
PPM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127.757
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120.926
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114.209
113.950
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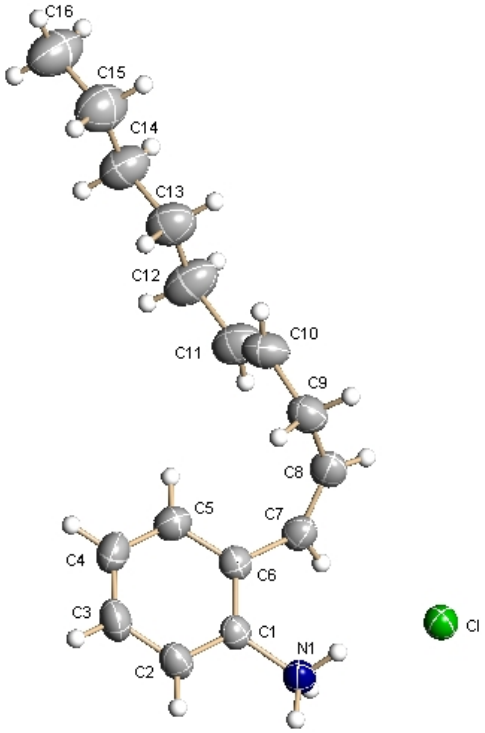
77.420
77.000
76.573
55.201
MeO
150
100
50
PPM

X-ray of **3al**·HCl




(CCDC 711923 contains the supplementary crystallographic data. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk /data request/cif.)

Table 1. Crystal data and structure refinement for cd26493.

| | |
|---|---|
| Identification code | cd26493 |
| Empirical formula | C16 H24 Cl N |
| Formula weight | 265.81 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Triclinic, P-1 |
| Unit cell dimensions | a = 5.4069(9) A alpha = 102.987(3) deg.<br>b = 9.6575(16) A beta = 95.655(3) deg.<br>c = 15.955(3) A gamma = 100.240(3) deg. |
| Volume | 790.5(2) A^3 |
| Z, Calculated density | 2, 1.117 Mg/m^3 |
| Absorption coefficient | 0.227 mm^-1 |
| F(000) | 288 |
| Crystal size | 0.486 x 0.382 x 0.097 mm |
| Theta range for data collection | 2.21 to 27.00 deg. |
| Limiting indices | -6<=h<=6, -12<=k<=6, -18<=l<=20 |
| Reflections collected / unique | 4680 / 3345 [R(int) = 0.0855] |
| Completeness to theta = 27.00 | 97.4 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 1.00000 and 0.76599 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3345 / 3 / 176 |
| Goodness-of-fit on F^2 | 0.947 |
| Final R indices [I>2sigma(I)] | R1 = 0.0532, wR2 = 0.1336 |
| R indices (all data) | R1 = 0.0698, wR2 = 0.1427 |
| Largest diff. peak and hole | 0.421 and -0.185 e.A^-3 |