Supplementary Information

Oxidative α-sulfonyloxylation of aryl ketones with sulfonic acids by lead tetraacetate

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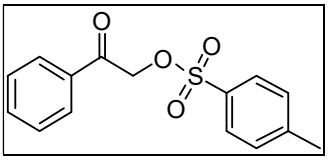
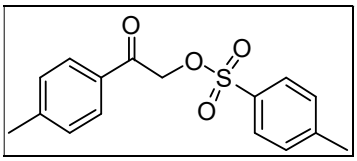
Analytical Data



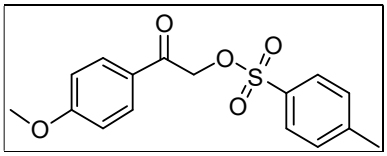
2-oxo-2-phenylethyl 4-methylbenzenesulfonate (3a)

Compound **3a** was obtained as white solid in 70% yield according to the general procedure. mp 100-102 ºC; IR (KBr film): 3069, 2920, 1706, 1596, 1364, 1187, 967 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.80-7.76 (m, 4H), 7.54 (t, J = 8 Hz, 1H), 7.40 (t, J = 8 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 5.20 (s, 2H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.3, 145.4, 134.2, 133.7, 132.6, 129.9, 128.9, 128.2, 128.0, 70.0, 21.7 ppm; MS (ES^+) calcd for $C_{15}H_{14}O_4S$ 290.0, found m/z 291.2 $[M + H]^+$.



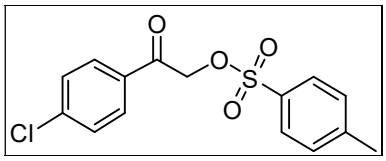
2-oxo-2-(p-tolyl)ethyl 4-methylbenzenesulfonate (3b)

Compound **3b** was obtained as white solid in 64% yield according to the general procedure. mp 90-92 ºC; IR (KBr Film): 3095, 2923, 1701, 1606, 1350, 1173, 964 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 8 Hz, 2H), 7.66 (d, J = 8 Hz, 2H), 7.27 (d, J = 8 Hz, 2H), 7.19 (d, J = 8 Hz, 2H), 5.17 (s, 2H), 2.37 (s, 3H), 2.34 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 144.3, 144.2, 131.6, 130.2, 128.9, 128.6, 127.1, 127.0, 68.9, 20.8, 20.7, ppm; MS (ES^+) calcd for $C_{16}H_{16}O_4S$ 304.0, found m/z 305.3 $[M+H]^+$.



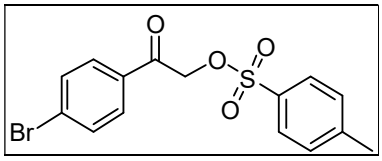
2-(4-methoxyphenyl)-2-oxoethyl-4-methylbenzenesulfonate (3c)

Compound **3c** was obtained as white solid in 68% yield according to the general procedure. mp 116-118 ºC; IR (KBr Film): 3064, 2928, 1668, 1601, 1547, 1362, 1312, 1177, 972 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79-7.775 (m, 4H), 7.28 (d, J = 8 Hz, 2H), 6.86 (d, J = 8.0 Hz, 2H), 5.14 (s, 2H), 3.80 (s, 3H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.2, 163.8, 144.8, 132.1, 129.9, 129.4, 127.6, 126.3, 113.6, 69.3, 55.1, 21.2 ppm; MS (ES^+) calcd for $C_{16}H_{16}O_5S$ 320.0, found m/z 321.2 $[M + H]^+$.



2-(4-chlorophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3d)

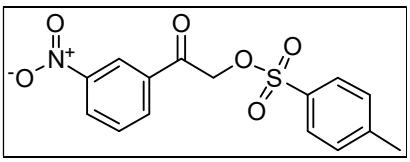
Compound **3d** was obtained as white solid in 75% yield according to the general procedure. mp 98-100 ºC; IR (KBr Film): 3068, 2966, 1702, 1593, 1361, 1174, 988, 871 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8 Hz, 2H), 7.72 (d, J = 8 Hz, 2H), 7.38 (d, J = 8 Hz, 2H), 7.28 (d, J = 8 Hz, 2H), 5.14 (s, 2H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.5, 145.5, 140.8, 132.5, 132.1, 130.0, 129.5, 129.3, 128.1, 69.8, 21.7 ppm; MS (ES^+) calcd for $C_{15}H_{13}ClO_4$ 324.0, found m/z 347.2 $[M+Na]^+$.



2-(4-bromophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3e)

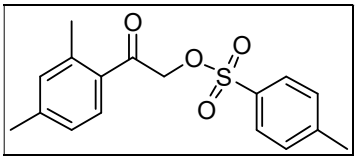
Compound **3e** was obtained as white solid in 73% yield according to the general procedure. mp 126-128 ºC; IR (KBr Film): 3099, 2920, 1708, 1589, 1368, 1192, 970, 554 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8 Hz, 2H), 7.64 (d, J = 8 Hz, 2H), 7.55 (d, J = 8 Hz, 2H), 7.28 (d, J = 8 Hz, 2H), 5.13 (s, 2H), 2.39 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.7, 145.5, 132.4, 132.4, 132.3, 130.0, 129.5, 128.1, 69.8, 21.7 ppm; MS (ES^+) calcd for $C_{15}H_{13}BrO_4S$ 369.9, found m/z

371.1 [M+2].



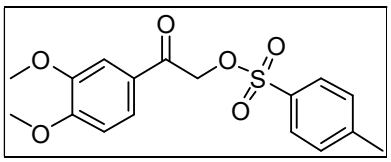
2-(3-nitrophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3f)

Compound **3f** was obtained as white solid in 71% yield according to the general procedure. mp 116-118 ºC; IR (KBr Film): 3090, 2929, 1712, 1615, 1524, 1362, 1173, 970 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (t, J = 2 Hz , 1H), 8.47-8.44 (m, 1H), 8.22-8.19 (m, 1H), 7.83 (d, J = 8 Hz, 2H), 7.71 (t, J = 8 Hz, 1H), 7.36 (d, J = 8 Hz, 2H), 5.25 (s, 2H), 2.45 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.2, 148.4, 145.8, 135.0, 133.8, 132.2, 130.3, 130.1, 128.3, 128.2, 123.1, 70.0, 21.7 ppm. MS (ES^+) calcd for $C_{15}H_{13}NO_6S$ 335.3, found m/z 336.2 $[M + H]^+$.



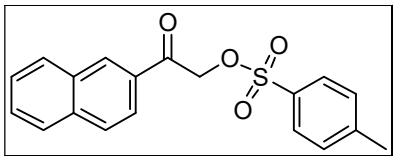
2-(2,4-dimethylphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3g)

Compound **3g** was obtained as white solid in 68% yield according to the general procedure. mp 55-57 ºC; IR (KBr Film): 3068, 2978, 1707, 1607, 1564, 1361, 1173, 972 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, J = 8 Hz, 2H), 7.7 (d, J = 8 Hz, 1H), 7.34 (d, J = 8 Hz, 2H), 7.07-7.05 (m, 2H), 5.12 (s, 2H), 2.45 (s, 3H), 2.7 (s, 3H), 2.36 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.7, 145.2, 17.5, 141.4, 140.0, 133.3, 132.7, 129.9, 128.9, 128.1, 126.5, 70.8, 21.7, 21.5, 21.3 ppm. MS (ES^+) calcd for $C_{17}H_{18}O_4S$ 318.3, found m/z 319.3 $[M + H]^+$.



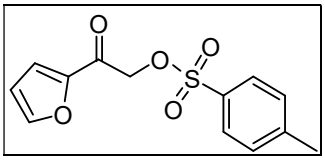
2-(3,4-dimethoxyphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3h)

Compound **3h** was obtained as white solid in 64% yield according to the general procedure. mp 117-119 ºC; IR (KBr Film): 3069, 2936, 177, 1678, 1593, 1355, 1300, 1269, 1177, 993 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 8 Hz, 2H), 7.40-7.35 (m, 2H), 7.28 (d, J = 8 Hz, 2H), 6.81 (d, J = 8 Hz, 1H), 5.16 (s, 3H), 3.88 (s, 3H), 3.85 (s, 3H), 2.38(s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 154.2, 149.4, 145.3, 132.7, 129.9, 128.2, 126.9, 122.8, 110.2, 110.1, 69.8, 56.2, 56.1, 21.7 ppm; MS (ES^+) calcd for $C_{17}H_{18}O_6S$ 350.4, found m/z 351.3 $[M + H]^+$.



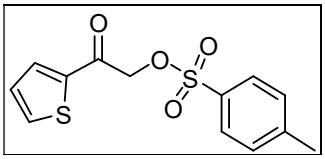
2-(naphthalen-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3i)

Compound **3i** was obtained as white solid in 66% yield according to the general procedure. mp 118-120 ºC; IR (KBr Film): 3068, 2953, 1699, 1596, 1372, 1186, 991 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.35 (s, 1H), 7.94 (d, J = 8 Hz, 1H), 7.89-7.87 (m, 5H), 7.66-7.56 (m, 2H), 7.34 (d, J = 8 Hz, 2H), 5.40 (s, 2H), 2.44 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.3, 145.3, 136.0, 132.7, 132.3, 131.1, 130.0, 129.9, 129.6, 129.2, 128.9, 128.2, 127.9, 127.2, 123.3, 70.0, 21.7 ppm; MS (ES^+) calcd for $C_{19}H_{16}O_4S$ 340.1, found m/z 341.3 $[M+H]^+$.



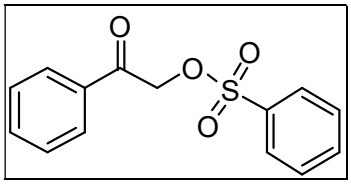
2-(furan-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3j)

Compound **3j** was obtained as white solid in 59% yield according to the general procedure. mp 90-92 ºC; IR (KBr Film): 3069, 2920, 1708, 1589, 1367, 1192, 970 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 8 Hz, 2H), 7.54 (d, J = 1.2 Hz, 1H), 7.30-7.26 (m, 3H), 6.52-6.51 (m, 1H), 5.02 (s, 2H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 179.4, 149.9, 147.3, 145.4, 132.4, 130.0, 128.1, 119.1, 112.8, 69.4, 21.7 ppm; MS (ES^+) calcd for $C_{13}H_{12}O_5S$ 280.0, found m/z 281.2 $[M+H]^+$.



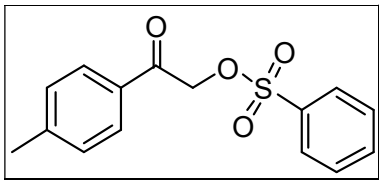
2-oxo-2-(thiophen-2-yl)ethyl 4-methylbenzenesulfonate (3k)

Compound **3k** was obtained as white solid in 62% yield according to the general procedure. mp 84-86 ºC; IR (KBr Film): 3088, 2958, 1683, 1595, 1383, 1186, 924, 847 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 8 Hz , 2H), 7.95 (dd, J = 4.0 Hz (0.8,0.8 Hz), 1H), 7.88 (dd, J = 4.0 Hz (0.8, 0.8 Hz), 1H), 7.51 (d, J = 8.0 Hz, 2H), 7.32-7.30 (m,1H), 5.24 (s, 2H), 2.60 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 183.7, 145.5, 140.0, 135.2, 133.2, 132.3, 130.0, 128.5, 128.2, 69.9, 21.7 ppm; MS (ES^+) calcd for $C_{13}H_{12}O_4S_2$ 296.0, found m/z 297.2 $[M+H]^+$.



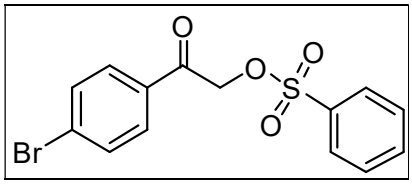
2-oxo-2-phenylethyl benzenesulfonate (3l)

Compound **3l** was obtained as white solid in 77% yield according to the general procedure. mp 78-80 ºC; IR (KBr Film): 3069, 2960, 1702, 1590, 1372, 1189, 967 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, J = 8 Hz, 2H), 7.77 (d, J = 8 Hz, 2H), 7.61 (t, J = 8 Hz, 1H), 7.56-7.48 (m, 3H), 7.41 (t, J = 8 Hz, 2H), 5.24 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 135.7, 134.3, 134.2, 129.3, 129.0, 128.6, 128.1, 128.0, 70.1 ppm; MS (ES^+) calcd for $C_{14}H_{12}O_4S$ 276.3, found m/z 277.3 $[M + H]^+$.



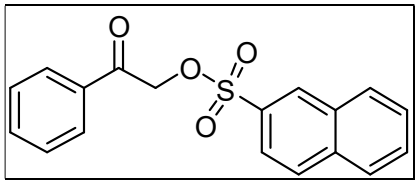
2-oxo-2-(p-tolyl)ethyl benzenesulfonate (3m)

Compound **3m** was obtained as white solid in 74% yield according to the general procedure. mp 93-95 ºC; IR (KBr Film): 3087, 2956, 1701, 1605, 1371, 1189, 967 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, J = 8 Hz, 2H), 7.67 (d, J = 8 Hz, 2H), 7.61 (t, J = 8 Hz, 1H), 7.50 (t, J = 8 Hz, 2H), 7.20 (d, J = 12 Hz, 2H), 5.21 (s, 2H), 2.34 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.7, 145.4, 135.7, 134.2, 131.2, 129.6, 129.3, 128.1, 128.0, 70.0, 21.8 ppm. HRMS calcd for $C_{15}H_{14}O_4S$ $[M + H]^+$ 291.0691, found, 291.0702.



2-(4-bromophenyl)-2-oxoethyl benzenesulfonate (3n)

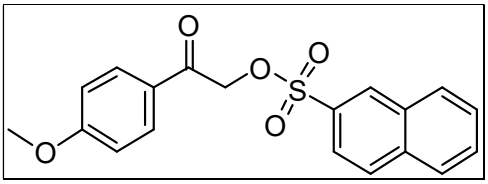
Compound **3n** was obtained as white solid in 81% yield according to the general procedure. mp 108-110 ºC; IR (KBr Film): 3062, 2963, 1699, 1585, 1369, 1189, 972, 556 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 8 Hz, 2H), 7.71-7.66 (m, 3H), 7.63-7.55 (m, 4H), 5.24 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.5, 135.5, 134.3, 132.3, 131.9, 129.6, 129.5, 129.4, 128.1, 69.9 ppm; HRMS calcd for $C_{14}H_{11}BrO_4S$ $[M + H]^+$ 354.9640, found, 354.9644.



2-oxo-2-phenylethyl naphthalene-2-sulfonate (3o)

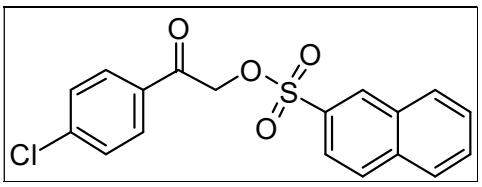
Compound **3o** was obtained as white solid in 84% yield according to the general procedure. mp 84-86 ºC; IR (KBr Film): 3058, 2962, 1707, 1592, 1369, 1175, 967 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.54 (s, 1H), 7.99 (t, J = 8 Hz, 2H), 7.93 (dd, J =1.6, 1.6 Hz, 2H), 7.81 (dd, J = 0.8, 1.2 Hz, 2H), 7.71-7.57 (m, 3H), 7.44 (t, J = 8 Hz, 2H), 5.32 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 135.4, 134.2,

133.7, 132.4, 131.9, 130.0, 129.8, 129.6, 129.4, 128.9, 128.0, 128.0, 127.9, 122.6, 70.2 ppm; MS (ES^+) calcd for $C_{18}H_{14}O_4S$ 326.4, found m/z 327.3 $[M + H]^+$.



2-(4-methoxyphenyl)-2-oxoethyl naphthalene-2-sulfonate (3p)

Compound **3p** was obtained as white solid in 80% yield according to the general procedure. p 115-117 ºC; IR (KBr Film): 3059, 2927, 1687, 1601, 1361, 1247, 1174, 973 cm^{-1}; m^1H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 7.93 (t, J = 8 Hz, 2H), 7.87 (dd, J =1.6, 1.6 Hz, 2H), 7.74 (d, J = 12 Hz, 2H), 7.65-7.55 (m, 2H), 6.84 (d, J = 12 Hz, 2H), 5.19 (s, 2H), 3.79 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.6, 164.3, 135.4, 132.5, 132.3, 131.9, 130.4, 130.0, 129.7, 129.5, 129.4, 128.0, 127.8, 122.7, 114.1, 70.0, 55.6 ppm; HRMS calcd for $C_{19}H_{16}ClO_4S$ $[M + H]^+$ 357.0797, found, 357.0816.

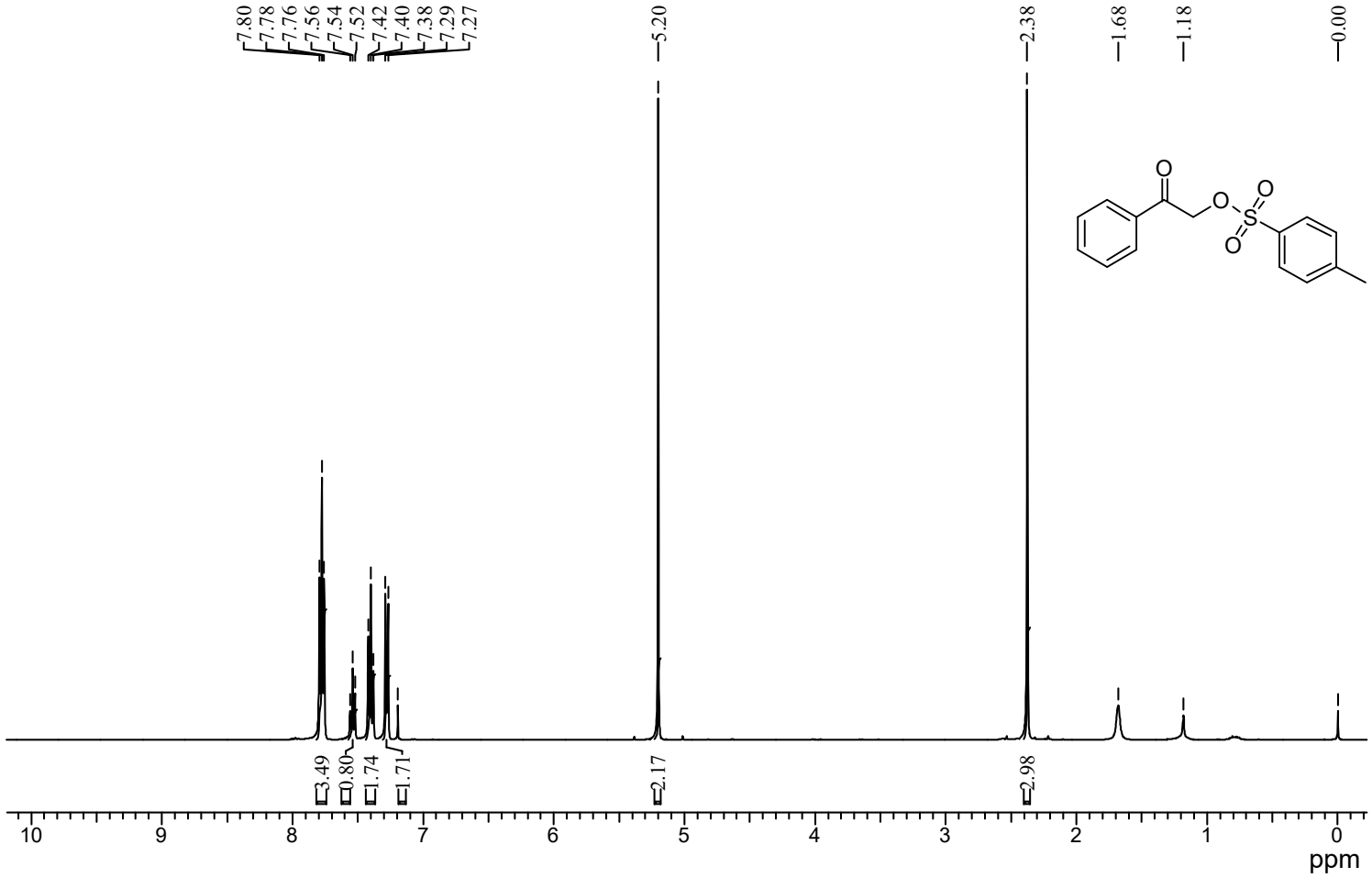


2-(4-chlorophenyl)-2-oxoethyl naphthalene-2-sulfonate (3q)

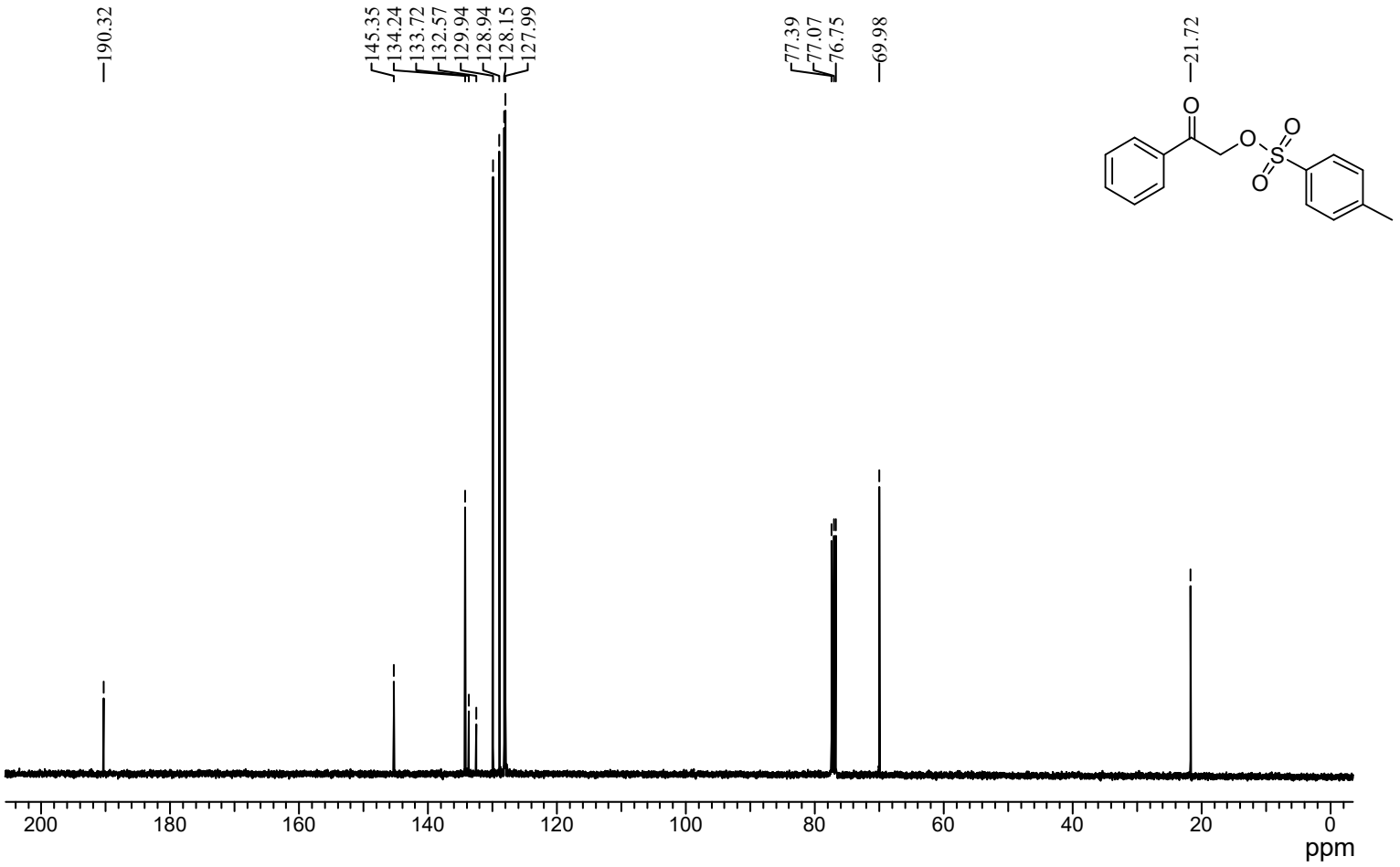
Compound **3q** was obtained as white solid in 89% yield according to the general procedure. mp 56-58 ºC; IR (KBr Film): 3070, 2928, 1698, 1591, 1365, 1175, 999, 724 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (s, 1H), 7.93 (t, J = 8 Hz, 2H), 7.88-7.83 (m, 2H), 7.69 (d, J = 12 Hz, 2H), 7.66-7.57 (m, 2H), 7.34 (d, J = 8 Hz, 2H), 5.19 (s, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.4, 135.5, 132.3,130.1, 129.8, 129.7, 129.7, 129.5, 129.4, 129.3, 129.2, 128.9, 128.1, 127.9, 122.6, 70.1 ppm; HRMS calcd for $C_{18}H_{13}ClO_4S$ $[M + H]^+$ 361.0301, found, 361.0313.

Spectral Data

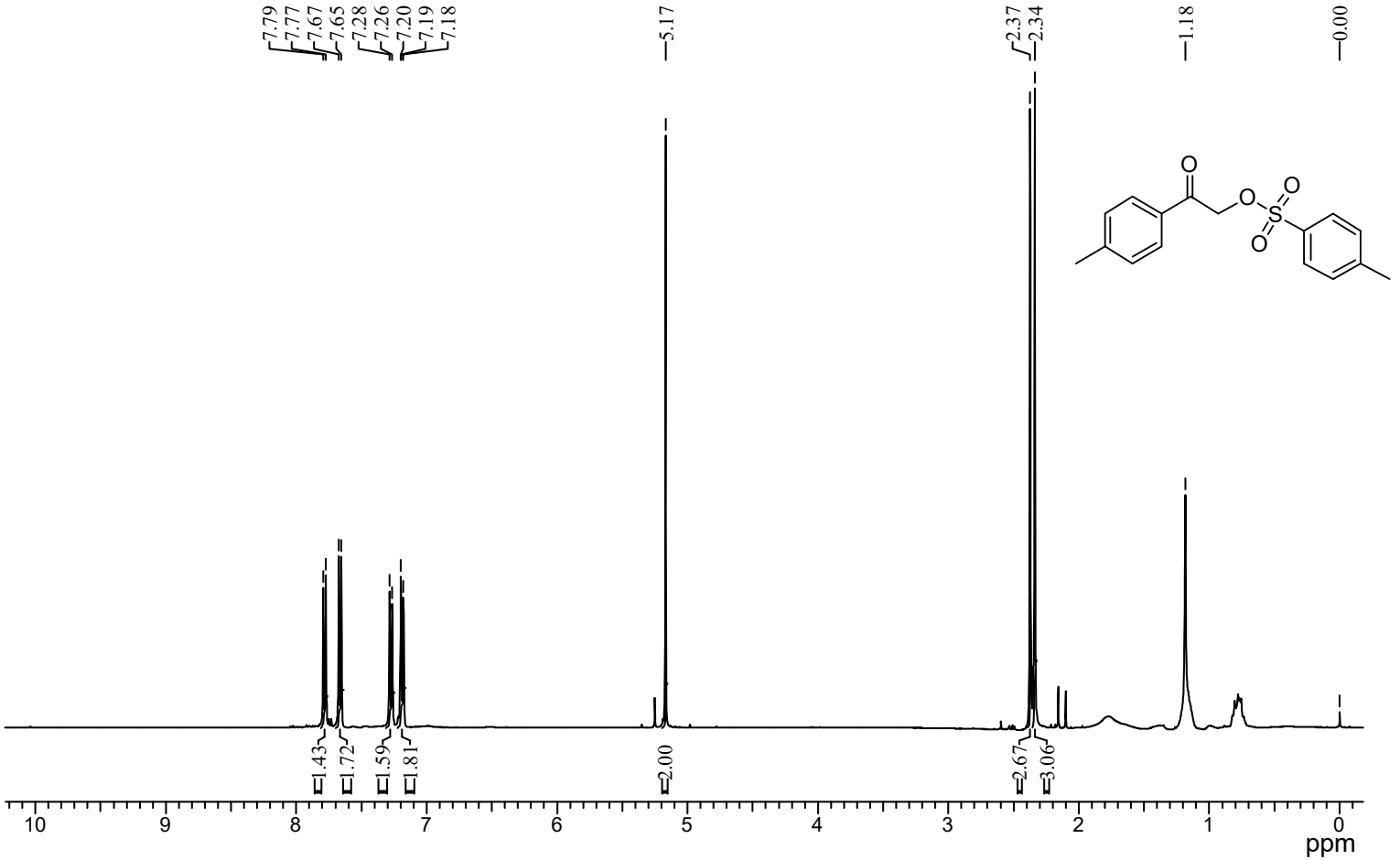
2-oxo-2-phenylethyl 4-methylbenzenesulfonate (3a): ^{1}H NMR (400 MHz, $CDCl_3$)



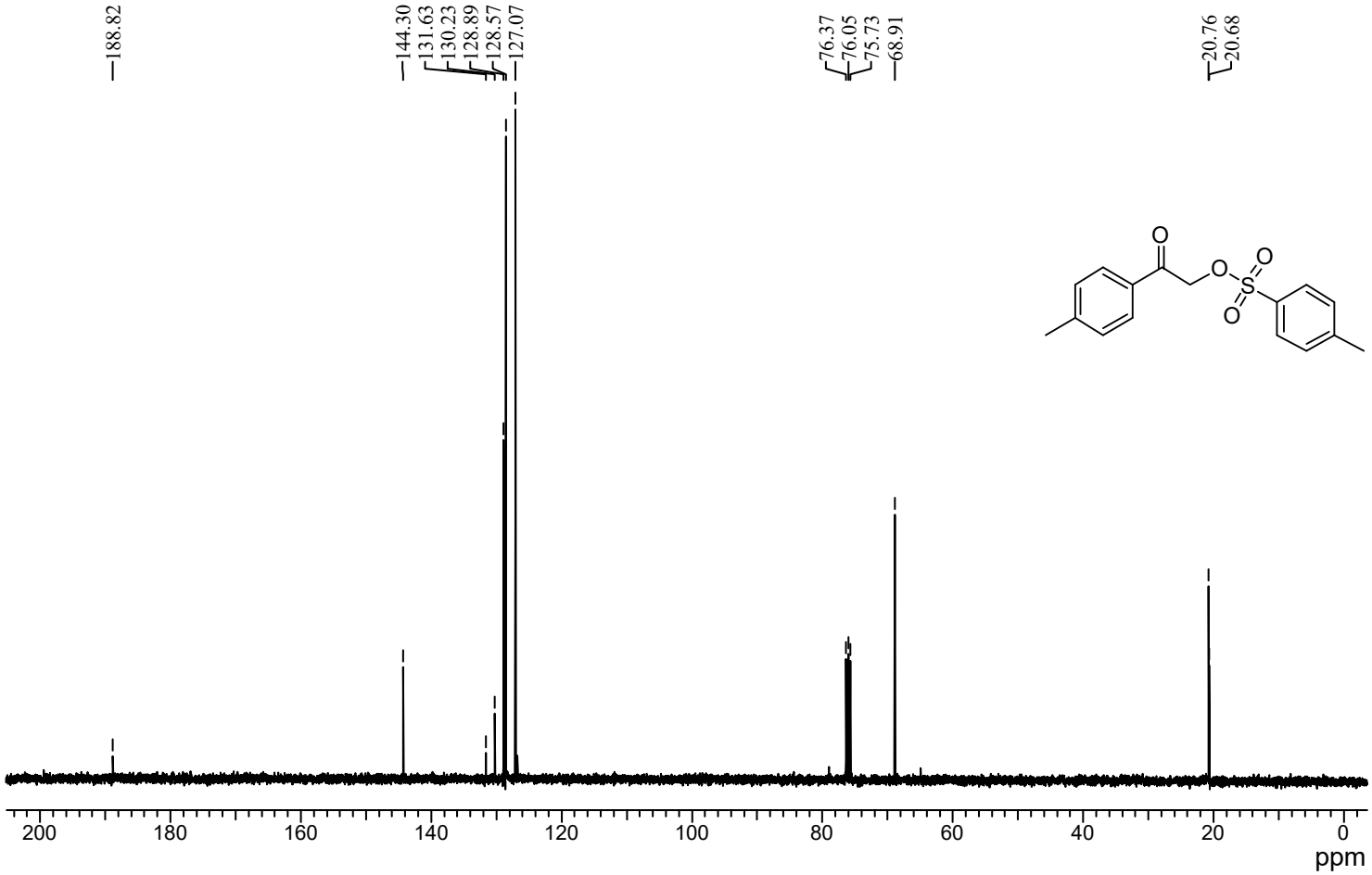
2-oxo-2-phenylethyl 4-methylbenzenesulfonate (3a): ^{13}C NMR (100 MHz, $CDCl_3$)



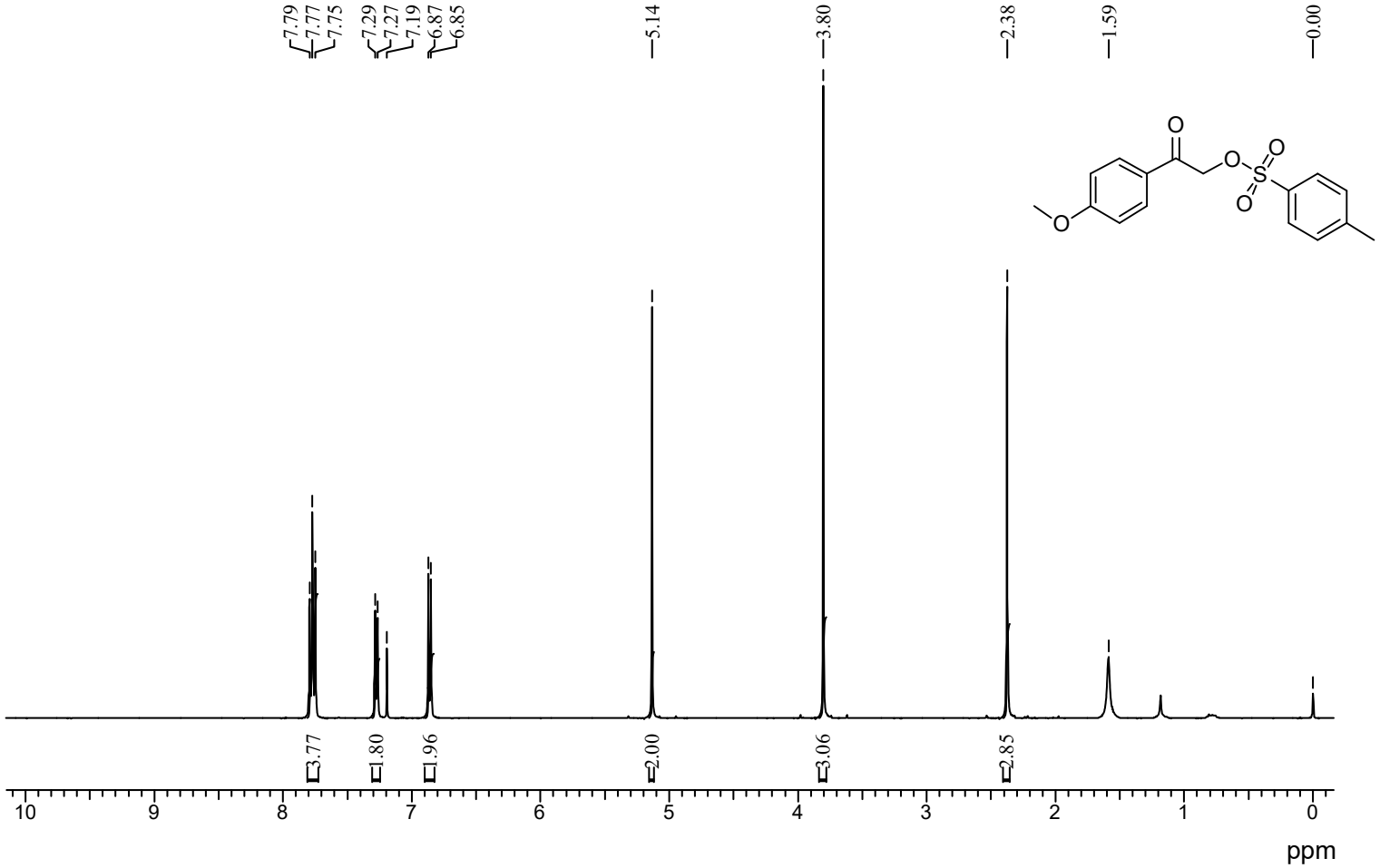
2-oxo-2-(*p*-tolyl)ethyl 4-methylbenzenesulfonate (3b): ^{1}H NMR (400 MHz, $CDCl_3$)



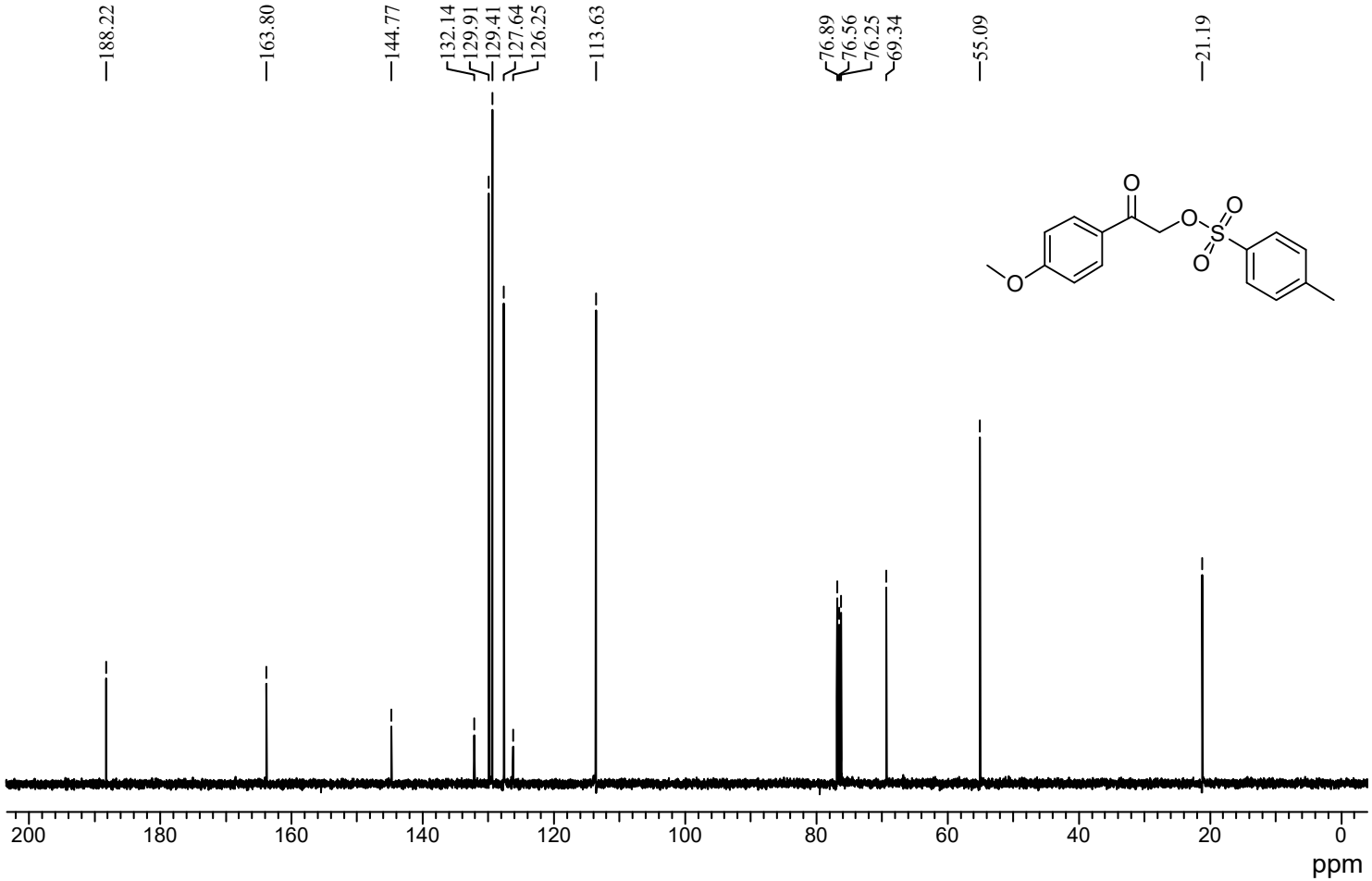
2-oxo-2-(*p*-tolyl)ethyl 4-methylbenzenesulfonate (3b): ^{13}C NMR (100 MHz, $CDCl_3$)



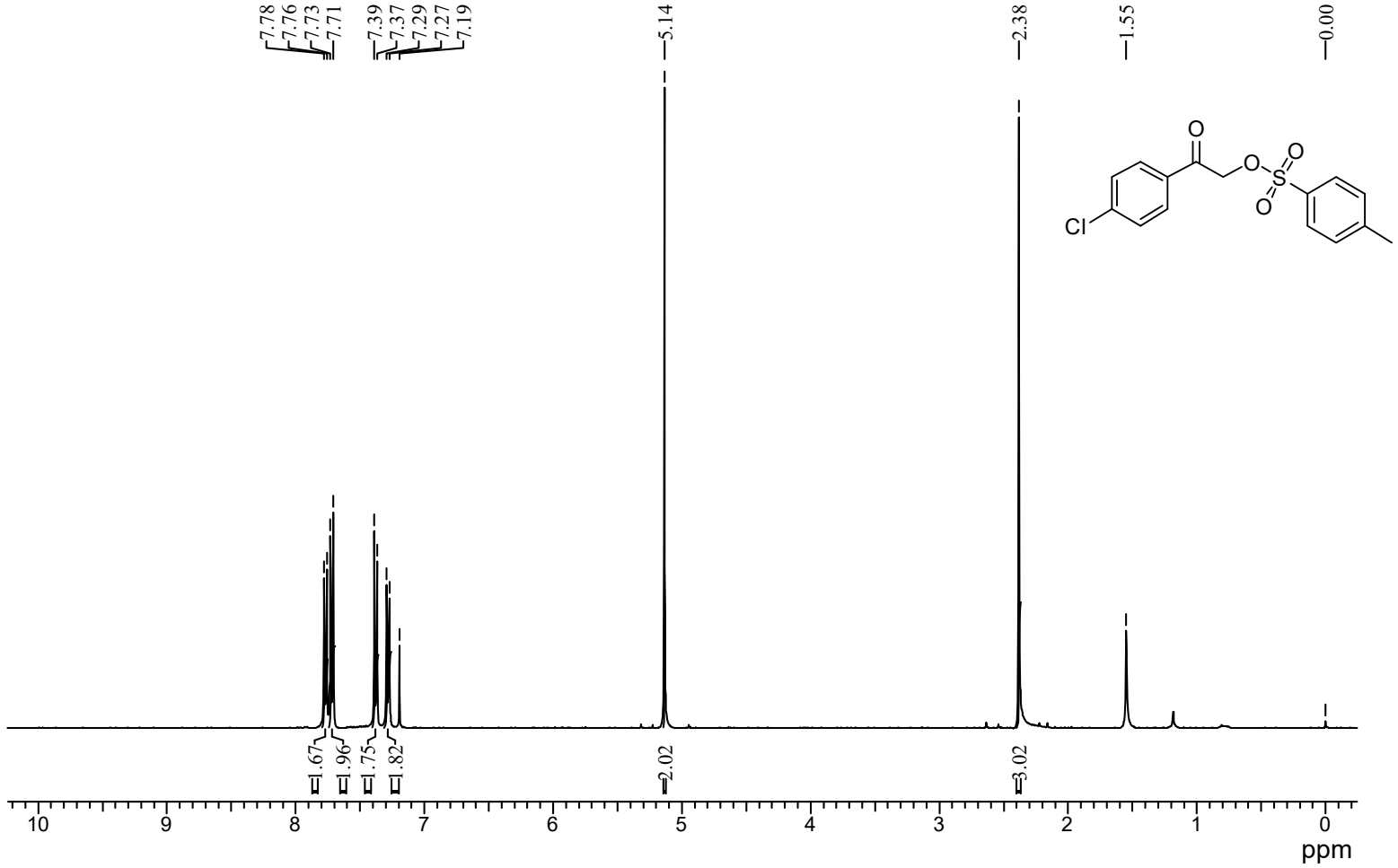
2-(4-methoxyphenyl)-2-oxoethyl-4-methylbenzenesulfonate (3c): ^{1}H NMR (400 MHz, $CDCl_3$)



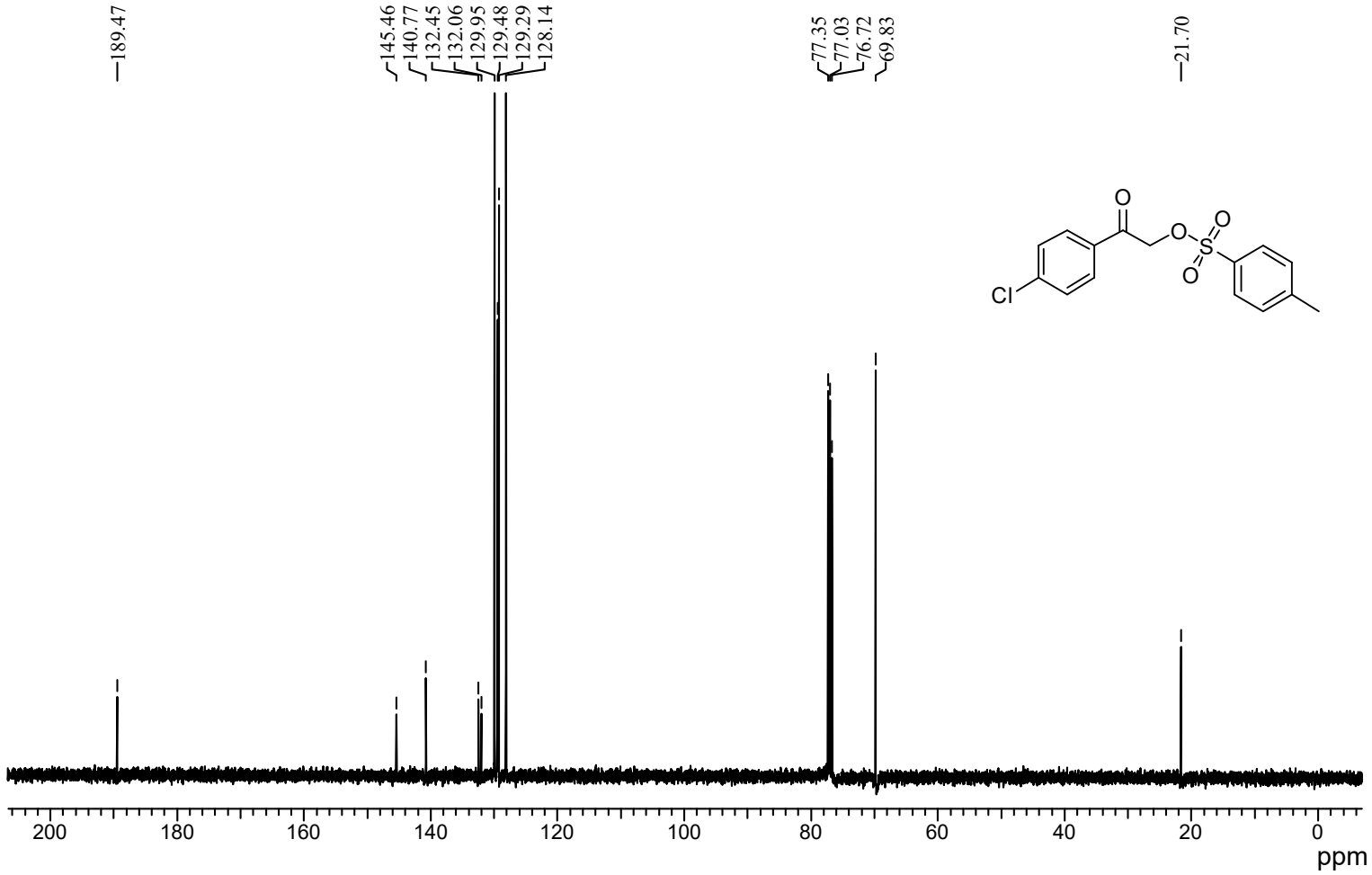
2-(4-methoxyphenyl)-2-oxoethyl-4-methylbenzenesulfonate (3c): ^{13}C NMR (100 MHz, $CDCl_3$)



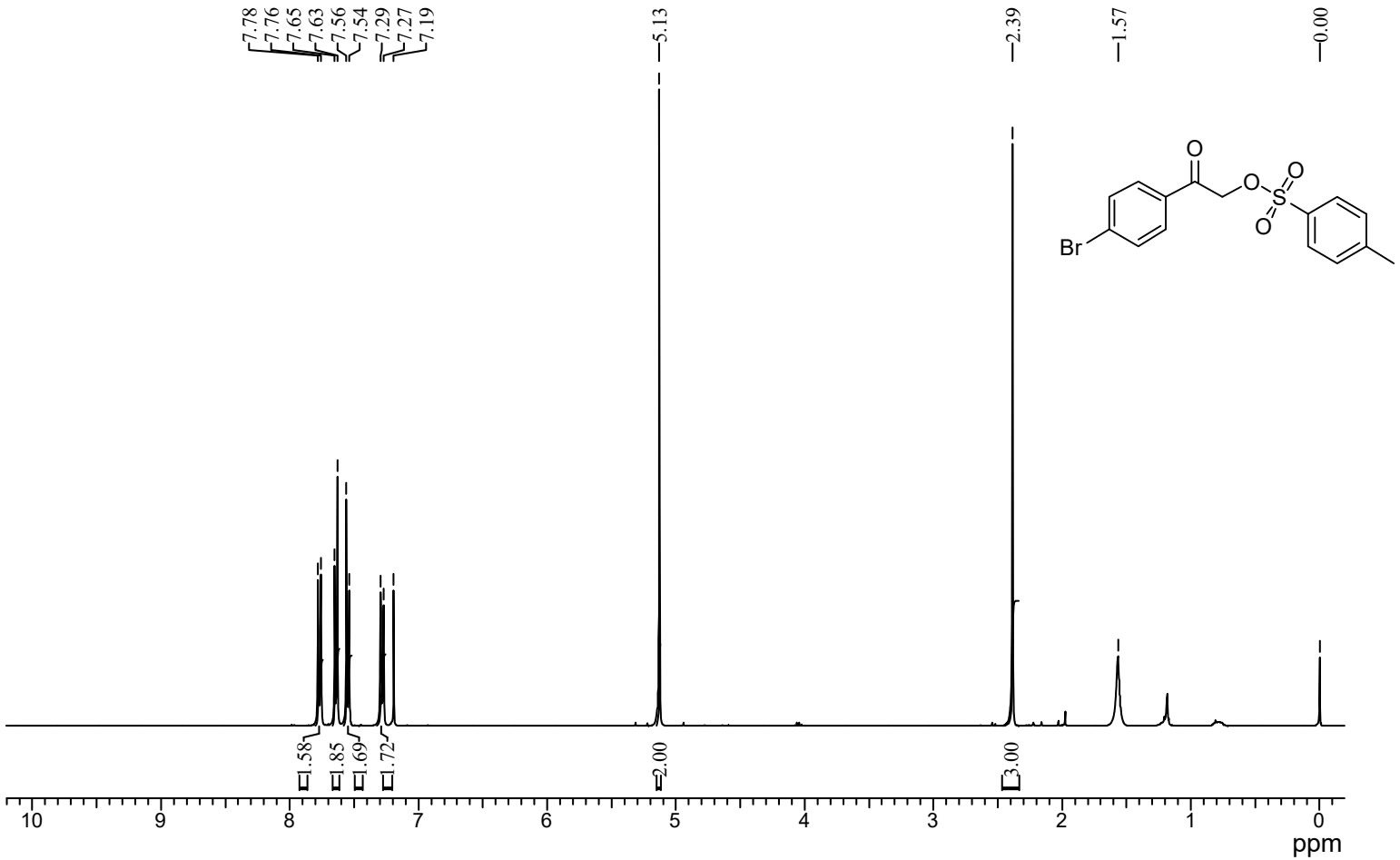
2-(4-chlorophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3d): ^{1}H NMR (400 MHz, $CDCl_3$)



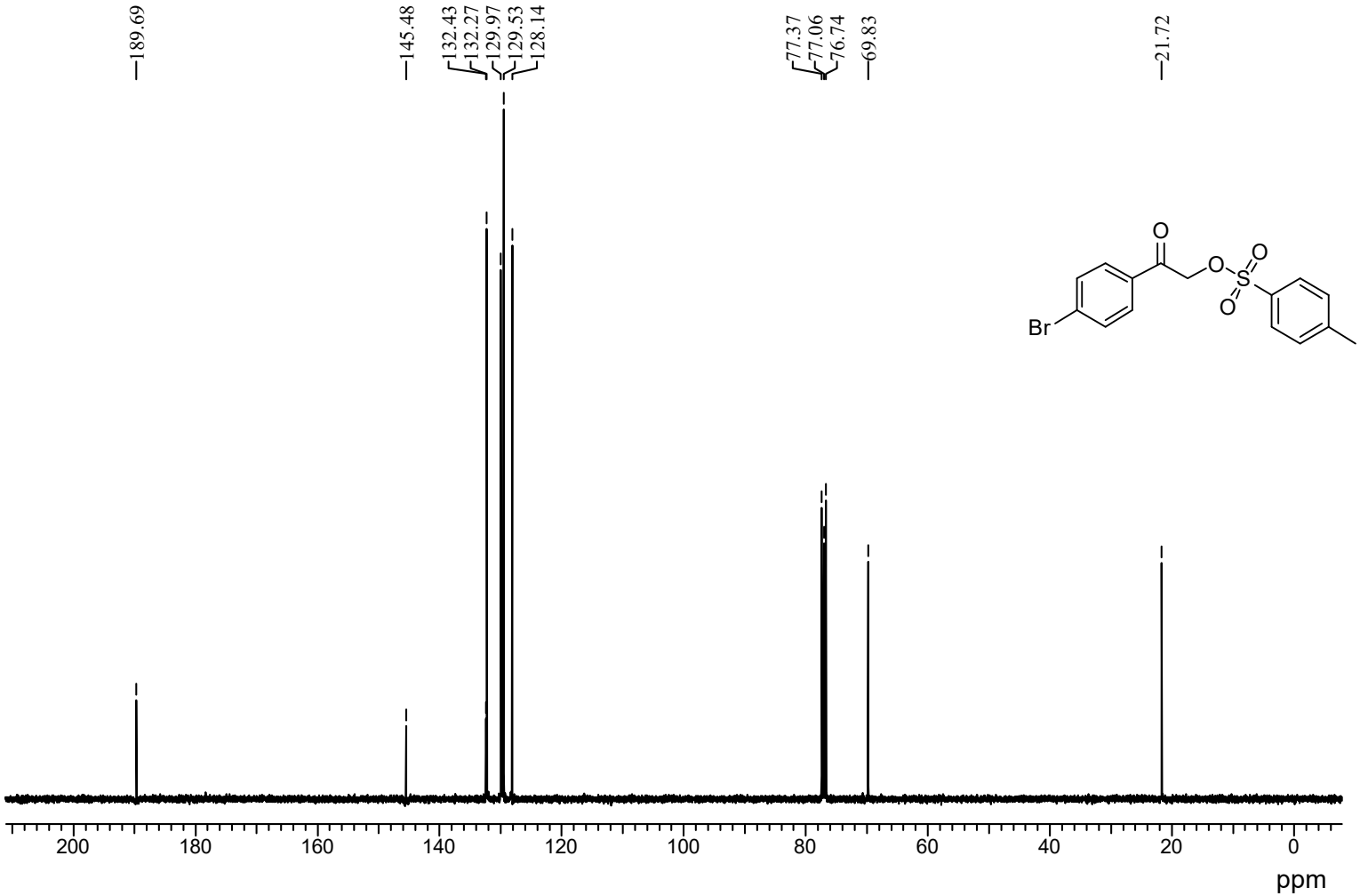
2-(4-chlorophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3d): ^{13}C NMR (100 MHz, $CDCl_3$)



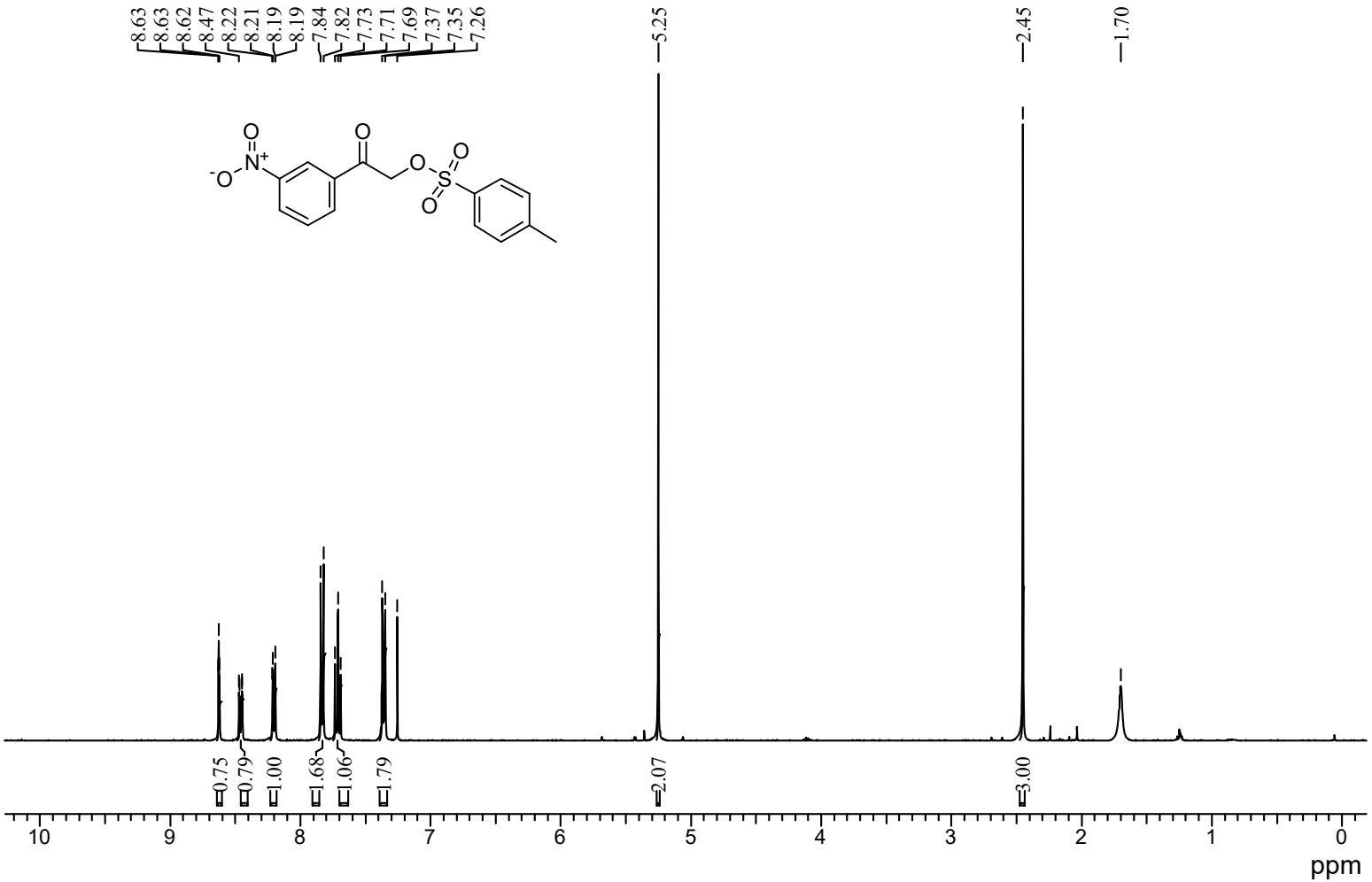
2-(4-bromophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3e): ^{1}H NMR (400 MHz, $CDCl_3$)



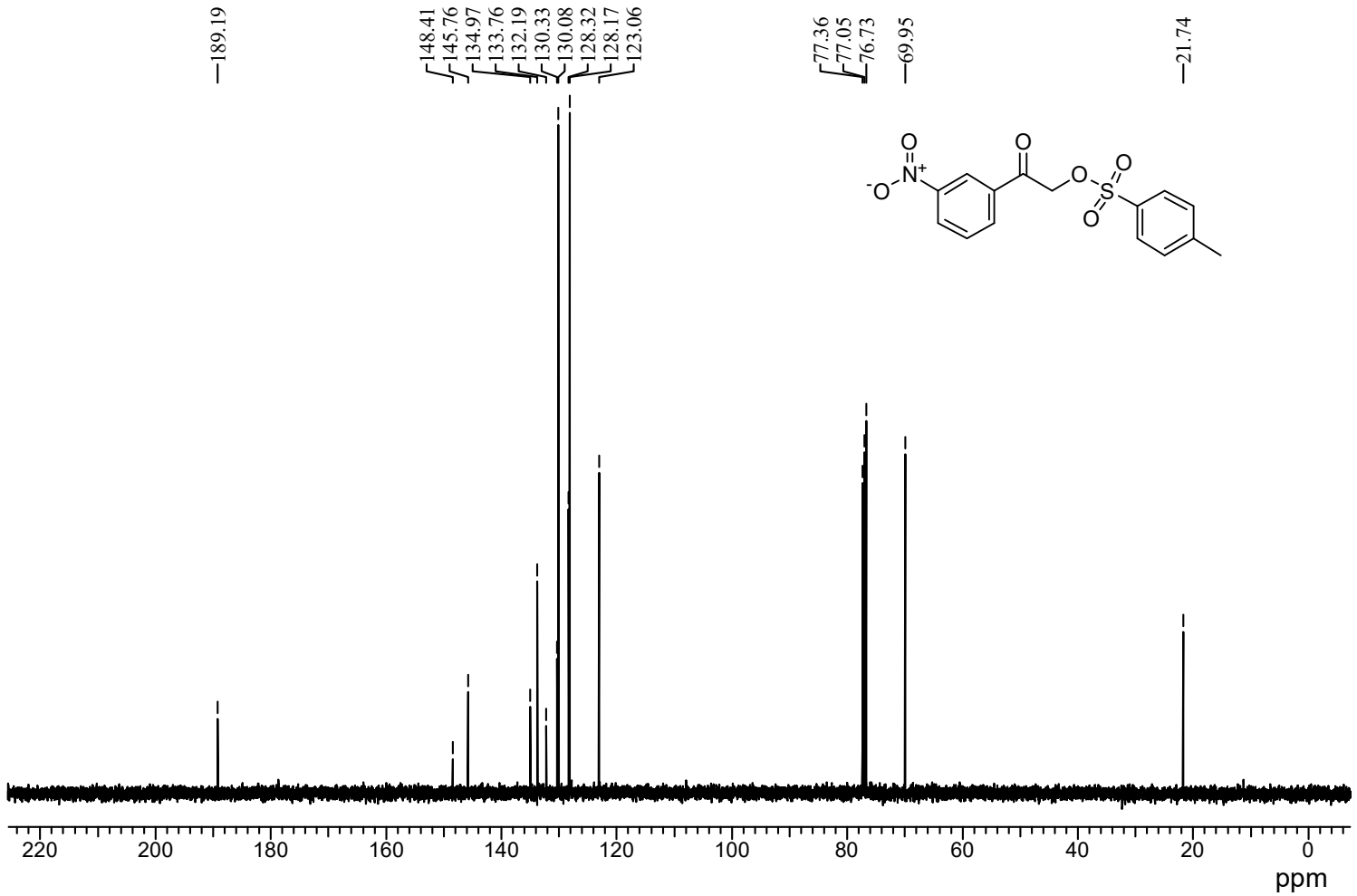
2-(4-bromophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3e): ^{13}C NMR (100 MHz, $CDCl_3$)



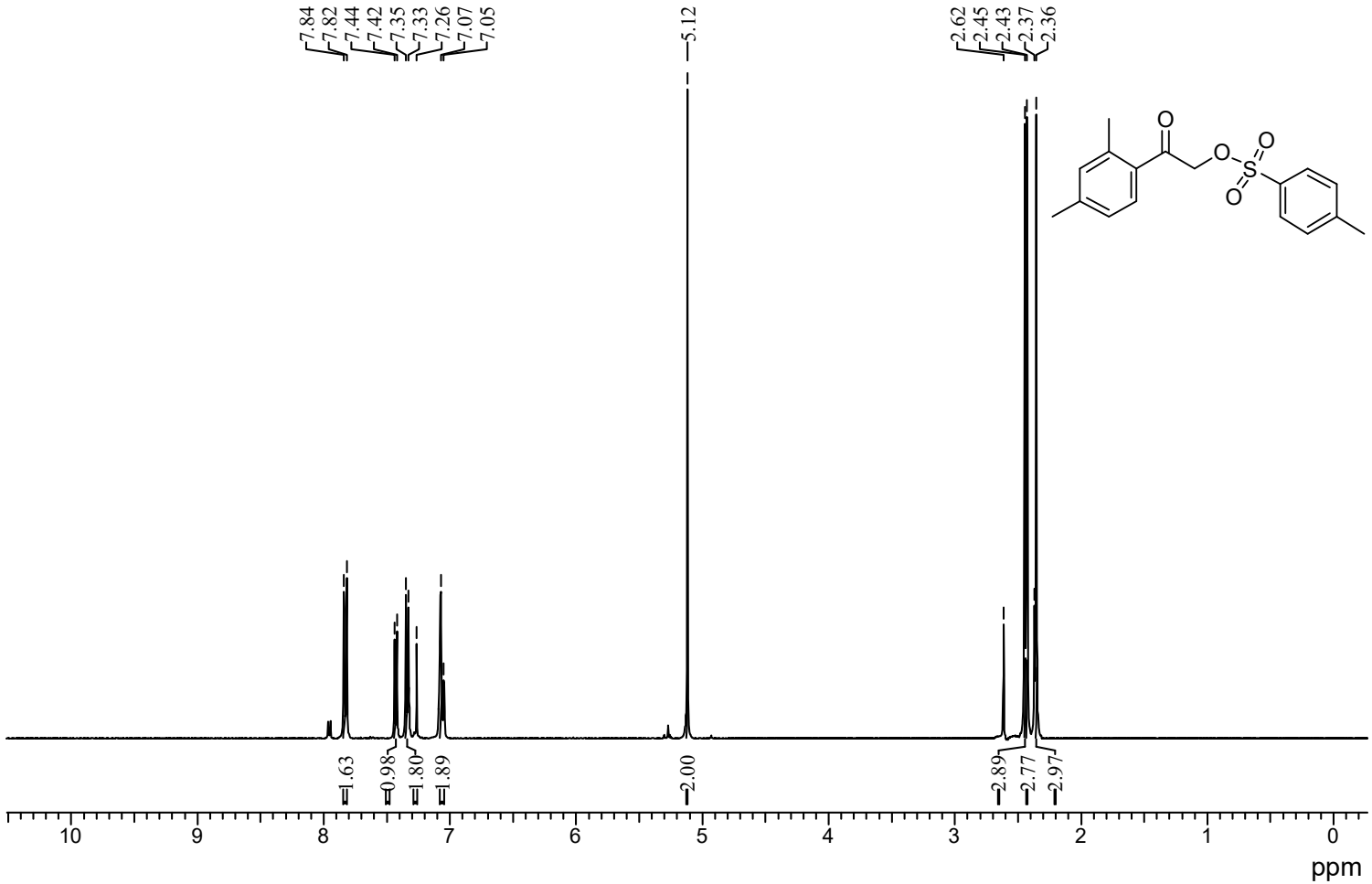
2-(3-nitrophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3f): ^{1}H NMR (400 MHz, $CDCl_3$)



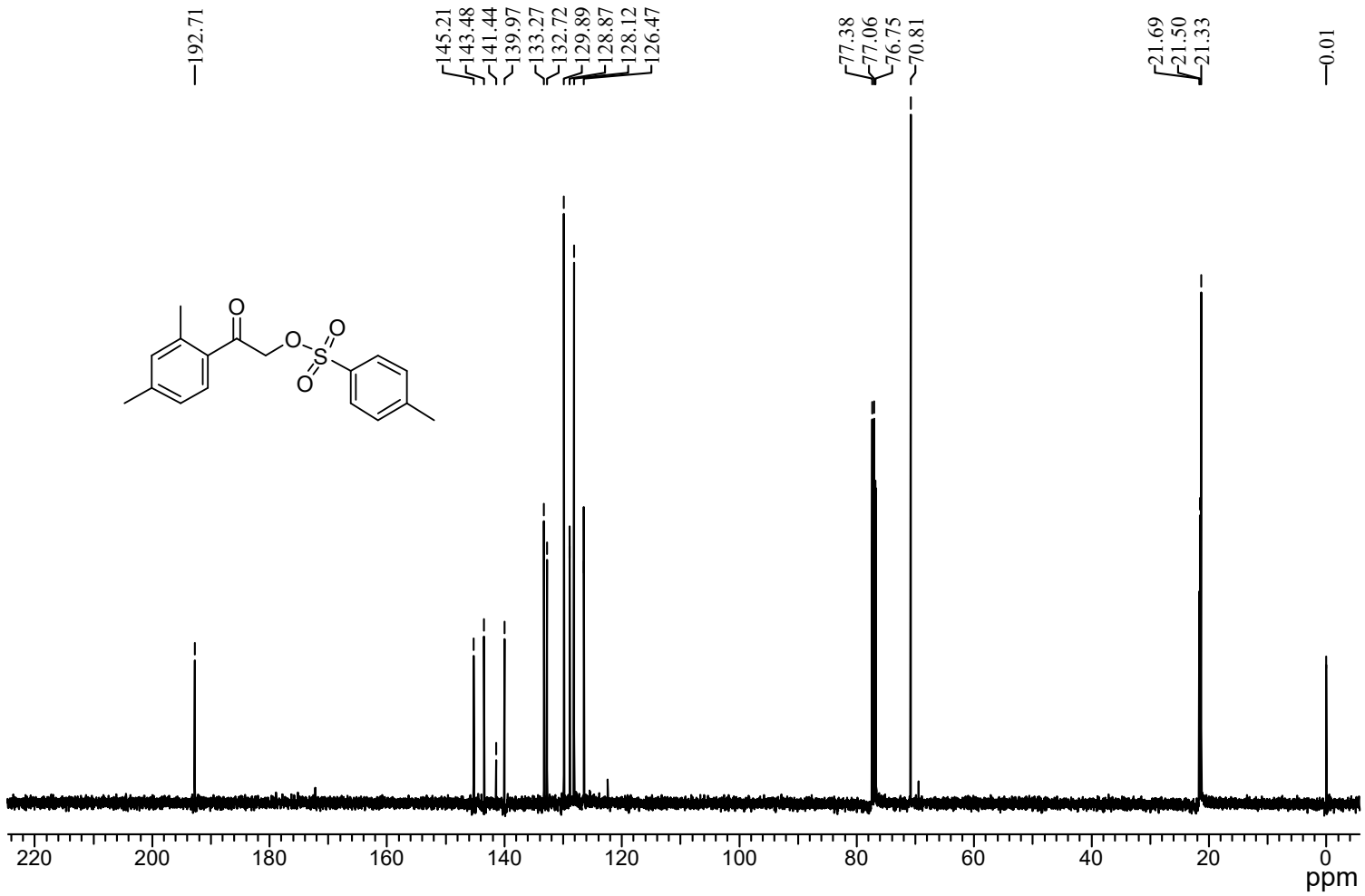
2-(3-nitrophenyl)-2-oxoethyl 4-methylbenzenesulfonate (3f): ^{13}C NMR (100 MHz, $CDCl_3$)



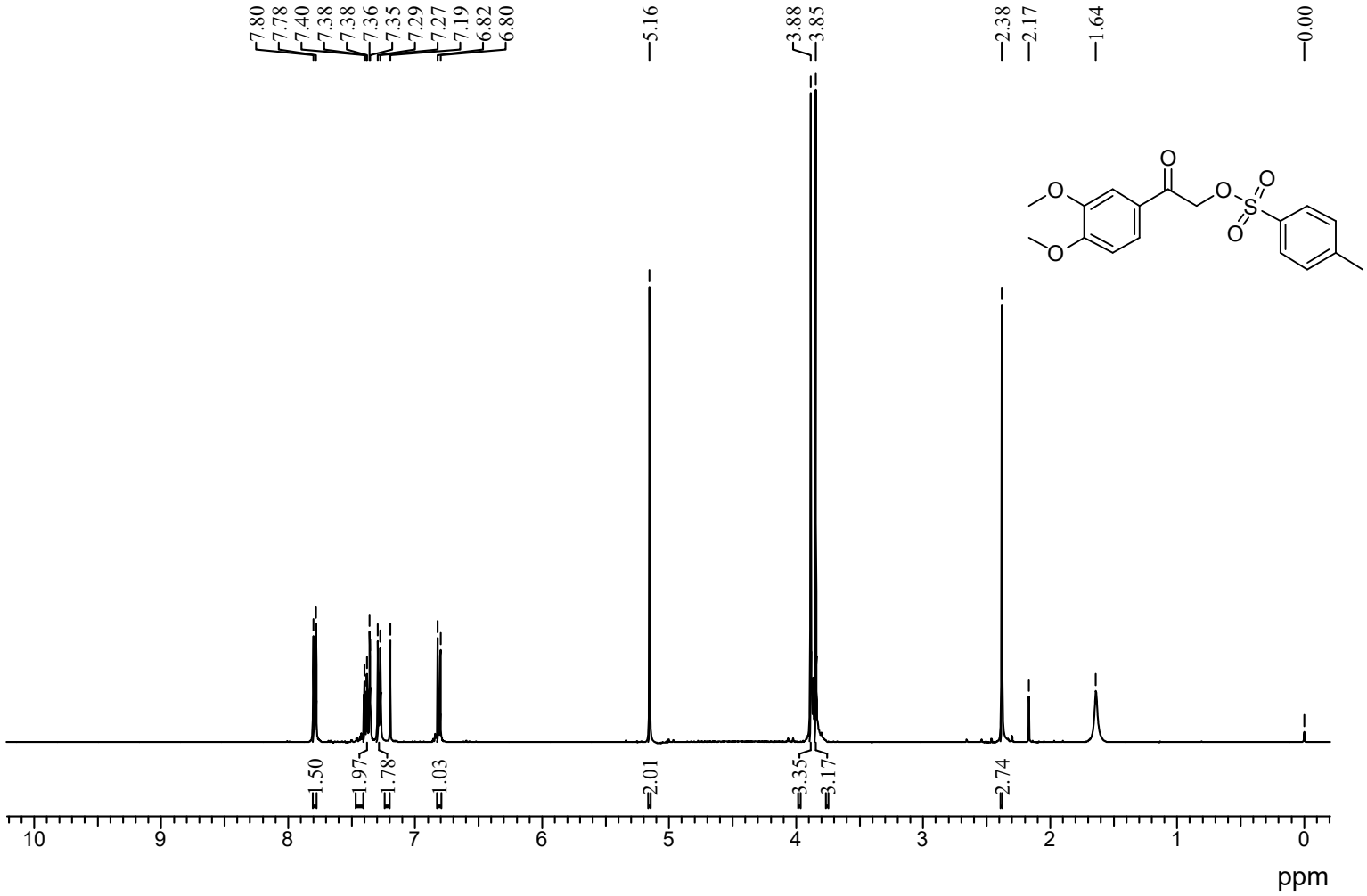
2-(2,4-dimethylphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3g): ^{1}H NMR (400 MHz, $CDCl_3$)



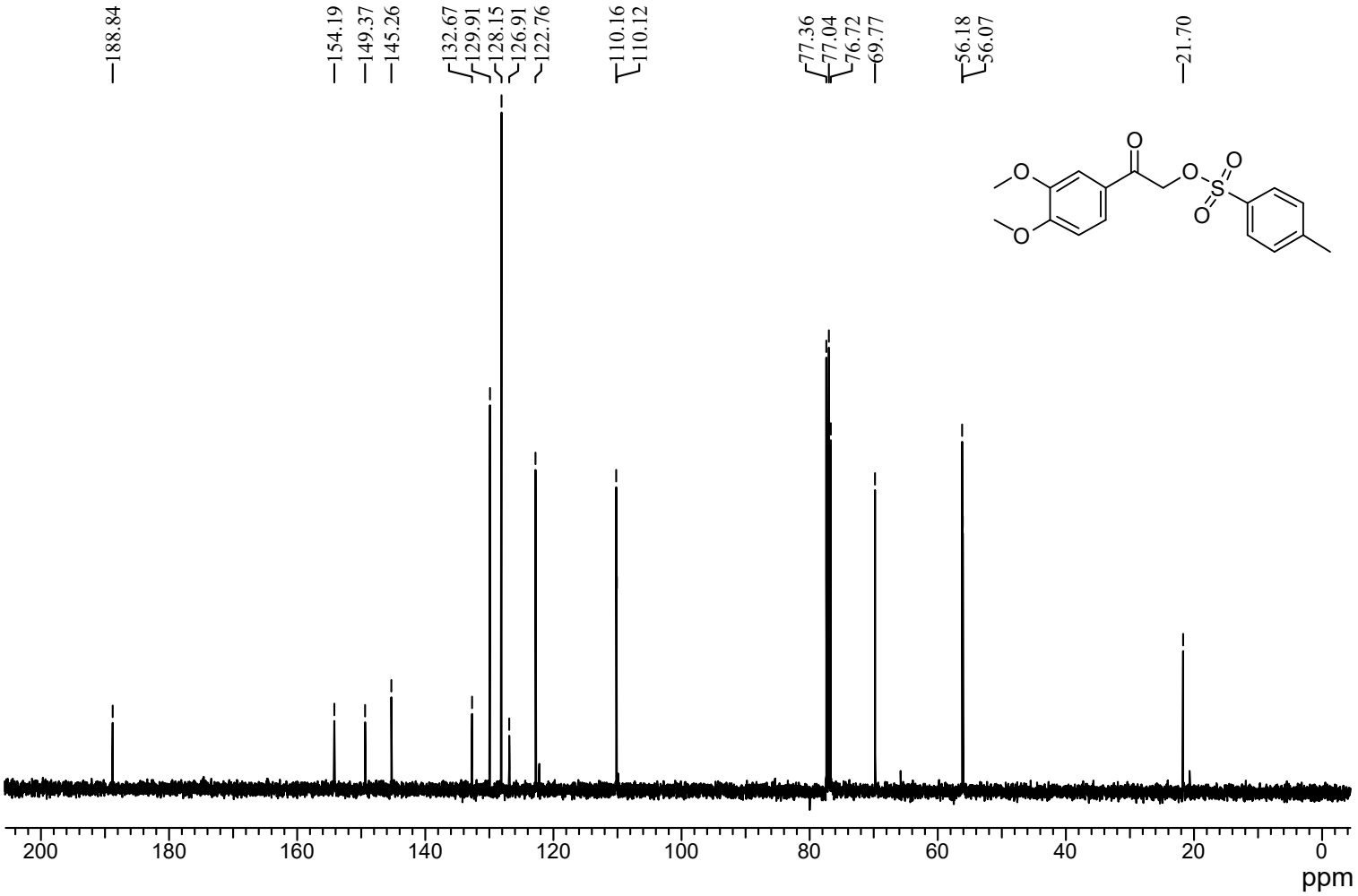
2-(2,4-dimethylphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3g): ^{13}C NMR (100 MHz, $CDCl_3$)



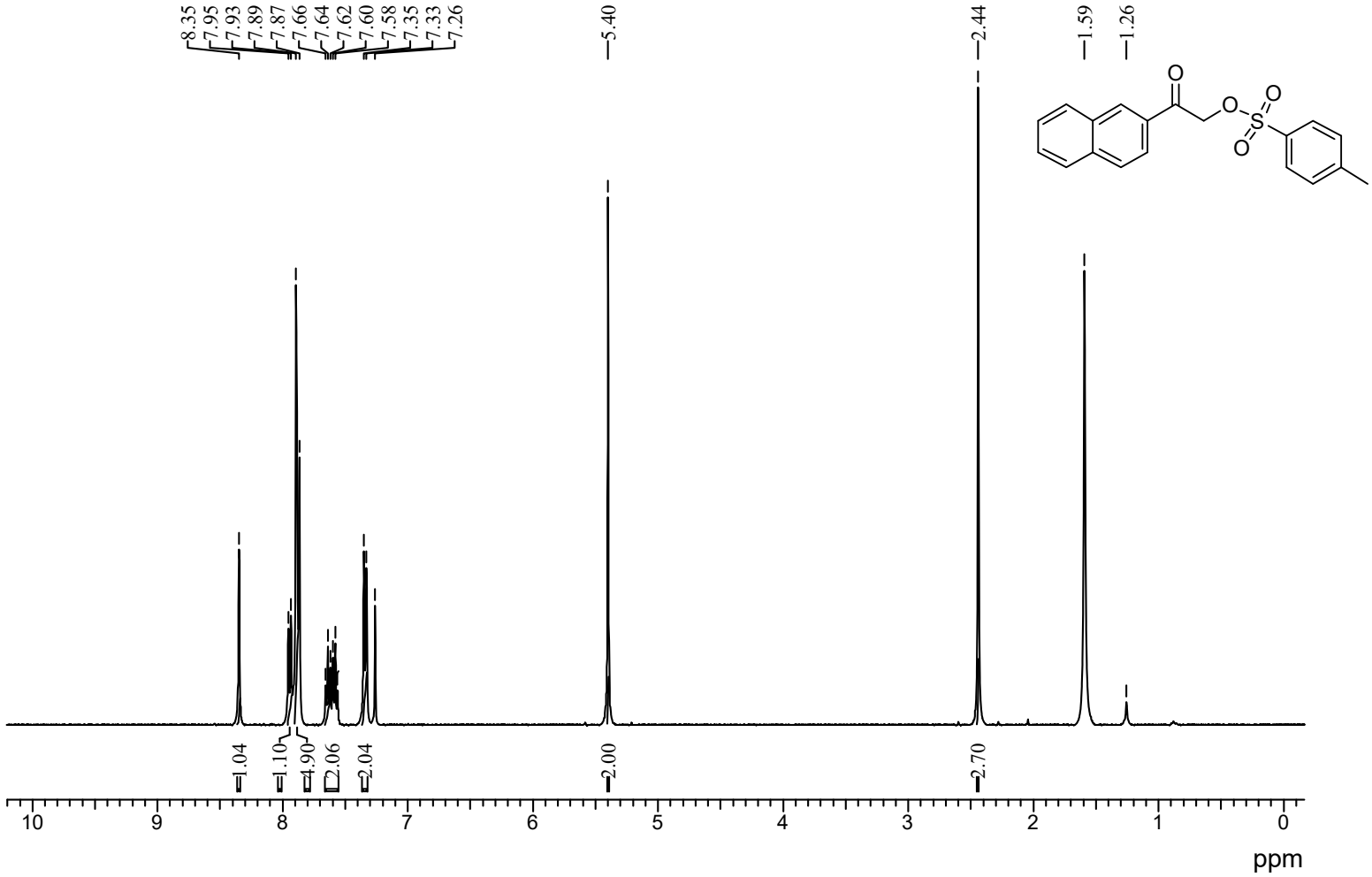
2-(3,4-dimethoxyphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3h): ^{1}H NMR (400 MHz, $CDCl_3$)



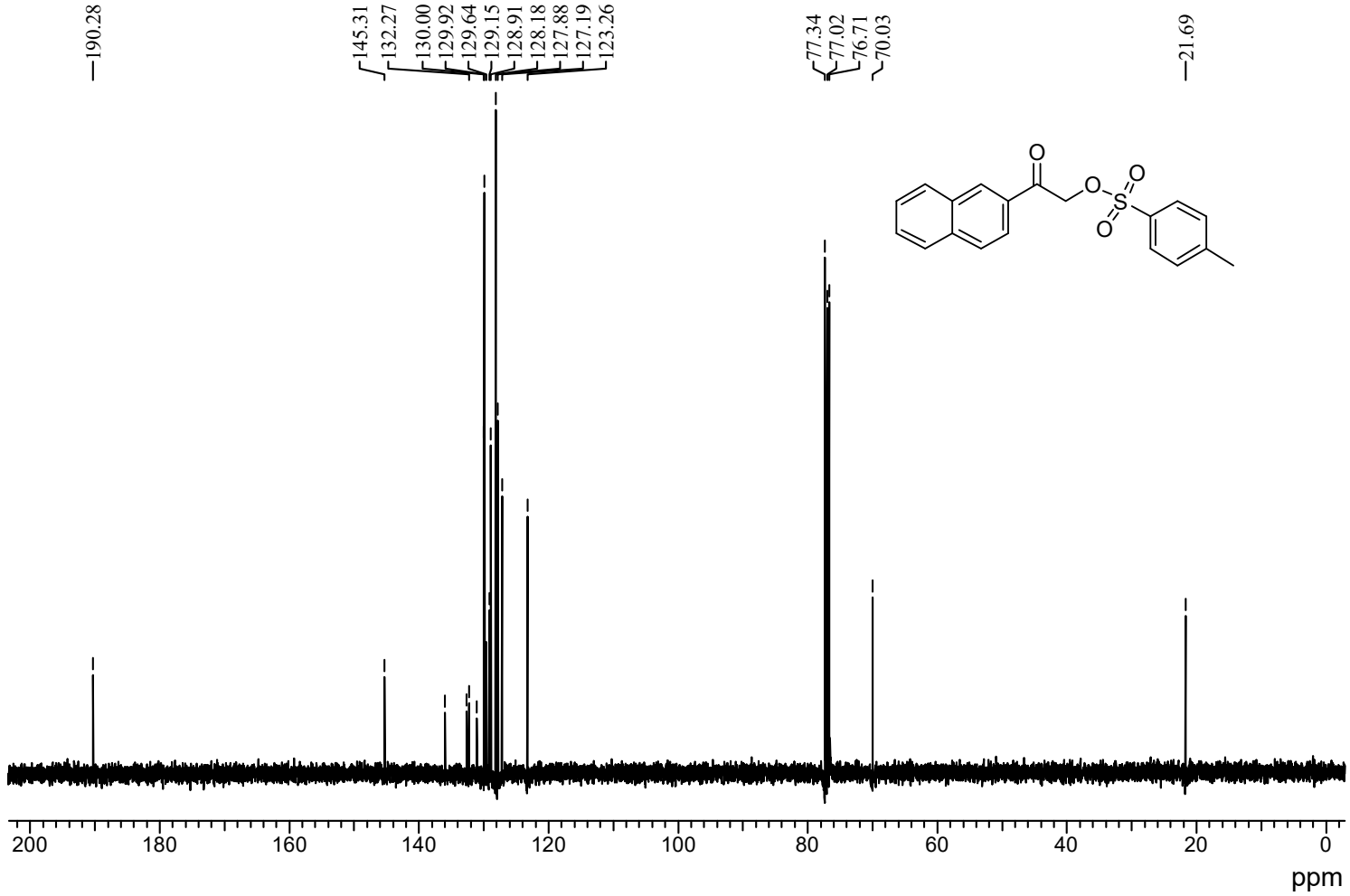
2-(3,4-dimethoxyphenyl)-2-oxoethyl 4-methylbenzenesulfonate (3h): ^{13}C NMR (100 MHz, $CDCl_3$)



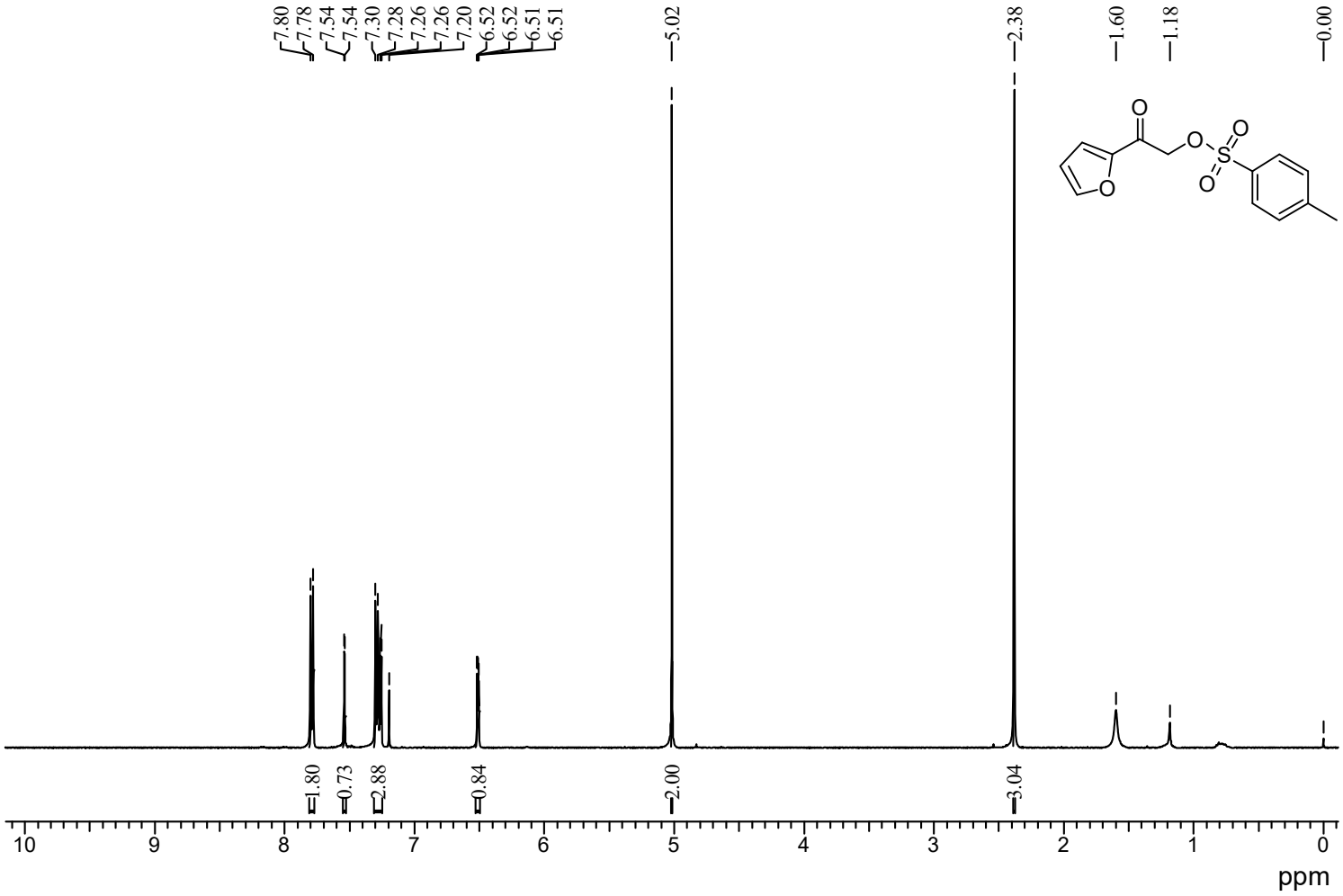
2-(naphthalen-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3i): ^{1}H NMR (400 MHz, $CDCl_3$)



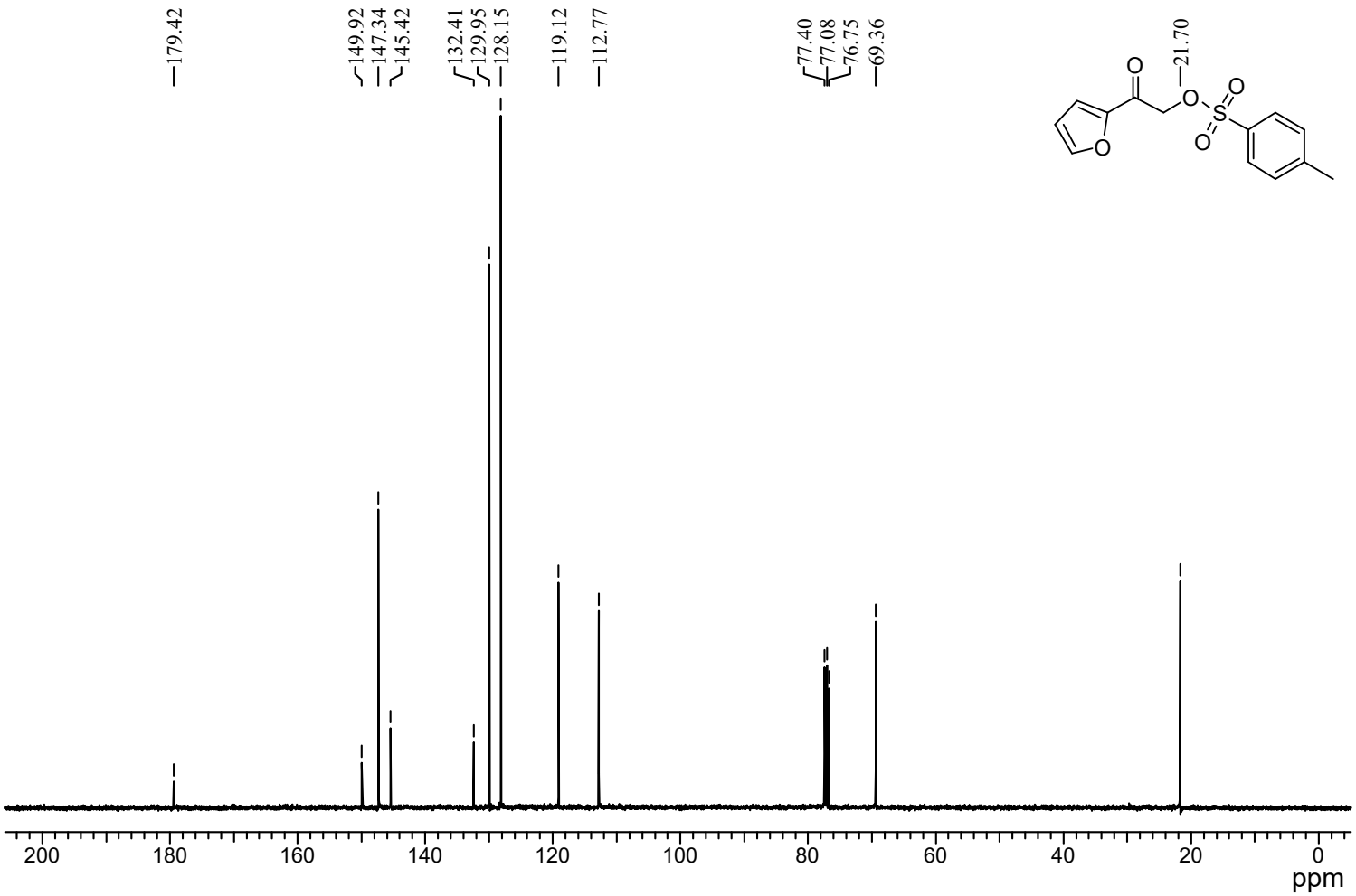
2-(naphthalen-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3i): ^{13}C NMR (100 MHz, $CDCl_3$)



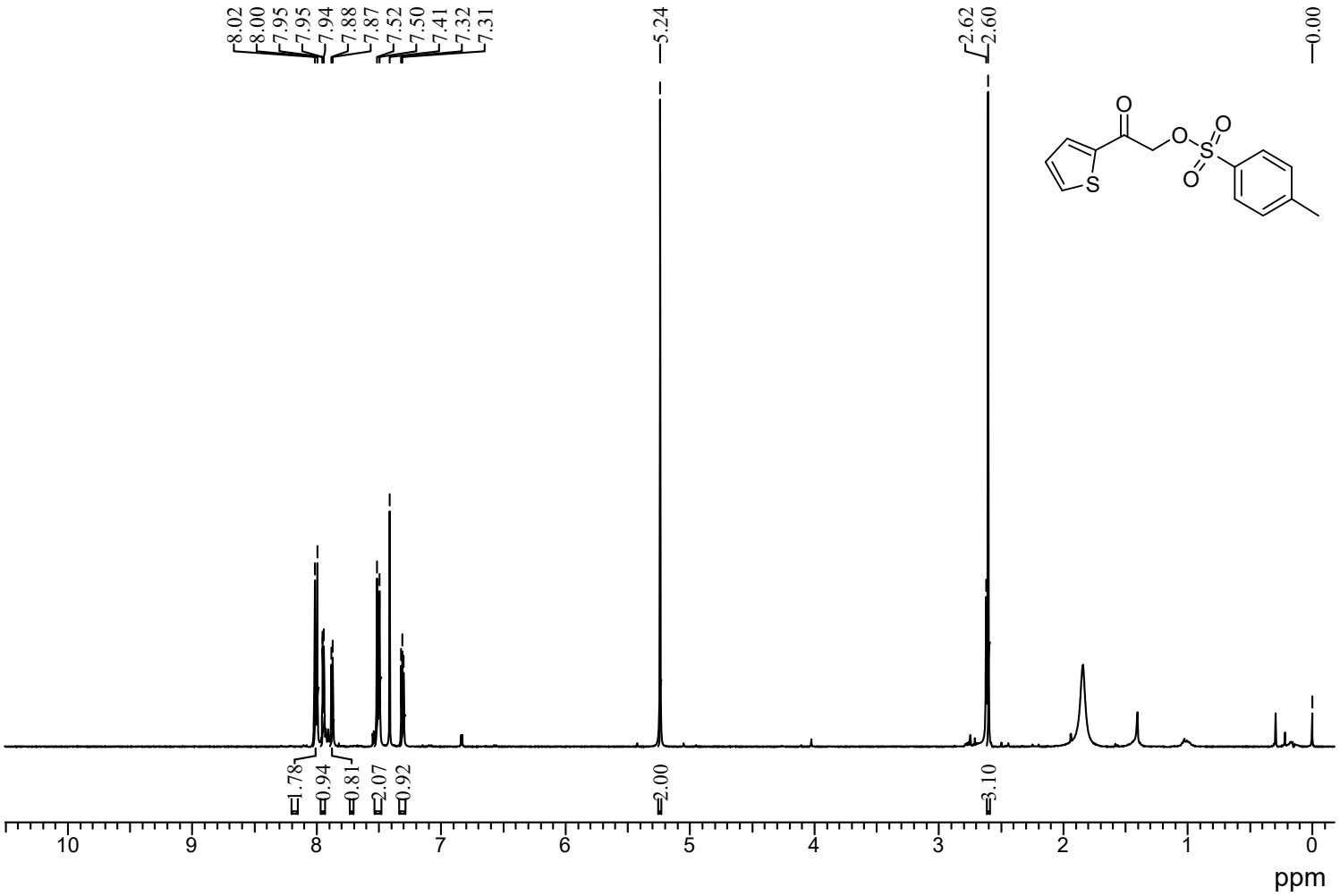
2-(furan-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3j): ^{1}H NMR (400 MHz, $CDCl_3$)



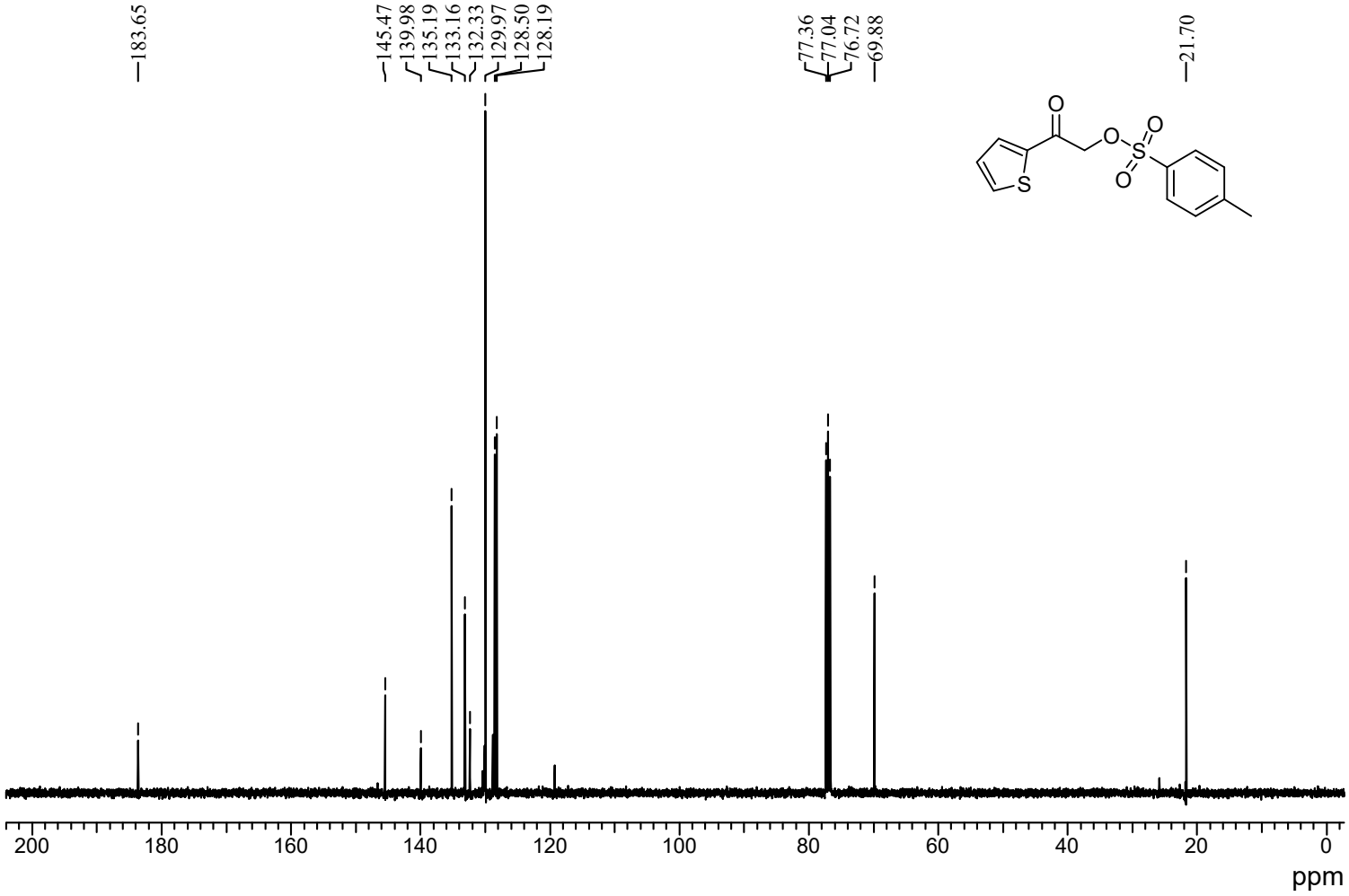
2-(furan-2-yl)-2-oxoethyl 4-methylbenzenesulfonate (3j): ^{13}C NMR (100 MHz, $CDCl_3$)



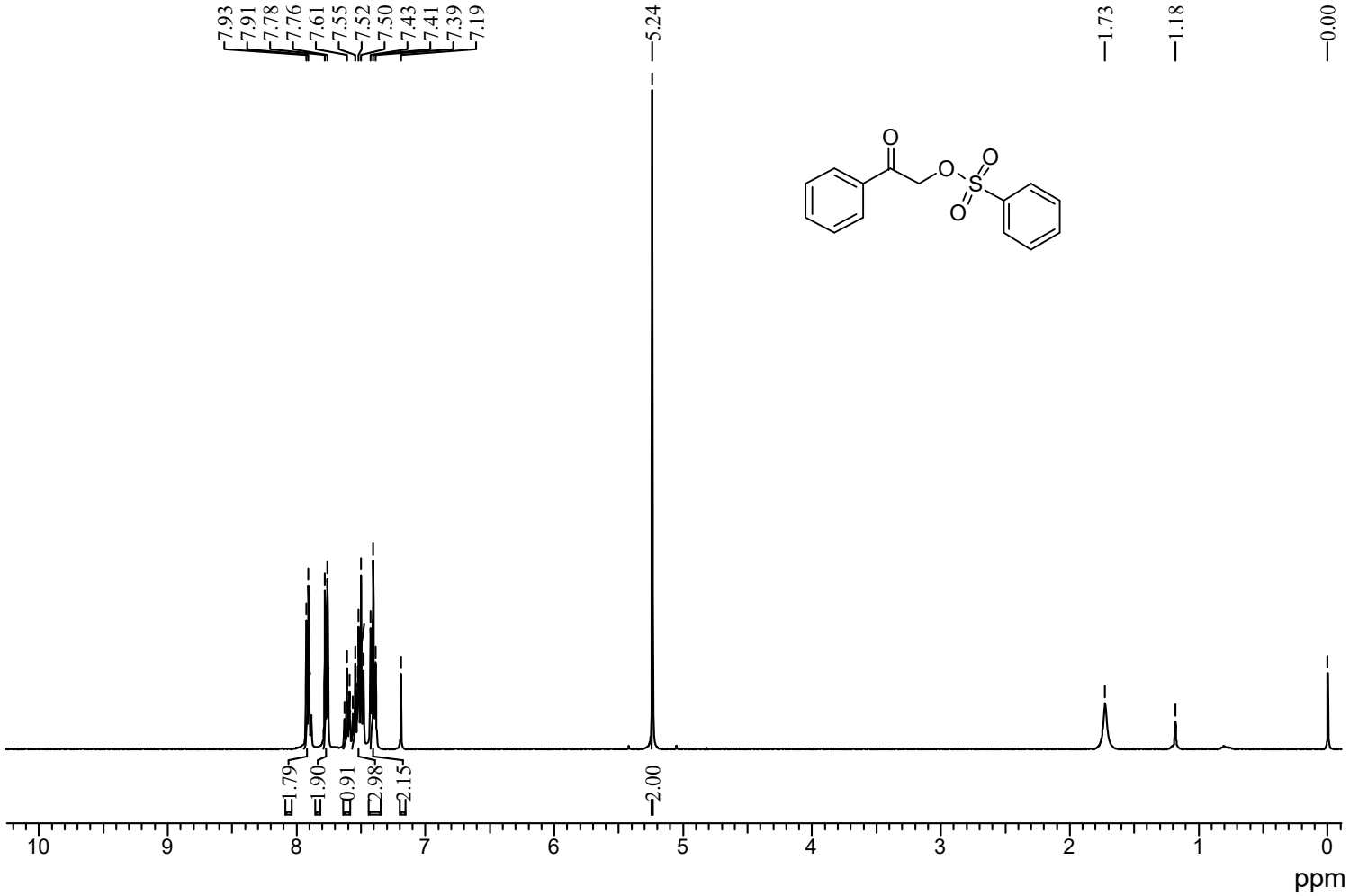
2-oxo-2-(thiophen-2-yl)ethyl 4-methylbenzenesulfonate (3k): ^{1}H NMR (400 MHz, $CDCl_3$)



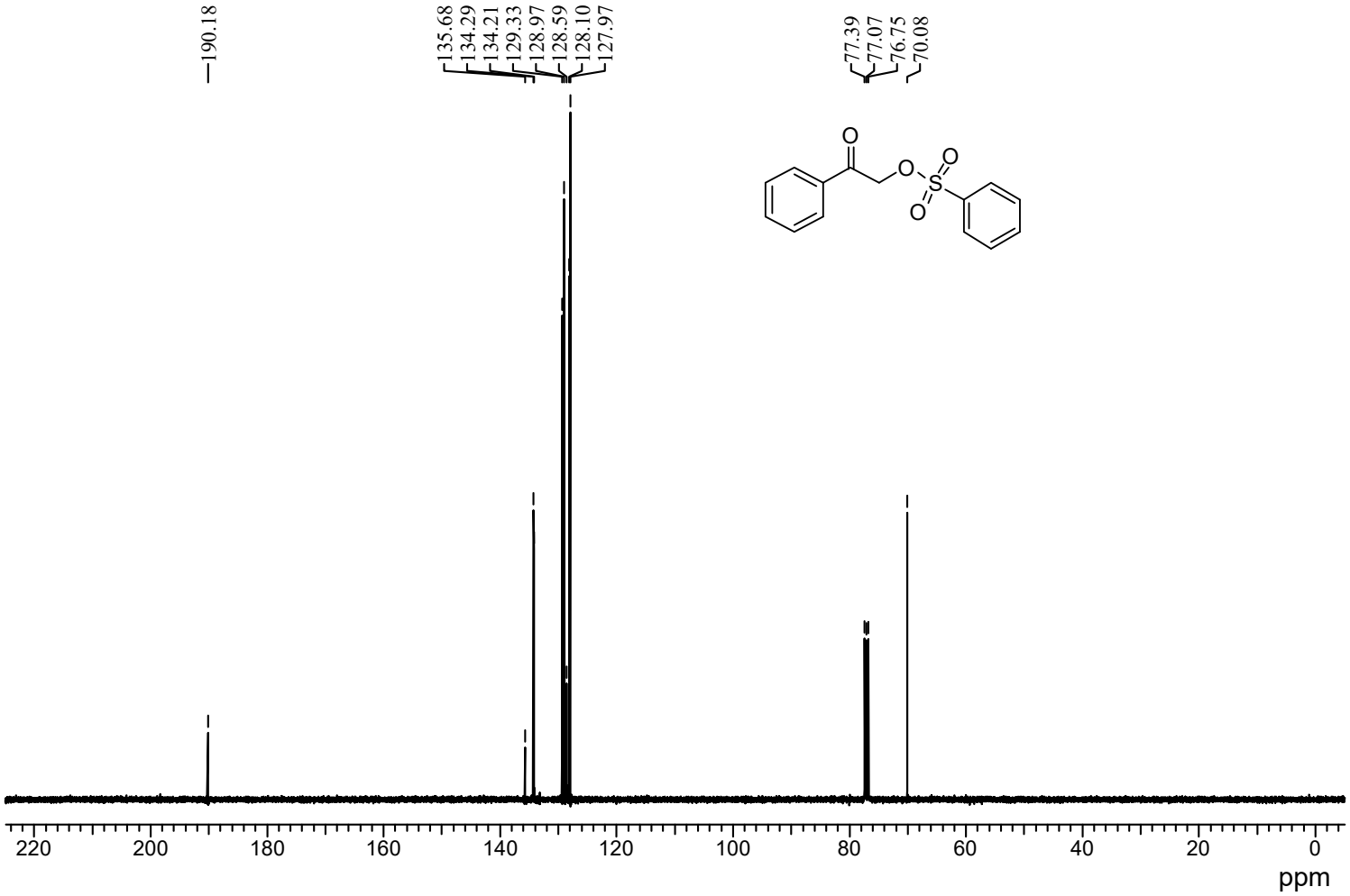
2-oxo-2-(thiophen-2-yl)ethyl 4-methylbenzenesulfonate (3k): ^{13}C NMR (100 MHz, $CDCl_3$)



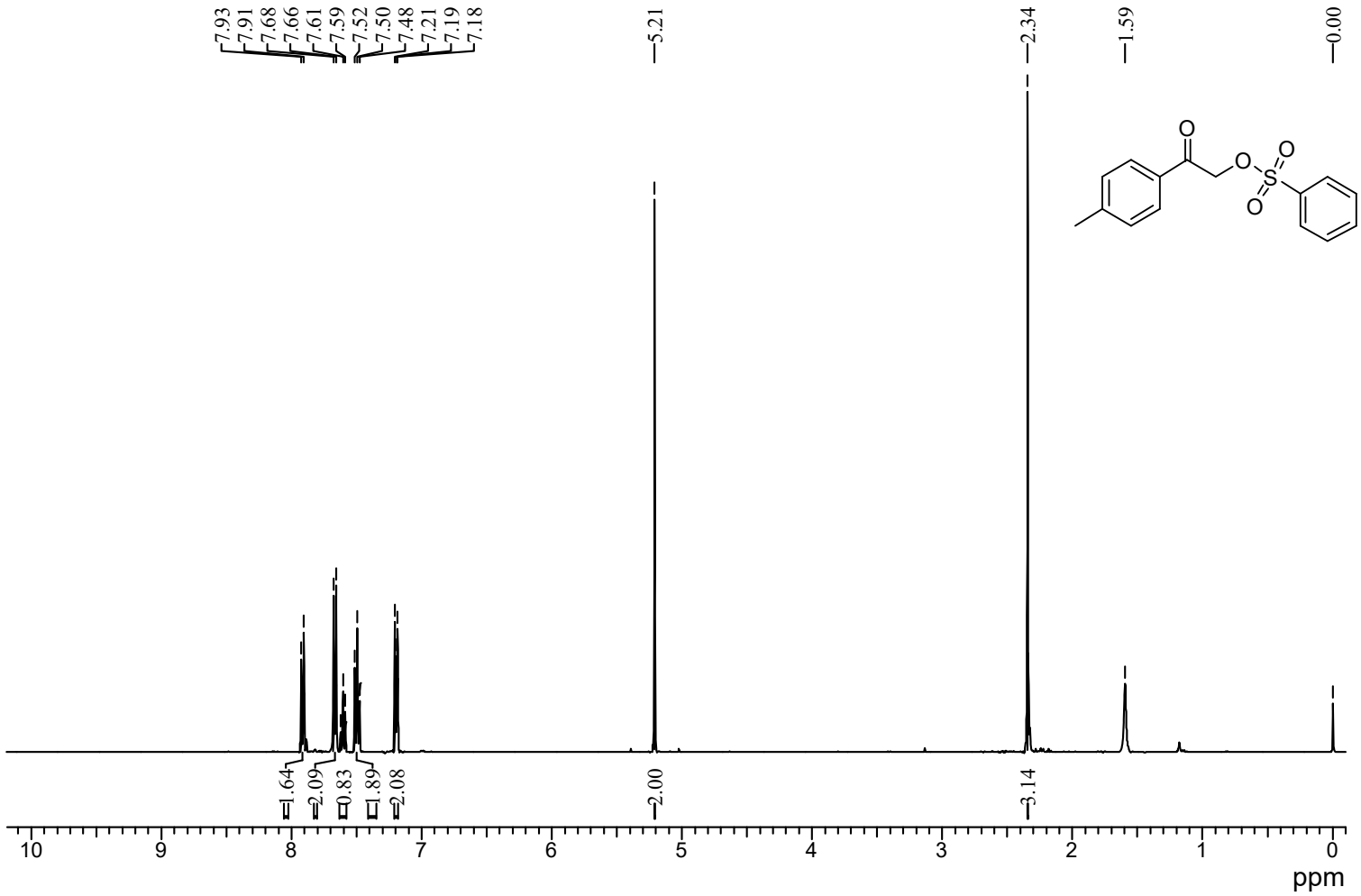
2-oxo-2-phenylethyl benzenesulfonate (3l): ^{1}H NMR (400 MHz, $CDCl_3$)



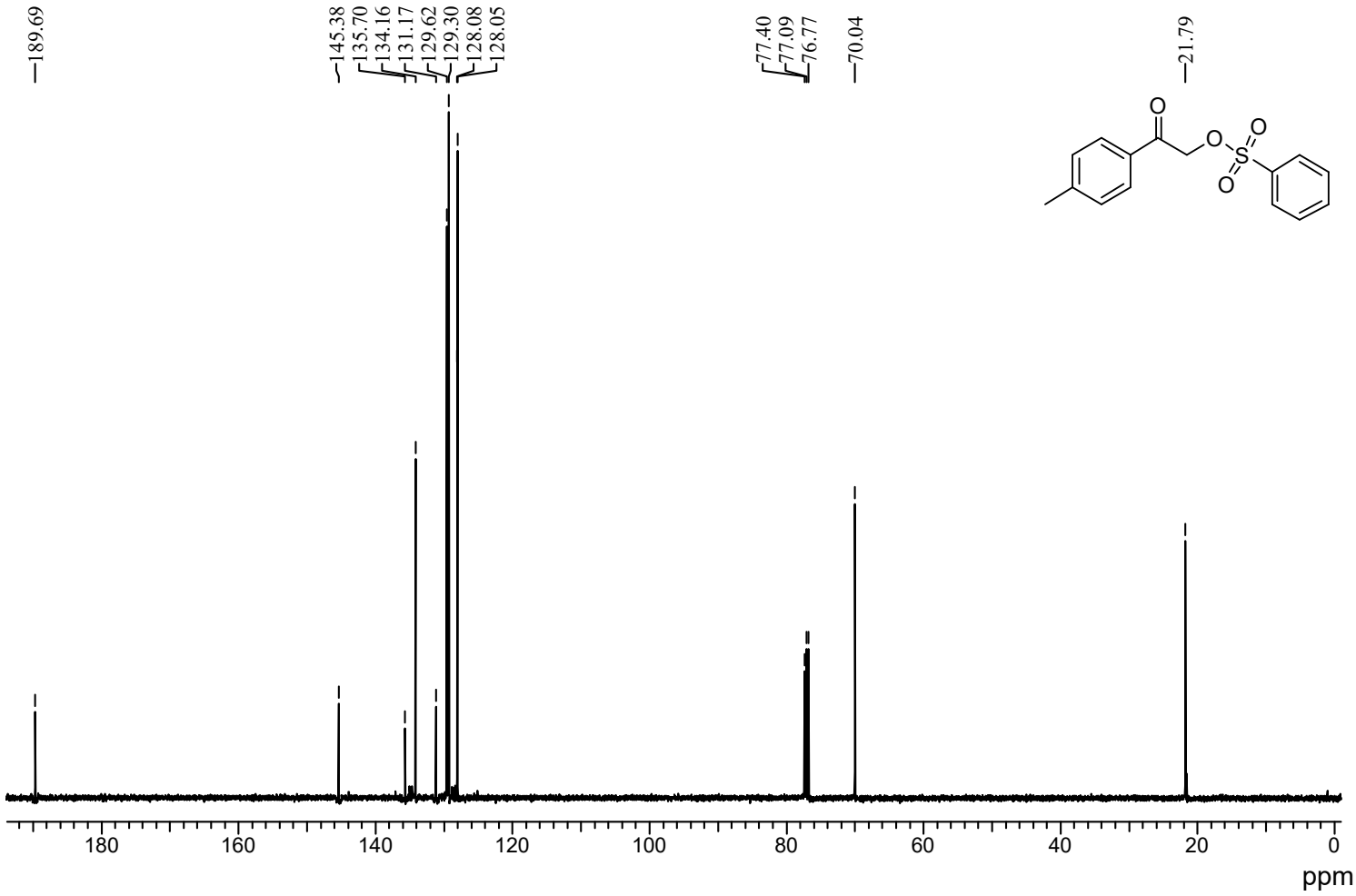
2-oxo-2-phenylethyl benzenesulfonate (3l): ^{13}C NMR (100 MHz, $CDCl_3$)



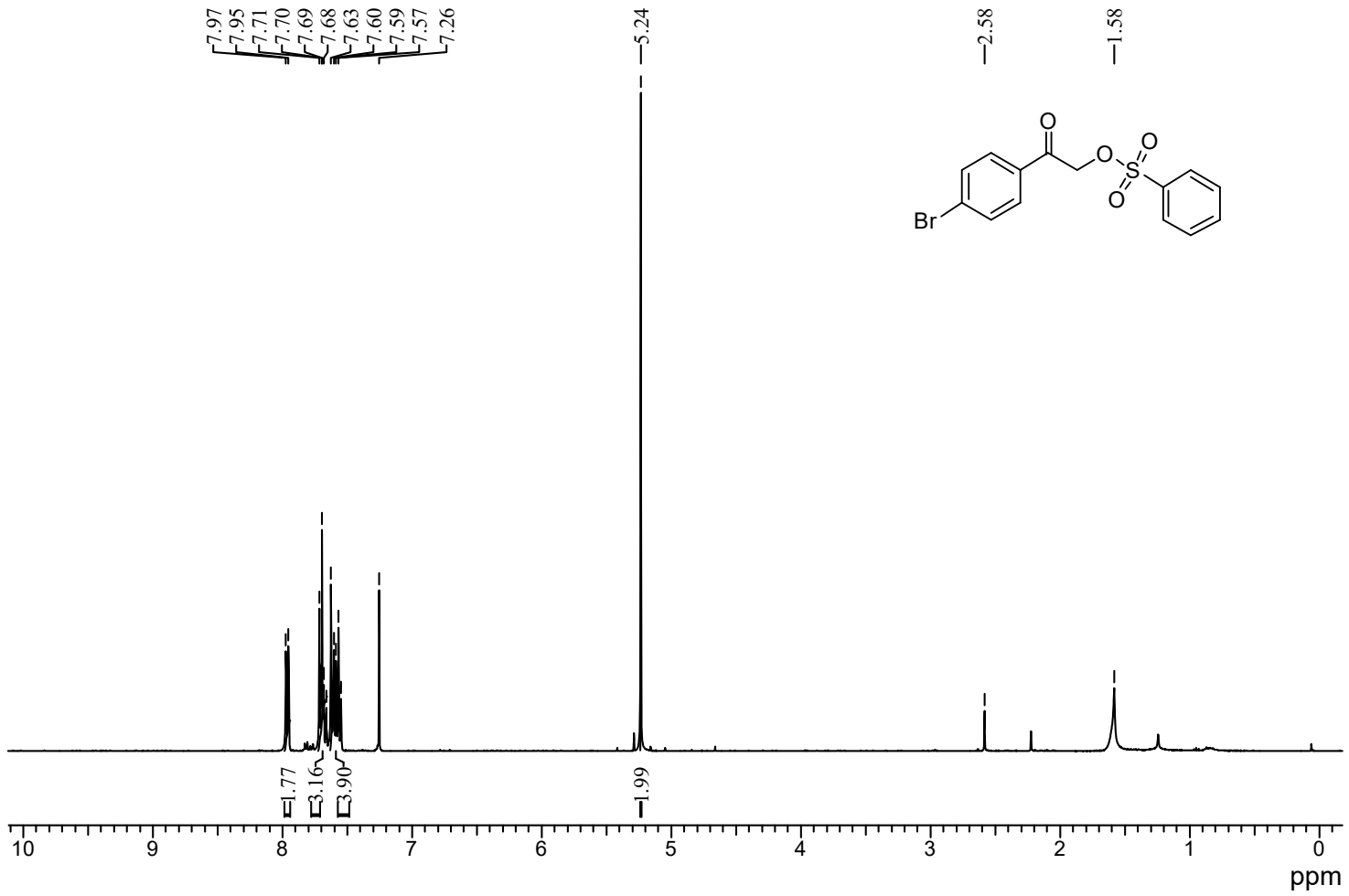
2-oxo-2-(p-tolyl)ethyl benzenesulfonate (3m): ^{1}H NMR (400 MHz, $CDCl_3$)



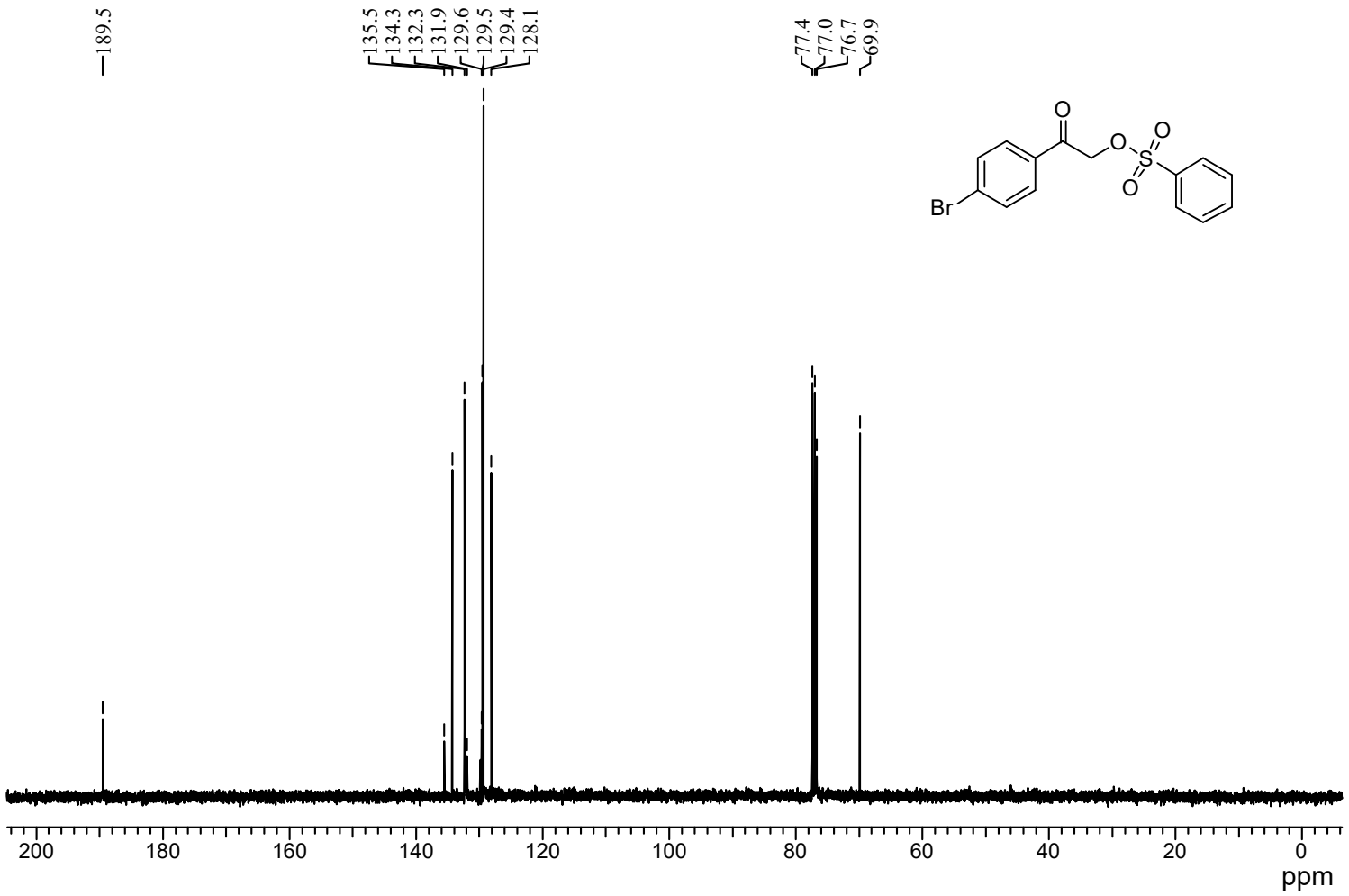
2-oxo-2-(p-tolyl)ethyl benzenesulfonate (3m): ^{13}C NMR (100 MHz, $CDCl_3$)



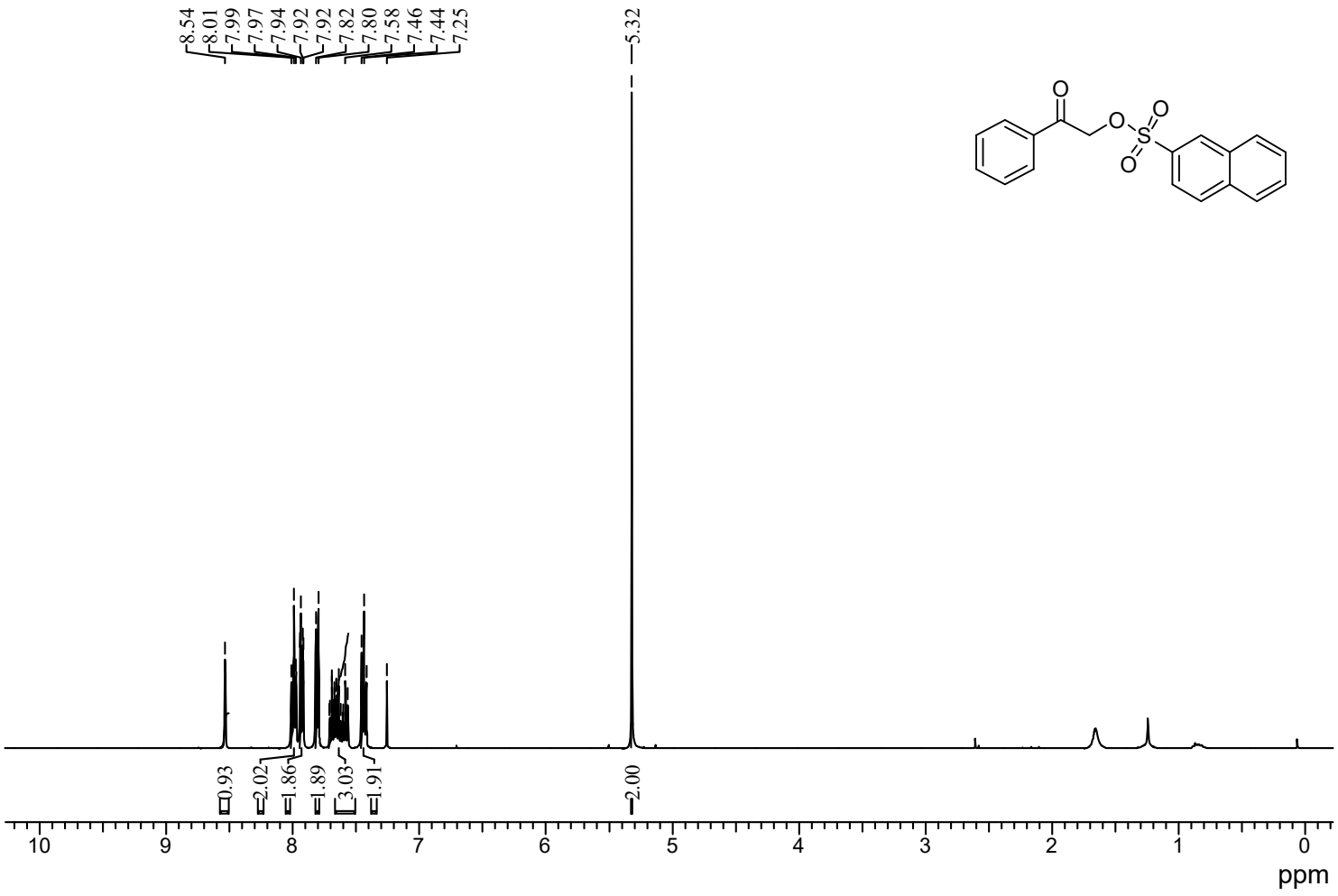
2-(4-bromophenyl)-2-oxoethyl benzenesulfonate (3n): ^{1}H NMR (400 MHz, $CDCl_3$)



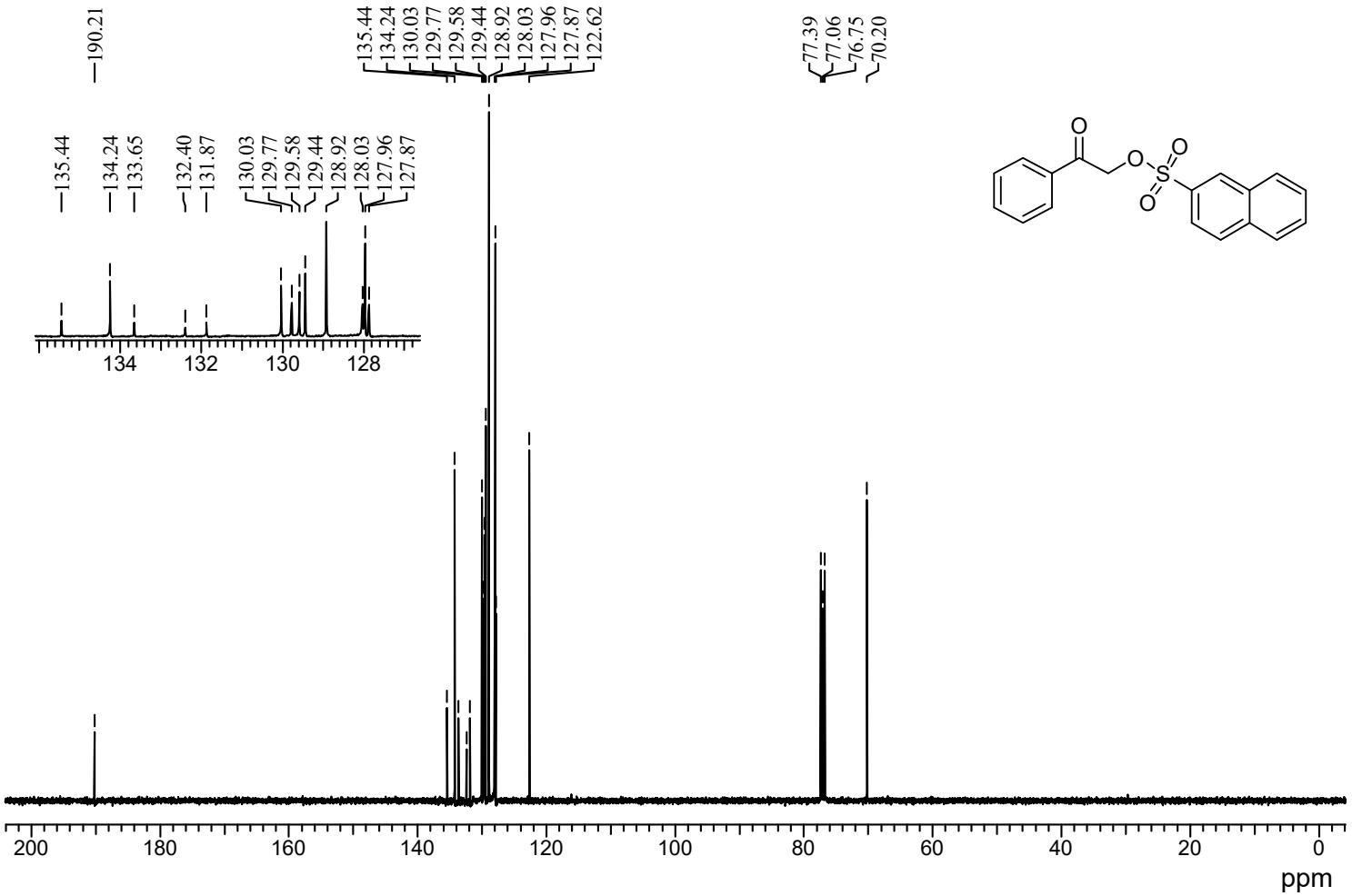
2-(4-bromophenyl)-2-oxoethyl benzenesulfonate (3n): ^{13}C NMR (100 MHz, $CDCl_3$)



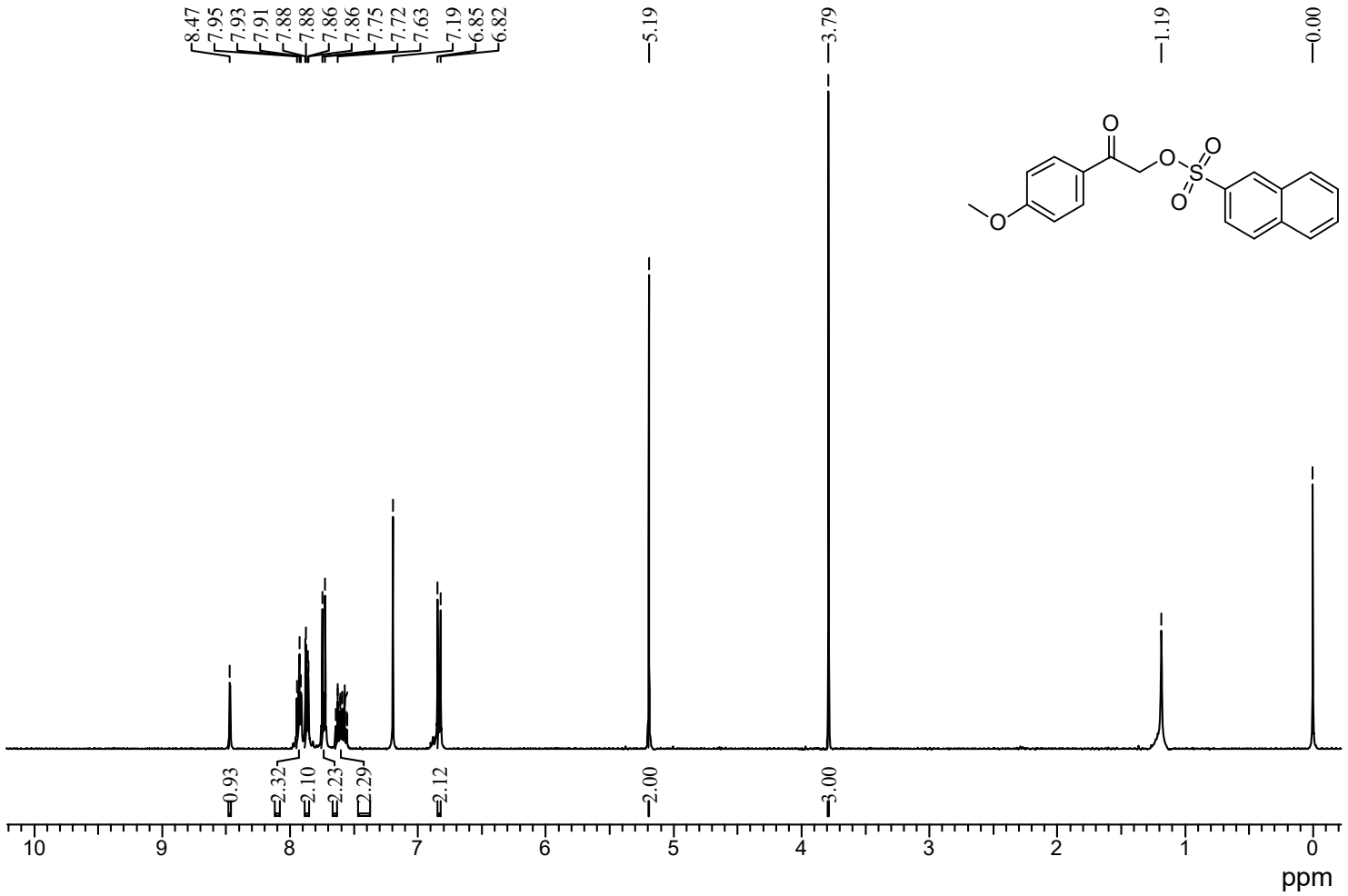
2-oxo-2-phenylethyl naphthalene-2-sulfonate (3o): ^{1}H NMR (400 MHz, $CDCl_3$)



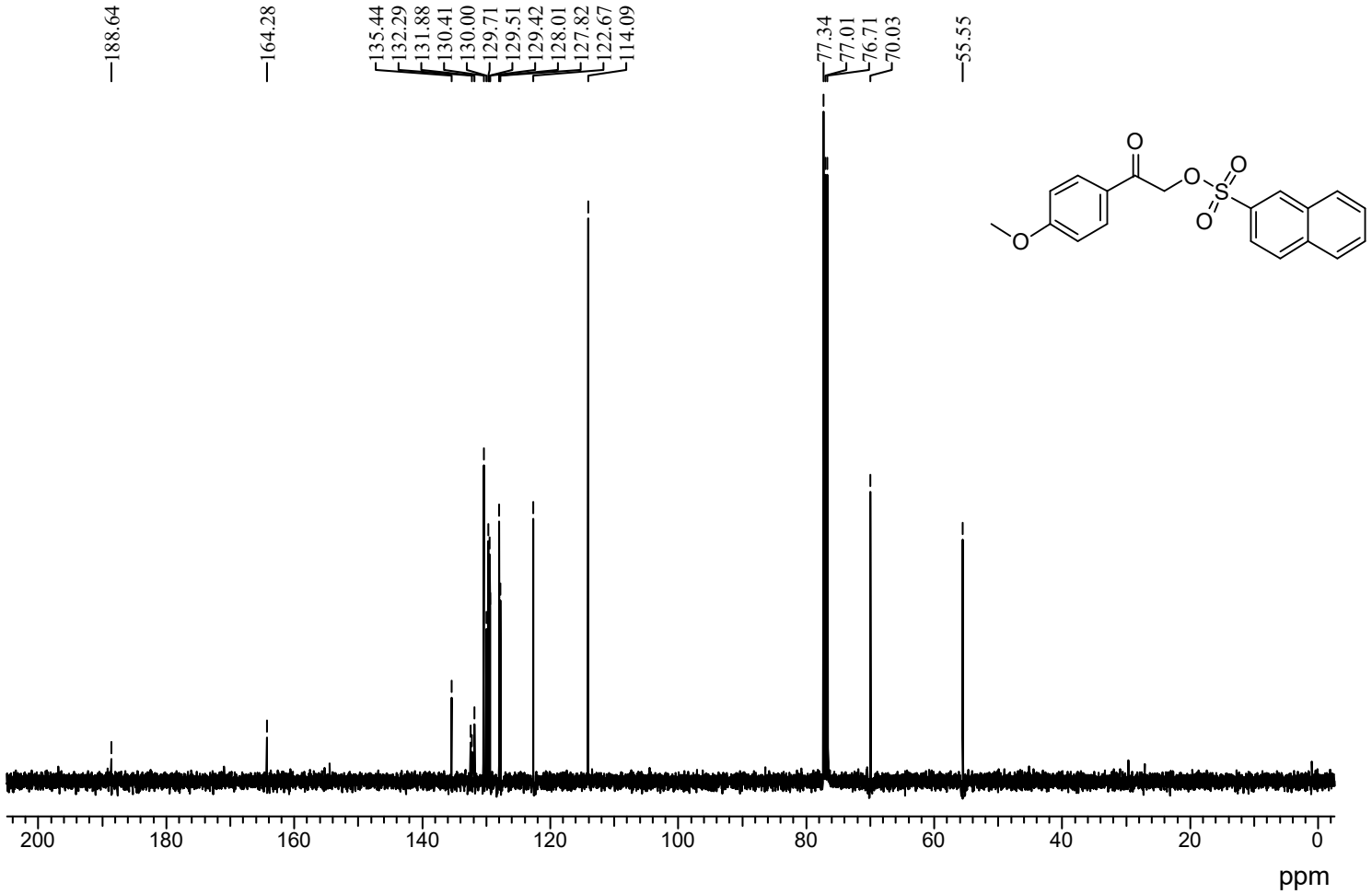
2-oxo-2-phenylethyl naphthalene-2-sulfonate (3o): ^{13}C NMR (100 MHz, $CDCl_3$)



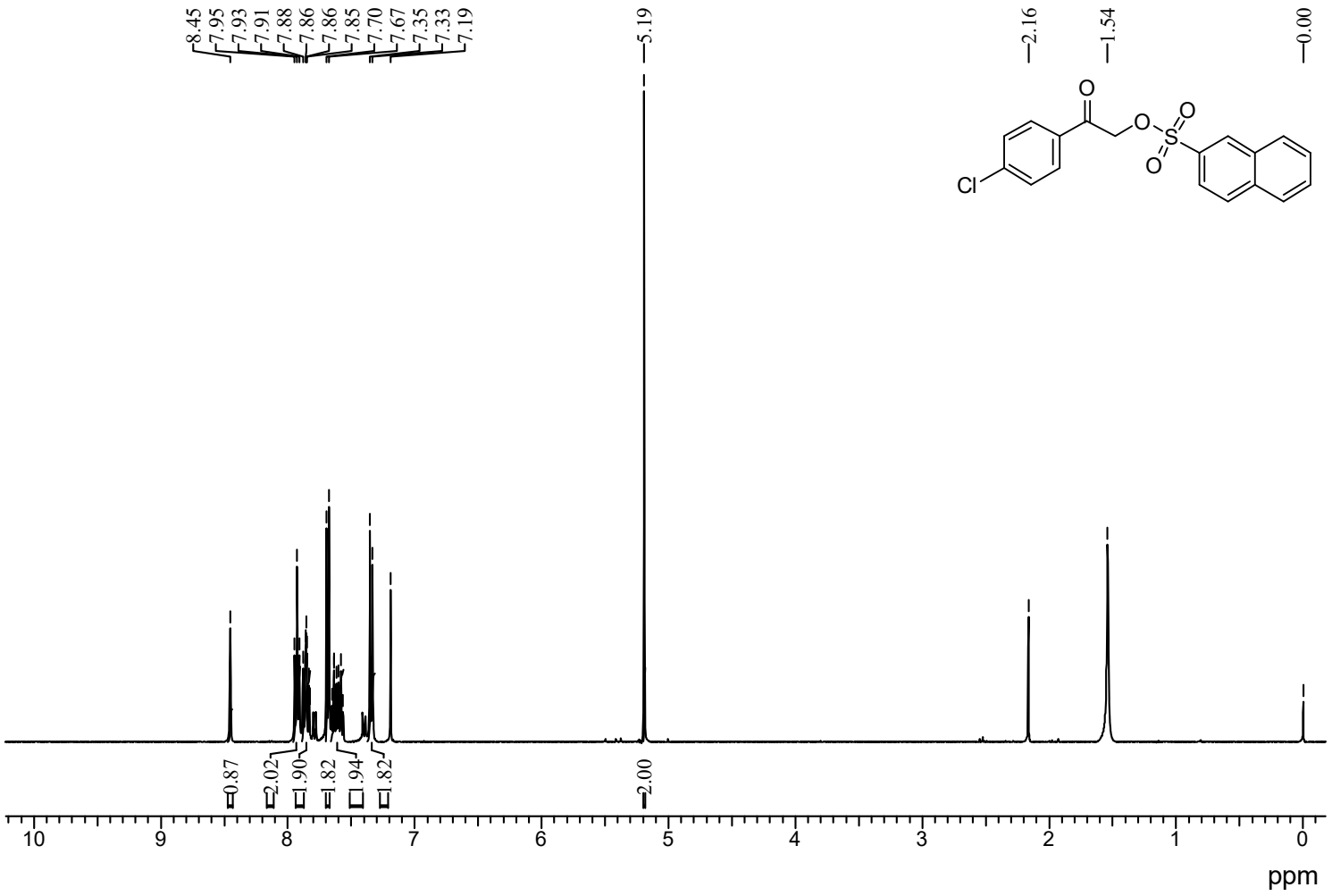
2-(4-methoxyphenyl)-2-oxoethyl naphthalene-2-sulfonate (3p): ^{1}H NMR (400 MHz, $CDCl_3$)



2-(4-methoxyphenyl)-2-oxoethyl naphthalene-2-sulfonate (3p): ^{13}C NMR (100 MHz, $CDCl_3$)



2-(4-chlorophenyl)-2-oxoethyl naphthalene-2-sulfonate (3q): ^{1}H NMR (400 MHz, $CDCl_3$)



2-(4-chlorophenyl)-2-oxoethyl naphthalene-2-sulfonate (3q): ^{13}C NMR (100 MHz, $CDCl_3$)