Electronic Supplementary Information

Synthesis of 2-Fluoroalkylbenzimidazoles via Copper(I)-catalyzed Tandem Reactions

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General:

Melting points were measured on a Melt-Temp apparatus andw uncorrected. ^{1}H NMR spectra were recorded in $CDCl_3$ on a Bruker AM-300 spectrometer (300 MHz) with TMS as internal standard. ^{19}F NMR spectra were taken on a Bruker AM-300 (282 MHz) spectrometer using $CFCl_3$ as external standard. ^{13}C NMR spectra were taken on a Bruker AM-400 (100 MHz) spectrometer. IR spectra were obtained with a Nicolet AV-360 spectrophotometer. Solvents and reagents were purchased from commercial sources and used as received. DMF was distilled from calcium hydride. All reactions were carried out under a nitrogen atmosphere in a Schlenk tube, with a stir bar and capes with a Teflon screw-cap. TLC analysis was performed on silica gel plates, column chromatography over silica gel (mesh 200-300) and petroleum ether/ethyl acetate combination was used as the eluent. The imidoyl chloride was synthesized according to the literature.[1]

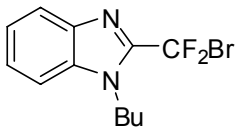
General procedure for benzimidazoles synthesis.

Method A: A Schlenk tube was charged with CuI (8 mg, 0.04mmol), and K_2CO_3 (220 mg, 1.6mmol), evacuated and backfilled with nitrogen. Amine (0.5mmol), DMF (2ml) and imidoyl chloride (0.4mmol) was successively added. Then the reaction mixture was stirred at 60^{o}C for 3h. The mixture was partitioned between ethyl acetate and water, the organic layer was washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The residue was purified by column chromatography on silica gel to provide the desired product.

Method B: A Schlenk tube was charged with CuI (8 mg, 0.04mmol), and K_3PO_4 (339 mg, 1.6mmol), evacuated and backfilled with nitrogen. Amine (0.5mmol), DMF (2ml) and imidoyl chloride (0.4mmol) was successively added. Then the reaction mixture was stirred at 60^{o}C for 3h. the mixture was partitioned between ethyl acetate and water, the organic layer was washed with brine, dried over $MgSO_4$, and concentrated

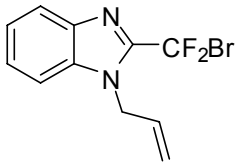
in vacuo. The residue was purified by column chromatography on silica gel to provide the desired product.

2-(bromodifluoromethyl)-1-butyl-1*H*-benzo[*d*]imidazole **(3a)**



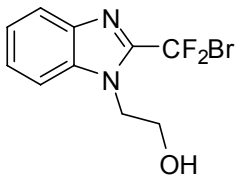
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, J = 7.9 Hz, 1H), 7.22-7.35 (m, 3H), 4.20-4.28 (m, 2H), 1.72-1.86 (m, 2H), 1.28-1.45 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -46.10 (s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.8 (t, J = 28.3 Hz), 140.9, 135.5, 125.0, 123.4, 121.5, 111.7 (t, J = 299,8 Hz), 110.5, 45.1, 31.6, 20.0, 13.5; IR (film): 3059, 2962, 2935, 1615, 1589, 1501, 1457, 1455, 1253, 1177, 1141, 1082, 910 cm^{-1}; MS: m/z (%): 302 (10.60) [M$^+$], 181 (100.00); Anal. Cacld. For $C_{12}H_{13}BrF_2N_2$: C, 47.54; H, 4.32; N, 9.24; Found: C, 47.68; H, 4.61; N, 9.30.

1-allyl-2-(bromodifluoromethyl)-1*H*-benzo[*d*]imidazole **(3b)**



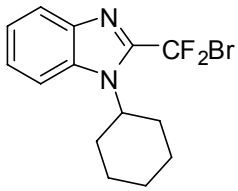
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84-7.91 (m, 1H), 7.31-7.43 (m, 3H), 5.88-6.05 (m, 1H), 5.27 (dt, J_1 = 10.2 Hz, J_2 =1.5 Hz, 1H), 5.13 (dt, J_1 = 17.3 Hz, J_2 = 1.5 Hz, 1H), 4.98 (d, J = 5.4 Hz, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -46.09 (s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.9 (t, J = 22.8 Hz), 140.8, 135.5, 130.8, 125.2, 123.6, 121.5, 118.4, 111.5 (t, J = 239.9 Hz), 110.8, 47.4; IR (film): 3087, 3068, 2928, 1647, 1615, 1589, 1503, 1464, 1412, 1254, 1171, 1141, 929cm^{-1}; MS (ESI): m/z: 287 [M + H$^+$]; HRMS Calcd for $C_{11}H_9N_2BrF_2$: 285.9917, Found：285.9920.

2-(2-(bromodifluoromethyl)-1*H*-benzo[*d*]imidazol-1-yl)ethanol **(3c)**



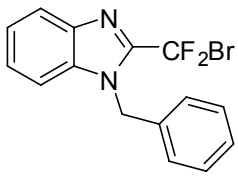
White solid, mp 84-85 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.22-7.71 (m, 4H), 4.43 (m, 2H), 3.97 (m, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -46.46 (s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.7 (t, *J* = 28.9 Hz), 140.2, 136.0, 125.2, 123.6, 120.7, 111.4, 111.3 (t, *J* = 299.9 Hz), 60.7 ,47.3; IR (film): 3298, 3059, 2896, 1612, 1590, 1501, 1475, 1255, 1166, 1141, 1055, 921; MS: m/z (%): 290 (19.54) [M^+], 145(100); HRMS Calcd for $C_{10}H_9N_2OBrF_2$: 289.9866, Found: 289.9863.

2-(bromodifluoromethyl)-1-cyclohexyl-1*H*-benzo[*d*]imidazole **(3d)**



White solid, mp 91-93 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.81 (m, 1H), 7.52-7.61 (m, 1H), 7.16-7.31 (m, 2H), 4.40-4.65 (m, 1H), 1.09-2.31 (m, 10H); ^{19}F NMR (282MHz, $CDCl_3$): δ -46.30 (s);^{13}C NMR (100 MHz, $CDCl_3$): δ 144.7, 141.5, 134.0, 124.5, 123.0, 121.9, 113.5, 111.3 (t, *J* = 240.3 Hz), 57.8, 30.7, 25.8, 25.1; IR (KBr): 3062, 2932, 2860, 1604, 1585, 1502, 1455, 1413, 1252, 1176, 1143, 1086, 927; MS (ESI): m/z: 329 [M + H^+]; Anal. Cacld. For $C_{14}H_{15}BrF_2N_2$: C, 51.08; H, 4.59; N, 8.51; Found: C, 51.17; H, 4.70; N, 8.52.

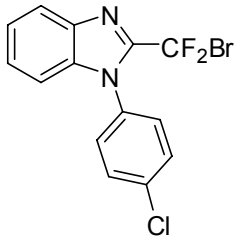
1-Benzyl-2-(bromodifluoromethyl)-1*H*-benzo[*d*]imidazole **(3e)**



White solid, mp 65-66 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.1 Hz, 1H), 6.94-7.28 (m, 8H), 5.48 (s, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -45.77 (s); ^{13}C NMR

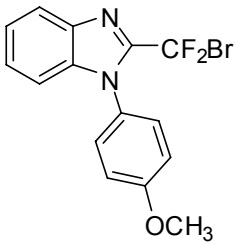
(100 MHz, $CDCl_3$): δ 145.2, 140.8, 135.7, 134.7, 128.7, 127.9, 126.1, 125.3, 123.6, 121.5, 111.5, 111.0 (t, J = 301.8 Hz), 48.5; IR (KBr): 3088, 3062, 1614,1589, 1498, 1451, 1260, 1167 ,1135 ,919; MS (ESI): m/z: 337 [M + H^+]; Anal. Cacld. For $C_{15}H_{14}BrF_2N_2$: C, 53.43, H, 3.29, N, 8.31; Found: C, 53.52, H, 3.60, N, 8.22.

2-(bromodifluoromethyl)-1-(4-chlorophenyl)-1*H*-benzo[*d*]imidazole **(3g)**



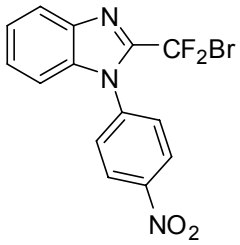
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.92 (d, J = 7.8 Hz, 1H), 7.59-7.10 (m, 7H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -44.45 (s); ^{13}C NMR (100 MHz , $CDCl_3$): δ 145.2 (t, J = 22.7 Hz), 140.5, 137.4, 136.1, 133.3, 129.9, 129.4, 125.9, 124.2, 121.5, 111.3 (t, J = 240.5 Hz), 110.9; IR (KBr): 3089, 3057, 1612, 1589, 1501, 1451, 1406, 1261, 1199, 1144, 1092, 991; MS (ESI): m/z: 357 [M + H^+]; HRMS Calcd for $C_{14}H_8N_2ClBrF_2$: 355.9527, Found: 355.9529.

2-(bromodifluoromethyl)-1-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazole **(3h)**



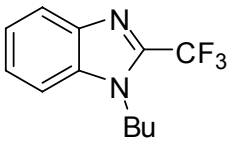
White solid, mp 94-96 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.89-7.95 (m, 1H), 7.32-7.43 (m, 4H), 7.03-7.11 (m, 3H), 3.91(s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -44.50(s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.4, 145.6, 140.4, 137.9, 129.3, 127.1 ,125.6 ,123.9, 121.3, 114.7, 111.3 (t, J = 301.4 Hz), 111.2, 55.6; IR (KBr): 2958, 2933, 1610, 1587, 1514, 1441, 1253, 1141, 1109, 989; MS: m/z (%):352 (14.11) [M^+], 273 (100); Anal. Cacld. For $C_{15}H_{11}BrF_2N_2O$: C, 51.01; H, 3.14, N, 7.93; Found: C, 50.94; H, 3.42; N, 7.86.

2-(bromodifluoromethyl)-1-(4-nitrophenyl)-1*H*-benzo[*d*]imidazole **(3i)**



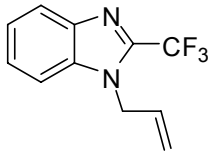
Yellow solid, mp 133-134 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.49 (d, J = 8.8 Hz, 2H), 7.96 (d, J = 6.8 Hz, 1H), 7.70 (d, J = 8.7 Hz, 2H), 7.42-7.46 (m, 2H), 7.10 (d, J = 7.1 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -44.3 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 148.4, 144.9 (t, J = 28.9 Hz), 140.5, 140.3, 136.9, 129.2, 126.4, 125.3, 124.7, 124.0, 111.1 (t, J = 300.8 Hz), 110.6; IR (KBr): 3111, 3084, 1610, 1595, 1525, 1407, 1353, 754; MS: m/z (%):367 (8.58) [M^+], 242 (100); Anal. Cacld. For $C_{14}H_8BrF_2N_3O_2$: C, 45.68; H, 2.19; N, 11.41; Found: C, 45.96; H, 2.34; N, 11.42.

1-butyl-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3j)**



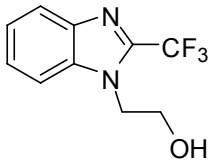
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83 (d, J = 8.0 Hz, 1H), 7.28-7.41 (m, 3H), 4.21-4.29 (m, 2H), 1.75-1.87 (m, 2H), 1.32-1.46 (m, 2H), 0.94 (t, J = 7.5 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -62.49 (s); ^{13}C NMR (100 MHz, $CDCl_3$): δ135.9, 135.2 (q, J = 38.0 Hz), 130.2, 119.9, 118.2, 114.0 (q, J = 270.3 Hz), 116.3, 105.3, 39.7, 26.7, 14.8, 8.3; IR (film): 3050, 2964, 2938, 2876, 1583, 1521, 1479, 1456, 1268, 1198, 746; MS: m/z (%): 242 (70.78) [M^+], 199 (100); HRMS Calcd for $C_{12}H_{13}N_2F_3$: 242.1031, Found: 242.1034.

1-allyl-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3k)**[2]



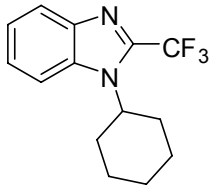
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34-7.89 (m, 4H), 5.88-6.03 (m, 1H), 5.27 (d, *J* = 11.0 Hz, 1H), 5.11 (d, *J* = 17.4 Hz, 1H), 4.93 (d, *J* = 5.0 Hz, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -62.53 (s); MS(ESI): m/z: 227.1 [M + H^+].

2-(2-(trifluoromethyl)-1*H*-benzo[*d*]imidazol-1-yl)ethanol **(3l)**[2]



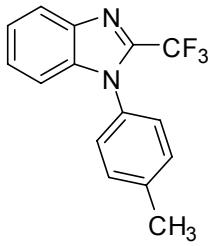
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.15-7.85 (m, 4H), 4.43 (t, *J* =5.5 Hz, 2H), 3.98(t, *J* =5.5 Hz, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -61.89 (s); MS (ESI): m/z: 231.1 [M^+ + H].

1-cyclohexyl-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3m)**[2]



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.88 (d, *J* = 7.3 Hz, 1H), 7.68 (d, *J* = 7.3 Hz, 1H), 4.33-4.53 (m, 1H), 1.22-2.48 (m, 10H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -62.06 (s); MS (ESI): m/z: 269.2 [M^+ + H].

1-p-tolyl-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3n)**

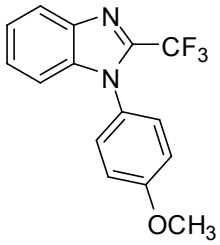


White solid, mp 56-58 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.82 (d, *J* = 6.6 Hz, 1H),

7.00-7.32 (m, 7H), 2.36 (s, 3H); ^{19}F NMR ($CDCl_3$): δ -60.54(s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.7 (q, J = 38.2 Hz), 135.4, 134.9, 132.1, 126.5, 125.1, 121.9, 120.5, 113.7 (q, J = 207.6 Hz), 118.7, 116.1, 106.0, 16.0; IR (KBr): 3064, 2927, 1609, 1589, 1514, 1453, 1264, 753;

MS (ESI): m/z: 277.1 [M^+ + H]. HRMS Calcd for $C_{15}H_{11}N_2F_3$: 276.0874, Found: 276.0877.

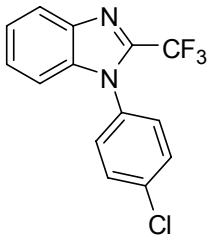
1-(4-methoxyphenyl)-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3o)**



White solid, mp 83-84 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79-7.87 (m, 1H), 6.92-7.34 (m, 7H), 3.81 (s, 3H);

^{19}F NMR (282 MHz, $CDCl_3$): δ -60.59 (s); ^{13}C NMR (100 MHz, $CDCl_3$): δ160.4, 141.0 (q, J = 37.3 Hz), 140.5, 137.5, 128.5, 126.7, 125.6, 123.8, 120.2, 118.9 (q, J = 270.3 Hz), 114.8, 111.1, 55.5; IR (KBr): 3064, 3016, 2968, 1612, 1514, 1456, 1417, 755; MS (ESI): m/z: 293.1[M^+ + H]; Anal. Cacld. For $C_{15}H_{11}F_3N_2$: C, 61.64, H, 3.60, N, 9.59; Found: C, 61.63, H, 3.60, N, 9.57.

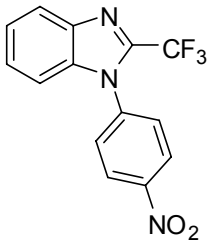
1-(4-chlorophenyl)-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3p)**



White solid, mp 80-81 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.04 – 7.87 (m, 1H), 7.57 (d, J = 8.7, 2H), 7.47 – 7.31 (m, 4H), 7.22 – 7.06 (m, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -60.63 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 140.6, 140.5 (q, J = 38.4 Hz), 136.9,

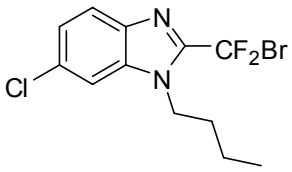
136.0, 132.8, 130.0, 128.7, 125.9, 124.1, 121.4, 118.7 (q, J = 270.6 Hz), 110.8; IR (KBr): 3091, 3058, 1592, 1528, 1497, 1451, 1263, 746; MS: m/z (%): 296 (100) [M^+]; Cacld. For $C_{14}H_8F_3N_3O_2$: C, 56.68; H, 2.72; N, 9.44; Found: C, 56.94; H, 2.95; N, 9.51.

1-(4-nitrophenyl)-2-(trifluoromethyl)-1*H*-benzo[*d*]imidazole **(3q)**



White solid, mp 146-148 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ 8.49 (d, J = 8.8 Hz, 2H), 7.96 (m, 1H), 7.70 (d, J = 8.7 Hz, 2H), 7.58 – 7.35 (m, 2H), 7.22 (m, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -60.23 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 148.3, 140.7, 140.2 (q, J = 38.5 Hz),139.8, 136.4, 128.4, 126.5, 125.2, 124.6, 121.7, 118.6 (q, J = 270.7 Hz), 110.6; IR (KBr): 3118, 3084, 1612, 1597, 1526, 1502, 1355, 1205, 757; MS: m/z (%): 307 (100) [M^+]; Cacld. For $C_{14}H_8F_3N_3O_2$: C, 54.73; H, 2.62; N, 13.68; Found: C, 54.74; H, 2.58; N, 13.68.

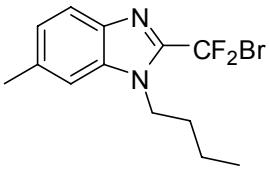
2-(bromodifluoromethyl)-1-butyl-6-chloro-1*H*-benzo[*d*]imidazole **(3r)**



White solid, mp 45-46 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ 7.71 (d, J = 8.7 Hz, 1H), 7.37-7.24 (m, 5H), 4.23 (m, 2H), 1.98 – 1.69 (m, 2H), 1.51 – 1.30 (m, 2H), 0.96 (d, J = 7.3 Hz, 3H);. ^{19}F NMR (282 MHz, $CDCl_3$): -45.72 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 145.9, 139.7, 136.3, 131.3, 124.7, 122.8, 111.6 (t, J = 300 Hz), 110.8, 45.7, 31.8, 20.3, 13.8; IR (film): 2965, 2934, 2877, 1612, 1579, 1498, 1483, 1417, 1131,

772; MS: m/z (%): 336 (12.04) [M^+], 257 (100); Cacld. For $C_{12}H_{12}BrClF_2N_2$: C, 42.69; H, 3.58; N, 8.30; Found: C, 42.66; H,3.54; N, 8.38.

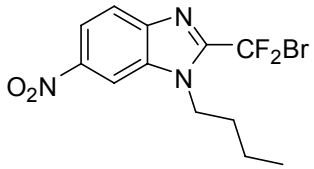
2-(bromodifluoromethyl)-1-butyl-6-methyl-1*H*-benzo[*d*]imidazole **(3s)**



White solid, mp 39-40 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ 8.28 (d, J = 8.3 Hz, 1H), 7.87 – 7.63 (m, 2H), 4.94 – 4.73 (m, 2H), 3.07 (s, 3H), 2.41 (m, 2H), 2.01 (m, 2H), 1.55 (t, J = 7.3 Hz, 3H).

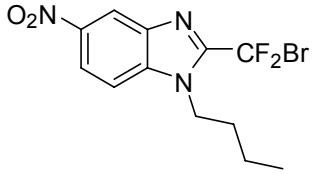
^{19}F NMR (282 MHz, $CDCl_3$): δ -44.98 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 144.6 (t, J = 38.2 Hz), 139.3, 136.0, 135.7, 125.6, 121.2, 112.1 (t, J = 300 Hz), 110.4, 45.3, 31.9, 22.2, 20.3, 13.8; IR (film):3034, 2962, 2935, 2874, 1624, 1585, 1505, 1476, 1233, 1177; MS: m/z (%): 316 (10.45) [M^+], 237 (100); Cacld. For $C_{13}H_{15}BrF_2N_2$: C, 49.23; H, 4.77; N, 8.83; Found: C, 48.94; H, 4.80; N, 8.93.

2-(bromodifluoromethyl)-1-butyl-6-nitro-1*H*-benzo[*d*]imidazole **(3t)**



White solid, mp 90-91 ^oC; ^1H NMR (300 MHz, $CDCl_3$): δ 8.41 (s, 1H), 8.28 (d, J = 9.0 Hz, 1H), 7.96 (d, J = 9.0
hz, 1H), 4.42 (m, 2H), 2.02 – 1.82 (m, 2H), 1.60 – 1.40 (m, 2H), 1.03 (t, J = 7.3 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): -46.99 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 149.1 (t, J = 29.0 Hz), 145.2, 144.8, 122.0, 119.0, 110.9 (t, J = 301.5 Hz), 107.7, 45.9, 31.8, 20.0, 13.5; IR (KBr): 3086, 2960, 2874, 1617, 1597, 1521, 1350, 1186, 1138, 735; MS (ESI): m/z: 347.8 [M^+ + H]; Cacld. For $C_{12}H_{12}BrF_2N_3O_2$: C, 41.40; H, 3.47; N, 12.07; Found: C, 41.41; H, 3.63; N, 11.98.

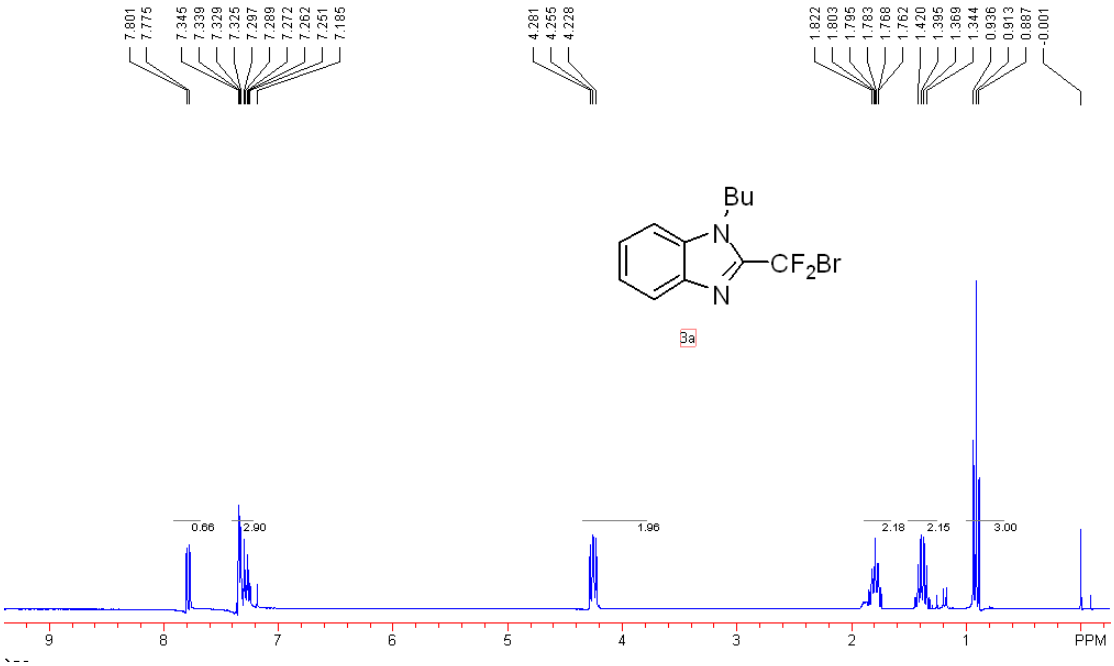
2-(bromodifluoromethyl)-1-butyl-5-nitro-1*H*-benzo[*d*]imidazole **(3u)**



White solid, mp 69-71 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.78 (d, J = 2.1, 1H), 8.34 (dd, J = 9.1, 2.1 Hz, 1H), 7.54 (d, J = 9.0, 1H), 4.63 – 4.20 (m, 2H), 2.15 – 1.75 (m, 2H), 1.60 – 1.30 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): -44.65 (s); ^{13}C NMR (100 MHz, $CDCl_3$): 148.3 (t, J = 29.0 Hz), 144.5, 140.1, 139.3, 120.5, 118.3, 110.9 (t, J = 300.7 Hz), 45.9, 31.7, 20.0, 13.5; IR (KBr): 3105, 2967, 2873, 1698, 1618, 1528, 1518, 1335, 738; MS (ESI): m/z: 347.9 [M^+ + H]; Cacld. For $C_{12}H_{12}BrF_2N_3O_2$: C, 41.40; H, 3.47; N, 12.07; Found: C, 41.13; H, 3.85; N, 12.07.

Reference：

1. Tamura, K.; Mizukami, H.; Maeda, K.; Watanabe, H.;Uneyama, K. *J. Org. Chem.* 1993, **58,** 32–35.
2. Zou, B.; Yuan, Q.; Ma, D. *Angew. Chem., Int. Ed.* **2007,** *46,* 2598-2601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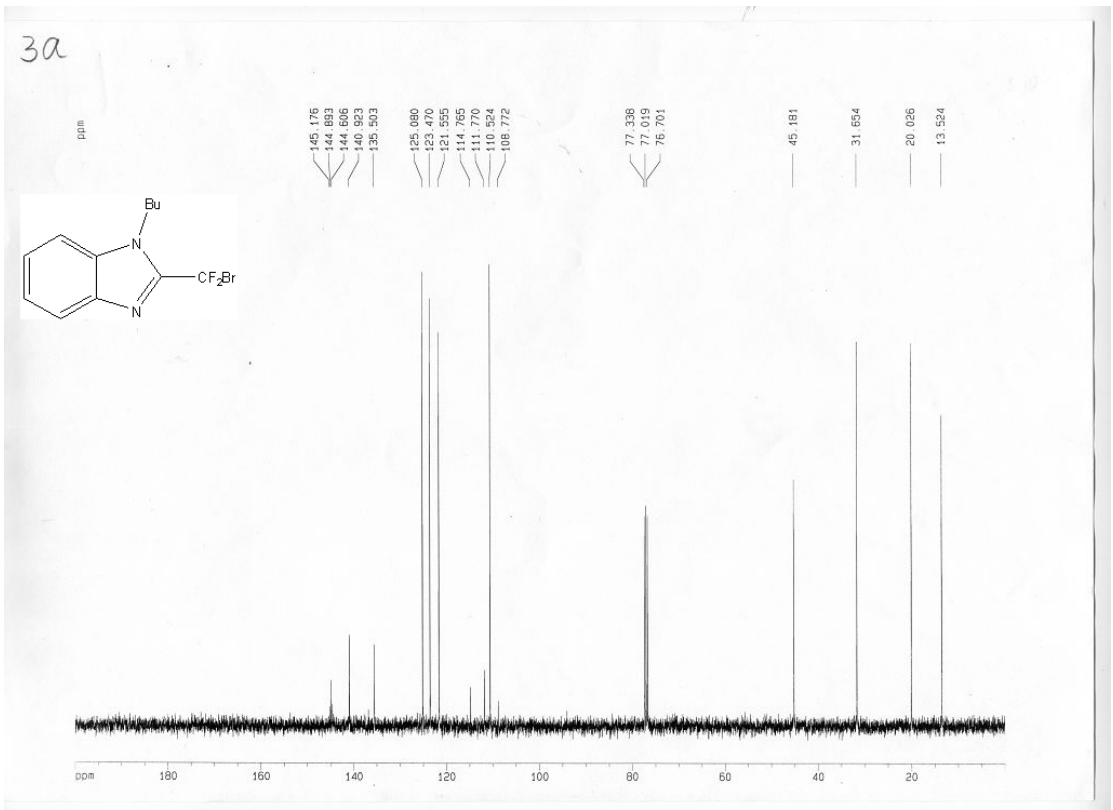
7.345
7.339
7.329
7.325
7.297
7.289
7.272
7.262
7.251
7.185
4.281
4.255
4.228
1.822
1.803
1.795
1.783
1.768
1.762
1.420
1.395
1.369
1.344
0.936
0.913
0.887
-0.001
Bu
N
N
CF2Br
3a
0.66
2.90
1.96
2.18
2.15
3.00
9
8
7
6
5
4
3
2
1
PPM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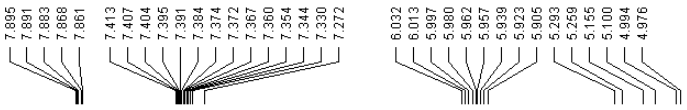
144.893
144.606
140.923
135.503
125.080
123.470
121.555
114.765
111.770
110.524
108.772
77.336
77.019
76.701
45.181
31.654
20.026
13.524
Bu
N
N
CF2Br
ppm
180
160
140
120
100
80
60
40
20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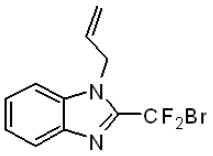
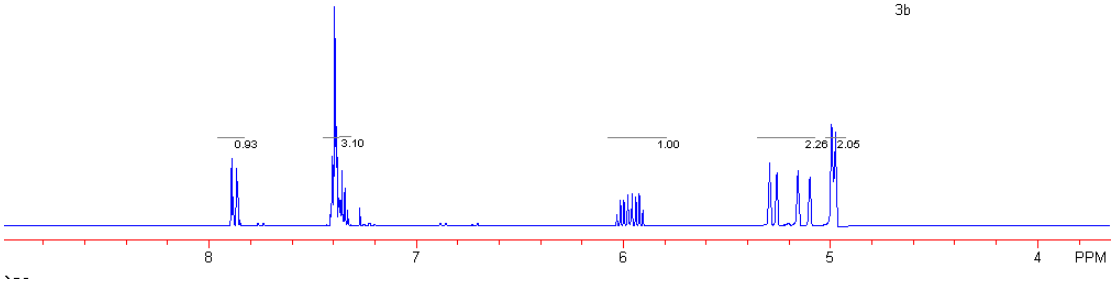
7.883
7.868
7.861
7.413
7.407
7.404
7.395
7.391
7.384
7.374
7.372
7.367
7.360
7.354
7.344
7.330
7.272
6.032
6.013
5.997
5.980
5.962
5.957
5.939
5.923
5.905
5.293
5.259
5.155
5.100
4.994
4.976


N
N
CF2Br

3b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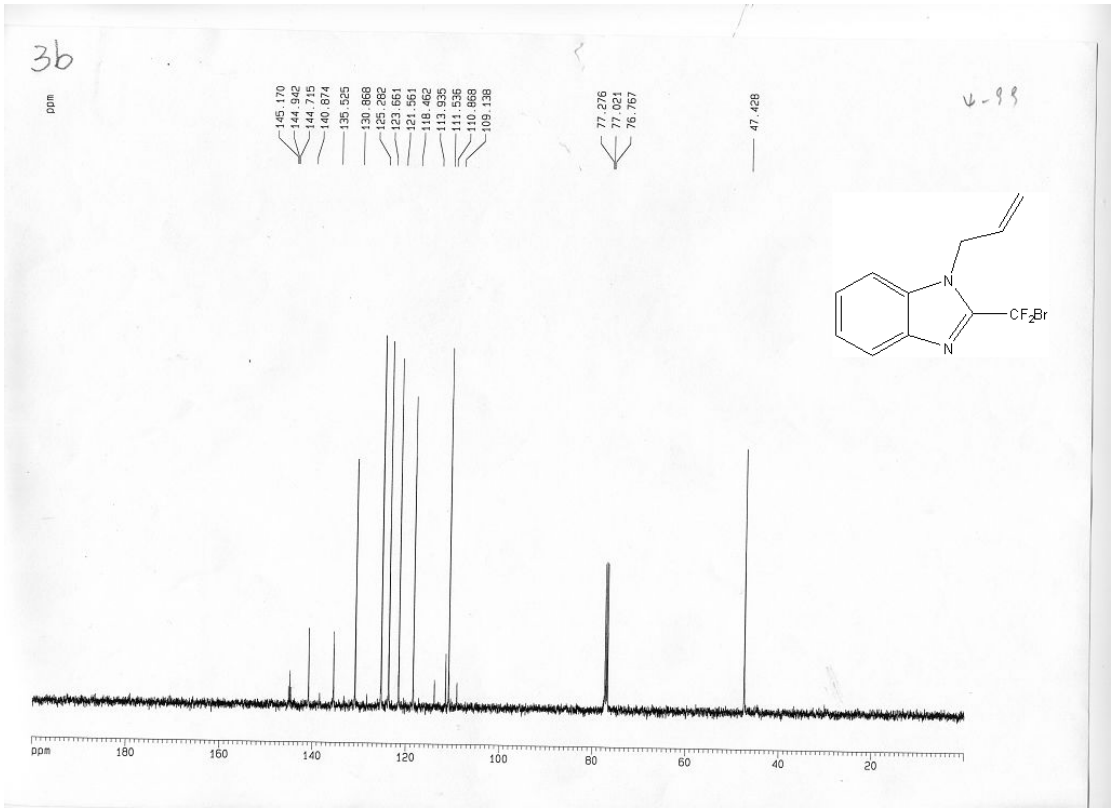
1.00
2.26
2.05
8
7
6
5
4
PPM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ppm
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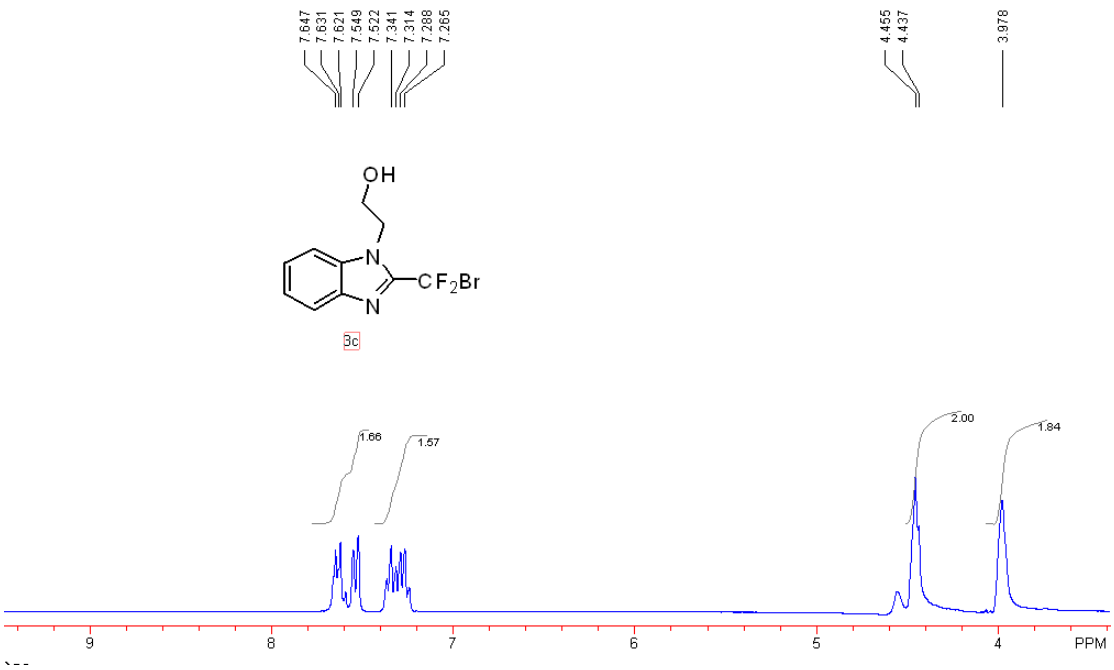
144.715
140.874
135.525
130.868
125.282
123.661
121.561
118.462
113.935
111.536
110.868
109.138
77.276
77.021
76.767
47.428
N
N
CF2Br
ppm
180
160
140
120
100
80
60
40
20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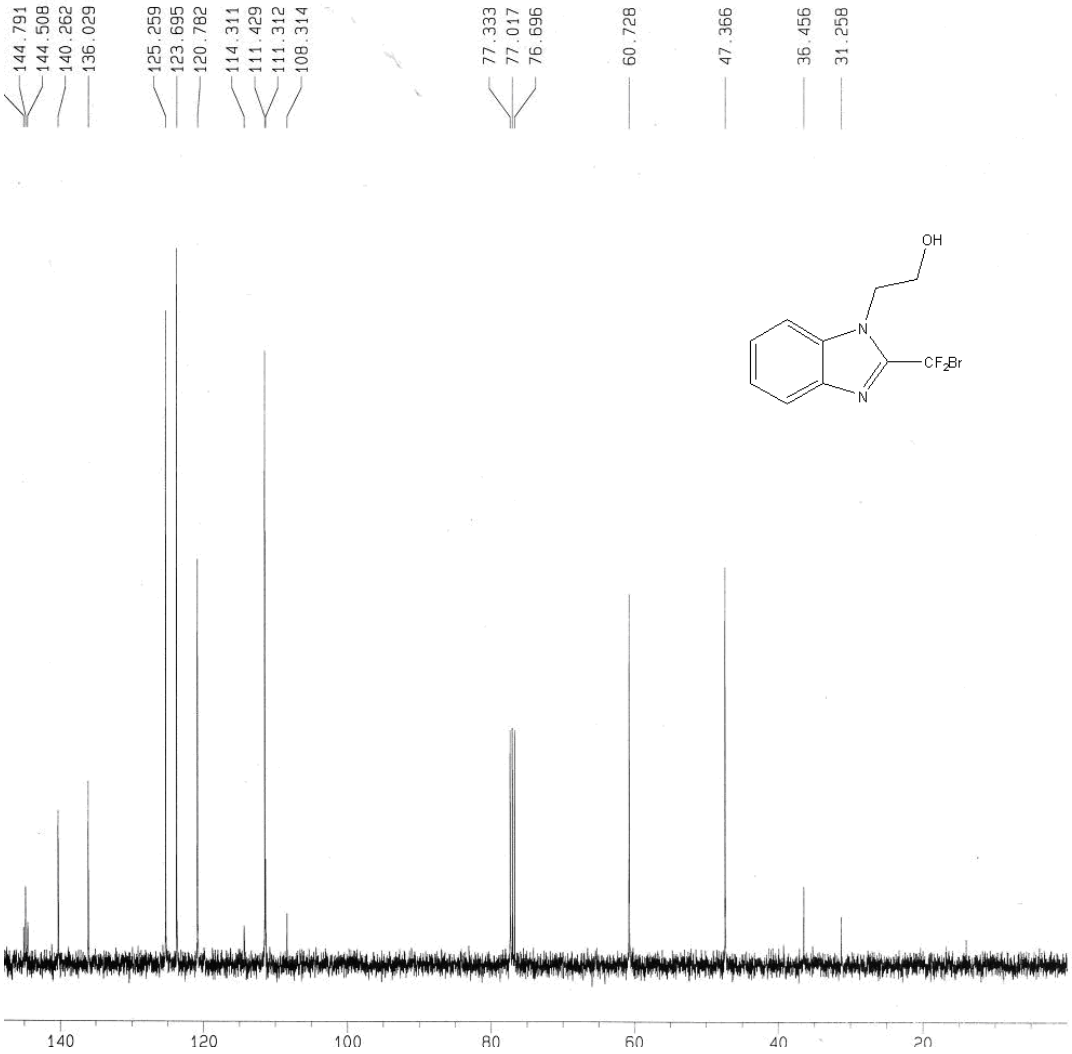
7.621
7.549
7.522
7.341
7.314
7.288
7.265
4.455
4.437
3.978
OH
N
N
CF2Br
3c
1.66
1.57
2.00
1.84
9
8
7
6
5
4
PPM

3C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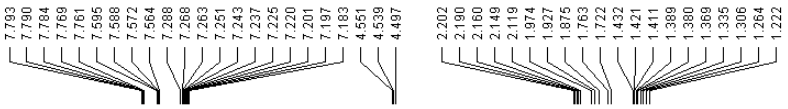
140.262
136.029
125.259
123.695
120.782
114.311
111.429
111.312
108.314
77.333
77.017
76.696
60.728
47.366
36.456
31.258
OH
N
N
CF2Br
140
120
100
80
60
40
20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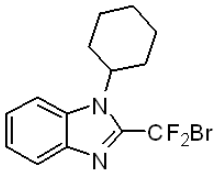
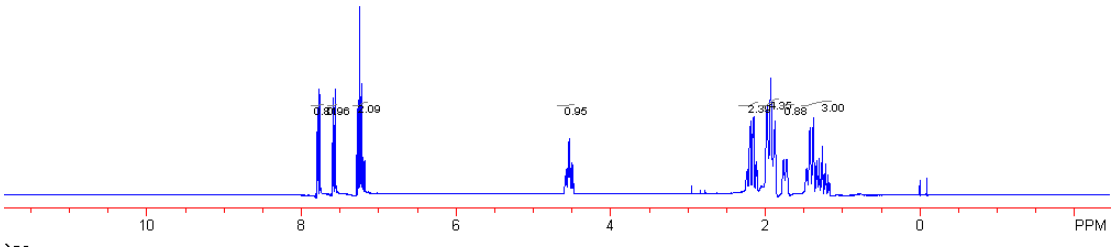
7.784
7.769
7.761
7.595
7.588
7.572
7.564
7.288
7.268
7.263
7.251
7.243
7.237
7.225
7.220
7.201
7.197
7.183
4.551
4.539
4.497
2.202
2.190
2.160
2.149
2.119
1.974
1.927
1.875
1.763
1.722
1.432
1.421
1.411
1.389
1.380
1.369
1.335
1.306
1.264
1.222


N
CF2Br
N

3d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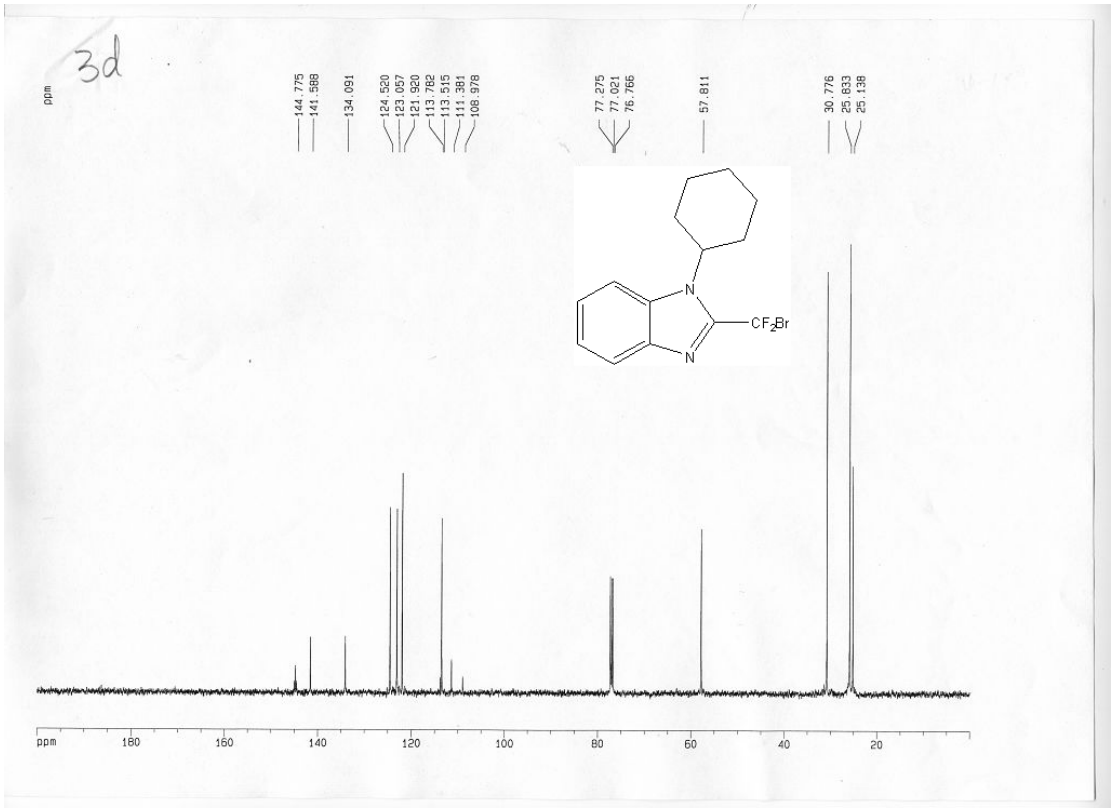
10
8
6
4
2
0
PPM


3d
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144.775
141.588
134.091
124.520
123.057
121.920
113.782
113.515
111.381
108.978
77.275
77.021
76.766
57.811
30.776
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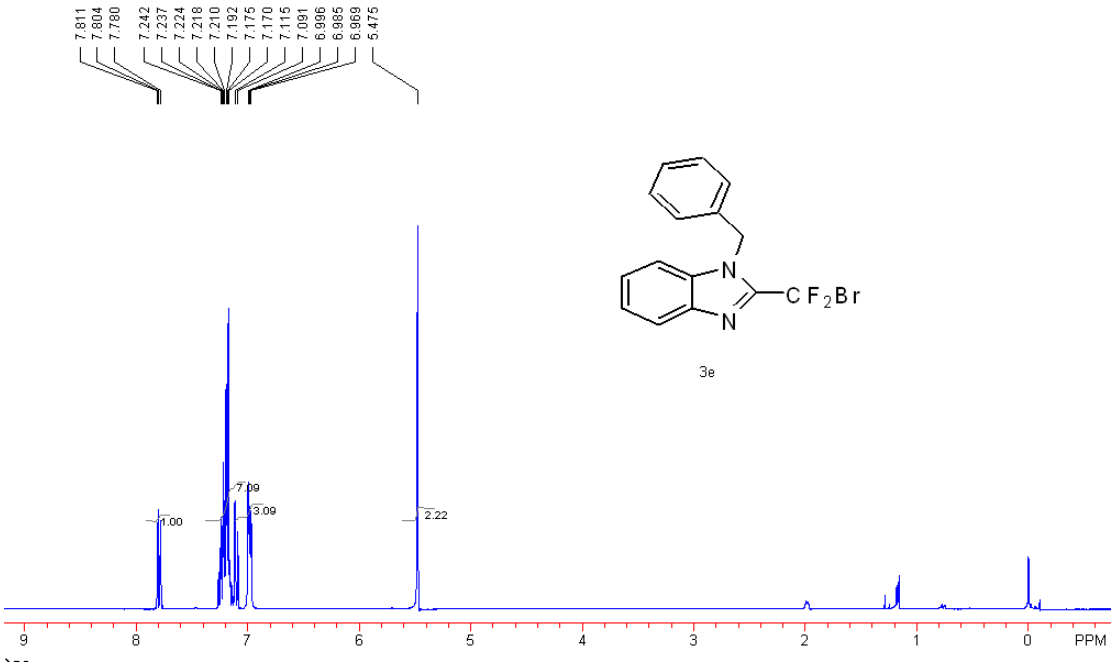
25.138
N
CF2Br
N
ppm
180
160
140
120
100
80
60
40
20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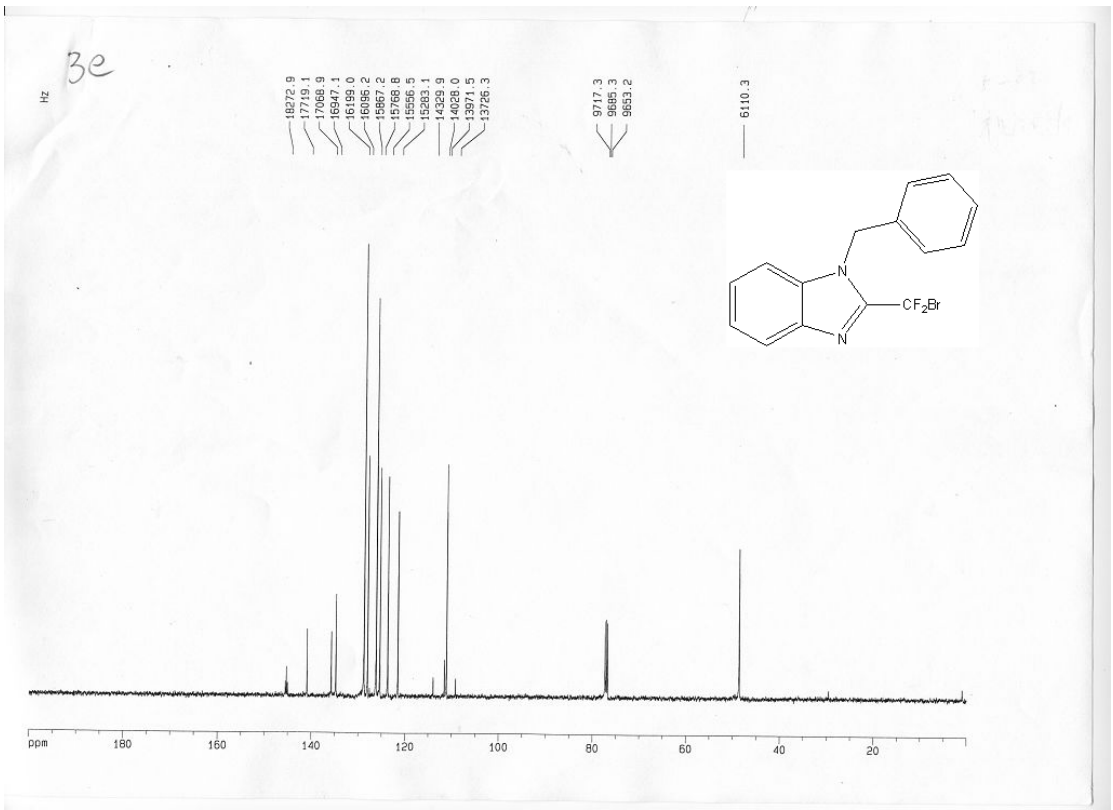
7.804
7.780
7.242
7.237
7.224
7.218
7.210
7.192
7.175
7.170
7.115
7.091
6.996
6.985
6.969
5.475
N
N
C F 2 B r
3e
1.00
3.09
2.22
9
8
7
6
5
4
3
2
1
0
PPM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Hz
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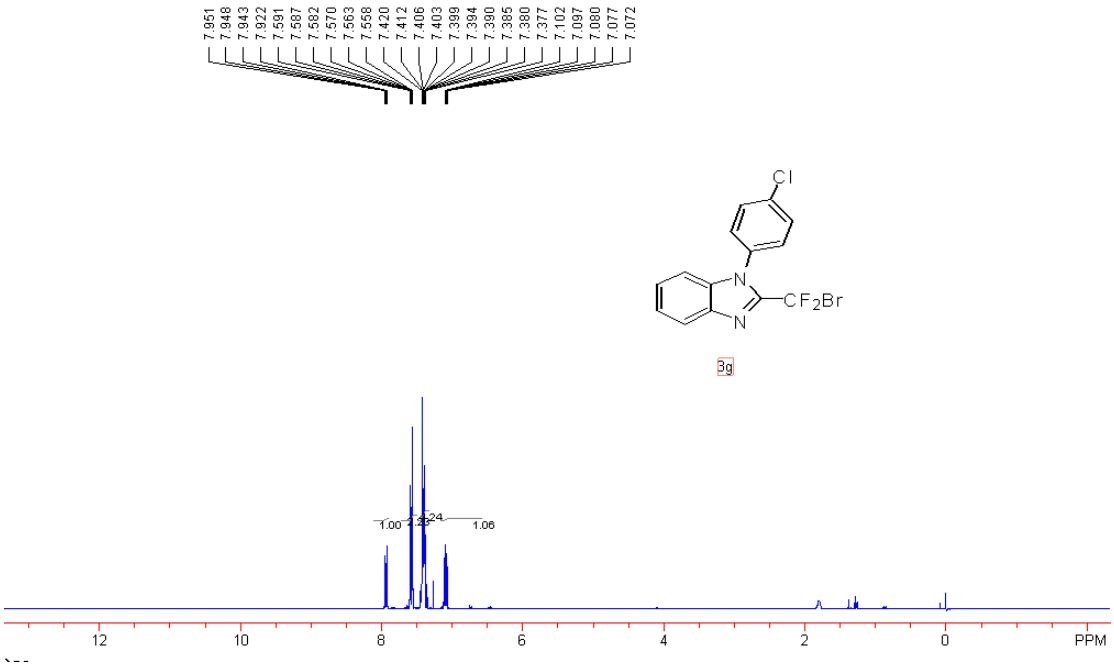
17719.1
17068.9
16947.1
16199.0
16096.2
15867.2
15768.8
15556.5
15283.1
14329.9
14028.0
13971.5
13726.3
9717.3
9685.3
9653.2
6110.3
N
N
CF2Br
ppm
180
160
140
120
100
80
60
40
20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7.922
7.591
7.587
7.582
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7.563
7.558
7.420
7.412
7.406
7.403
7.399
7.394
7.390
7.385
7.380
7.377
7.102
7.097
7.080
7.077
7.072
Cl
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N
CF2Br
3g
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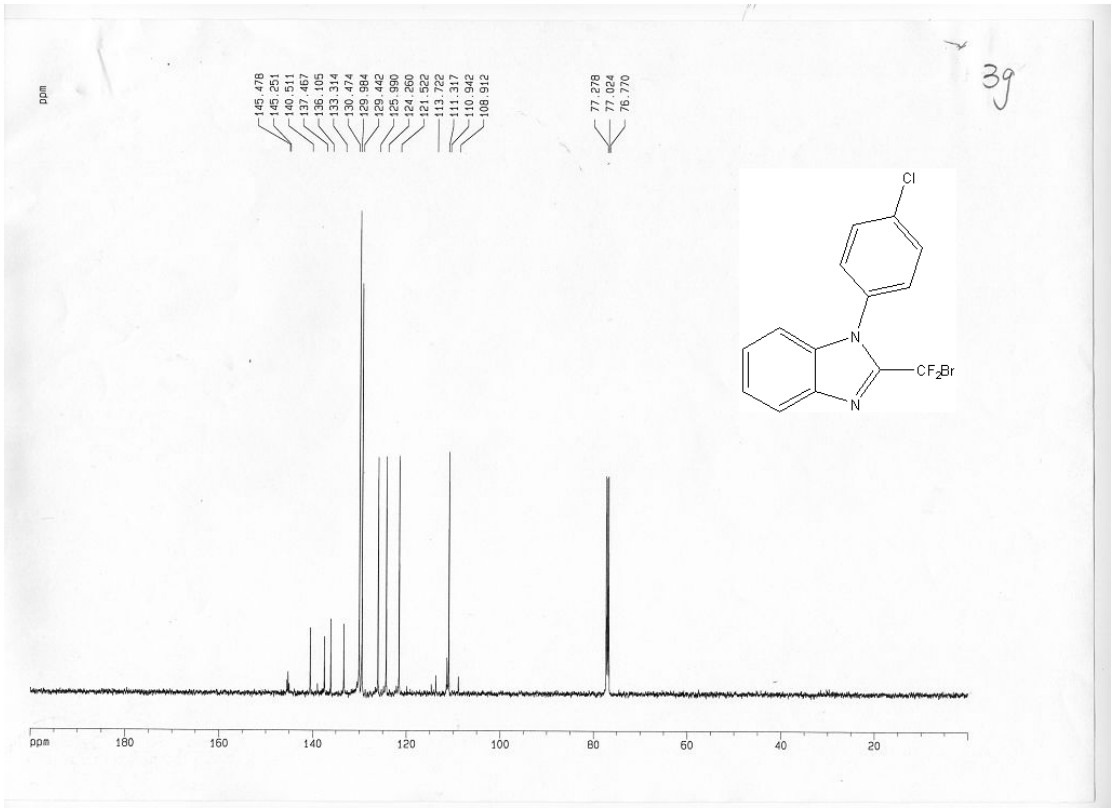
2.24
1.06
12
10
8
6
4
2
0
PPM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140.511
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129.442
125.990
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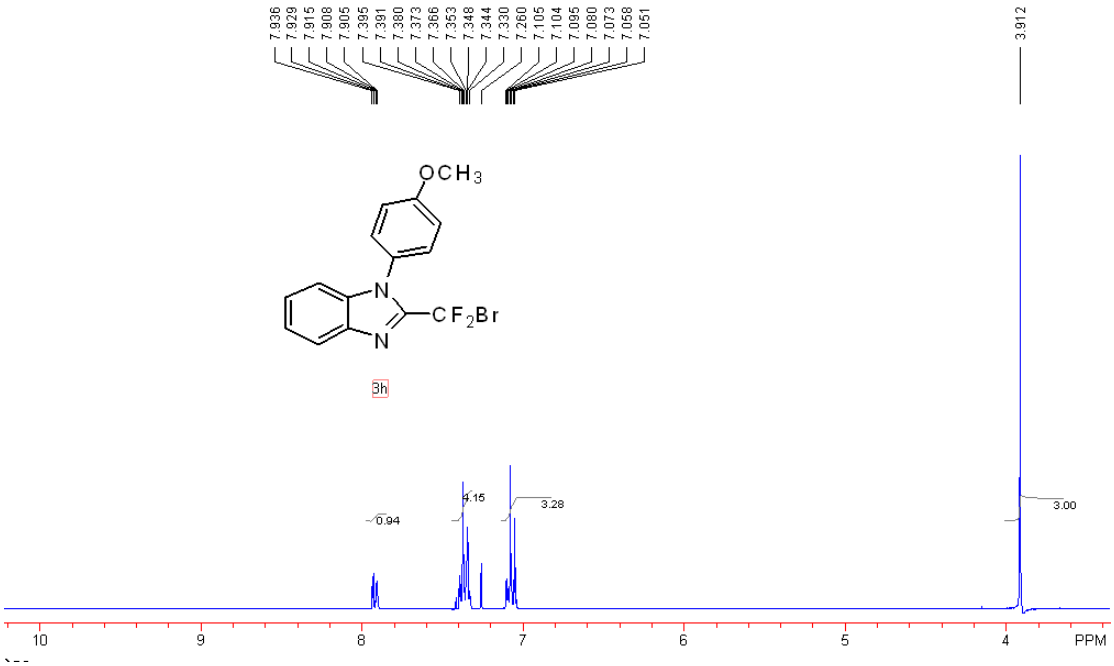
111.317
110.942
108.912
77.278
77.024
76.770
3g
Cl
N
N
CF2Br
ppm
180
160
140
120
100
80
60
40
20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7.905
7.395
7.391
7.380
7.373
7.366
7.353
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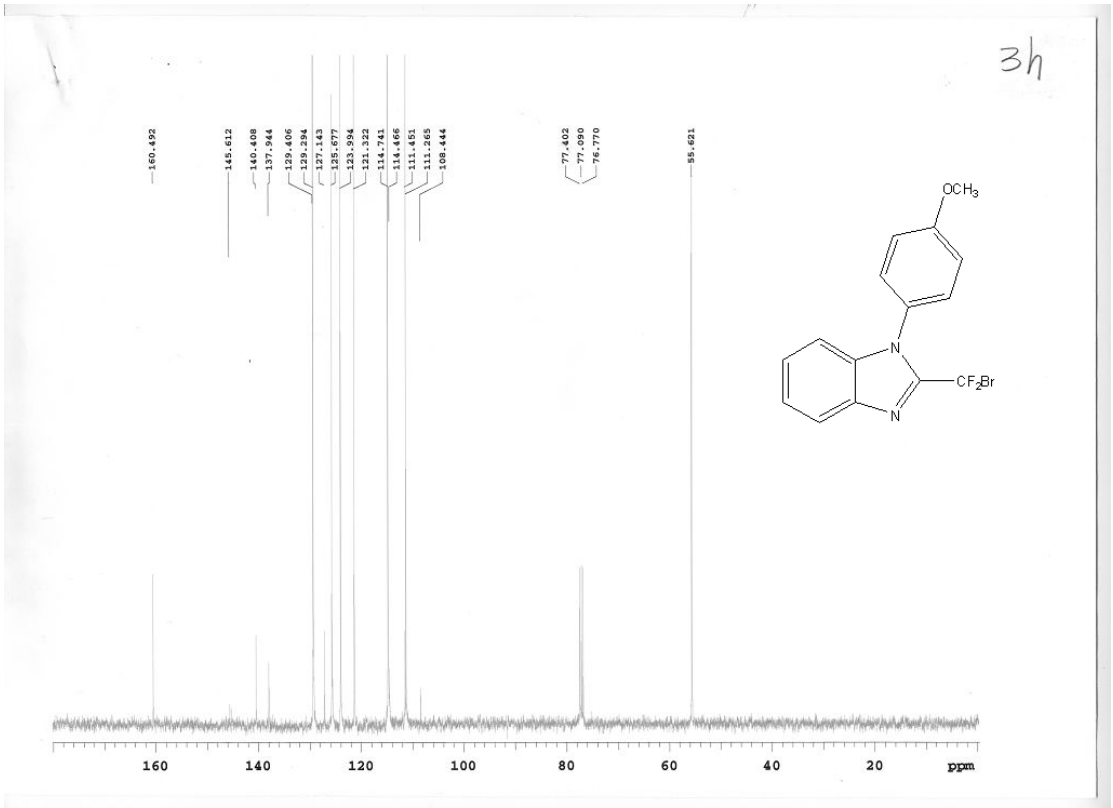
7.330
7.260
7.105
7.104
7.095
7.080
7.073
7.058
7.051
3.912
OCH3
N
CF2Br
N
3h
0.94
4.15
3.28
3.00
10
9
8
7
6
5
4
PPM


3h
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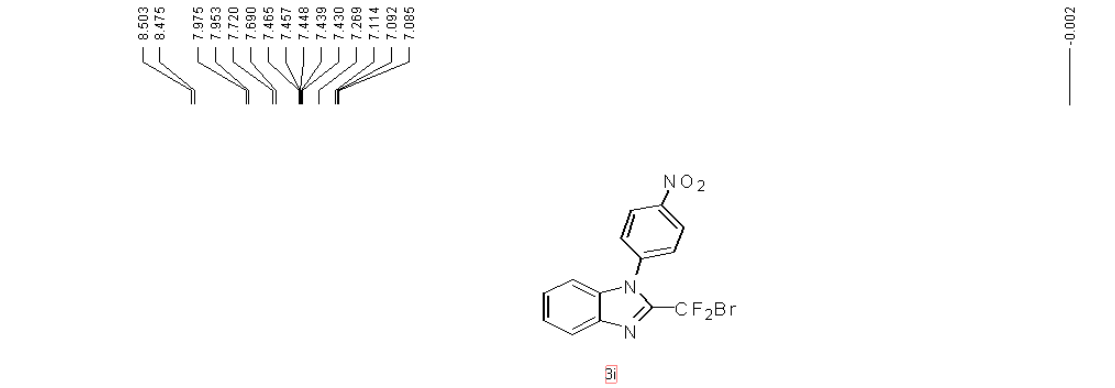
140.408
137.944
129.406
129.294
127.143
125.677
123.994
121.322
114.741
114.466
111.451
111.265
108.444
77.402
77.090
76.770
55.621
OCH3
N
CF2Br
N
160
140
120
100
80
60
40
20
ppm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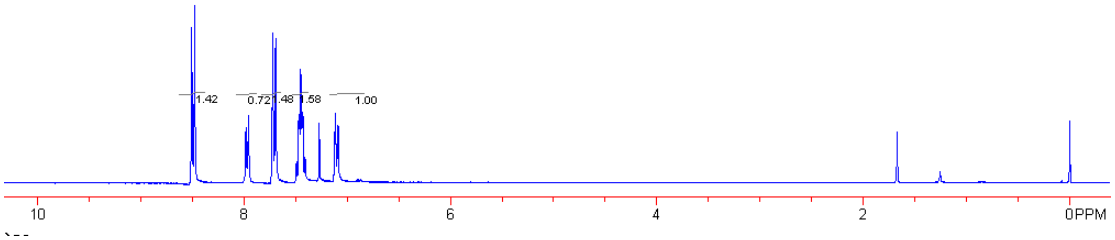
7.953
7.720
7.690
7.465
7.457
7.448
7.439
7.430
7.269
7.114
7.092
7.085
-0.002

NO2
N
N
CF2Br

3i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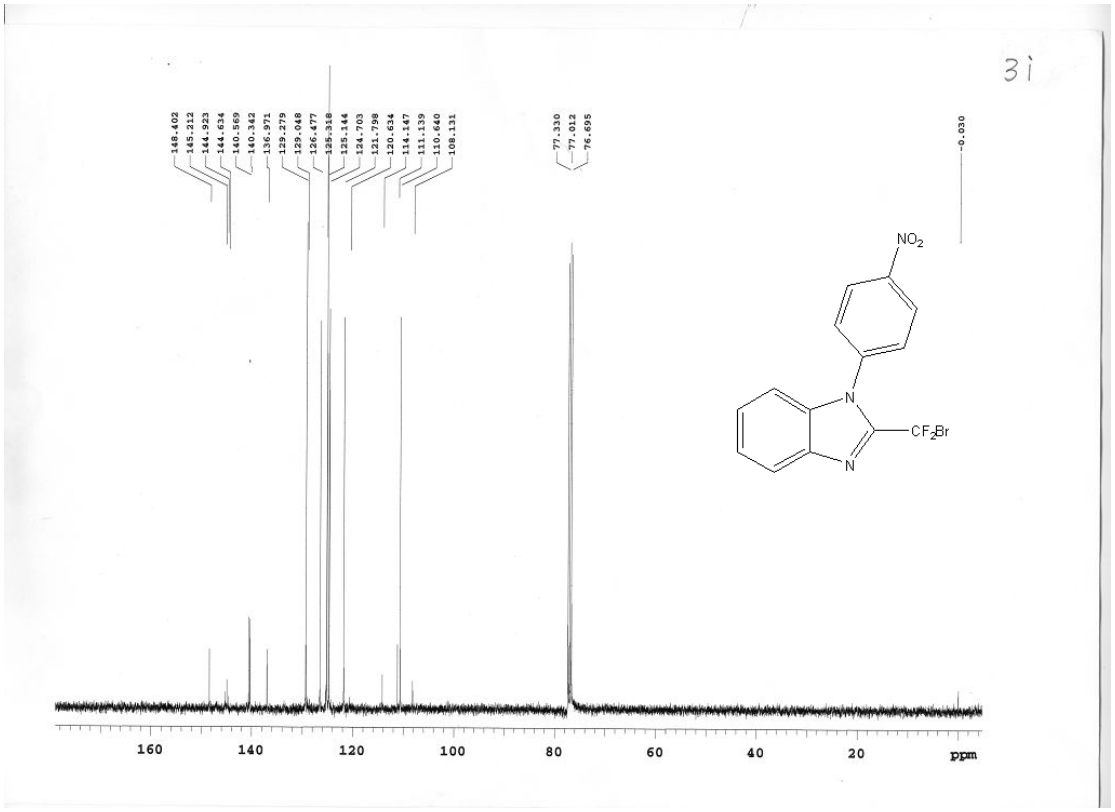
1.58
1.00
10
8
6
4
2
0PPM


3i
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140.569
140.342
136.971
129.279
129.048
126.477
125.318
125.144
124.703
121.798
120.634
114.147
111.139
110.640
108.131
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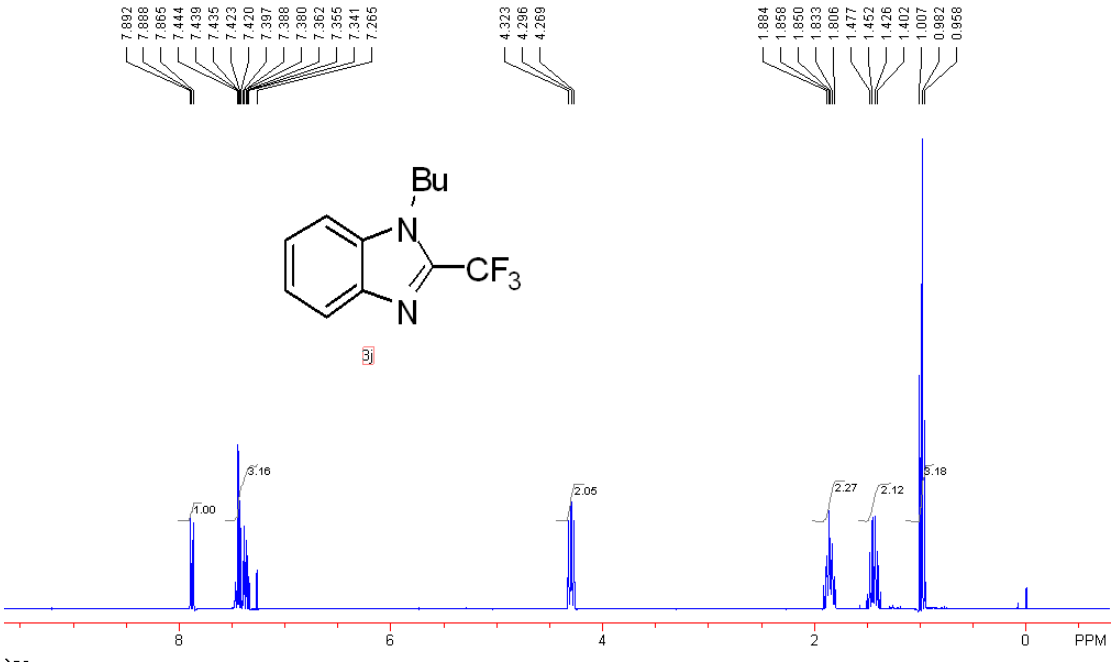
76.695
-0.030
NO2
N
N
CF2Br
160
140
120
100
80
60
40
20
ppm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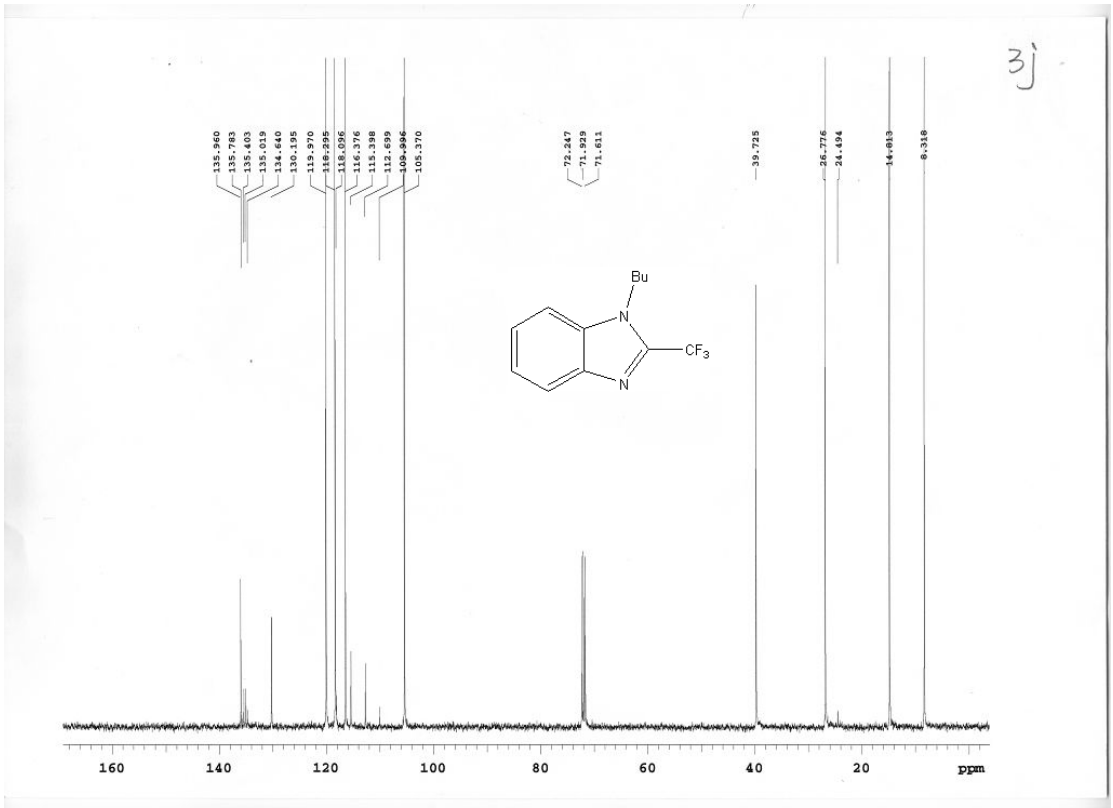
7.888
7.865
7.444
7.439
7.435
7.423
7.420
7.397
7.388
7.380
7.362
7.355
7.341
7.265
4.323
4.296
4.269
1.884
1.858
1.850
1.833
1.806
1.477
1.452
1.426
1.402
1.007
0.982
0.958
Bu
N
CF3
N
3j
1.00
3.16
2.05
2.27
2.12
3.18
8
6
4
2
0
PPM


3j
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112.699
109.996
105.370
72.247
71.929
71.611
39.735
26.776
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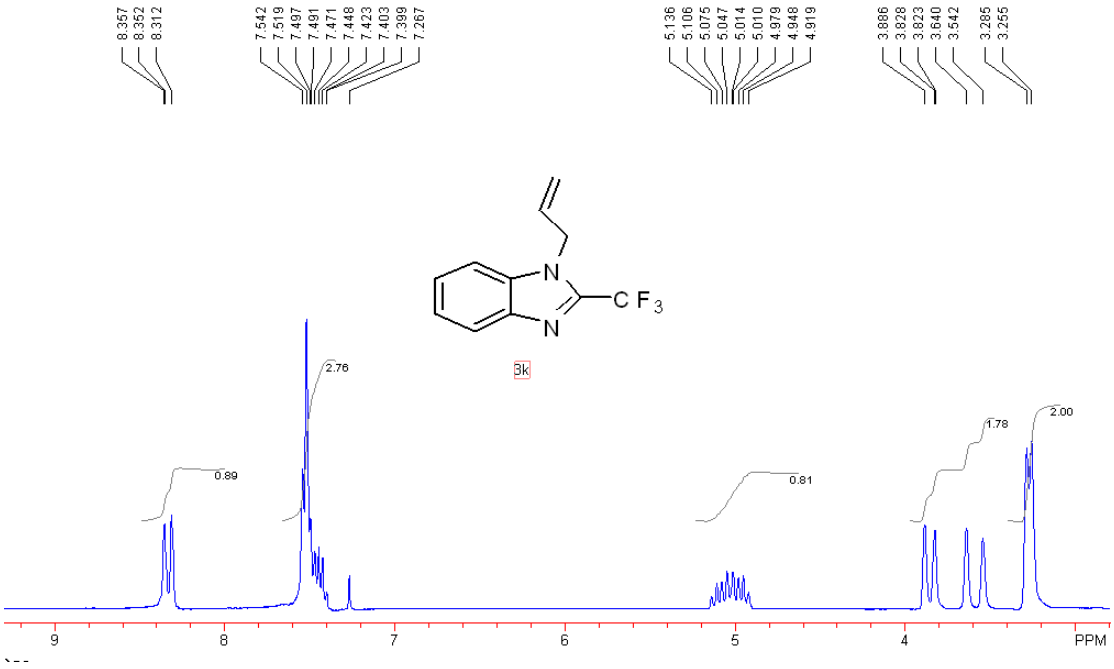
8.318
Bu
N
CF3
N
160
140
120
100
80
60
40
20
ppm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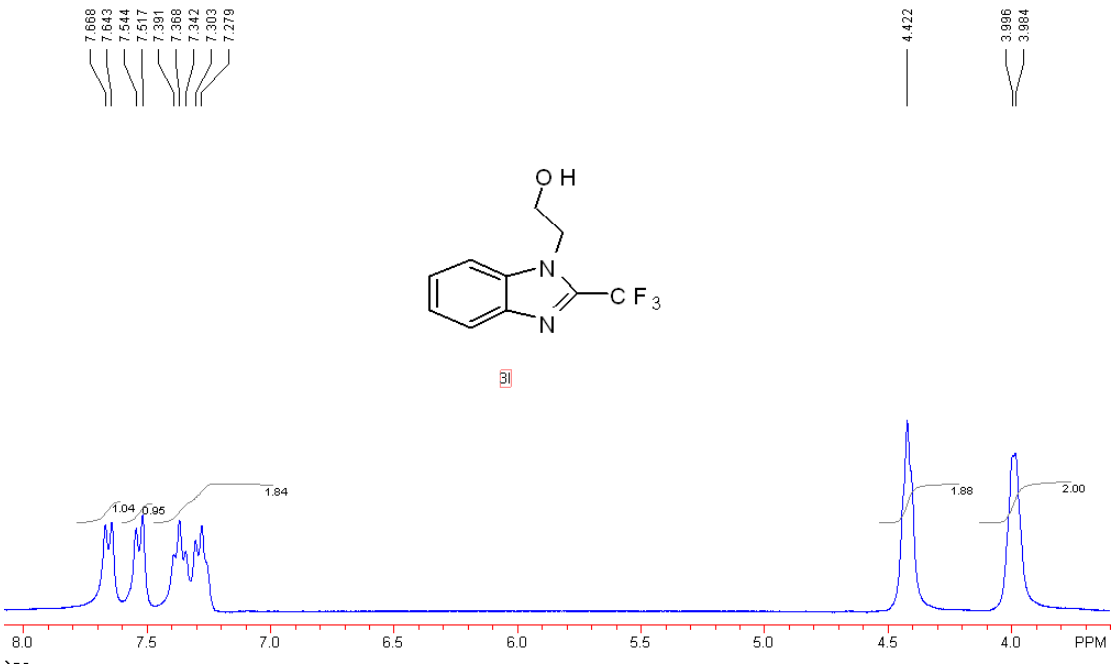
7.519
7.497
7.491
7.471
7.448
7.423
7.403
7.399
7.267
5.136
5.106
5.075
5.047
5.014
5.010
4.979
4.948
4.919
3.886
3.828
3.823
3.640
3.542
3.285
3.255
N
C F 3
N
3k
2.76
0.89
0.81
1.78
2.00
9
8
7
6
5
4
PPM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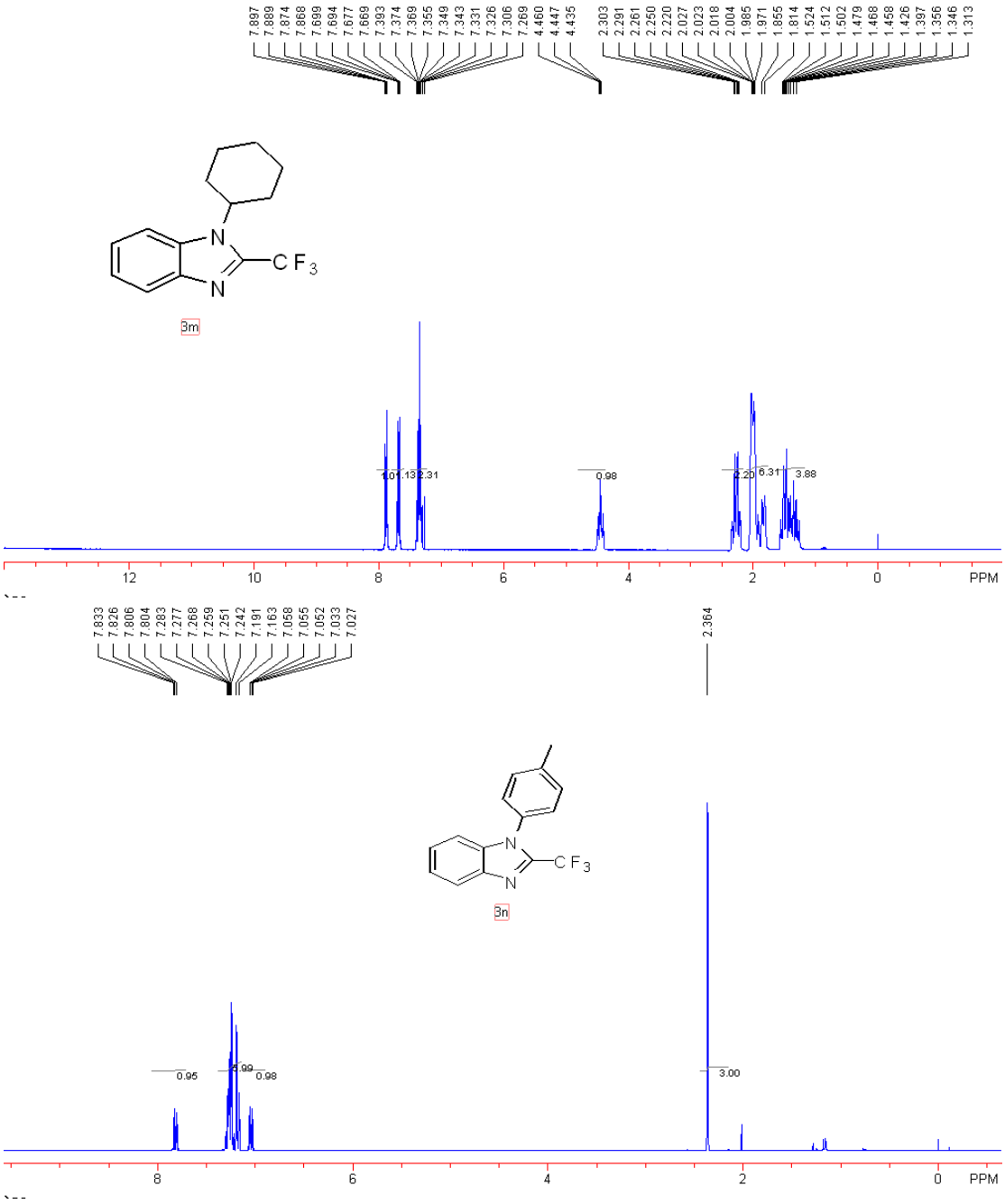
7.517
7.391
7.368
7.342
7.303
7.279
4.422
3.996
3.984
O H
N
C F 3
N
3l
1.04
0.95
1.84
1.88
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
PPM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7.889
7.874
7.868
7.699
7.694
7.677
7.669
7.393
7.374
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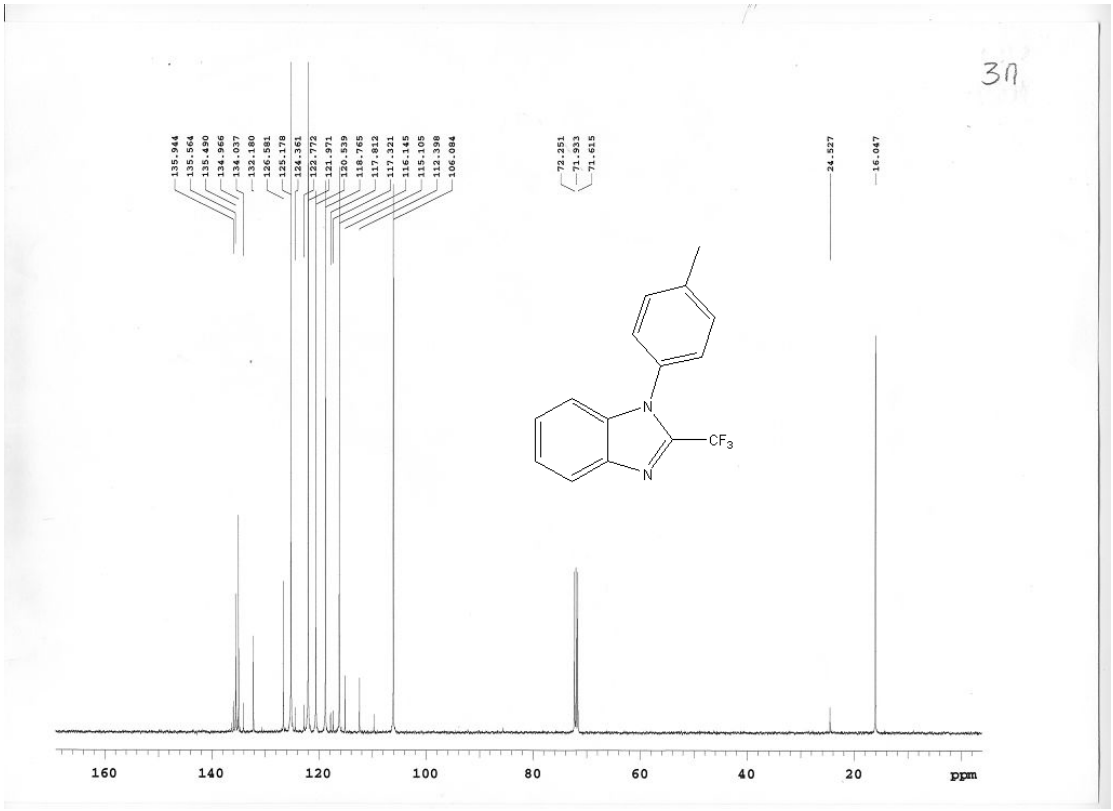
7.355
7.349
7.343
7.331
7.326
7.306
7.269
4.460
4.447
4.435
2.303
2.291
2.261
2.250
2.220
2.027
2.023
2.018
2.004
1.985
1.971
1.855
1.814
1.524
1.512
1.502
1.479
1.468
1.458
1.426
1.397
1.356
1.346
1.313
N
N
C F 3
3m
1.01
1.13
2.31
0.98
2.20
6.31
3.88
12
10
8
6
4
2
0
PPM
7.833
7.826
7.806
7.804
7.283
7.277
7.268
7.259
7.251
7.242
7.191
7.163
7.058
7.055
7.052
7.033
7.027
2.364
N
N
C F 3
3n
0.95
2.99
0.98
3.00
8
6
4
2
0
PPM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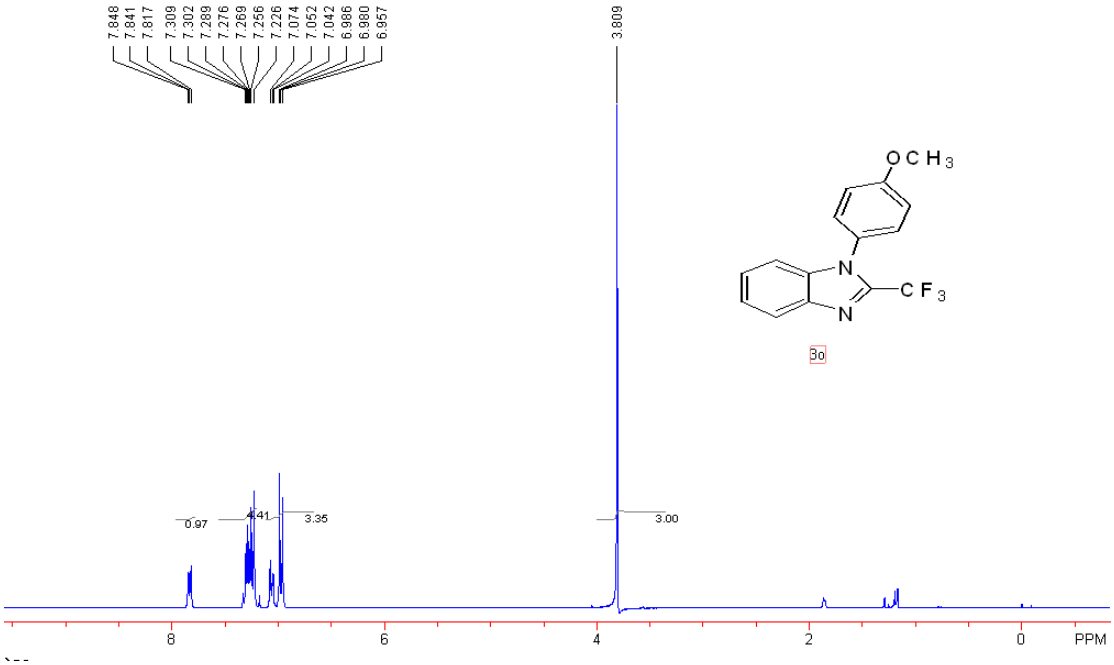
135.564
135.490
134.966
134.037
132.180
126.581
125.178
124.361
122.772
121.971
120.539
118.765
117.812
117.321
116.145
115.105
112.398
106.084
72.251
71.933
71.615
24.527
16.047
N
CF3
N
160
140
120
100
80
60
40
20
ppm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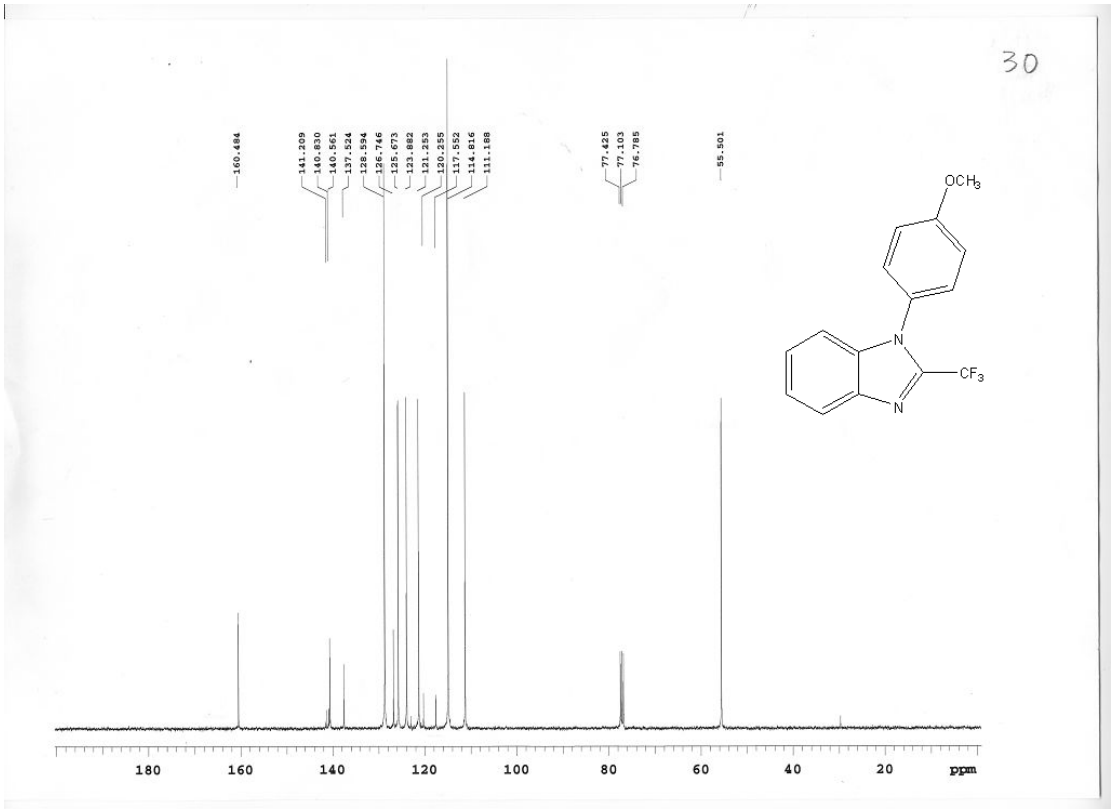
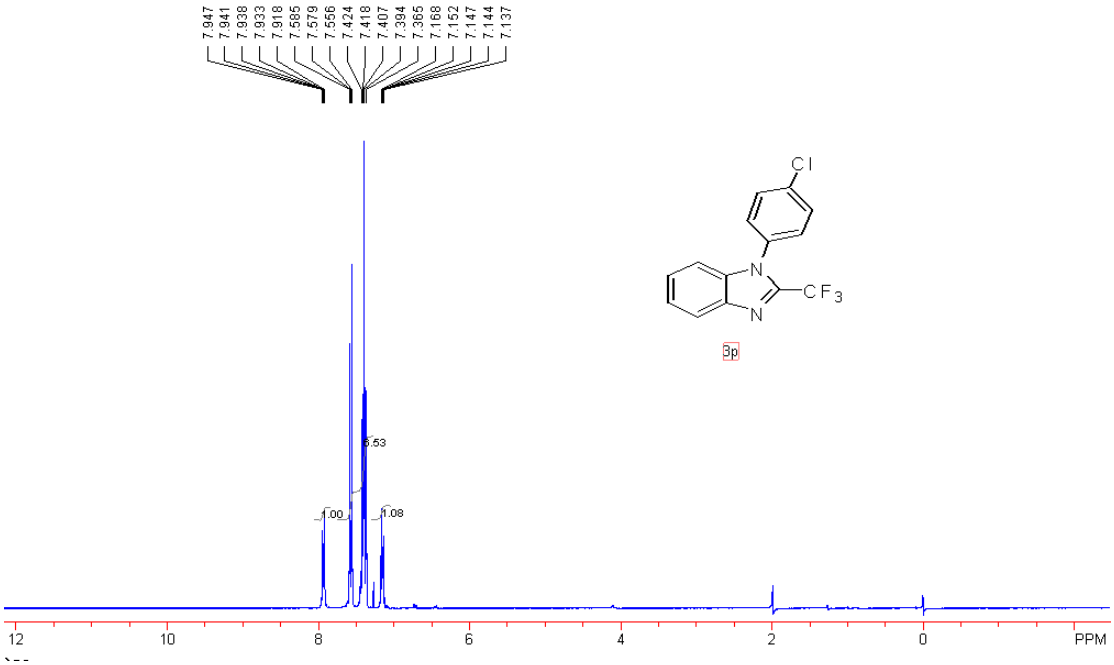
7.817
7.309
7.302
7.289
7.276
7.269
7.256
7.226
7.074
7.052
7.042
6.986
6.980
6.957
3.809
OCH3
N
CF3
N
3o
0.97
4.41
3.35
3.00
8
6
4
2
0
PPM


30
160.484
141.309
140.830
140.561
137.524
128.594
126.746
125.673
123.882
121.253
120.255
117.552
114.816
111.188
77.425
77.103
76.785
55.501
OCH3
N
CF3
N
180
160
140
120
100
80
60
40
20
ppm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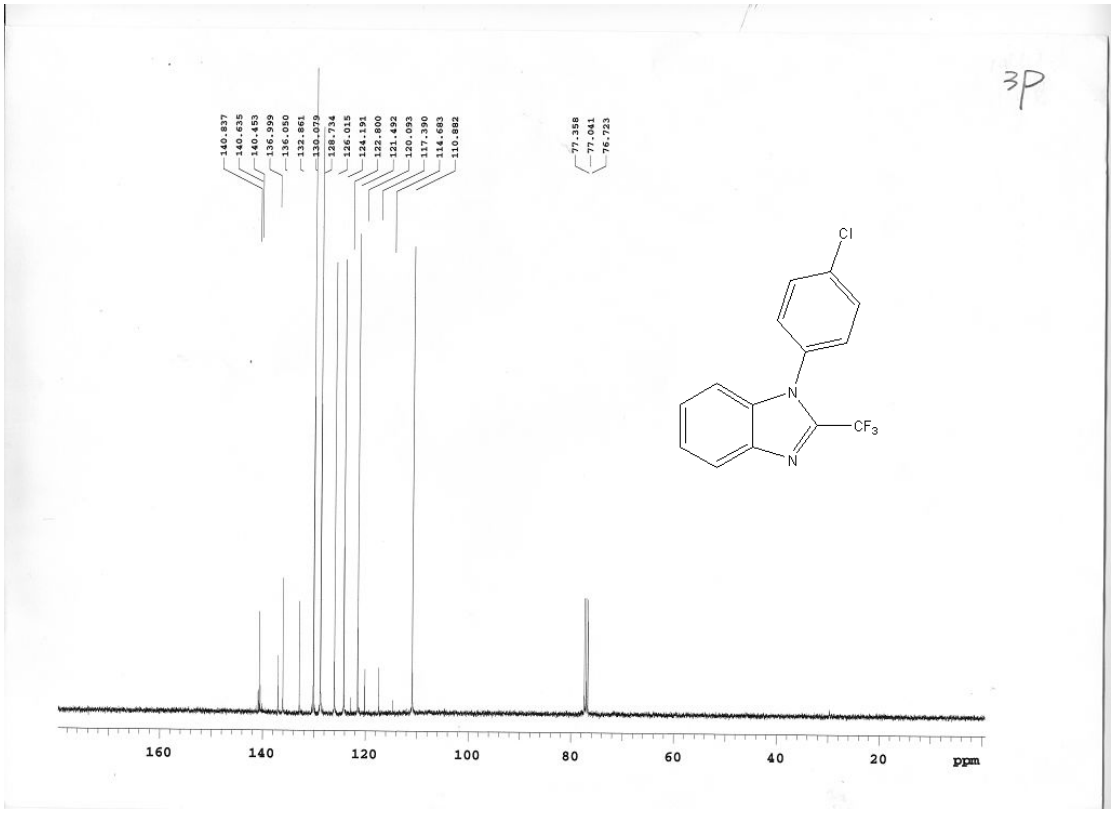
7.941
7.938
7.933
7.918
7.585
7.579
7.556
7.424
7.418
7.407
7.394
7.365
7.168
7.152
7.147
7.144
7.137
6.53
1.00
1.08
12
10
8
6
4
2
0
PPM

Cl
N
CF3
N

3p


3P
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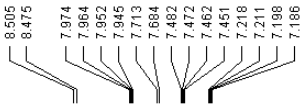
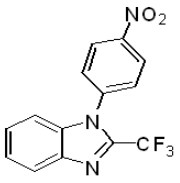
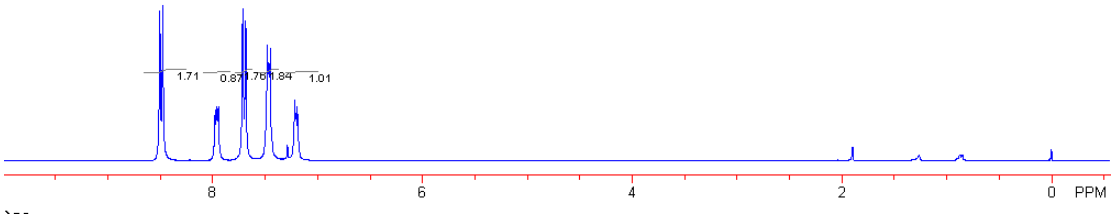
140.635
140.453
136.999
136.050
132.661
130.079
128.734
126.015
124.191
122.800
121.492
120.093
117.390
114.683
110.882
77.358
77.041
76.723
Cl
N
CF3
N
160
140
120
100
80
60
40
20
ppm


8.505
8.475
7.974
7.964
7.952
7.945
7.713
7.684
7.482
7.472
7.462
7.451
7.218
7.211
7.198
7.186


NO2
N
CF3
N

3q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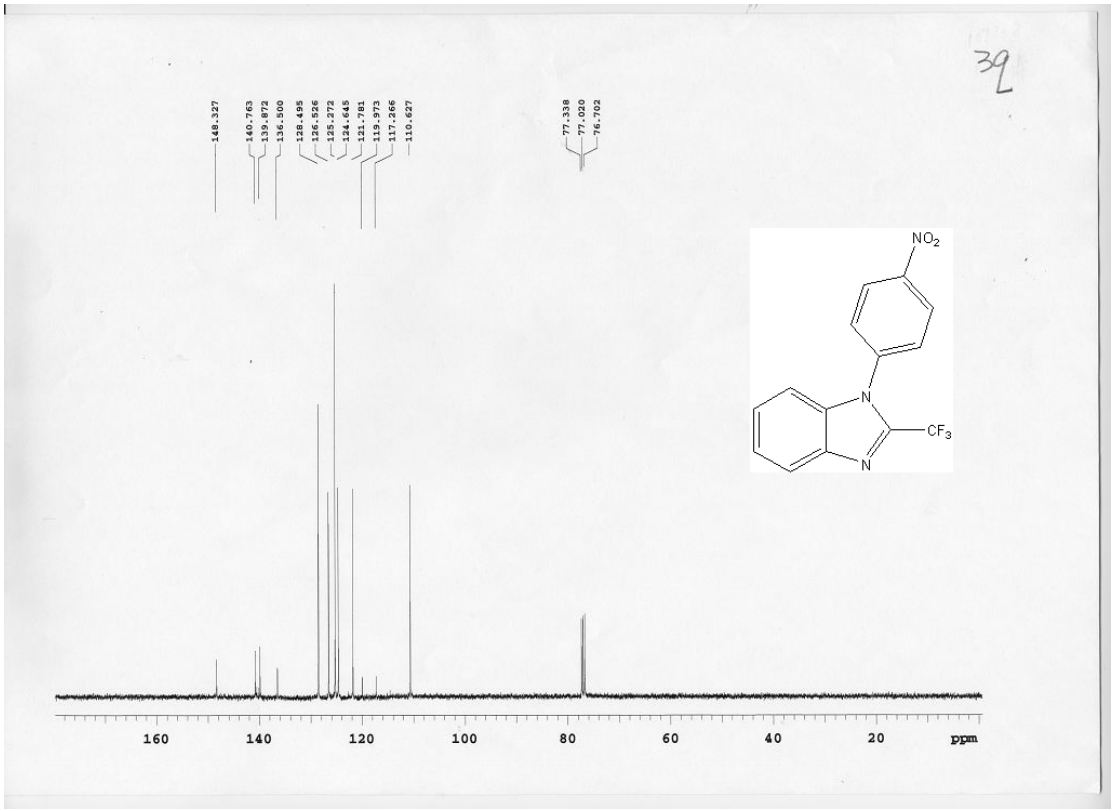
0.87
0.75
1.84
1.01
8
6
4
2
0
PPM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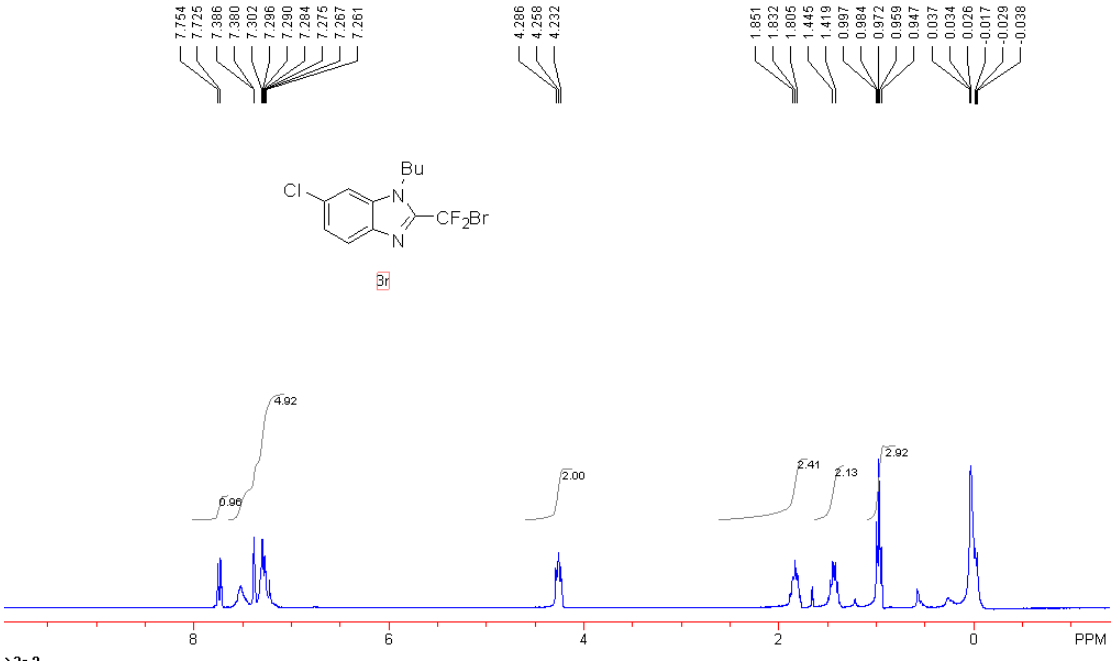
140.763
139.872
136.500
128.495
126.526
125.272
124.645
121.781
119.973
117.266
110.627
77.338
77.020
76.702
NO2
N
CF3
N
160
140
120
100
80
60
40
20
ppm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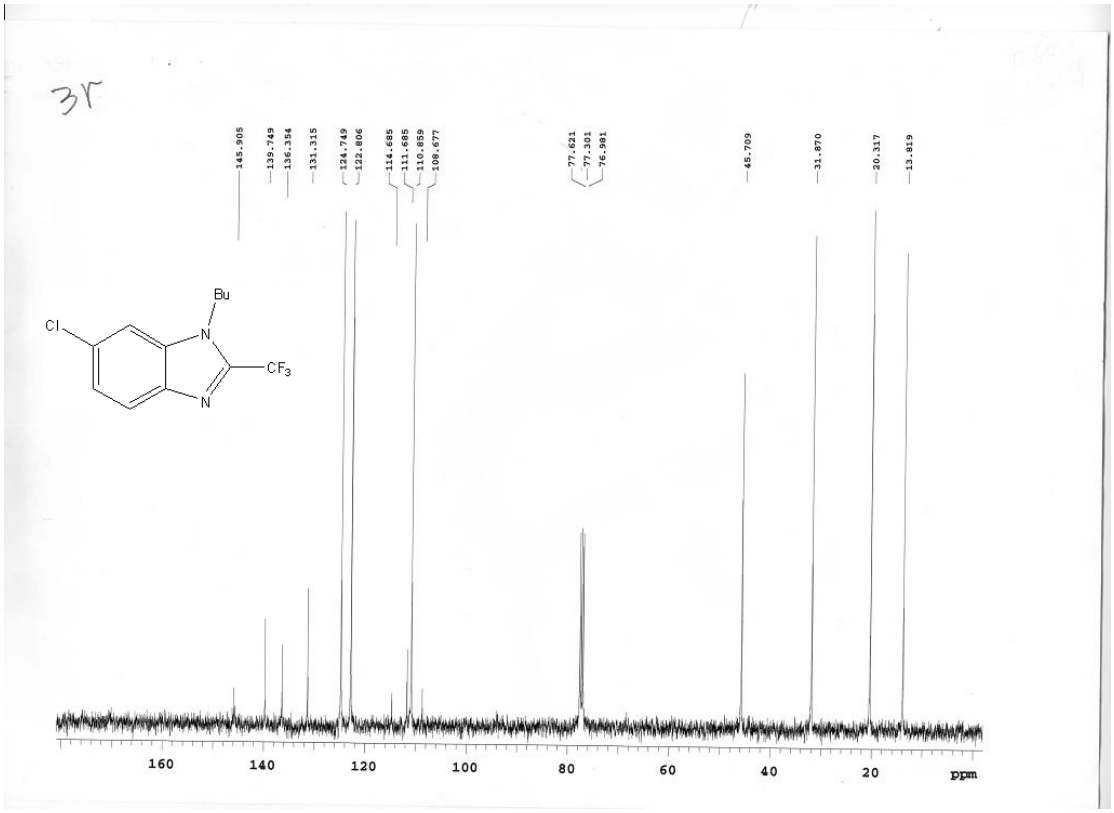
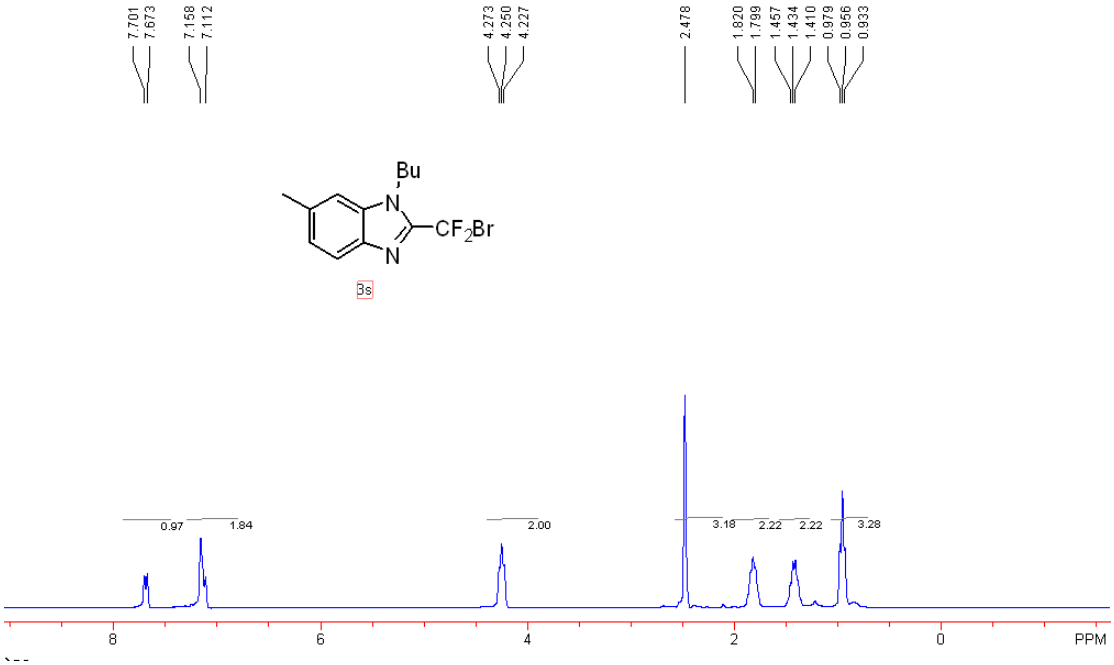
7.386
7.380
7.302
7.296
7.290
7.284
7.275
7.267
7.261
4.286
4.258
4.232
1.851
1.832
1.805
1.445
1.419
0.997
0.984
0.972
0.959
0.947
0.037
0.034
0.026
-0.017
-0.029
-0.038
Bu
Cl
N
CF2Br
N
3r
4.92
0.96
2.00
2.41
2.13
2.92
8
6
4
2
0
PPM


3r
145.905
139.749
136.354
131.315
124.749
122.806
114.685
111.685
110.859
108.677
77.621
77.301
76.981
45.709
31.870
20.317
13.819
Bu
Cl
N
CF3
N
160
140
120
100
80
60
40
20
ppm


7.701
7.673
7.158
7.112
4.273
4.250
4.227
2.478
1.820
1.799
1.457
1.434
1.410
0.979
0.956
0.933
Bu
N
CF2Br
N
3s
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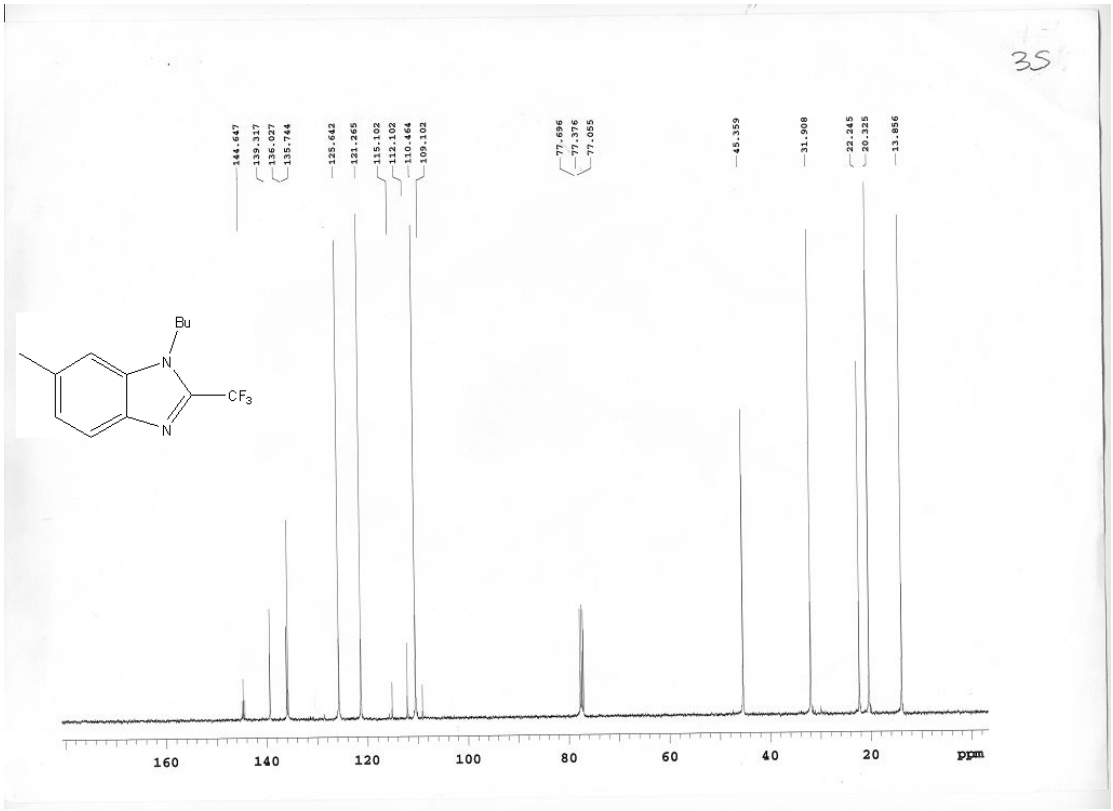
1.84
2.00
3.18
2.22
2.22
3.28
8
6
4
2
0
PPM


3S
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136.027
135.744
125.642
121.265
115.102
112.102
110.464
109.102
77.696
77.376
77.055
45.359
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22.245
20.325
13.856
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N
CF3
N
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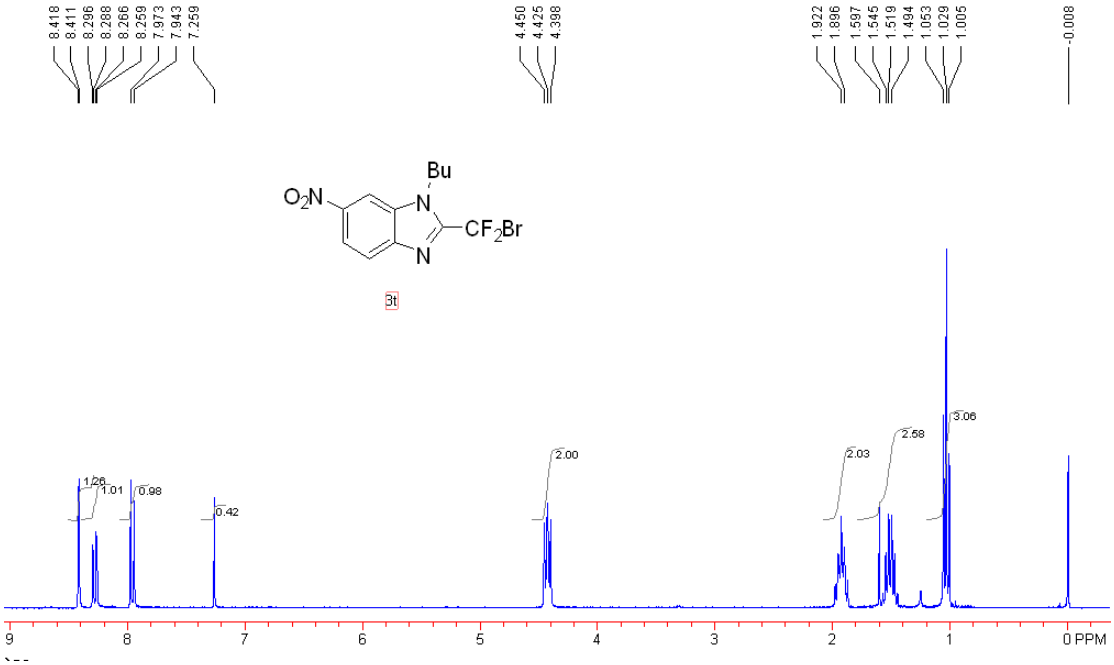
140
120
100
80
60
40
20
ppm


8.418
8.411
8.296
8.288
8.266
8.259
7.973
7.943
7.259
4.450
4.425
4.398
1.922
1.896
1.597
1.545
1.519
1.494
1.053
1.029
1.005
-0.008
Bu
O2N
N
CF2Br
N
3t
1.26
1.01
0.98
0.42
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2.03
2.58
3.06
9
8
7
6
5
4
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2
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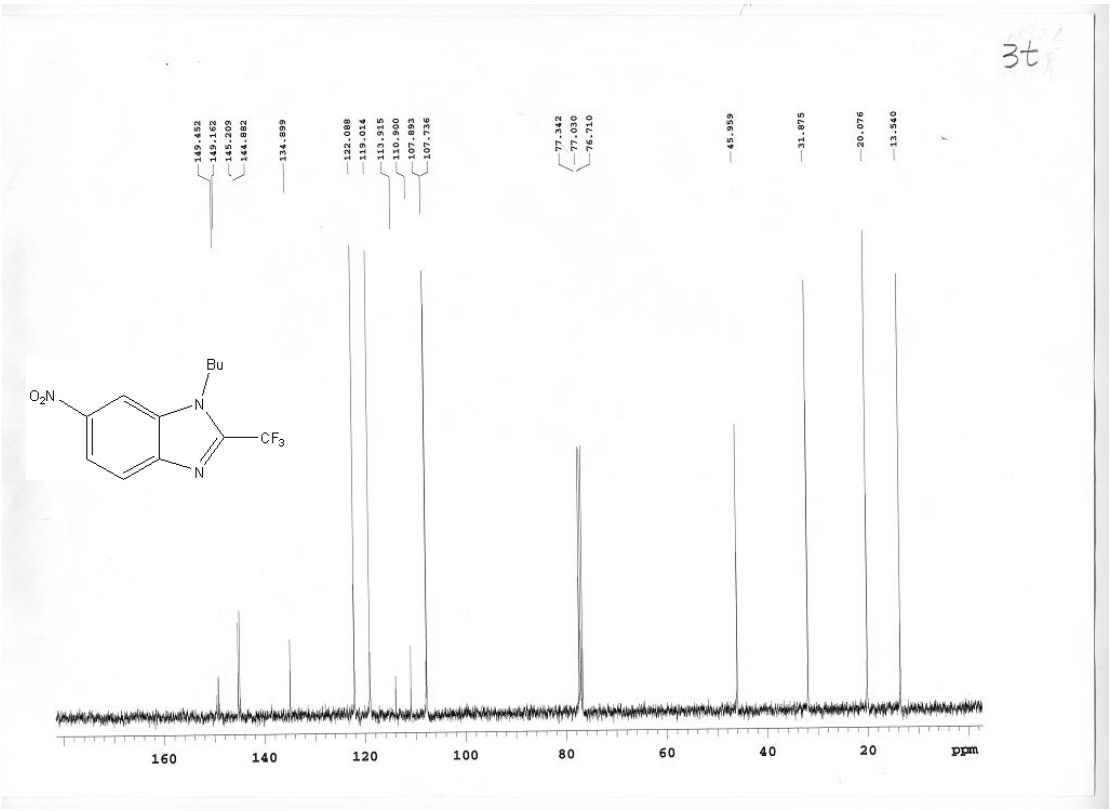
0 PPM


3t
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145.209
144.882
134.899
122.088
119.014
113.915
110.900
107.893
107.736
77.342
77.030
76.710
45.959
31.875
20.076
13.540
Bu
N
O_2N
CF_3
N
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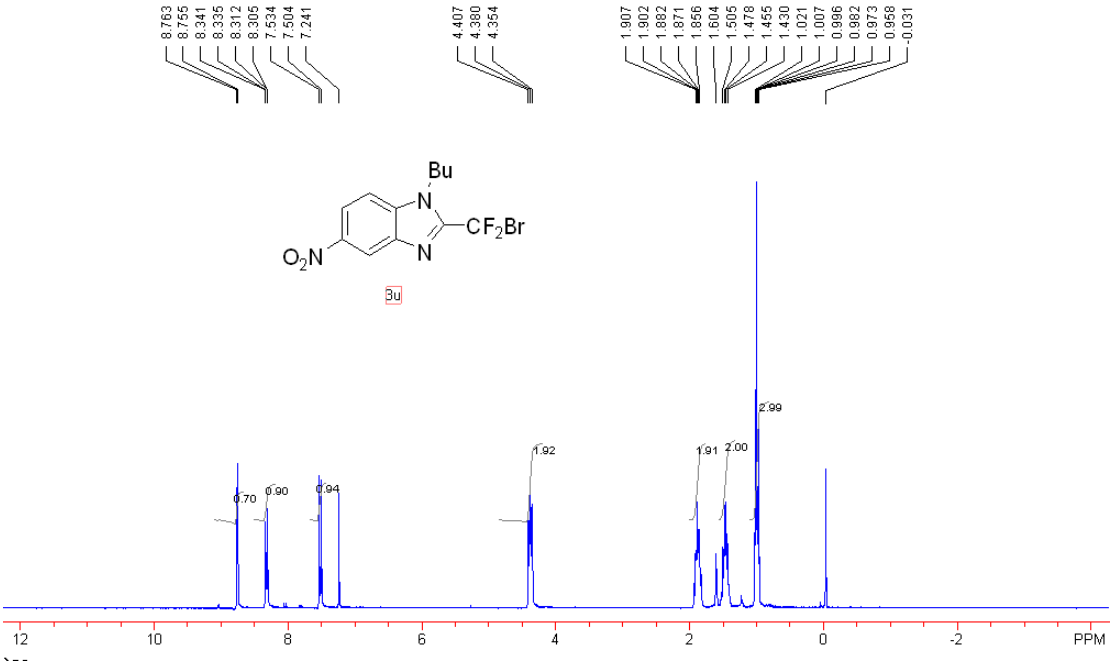
140
120
100
80
60
40
20
ppm


8.763
8.755
8.341
8.335
8.312
8.305
7.534
7.504
7.241
4.407
4.380
4.354
1.907
1.902
1.882
1.871
1.856
1.604
1.505
1.478
1.455
1.430
1.021
1.007
0.996
0.982
0.973
0.958
-0.031
Bu
N
CF_2Br
O_2N
N
3u
0.70
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10
8
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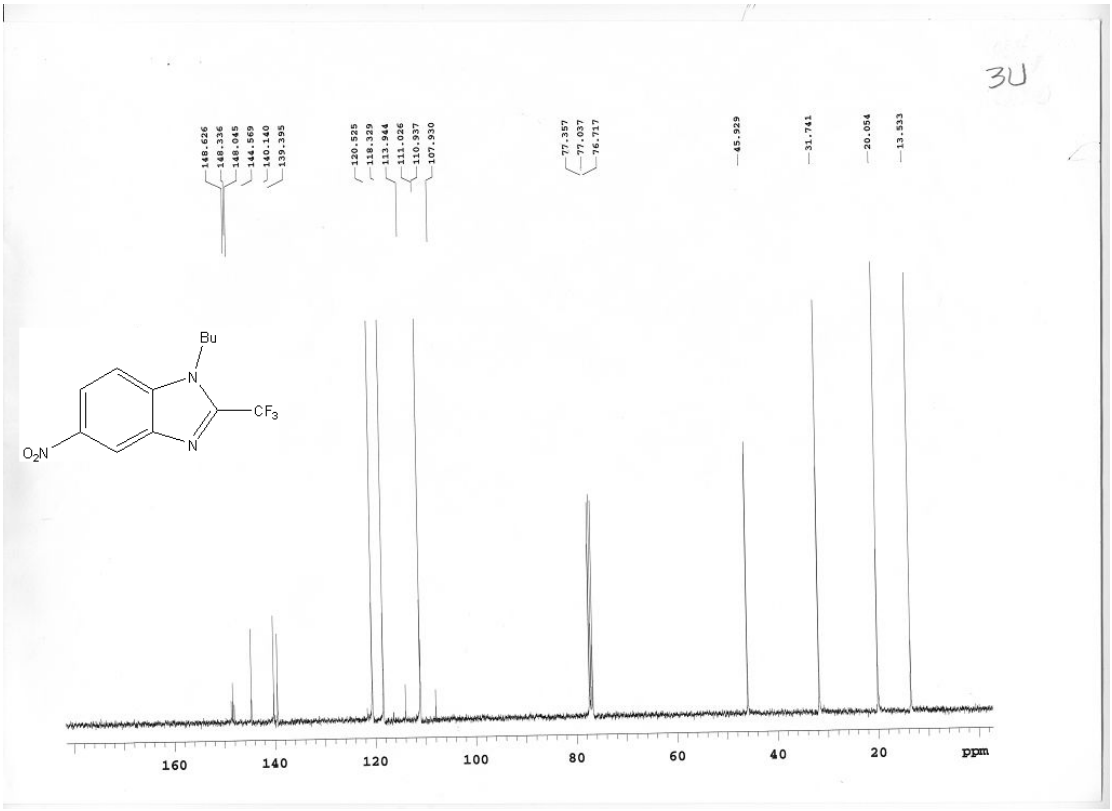
PPM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148.626
148.336
148.045
144.569
140.140
139.395
120.525
118.329
113.944
111.026
110.937
107.930
77.357
77.037
76.717
45.929
31.741
20.054
13.533
Bu
N
CF3
O2N
N
160
140
120
100
80
60
40
20
ppm