Supporting Information

Highly efficient catalyst-free protocol for C-H bond activation: sulfamidation of alkyl aromatics and aldehydes

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CONTENTS

General Remarks

All reagents and starting materials were purchased from commercial sources. Solvents were dried before use. ^{1}H NMR and ^{13}C NMR spectra were recorded in Bruker Ultrashield 300 NMR spectrometer. Chemical shifts are given in δ units relative to the tetramethylsilane (TMS) signal as an internal reference in $CDCl_3$. Coupling constants (*J*) are reported in hertz. Mass spectra (ESI-MS) were recorded in Water ZQ-4000 mass spectrometer. Elemental analysis was carried out using Perkin-Elmer elemental analyzer. IR spectra were recorded in IR Affinity-1 (SHIMADZU) spectrometer.

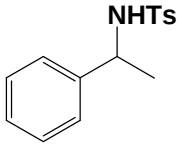
Preparation of *N*,*N*-dibromo-*p*-toluene sulfonamide ($TsNBr_2$)

The reagent *N*,*N*-dibromo-*p*-toluene sulfonamide was prepared from chloramine-T.$3H_2O$ by following literature procedure[1] as follows.

Bromine (2 ml) was added drop wise to a solution of chloramine-T.$3H_2O$ (10 g) in water (200 ml) with constant stirring. The golden yellow precipitate of *N*,*N*-dibromo-*p*-toluene sulfonamide was filtered under suction, washed with water and dried in a desiccator over P_2O_5 for 24 h.

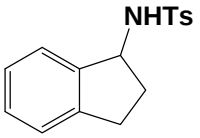
SPECTRAL DATA

4-Methyl-*N*-(1-phenylethyl)benzenesulfonamide (1b) [2]



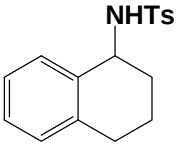
White solid; mp. 78-80 °C (lit[2] 77-79 °C); IR (KBr, cm^{-1}) : 3251, 1593, 1492, 1435, 1323, 1157, 1083; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.62 (d, *J*=9 Hz, 2H), 7.18-7.10 (m, 7H), 5.31-5.25 (br, 1H), 4.48-4.43 (m, 1H), 2.38 (s, 3H), 1.41 (d, *J*=6 Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.1, 142.1, 137.6, 129.4, 128.5, 127.4, 127.1, 126.1, 53.6, 23.6, 21.5.

***N*-[1-(2,3-Dihydro-1*H*-inden-1-yl)ethyl]-4-methylbenzenesulfonamide (2b)**[2,3]



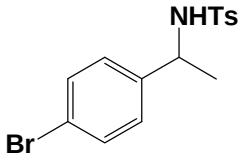
White solid; mp. 141-143 °C (lit[3] 141-142 °C); IR (KBr, cm^{-1}) : 3263, 1597, 1454, 1423, 1315, 1161, 1091, 1064; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83 (d, *J*=9 Hz, 2H), 7.34 (d, *J*=6 Hz, 2H), 7.21-7.09 (m, 4H), 4.87-4.81 (m, 2H), 2.95-2.85 (m, 1H), 2.79-2.68 (m, 1H), 2.46 (s, 3H), 2.37-2.27 (m, 1H), 1.78-1.73 (m, 1H); ^{13}C NMR (75MHz, $CDCl_3$): 143.4, 142.8, 142.0, 138.2, 129.7, 128.2, 127.1, 126.8, 124.8, 124.1, 58.7, 34.6, 29.9, 21.5.

4-Methyl-*N*-[1-(1,2,3,4-tetrahydronaphthalen-1-yl)ethyl]benzenesulfonamide (3b)[4]



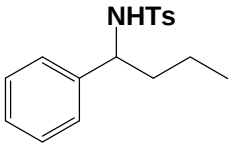
White solid; mp. 135-137 °C; IR (KBr, cm^{-1}): 3251, 2947, 2924, 1593, 1442, 1319, 1157, 1083 ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83 (d, *J*=9 Hz, 2H), 7.35 (d, *J*=6 Hz, 2H), 7.18-7.03 (m, 3H), 6.94 (d, *J*=9 Hz, 1H), 4.75-4.73 (br, 1H), 4.46 (br, 1H), 2.81-2.61 (m, 2H), 2.47 (s, 3H), 1.83-1.67 (m, 4H);^{13}C NMR (75MHz, $CDCl_3$): 143.4, 138.4, 137.5, 135.6, 129.7, 129.2, 128.7, 127.6, 127.1, 126.2, 51.8, 30.7, 28.8, 21.6, 19.1.

_N_-[1-(4-Bromophenyl)ethyl]-4-methylbenzenesulfonamide (4b)[5,6]



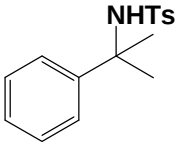
White solid; mp. 142-144 °C; IR (KBr, cm^{-1}) : 3250, 2972, 2925, 1600, 1447, 1334, 1162, 1089, 1016; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.57 (d, *J*=9 Hz, 2H), 7.27 (d, *J*=9 Hz, 2H), 7.17 (d, *J*=9 Hz, 2H), 6.96 (d, *J*=9 Hz, 2H), 5.24 (d, *J*=6 Hz, 1H), 4.44-4.40 (m, 1H), 2.40 (s, 3H), 1.37 (d, *J*=9 Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.4, 141.1, 137.4, 131.5, 129.5, 128.0, 127.1, 121.3, 53.1, 23.4, 21.5.

4-Methyl-_N_-(1-phenylbutyl)benzenesulfonamide (5b)[5]



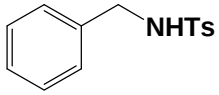
White solid; mp. 80-82 °C (lit[5] 82-83 °C); IR (KBr, cm^{-1}): 3774, 3575, 3277, 2925, 2866, 1600, 1454, 1321, 1162, 1096, 1049; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.53 (d, *J*=9 Hz, 2H), 7.14-7.01 (m, 7H), 5.19 (br, 1H), 4.30-4.23 (m, 1H), 2.35 (s, 3H), 1.71-1.62 (m, 2H), 1.30-1.15 (m, 2H), 0.82 (t, *J*=6 Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 142.8, 141.0, 137.6, 129.2, 128.3, 127.2, 127.0, 126.4, 58.1, 39.7, 21.4, 19.1, 13.5.

4-Methyl-_N_-(2-phenylpropan-2-yl)benzenesulfonamide (7b)[7,8]



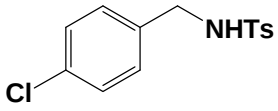
White solid; mp. 137-139 °C (lit[7] 138-141 °C); IR (KBr, cm^{-1}): 3267, 2981, 1597, 1492, 1431, 1319, 1149, 1087, 979; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.57 (d, *J*=9 Hz, 2H), 7.33-7.30 (m, 2H), 7.20-7.14 (m, 5H), 5.47 (s, 1H), 2.39 (s, 3H), 1.63 (s, 6H); ^{13}C NMR (75MHz, $CDCl_3$): 145.2, 142.7, 139. 8, 129.3, 128.2, 127.0, 126.9, 125.5, 58.6, 29.8, 21.5.

_N_-Benzyl-4-methylbenzenesulfonamide (8b)[2]



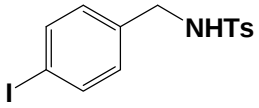
White solid; m.p. 111-113 °C (lit[2] 111-112 °C); IR (KBr, cm^{-1}): 3267, 1597, 1492, 1454, 1323, 1161, 1087, 1056; ^1H NMR (300 MHz, $CDCl_3$): δ 7.74 (d, *J*=9 Hz, 2H), 7.29-7.20 (m, 7H), 5.22 (br, 1H), 4.09 (d, *J*=6 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.3, 136.7, 136.3, 129.6, 128.5, 127.8, 127.6, 127.0, 47.0, 21.4.

_N_-(4-Chlorobenzyl)-4-methylbenzenesulfonamide (9b)



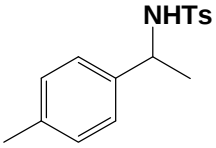
White solid; m.p. 101-103 °C ; IR (KBr, cm^{-1}): 3237, 1606, 1447, 1321, 1162, 1089; ^1H NMR (300 MHz, $CDCl_3$): δ 7.72 (d, *J*=6 Hz, 2H), 7.28 (d, *J*=9 Hz, 2H), 7.22 (d, *J*=6 Hz, 2H), 7.12 (d, *J*=9 Hz, 2H), 5.08 (t, *J*= 6 Hz, 1H), 4.07 (d, *J*=9 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.6, 136.7, 134.8, 133.6, 129.7, 129.2, 128.7, 127.1, 46.5, 21.5; ESI-MS (m/z, %): m/z 318 [$M+Na^+$, 100] ; Anal.calcd. for $C_{14}H_{14}ClNO_2S$ (%): C, 56.85; H, 4.77; N, 4.74. Found: C, 56.79; H, 4.82; N, 4.80.

_N_-(4-Iodobenzyl)-4-methylbenzenesulfonamide (10b)



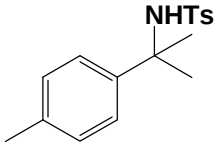
White solid; m.p. 135-137 °C ; IR (KBr, cm^{-1}) : 3257, 2938, 1599, 1427, 1327, 1155, 1095, 1015;^1H NMR (300 MHz, $CDCl_3$): δ7.71 (d, *J*=9 Hz, 2H), 7.57 (d, *J*=9 Hz, 2H), 7.29 (d, *J*=9 Hz, 2H), 6.94 (d, *J*=9 Hz, 2H), 4.94-5.02 (br, 1H), 4.06 (d, *J*=6 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.6, 137.6, 136.7, 136.0, 129.7, 127.1, 93.3, 46.6, 21.5; ESI-MS (m/z, %): 413[$M+3+Na^+$, 100], 261[M-I, 5], 256[(M-Ts)+1+ Na^+, 9]; Anal.calcd. for $C_{14}H_{14}INO_2S$ (%): C, 43.42; H, 3.64; N, 3.62. Found: C, 43.34; H, 3.68; N, 3.69.

4-Methyl-*N*-[1-(4-methylphenyl)ethyl]benzenesulfonamide (11b)[7]



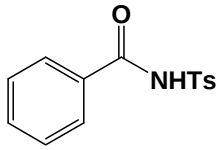
White solid; mp. 110-112 °C (lit[7] 108-111 °C); IR (KBr, cm^{-1}): 3251, 1597, 1512, 1435, 1375, 1327, 1083, 1022; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.63 (d, *J*=9 Hz, 2H), 7.19 (d, *J*=9 Hz, 2H), 7.00-6.97 (s, 4H), 4.89-4.85 (br, 1H), 4.42 (br, 1H), 2.40 (s, 3H), 2.28 (s, 3H), 1.41 (d, *J*=6 Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$): 143.0, 139.0, 137.6, 137.1, 129.4, 129.1, 127.1, 126.0, 53.3, 23.4, 21.4, 20.9.

4-Methyl-*N*-[2-(4-methylphenyl)propan-2-yl]benzenesulfonamide (12b)[12]



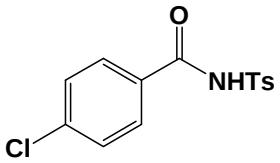
White solid; m.p. 116-117 °C; IR (KBr, cm^{-1}): 3263, 2978, 2924, 1597, 1512, 1431, 1381, 1323, 1149, 1091, 979; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (d, *J*=9 Hz, 2H), 7.20-7.14 (m, 4H), 6.98 (d, *J*=9 Hz, 2H), 5.15 (s, 1H), 2.40 (s, 3H), 2.29 (s, 3H), 1.61 (s, 6H); ^{13}C NMR (75MHz, $CDCl_3$): 142.6, 142.2, 139.8, 136.7, 129.2, 128.8, 127.0, 125.4, 58.4, 29.8, 21.5, 20.9.

N-tosylbenzamide (13b)[9]



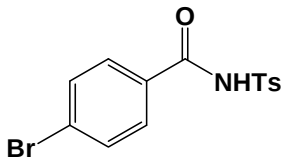
White solid; mp: 85-87 °C; IR (KBr, cm^{-1}): 3259, 1705, 1597, 1423, 1334, 1165, 1060; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.0 (d, *J* =7.9 Hz, 2H), 7.84 (d, *J* =8.3 Hz, 2H), 7.49 (t, *J* =7.5 Hz, 1H), 7.41-7.22 (m, 4H), 5.49 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.3, 144.8, 135.7, 133.2, 129.5, 129.4, 128.6, 128.3, 128.0, 21.5.

4-chloro-N-tosylbenzamide (14b)[10]



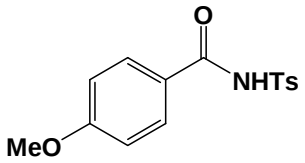
White solid; mp: 130-133 °C; IR (KBr, cm^{-1}): 3257, 1698, 1592, 1433, 1320, 1161, 1088; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.28 (br, 1H), 8.02 (d, *J* = 7.9 Hz, 2H), 7.86-7.68 (m, 2H), 7.48-7.28 (m, 4H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.5, 145.5, 140.0, 135.1, 129.8, 129.7, 129.2, 128.7, 126.4, 21.7.

4-bromo-N-tosylbenzamide (15b)[11]



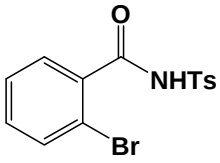
White solid; mp: 115-117 °C; IR (KBr,cm^{-1}): 3259, 1701, 1589, 1527, 1442, 1330, 1161, 1072; ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.85 (d, *J* = 7.9 Hz, 2H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.36 (s, 3H), 1.17 (br, 1H); ^{13}C NMR (75 MHz, $CDCl_3$ + DMSO-d_6): δ 164.2, 143.9, 136.1, 131.1, 130.2, 129.9, 128.9, 127.7, 127.3, 21.1.

4-methoxy-N-tosylbenzamide (16b) [9]



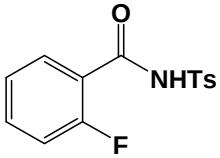
White solid; mp: 142-144 °C; IR (KBr, cm^{-1}): 3246, 1666, 1604, 1438, 1342, 1257, 1165, 1080; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.09 (br, 1H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 3.84 (s, 3H), 2.44 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 163.7, 163.6, 145.1, 135.6, 129.9, 129.6, 128.7, 123.3, 114.1, 55.5, 21.9.

2-bromo-N-tosylbenzamide (17b)



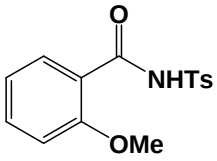
Light yellowish oil; IR (neat, cm^{-1}): 3383, 1719, 1600, 1427, 1354, 1169, 1089; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.54-7.48 (m, 2H), 7.36-7.26 (m, 3H), 5.21 (s, 1H), 2.44(s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 164.5, 145.3, 134.4, 133.6, 132.6, 130.0, 129.5, 128.6, 127.7, 126.3, 21.7; MS (ES) m/z 376 [M+Na$^+$, 100], 378[M+2+Na$^+$, 100]; Anal.calcd. for $C_{14}H_{12}BrNO_3S$ (%): C, 47.47; H, 3.41; N, 3.95; Found: C, 47.52; H, 3.35; N, 4.01;

2-fluro-N-tosylbenzamide (18b)



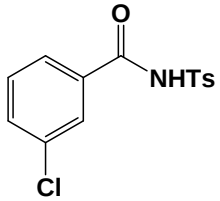
White solid; mp: 97-99 °C; IR (KBr, cm^{-1}): 3250, 2925, 1699, 1613, 1454, 1348, 1169, 1082; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.04 (br, 1H), 8.05-7.94 (m, 3H), 7.58-7.54 (m, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.30-7.22 (m, 1H), 7.18-7.11 (m, 1H), 2.43 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 162.4, 160.4, 159.1, 145.2, 135.5, 135.4, 132.3, 129.5, 128.7, 125.3, 125.2, 118.7, 118.5, 116.5, 116.2, 21.7; MS (ES) m/z 316 [M+Na$^+$, 100], 317[M+1+Na$^+$, 20]; Anal.calcd. for $C_{14}H_{12}FNO_3S$ (%): C, 57.33; H, 4.12; N, 4.78; Found: C, 57.25; H, 4.15; N, 4.75.

2-methoxy -N-tosylbenzamide (19b)



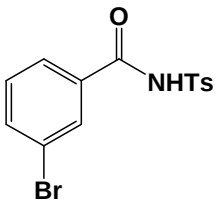
White solid; mp: 92-94 °C; IR (KBr, cm^{-1}):3232 , 1685, 1597, 1446, 1423, 1327, 1250, 1149, 1091, 1014; ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.4 (s, 1H), 8.06-8.02 (m, 3H), 7.54-7.48 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.06-6.98 (m, 2H), 4.03 (s, 3H), 2.41 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 162.3, 157.7, 144.8, 135.8, 135.1, 132.5, 129.4, 128.5, 121.6, 118.6, 111.6, 56.4, 21.6; MS (ES) m/z 328 [$M+Na^+$, 100]; Anal.calcd. for $C_{15}H_{15}NO_4S$ (%): C, 59.00; H, 4.95; N, 4.59; Found: C, 59.15; H, 5.00; N, 4.50.

3-chloro-N-tosylbenzamide (20b)



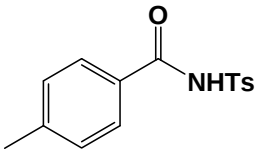
White solid; IR (KBr, cm^{-1}): 3275, 1688, 1597, 1423, 1324, 1175, 1082; ^{1}H NMR (300 MHz, DMSO-d_6): δ 7.85 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.9 Hz, 2H), 7.42-7.39 (m, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.9 Hz, 2H), 2.30 (s, 3H), 1.22 (s, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): δ 168.0, 143.1, 141.5, 139.5, 132.2, 129.5, 129.3, 128.1, 128.0, 126.8, 126.7, 20.8; MS (ES) m/z 332 [$M+Na^+$, 100]; Anal.calcd. for $C_{14}H_{12}ClNO_3S$ (%): C, 54.28; H, 3.90; N, 4.52; Found: C, 54.33; H, 3.85; N, 4.50;

3-bromo-N-tosylbenzamide (21b)



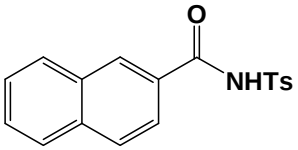
White solid; mp: 99-101 °C; IR (KBr, cm^{-1}): 3286, 1697, 1589, 1419, 1334, 1165, 1072; ^{1}HNMR (300 MHz, $CDCl_3$): δ 8.05 (s, 1H), 7.93-7.91 (m, 2H), 7.81 (d, *J* = 8.7 Hz, 1H), 7.74-7.69 (m, 1H), 7.60-7.46 (m, 1H), 7.29-7.10 (m, 2H), 5.85 (br, 1H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$ +DMSO-d_6): δ 164.7, 144.1, 135.3, 133.9, 131.4, 129.7, 129.2, 129.1, 127.9, 127.1, 125.9, 21.4; MS (ES) m/z 376 [$M+Na^+$, 100], 378 [$M+2+Na^+$, 99]; Anal.calcd. for $C_{14}H_{12}BrNO_3S$ (%): C, 47.47; H, 3.41; N, 3.95; Found: C, 47.44; H, 3.45; N, 4.00.

4-methyl-N-tosylbenzamide (22b) [10]



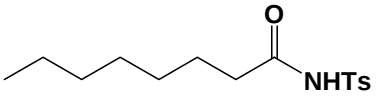
White solid; mp: 92-95 °C; IR (KBr, cm^{-1}): 3259, 1688, 1597, 1438, 1342, 1165, 1080; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.02 (d. *J* = 7.6 Hz, 2H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 2H), 5.22 (br, 1H), 2.41 (s, 3H), 2.36 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 165.1, 144.8, 144.1, 139.0, 135.8, 129.5, 129.4, 128.4, 128.0, 21.6, 21.5.

N-tosyl-2-napthamide (23b)



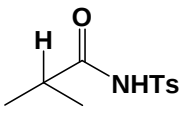
White solid; mp: 106-109 °C; IR (KBr, cm^{-1}): 3259, 1674, 1597, 1477, 1446, 1342, 1165, 1072; ^{1}H NMR (300 MHz, DMSO-d_6): δ 12.61 (br, 1H), 8.56 (s, 1H), 8.06-7.83 (m, 4H), 7.72-7.59 (m, 3H), 7.43-7.29 (m, 3H), 2.37 (s, 3H); ^{13}CNMR (75 MHz, DMSO- d_6): δ 166.9, 143.9, 137.2, 134.8, 131.8, 129.7, 129.5, 129.4, 128.5, 128.1, 127.8, 127.7, 127.0, 124.3, 21.1; MS (ES) m/z 348 [M+Na^+, 100]; Anal.calcd. for $C_{18}H_{15}NO_3S$ (%): C, 66.44; H, 4.65; N, 4.30; Found: C, 66.50; H, 4.70; N, 4.20.

N-tosyloctanamide (24b)



White solid; mp: 70-71 °C; IR (KBr, cm^{-1}): 3305, 2924, 2850, 1728, 1597, 1423, 1334, 1172, 1083; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.22 (br, 1H), 7.94 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 2.43 (s, 3H), 2.24 (t, *J* = 6Hz, 2H), 1.55-1.51 (m, 2H), 1.41-1.23 (m, 8H), 0.85 (t, *J* = 6Hz, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 171.4, 145.0, 135.5, 129.5, 128.2, 36.2, 31.5, 28.8, 28.7, 24.2, 22.5, 21.6, 14.0; MS (ES) m/z 298 [M+H^+, 100]; Anal.calcd. for $C_{15}H_{23}NO_3S$ (%): C, 60.58; H, 7.79; N, 4.71; Found: C, 60.51; H, 7.85; N, 4.68.

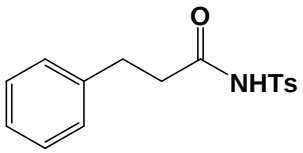
N-tosylisobutyramide (25b) [11]



White solid; mp: 114-115 °C; IR (KBr, cm^{-1}): 3257, 2972, 1739, 1606, 1447, 1328, 1182, 1082; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.86 (br, 1H), 7.95 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H),

2.45 (s, 3H), 1.11 (s, 3H), 1.09 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 174.6, 145.1, 135.4, 129.6, 128.3, 35.6, 21.7, 18.5.

3-phenyl-N-prpanamide (26b)[9]



White solid; mp: 110-112^{0}C; IR (KBr, cm^{-1}): 3124, 1681, 1597, 1458, 1342, 1134, 1087; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.05 (br, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 7.25-7.17 (m, 3H), 7.08-7.05 (m, 2H), 2.87 (t, *J* = 6 Hz, 2H), 2.56 (t, *J* = 6 Hz, 2H), 2.45 (s, 3H); ^{13}CNMR (75 MHz, $CDCl_3$): δ 170.4, 145.1, 135.6, 135.3, 129.6, 128.5, 128.3, 128.2, 126.3, 37.8, 30.2, 21.7.

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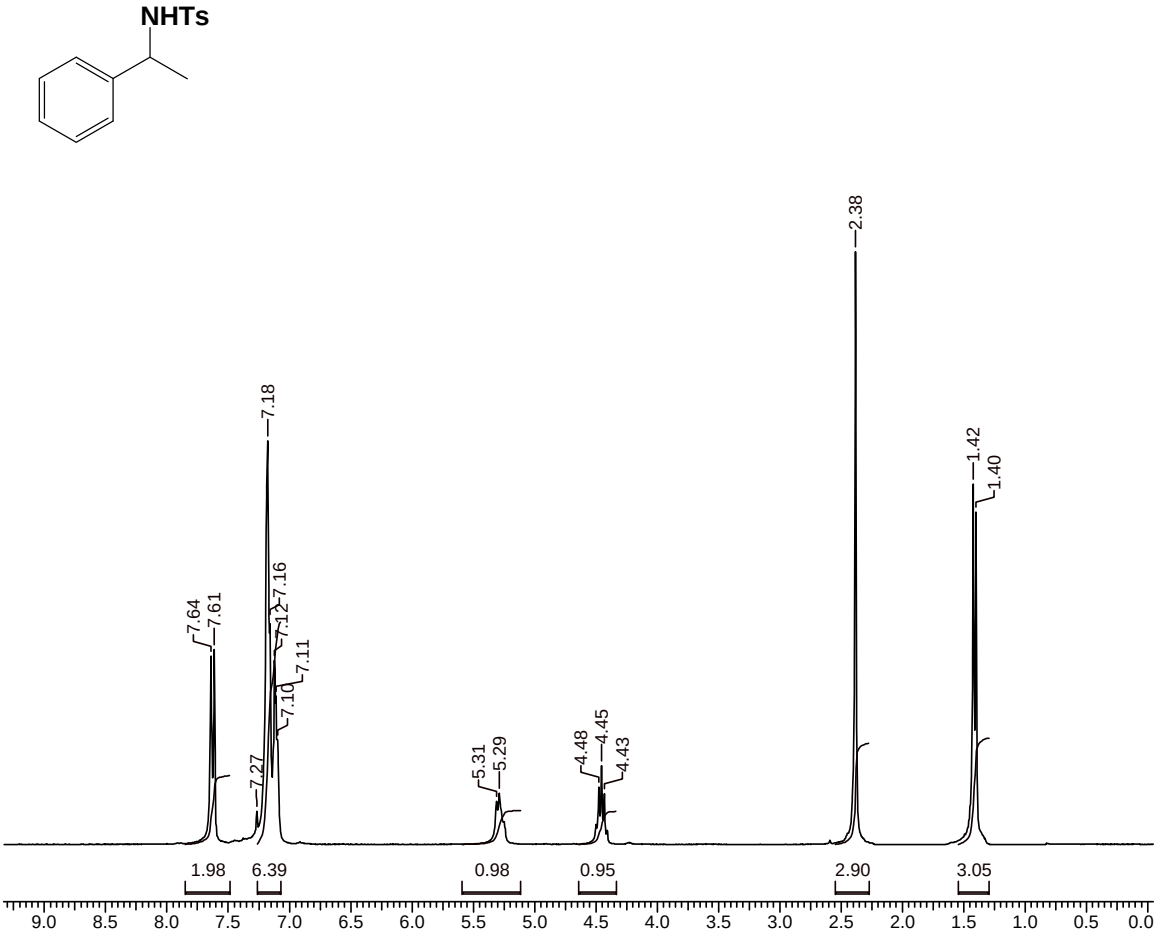
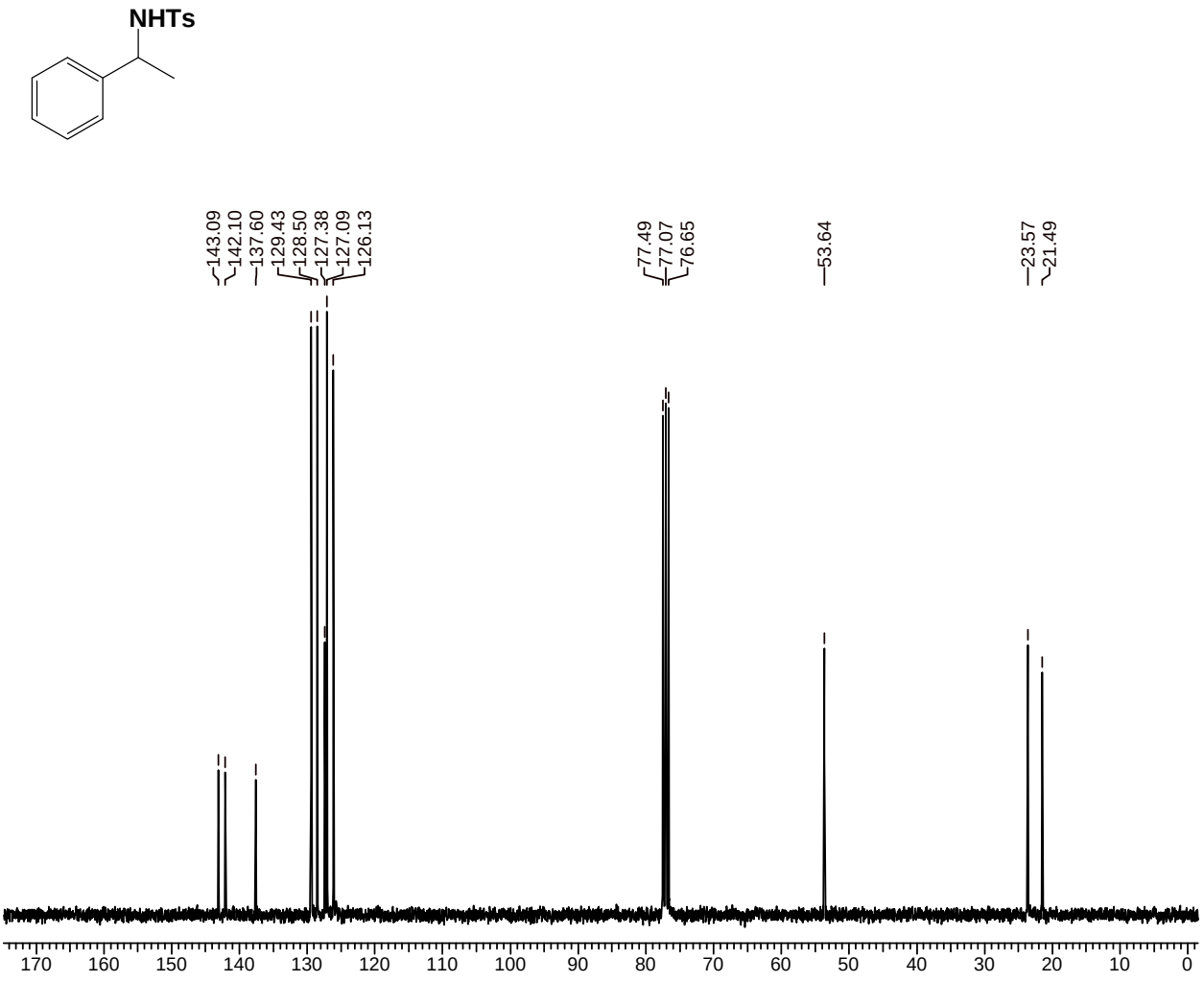
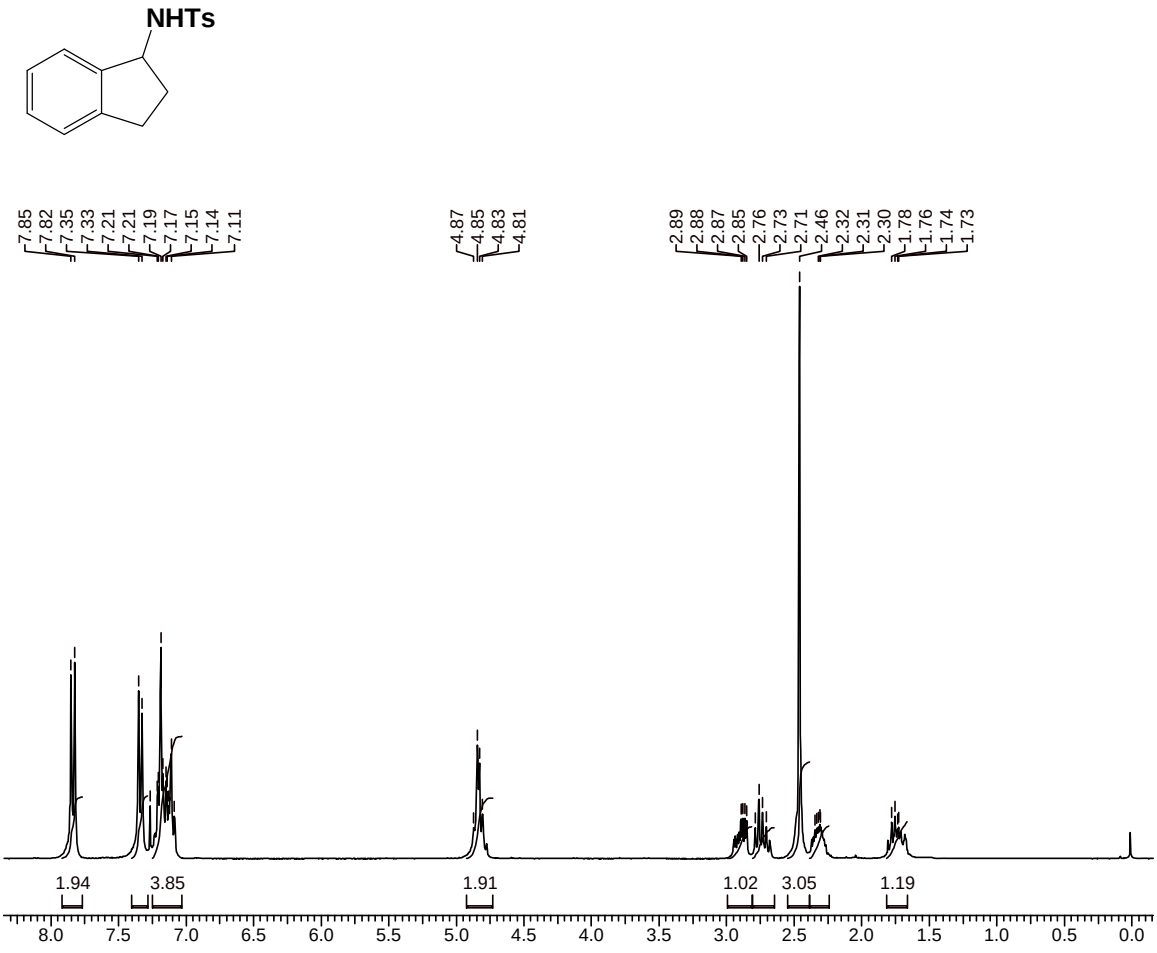
NMR SPECTRA

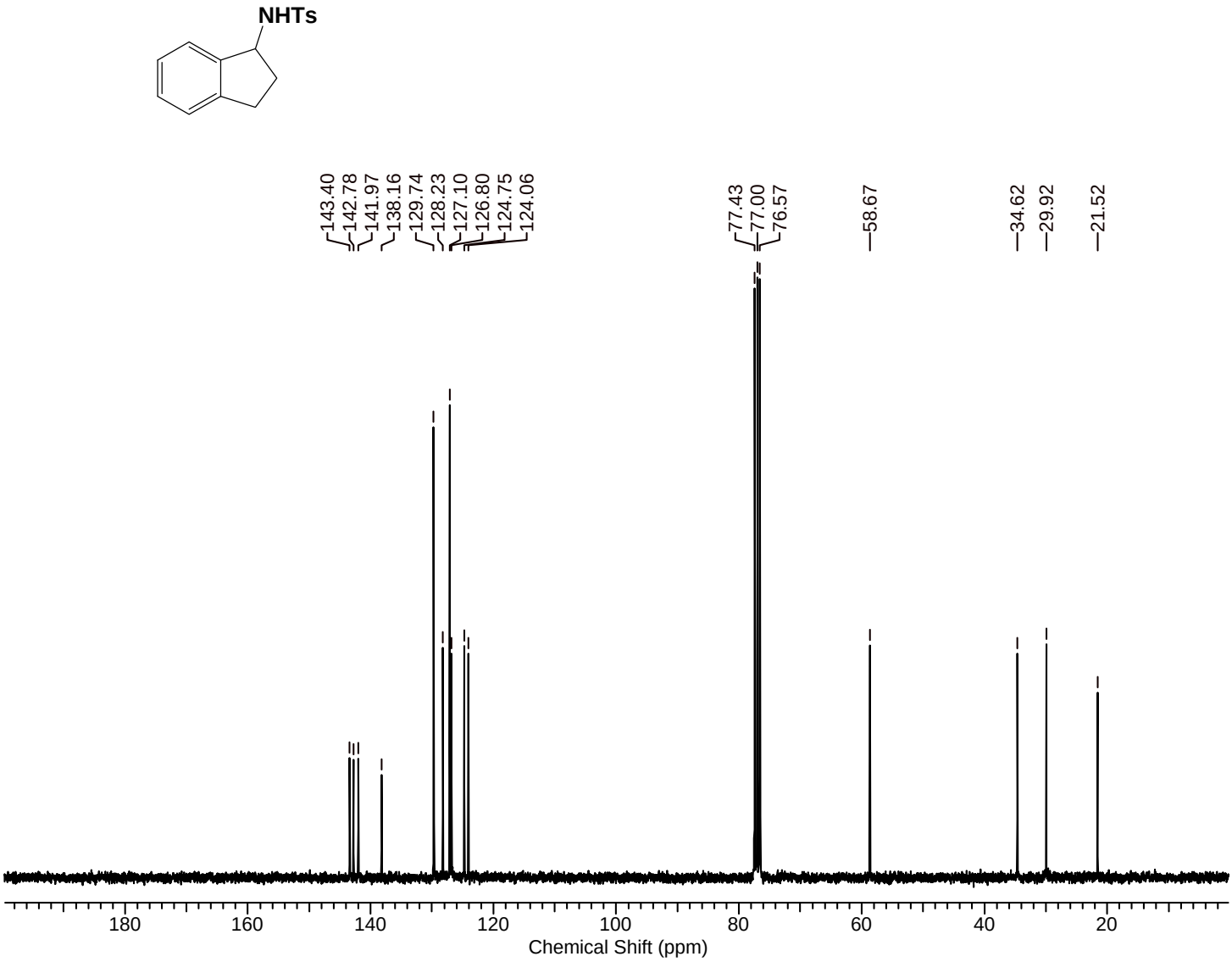
4-Methyl-*N*-(1-phenylethyl)benzenesulfonamide (1b)



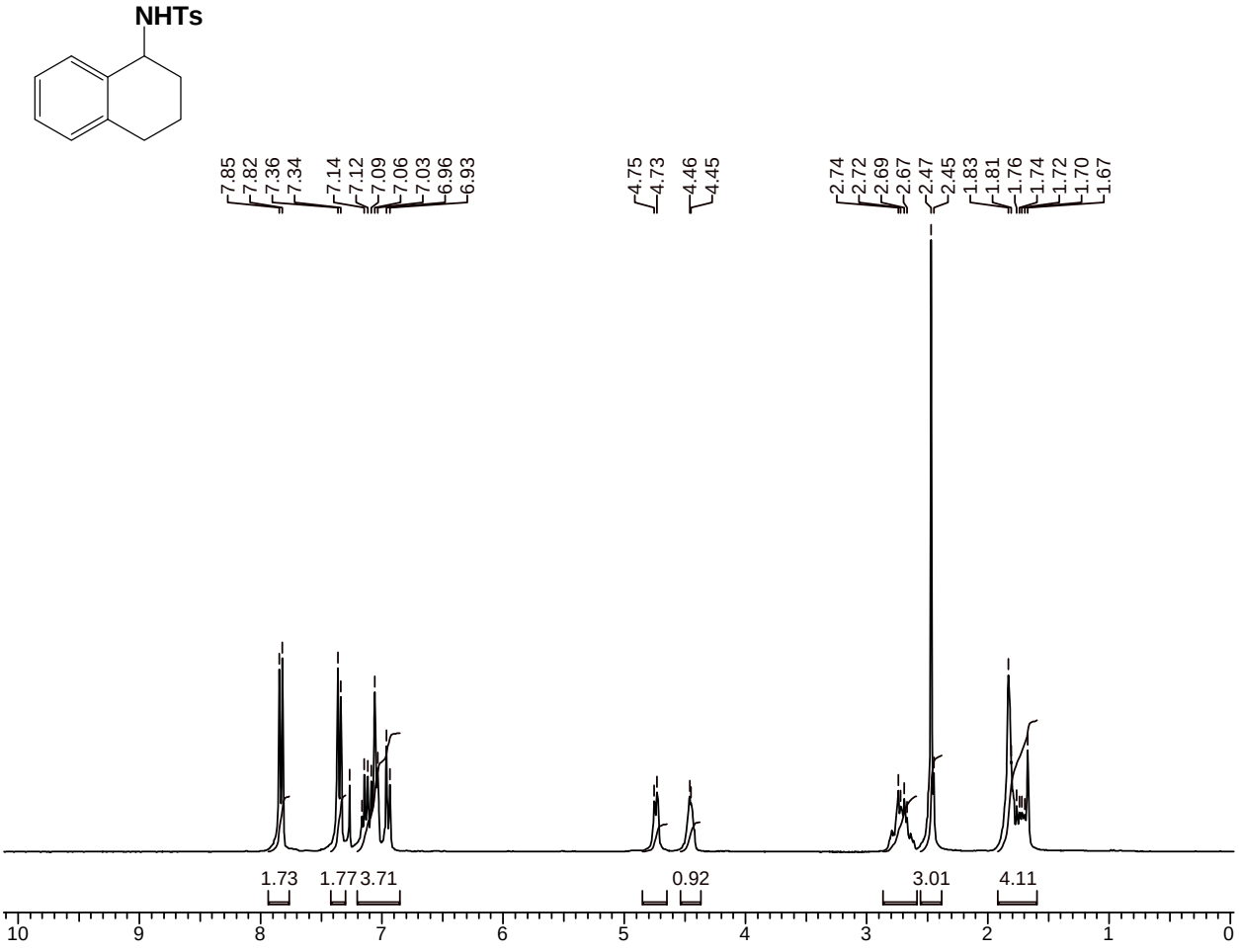


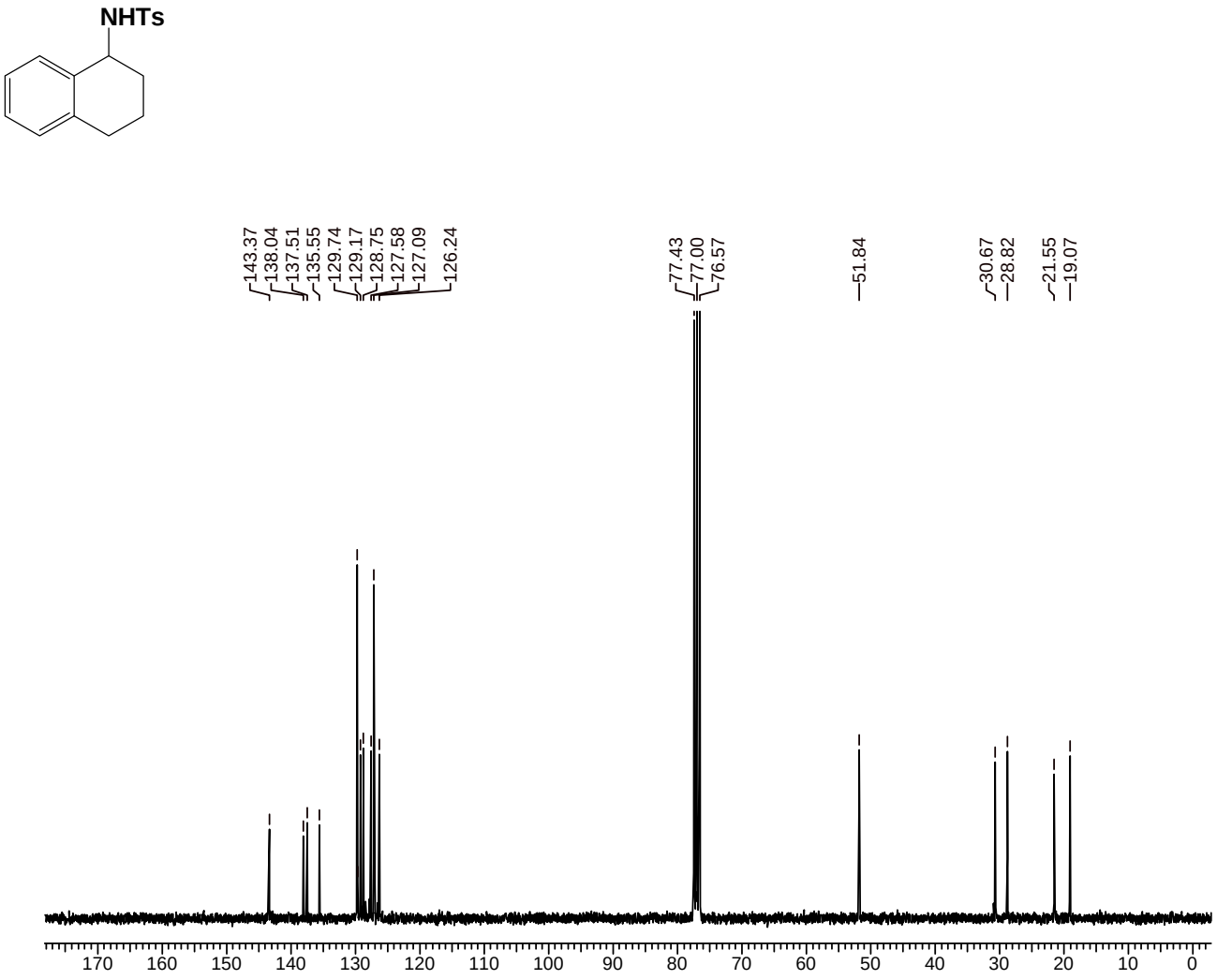
_N_-[1-(2,3-Dihydro-1_H_-inden-1-yl)ethyl]-4-methylbenzenesulfonamide (2b)



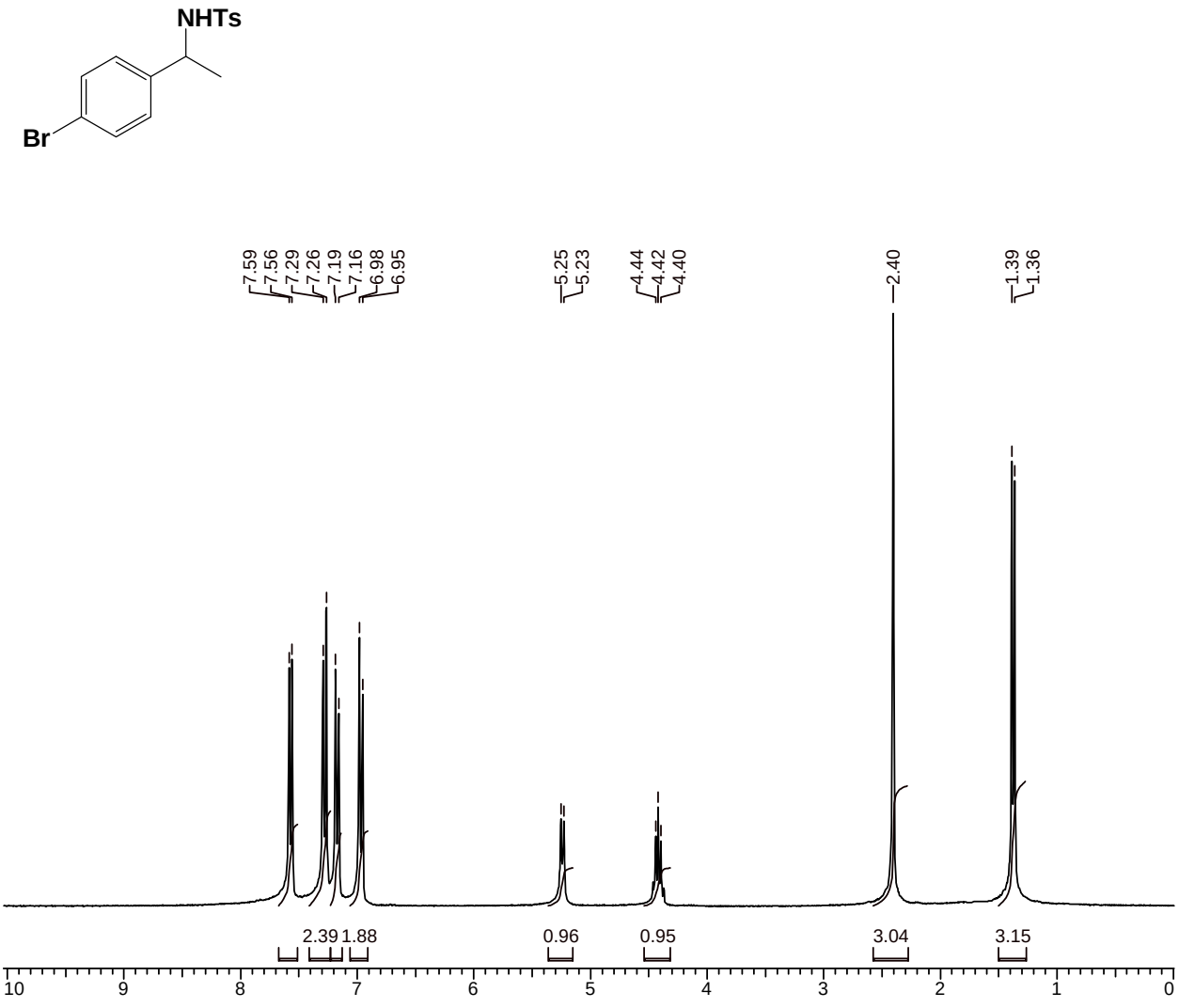


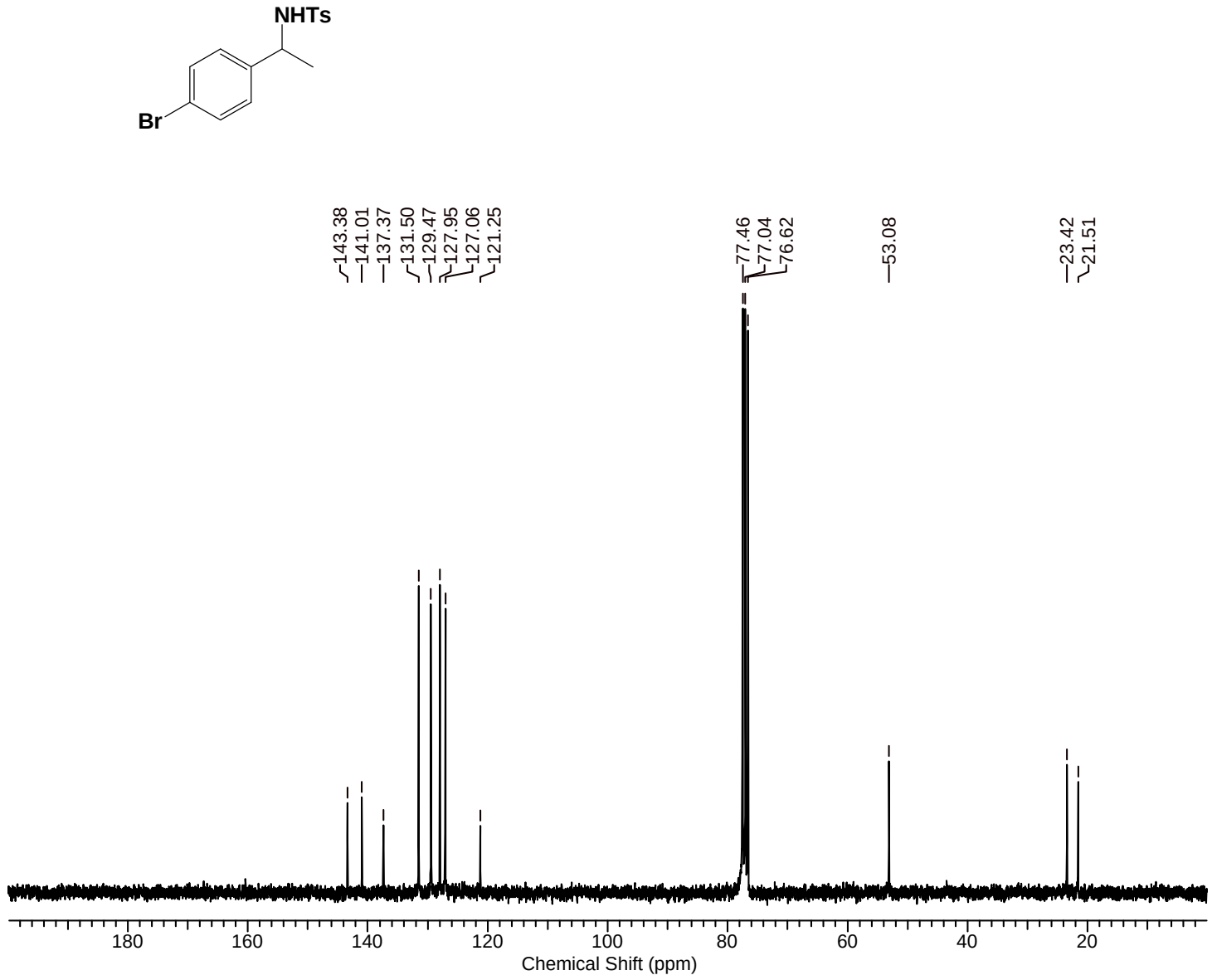
4-Methyl-*N*-[1-(1,2,3,4-tetrahydronaphthalen-1-yl)ethyl]benzenesulfonamide (3b)



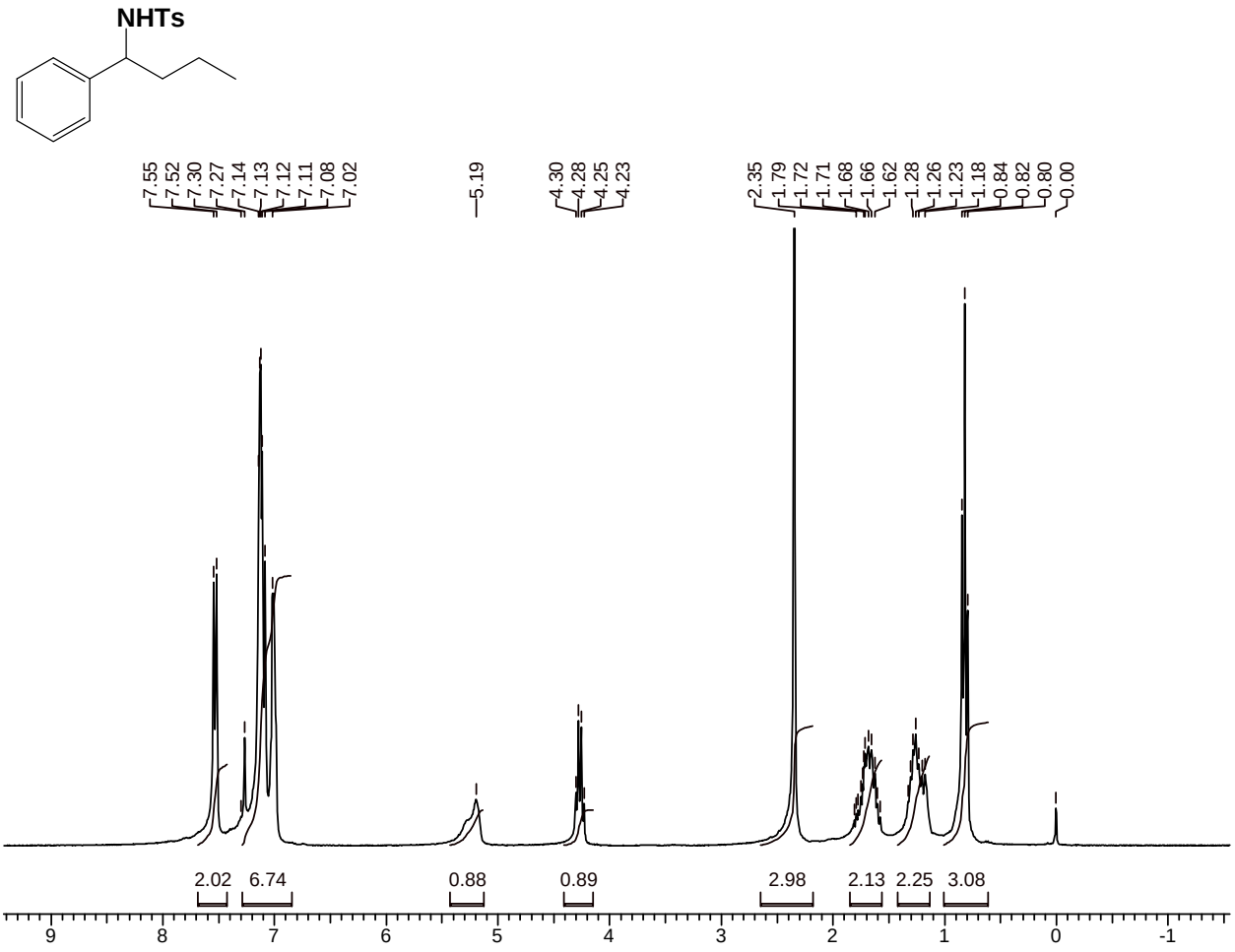


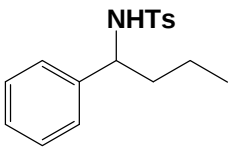
_N_-[1-(4-Bromophenyl)ethyl]-4-methylbenzenesulfonamide (4b)

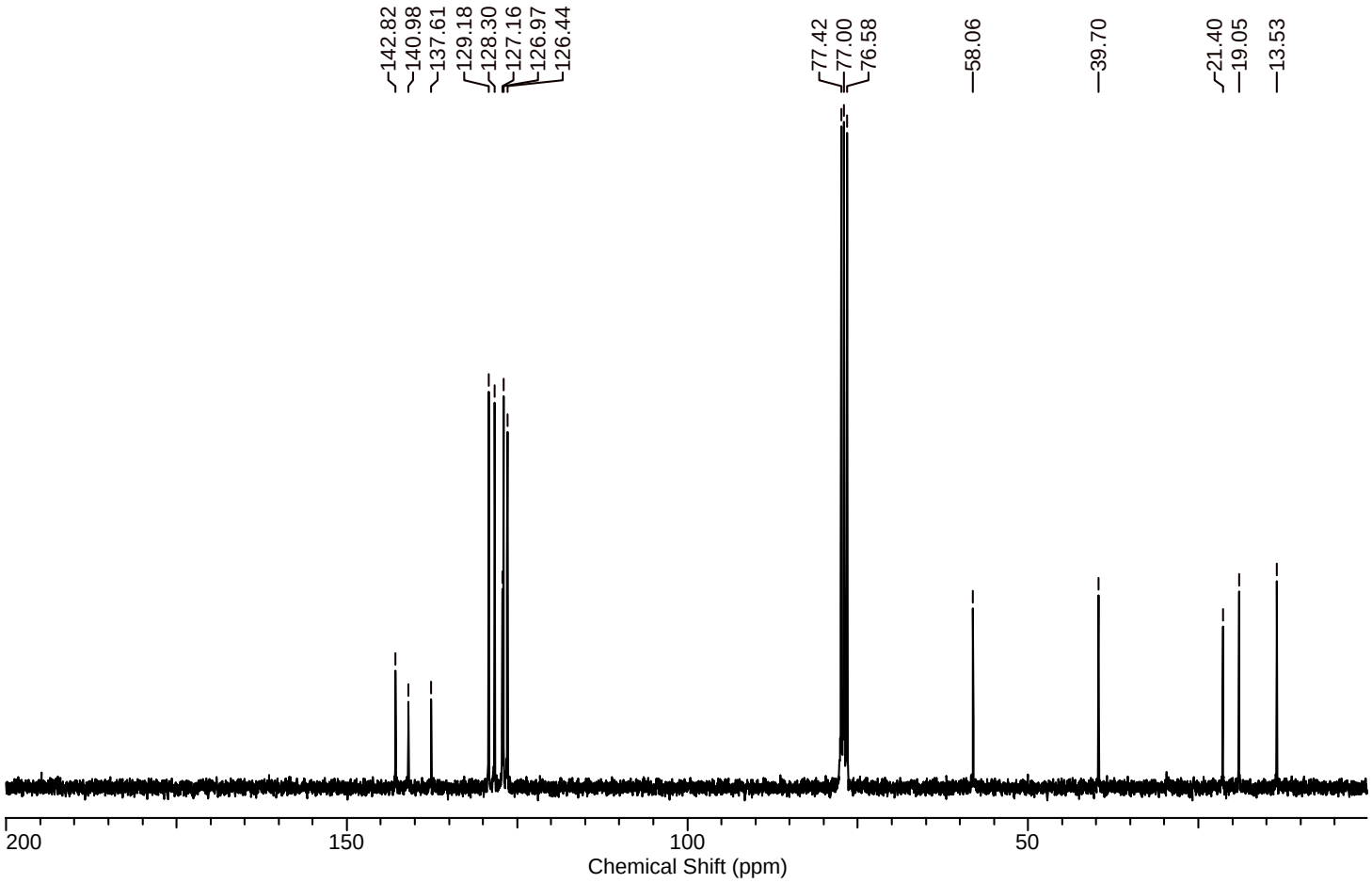




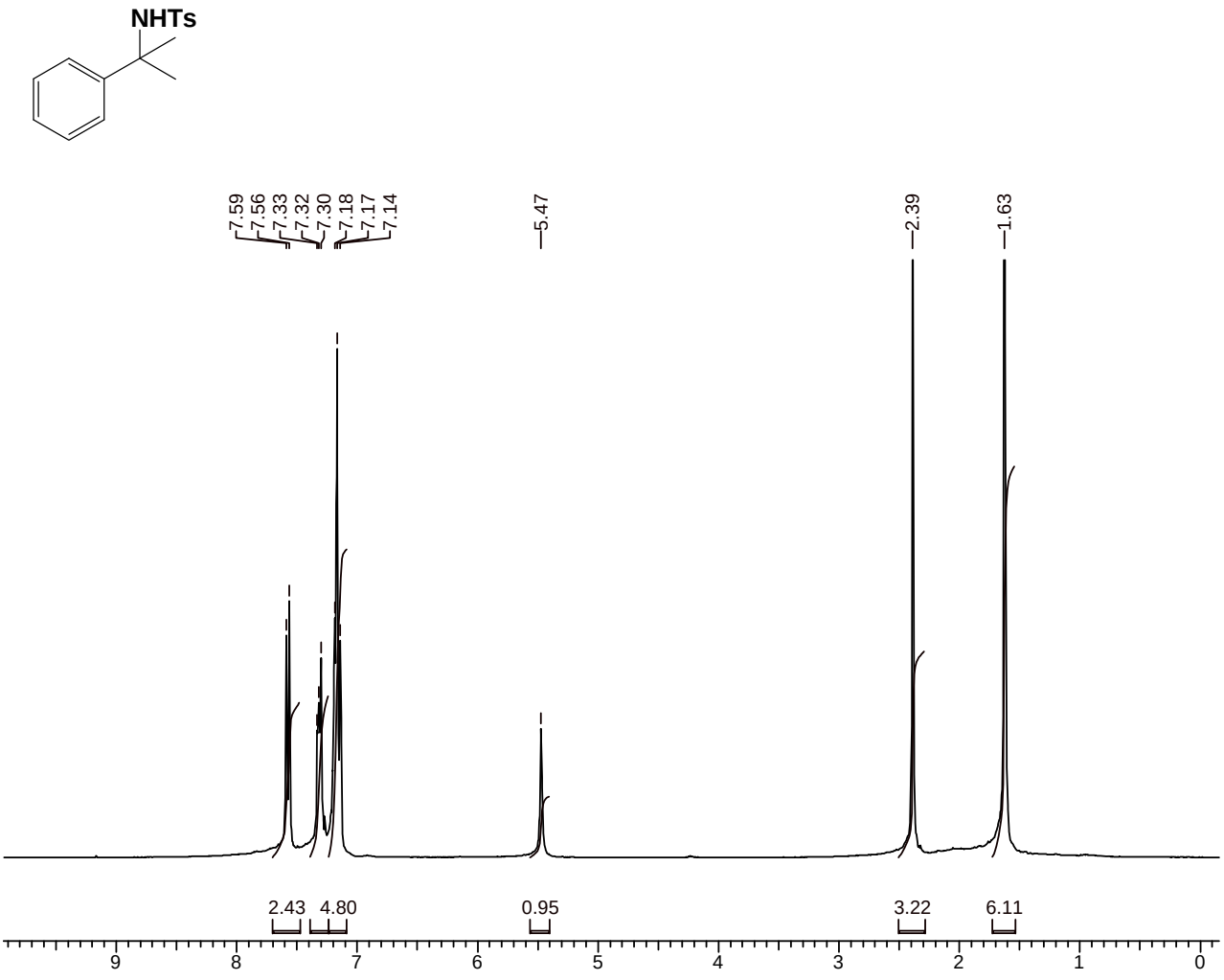
4-Methyl-*N*-(1-phenylbutyl)benzenesulfonamide (5b)

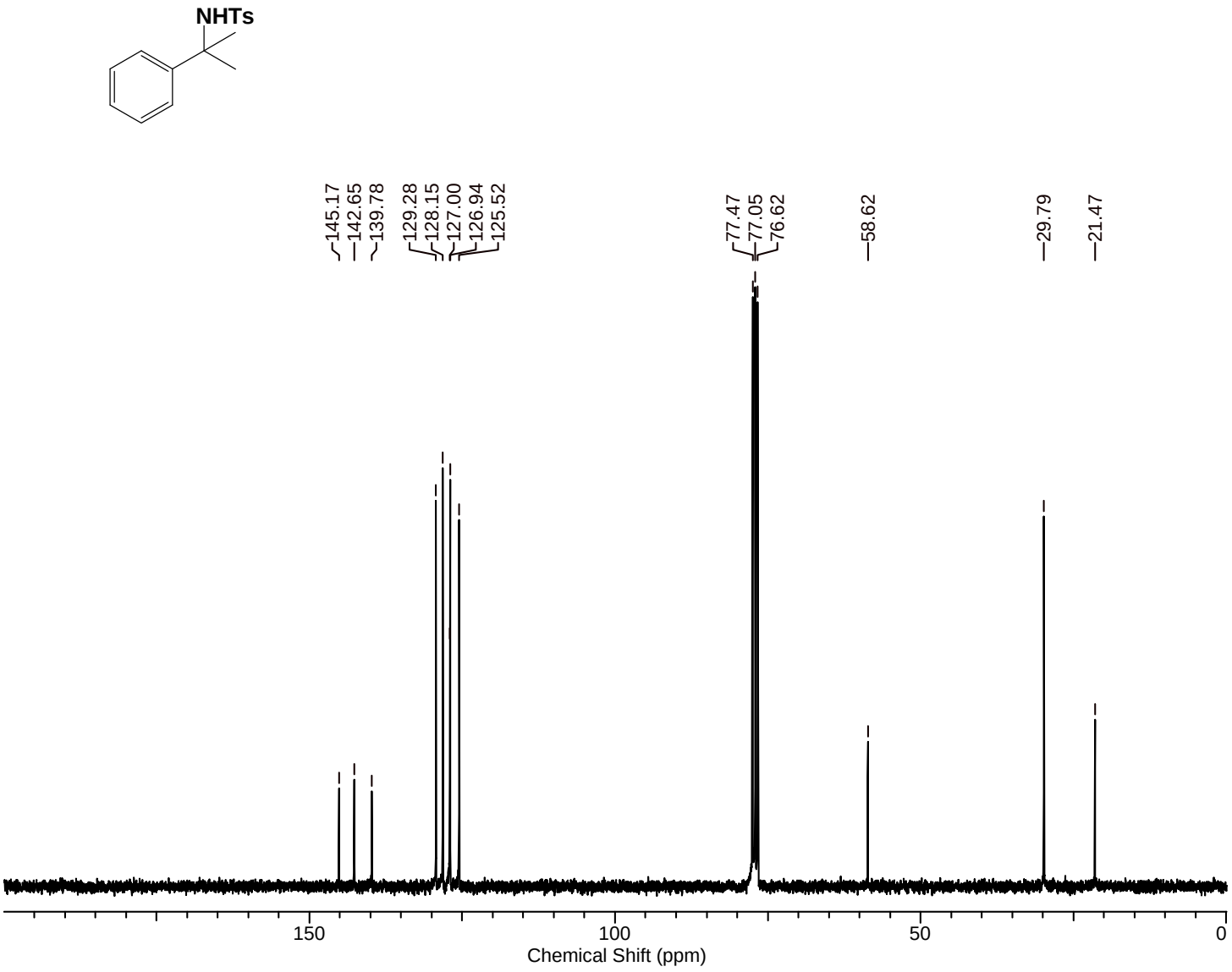




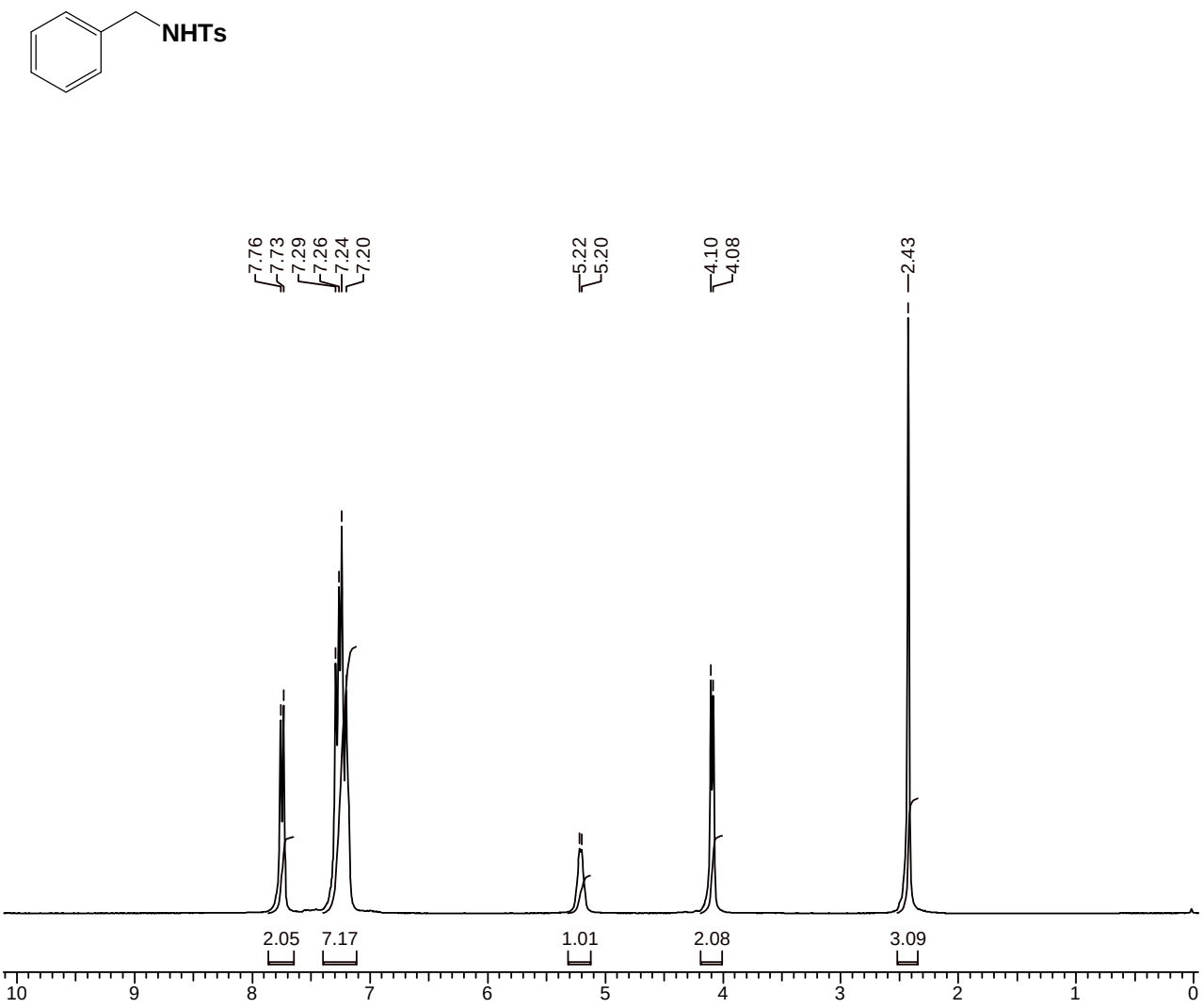


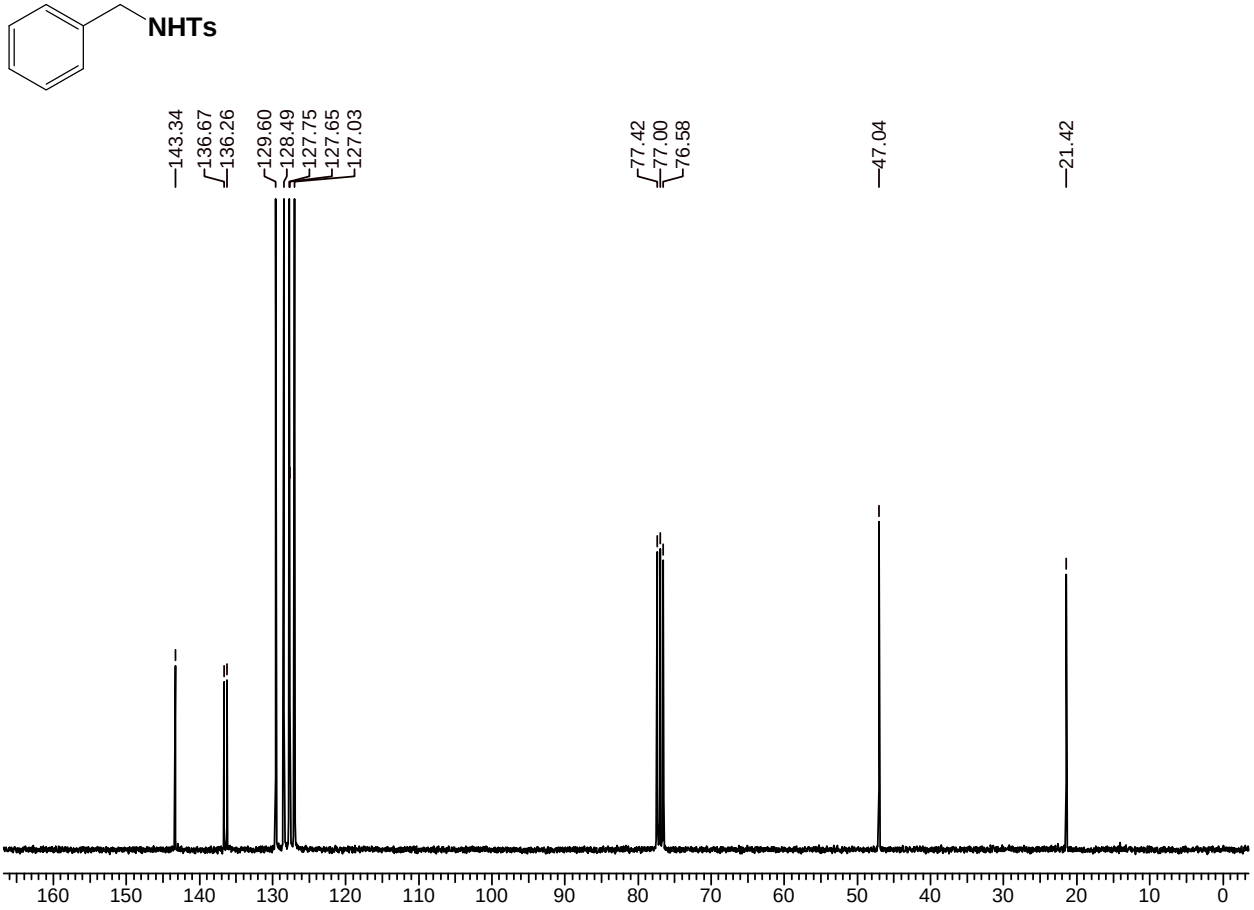
4-Methyl-*N*-(2-phenylpropan-2-yl)benzenesulfonamide (7b)



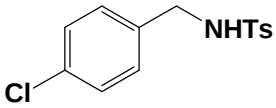


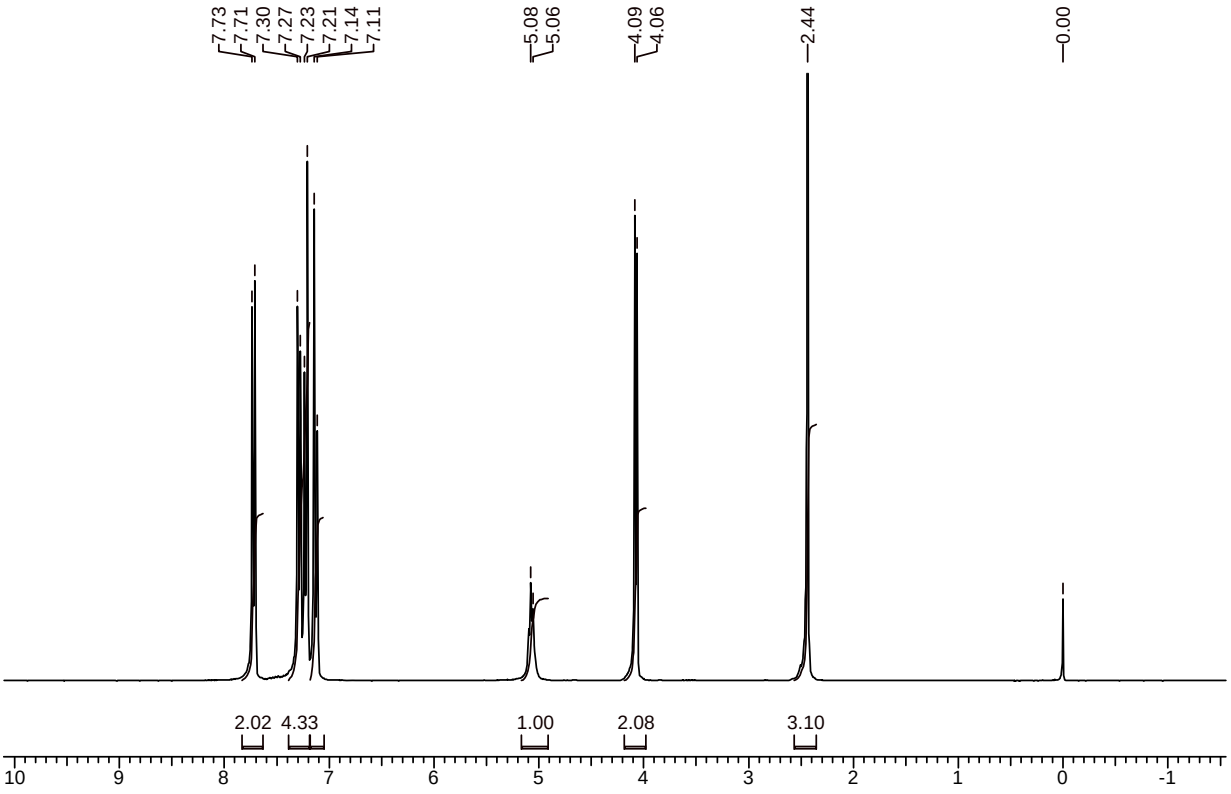
N-Benzyl-4-methylbenzenesulfonamide (8b)

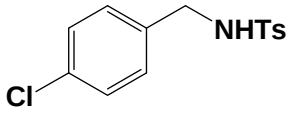


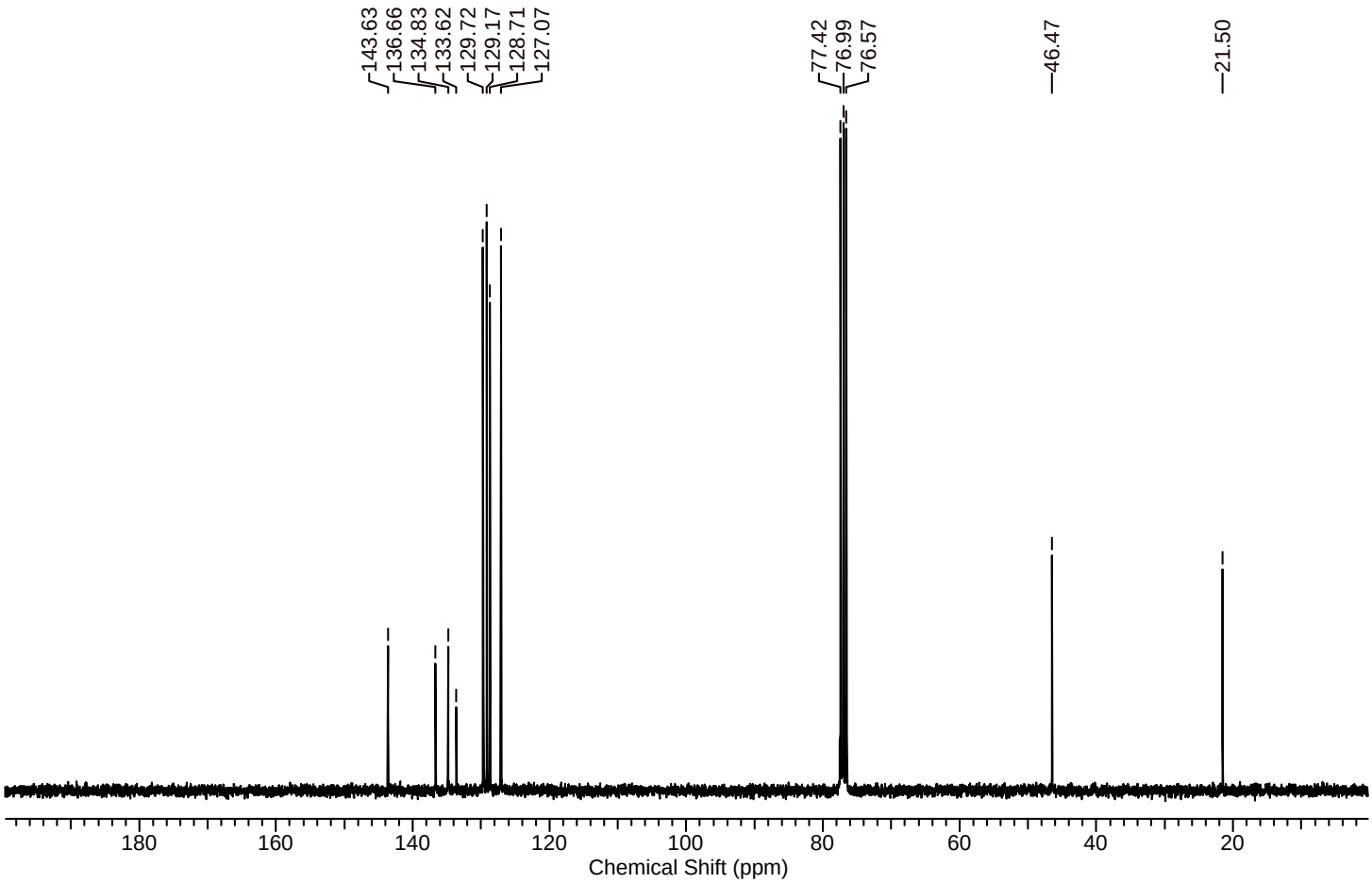


_N_-(4-Chlorobenzyl)-4-methylbenzenesulfonamide (9b)

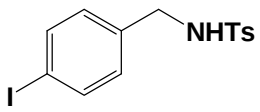


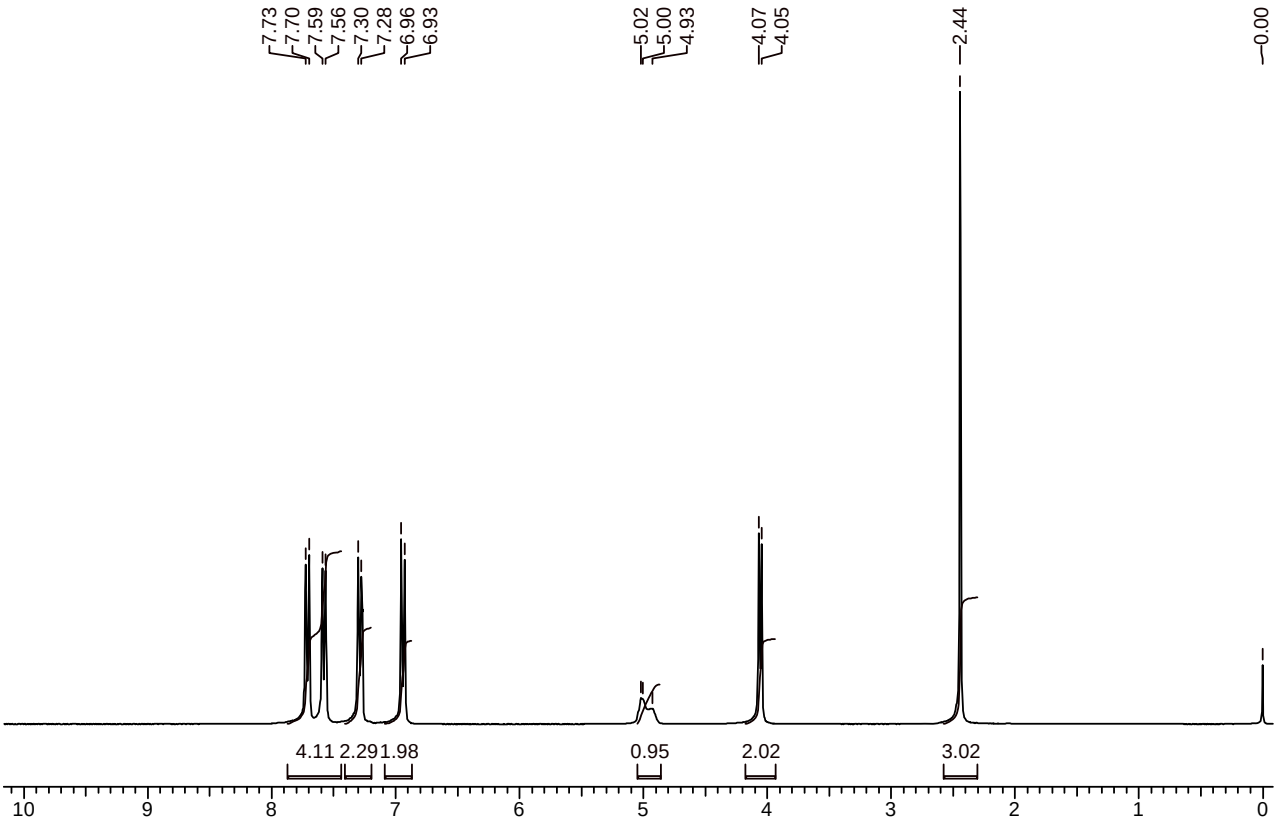


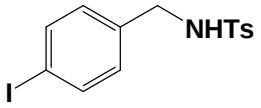


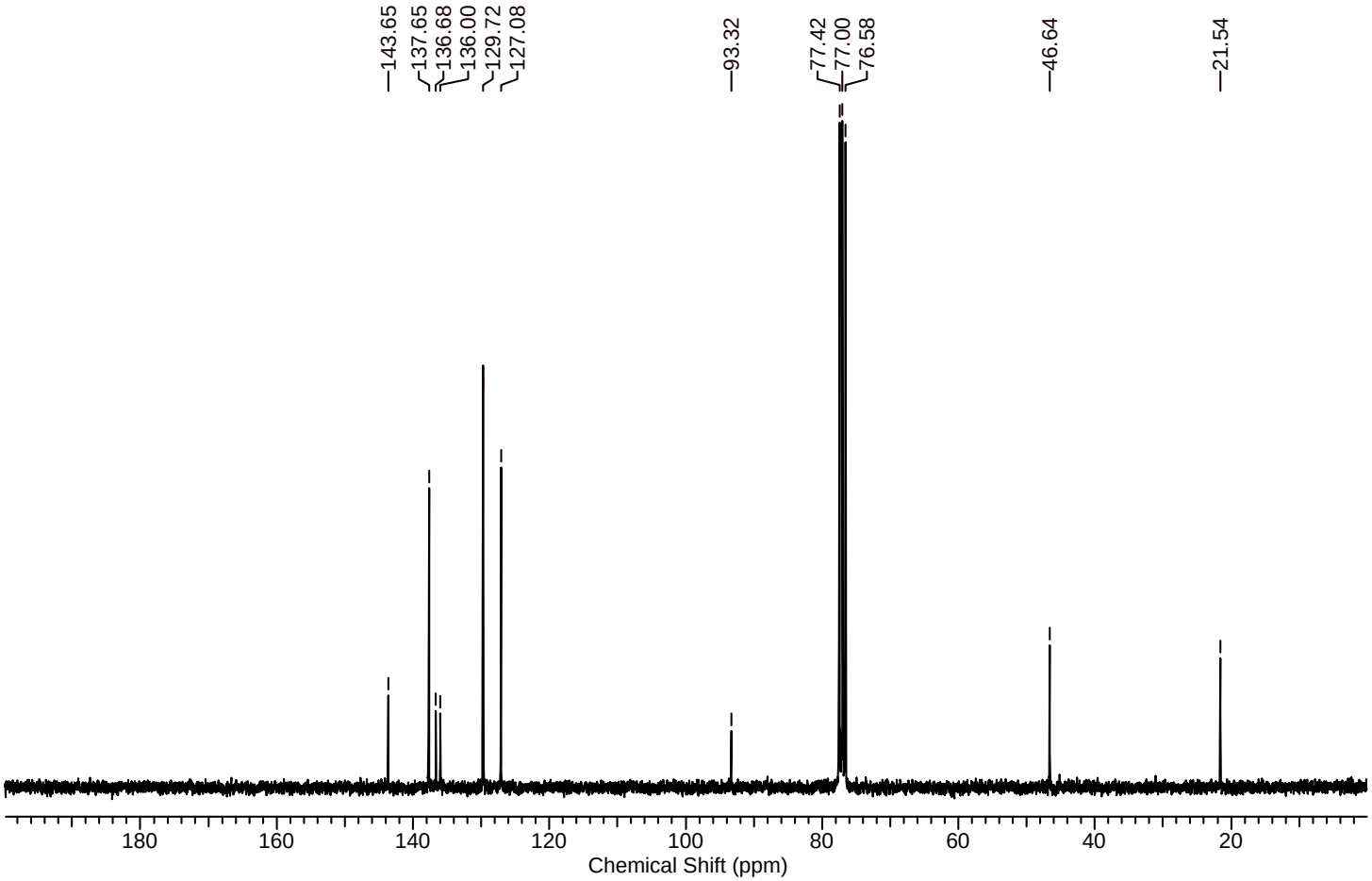


_N_-(4-Iodobenzyl)-4-methylbenzenesulfonamide (10b)

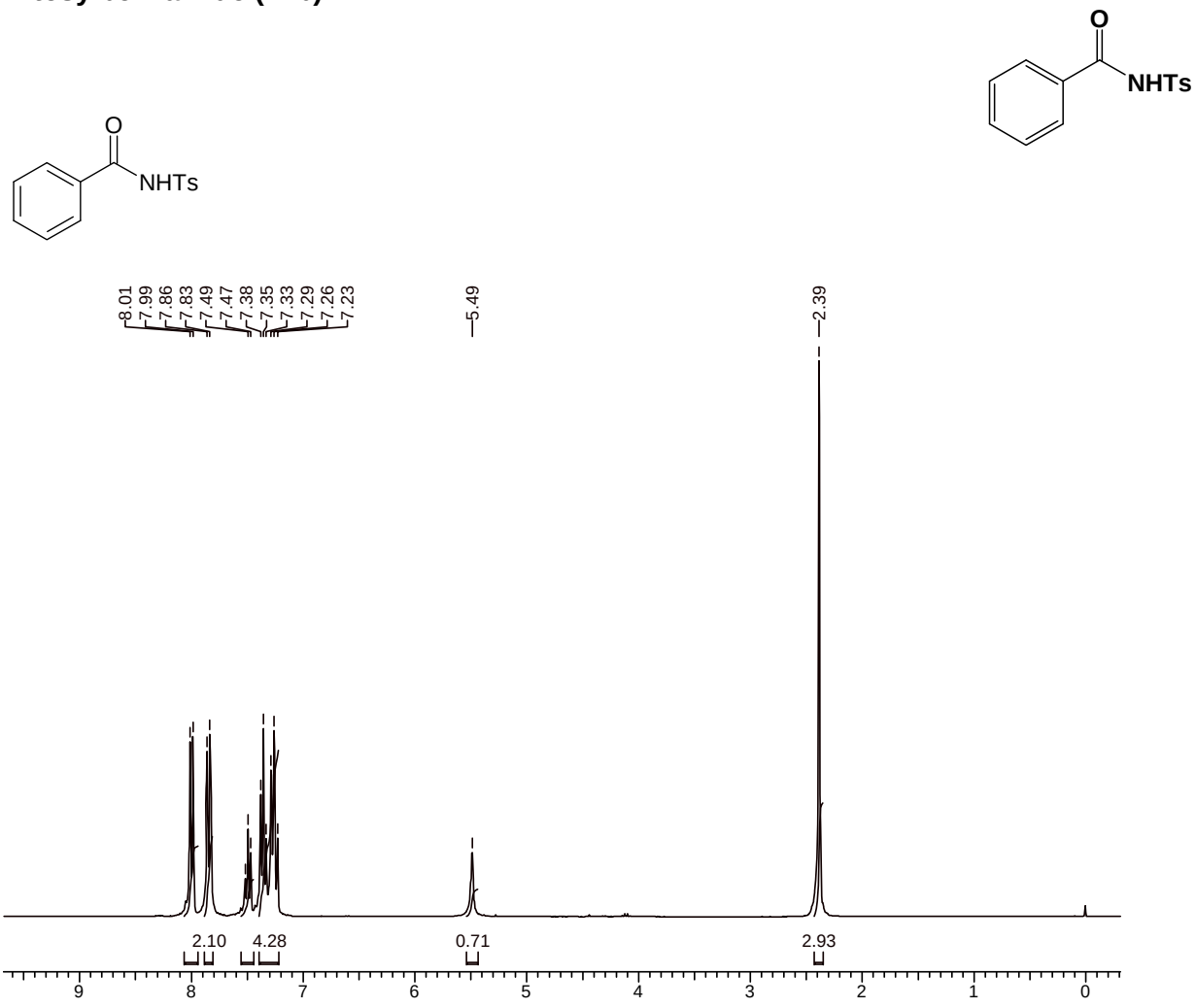


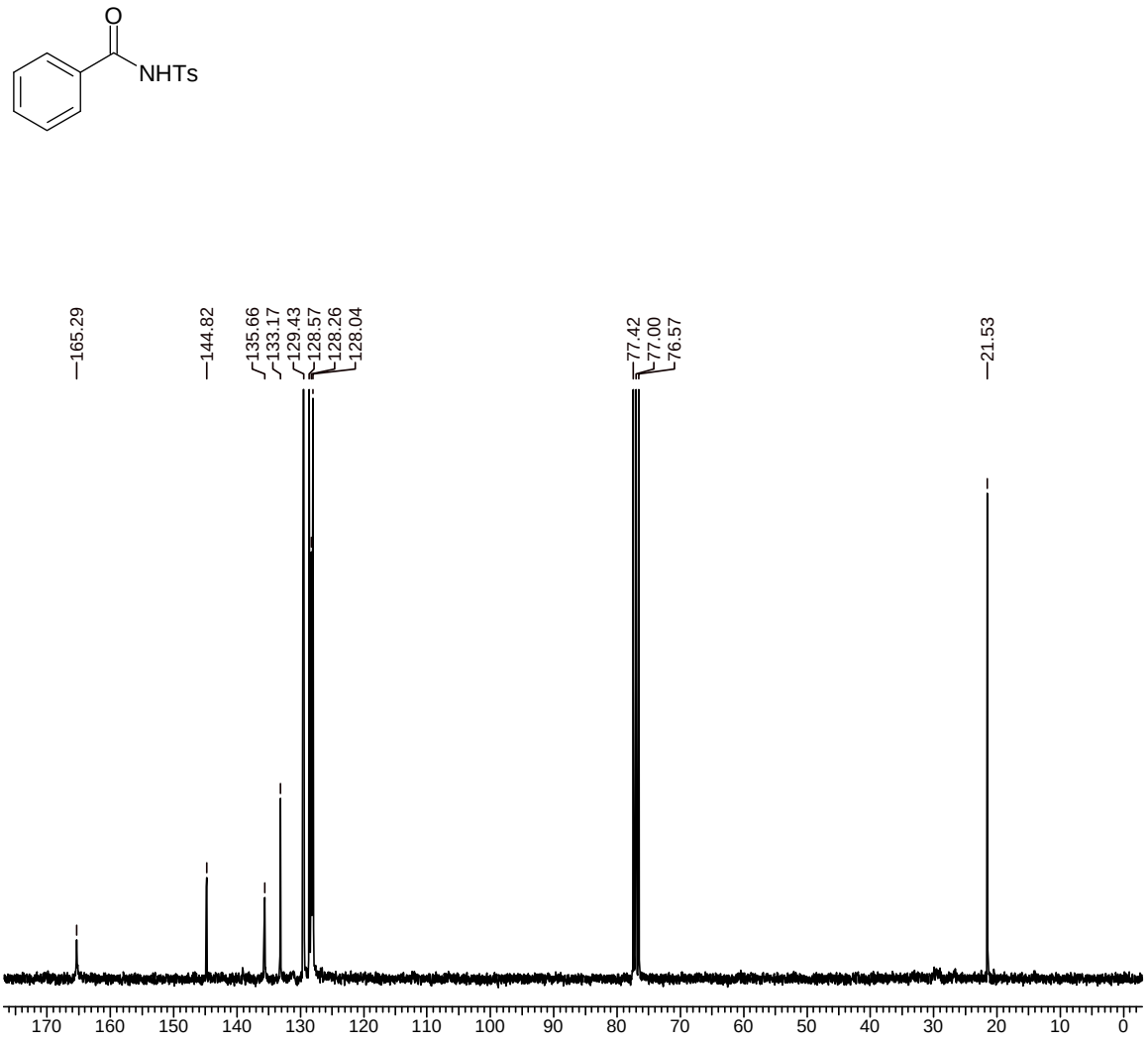




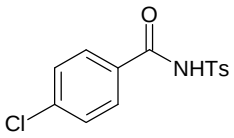


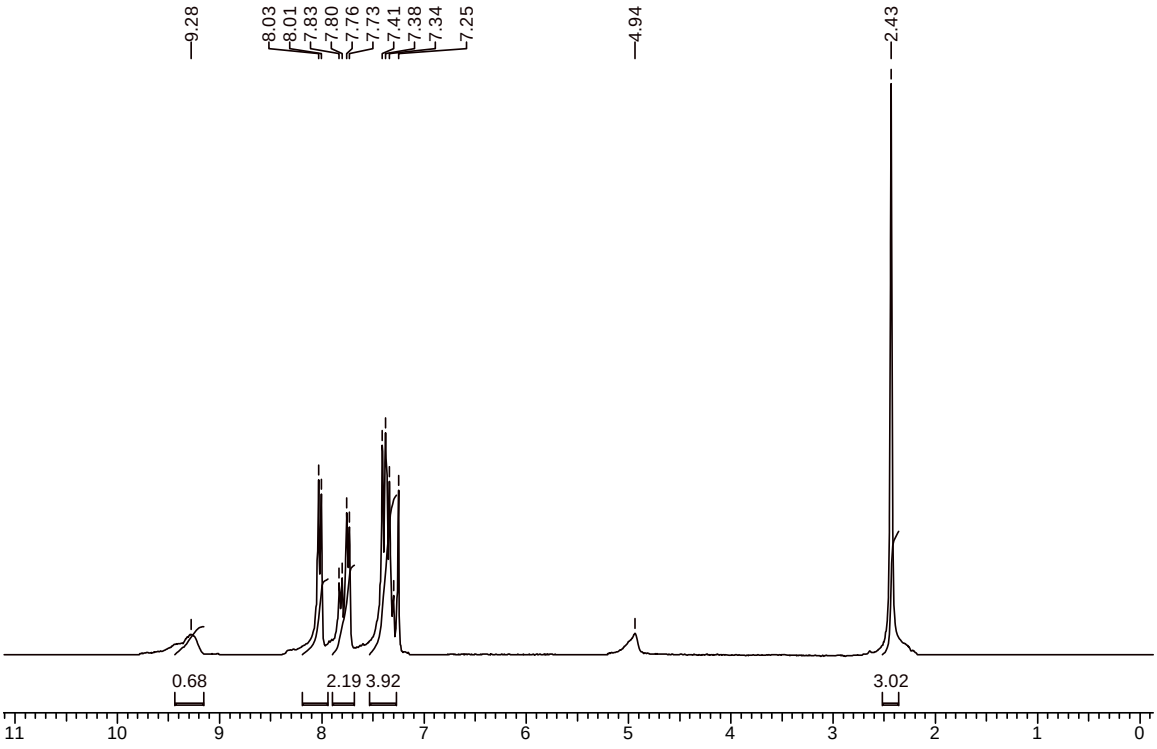
N-tosylbenzamide (11b)

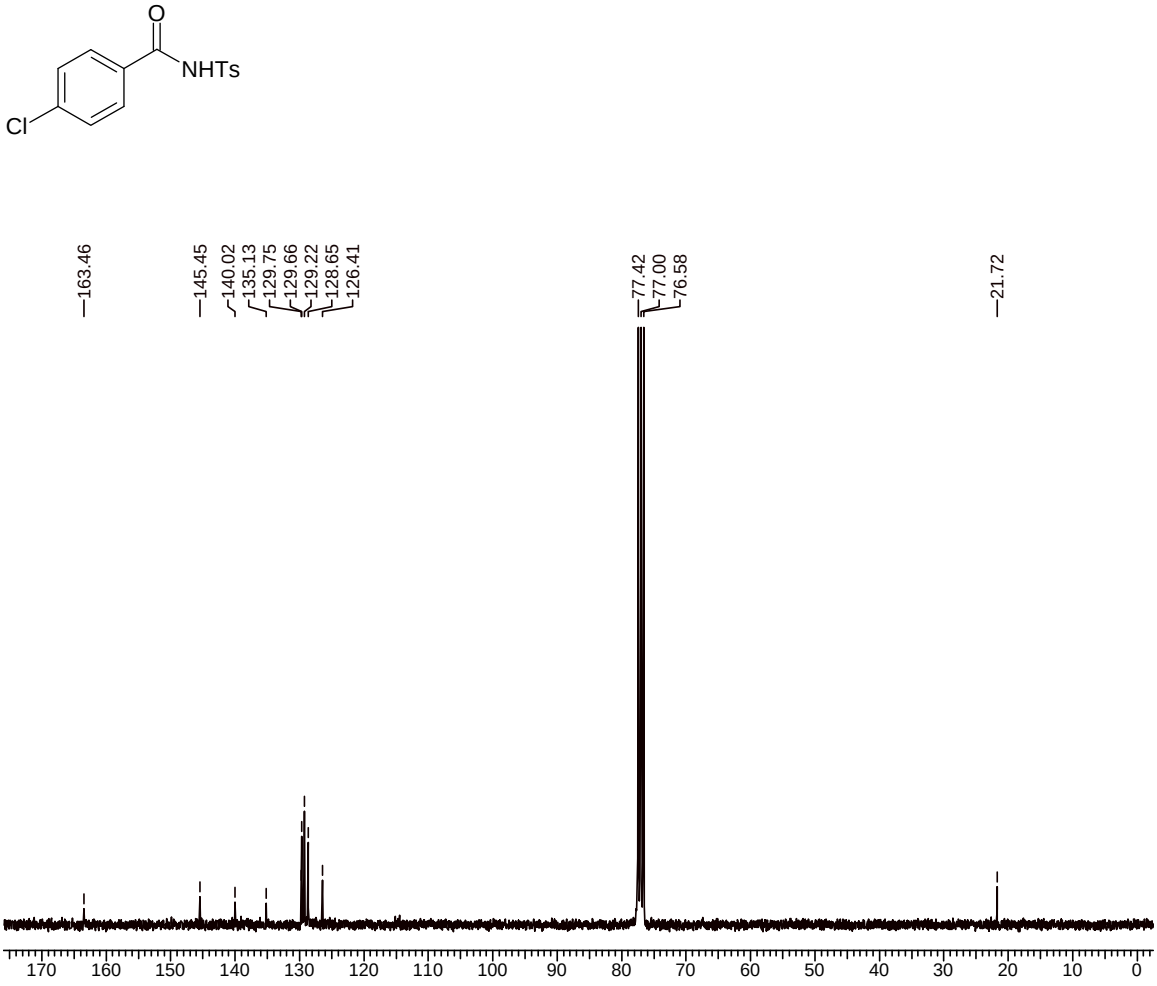




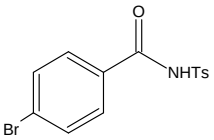
4-chloro-N-tosylbenzamide (12b)

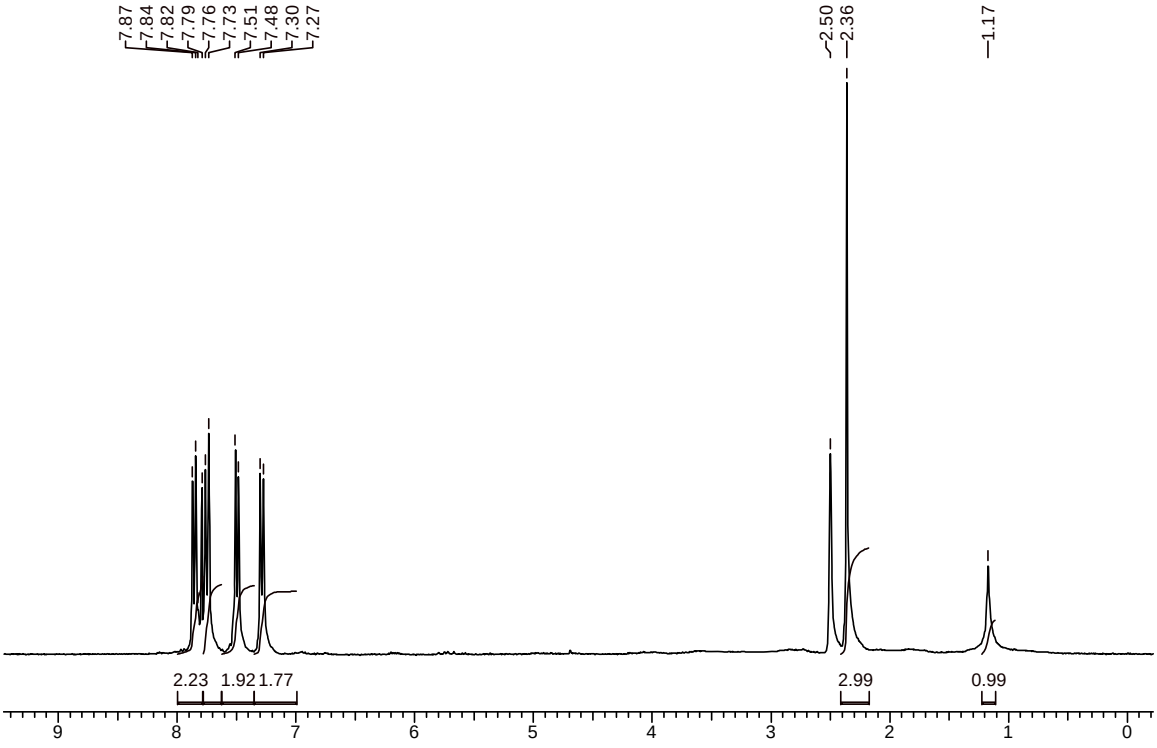


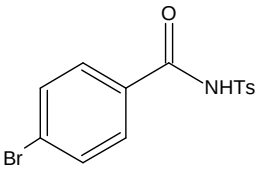


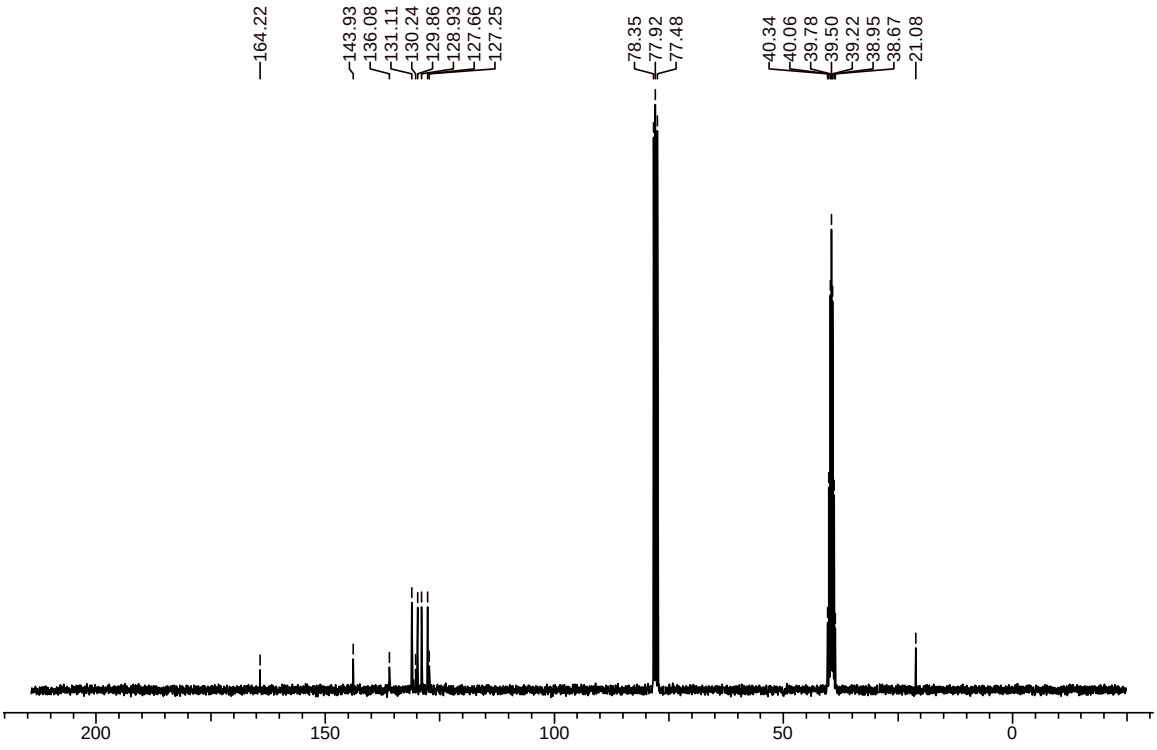


4-bromo-N-tosylbenzamide (13b)

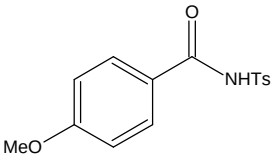


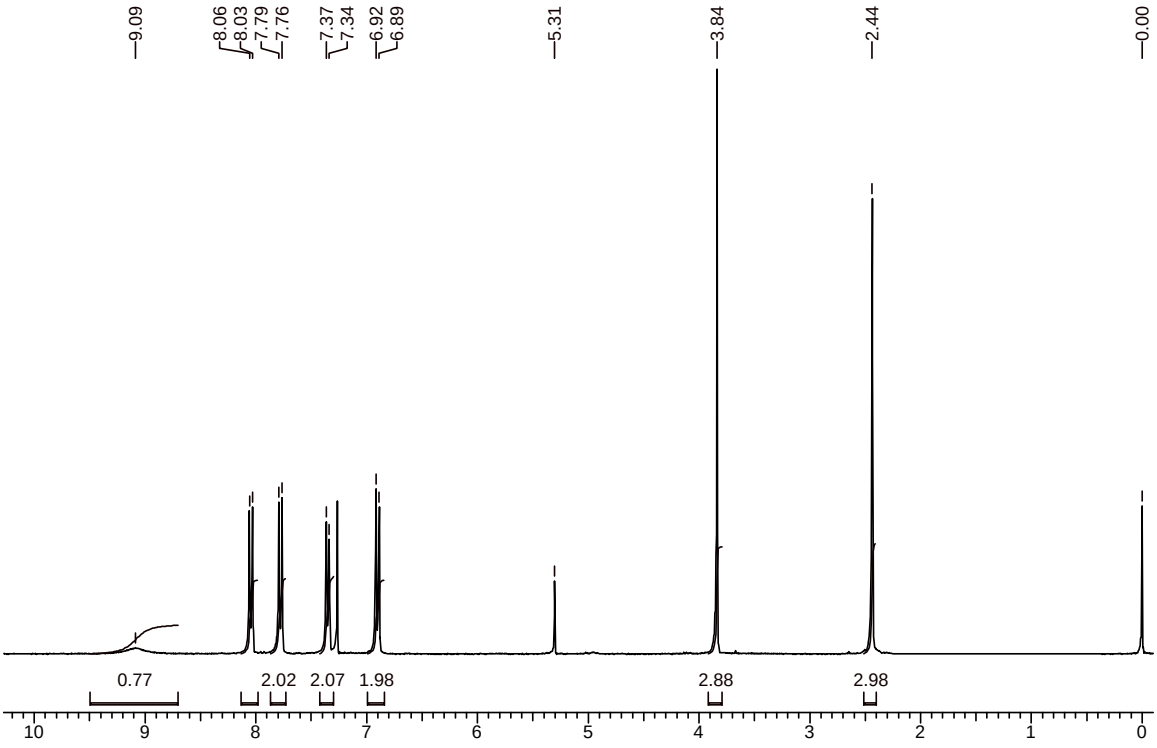


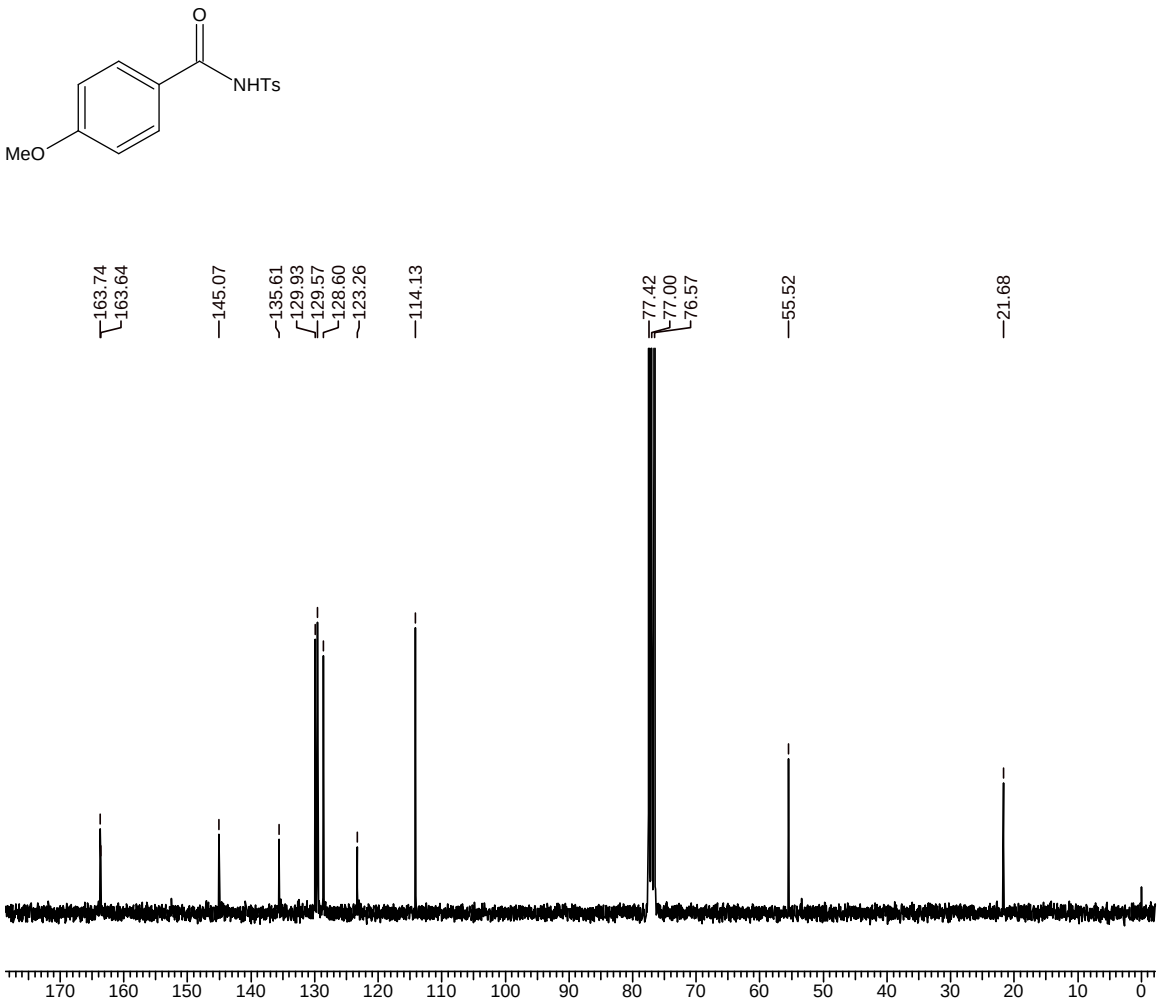

O
NHTs
Br


164.22
143.93
136.08
131.11
130.24
129.86
128.93
127.66
127.25
78.35
77.92
77.48
40.34
40.06
39.78
39.50
39.22
38.95
38.67
21.08
200
150
100
50
0

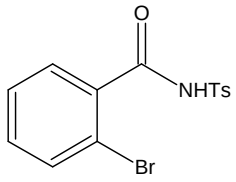
4-methoxy-N-tosylbenzamide (14b)

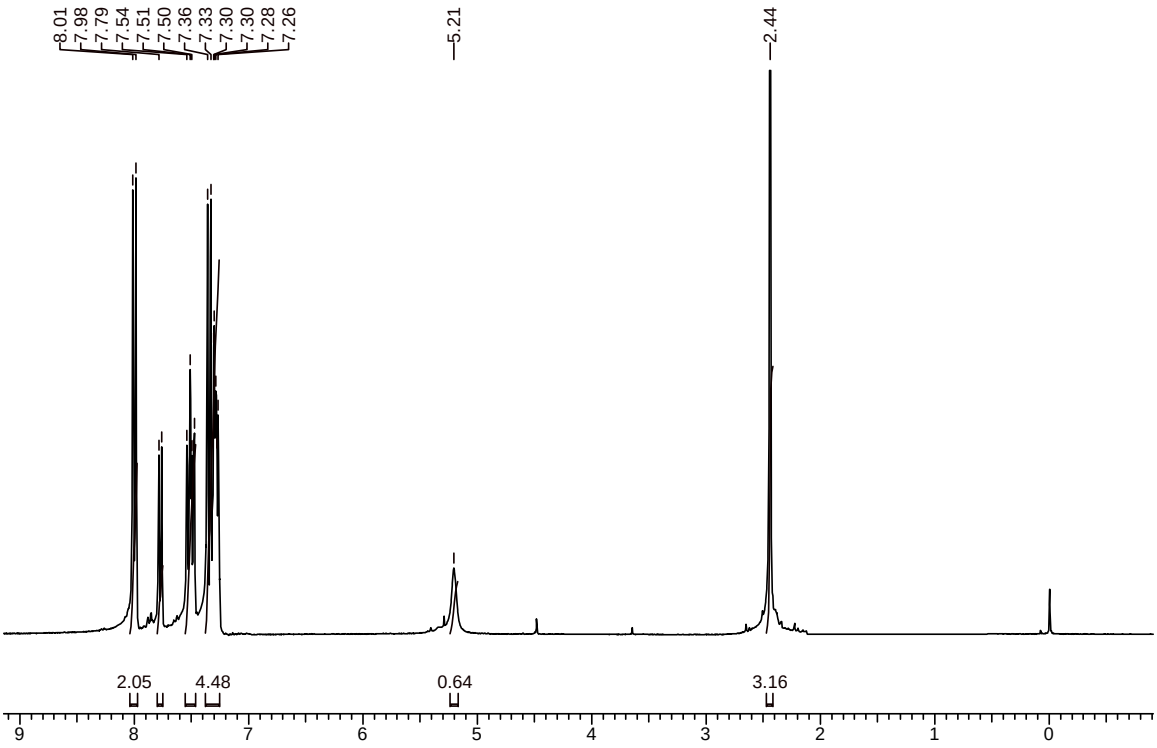


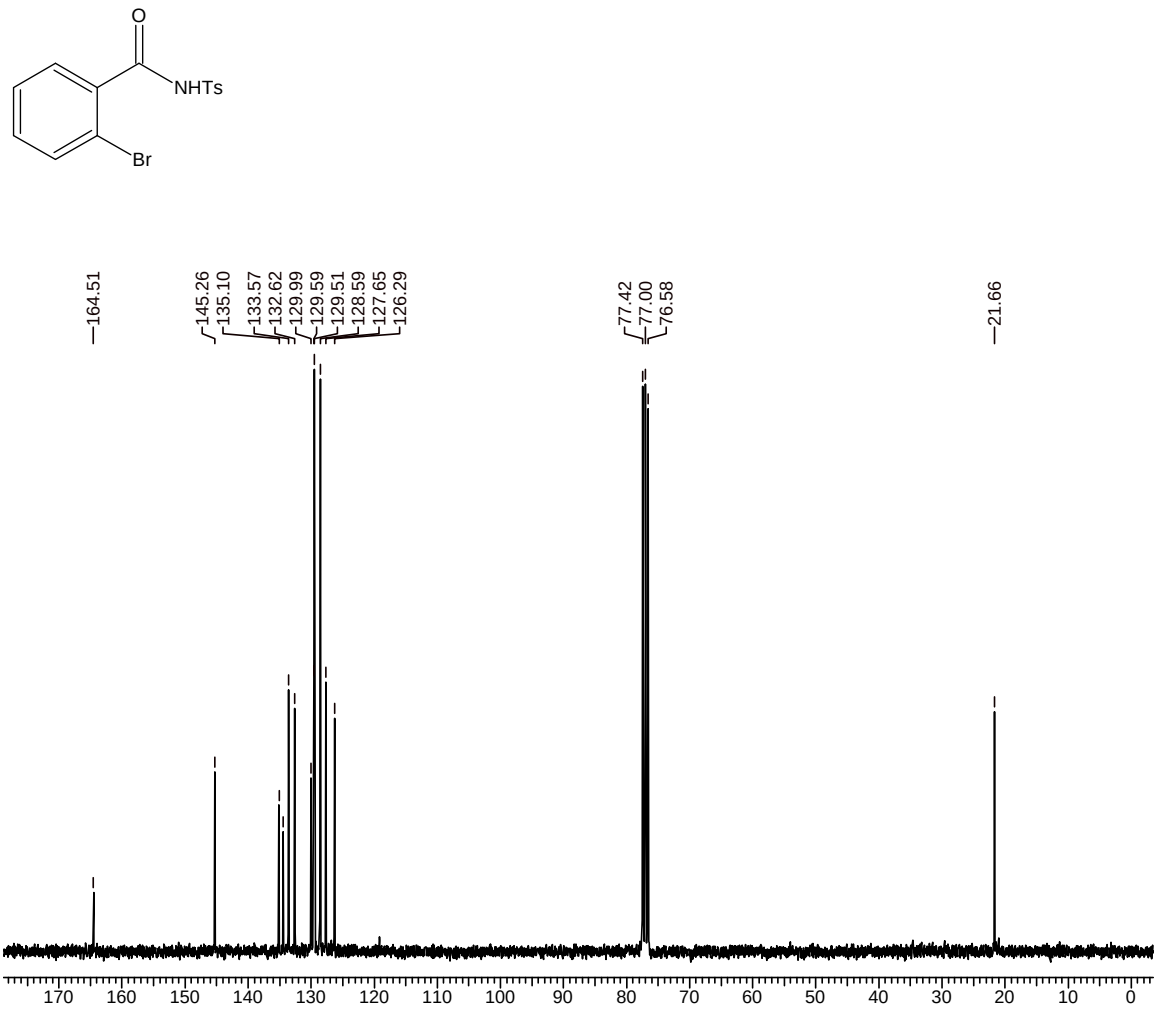




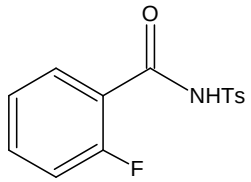
2-bromo-N-tosylbenzamide (15b)

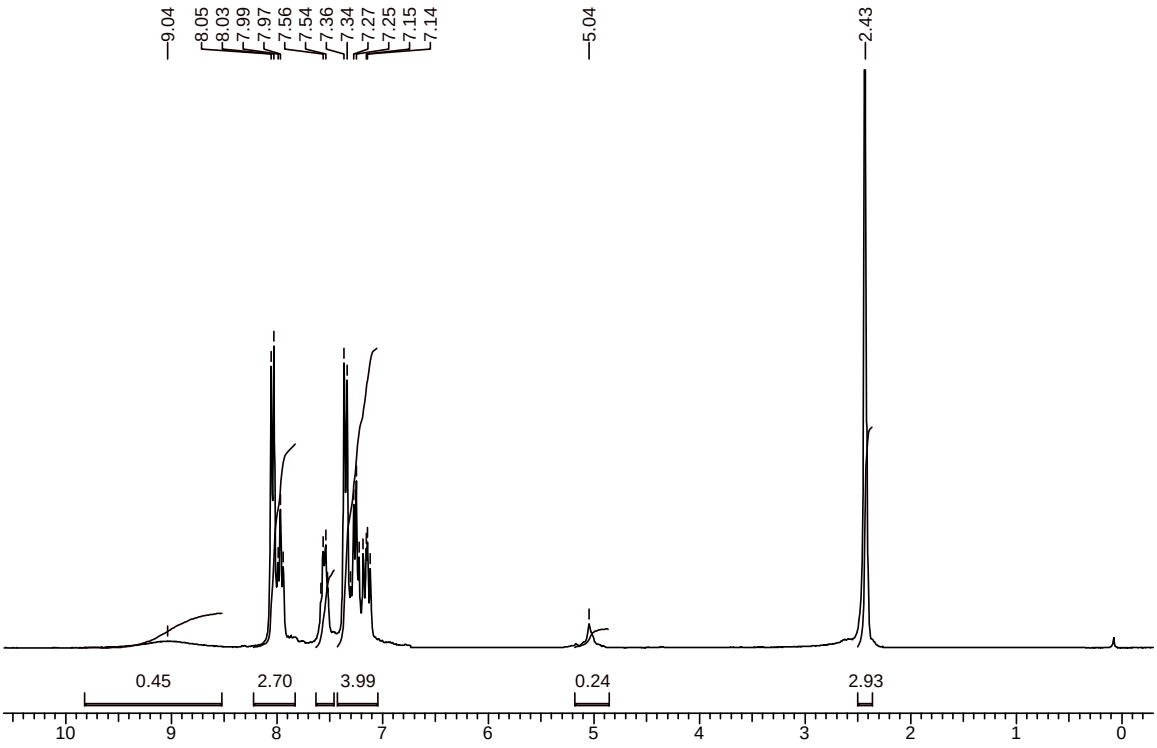


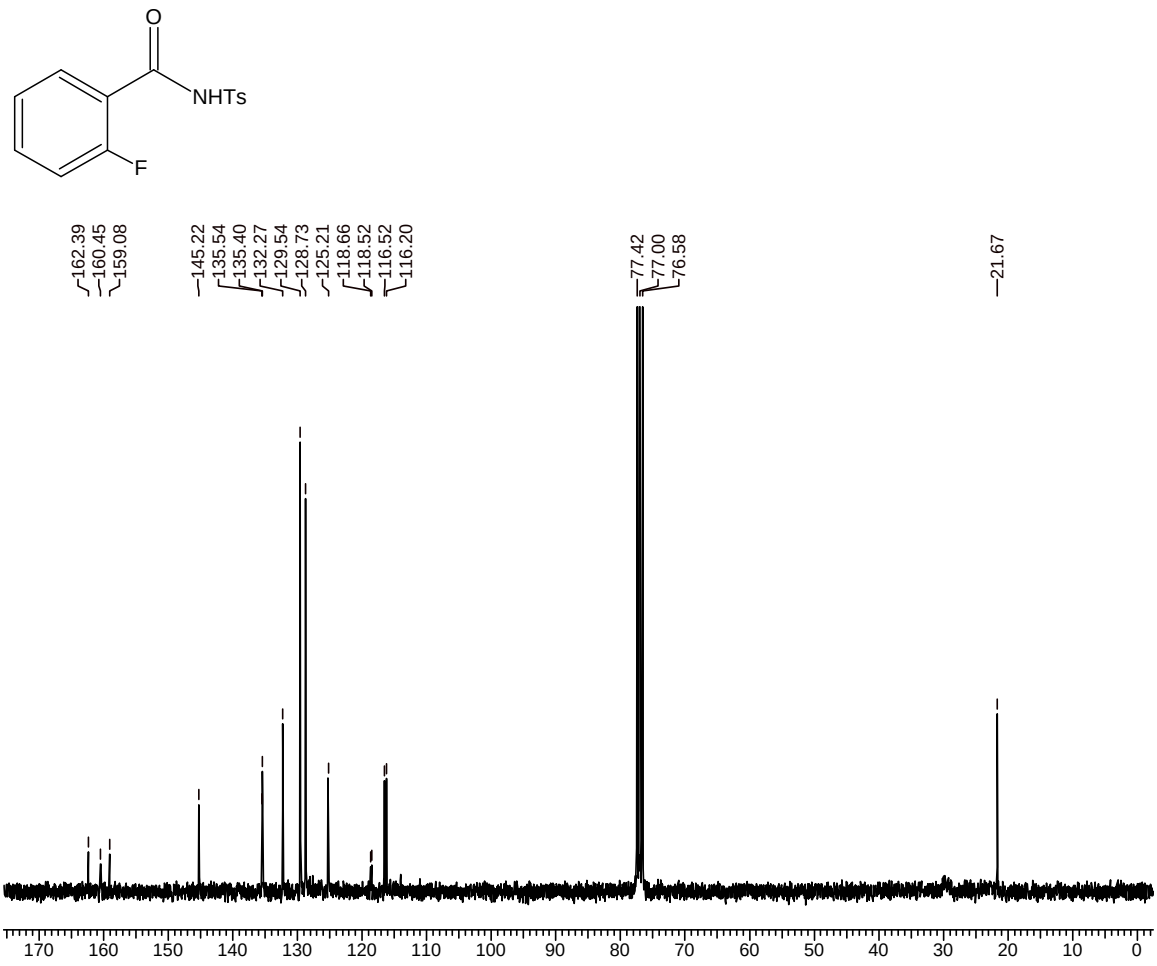




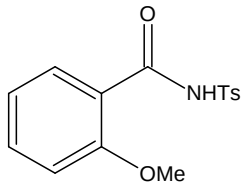
2-fluro-N-tosylbenzamide (16b)

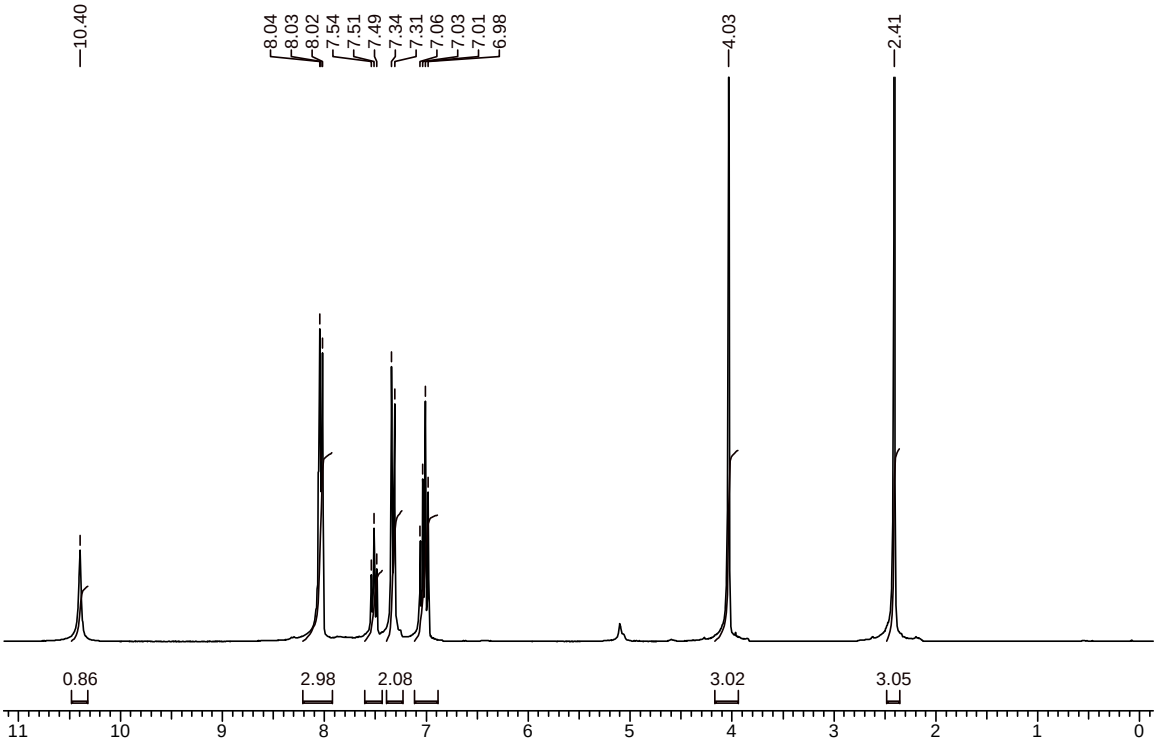


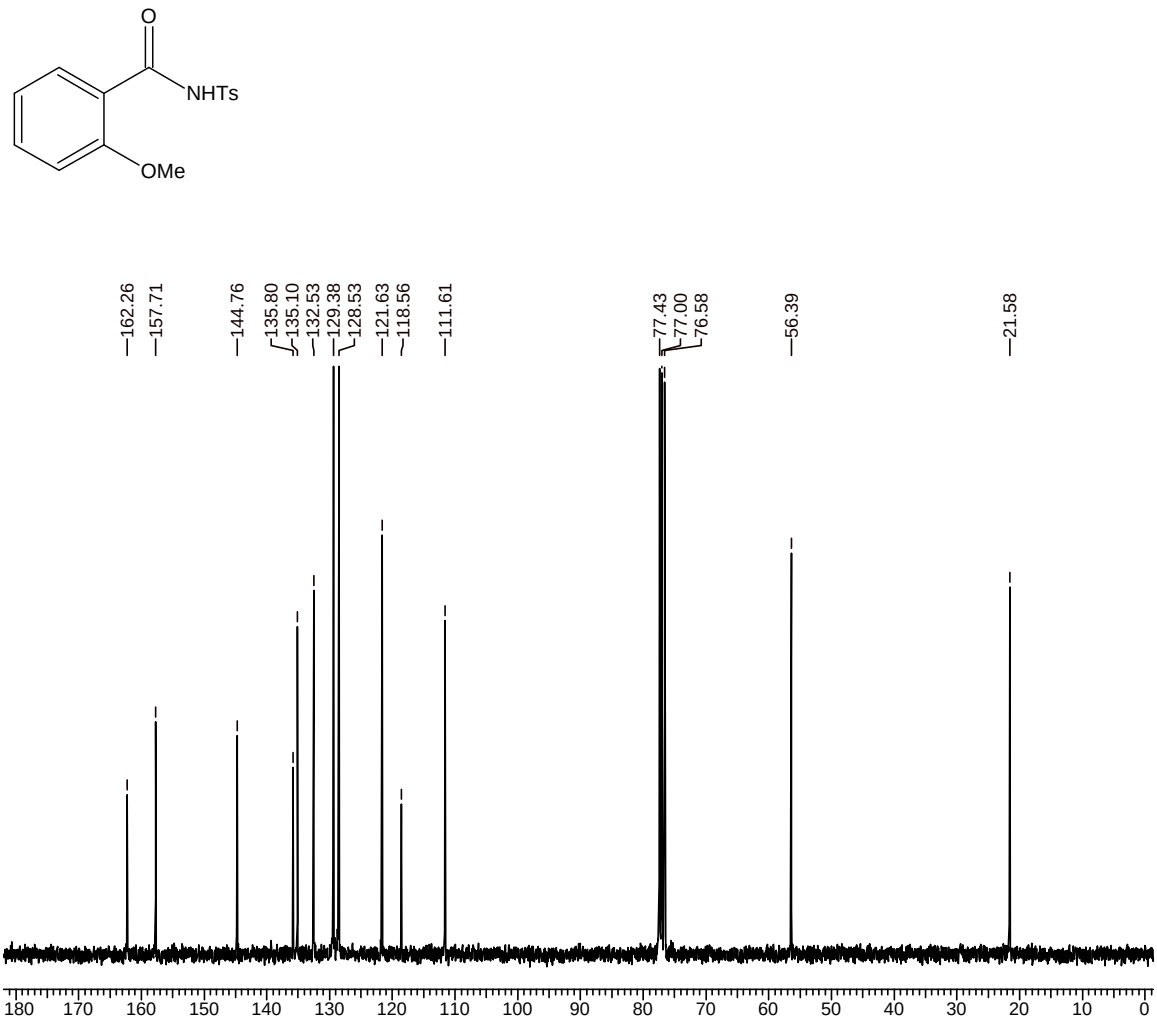




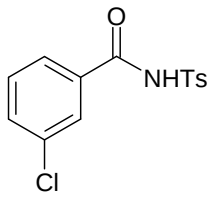
2-methoxy –N-tosylbenzamide (17b)

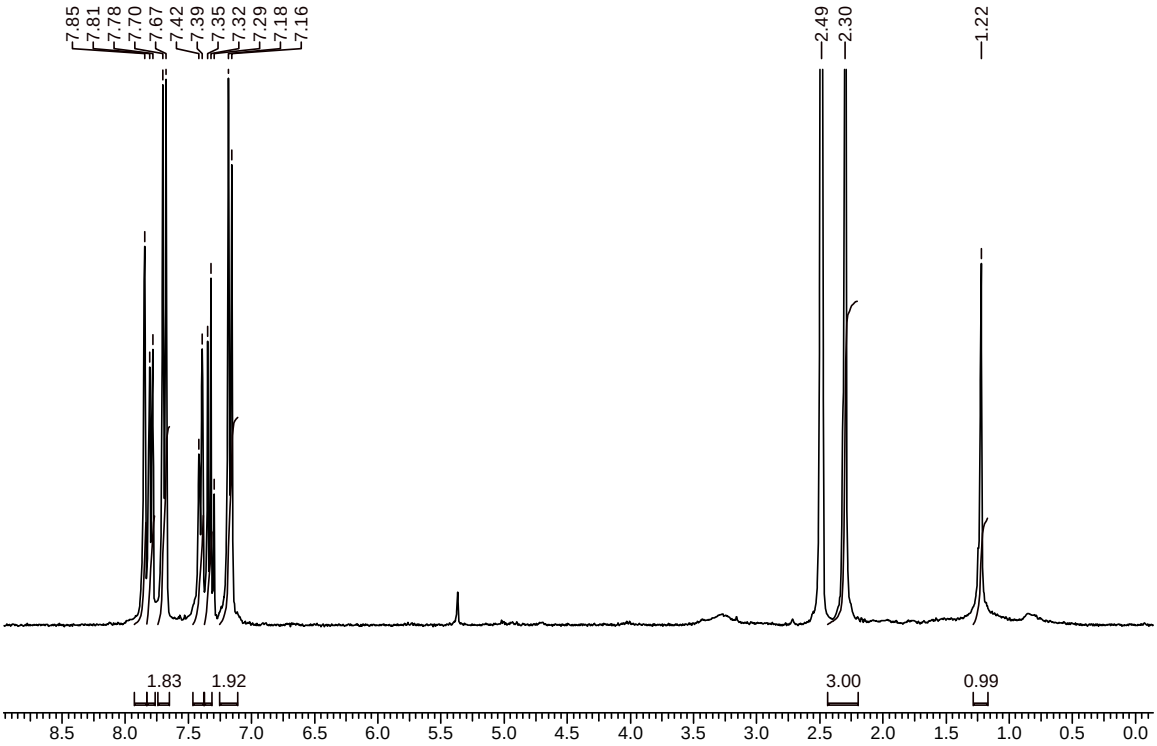


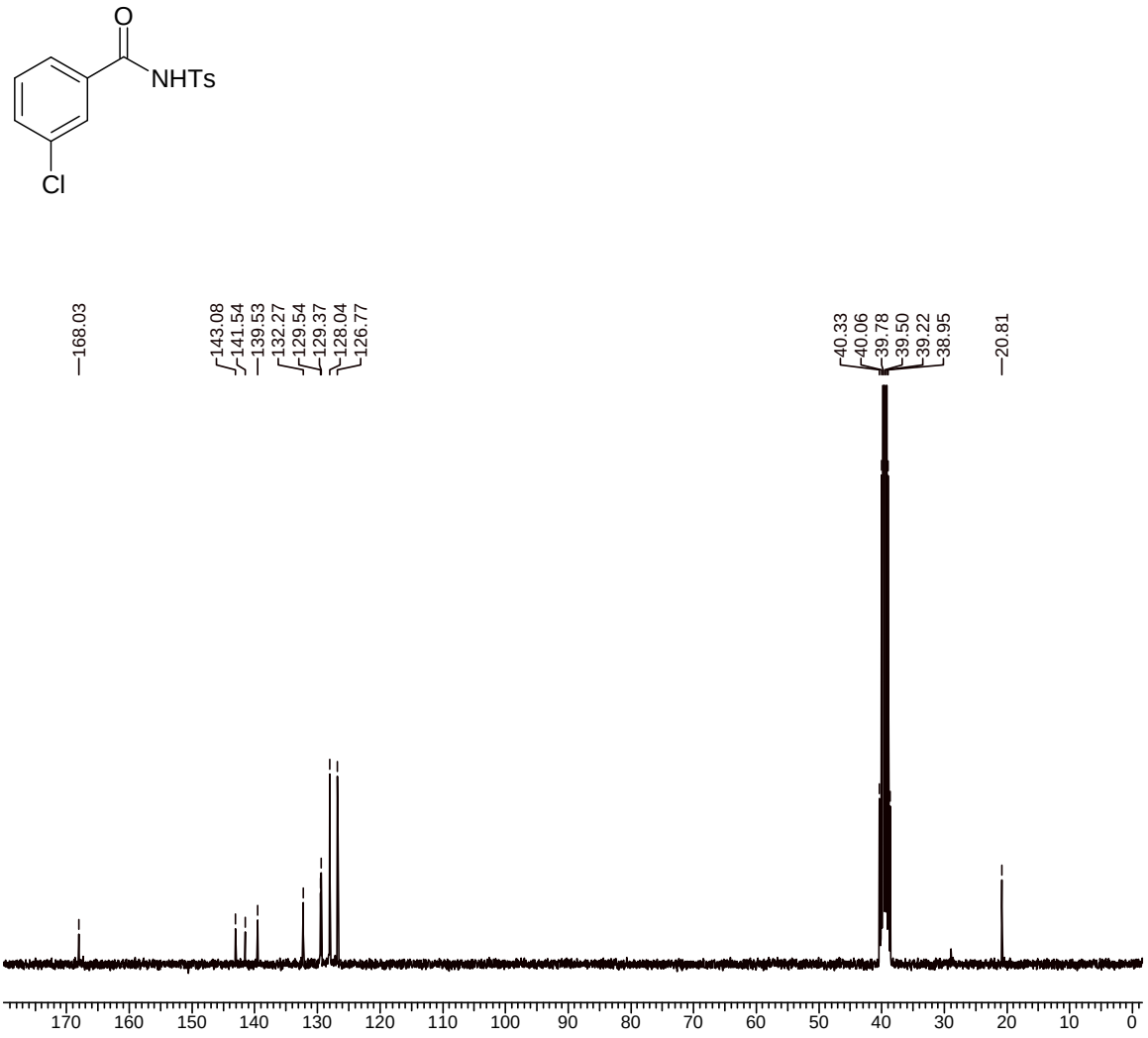




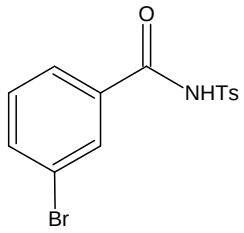
3-chloro-N-tosylbenzamide (18b)

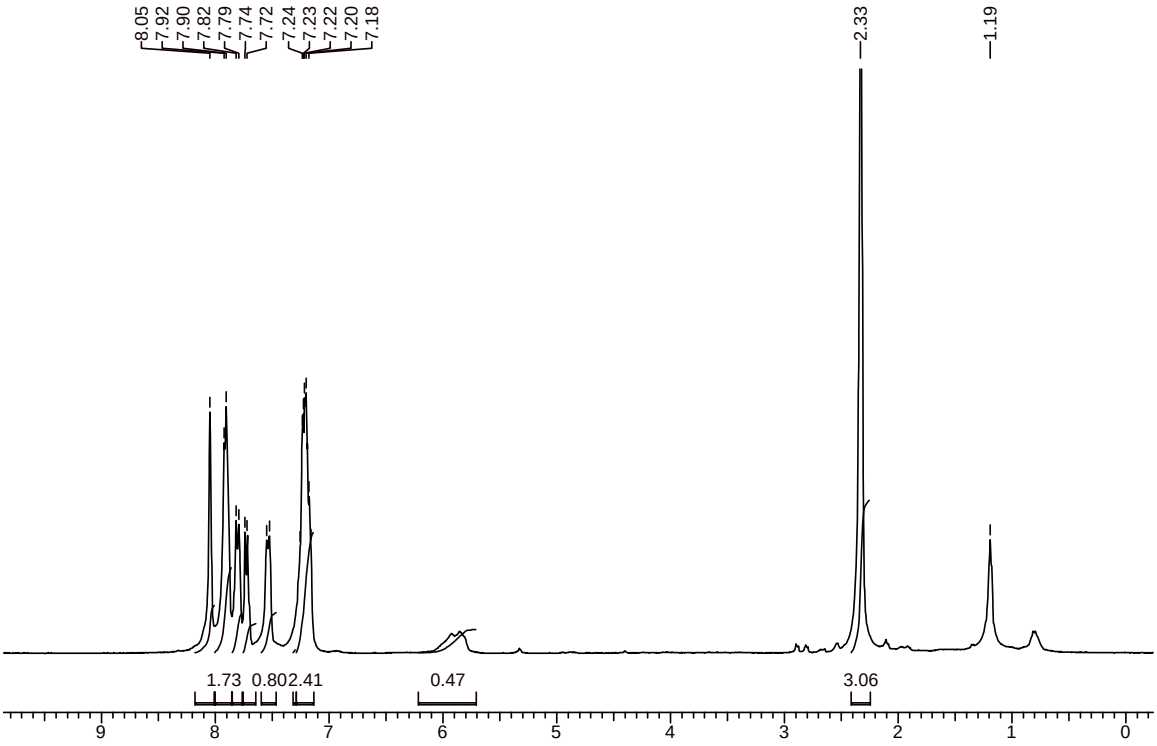


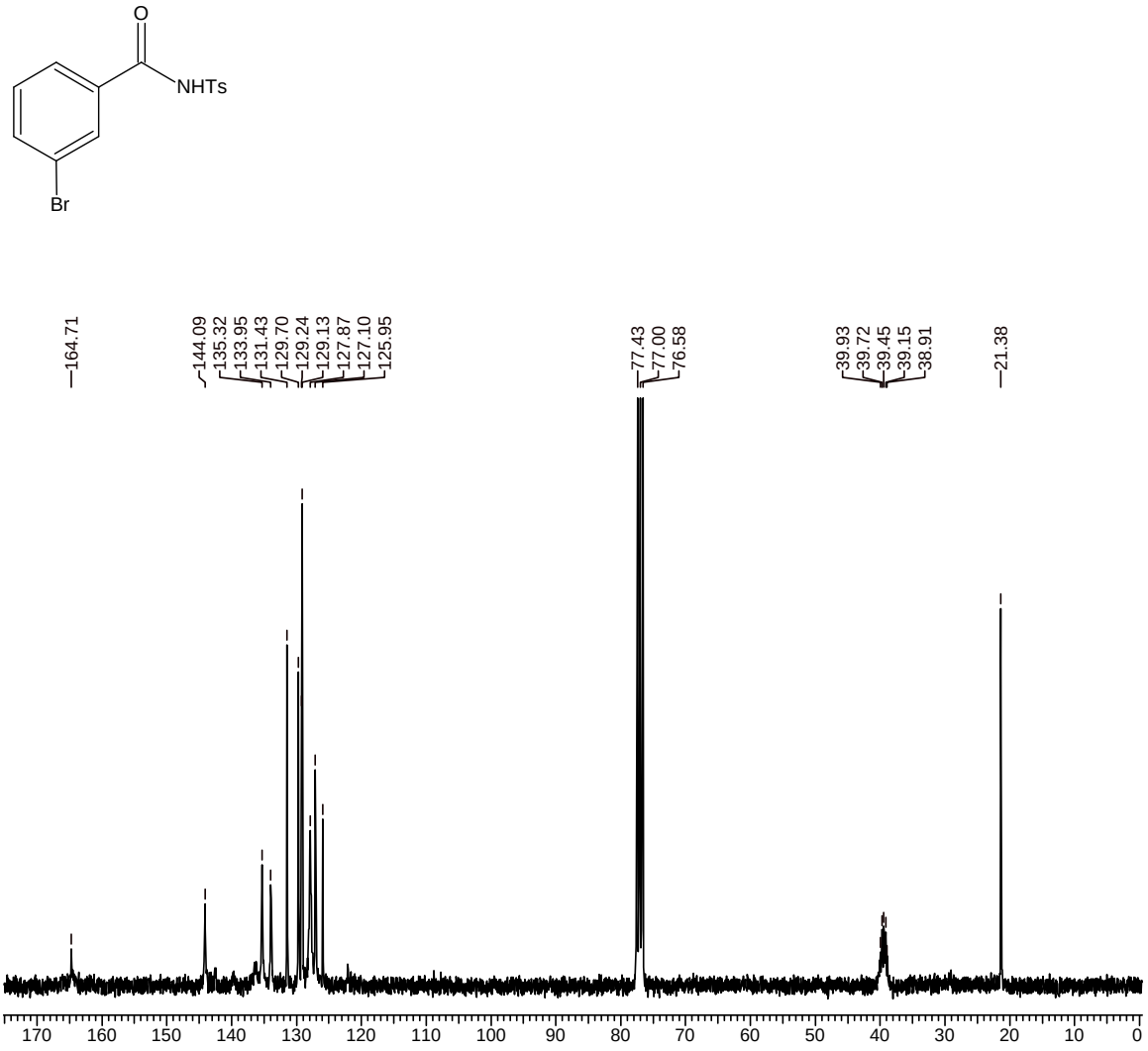




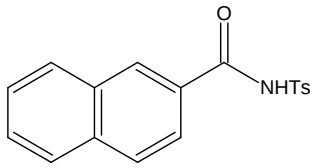
3-bromo-N-tosylbenzamide (19b)

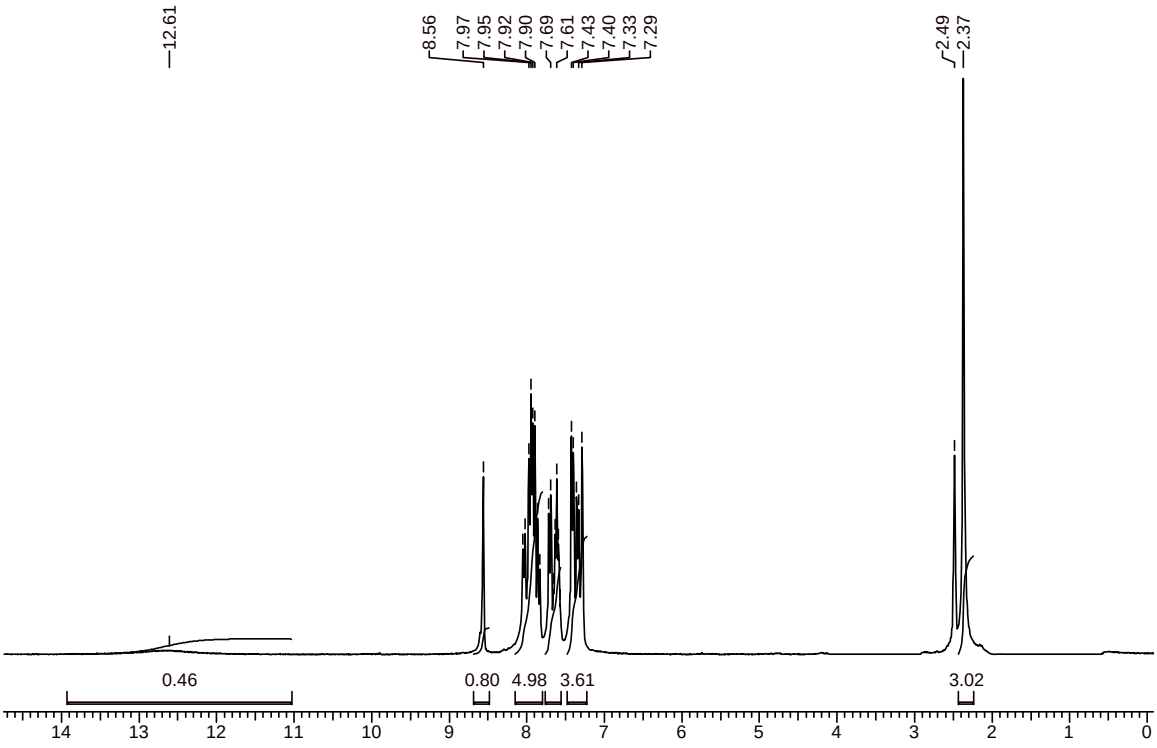


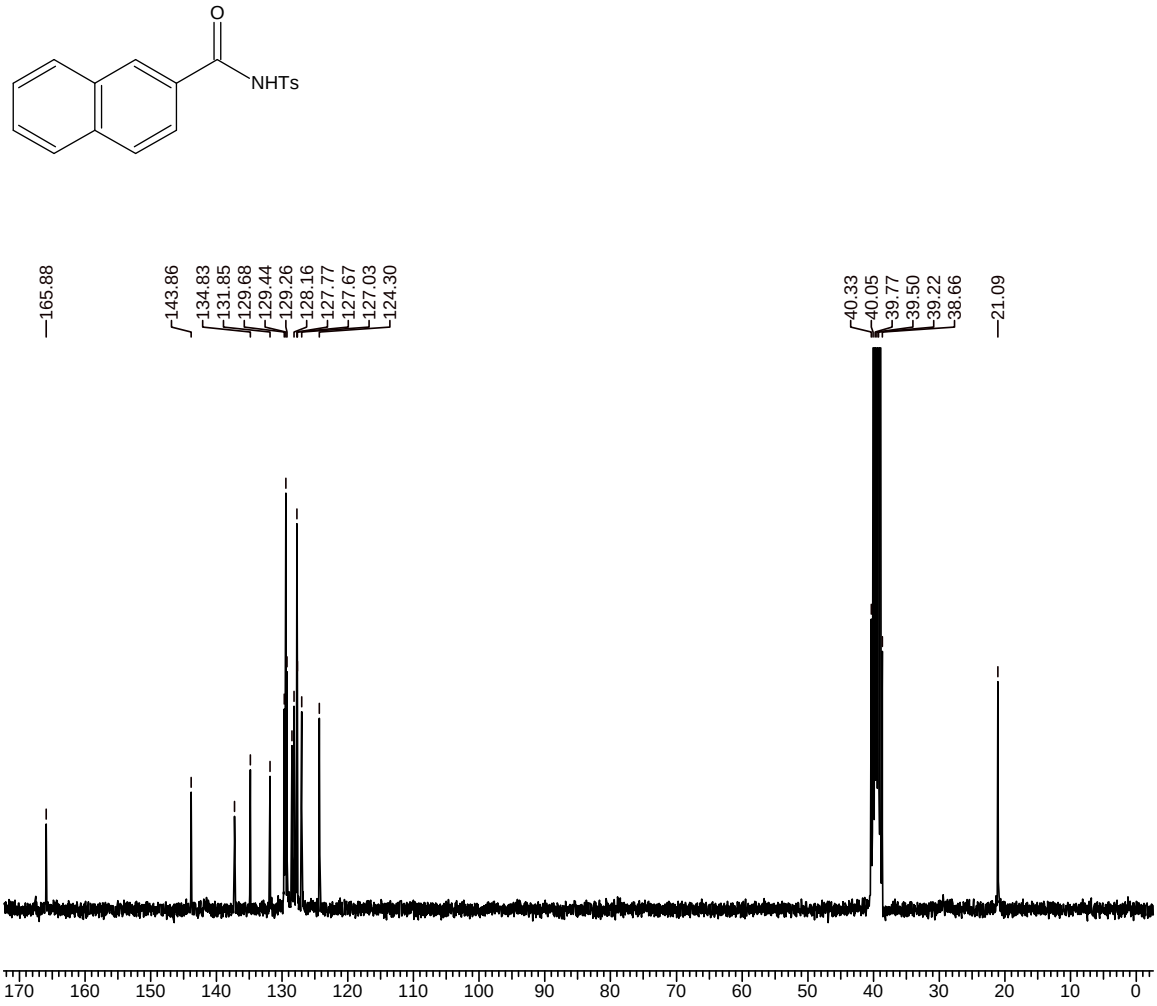




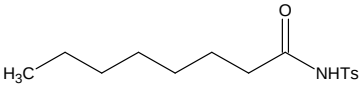
N-tosyl-2-napthamide (20b)

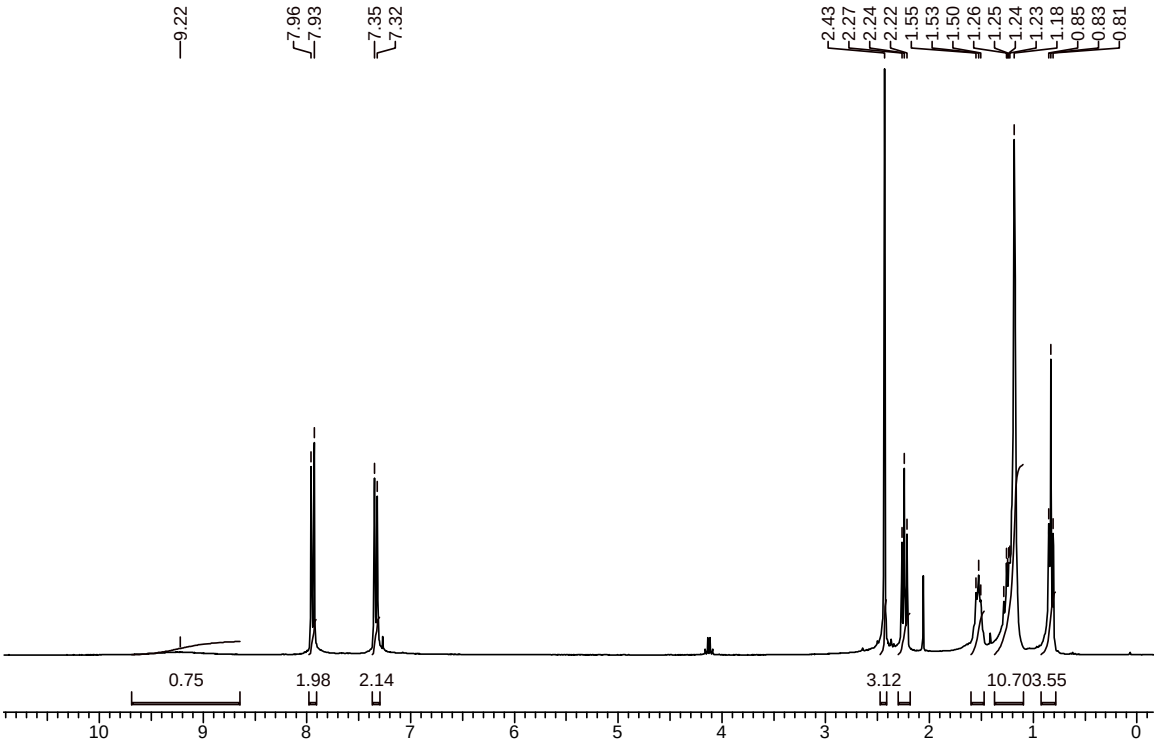


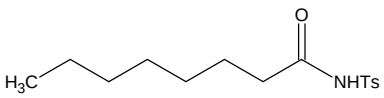


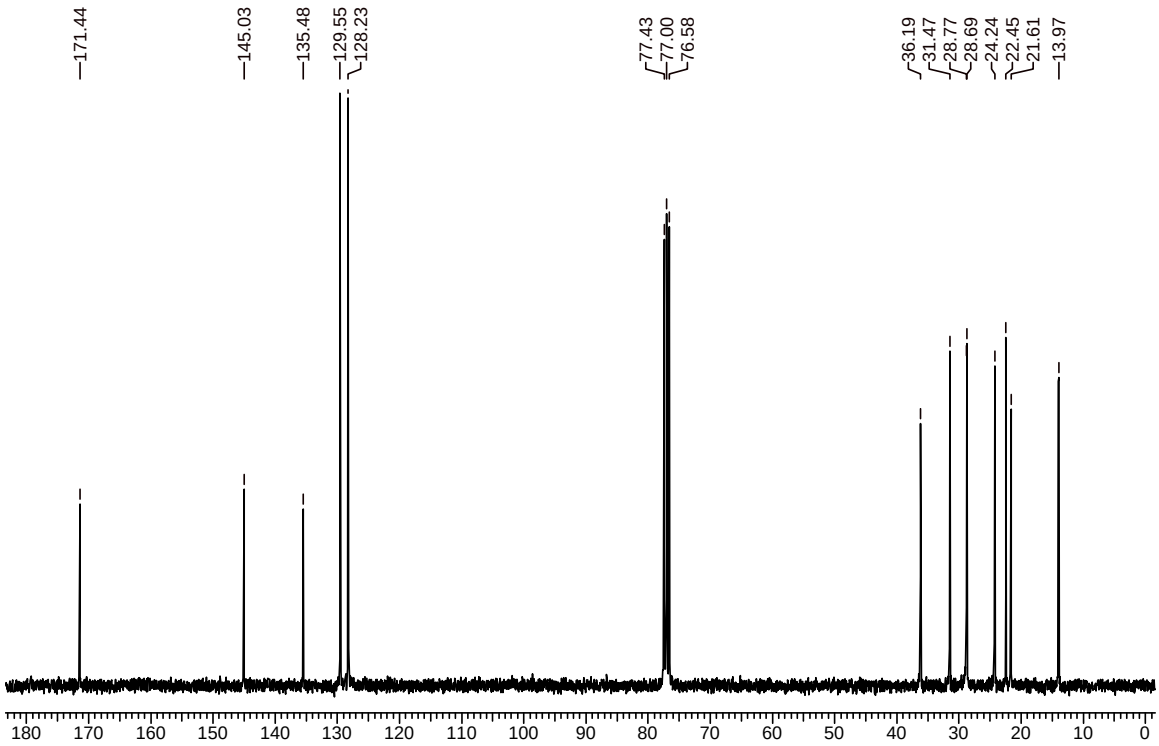


N-tosyloctanamide (21b)

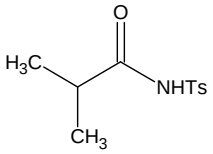


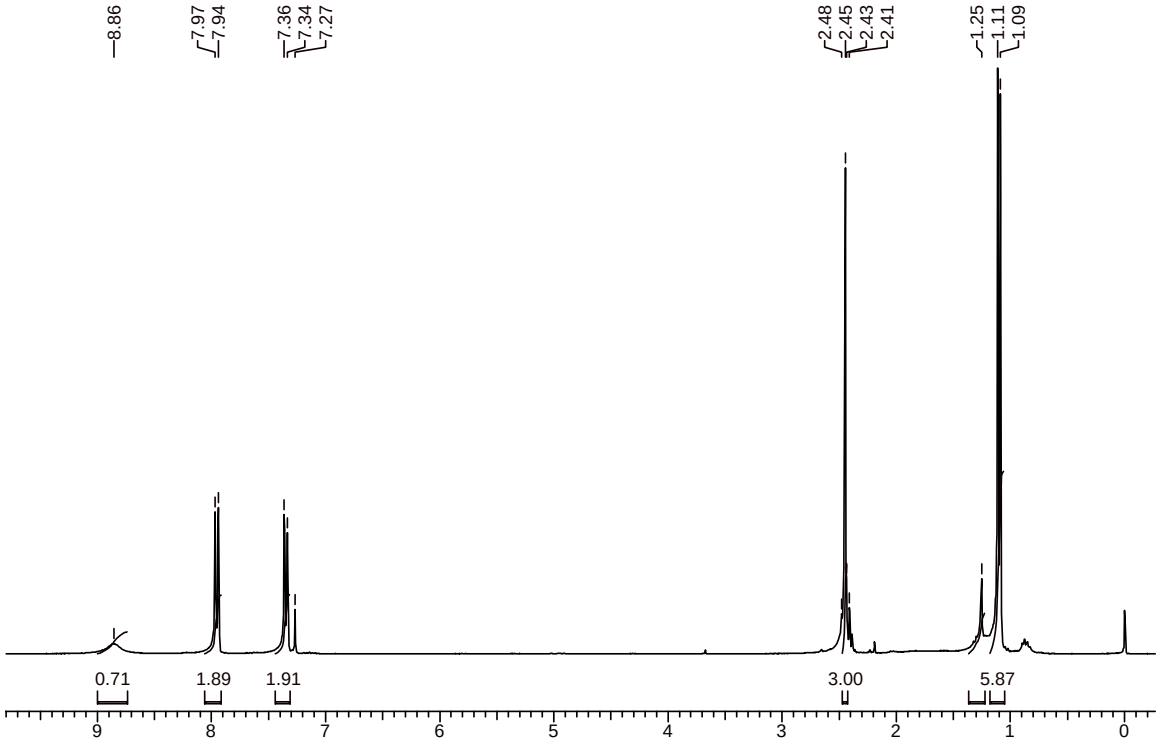


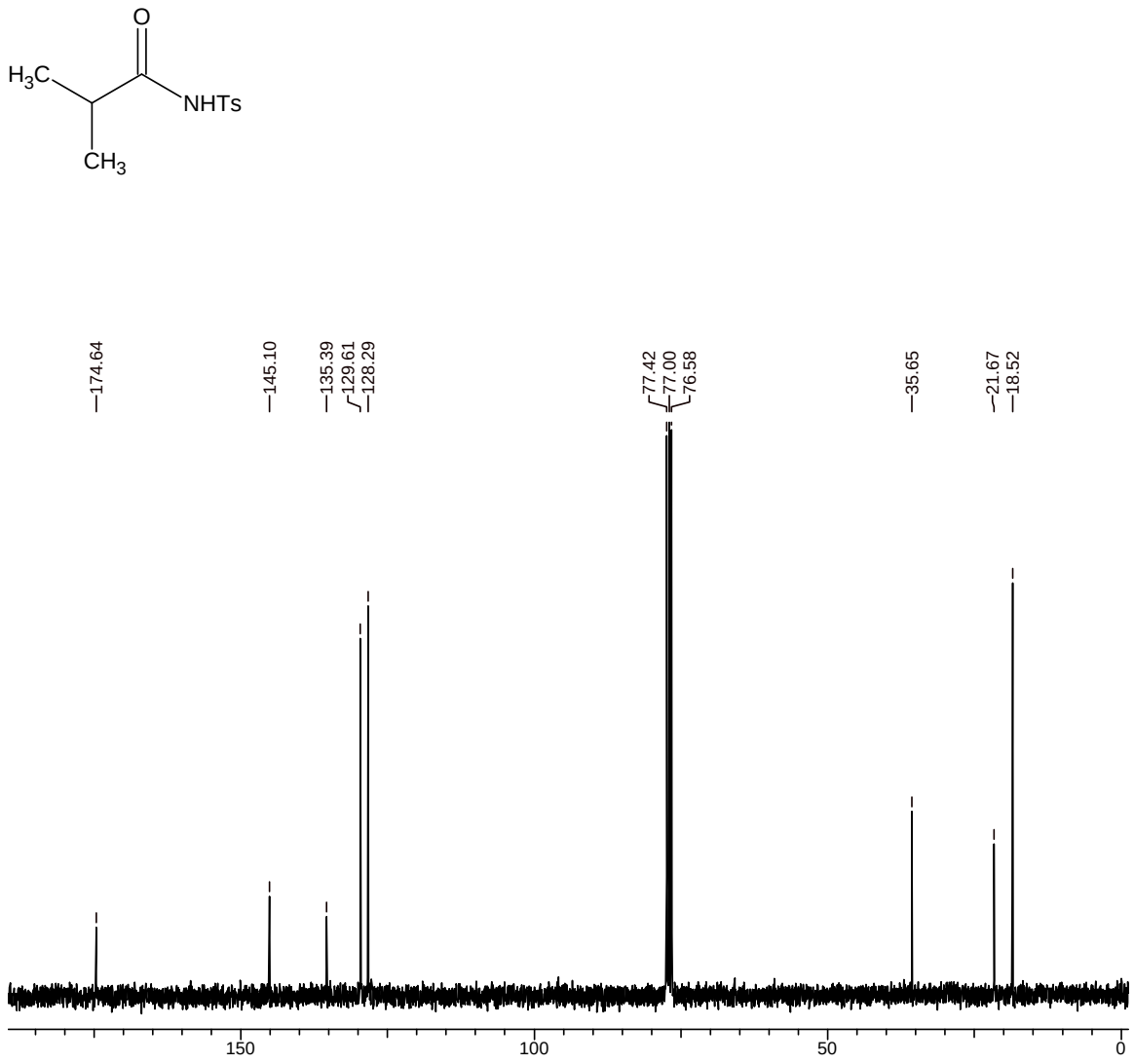




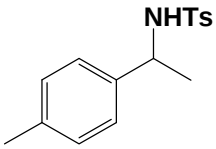
N-tosylisobutyramide (22b)

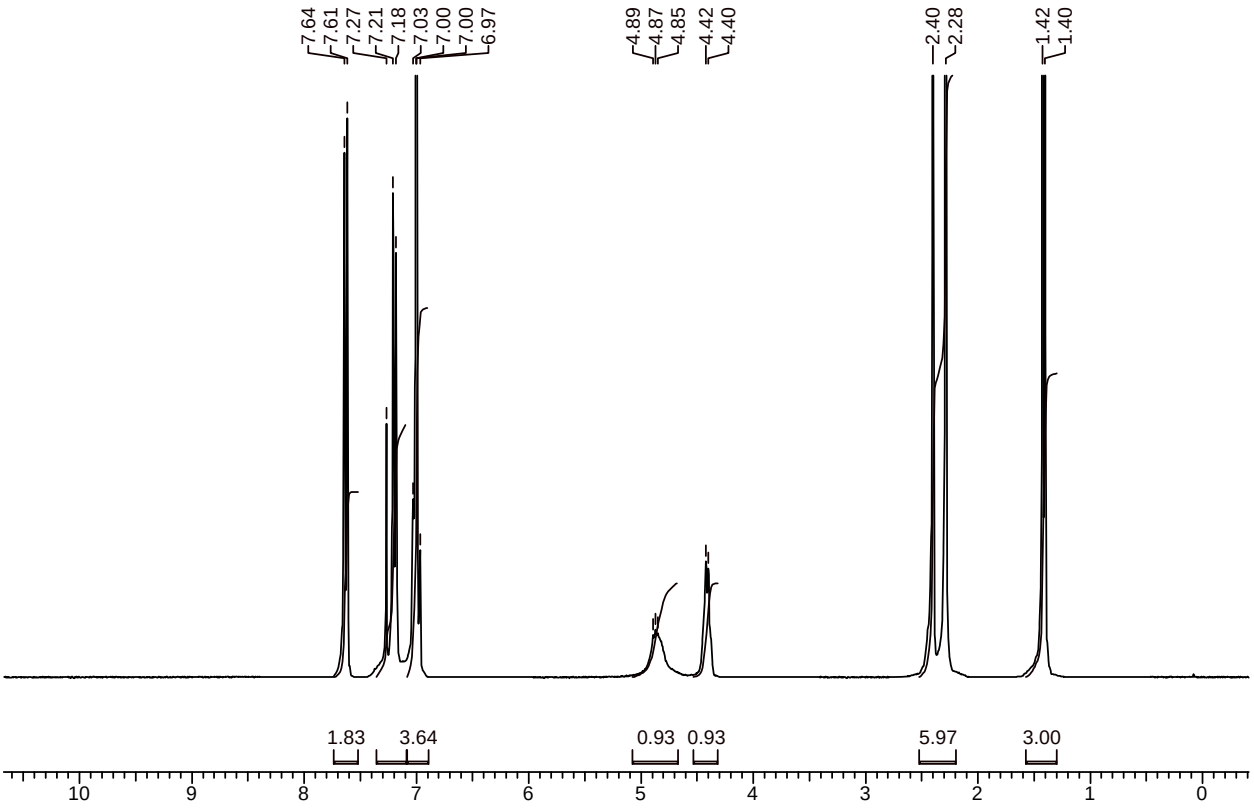


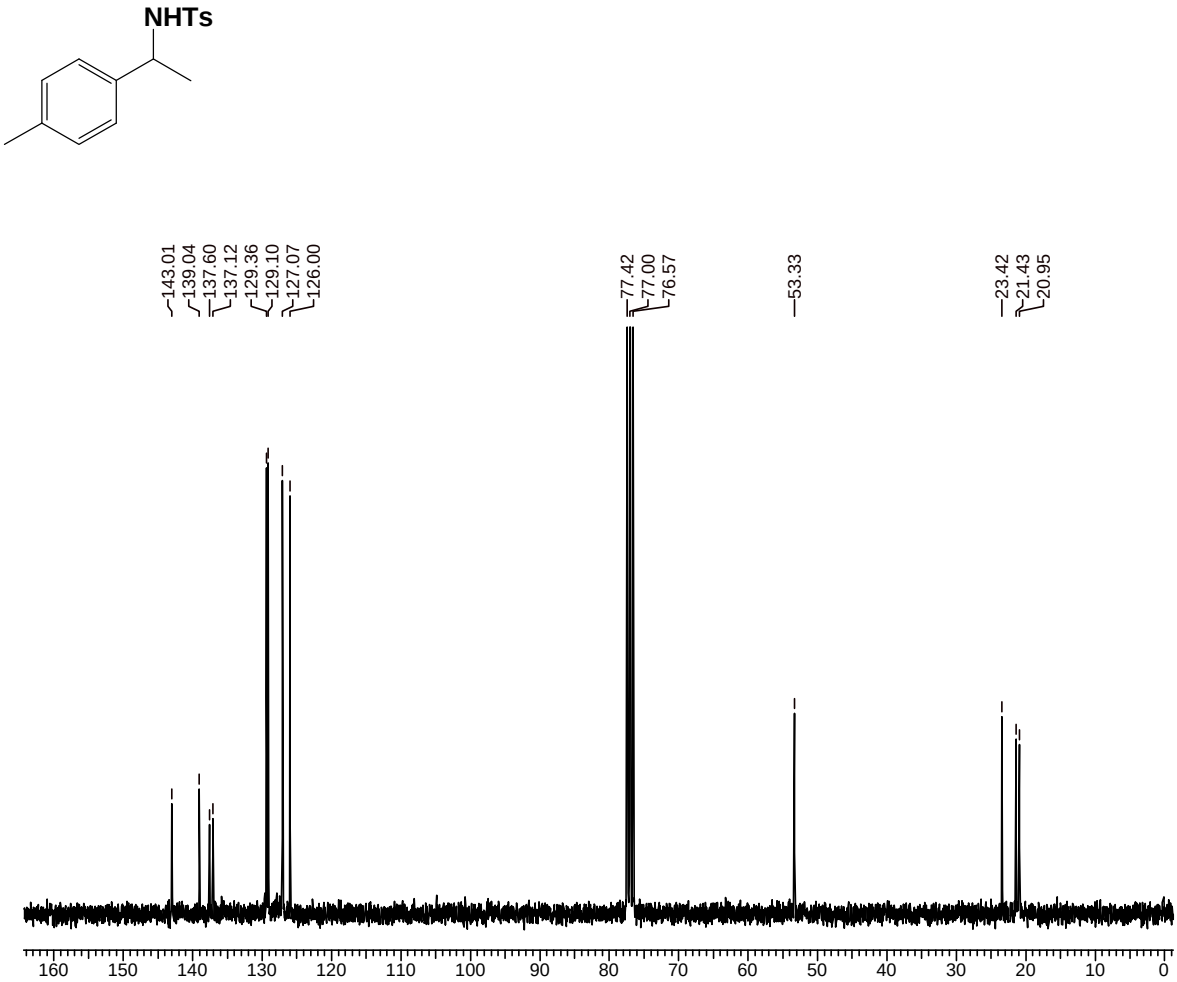




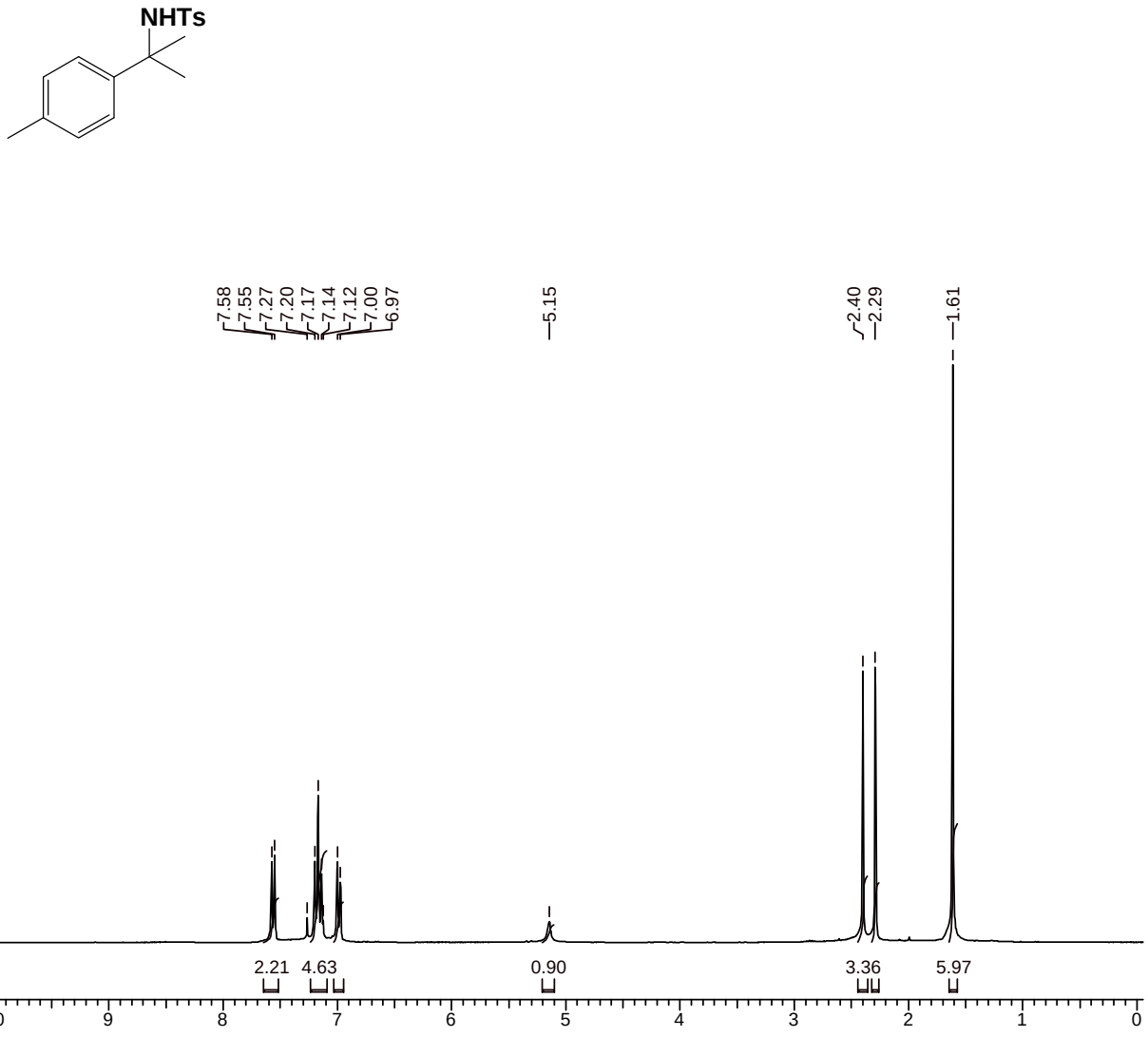
4-Methyl-*N*-[1-(4-methylphenyl)ethyl]benzenesulfonamide (23b)

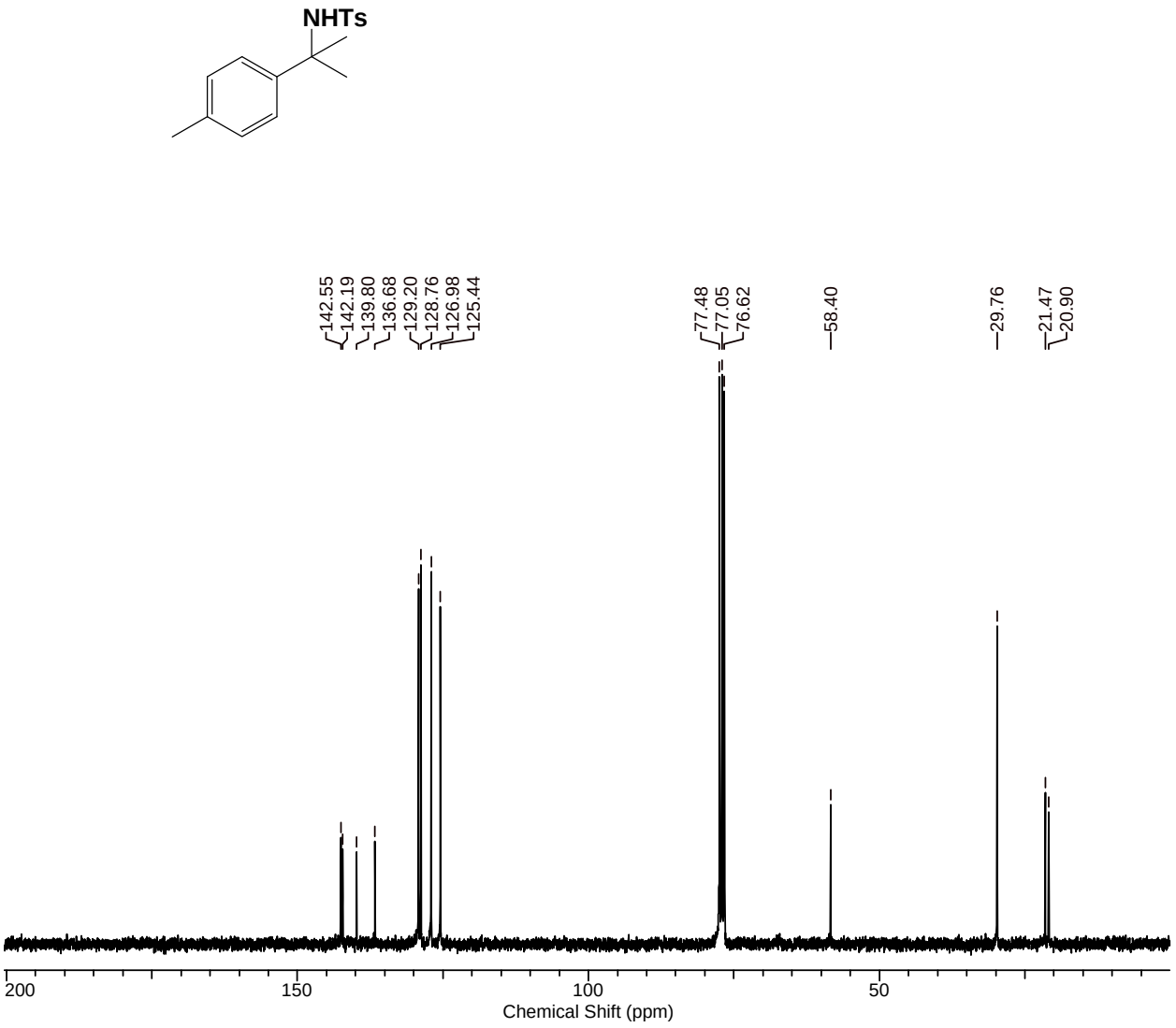




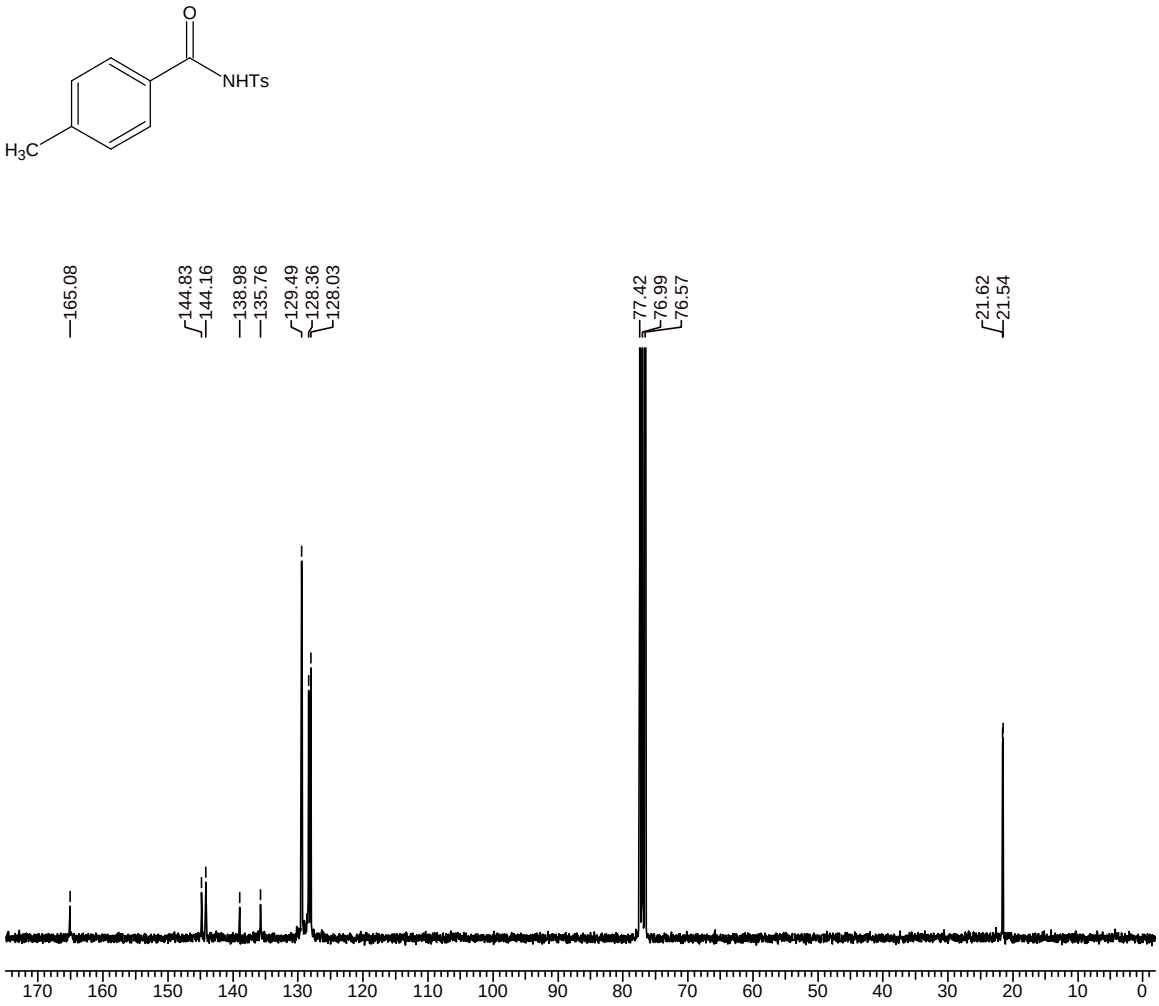


4-Methyl-*N*-[2-(4-methylphenyl)propan-2-yl]benzenesulfonamide (24b)

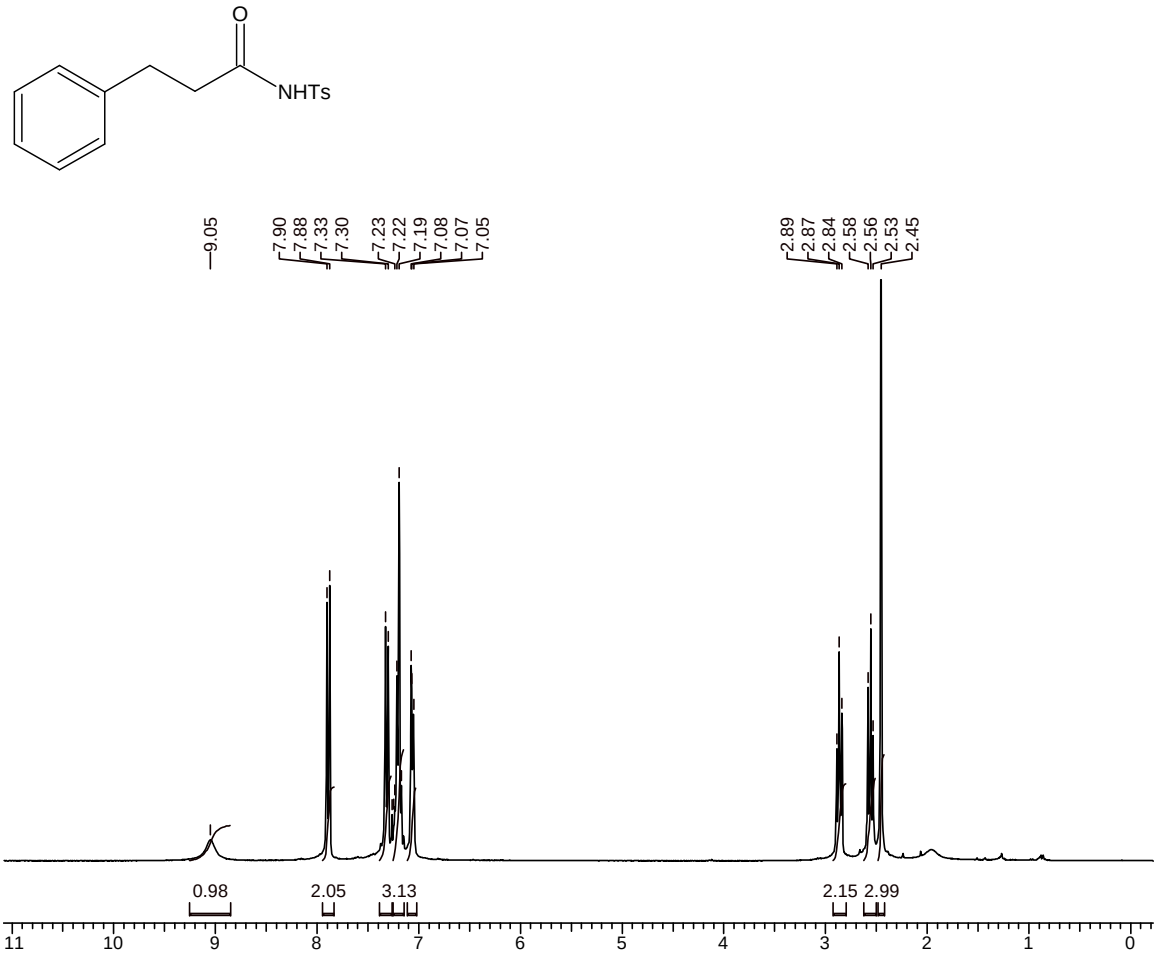


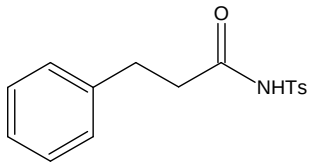


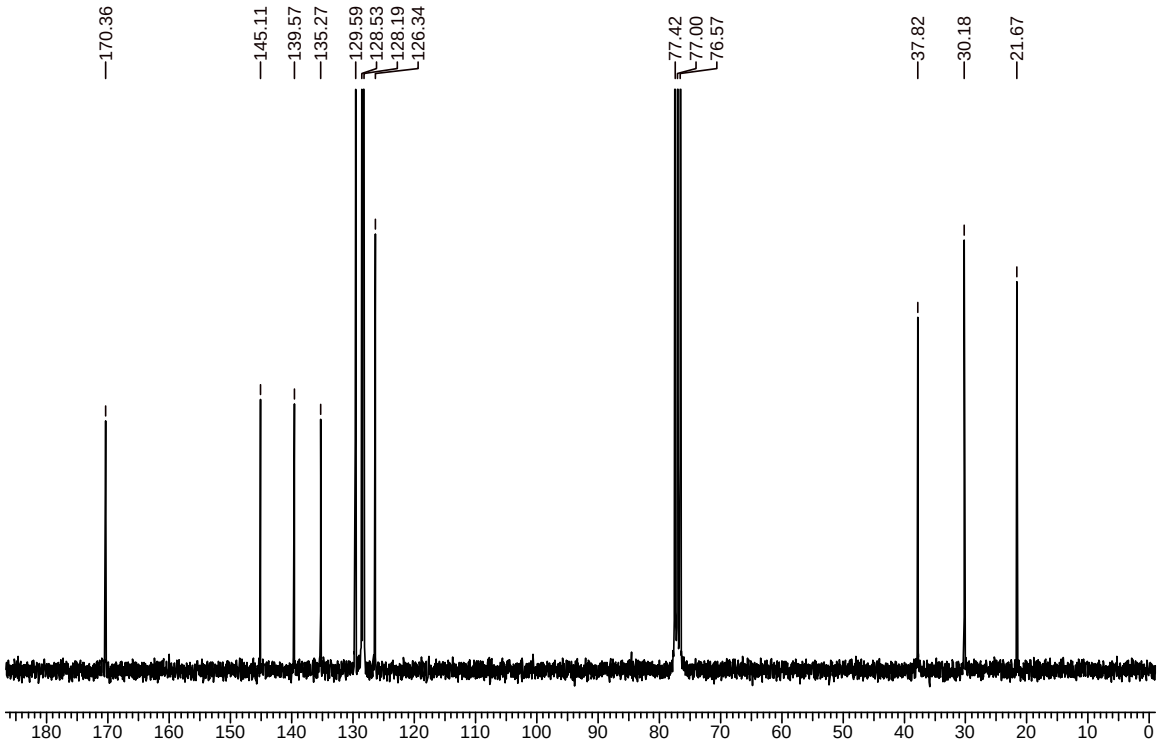
4-methyl-N-tosylbenzamide (25b)



3-phenyl-N-prpanamide (26b)

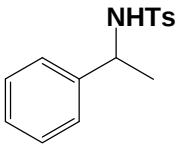




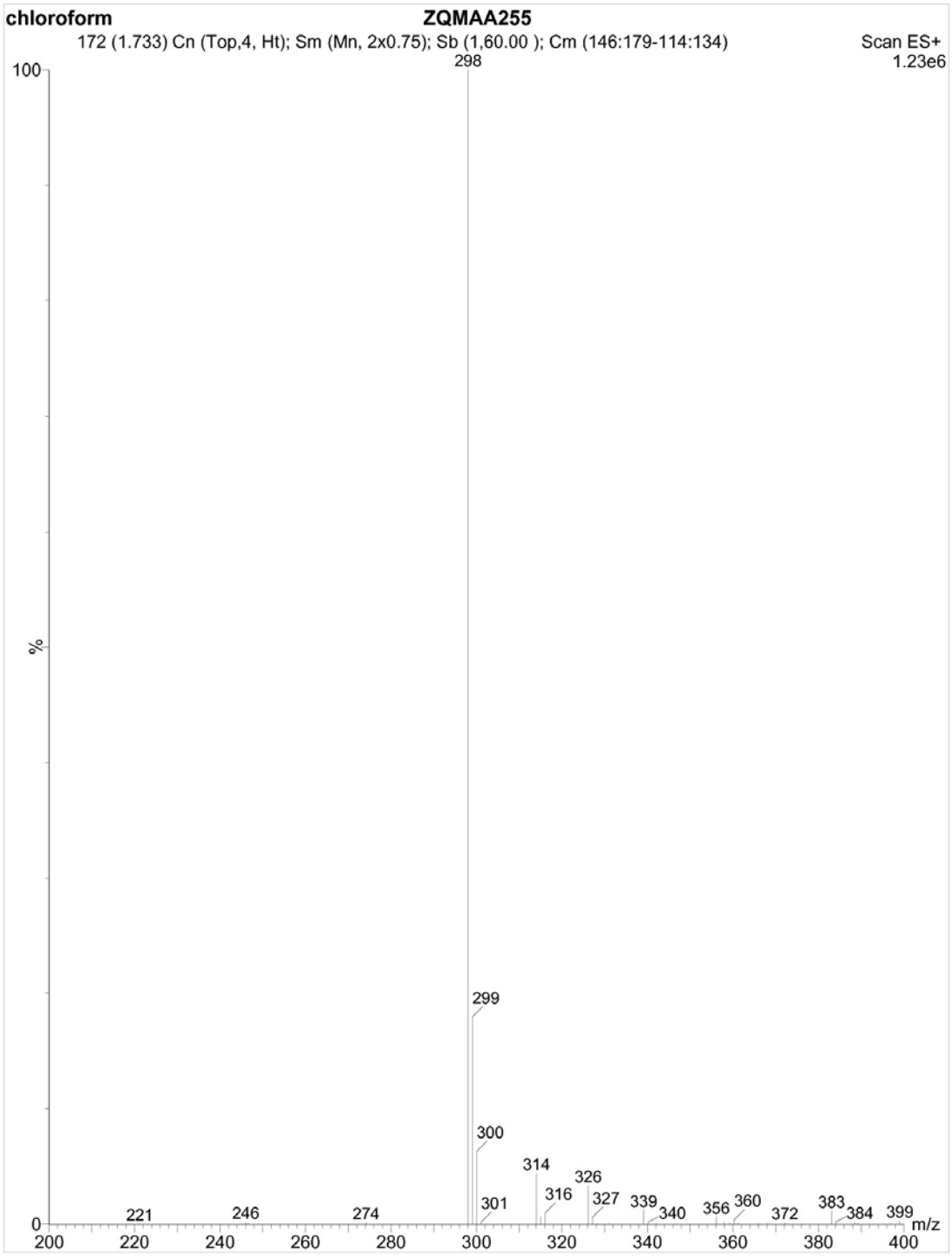


Mass Spectra

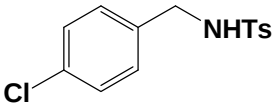
Benzylic amination reaction

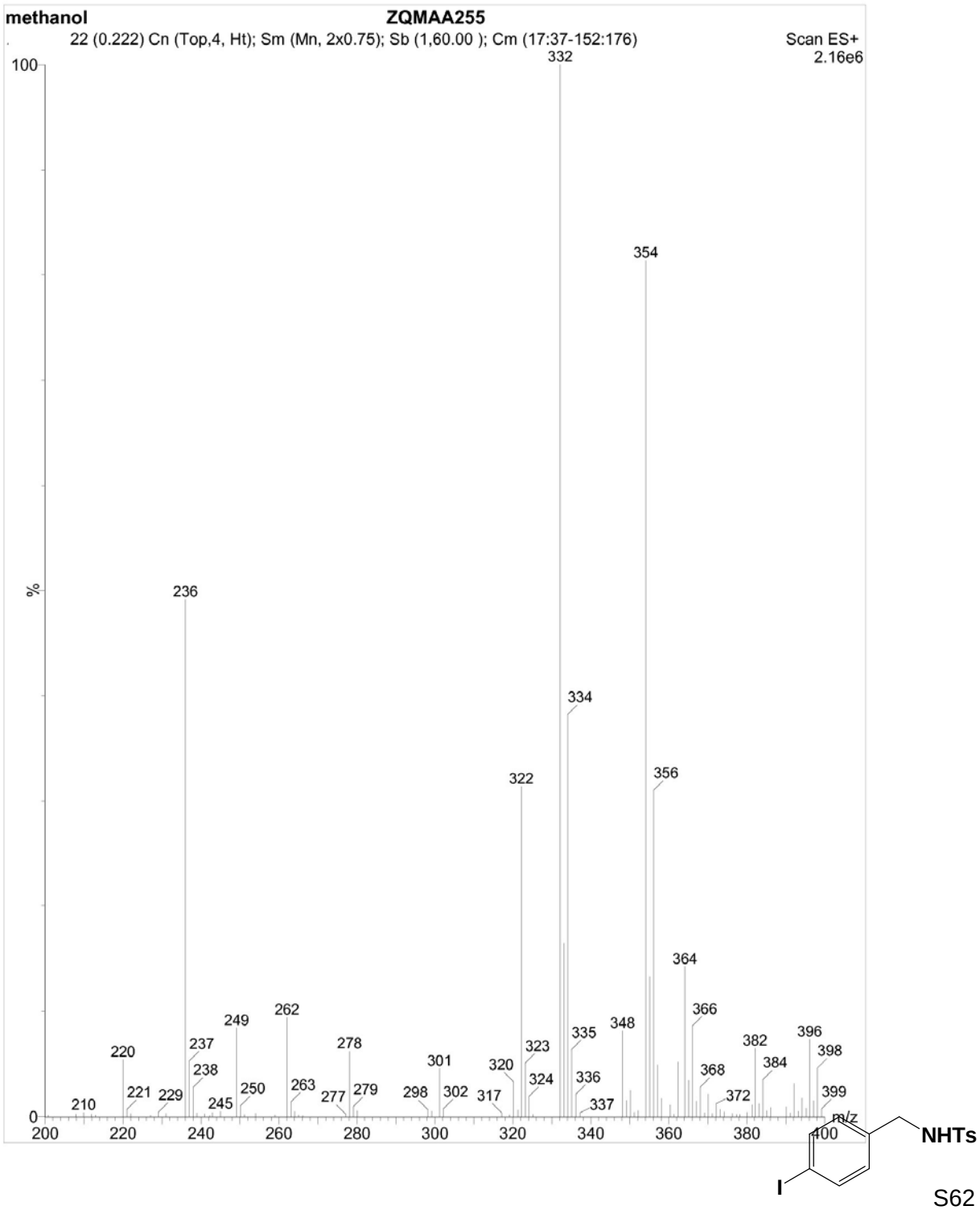


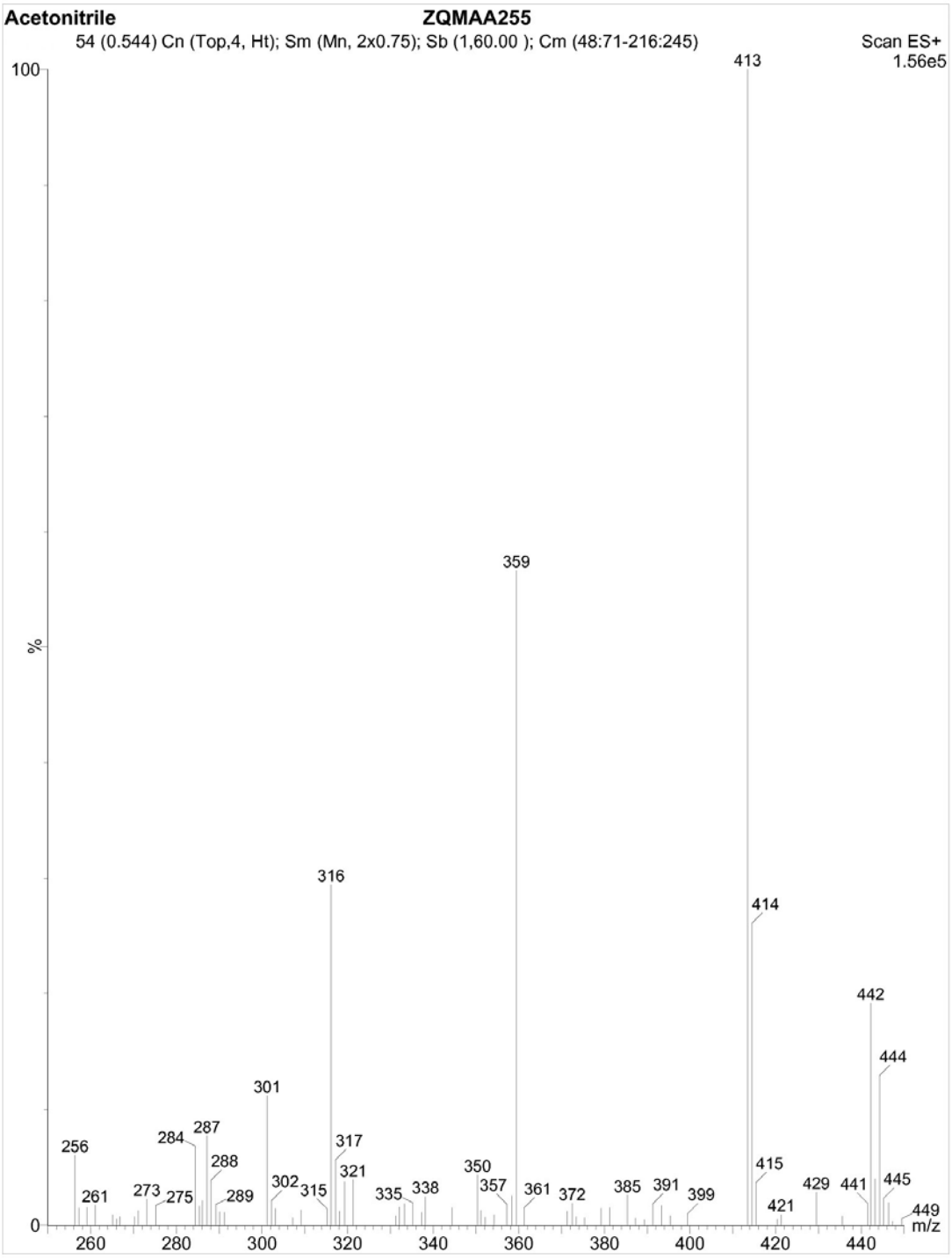
4-Methyl-*N*-(1-phenylethyl)benzenesulfonamide 6b



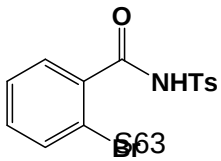
N-(4-Chlorobenzyl)-4-methylbenzenesulfonamide 9b

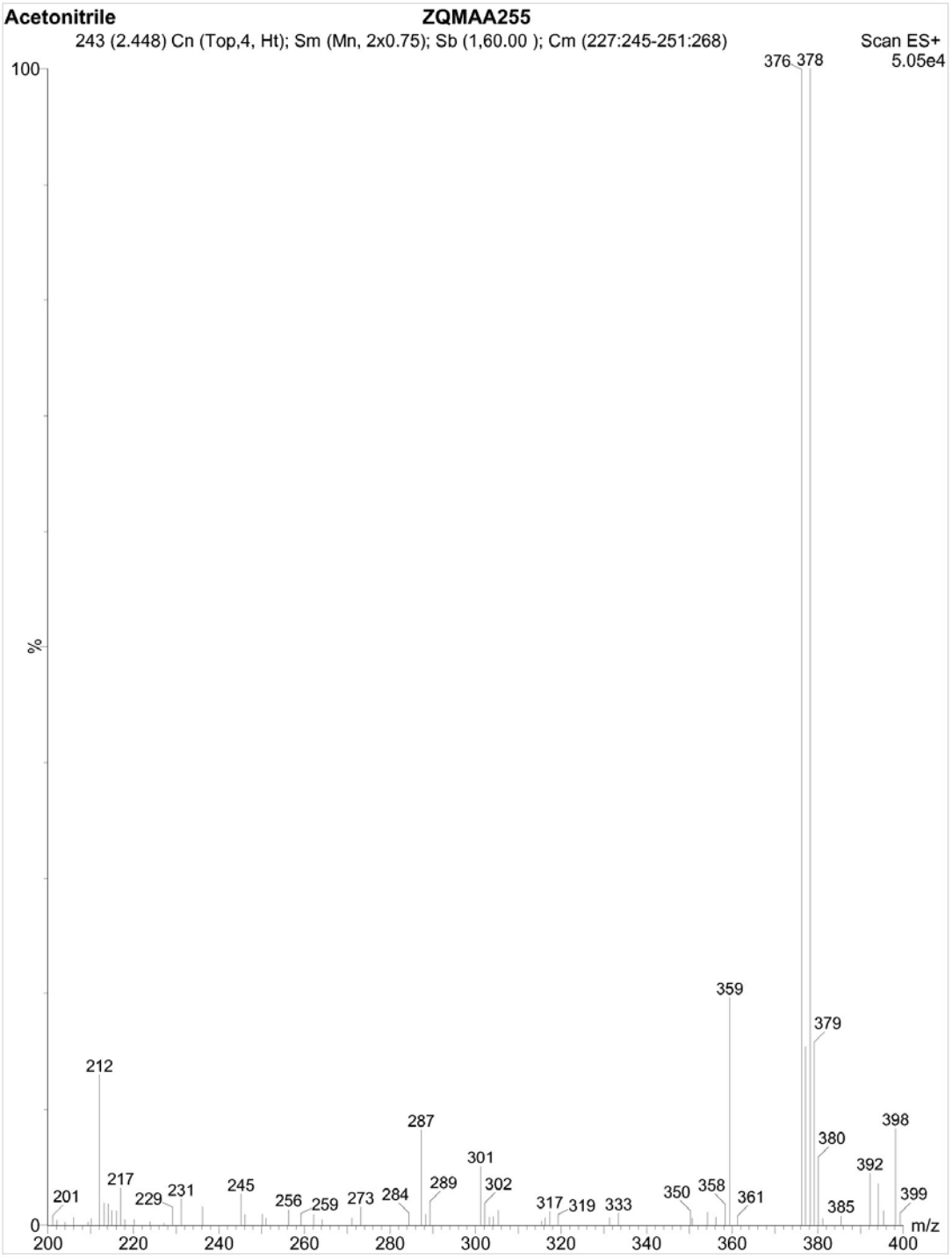


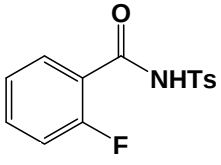


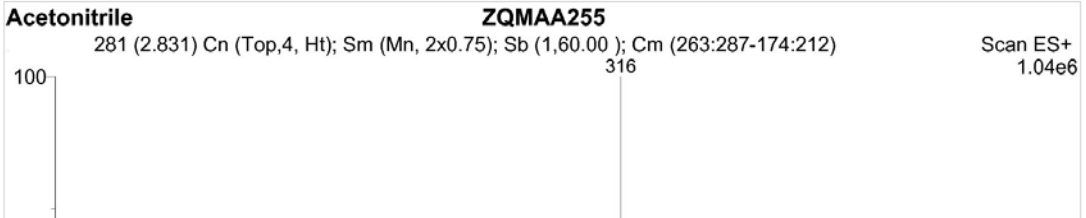


2-bromo-N-tosylbenzamide 7b

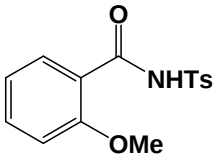


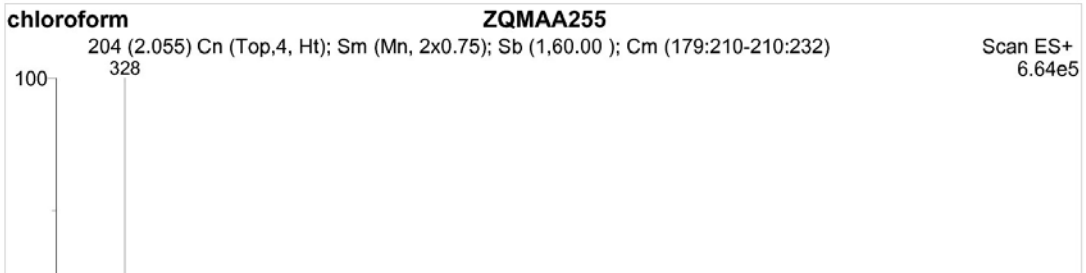

Acetonitrile
ZQMAA255
243 (2.448) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (1,60.00); Cm (227:245-251:268)
Scan ES+
5.05e4
100
%
0
376
378
359
379
212
287
398
380
301
392
217
289
302
201
229
231
245
256
259
273
284
317
319
333
350
358
361
385
399
m/z
200
220
240
260
280
300
320
340
360
380
400


O
NHTs
F

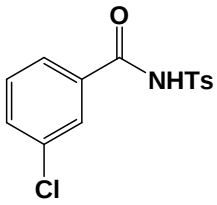

Acetonitrile
ZQMAA255
281 (2.831) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (1,60.00); Cm (263:287-174:212)
Scan ES+
1.04e6
100
316

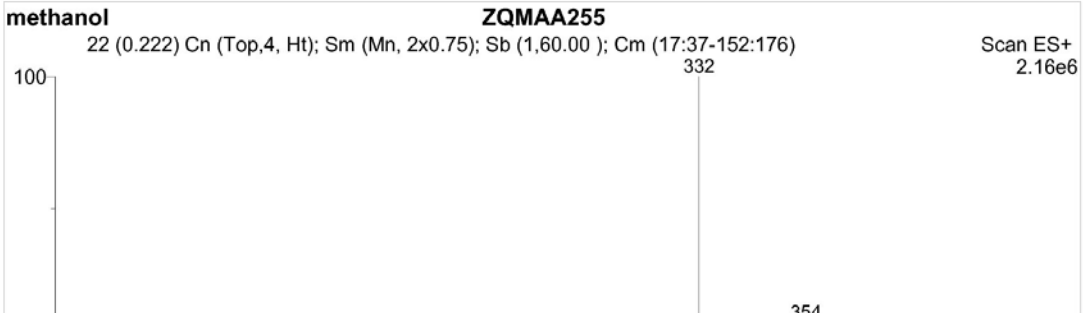
2-methoxy –N-tosylbenzamide 9b



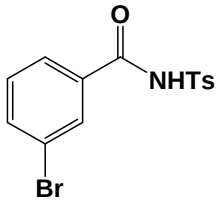


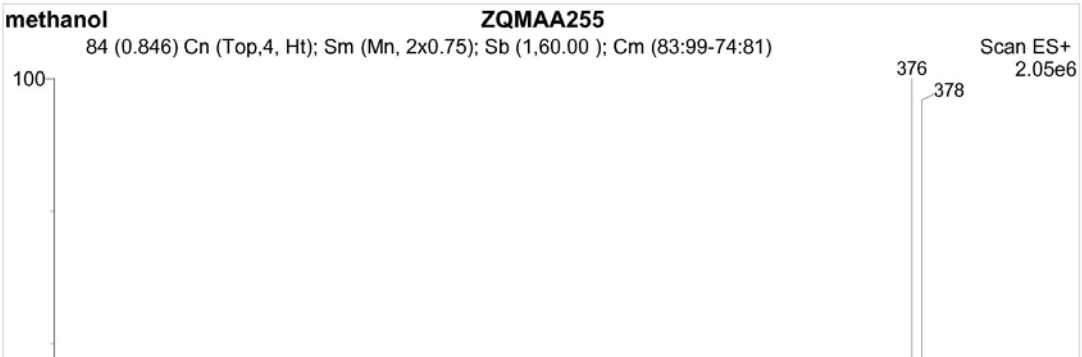
3-chloro-N-tosylbenzamide 10b



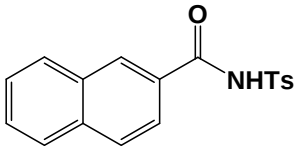


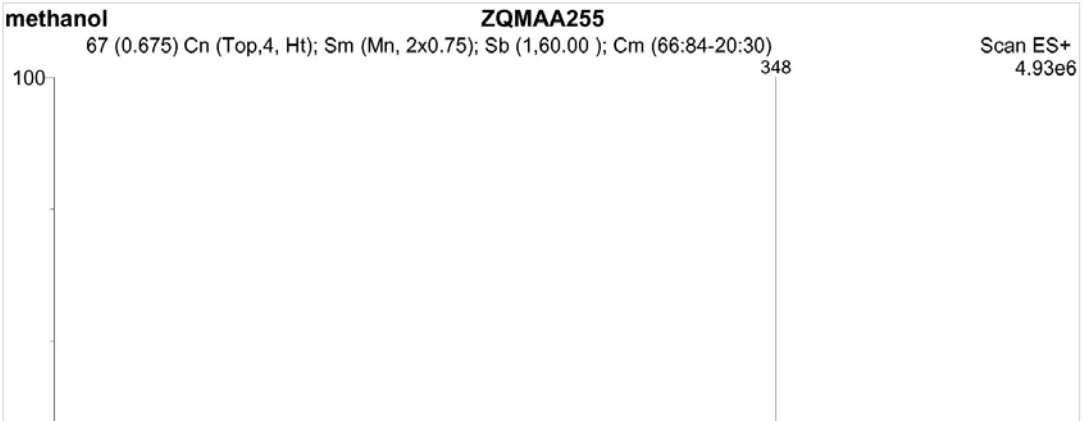
3-bromo-N-tosylbenzamide 11b





N-tosyl-2-napthamide 12b





N-tosyloctanamide 14b