Supporting Information

Flexible and Practical Synthesis of Anthracenes through Gold-Catalyzed Cyclization of o-Alkynyldiarylmethanes

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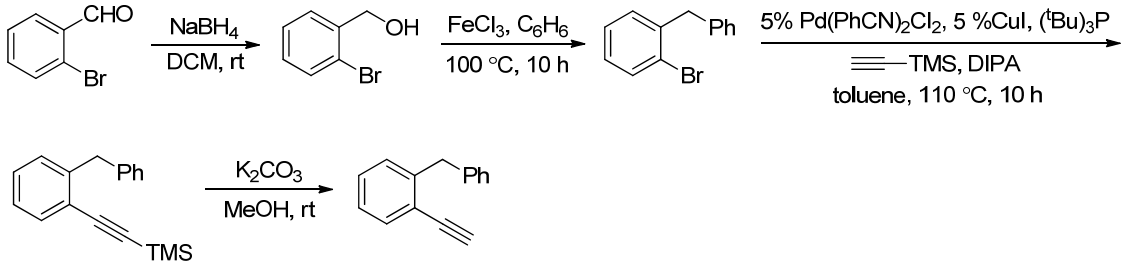
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade) and anhydrous 1, 2-dichloroethane (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass QTOF2 Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

^{1}H NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

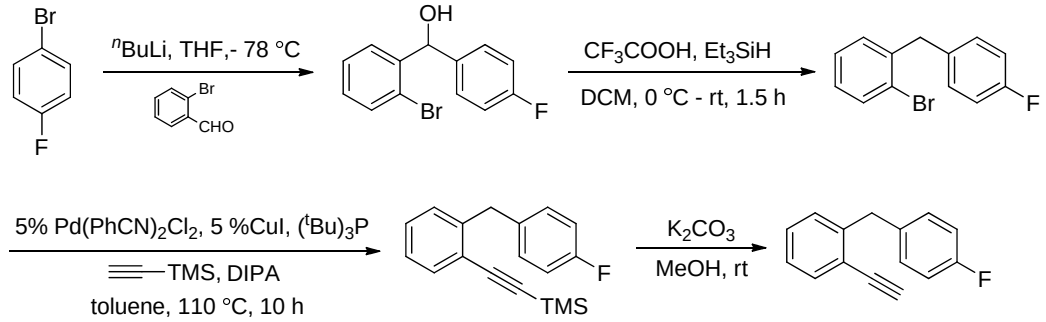
^{13}C NMR spectra were recorded on on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

Representative synthetic procedures for the preparation of starting materials: [1,2]

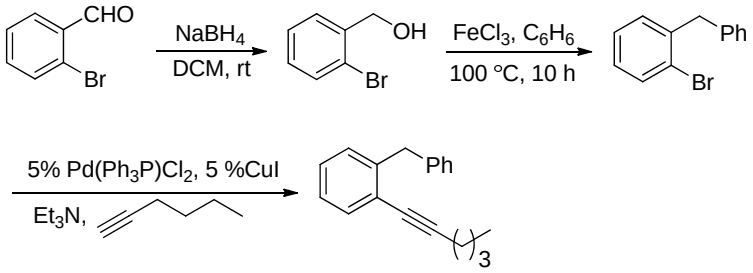
(a) Procedure for the preparation of 1-benzyl-2-ethynylbenzene (**1a**)



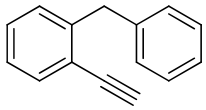
(b) Procedure for the preparation of 1-benzyl-2-ethynylbenzene (**1f**)



(c) Procedure for the preparation of 1-benzyl-2-ethynylbenzene (**1n**)



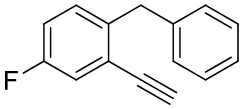
1-benzyl-2-ethynylbenzene (1a)



1a

This compound is known and the spectroscopic data match those reported.[1] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.5 (dd, 1H, *J* = 1.0 Hz, *J* = 7.5 Hz), 7.29 – 7.11 (m, 8H), 4.18 (s, 2H), 3.25 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.6, 140.4, 132.8, 129.3, 128.9, 128.4, 126.1, 126.0, 121.8, 82.5, 81.1, 39.9.

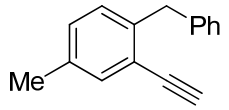
1-benzyl-2-ethynyl-4-fluorobenzene (1b)



1b

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 2H), 7.21 – 7.17 (m, 4H), 7.08 – 7.00 (m, 1H), 6.98 – 6.91 (m, 1H), 4.13 (s, 2H), 3.27 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6 (d, *J* = 243.6 Hz), 140.2, 139.5 (d, *J* = 23.0 Hz), 130.8 (d, *J* = 8.3 Hz), 128.9, 128.5, 126.2, 123.2 (d, *J* = 9.4 Hz), 119.2 (d, *J* = 22.8 Hz), 116.3 (d, *J* = 21.0 Hz), 82.0, 81.4 (d, *J* = 3.1 Hz), 39.2.

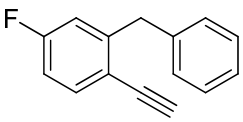
1-benzyl-2-ethynyl-4-methylbenzene (1c)



1c

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.38 – 7.23 (m, 5H), 7.16 – 7.08 (m, 2H), 4.23 (s, 2H), 3.30 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 140.6, 135.6, 133.3, 129.9, 129.3, 128.9, 128.3, 125.9, 121.6, 82.7, 80.6, 39.5, 20.7; IR (neat): 3289(bs), 3061, 3026, 2920, 2101, 1601, 1493, 1452, 1073, 837, 731, 697, 600; GCMS *m*/*z* 206 (M^+).

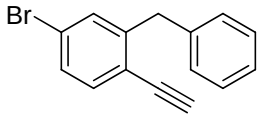
2-benzyl-1-ethynyl-4-fluorobenzene (1d)



1d

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (dd, 1H, *J* = 5.5 Hz, *J* = 8.5 Hz), 7.41 – 7.36 (m, 2H), 7.33 – 7.28 (m, 3H), 7.00 – 6.89 (m, 2H), 4.26 (s, 2H), 3.33 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.7 (d, *J* = 248.8 Hz), 146.5 (d, *J* = 7.5 Hz), 139.5, 134.6 (d, *J* = 8.8 Hz), 129.0, 128.5, 126.4, 117.8 (d, *J* = 2.5 Hz), 116.3 (d, *J* = 22.5 Hz), 113.4 (d, *J* = 22.5 Hz), 81.6, 80.9, 39.9.

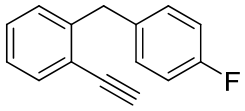
2-benzyl-4-bromo-1-ethynylbenzene (1e)



1e

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, 1H, *J* = 8.0 Hz), 7.30 – 7.26 (m, 4H), 7.23 – 7.19 (m, 3H), 4.13 (s, 2H), 3.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 139.4, 134.2, 132.4, 129.4, 128.9, 128.6, 126.4, 123.3, 120.8, 82.2, 81.6, 39.8; IR (neat): 3293(bs), 3061, 3026, 2922, 2106, 1583, 1472, 1110, 817, 730, 699; GCMS *m*/*z* 270 (M^+).

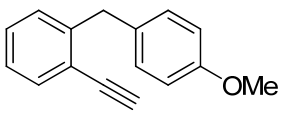
1-ethynyl-2-(4-fluorobenzyl) benzene (1f)



1f

This compound is known and the spectroscopic data match those reported.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, 1H, *J* = 7.2 Hz), 7.27 – 7.09 (m, 5H), 6.96 – 6.92 (m, 2H), 4.13 (s, 2H), 3.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4 (d, *J* = 243.0 Hz), 143.4, 136.0 (d, *J* = 4.0 Hz), 133.0, 130.3 (d, *J* = 8.0 Hz), 129.2, 129.1, 126.2, 121.8, 115.1 (d, *J* = 21.0 Hz), 82.4, 81.2, 39.2.

1-ethynyl-2-(4-methoxybenzyl) benzene (1g)

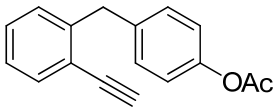


1g

This compound is known and the spectroscopic data match those reported.[1] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, 1H, *J* = 1.2 Hz, *J* = 7.6 Hz), 7.23 – 7.21 (m, 1H), 7.15 – 7.09 (m, 4H), 6.81 (d, 2H, *J* = 4.4 Hz), 4.11 (s, 2H), 3.74 (s, 3H), 3.25 (s, 1H) ; ^{13}C NMR

(100 MHz, $CDCl_3$) δ 157.9, 144.1, 132.9, 132.5, 129.9, 129.2, 128.9, 125.9, 121.6, 113.8, 82.5, 81.1, 55.1, 39.0.

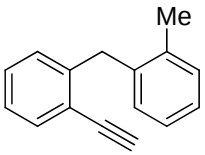
4-(2-ethynylbenzyl)phenyl acetate (1h)



1h

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, 1H, *J* = 1.2 Hz, *J* = 7.6 Hz), 7.27 – 7.10 (m, 5H), 7.01 – 6.95 (m, 2H), 4.16 (s, 2H), 3.25 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 149.0, 143.2, 137.9, 132.9, 129.8, 129.4, 129.0, 126.2, 121.8, 121.4, 82.4, 81.2, 39.3, 21.1; IR (neat): 3287, 3060, 2923, 2101, 1759 (s), 1505, 1483, 1369, 1217, 1197, 1017, 910, 759, 650; MS (ES^+) Calculated for $[C_{17}H_{14}NaO_2]^+$: 273.1; Found: 273.1.

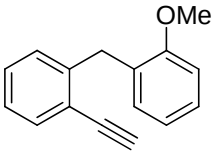
1-ethynyl-2-(2-methylbenzyl) benzene (1i)



1i

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, 1H, *J* = 7.6 Hz), 7.07 – 7.02 (m, 1H), 7.00 – 6.87 (m, 6H), 3.97 (s, 2H), 3.06 (s, 1H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 137.3, 135.4, 132.9, 129.3, 129.1, 128.9, 128.8, 125.9, 121.7, 82.6, 81.1, 39.5, 20.9; IR (neat): 3291(bs), 3048, 3020, 2920, 2101, 1513, 1481, 1446, 801, 757, 652, 604; GCMS *m*/*z* 206 (M^+).

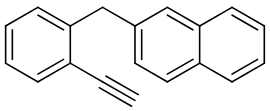
1-ethynyl-2-(2-methoxybenzyl) benzene (1j)



1j

This compound is known and the spectroscopic data match those reported.[2] ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (dd, 1H, *J* = 1.5 Hz, *J* = 7.5 Hz), 7.26 – 7.25 (m, 2H), 7.17 – 7.14 (m, 1H), 7.10 – 7.06 (m, 2H), 6.90 – 6.85 (m, 2H), 4.20 (s, 2H), 3.83 (s, 3H), 3.26 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.5, 143.6, 132.7, 130.5, 129.1, 128.8, 127.4, 125.7, 121.9, 120.5, 110.4, 99.9, 82.6, 80.9, 55.3, 33.9.

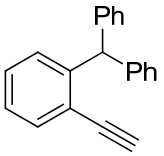
2-(2-ethynylbenzyl) naphthalene (1k)



1k

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 3H), 7.72 (s, 1H), 7.62 (dd, 1H, *J* = 1.2 Hz, *J* = 6.4 Hz), 7.53 – 7.43 (m, 3H), 7.33 – 7.29 (m, 1H), 7.26 – 7.21 (m, 2H), 4.43 (s, 2H), 3.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 137.9, 133.6, 132.9, 132.1, 129.4, 128.9, 127.9, 127.6, 127.57, 127.55, 127.2, 126.1, 125.9, 125.3, 121.9, 82.5, 81.3, 40.1; IR (neat): 3289(bs), 3054, 3021, 2919, 2104, 1632, 1599, 1508, 1482, 1446, 958, 813, 757, 654, 621; GCMS *m*/*z* 242 (M^+).

(2-ethynylphenyl)methylene) dibenzene (1l)

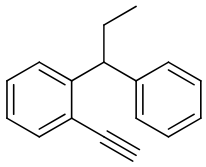


1l

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dd, 1H, *J* = 1.2 Hz, *J* = 7.6 Hz), 7.32 – 7.18 (m, 8H), 7.13 – 7.10 (m, 4H), 7.03 – 7.00 (m, 1H), 6.12 (s, 1H), 3.21 (s, 1H); ^{13}C NMR (100

MHz, $CDCl_3$) δ 146.4, 143.2, 133.1, 129.6, 129.5, 128.7, 128.2, 126.3, 126.2, 122.4, 82.2, 81.8, 54.2; IR (neat): 3292, 3060, 3021, 2919, 2104, 1597, 1493, 1482, 1445, 1246, 1114, 1028, 842, 756, 700; GCMS *m*/*z* 268 (M^+).

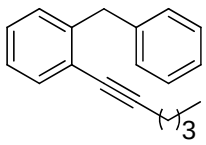
1-ethynyl-2-(1-phenylpropyl)benzene (1m)



1m

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, 1H, *J* = 0.8 Hz, *J* = 8.0 Hz), 7.31 – 7.22 (m, 6H), 7.18 – 7.09 (m, 2H), 4.50 (t, 1H, *J* = 7.6 Hz), 3.28 (s, 1H), 2.12 – 2.03 (m, 2H), 0.92 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 144.3, 133.0, 129.0, 128.2, 128.1, 126.8, 126.0, 125.7, 122.0, 82.8, 81.2, 49.7, 28.5, 21.6; IR (neat): 3292, 2962, 2929, 2101, 1599, 1492, 1478, 1447, 1383, 913, 743, 693; GCMS *m*/*z* 220 (M^+).

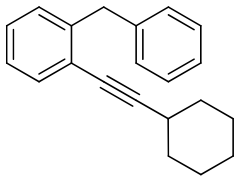
1-benzyl-2-(hex-1-ynyl)benzene (1n)



1n

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, 1H, *J* = 1.2 Hz, *J* = 10.8 Hz), 7.28 – 7.06 (m, 8H), 4.14 (s, 2H), 2.41 (t, 2H, *J* = 7.2 Hz), 1.59 – 1.52 (m, 2H), 1.47 – 1.38 (m, 2H), 0.91 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 140.8, 132.2, 129.2, 128.9, 128.3, 127.6, 125.9, 125.8, 123.8, 94.4, 79.4, 40.2, 30.8, 22.0, 19.2, 13.6; IR (neat): 3061, 3026, 2956, 2930, 2228, 1597, 1494, 1483, 1451, 912, 755, 696, 613; GCMS *m*/*z* 248 (M^+).

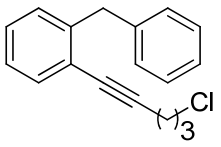
1-benzyl-2-(cyclohexylethynyl) benzene (1o)



1o

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, 1H, *J* = 2.4 Hz, *J* = 7.6 Hz), 7.28 – 7.08 (m, 8H), 4.15 (s, 2H), 2.65 – 2.58 (m, 1H), 1.91 – 1.79 (m, 2H), 1.75 – 1.68 (m, 2H), 1.56 – 1.47 (m, 3H), 1.38 – 1.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 140.9, 132.2, 129.2, 128.9, 128.3, 127.6, 126.0, 125.9, 123.8, 98.6, 79.4, 40.2, 32.7, 29.8, 26.0, 24.8; IR (neat): 3434, 2926, 2851, 2222, 1493, 1445, 1277, 1263, 1123, 918, 749; GCMS *m*/*z* 274 (M^+).

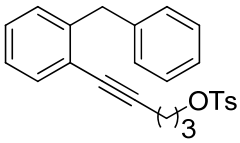
1-benzyl-2-(5-chloropent-1-ynyl)benzene (1p)



1p

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, 1H, *J* = 1.2 Hz, *J* = 7.2 Hz), 7.39 – 7.17 (m, 8H), 4.20 (s,2H), 3.66 (t, 2H, *J* = 6.4 Hz), 2.66 (t, 2H, *J* =6.8 Hz), 2.05 (t, 2H, *J* =6.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 140.6, 132.3, 129.4, 128.8, 128.3, 127.9, 126.0, 125.9, 123.3, 92.1, 80.4, 43.6, 40.2, 31.4, 17.0; IR (neat): 3061, 3025, 2957, 2921, 2225, 1598, 1494, 1484, 1449, 1290, 1029, 757, 732, 697, 653; GCMS *m*/*z* 268 (M^+).

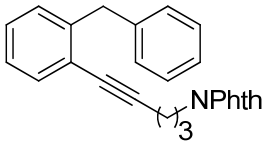
5-(2-benzylphenyl)pent-4-ynyl 4-methylbenzenesulfonate (1q)



1q

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, 2H, *J* = 8.8 Hz), 7.31 – 7.08 (m, 11H), 4.11 (t, 2H, *J* =6.0 Hz), 4.06 (s, 2H), 2.49 (t, 2H, *J* =6.8 Hz), 2.36 (s, 3H), 1.91 – 1.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 142.7, 140.6, 132.3, 130.0, 129.3, 128.8, 128.3, 128.0, 127.9, 126.0, 125.9, 123.2, 91.7, 80.6, 68.9, 40.2, 28.0, 21.5, 15.8; IR (neat): 2921, 2853, 2228, 1597, 1451, 1360, 1174, 1096, 927, 757, 662, 553; MS (ES^+) Calculated for $[C_{25}H_{24}NaO_3S]^+$: 427.1; Found: 427.1.

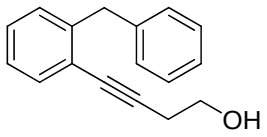
2-(5-(2-benzylphenyl)pent-4-ynyl)isoindoline-1,3-dione (1r)



1r

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dd, 2H, *J* = 2.8 Hz, *J* = 5.2 Hz), 7.65 (dd, 2H, *J* = 2.8 Hz, *J* = 5.2 Hz), 7.31 (d, 1H, *J* = 1.2 Hz), 7.23 – 7.27 (m, 2H), 7.21 – 7.13 (m, 4H), 7.10 – 7.04 (m, 2H), 4.12 (s, 2H), 3.81 (t, 2H, *J* = 6.8 Hz), 2.50 (t, 2H, *J* = 6.8 Hz), 2.02 – 1.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 142.7, 140.7, 135.9, 133.8, 132.2, 132.1, 129.1, 128.9, 128.3, 127.8, 125.9, 125.6, 123.1, 92.7, 80.1, 40.1, 37.3, 27.5, 17.4; IR (neat): 3025, 2925, 2228, 1771, 1709, 1394, 1370, 1112, 1025, 761, 716; (ES^+) Calculated for $[C_{26}H_{21}NNaO_2]^+$: 402.2; Found: 402.2.

3-(2-benzylphenyl)prop-2-yn-1-ol (1s)

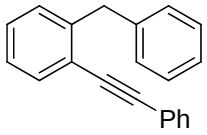


1s

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, 1H, *J* = 8.0 Hz), 7.29 – 7.12 (m, 8H), 4.14 (s, 2H), 3.28 – 3.67 (m, 2H), 2.64 (t, 2H, *J* = 6.0 Hz), 1.83 (t, 1H, *J* = 4.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 140.5, 132.3, 129.5, 128.7, 128.3, 128.1, 126.1, 126.0, 123.1, 90.6,

81.2, 61.1, 40.2, 23.9; IR (neat): 3388(bs), 3060, 3025, 2918, 2230, 1597, 1494, 1483, 1448, 1042, 757, 697; MS (ES^+) Calculated for $[C_{17}H_{16}NaO]^+$: 259.1; Found: 259.1.

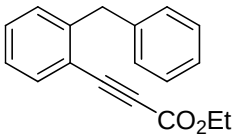
1-benzyl-2-(phenylethynyl)benzene (1t)



1t

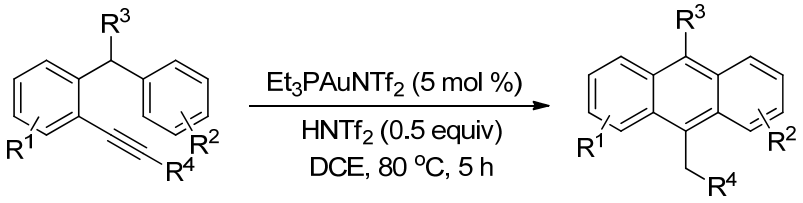
^1H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, 1H, *J* = 8.0 Hz), 7.48 – 7.45 (m, 2H), 7.34 – 7.30 (m, 3H), 7.27 – 7.26 (m, 4H), 7.24 – 7.15 (m, 4H), 4.24 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 140.6, 132.3, 131.5, 129.4, 128.9, 128.5, 128.4, 128.3, 128.2, 126.1, 126.0, 123.4, 122.9, 93.4, 88.4, 40.3; IR (neat): 3059, 3025, 2921, 2208, 1598, 1492, 1446, 1091, 1096, 1028, 754, 731, 689; MS (ES^+) Calculated for $[C_{21}H_{16}Na]^+$: 291.1; Found: 291.1.

ethyl 3-(2-benzylphenyl)propiolate (1u)



1u

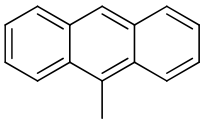
^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, 1H, *J* = 7.2 Hz), 7.34 – 7.15 (m, 8H), 4.27 (dd, 2H, *J* = 7.2 Hz, *J* = 14.4 Hz), 4.17 (s, 2H), 1.33 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 145.2, 139.7, 133.7, 130.7, 129.5, 129.0, 128.4, 126.2, 126.1, 119.2, 84.9, 84.5, 61.9, 40.0, 14.0; IR (neat): 3397, 3027, 2982, 2206, 1708, 1597, 1483, 1449, 1366, 1289, 1192, 1022, 759, 732, 697; MS (ES^+) Calculated for $[C_{18}H_{16}NaO_2]^+$: 287.1; Found: 287.1.



General procedure:

$HNTf_2$ (3.0 mL, 0.05 M in DCE), and $Et_3PAuNTf_2$ (9.0 mg, 0.015 mmol) were added to a solution of the 1-benzyl-2-ethynylbenzenes **1** (0.30 mmol) in DCE (3.0 mL) at room temperature. The reaction mixture was stirred at 80 ^oC and the progress of the reaction was monitored by TLC. The reaction typically took 5 h. Upon completion, the reaction diluted with DCM (30 mL) and washed with saturated aqueous $NaHCO_3$ (2 × 15 mL). The resulting solution was extracted again with DCM (30 mL) and the combined organic layers were dried with $MgSO_4$. The mixture was then concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired products **2**.

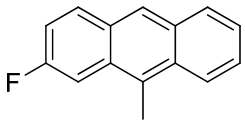
9-methylanthracene (2a)



2a

Compound **2a** was prepared in 72% yield according to the general procedure. This compound is known and the spectroscopic data match those reported.[3] ^1H NMR (500 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.24 (d, 2H, *J* = 8.0 Hz), 7.96 (d, 2H, *J* = 8.0 Hz), 7.49 – 7.41 (m, 4H), 3.05 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 131.4, 130.1, 130.0, 129.0, 125.3, 125.2, 124.8, 124.6, 13.9.

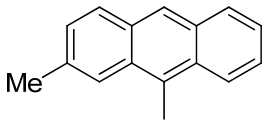
2-fluoro-9-methylanthracene (2b)



2b

Compound **2b** was prepared in 62% yield according to the general procedure. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (s, 1H), 8.20 (d, 1H, *J* = 8.8 Hz), 7.94 (d, 1H, *J* = 9.2 Hz), 7.92 (d, 1H, *J* = 9.2 Hz), 7.79 (dd, 1H, *J* = 2.4 Hz, *J* = 12.4 Hz), 7.52 –7.41 (m, 2H), 7.27 – 7.20 (m, 1H), 2.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4 (d, *J* = 244.8 Hz), 131.7 (d, *J* = 9.1 Hz), 130.9 (d, *J* = 2.1 Hz), 130.5, 130.4 (d, *J* = 8.4 Hz), 129.3 (d, *J* = 7.8 Hz), 129.1, 128.7, 125.8, 125.6 (d, *J* = 1.7 Hz), 124.7, 124.3, 116.6 (d, *J* = 27.5 Hz), 106.9 (d, *J* = 21.4 Hz), 14.0; IR (neat): 3049, 2923, 1905, 1634, 1486, 1455, 1255, 1188, 1174, 884, 849, 770, 739; GCMS *m*/*z* 210 (M^+).

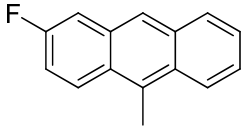
2,9-dimethylanthracene (2c)



2c

Compound **2c** was prepared in 60% yield according to the general procedure. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 –8.24 (m, 2H), 8.02 (s, 1H), 7.96 (d, 1H, *J* = 9.2 Hz), 7.89 (d, 1H, *J* = 8.4 Hz), 7.50 –7.39 (m, 2H), 7.30 (dd, 1H, *J* = 1.6 Hz, *J* = 8.4 Hz), 3.06 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 131.0, 130.4, 130.3, 130.1, 129.1, 128.9, 128.8, 127.6, 125.1, 125.0, 124.6, 124.4, 123.0, 22.5, 13.8; IR (neat): 3396, 3032, 2918, 2853, 1632, 1450, 1377, 1412, 1158, 876, 738; GCMS *m*/*z* 206 (M^+).

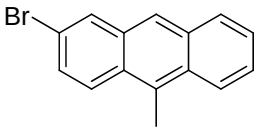
2-fluoro-10-methylanthracene (2d)



2d

Compound **2d** was prepared in 63% yield according to the general procedure. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 –8.24 (m, 3H), 7.97 –7.93 (m, 1H), 7.55 (dd, 1H, *J* = 2.4 Hz, *J* = 10.4 Hz), 7.52 –7.44 (m, 2H), 7.32 –7.27 (m, 1H), 3.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8 (d, *J* = 245.9 Hz), 132.2, 131.8 (d, *J* = 9.0 Hz), 130.9 (d, *J* = 1.9 Hz), 129.6 (d, *J* = 2.0 Hz), 128.6, 127.6 (d, *J* = 8.9 Hz), 127.5, 125.4, 125.2 (d, *J* = 0.9 Hz), 124.8, 124.4 (d, *J* = 7.1 Hz), 116.9 (d, *J* = 27.0 Hz), 110.3 (d, *J* = 19.8 Hz), 14.2; IR (neat): 3049, 2920, 1635, 1530, 1454, 1268, 1201, 1143, 970, 883, 804, 738; GCMS *m*/*z* 210 (M^+).

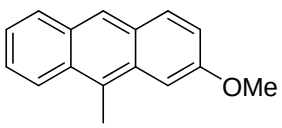
2-bromo-10-methylanthracene (2e)



2e

Compound **2e** was prepared in 68% yield according to the general procedure.^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 (d, 1H, *J* = 4.8 Hz), 8.21 (s, 1H), 8.15 –8.13 (m, 2H), 7.98 (d, 1H, *J* = 7.6 Hz), 7.55 –7.46 (m, 3H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.2, 132.0, 130.8, 130.5, 130.3, 128.9, 128.6, 128.3, 126.6, 125.6, 125.5, 124.7, 124.4, 119.1, 13.9; IR (neat): 3056, 2923, 2851, 1610, 1566, 1518, 1444, 1071, 917, 888, 801, 737; GCMS *m*/*z* 270 (M^+).

2-methoxy-9-methylanthracene (2g)

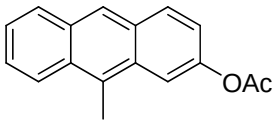


2g

Compound **2g** was prepared in 67% yield according to the general procedure. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 –8.22 (m, 2H), 7.96 (d, 1H, *J* = 8.4 Hz), 7.89 (d, 1H, *J* = 9.2 Hz), 7.51 –7.37 (m, 3H), 7.16 (dd, 1H, *J* = 2.4 Hz, *J* = 9.2 Hz), 3.99 (s, 3H), 3.01 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 131.0, 130.8, 130.5, 130.2, 129.1, 128.0, 127.6, 125.4, 125.3, 124.2, 123.9, 119.8, 100.8, 55.2, 14.1; IR (neat): 2996, 2933, 1626, 1464, 1434, 1283, 1218, 1178, 1162, 1022, 886, 744; GCMS *m*/*z* 222 (M^+).

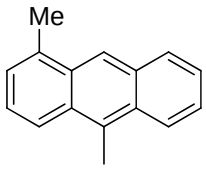
9-methylanthracen-2-yl acetate (2h)



2h

Compound **2h** was prepared in 63% yield according to the general procedure. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.25 (d, 1H, *J* = 8.8 Hz), 7.99 (t, 2H, *J* = 8.8 Hz), 7.94 (d, 1H, *J* = 2.0 Hz), 7.54 – 7.43 (m, 2H), 7.23 (dd, 1H, *J* =2.4 Hz, *J* = 9.2 Hz), 3.03 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 147.9, 131.4, 130.7, 130.4, 130.2, 129.9, 129.6, 129.1, 125.7, 125.4, 124.9, 124.5, 121.0, 114.9, 21.2, 14.1; IR (neat): 2923, 1758 (s), 1622, 1454, 1366, 1207, 1185, 1165, 912, 742; MS (ES^+) Calculated for $[C_{17}H_{14}NaO_2]^+$: 273.1; Found: 273.1.

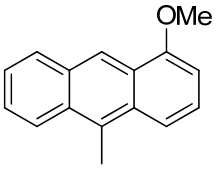
1,10-dimethylanthracene (2i)



2i

Compound **2i** was prepared in 62% yield according to the general procedure. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.25 –8.22 (m, 2H), 8.00 (s, 1H), 7.94 (d, 1H, *J* = 8.5 Hz), 7.87 (d, 1H, *J* = 8.5 Hz), 7.48 –7.38 (m, 2H), 7.28 (dd, 1H, *J* = 1.5 Hz, *J* = 8.5 Hz), 3.04 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.7, 131.0, 130.3, 130.2, 130.1, 129.1, 128.9, 127.6, 125.1, 125.0, 124.6, 124.3, 123.0, 22.5, 13.8; IR (neat): 3032, 2916, 2856, 1632, 1449, 1377, 1343, 1158, 876, 772, 739, 529; GCMS *m*/*z* 206 (M^+).

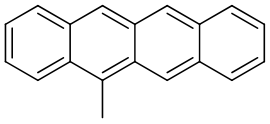
1-methoxy-10-methylanthracene (2j)



2j

Compound **2j** was prepared in 58% yield according to the general procedure. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.27 (d, 1H, *J* = 9.0 Hz), 8.06 (d, 1H, *J* = 8.0 Hz), 7.86 (d, 1H, *J* = 9.0 Hz), 7.53 –7.40 (m, 3H), 6.76 (d, 1H, *J* = 7.5 Hz), 4.09 (s, 3H), 3.08 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.9, 131.1, 130.9, 130.4, 129.7, 129.5, 125.5, 125.0, 124.8, 124.5, 124.4, 119.7, 117.1, 101.2, 55.6, 14.2; IR (neat): 3052, 2929, 1623, 1565, 1459, 1410, 1350, 1241, 1199, 1040, 794, 722; GCMS *m*/*z* 222 (M^+).

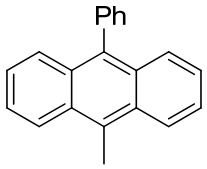
5-methyltetracene (2k)



2k

Compound **2k** was prepared in 68% yield according to the general procedure.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (t, 1H, *J* = 4.4 Hz), 8.32 (d, 1H, *J* = 8.8 Hz), 8.17 (s, 1H), 8.01 (d, 1H, *J* = 8.0 Hz), 7.82 –7.79 (m, 1H), 7.65 –7.50 (m, 6H), 3.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.8, 132.6, 131.4, 131.3, 131.2, 129.7, 128.7, 128.3, 128.0, 127.9, 126.8, 126.4, 125.8, 125.3, 125.2, 125.1, 125.0, 20.8; IR (neat): 3046, 2957, 1622, 1489, 1479, 1432, 1365, 1152, 1129, 1000, 883, 811, 748; GCMS *m*/*z* 242 (M^+).

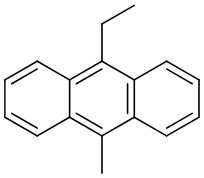
9-methyl-10-phenylanthracene (2l)



2l

Compound **2l** was prepared in 71% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, 2H, *J* = 8.8 Hz), 7.67 – 7.64 (m, 2H), 7.58 – 7.46 (m, 5H), 7.41 – 7.38 (m, 2H), 7.35 – 7.30 (m, 2H), 3.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 135.7, 131.5, 130.1, 130.0, 129.8, 128.3, 127.7, 127.3, 125.0, 124.7, 124.6, 14.2; IR (neat): 3063, 2924, 2852, 1600, 1442, 1460, 1388, 1275, 1261, 921, 753, 702, 643, 615; GCMS *m*/*z* 268 (M^+).

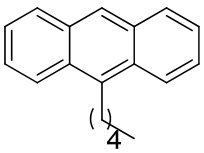
9-benzylanthracene (2m)



2m

Compound **2m** was prepared in 63% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.35 – 8.30 (m, 4H), 7.52 – 7.47 (m, 4H), 3.64 (q, 2H, *J* = 7.6 Hz), 3.01 (s, 3H), 1.45 (t, 3H, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.9, 130.1, 128.9, 128.5, 125.5, 124.9, 124.8, 124.7, 21.1, 15.6, 14.1; IR (neat): 2961, 2925, 2871, 1618, 1450, 1384, 1365, 1028, 913, 749; GCMS *m*/*z* 220 (M^+).

9-pentylanthracene (2n)

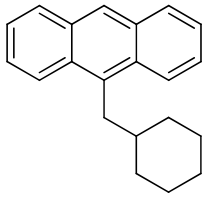


2n

Compound **2n** was prepared in 65% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.26 (d, 2H, *J* = 8.8 Hz), 7.99 (dd, 2H, *J* = 0.4 Hz, *J* = 8.4 Hz), 7.52 –7.42 (m, 4H), 3.59 (t, 2H, *J* = 8.0 Hz), 1.86 –1.78 (m, 2H), 1.61 –1.53 (m, 2H), 1.49 –1.39 (m, 2H), 0.94 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.5,

131.6, 129.5, 129.2, 125.4, 125.3, 124.7, 124.5, 32.5, 31.1, 28.0, 22.7, 14.1; IR (neat): 3054, 2950, 2924, 2853, 1621, 1465, 1445, 1351, 1155, 1011, 732; GCMS *m*/*z* 248 (M^+).

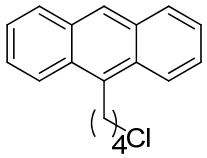
9-(cyclohexylmethyl)anthracene (2o)



2o

Compound **2o** was prepared in 66% yield according to the general procedure.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.27 (d, 2H, *J* = 8.8 Hz), 7.98 (dd, 2H, *J* = 0.4 Hz, *J* = 8.0 Hz), 7.50 – 7.42 (m, 4H), 3.50 (d, 2H, *J* = 6.8 Hz), 1.89 – 1.78 (m, 1H), 1.72 – 1.60 (m, 5H), 1.29 – 1.18 (m, 3H), 1.15 – 1.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.3, 131.6, 130.4, 129.1, 125.6, 125.2, 125.1, 124.7, 40.7, 35.2, 34.0, 26.5, 26.4. IR (neat): 3050, 2922, 2849, 1623, 1524, 1445, 1346, 1159, 879, 836, 729; GCMS *m*/*z* 274 (M^+).

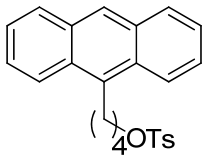
9-(4-chlorobutyl)anthracene (2p)



2p

Compound **2p** was prepared in 63% yield according to the general procedure.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.24 (d, 2H, *J* = 8.4 Hz), 7.99 (dt, 2H, *J* = 0.8 Hz, *J* = 8.4 Hz), 7.52 –7.42 (m, 4H), 3.65 –3.59 (m, 4H), 2.07 –1.93 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.2, 131.6, 129.6, 129.3, 125.8, 125.6, 124.8, 124.2, 44.8, 32.9, 28.4, 27.1; IR (neat): 3435 (bs), 3055, 2950, 2925, 1621, 1445, 1353, 1253, 1156, 886, 843, 733 ; GCMS *m*/*z* 268 (M^+).

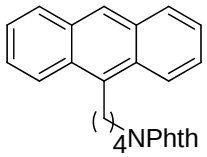
4-(anthracen-9-yl)butyl 4-methylbenzenesulfonate (2q)



2q

Compound **2q** was prepared in 65% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.16 (d, 2H, *J* = 9.2 Hz), 7.99 (d, 2H, *J* = 7.2 Hz), 7.75 (d, 2H, *J* = 8.0 Hz), 7.51 –7.42 (m, 4H), 7.28 –7.25 (m, 3H), 4.10 (t, 2H, *J* = 6.0 Hz), 3.58 (t, 2H, *J* = 8.0 Hz), 2.39 (s, 3H), 1.93 –1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 133.9, 133.3, 131.6, 129.8, 129.6, 129.3, 127.8, 125.9, 125.6, 124.8, 124.2, 70.3, 29.2, 27.1, 27.0, 21.5; IR (neat): 3390 (bs), 3052, 2924, 1602, 1442, 1357, 1175, 1097, 913, 733, 663; MS (ES^+) Calculated for $[C_{25}H_{24}NaO_3S]^+$: 427.1; Found: 427.1.

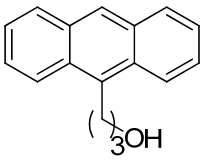
2-(4-(anthracen-9-yl)butyl)isoindoline-1,3-dione (2r)



2r

Compound **2r** was prepared in 70% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.24 (d, 2H, *J* = 8.8 Hz), 7.98 (d, 2H, *J* = 8.0 Hz), 7.83 (t, 2H, *J* = 5.2 Hz), 7.70 (dd, 2H, *J* = 2.8 Hz, *J* = 5.2 Hz), 7.51 –7.42 (m, 4H), 3.77 (t, 2H, *J* = 6.8 Hz), 3.65 (t, 2H, *J* = 8.0 Hz), 2.00 –1.93 (m, 2H), 1.91 –1.84 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 134.4, 133.9, 132.2, 131.6, 129.6, 129.2, 125.8, 125.5, 124.8, 124.4, 123.2, 37.9, 29.1, 28.4, 27.5; IR (neat): 3464, 3053, 2926, 1770, 1710(s), 1435, 1395, 1369, 1403, 719; MS (ES^+) Calculated for $[C_{26}H_{21}NNaO_2]^+$: 402.2; Found: 402.2.

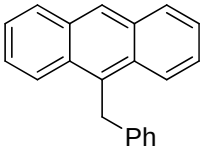
3-(anthracen-9-yl)propan-1-ol (2s)



2s

Compound **2s** was prepared in 79% yield according to the general procedure.[1]H NMR (400 MHz, $CDCl_3$) δ 8.32 (s, 1H), 8.28 (d, 2H, *J* = 8.8 Hz), 7.97 (t, 2H, *J* = 8.0 Hz), 7.51 –7.42 (m, 4H), 3.79 (t, 2H, *J* = 6.4 Hz), 3.71 (t, 2H, *J* = 7.6 Hz), 2.10 –2.03 (m, 2H), 1.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.2, 131.6, 129.6, 129.2, 125.7, 125.5, 124.8, 124.3, 62.6, 33.9, 24.0; IR (neat): 3360 (bs), 3051, 2926, 2884, 1622, 1445, 1348, 1157, 1061, 882, 731; GCMS *m*/*z* 236 (M^+).

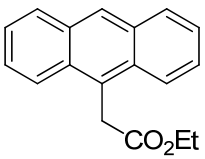
9-benzylanthracene (2t)



2t

Compound **2t** was prepared in 71% yield according to the general procedure. [1]H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.23 – 8.19 (m, 2H), 8.05 – 8.01 (m, 2H), 7.47 – 7.43 (m, 4H), 7.21 – 7.11 (m, 5H), 5.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 131.8, 131.7, 130.6, 129.1, 128.5, 128.1, 126.6, 126.0, 125.9, 124.9, 124.8, 33.5; IR (neat): 3082, 3055, 3026, 2921, 1621, 1601, 1492, 1444, 1074, 886, 845, 730, 703; GCMS *m*/*z* 268 (M^+).

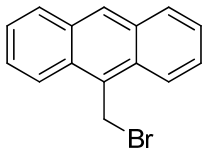
ethyl 2-(anthracen-9-yl)acetate (2u)



2u

Compound **2u** was prepared in 72% yield according to the general procedure. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.29 (d, 2H, *J* = 8.8 Hz), 8.02 (d, 2H, *J* = 8.4 Hz), 7.57 – 7.45 (m, 4H), 4.63 (s, 2H), 4.13 (dd, 2H, *J* = 6.8 Hz, *J* = 14.0 Hz), 1.90 (t, 3H, *J* = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 131.6, 130.6, 129.1, 127.3, 126.2, 126.1, 124.9, 124.4, 61.0, 34.1, 14.2; IR (neat): 3053, 2979, 2926, 1731 (s), 1625, 1446, 1366, 1254, 1158, 1030, 885, 841, 731; MS (ES^+) Calculated for $[C_{18}H_{16}NaO_2]^+$: 287.1; Found: 287.1.

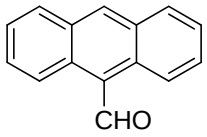
9-(bromomethyl)anthracene (5)



5

Compound **5** was prepared in 80% yield according to the literature procedure.[4] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.30 (dd, 2H, *J* = 0.4 Hz, *J* = 9.2 Hz), 8.04 (d, 2H, *J* = 8.8 Hz), 7.66 – 7.62 (m, 2H), 7.52 – 7.48 (m, 2H), 5.54 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.6, 129.7, 129.3, 129.2, 127.9, 126.8, 125.4, 123.5, 26.9; IR (neat): 3049, 2920, 1621, 1447, 1196, 1054, 882, 786, 729, 548, 487; GCMS *m*/*z* 270 (M^+).

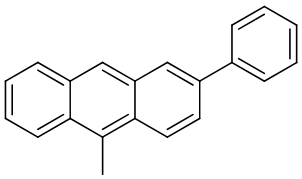
anthracene-9-carbaldehyde (6)



6

Compound **6** was prepared in 87% yield according to the literature procedure.[5] This compound is known and the spectroscopic data match those reported.[5] ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.54 (s, 1H), 9.00 (dd, 2H, *J* = 0.4 Hz, *J* = 9.2 Hz), 8.72 (s, 1H), 8.08 (d, 2H, *J* = 8.4 Hz), 7.71 – 7.67 (m, 2H), 7.58 – 7.54 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.9, 135.2, 132.2, 131.2, 129.3, 129.1, 125.7, 124.9, 123.6.

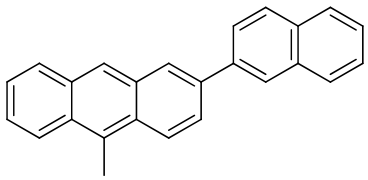
10-methyl-2-phenylanthracene (7)



7

Compound **7** was prepared in 85% yield according to the literature procedure.[6] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.34 (m, 2H), 8.28 (d, 1H, *J* = 9.2 Hz), 8.19 (d, 1H, *J* = 2.0 Hz), 8.00 (d, 1H, *J* = 7.6 Hz), 7.81 – 7.77 (m, 3H), 7.52 – 7.44 (m, 4H), 7.41 – 7.36 (m, 1H), 3.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 137.1, 131.9, 131.7, 130.3, 130.1, 129.3, 129.0, 128.9, 127.4, 127.3, 126.4, 125.6, 125.4, 125.3, 125.2, 124.9, 124.7, 13.9; IR (neat): 2917, 2849, 1446, 1434, 1262, 1177, 886, 732, 699; GCMS *m*/*z* 268 (M^+).

10-methyl-2-(naphthalen-2-yl)anthracene (8)



8

Compound **8** was prepared in 81% yield according to the literature procedure.[6] ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 – 8.38 (m, 2H), 8.33 – 8.28 (m, 2H), 8.23 (s, 1H), 8.03 – 7.88 (m, 6H), 7.55 – 7.45 (m, 4H), 3.13 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.1, 136.9, 133.8, 132.8, 131.9, 131.8, 130.4, 130.2, 129.4, 129.1, 128.6, 128.3, 127.7, 126.8, 126.4, 126.0, 125.9, 125.7, 125.6, 125.5, 125.4, 125.3, 125.0, 124.7, 14.0; IR (neat): 2919, 2849, 1621, 1596, 1366, 1351, 1275, 1260, 889, 806, 746; GCMS *m*/*z* 318 (M^+).

Reference:

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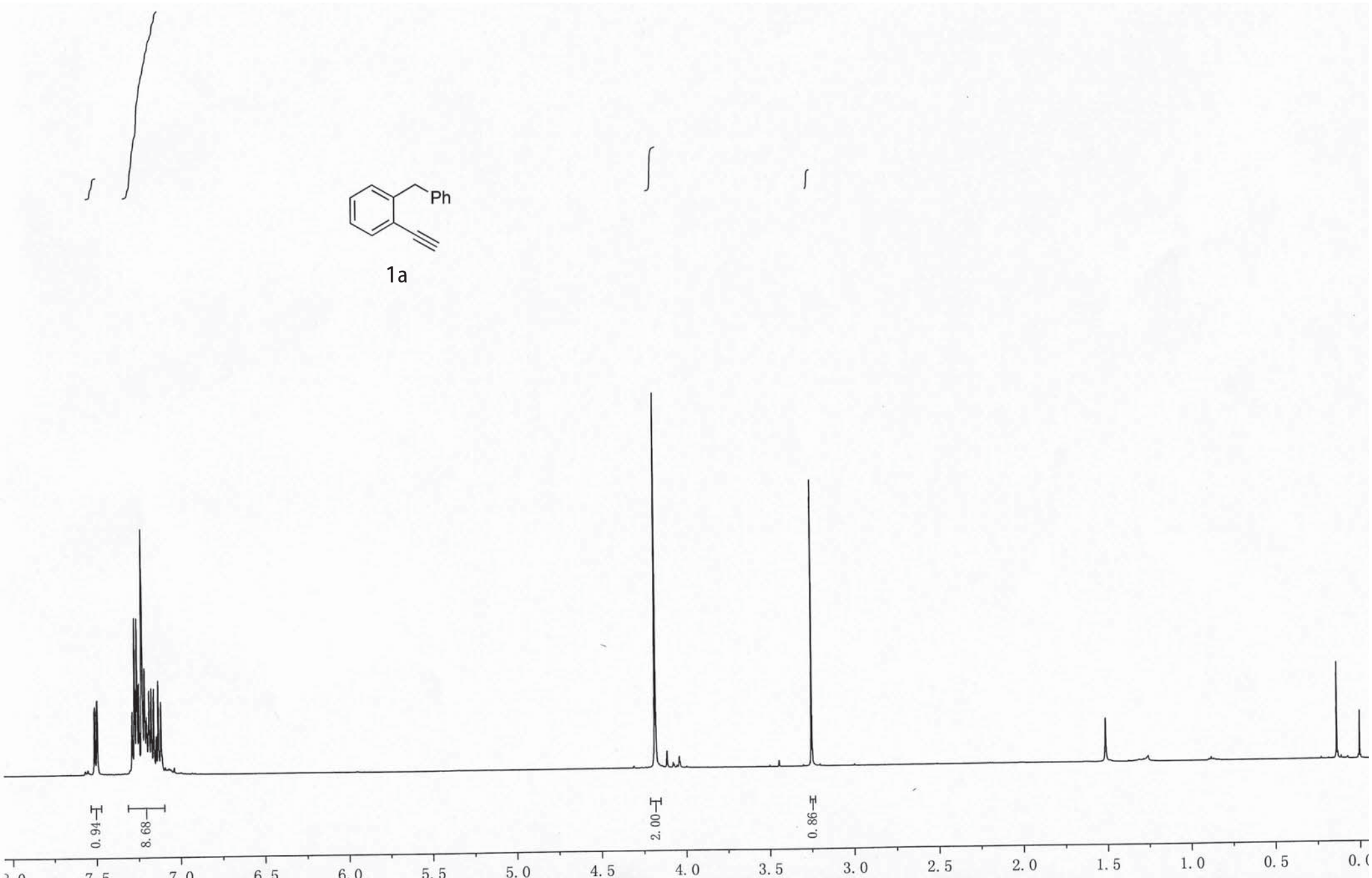
2. Odedra, A.; Datta, S.; Liu, R.-S. *J. Org. Chem.* **2007**, *72*, 3289.

3. Banciu, M. D.; Costea, C.; Draghici, C.; Banciu, A.; Mihaiescu, D.; Ciuculescu, D. *J. Anal. Appl. Pyrolysis.* **2003**, *67*, 359.
4. Andrus, M. B.; Ye, Z.; Zhang, J. *Tetrahedron Lett.* **2005**, *46*, 3839.
5. Karthikeyan, S.; Ramamurthy, V. *Tetrahedron Lett.* **2005**, *46*, 4495.
6. Jin, W.; Yamamoto, Y.; Fukushima, T.; Ishii, N.; Kim, J.; Kato, K.; Takata, M.; Aida, T. *J. Am. Chem. Soc.* **2008**, *130*, 9434.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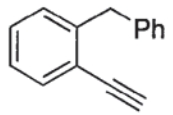
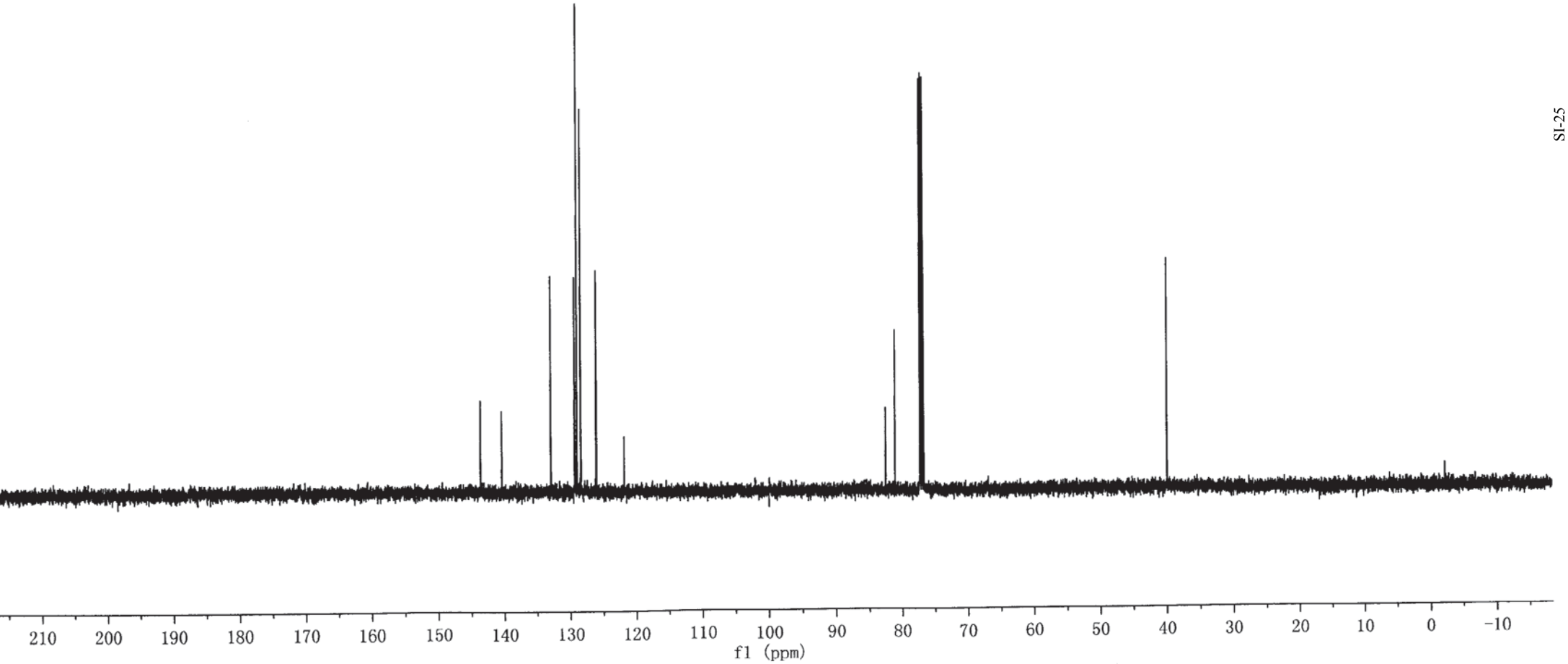
2.00
0.86


Ph

1a


210
200
190
180
170
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150
140
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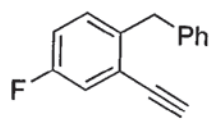
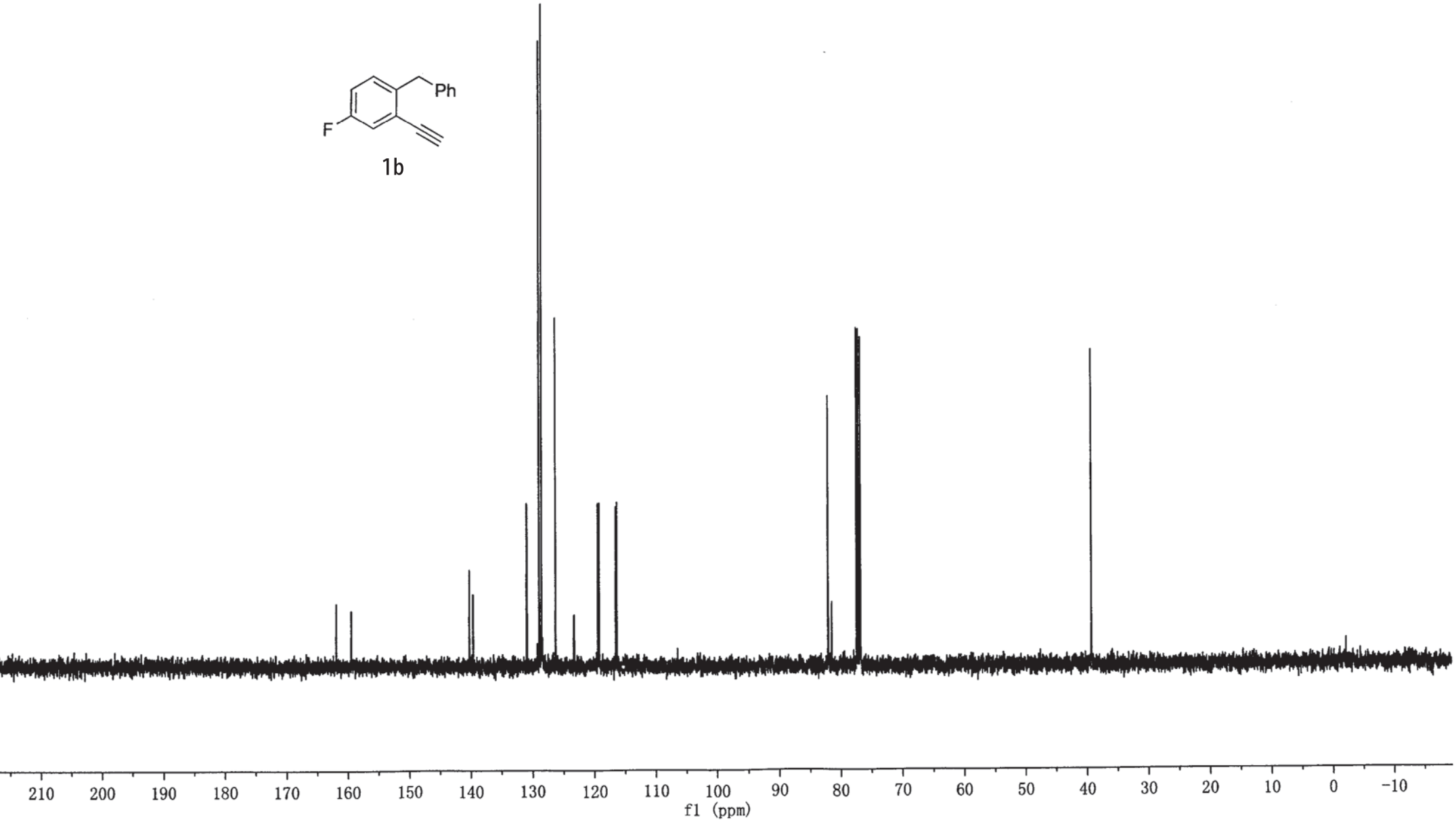
60
50
40
30
20
10
0
-10
f1 (ppm)



1b

Ph
F

1b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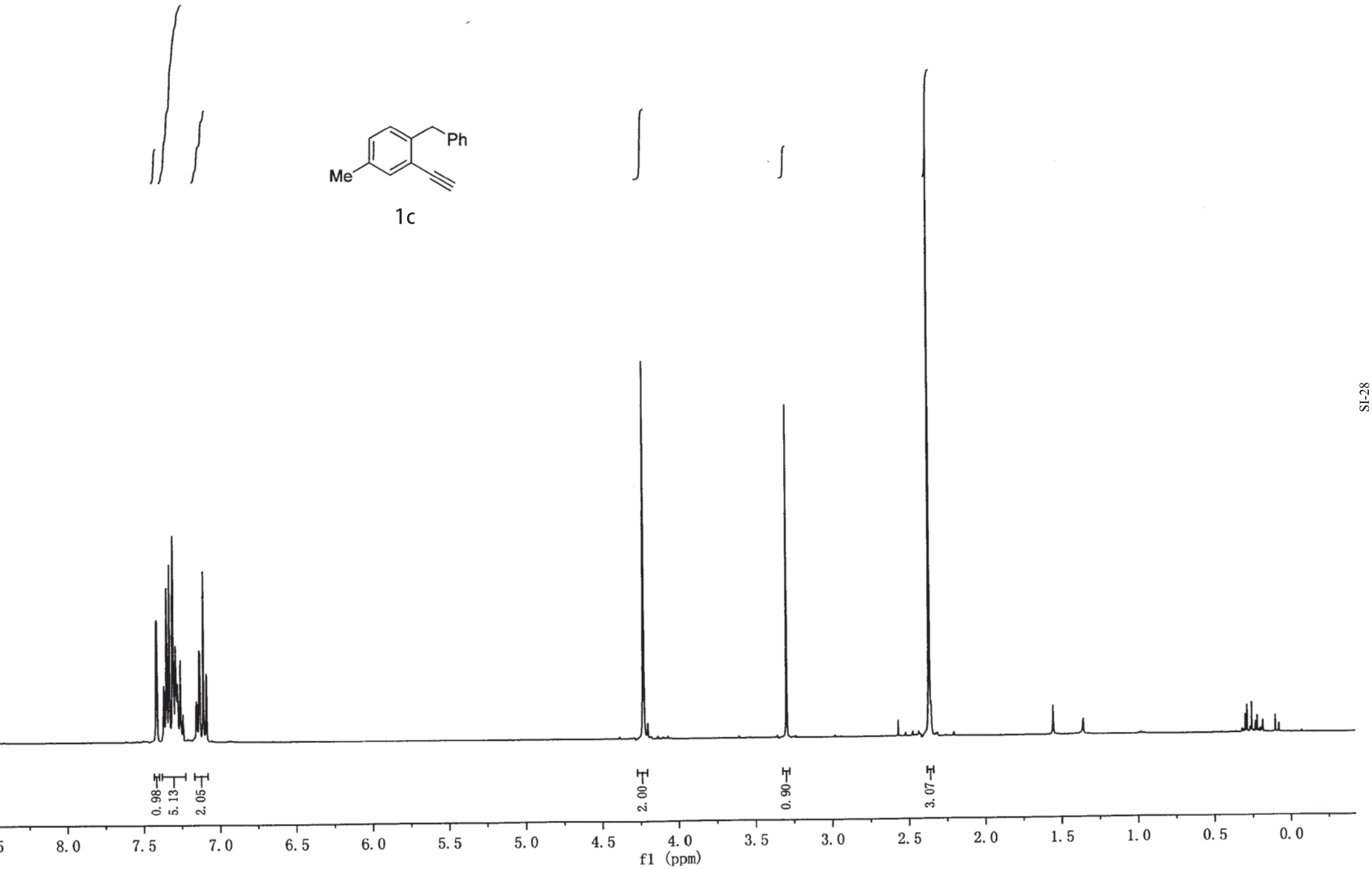
0
-10
f1 (ppm)


Ph
Me
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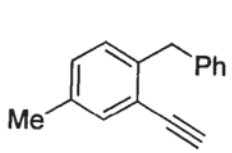
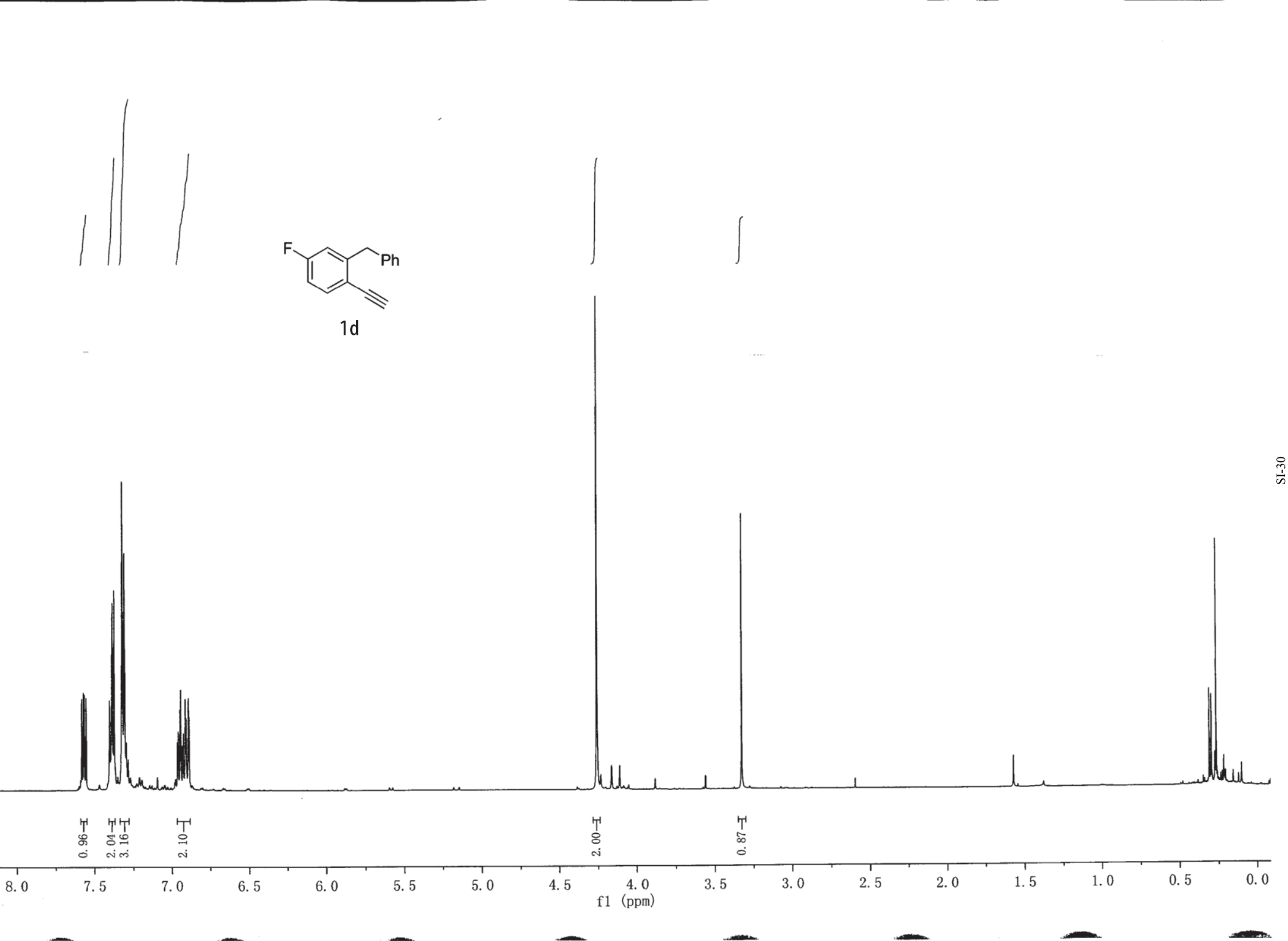
5.13
2.05
2.00
0.90
3.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph
Me

1c

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
Ph
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2.00
0.87
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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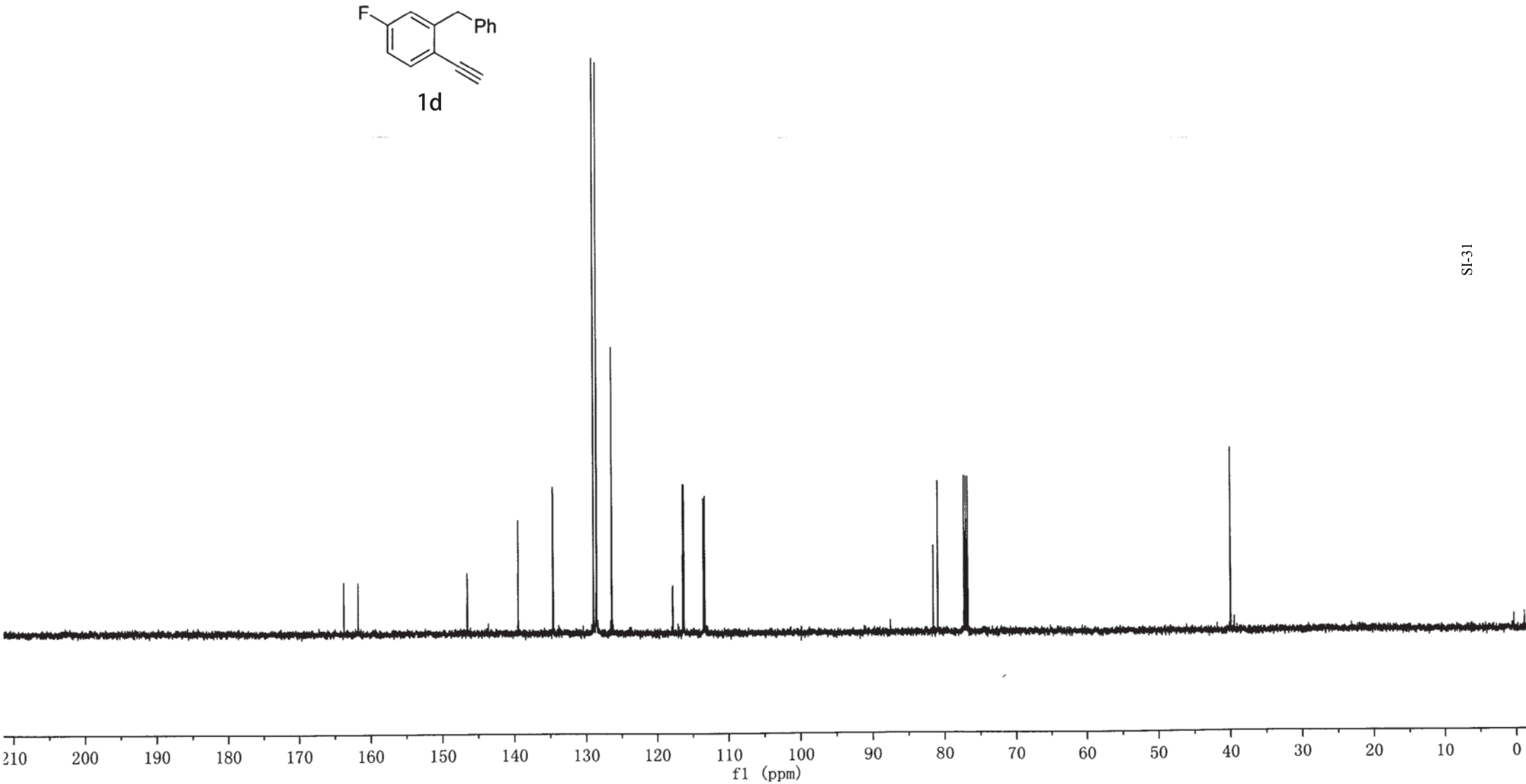
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


F
Ph
1d
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90
80
70
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50
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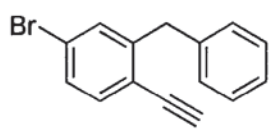
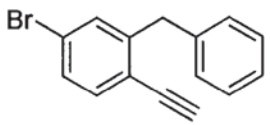
10
0
f1 (ppm)

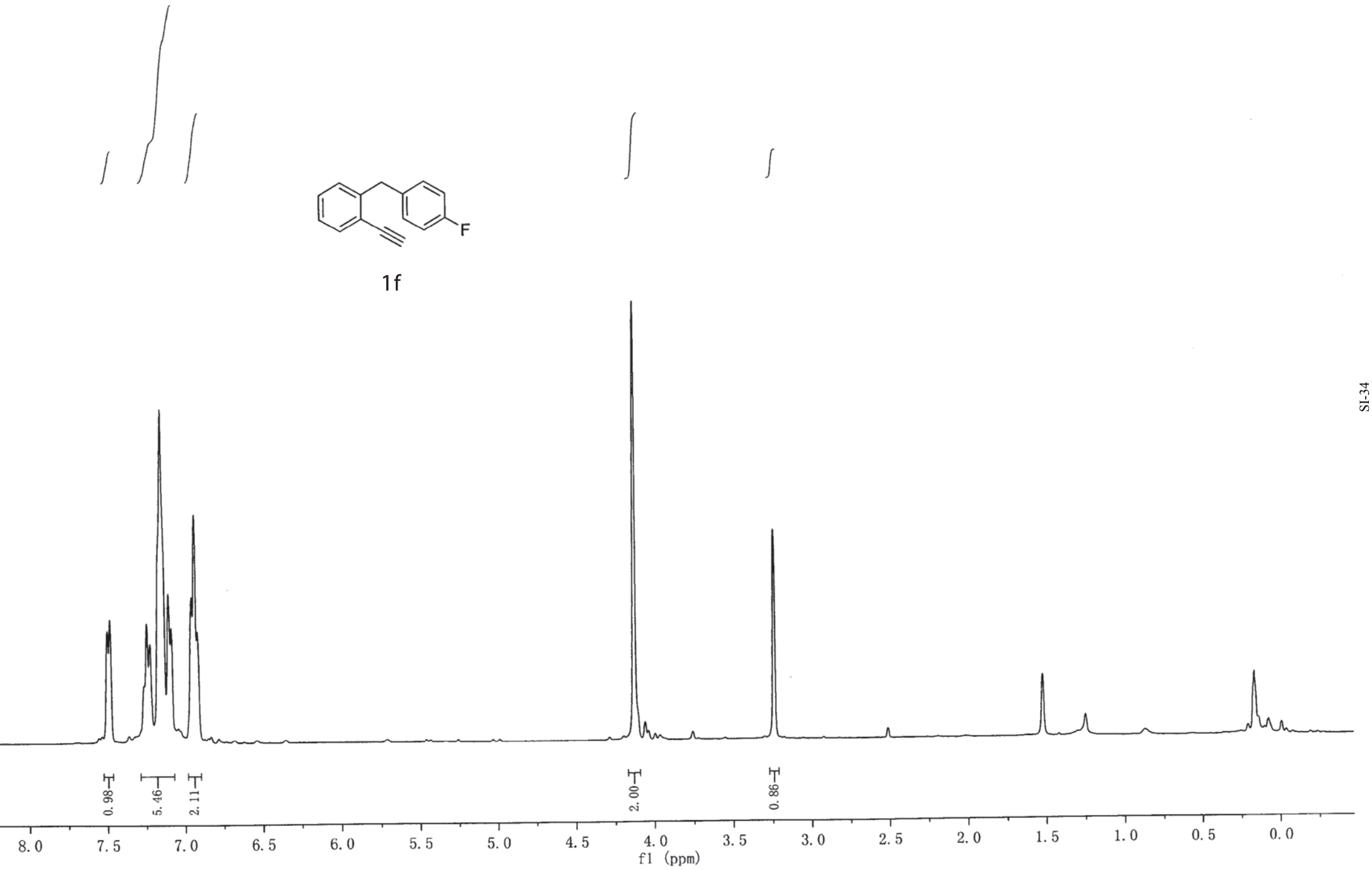


1e


Br

1e

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
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2.11
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0.86
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7.5
7.0
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4.5
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2.5
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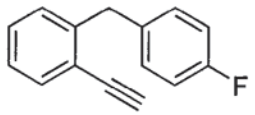
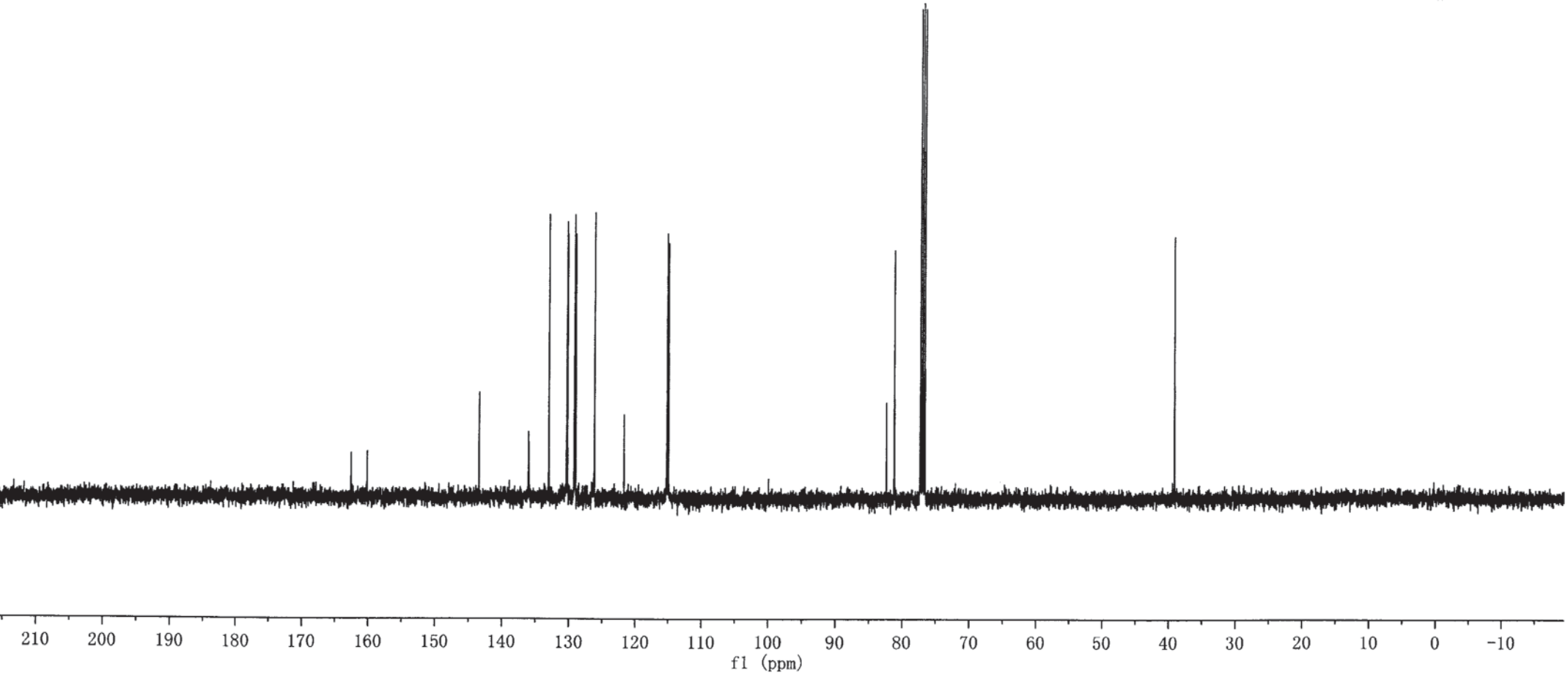
1.0
0.5
0.0
f1 (ppm)


F

1f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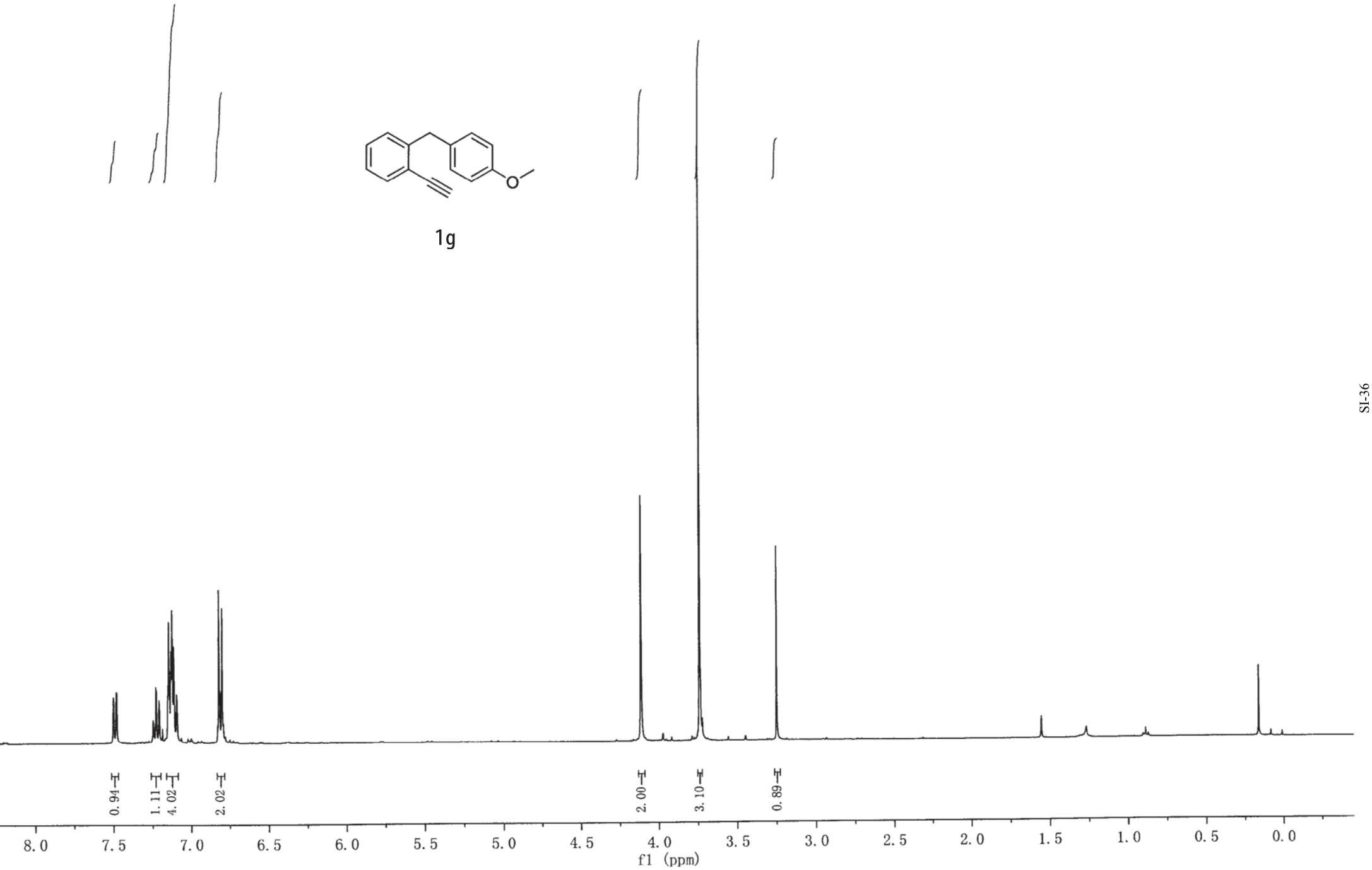
0
-10
f1 (ppm)


O
1g
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7.5
7.0
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6.0
5.5
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3.5
3.0
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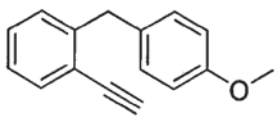
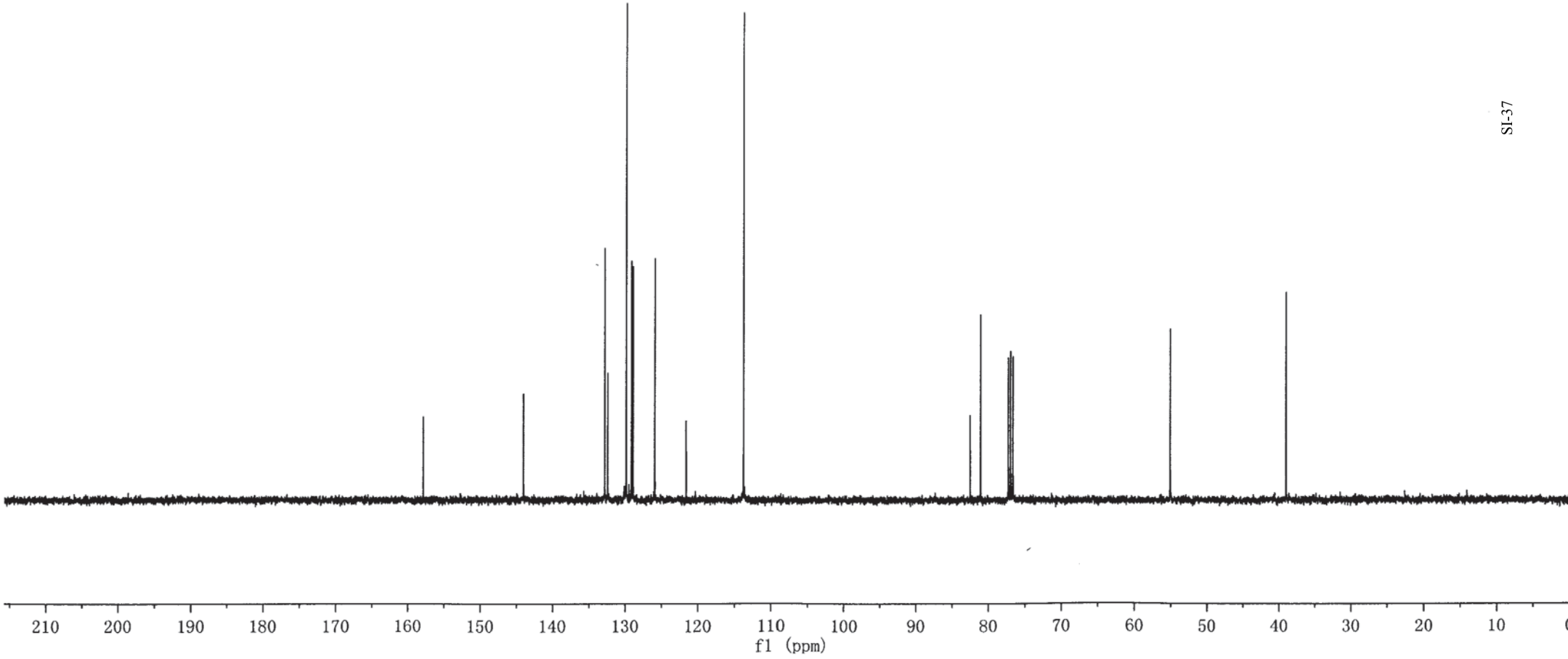
0.0
f1 (ppm)


O

1g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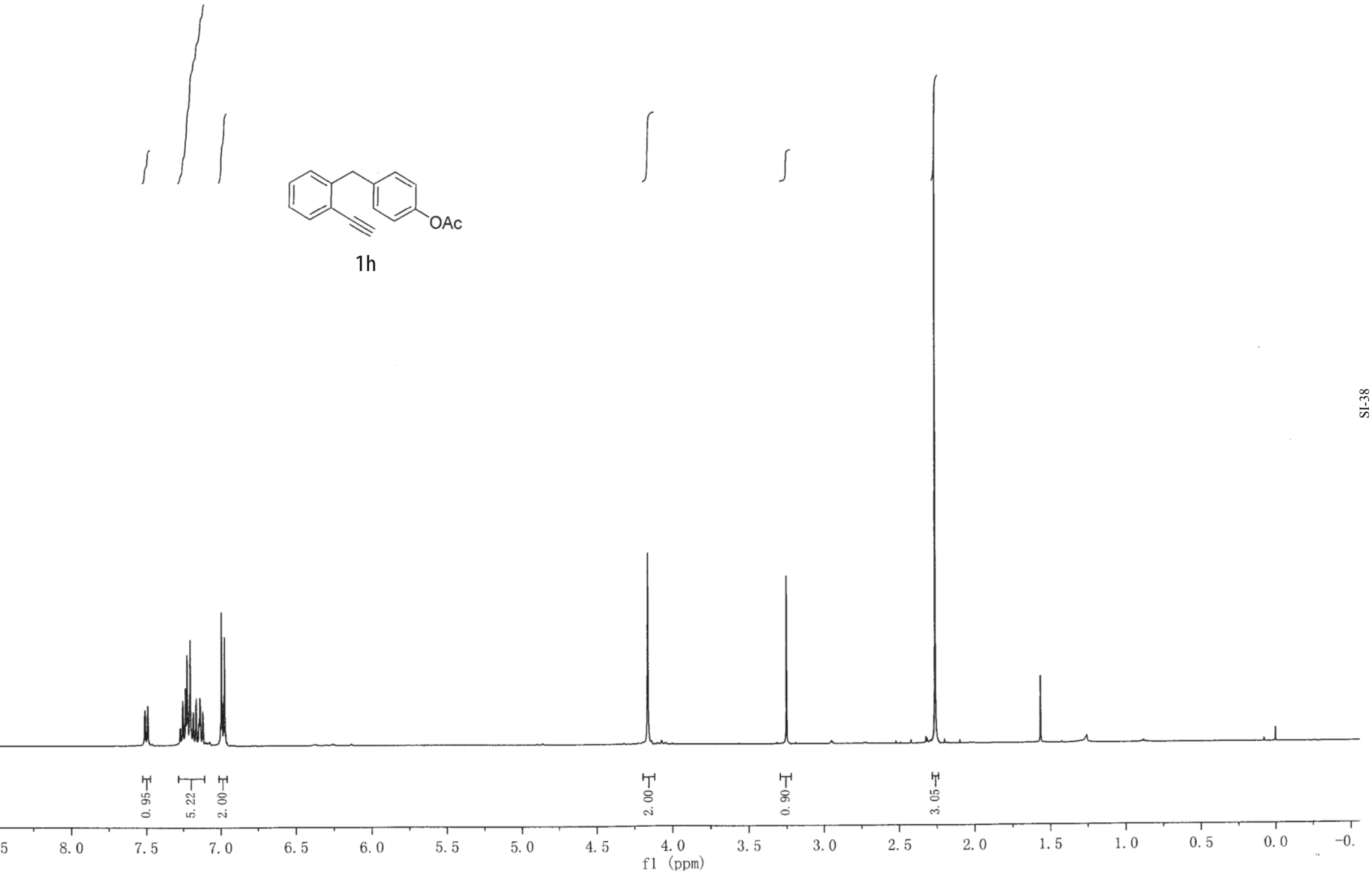
f1 (ppm)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3.0
2.5
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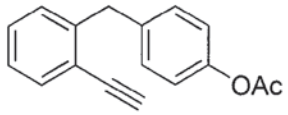
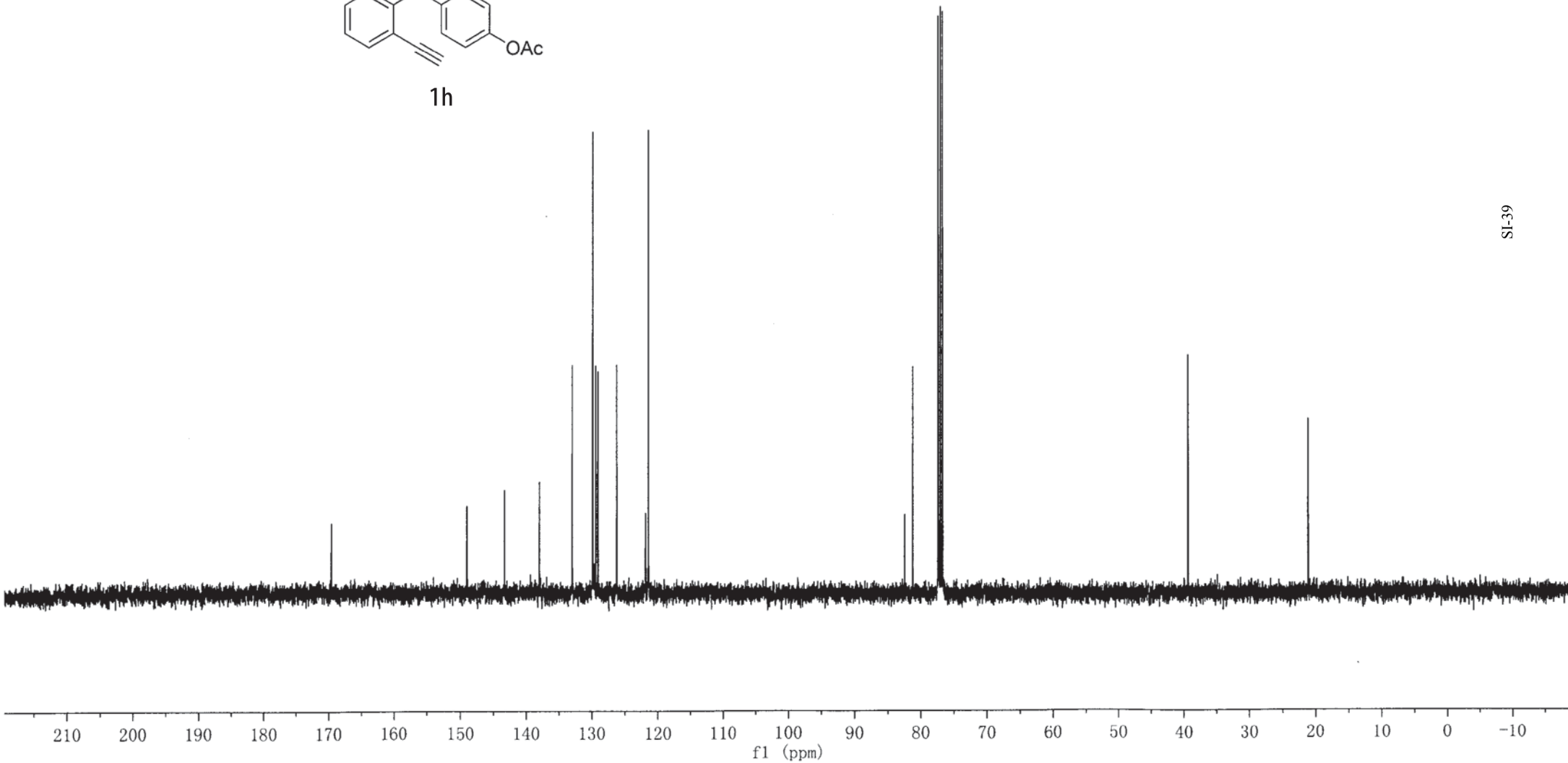
1.0
0.5
0.0
f1 (ppm)


OAc

1h


210
200
190
180
170
160
150
140
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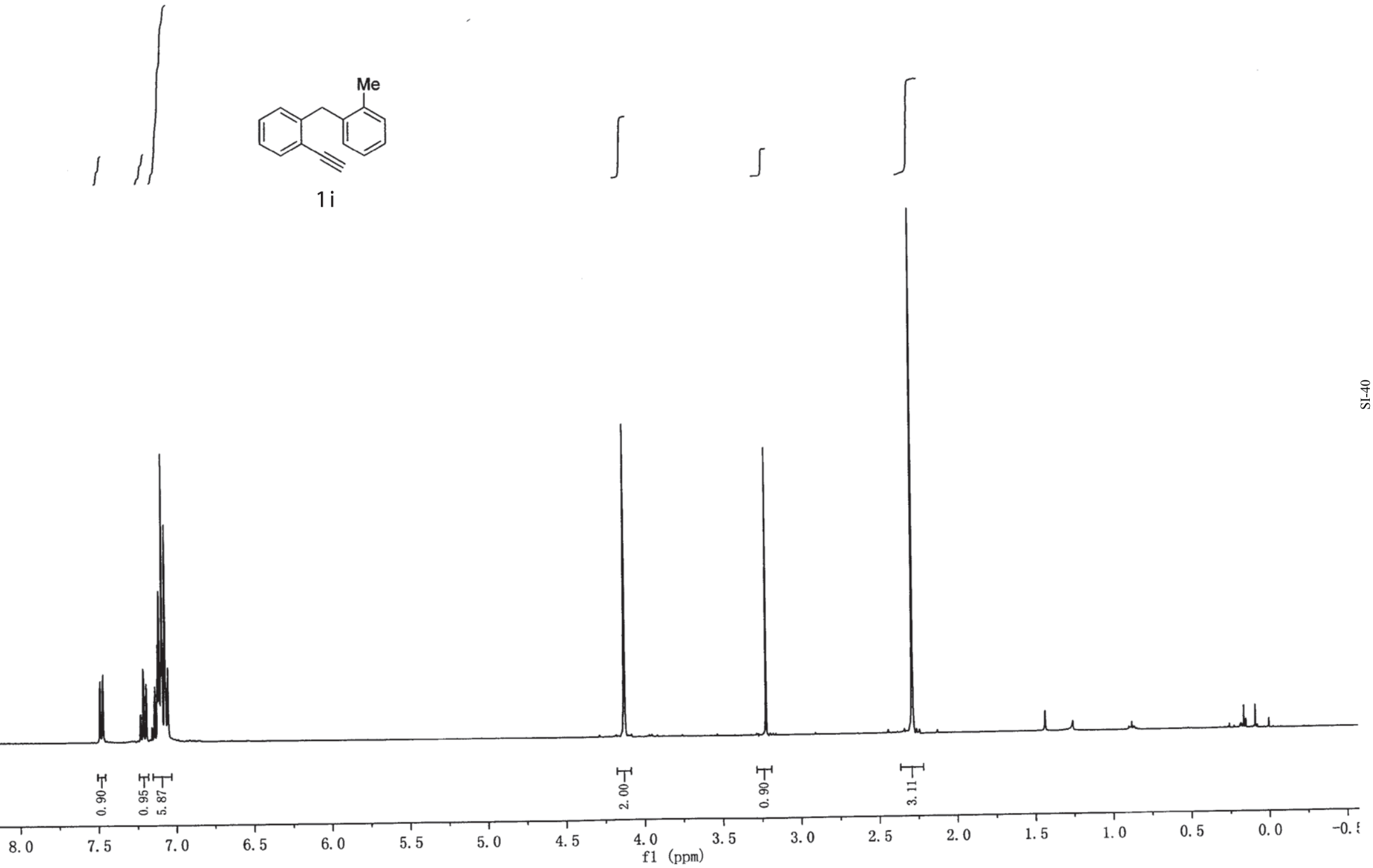
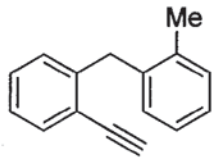
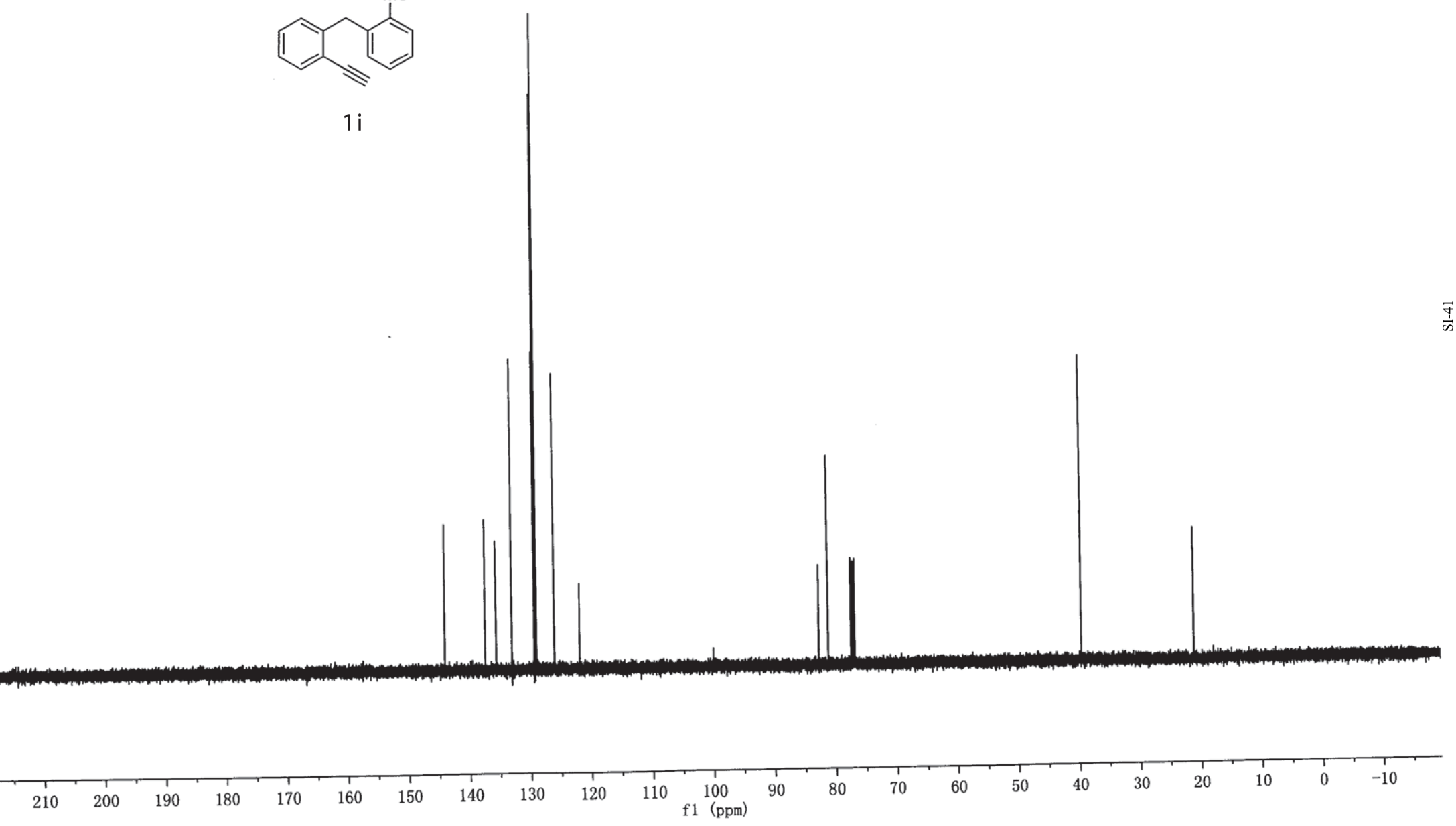
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
1i
0.90
0.95
5.87
2.00
0.90
3.11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Me

1i


210
200
190
180
170
160
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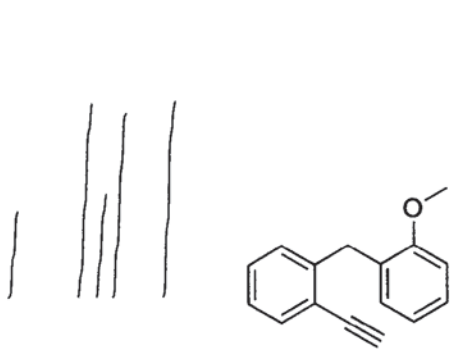
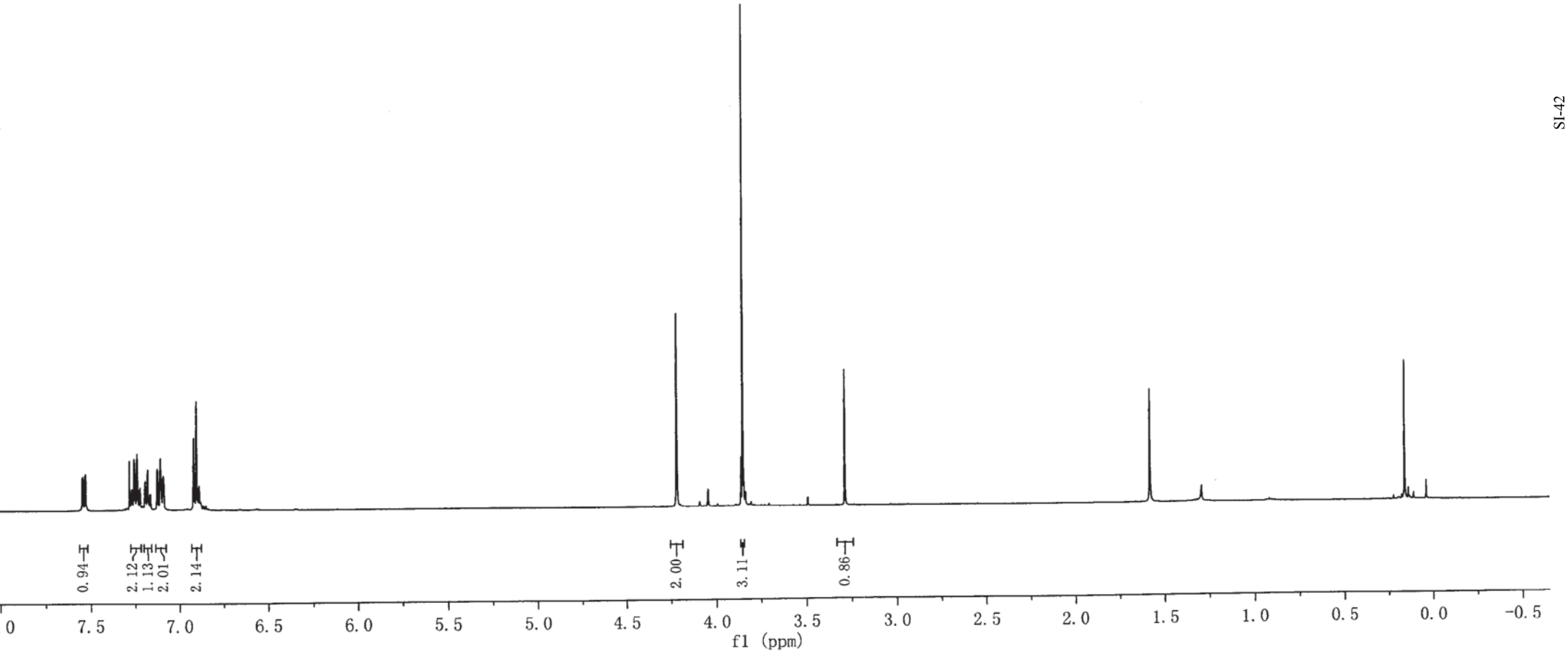
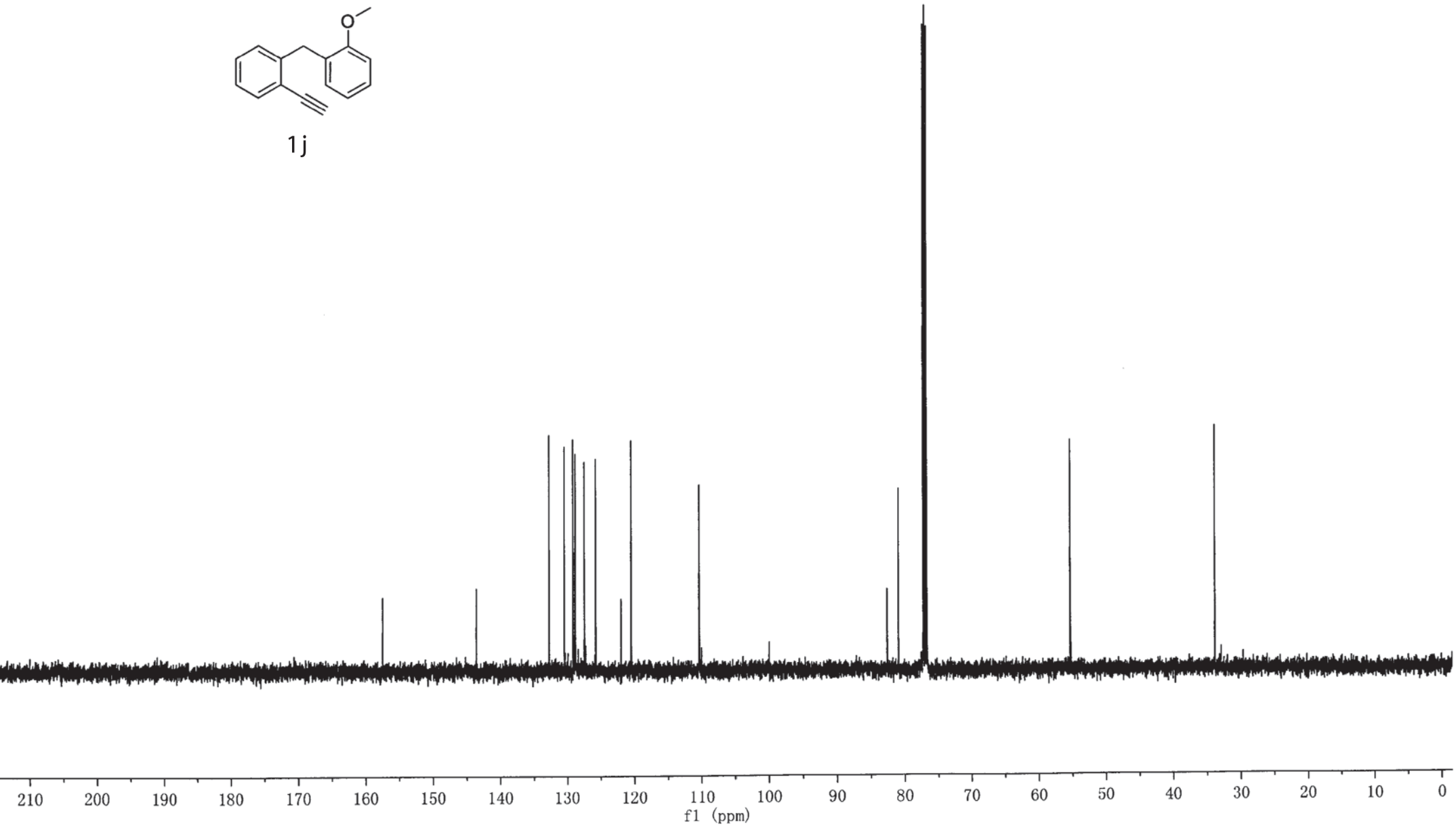
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

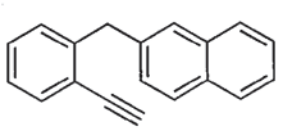


1j

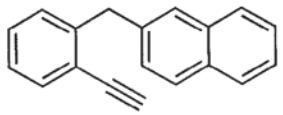

0.94
2.12
1.13
2.01
2.14
2.00
3.11
0.86
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

1j

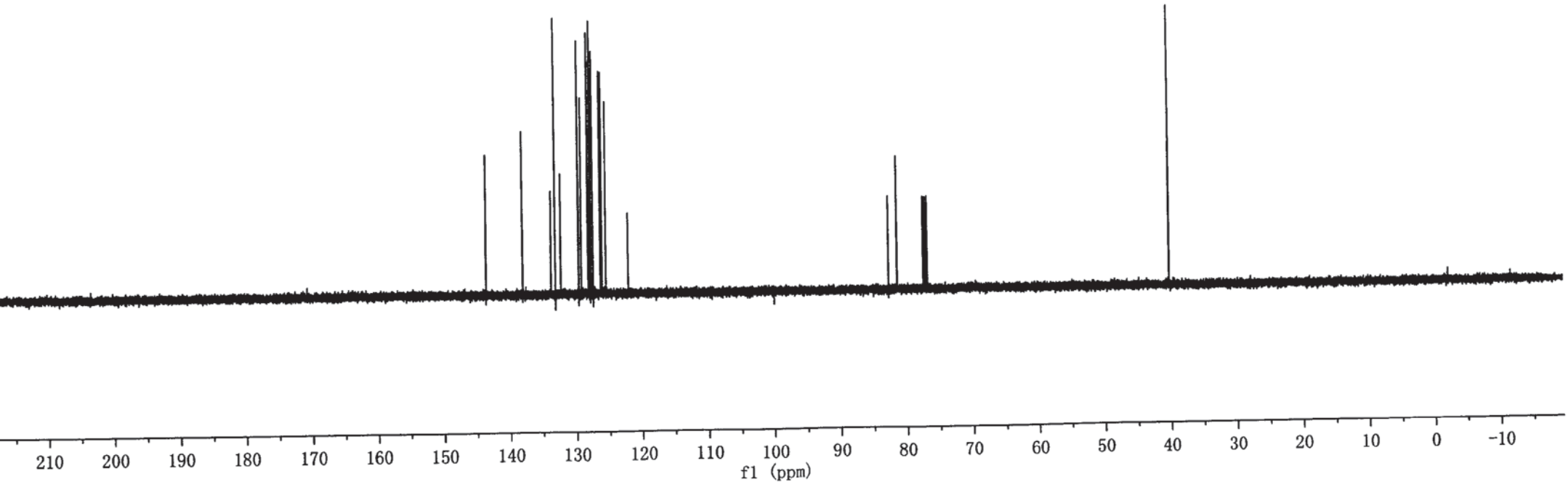

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

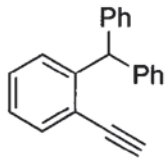


1k

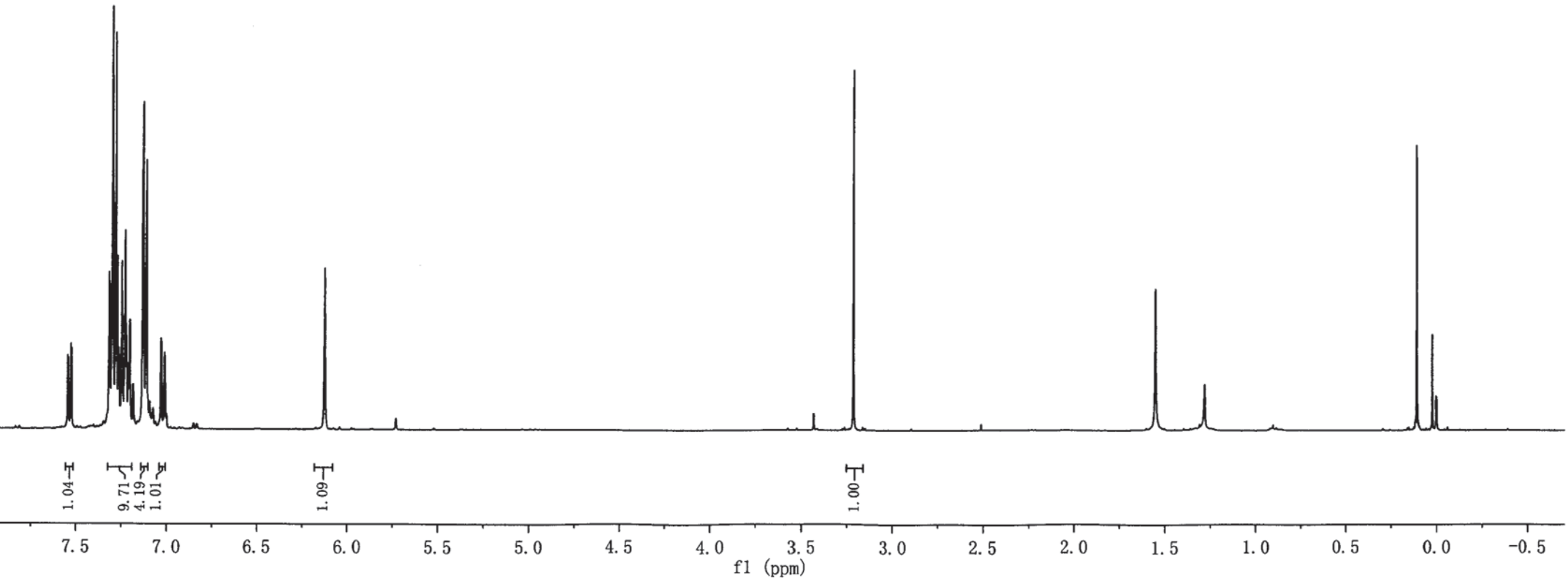


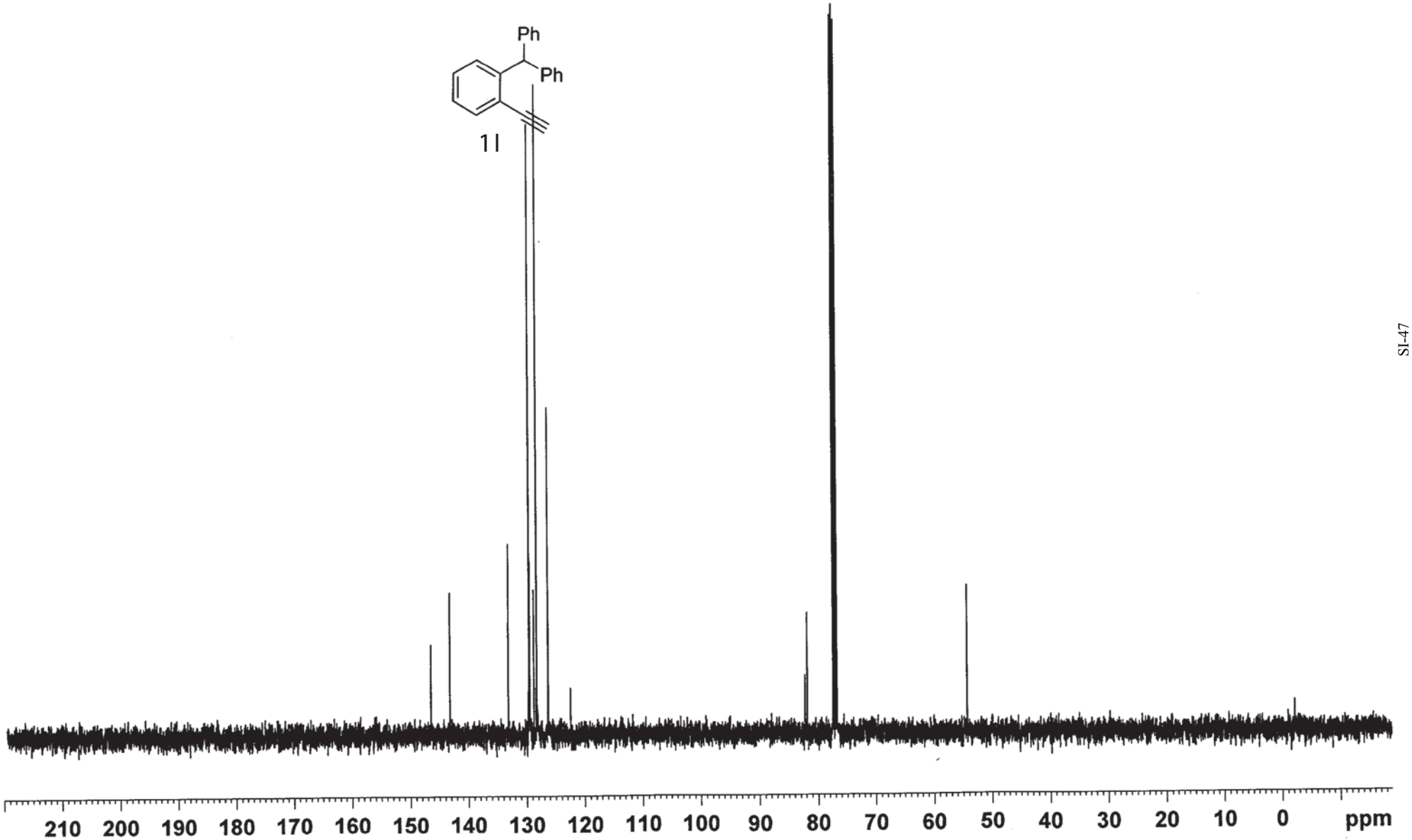
1k

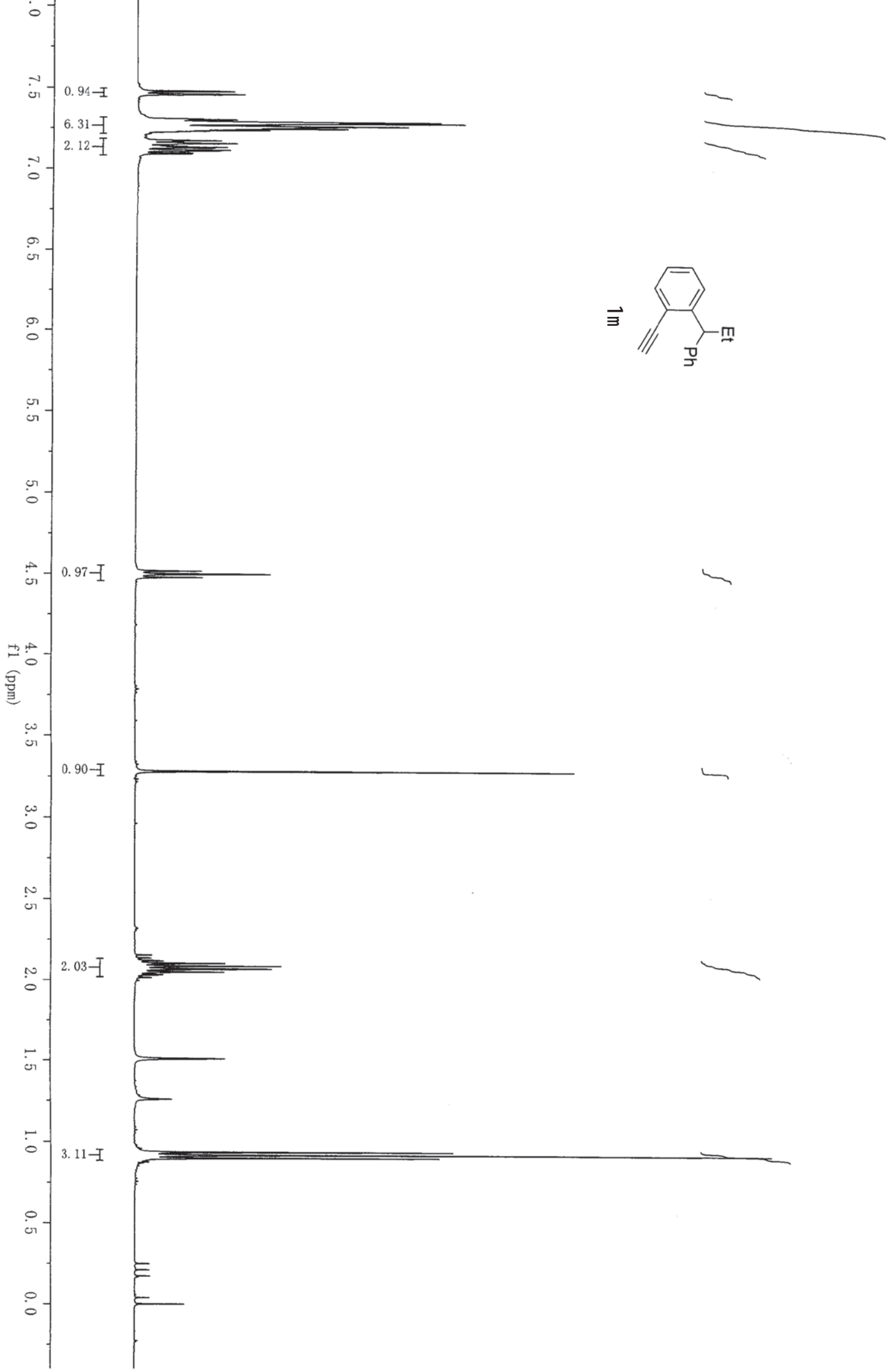

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

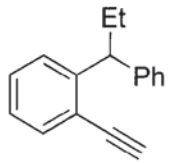

Ph
Ph

1l

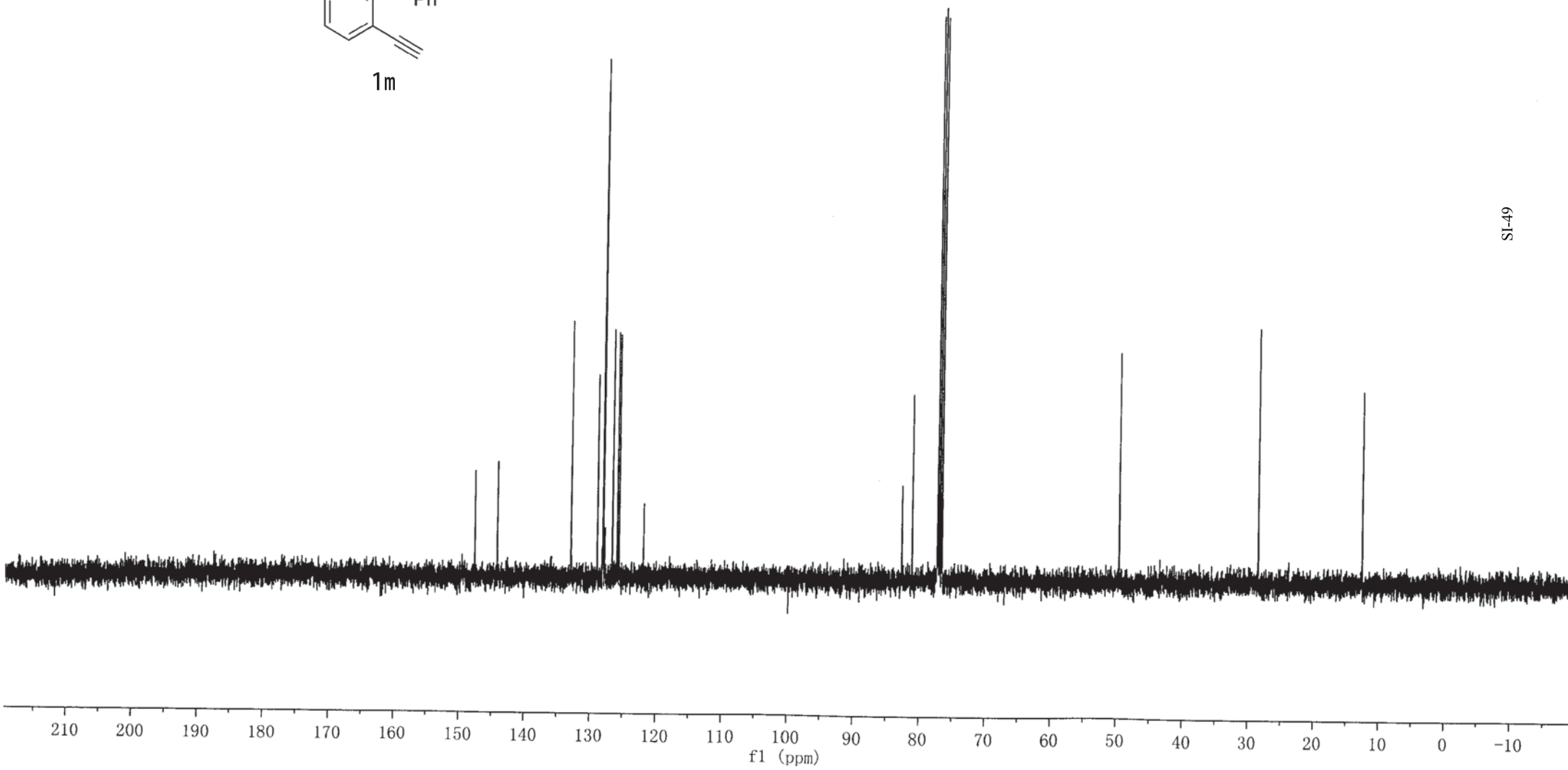

1.04
9.71
4.19
1.01
1.09
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

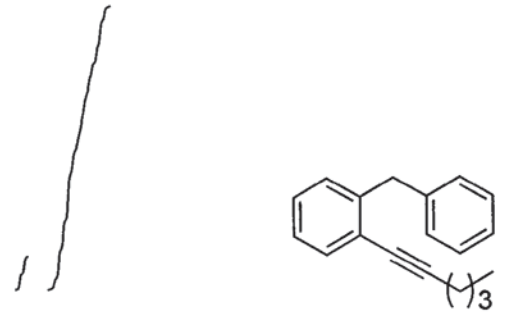

Ph
Ph
1l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


0.94
6.31
2.12
0.97
0.90
2.03
3.11
f1 (ppm)
1m
Et
Ph

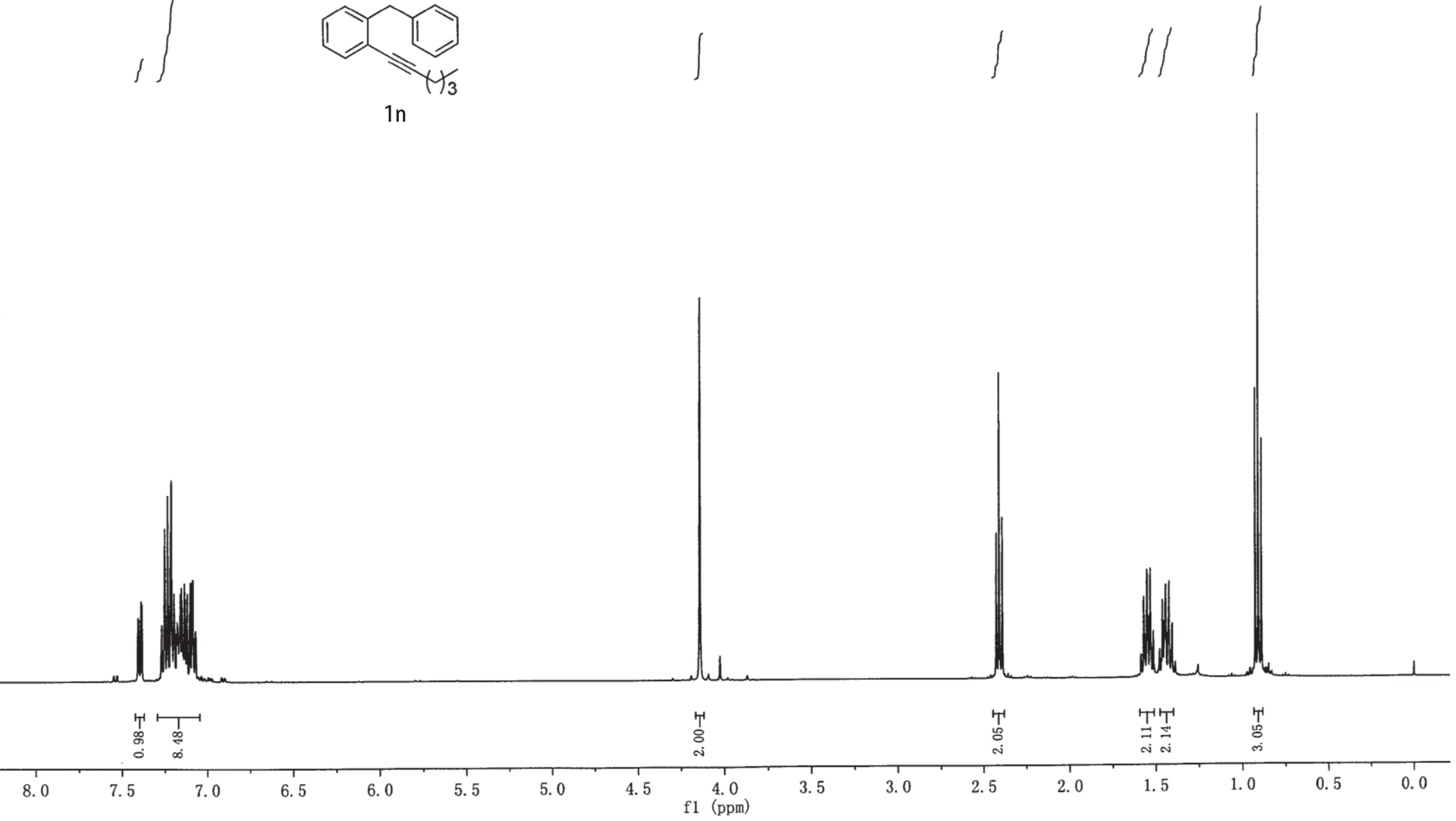

Et
Ph

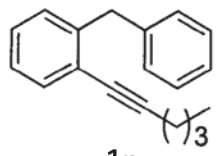
1m


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

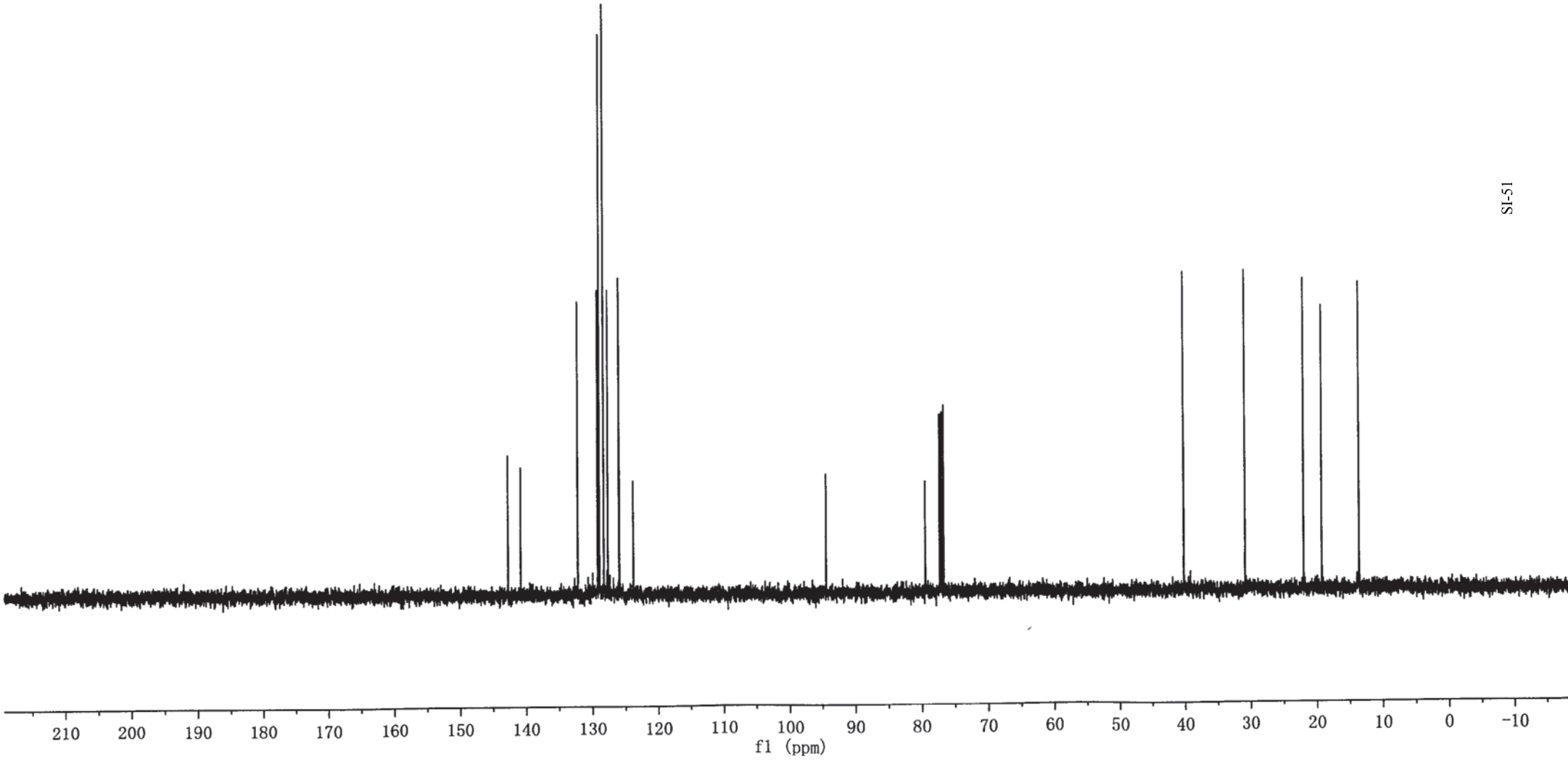


1n

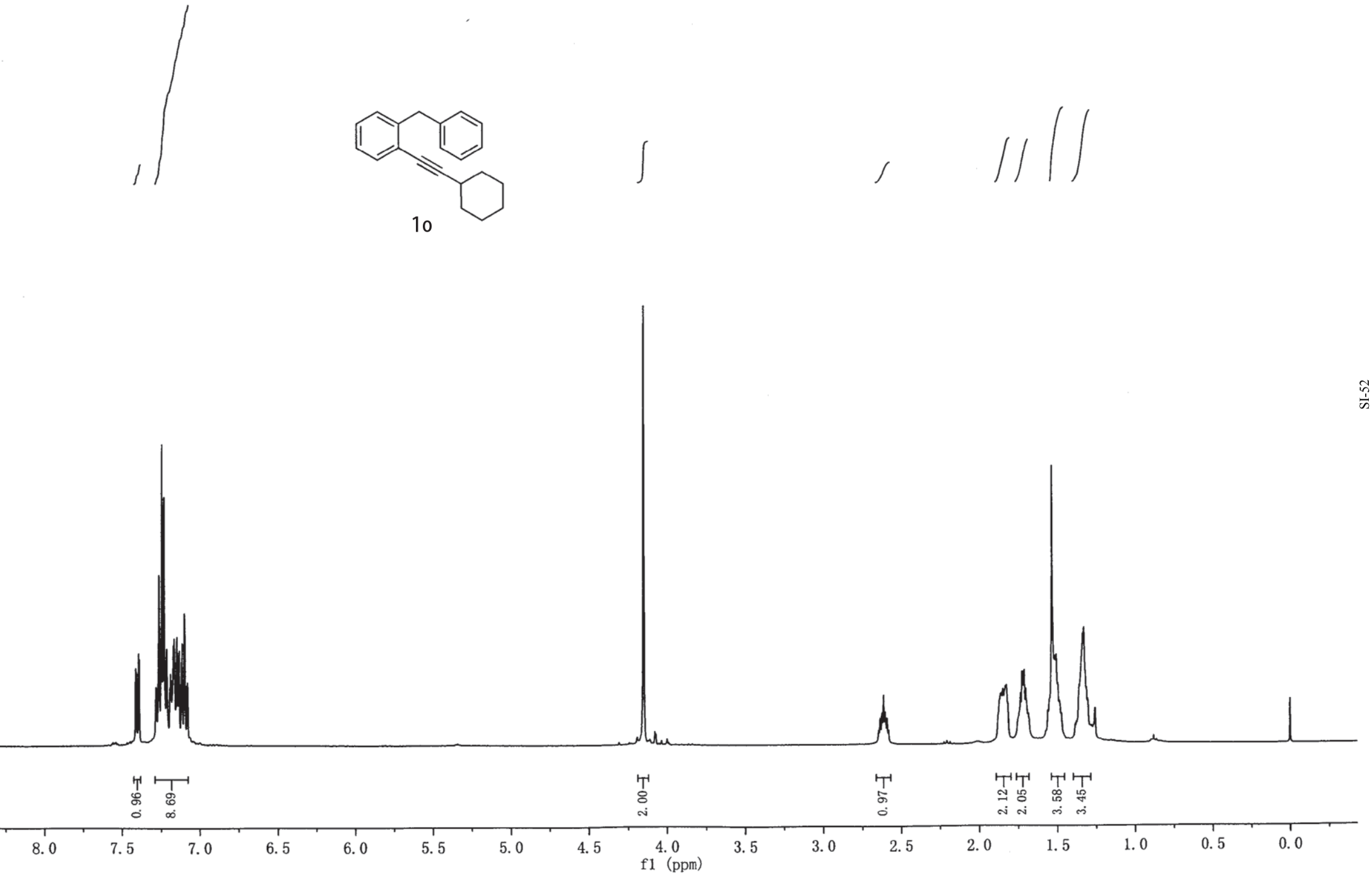

0.98
8.48
2.00
2.05
2.11
2.14
3.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

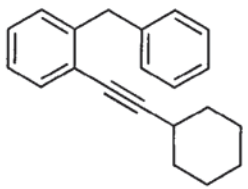


1n


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

1o

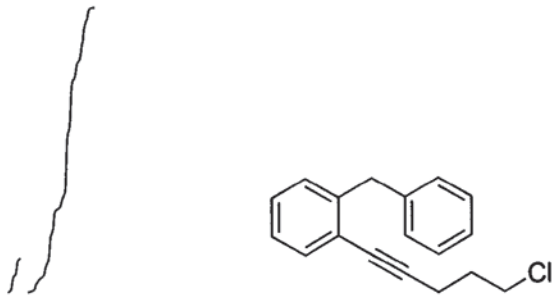

0.96
8.69
2.00
0.97
2.12
2.05
3.58
3.45
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



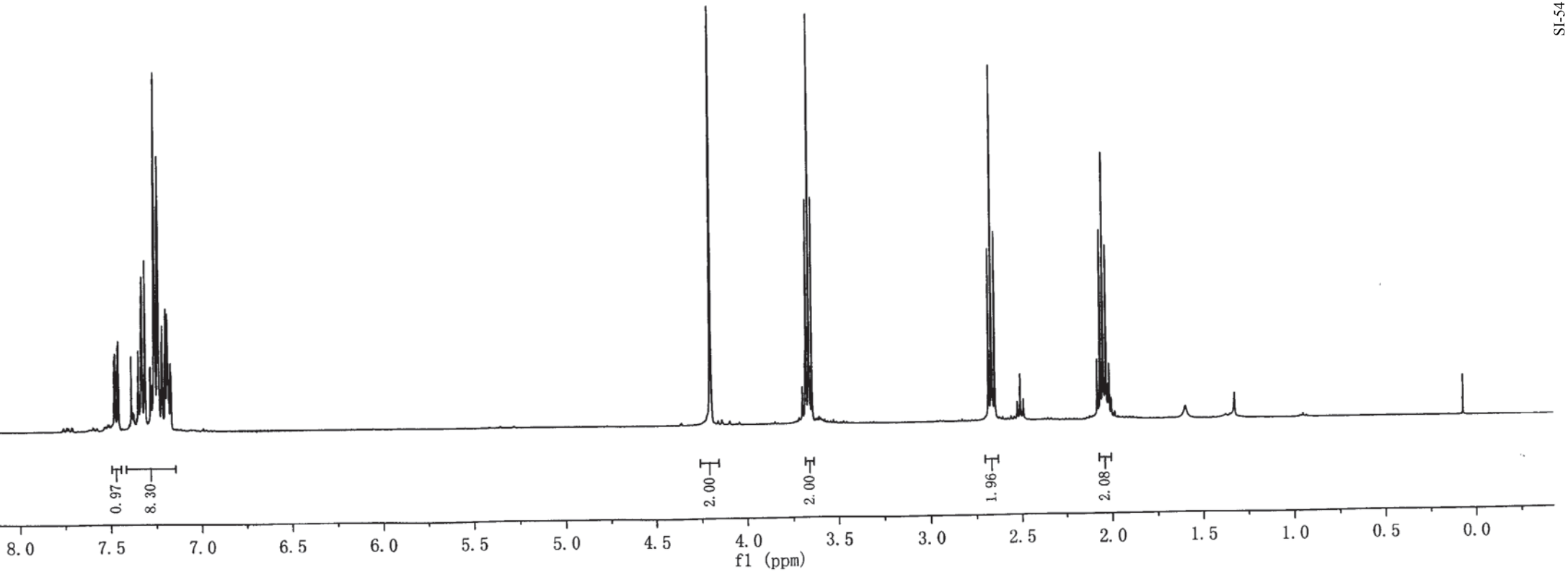
1o

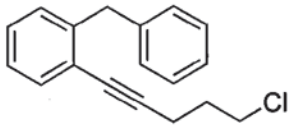
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

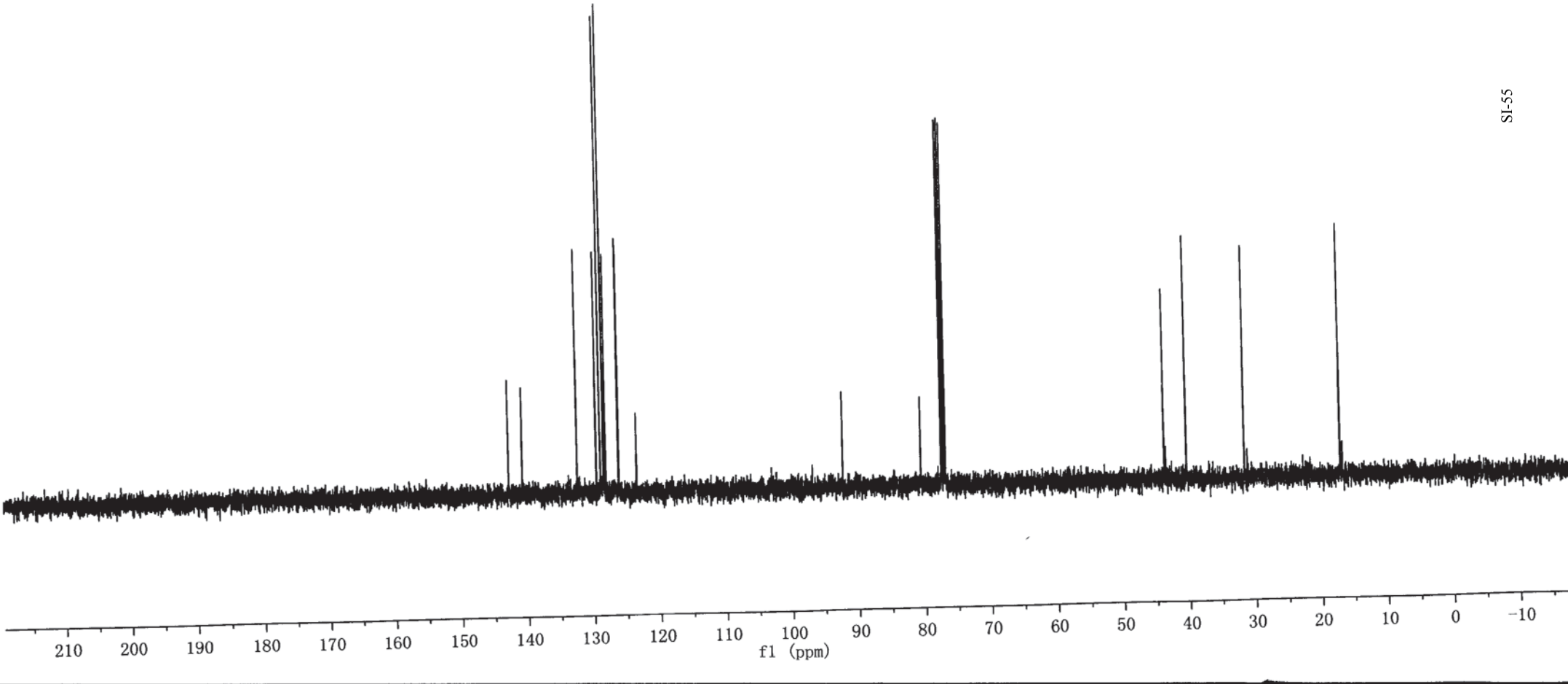

Cl

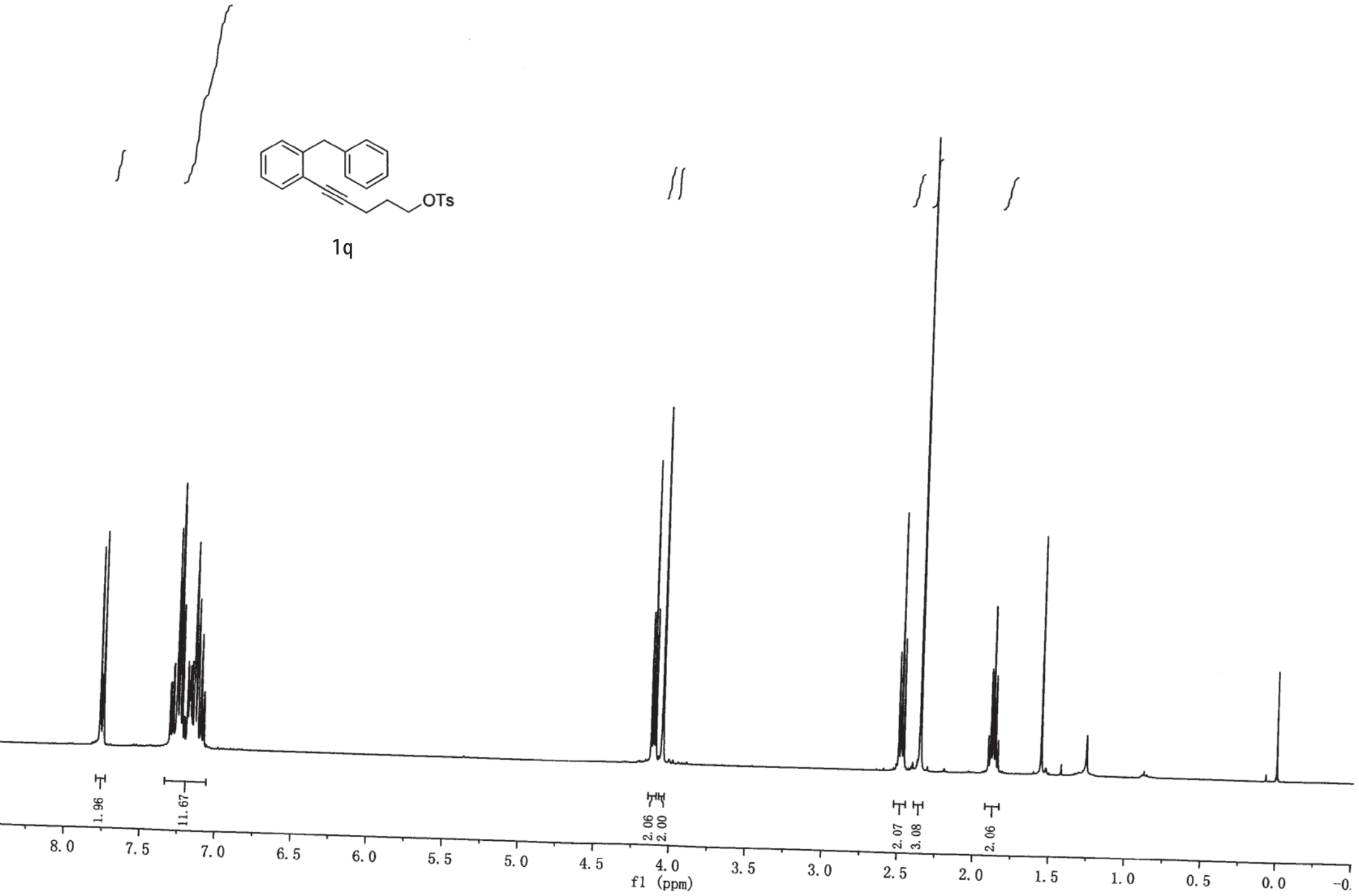
1p

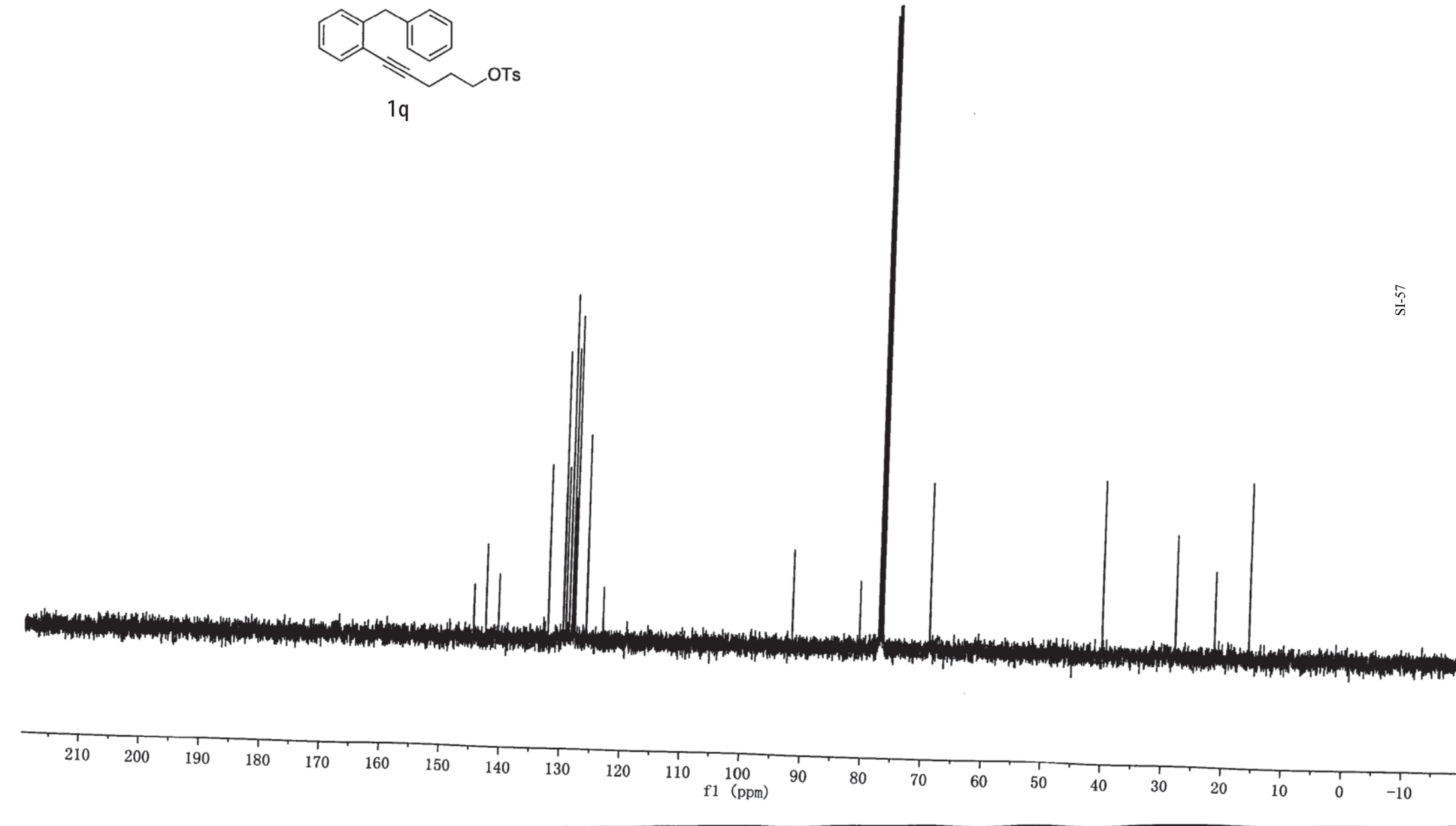

0.97
8.30
2.00
2.00
1.96
2.08
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

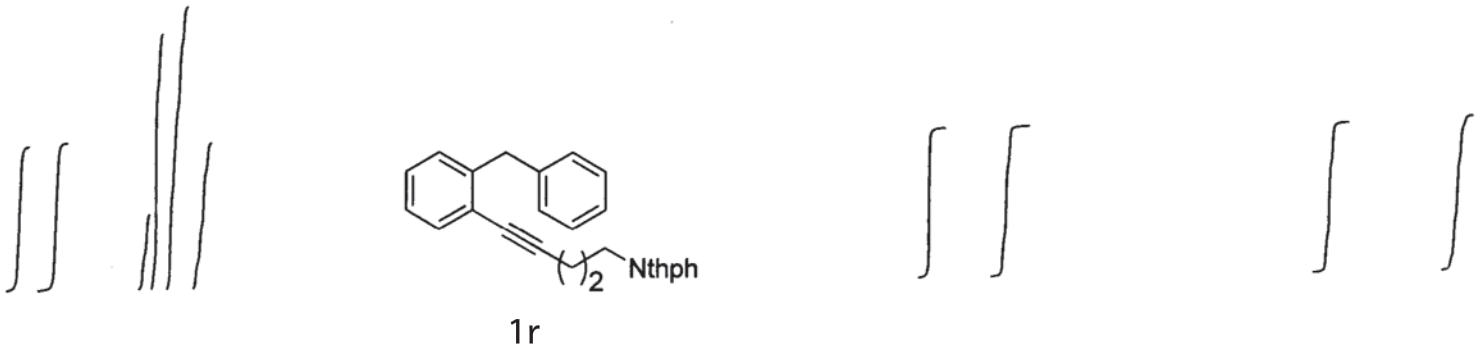

Cl

1p

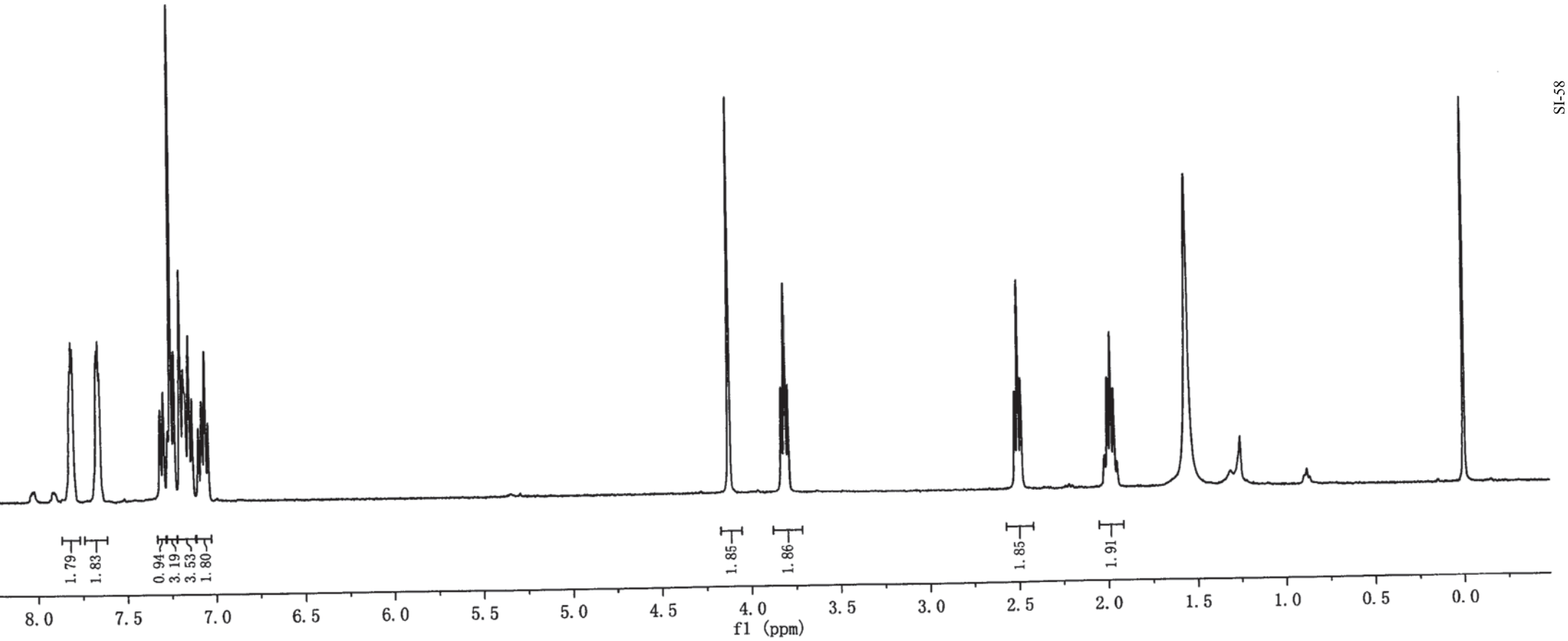

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

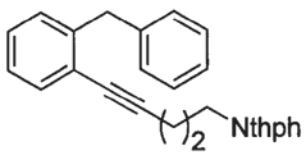

OTs
1q
1.96
11.67
2.06
2.00
2.07
3.08
2.06
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


OTs
1q
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

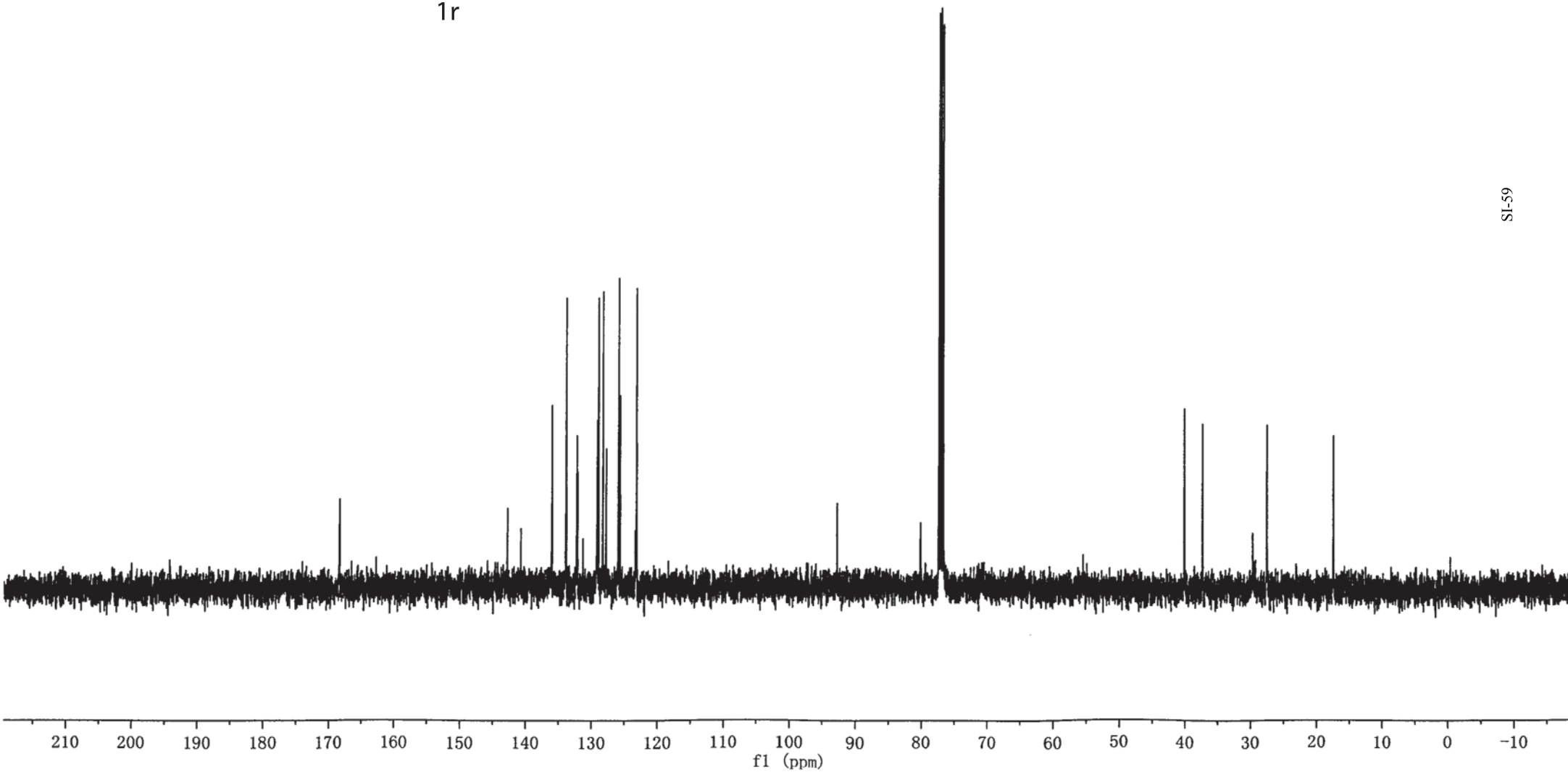

Nthph
2

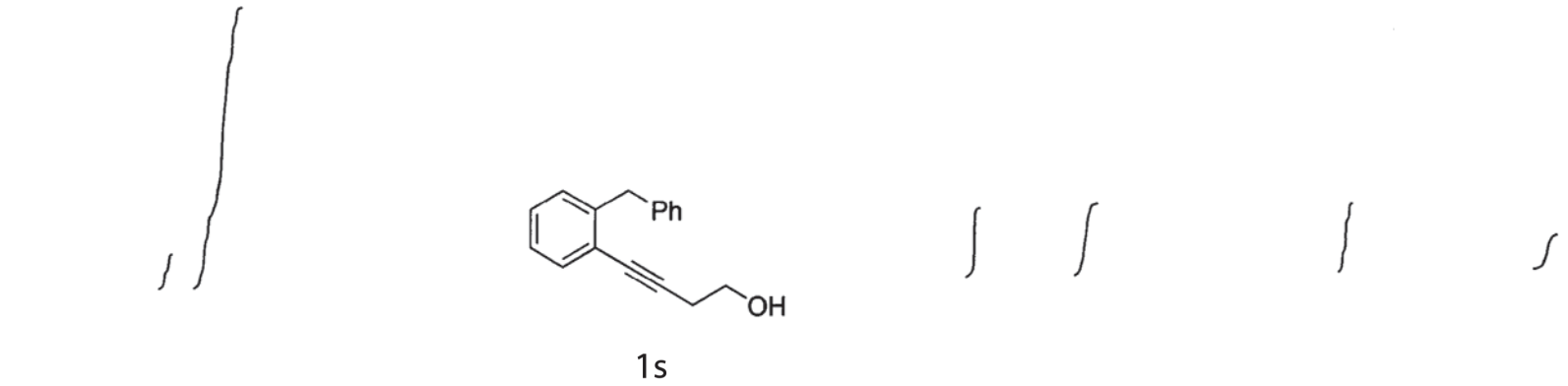
1r


1.79
1.83
0.94
3.19
3.53
1.80
1.85
1.86
1.85
1.91
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

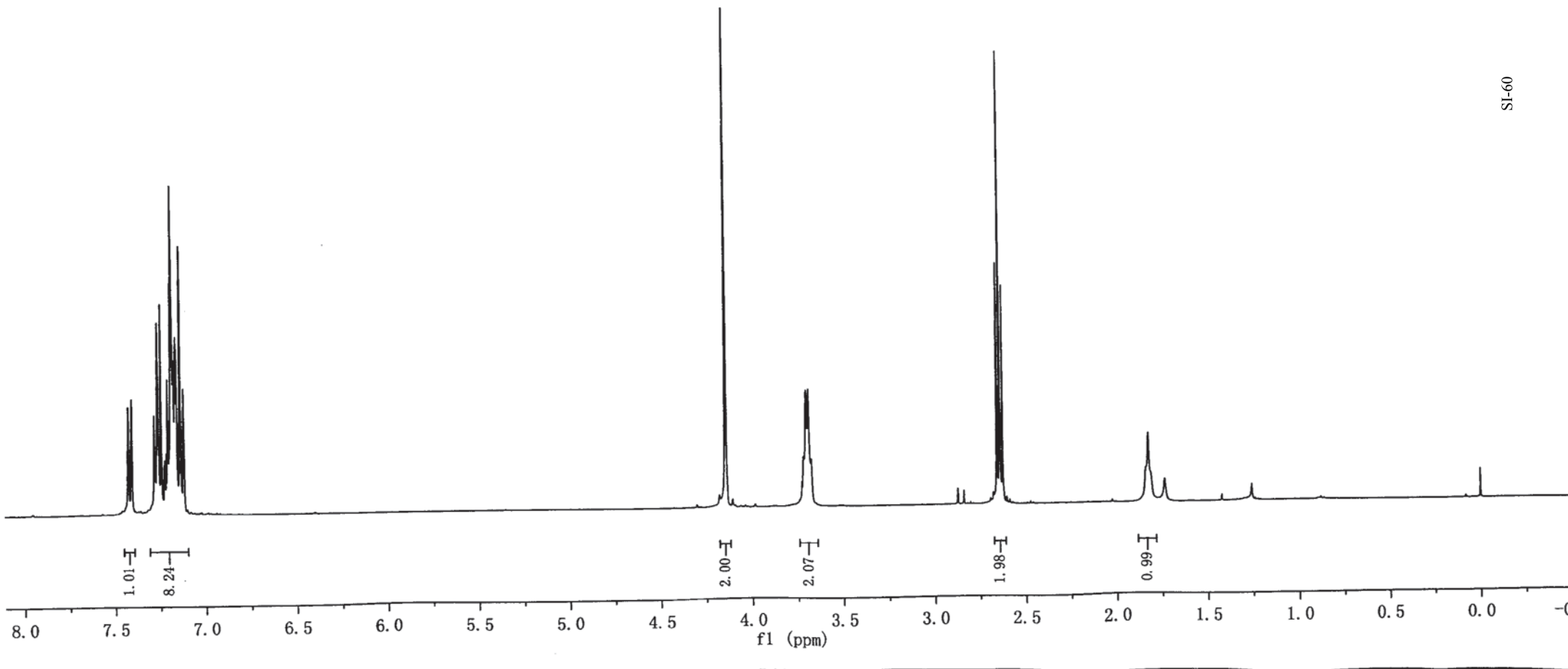

Nthph
2

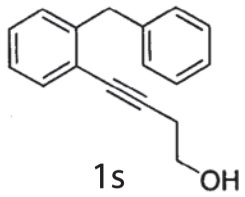
1r

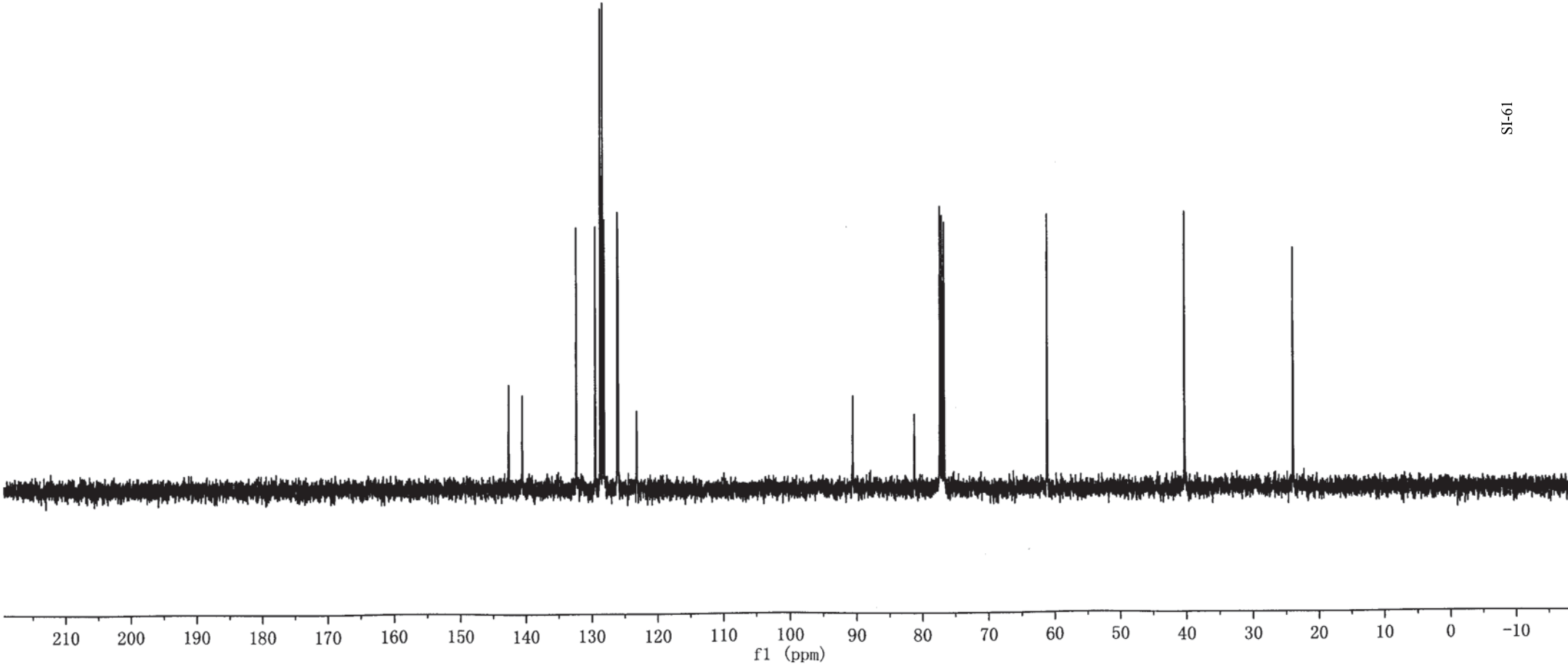

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

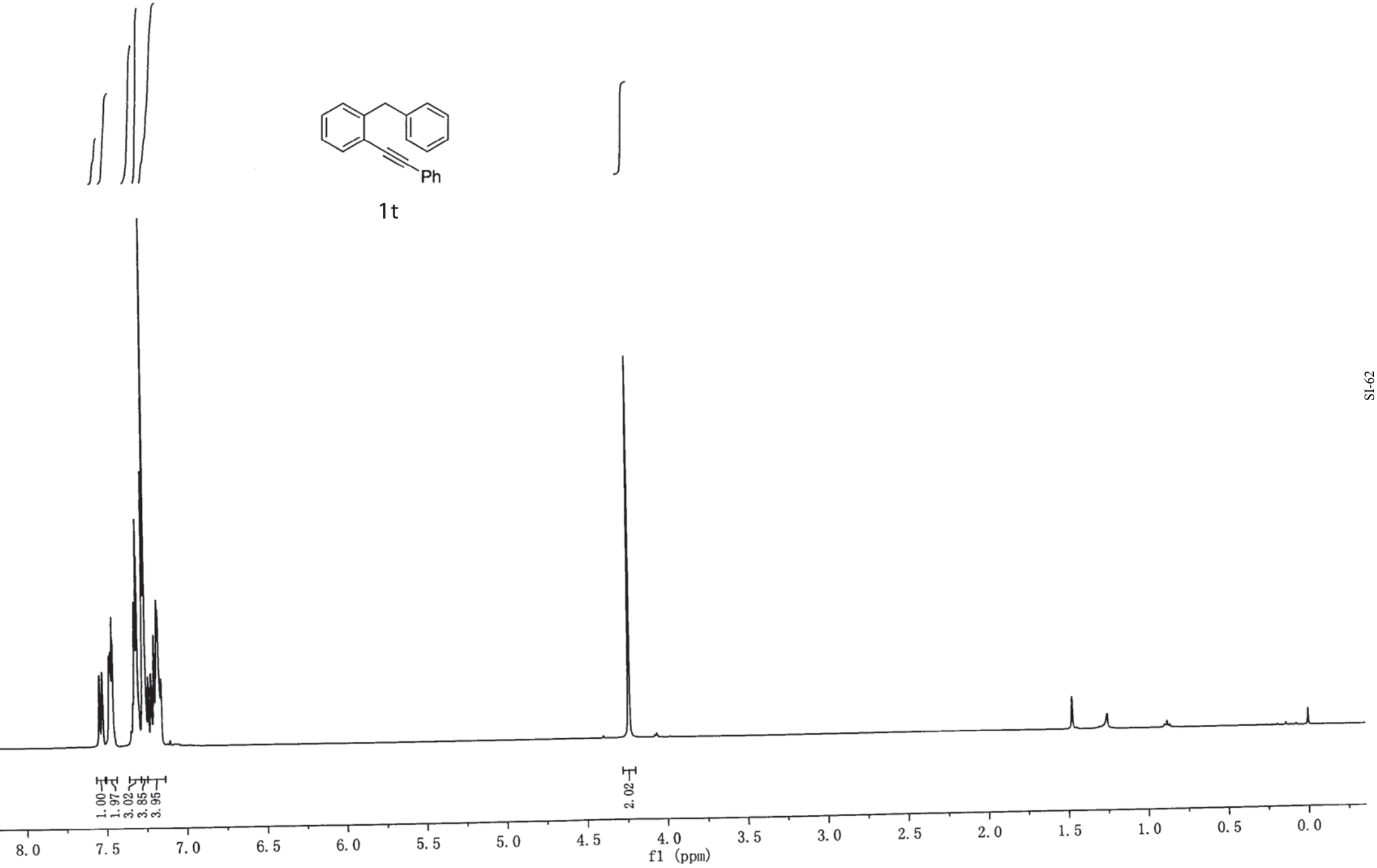

Ph
OH

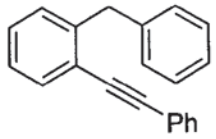
1s


1.01
8.24
2.00
2.07
1.98
0.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

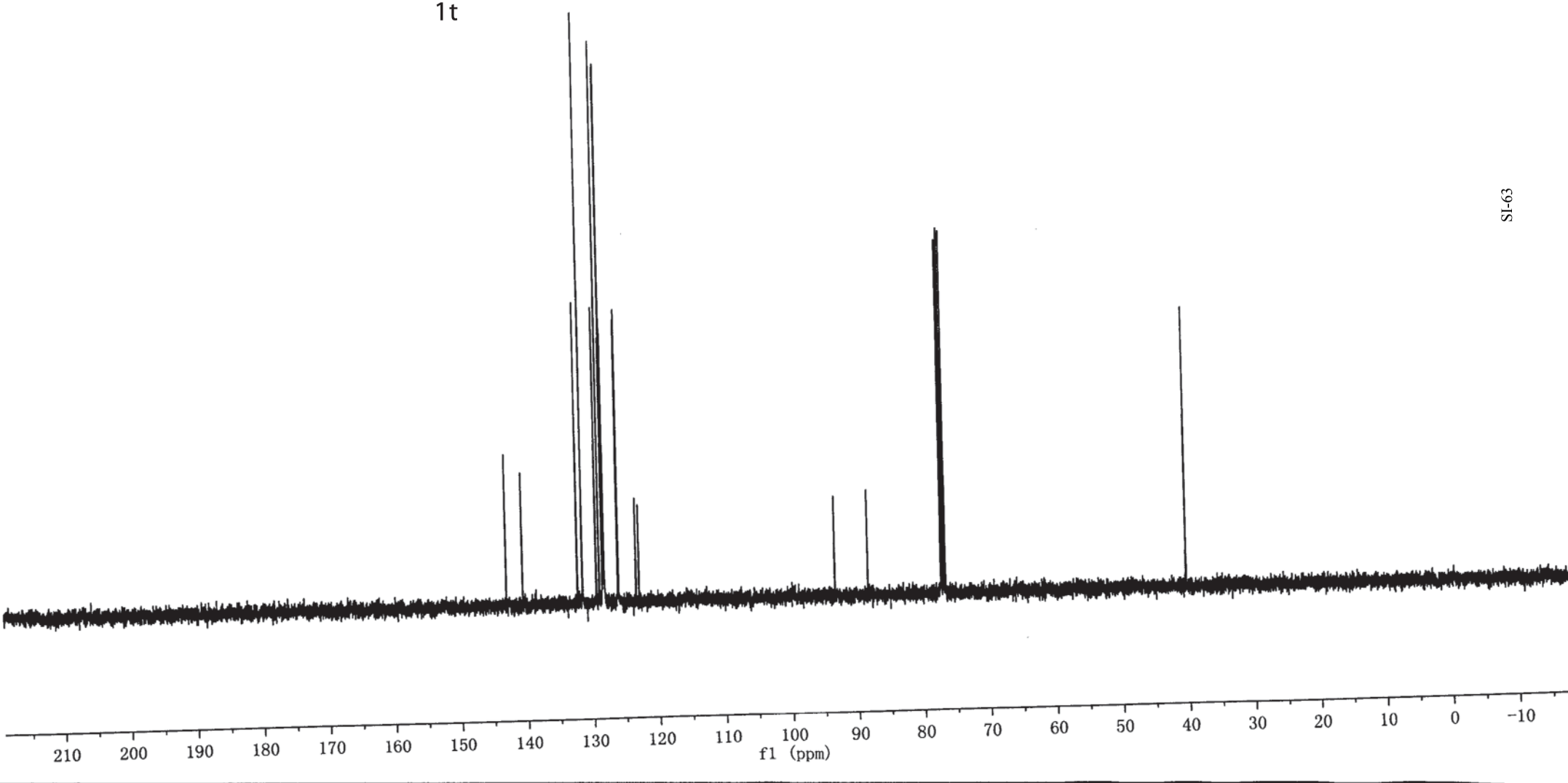

1s
OH

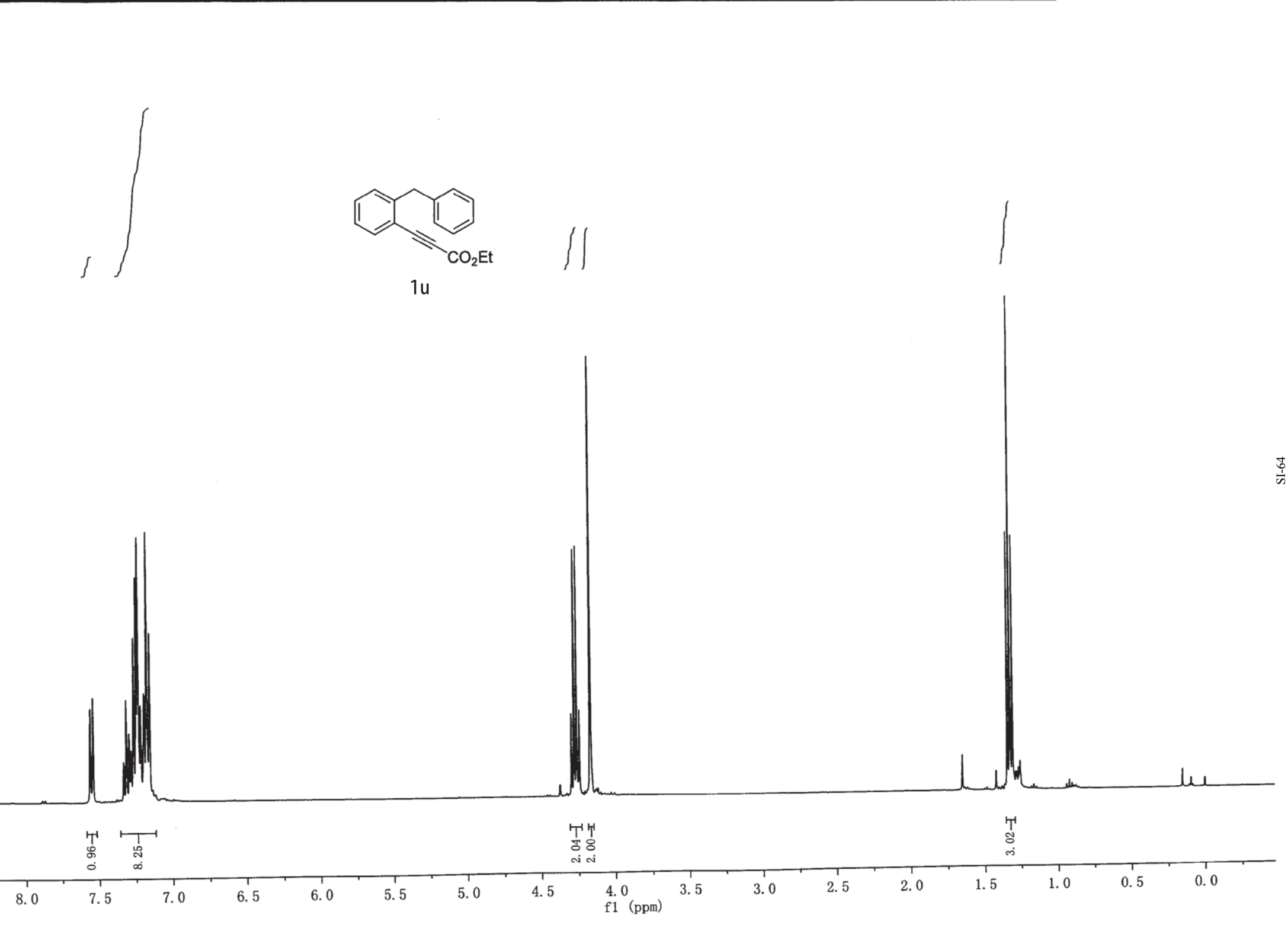

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

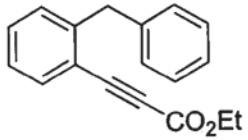

Ph
1t
1.00
1.97
3.02
3.85
3.95
2.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph

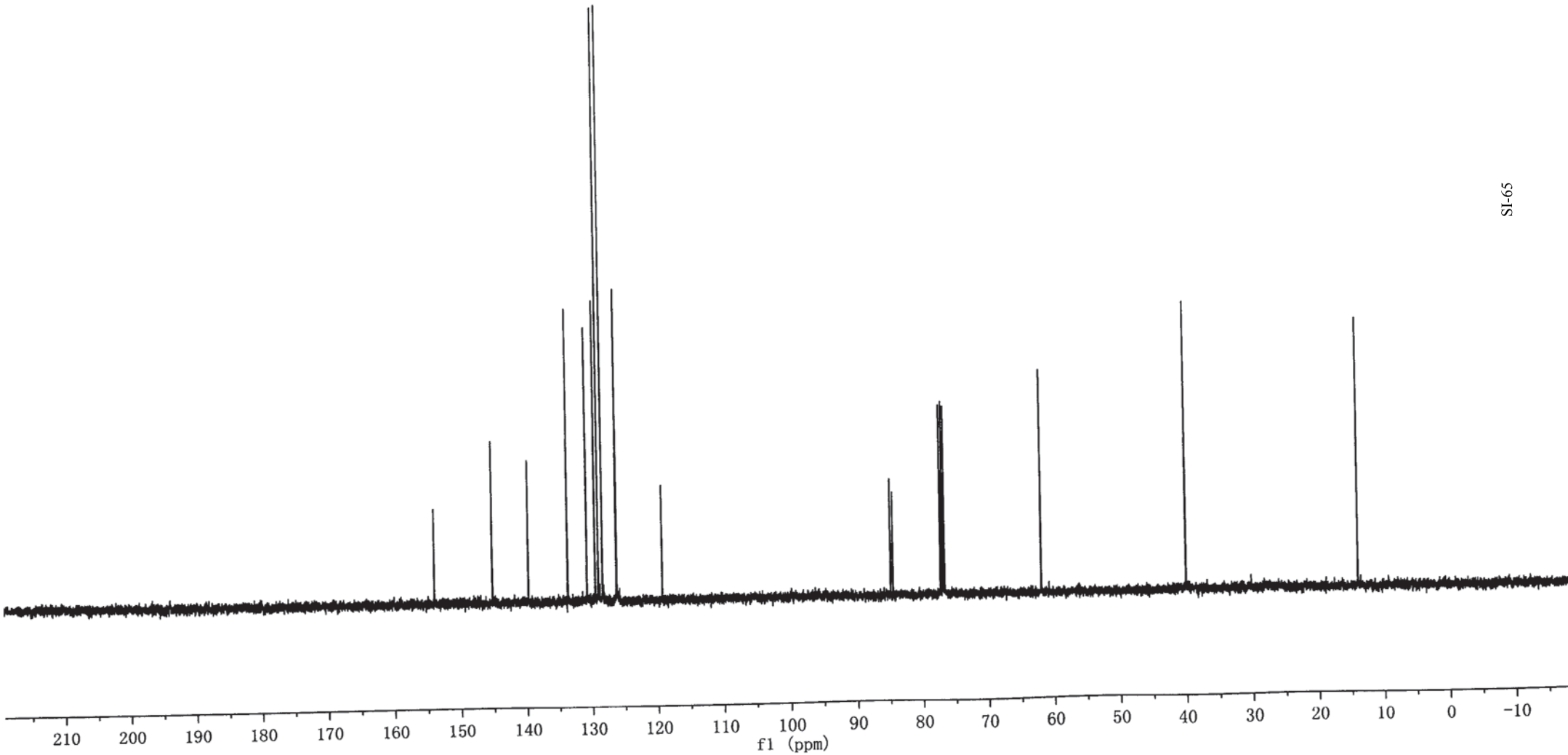
1t

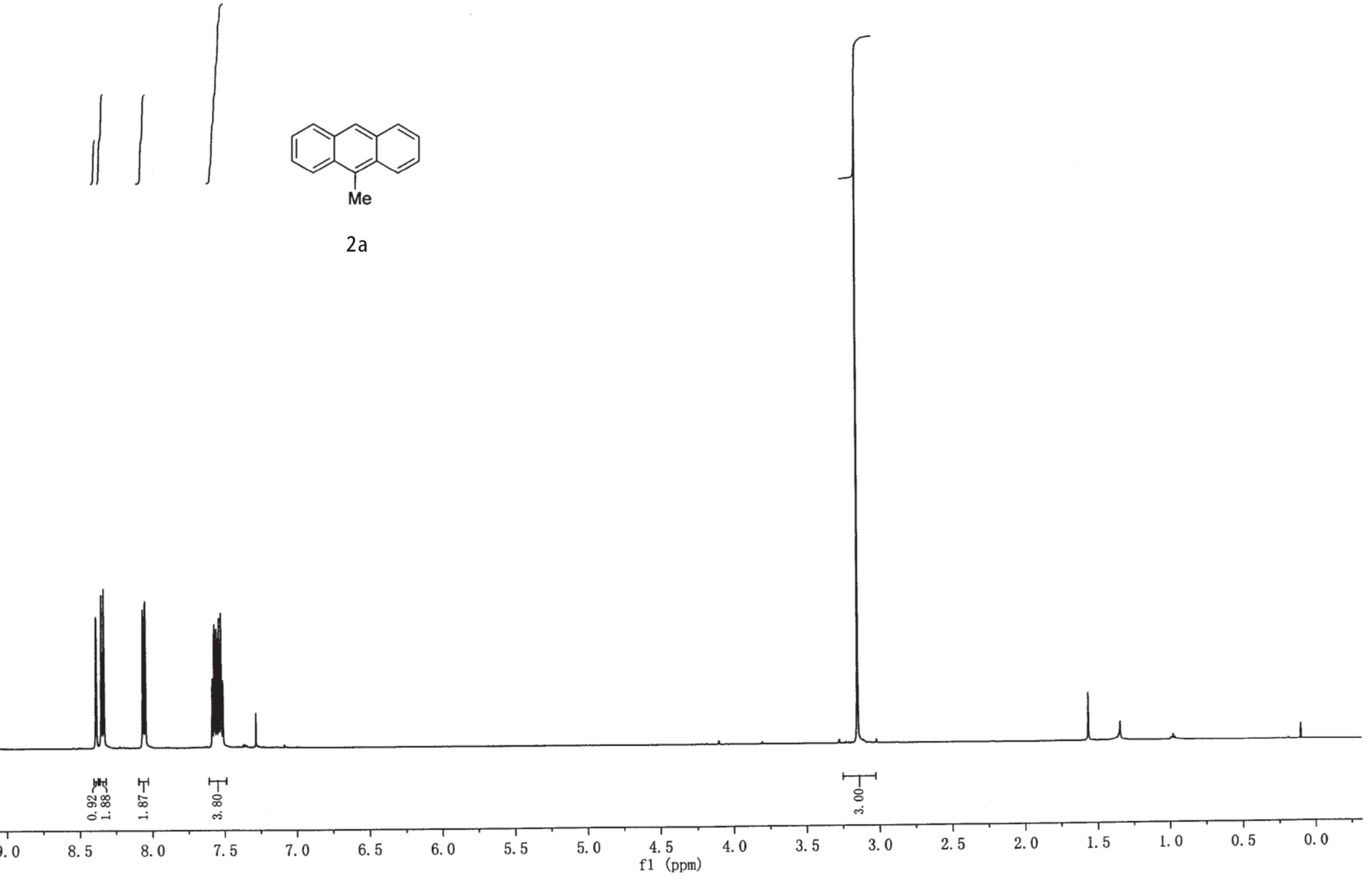

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

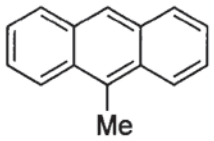

CO2Et
1u
0.96
8.25
2.04
2.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CO2Et

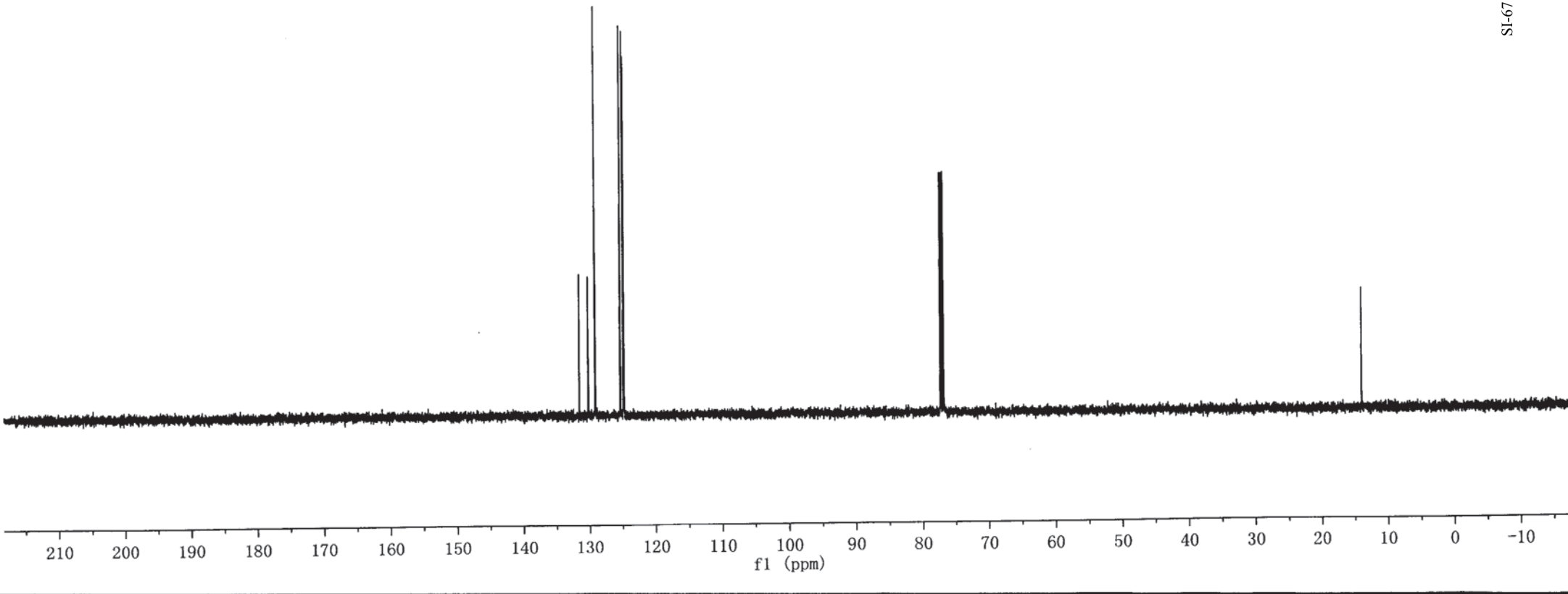
1u


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
2a
0.92
1.88
1.87
3.80
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

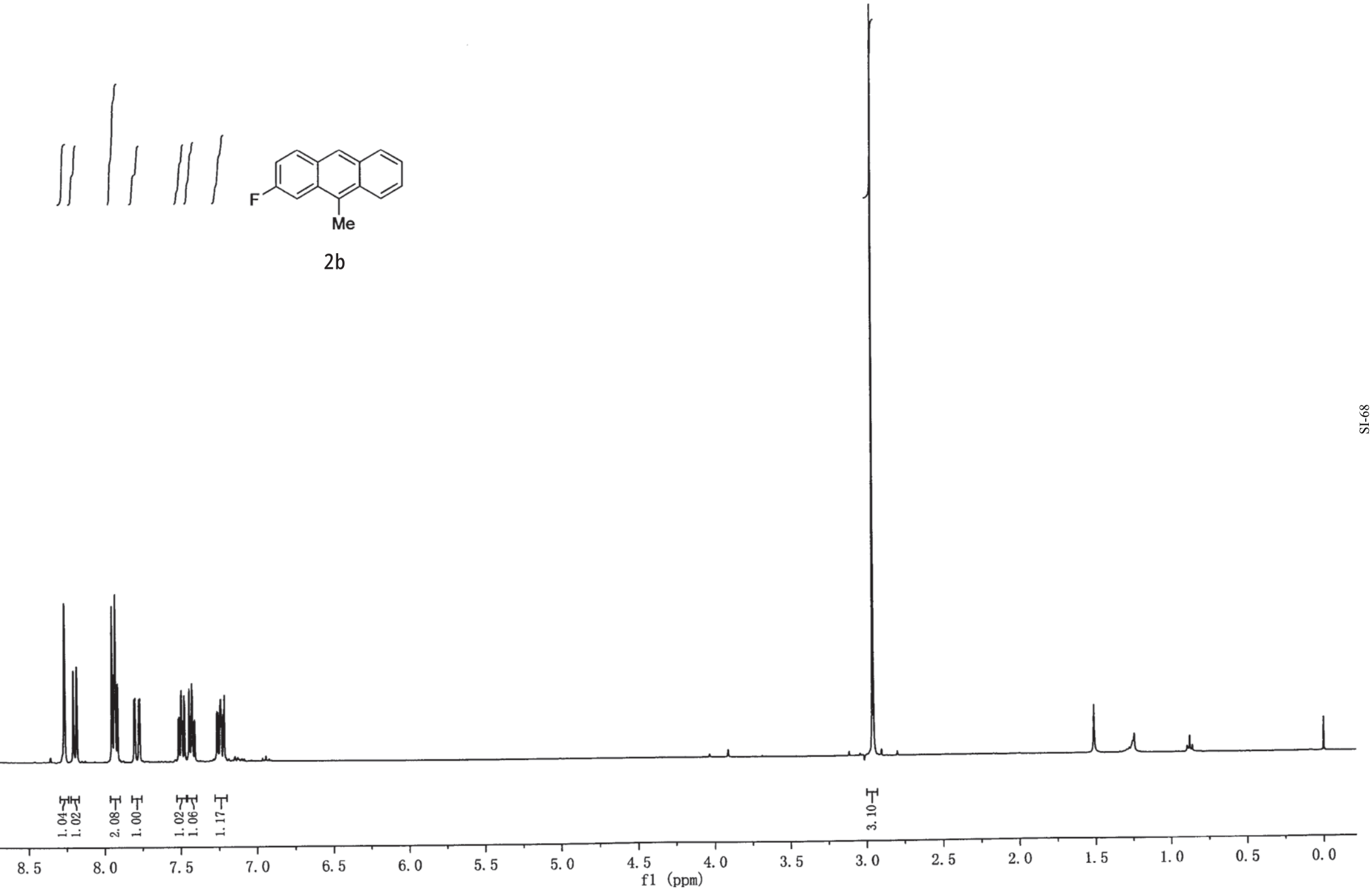

Me

2a


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

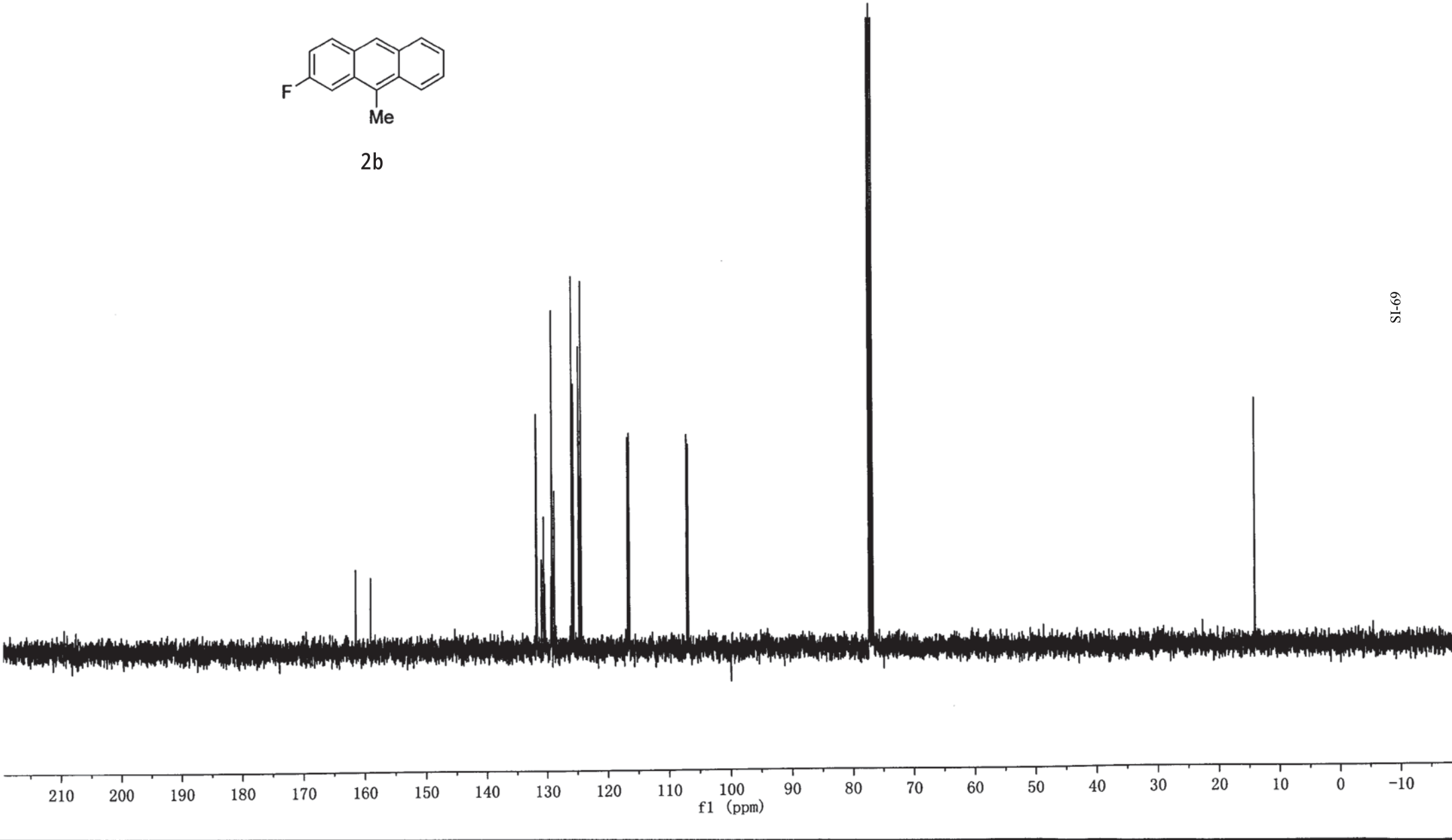
F
Me

2b


1.04
1.02
2.08
1.00
1.02
1.06
1.17
3.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

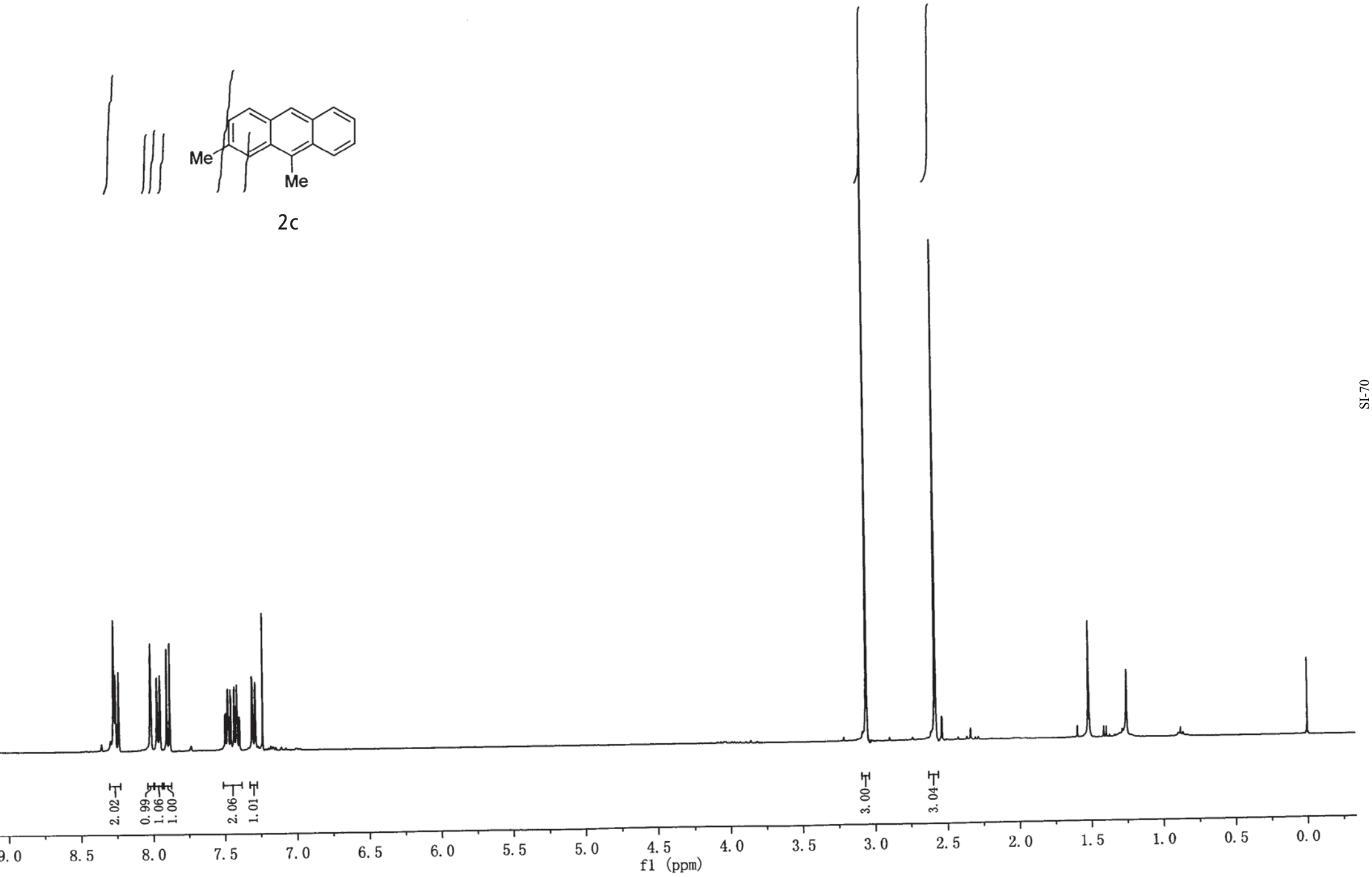
F
Me

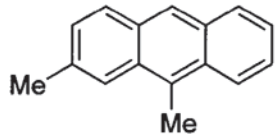
2b


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

Me
Me

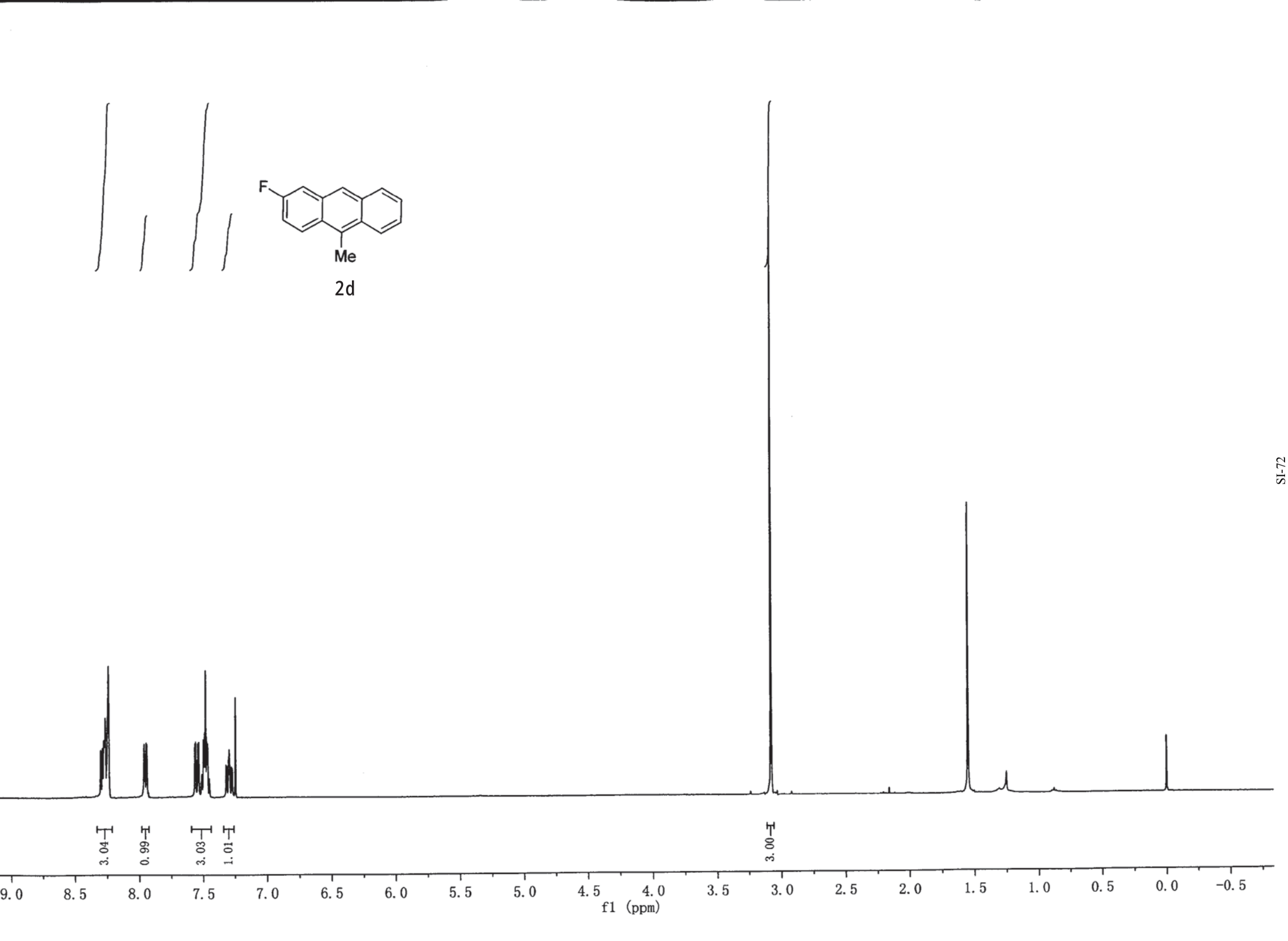
2c

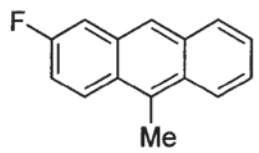

2.02
0.99
1.06
1.00
2.06
1.01
3.00
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Me
Me

2c

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F
Me
2d
3.04
0.99
3.03
1.01
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



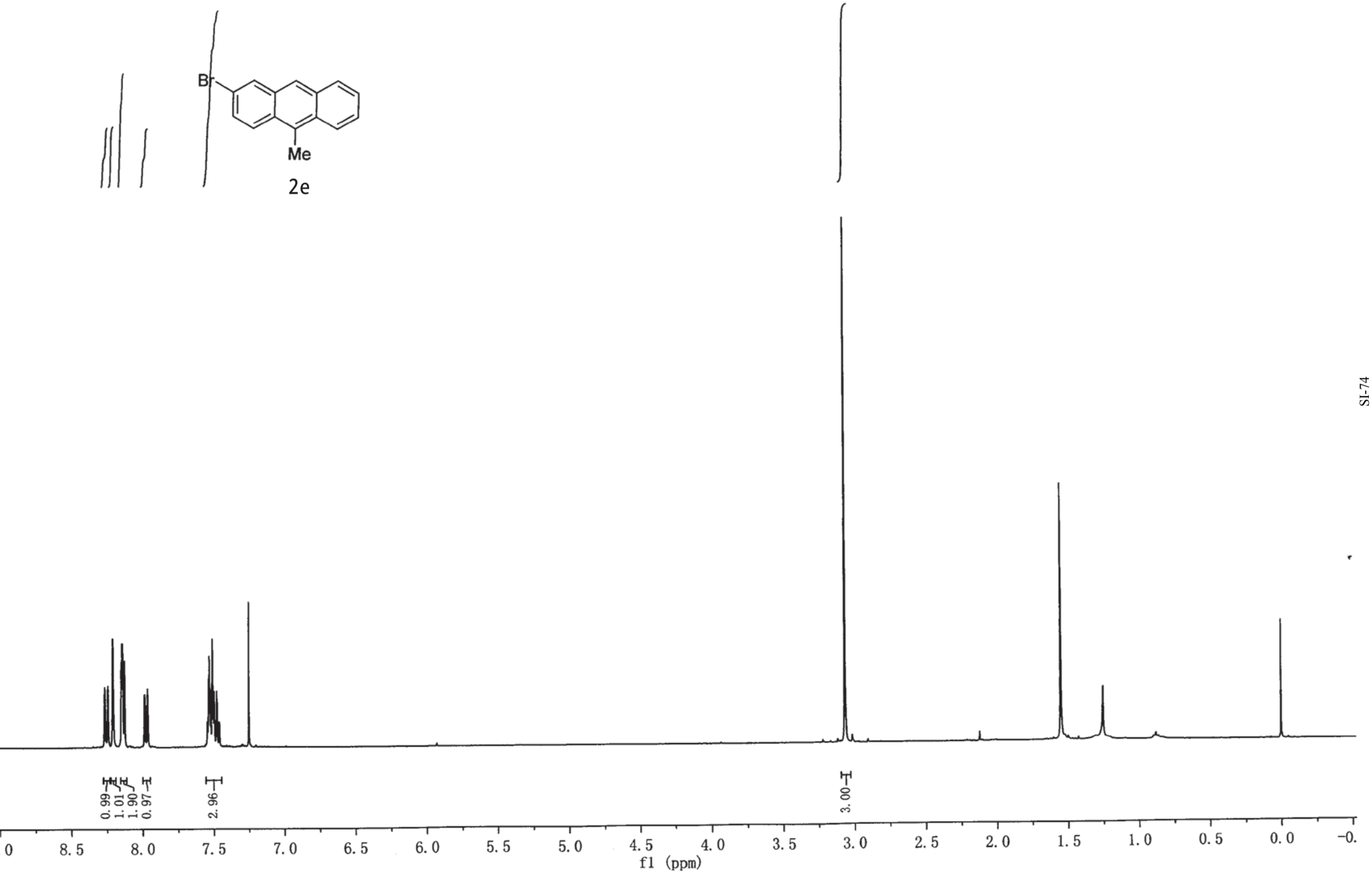
2d

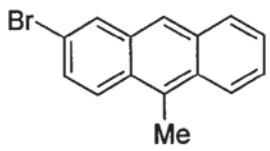
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10

f1 (ppm)

Br
Me

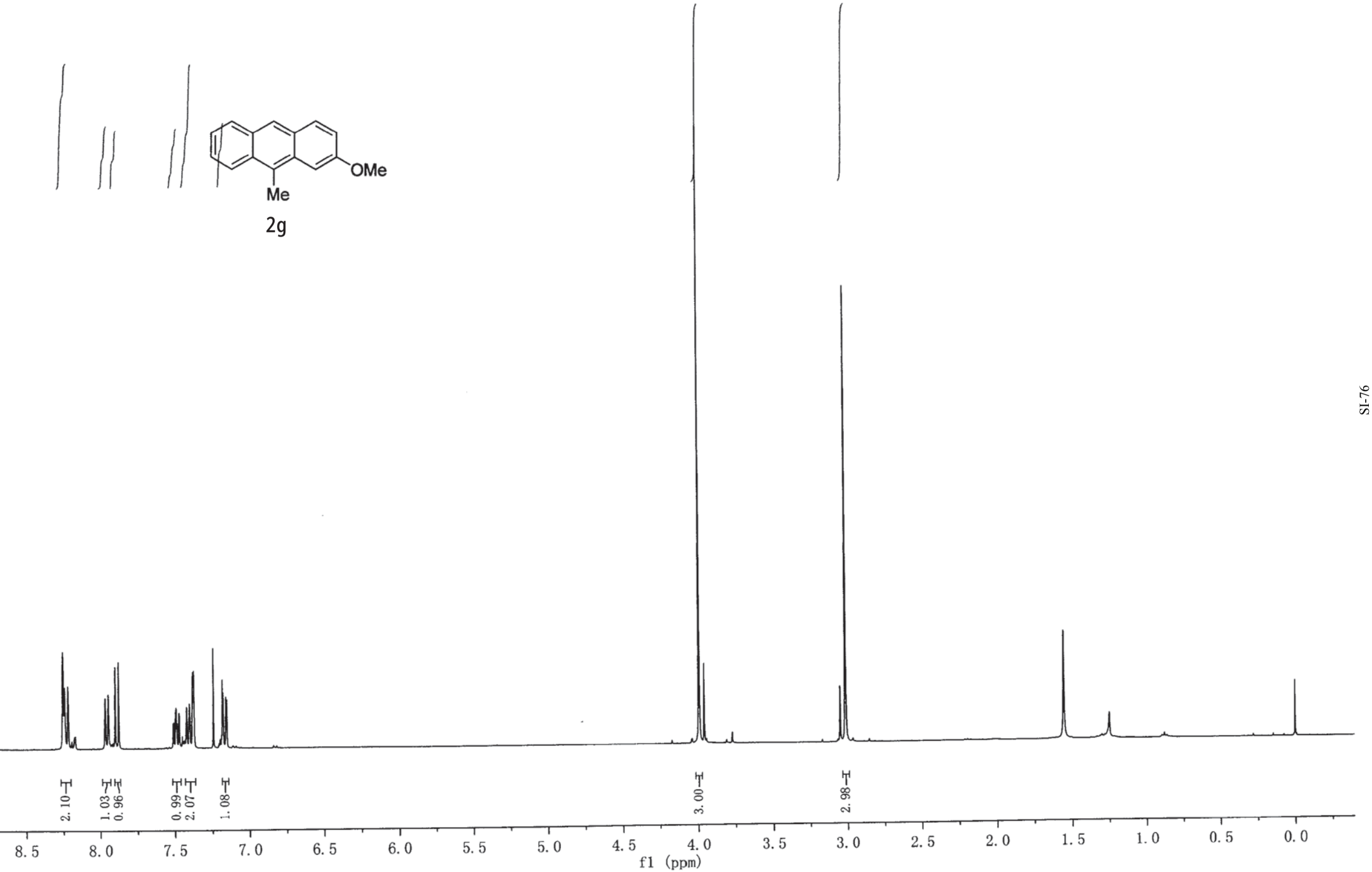
2e

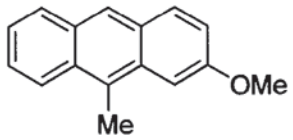

0.99
1.01
1.90
0.97
2.96
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Br
Me

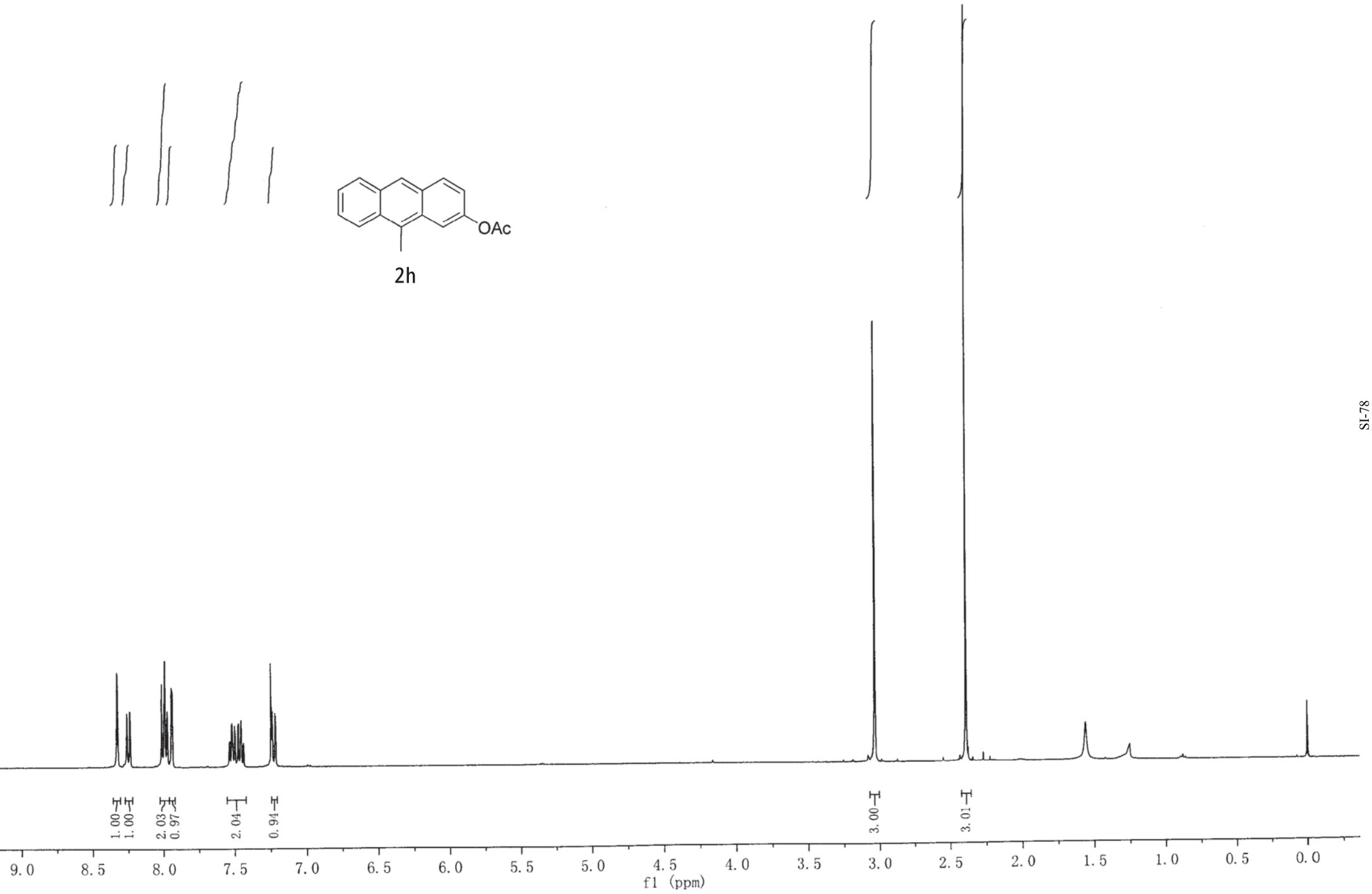
2e

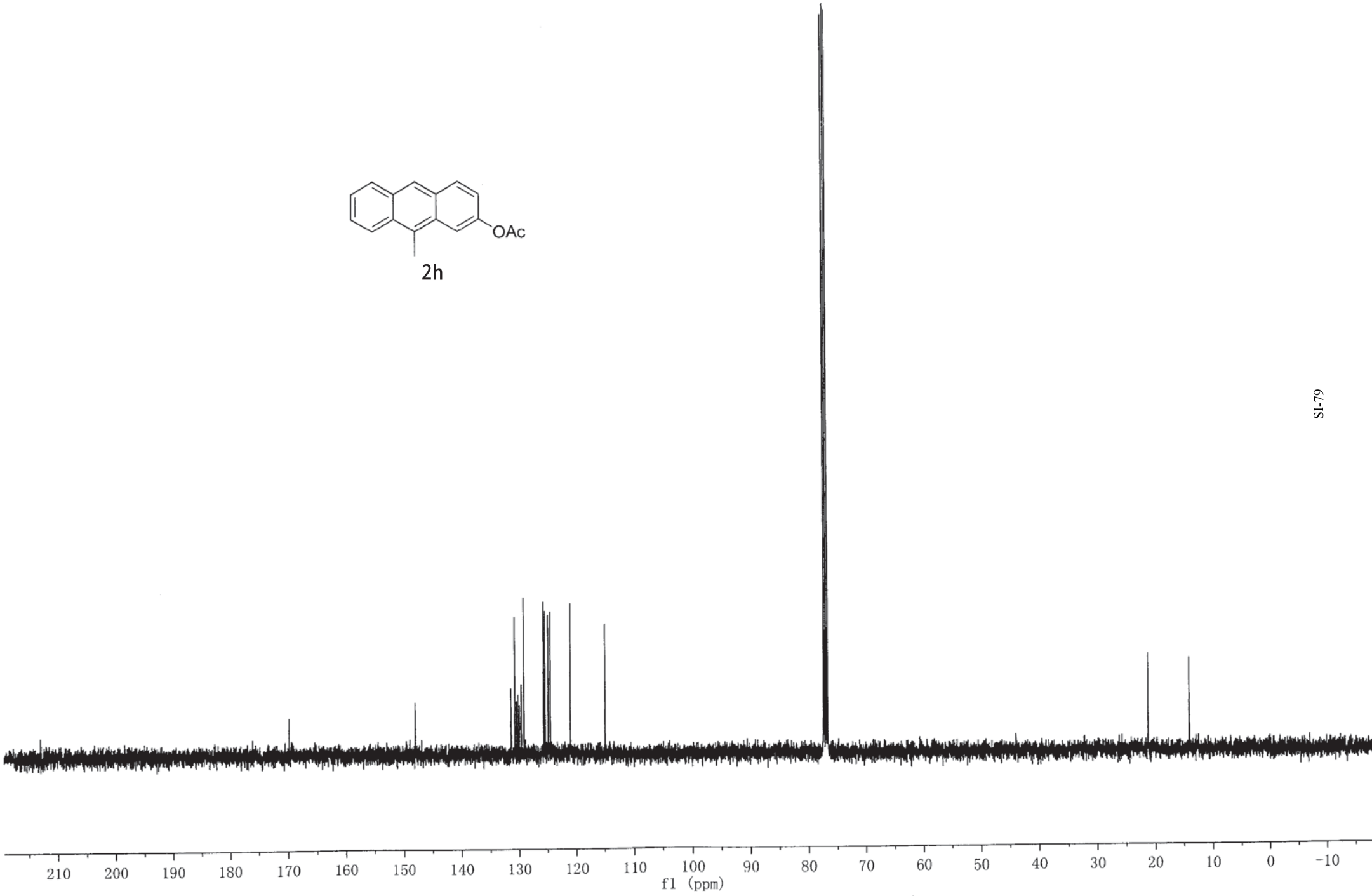
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

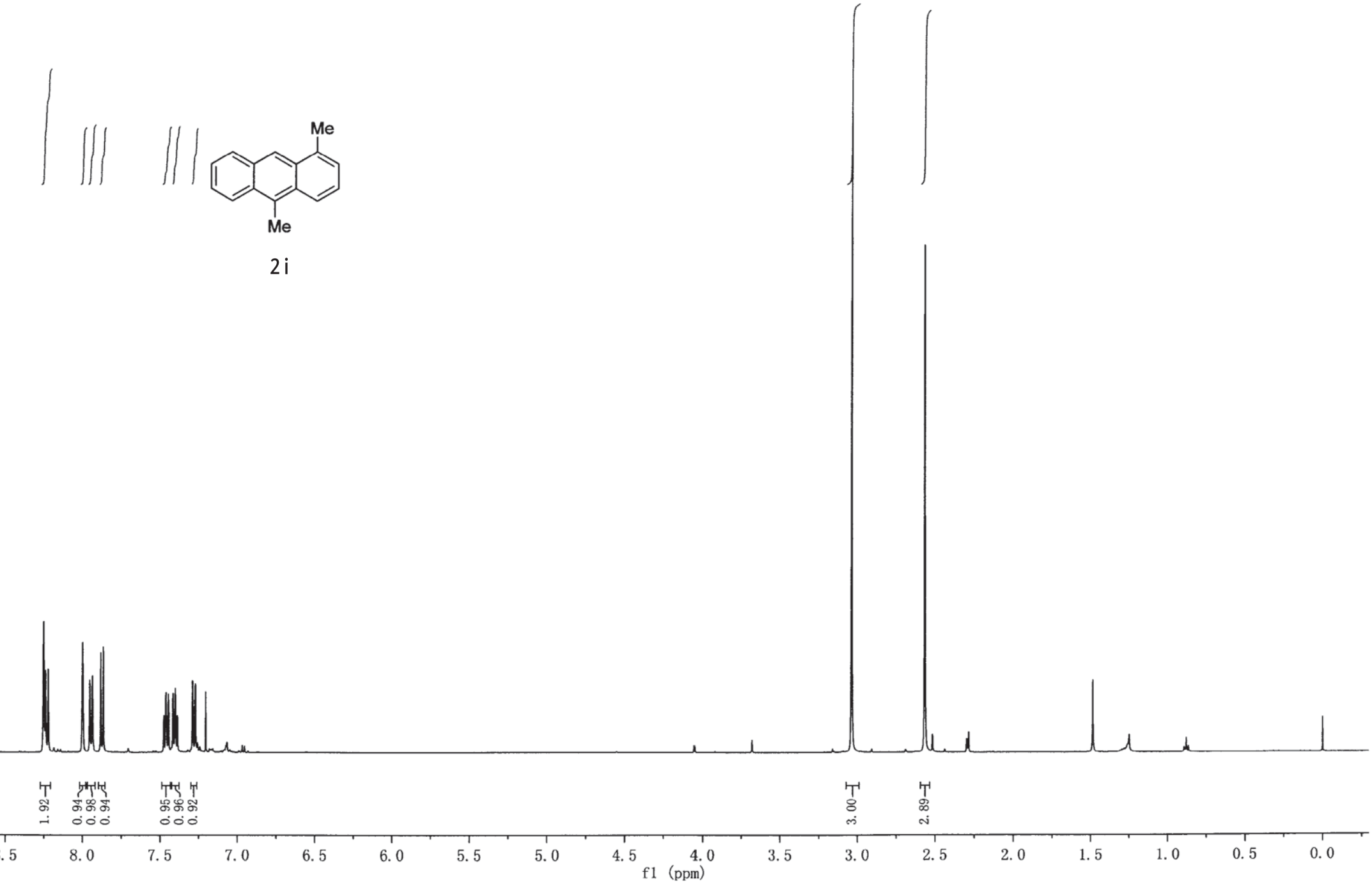

OMe
Me
2g
2.10
1.03
0.96
0.99
2.07
1.08
3.00
2.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

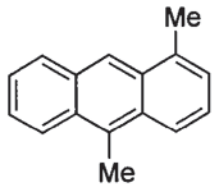


2g

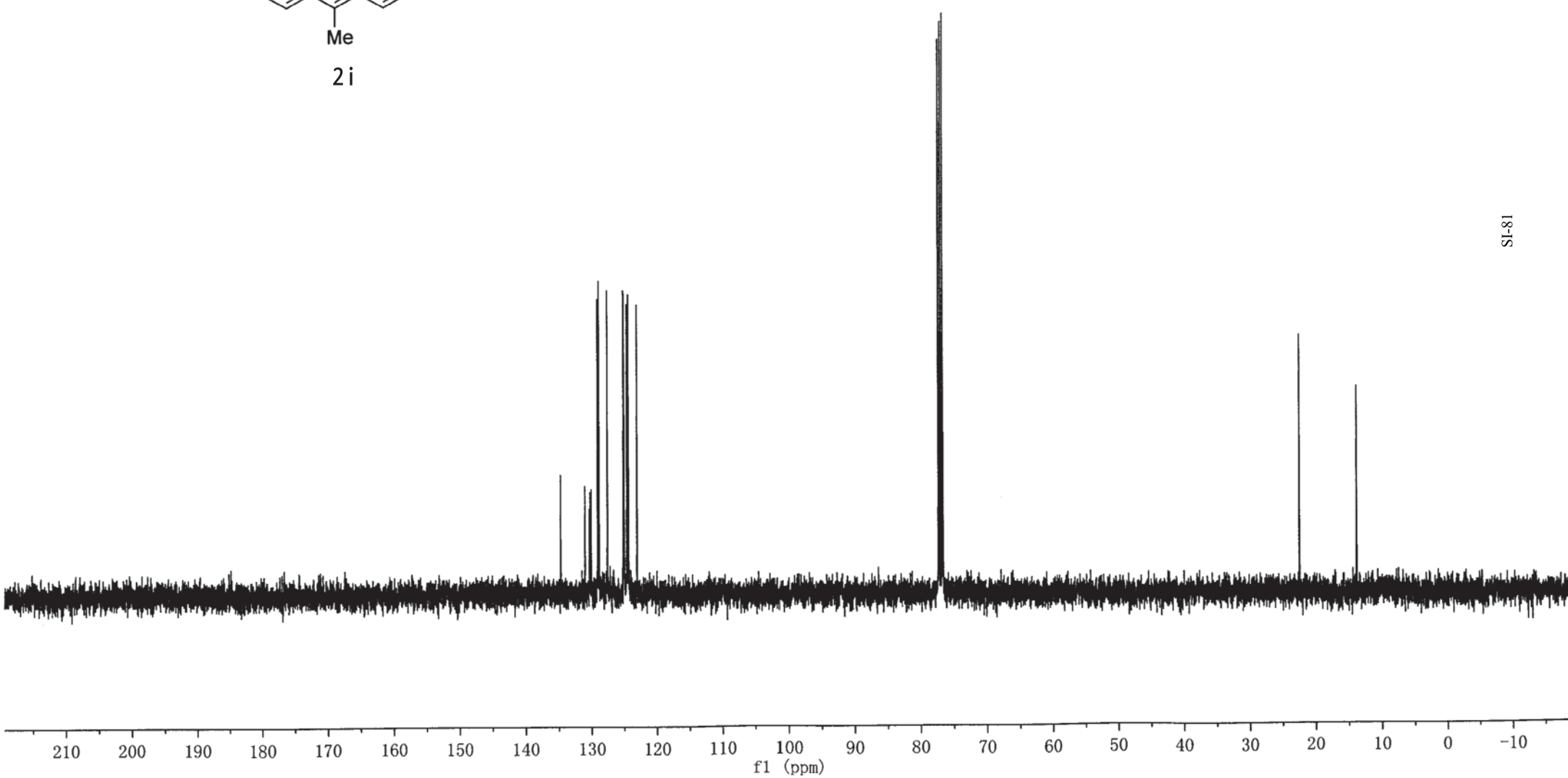

OAc
2h
1.00
1.00
2.03
0.97
2.04
0.94
3.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

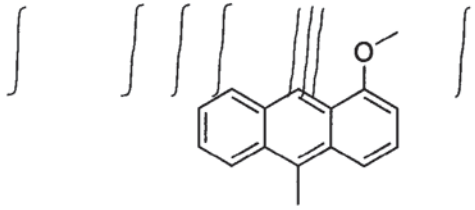

OAc
2h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
Me
2i
1.92
0.94
0.98
0.94
0.95
0.96
0.92
3.00
2.89
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

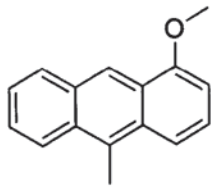

Me
Me

2i

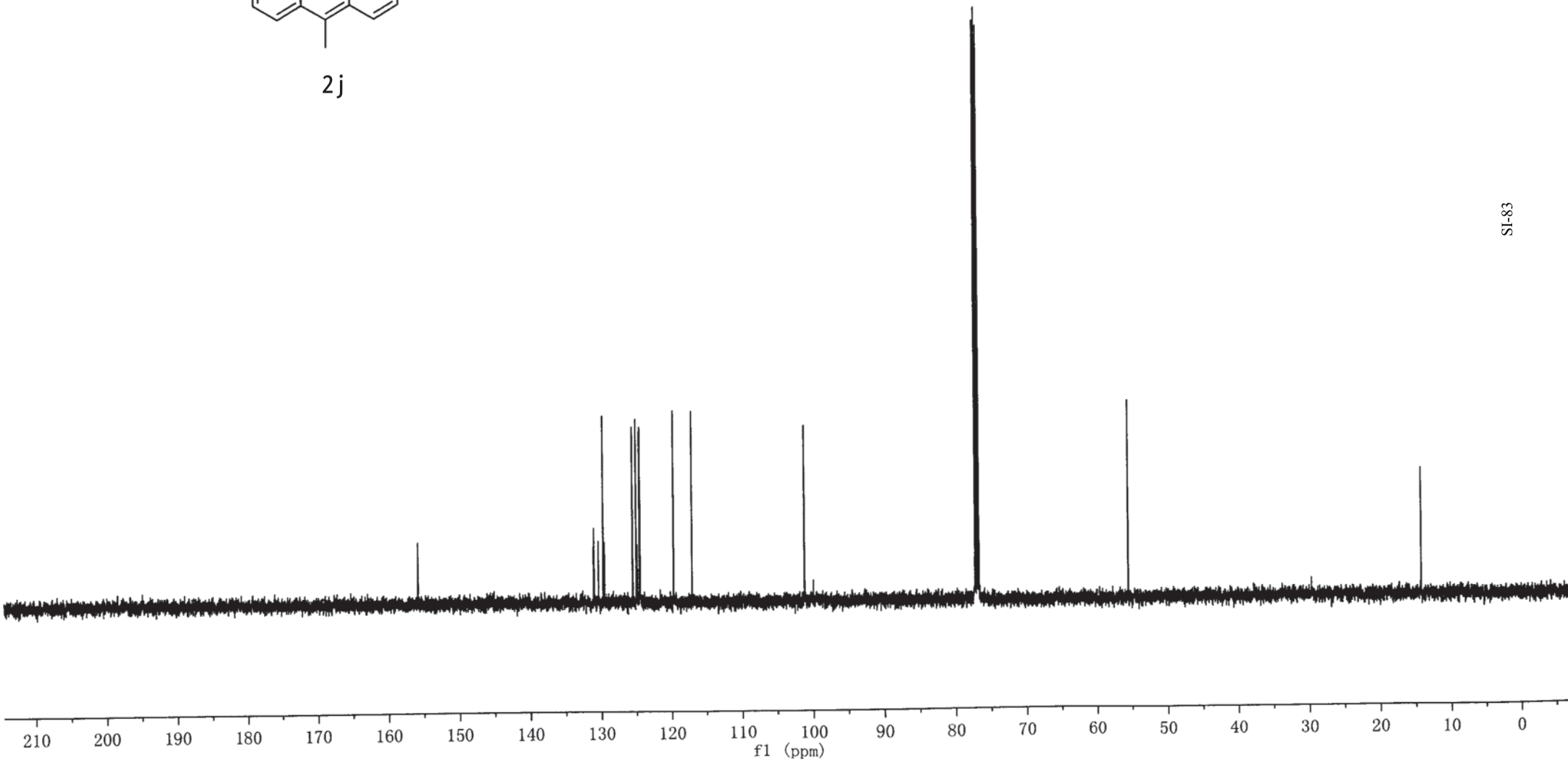

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

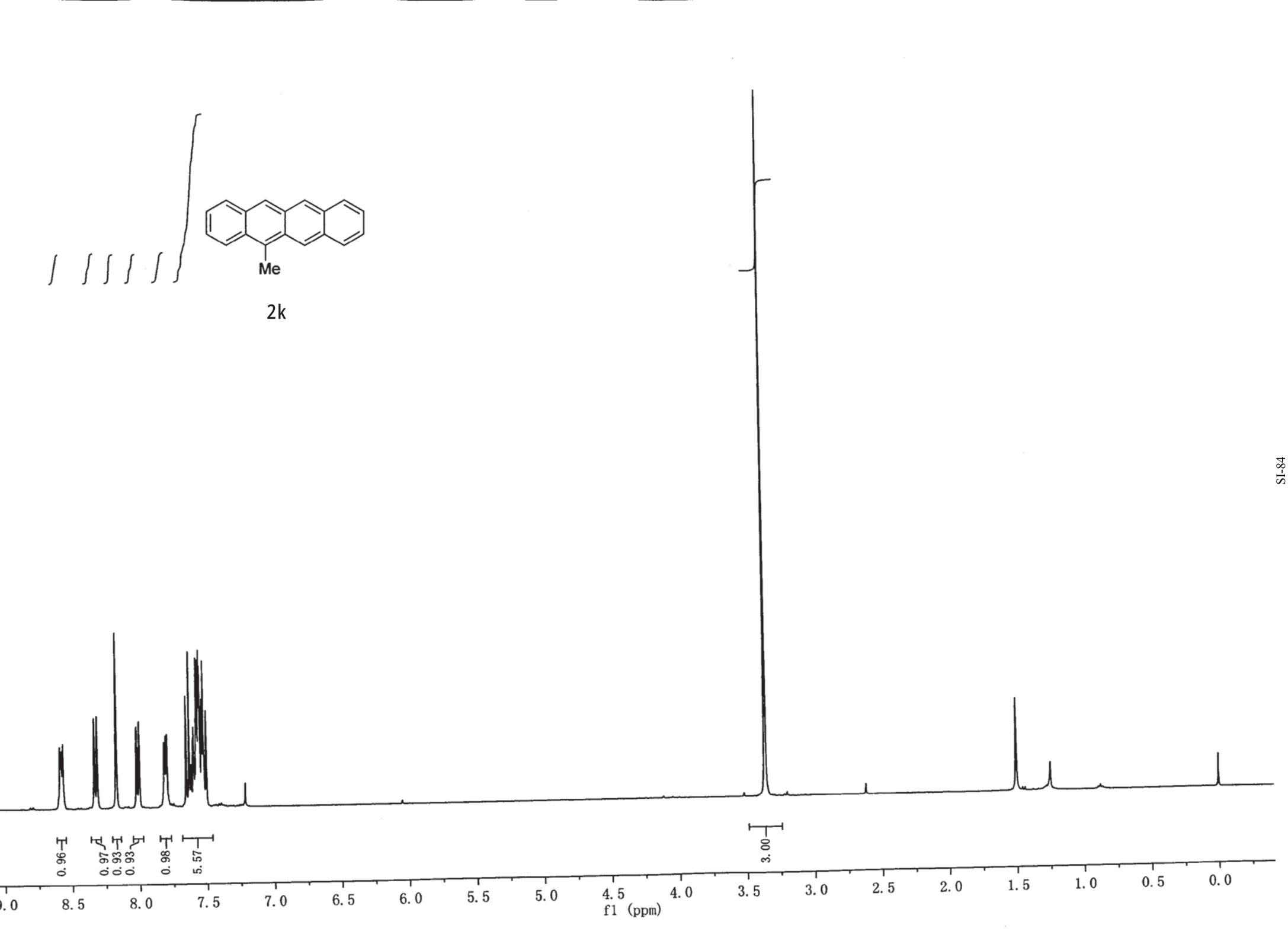


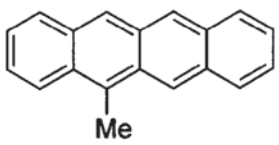
2j



2j

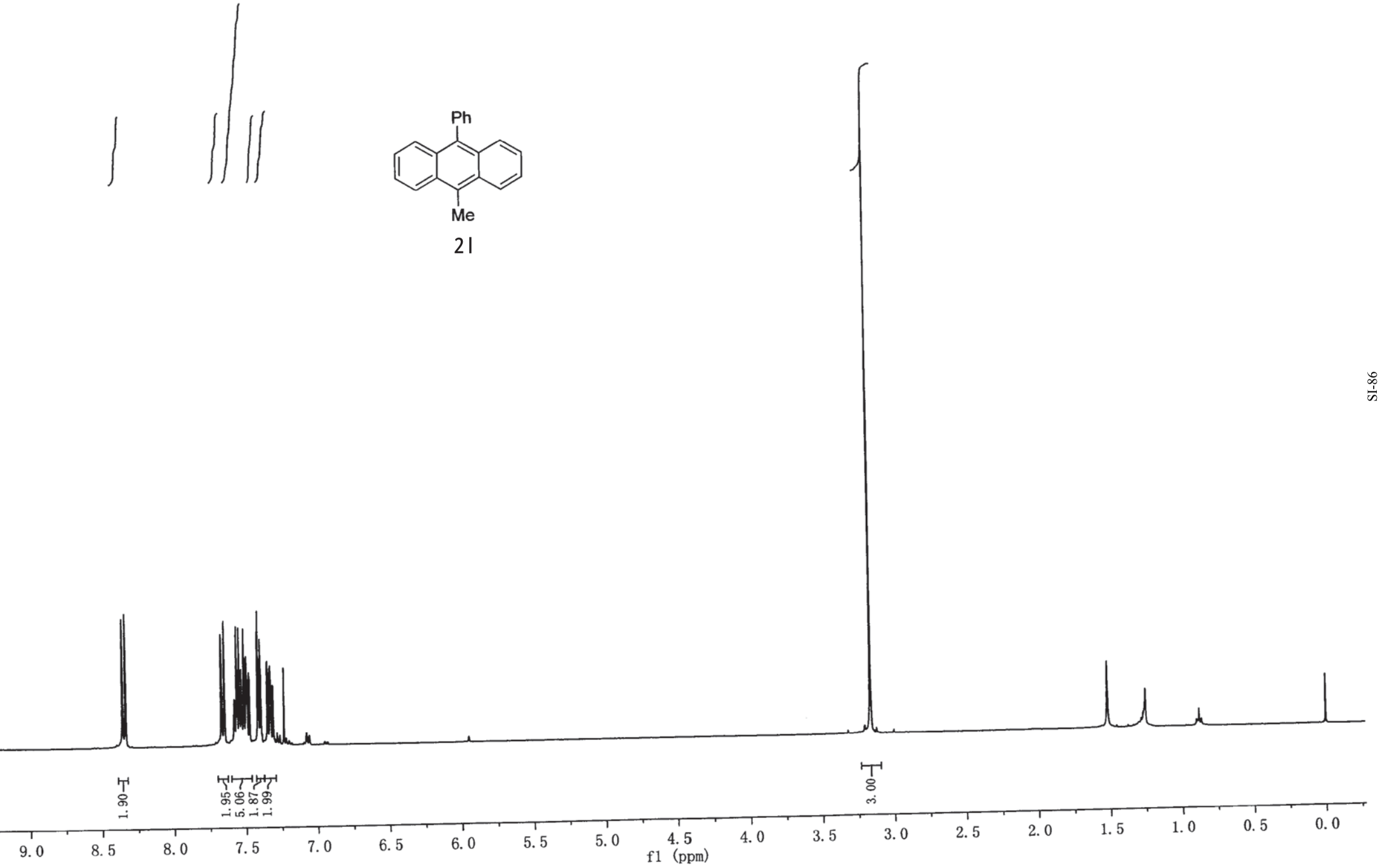

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Me
2k
0.96
0.97
0.93
0.93
0.98
5.57
3.00
f1 (ppm)


Me

2k

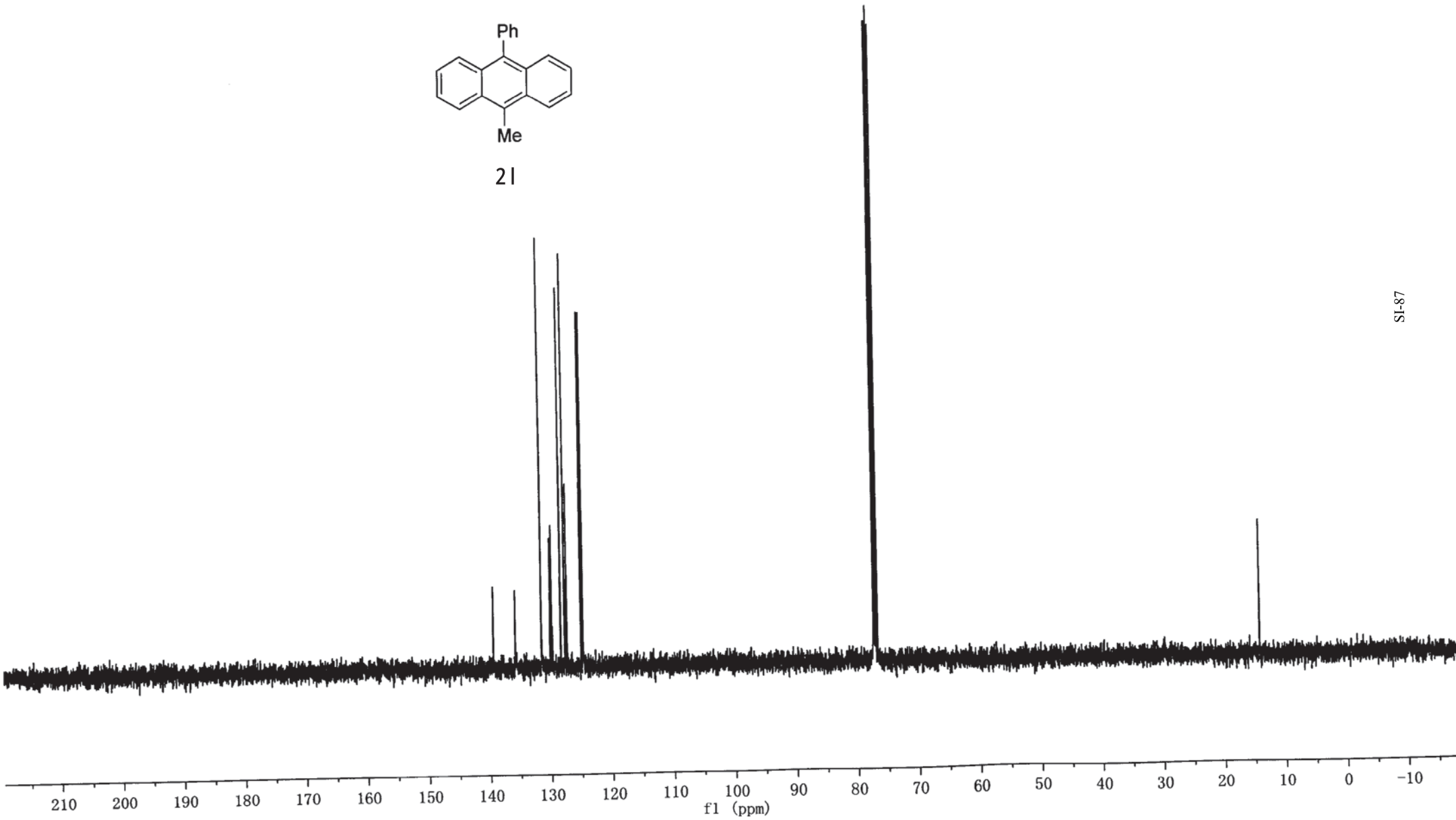
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

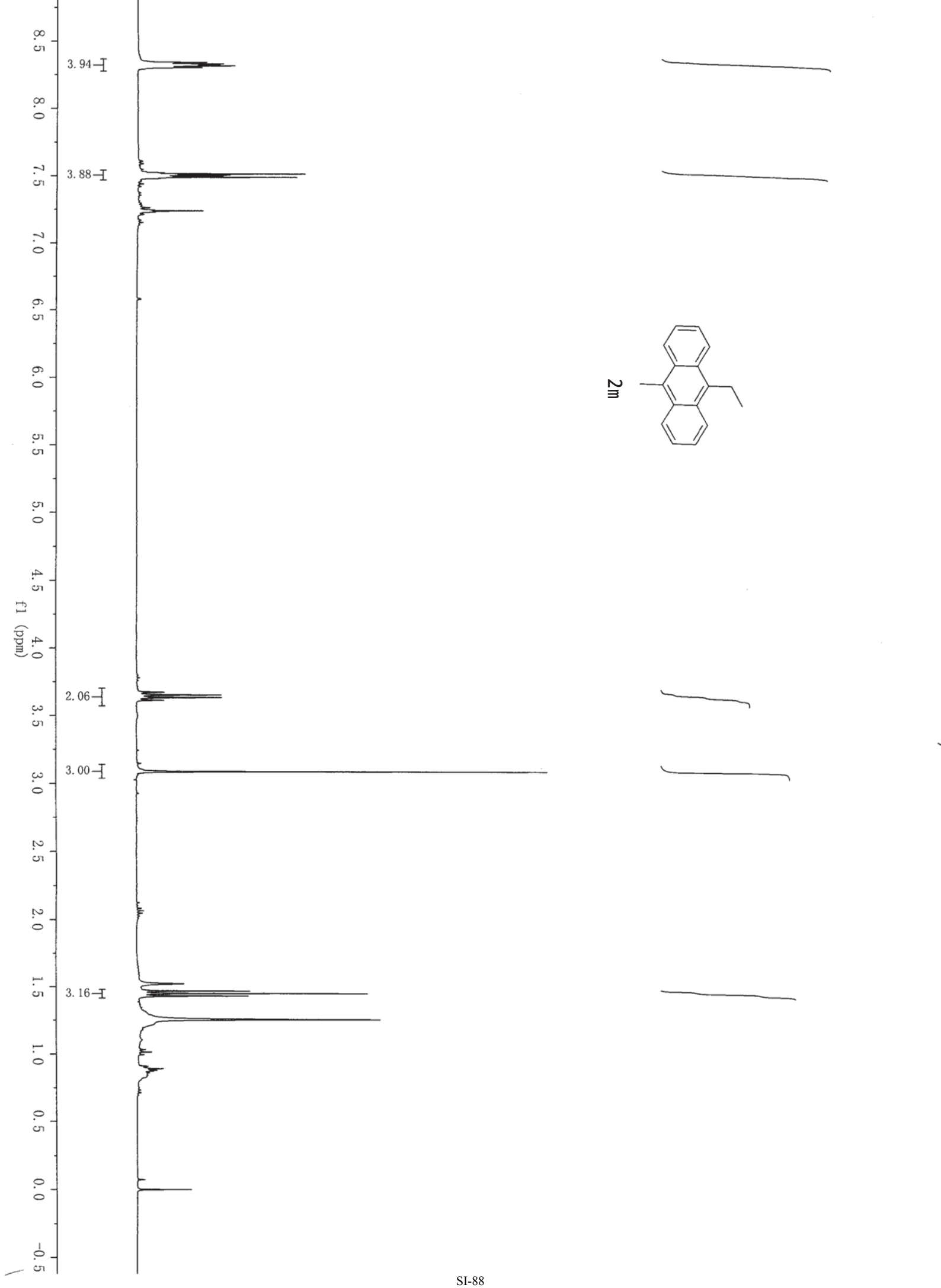

Ph
Me
1.90
1.95
5.06
1.87
1.99
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

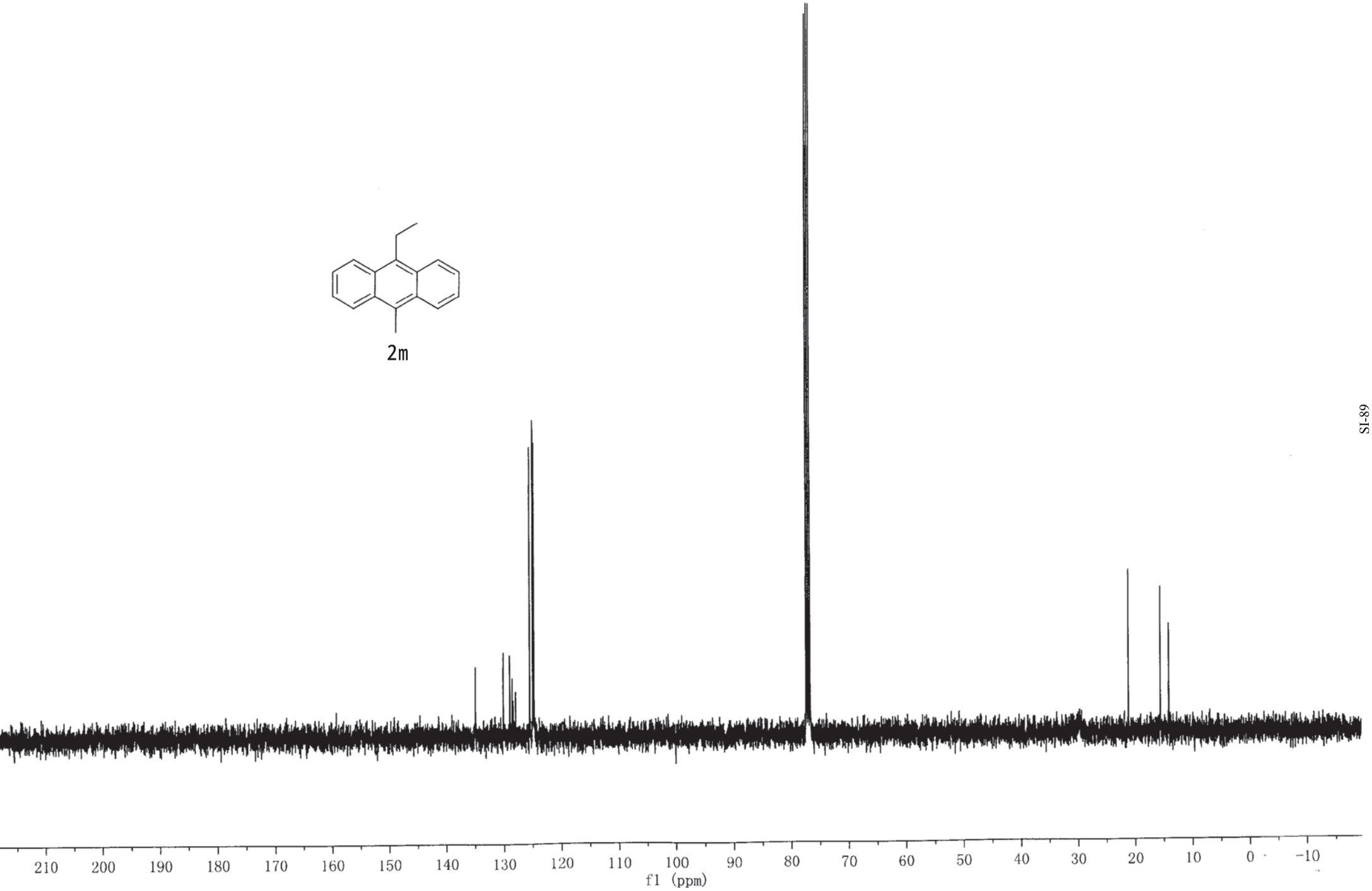
21

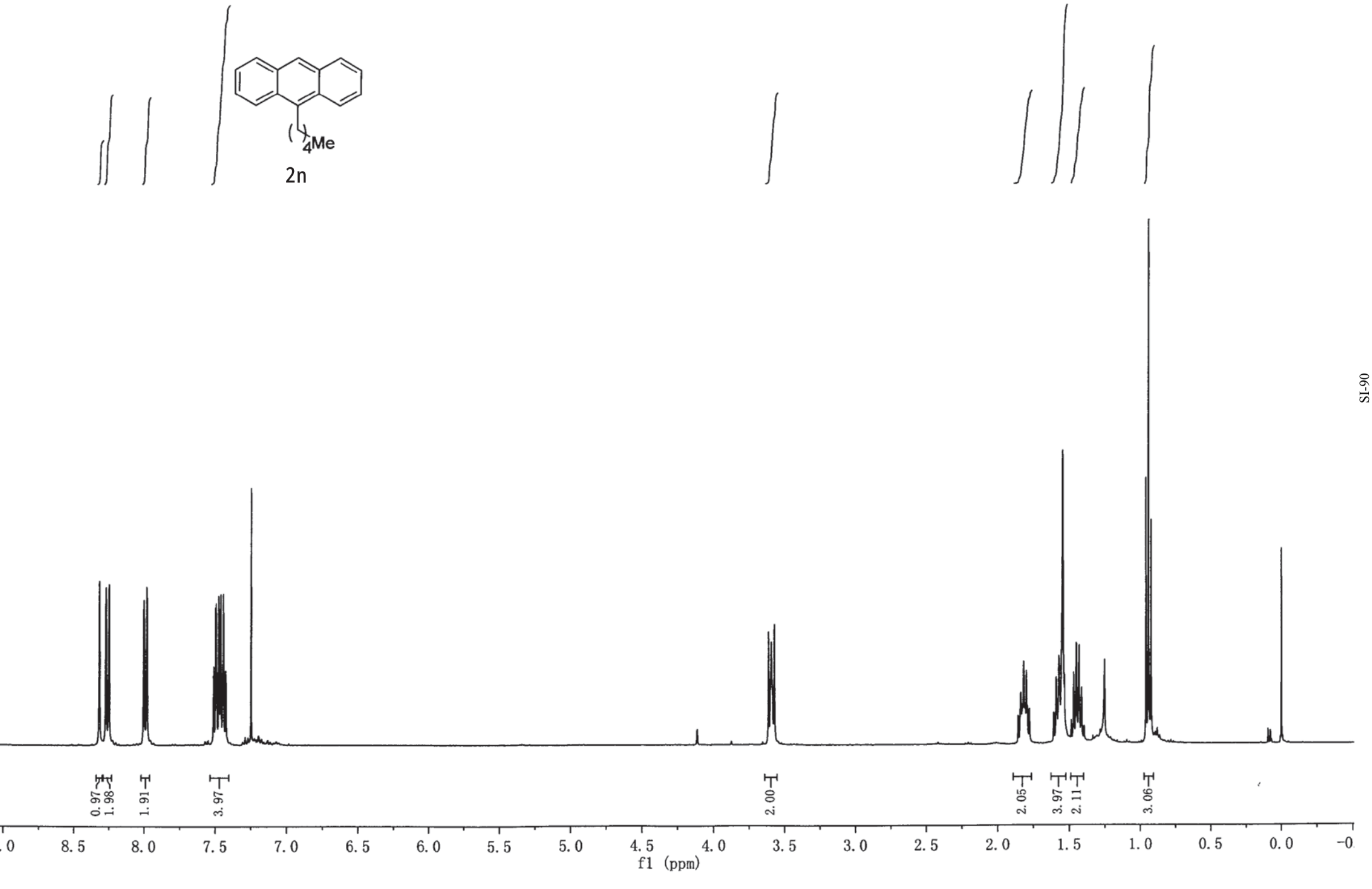
Ph
Me

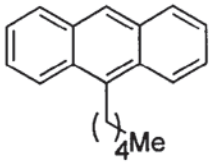
21


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


3.94
3.88
2.06
3.00
3.16
f1 (ppm)
2m

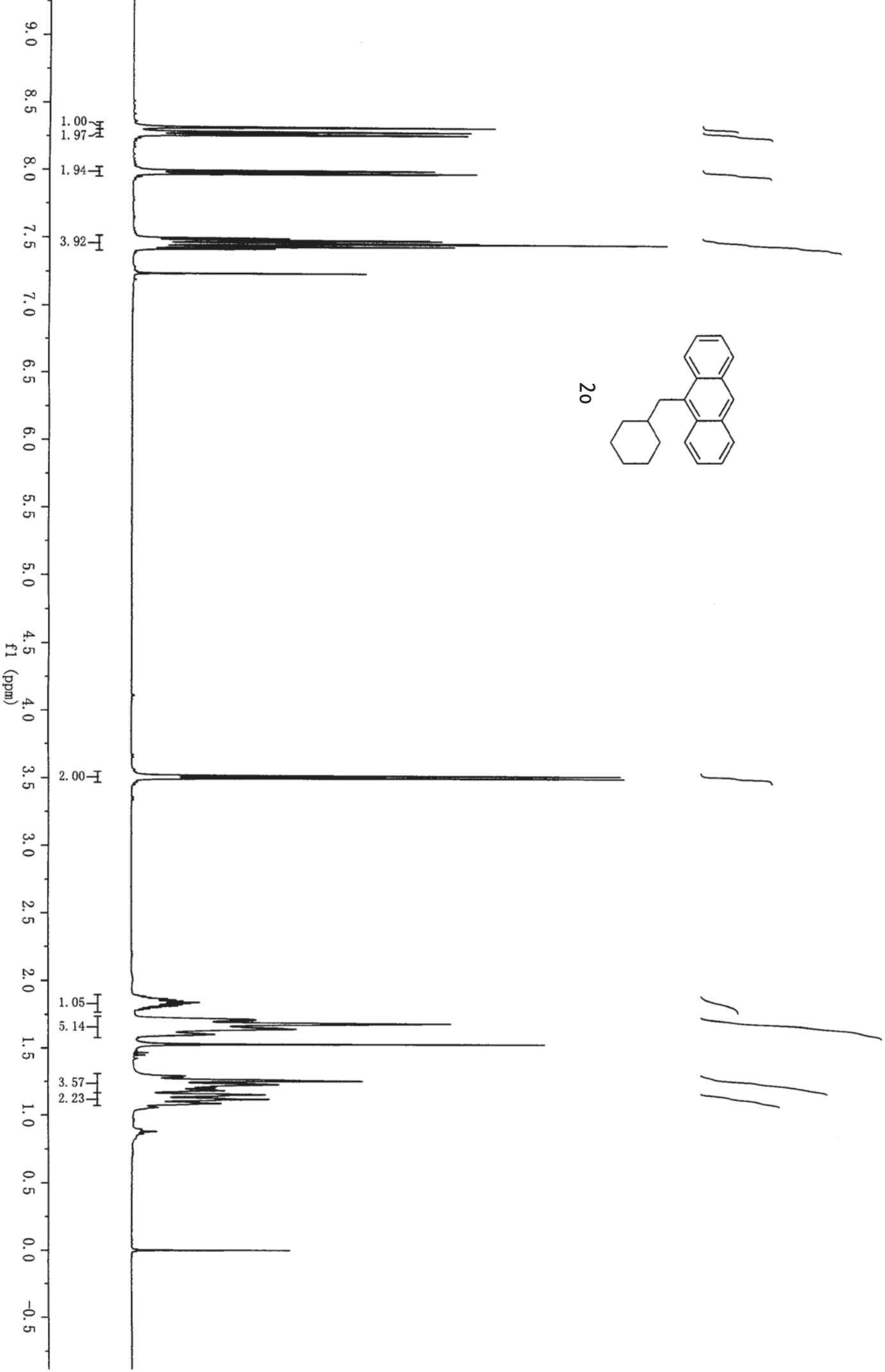

2m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


4Me
2n
0.97
1.98
1.91
3.97
2.00
2.05
3.97
2.11
3.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

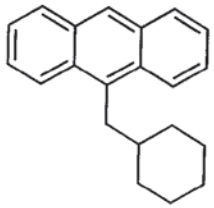

4Me

2n

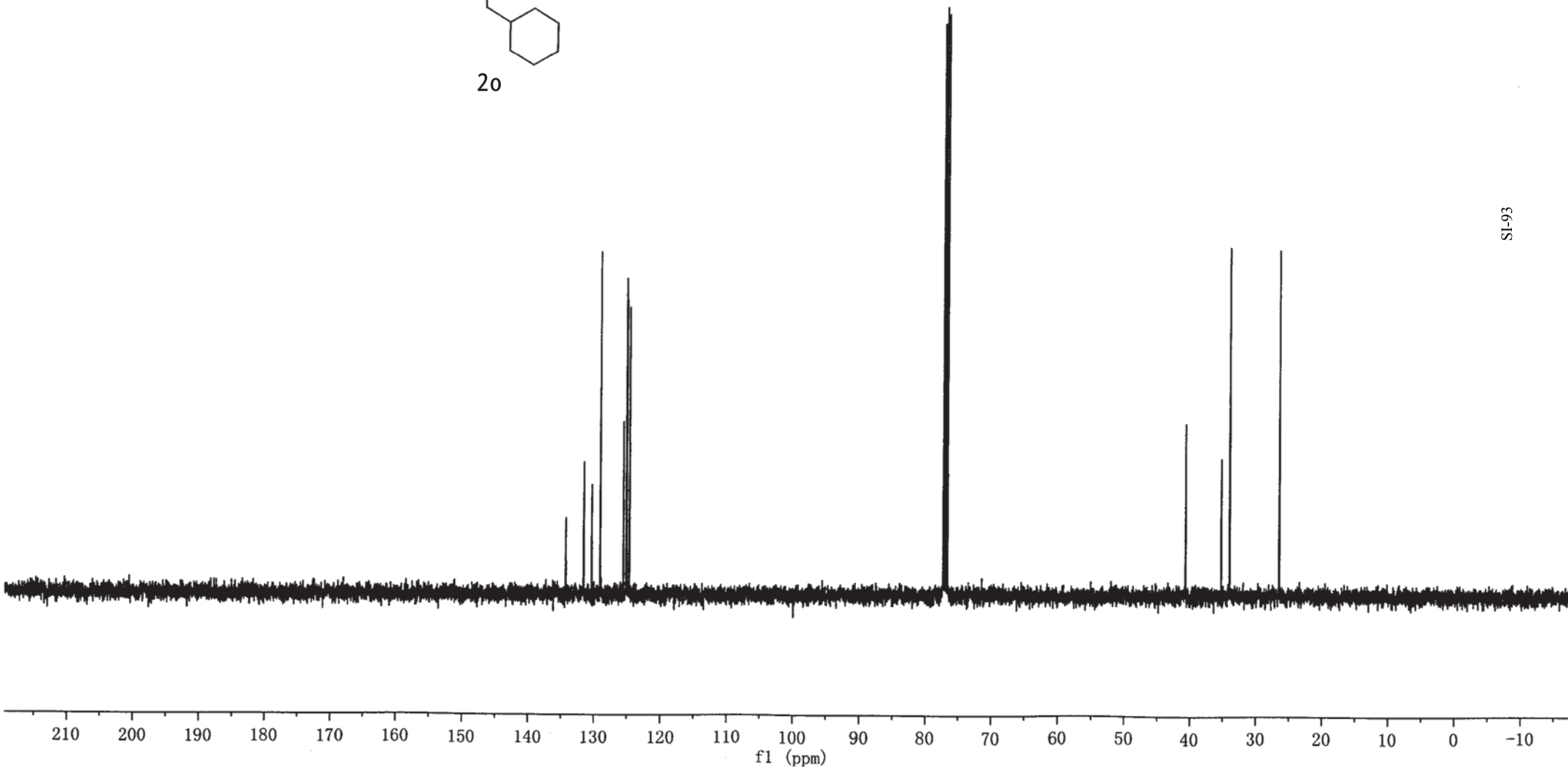
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

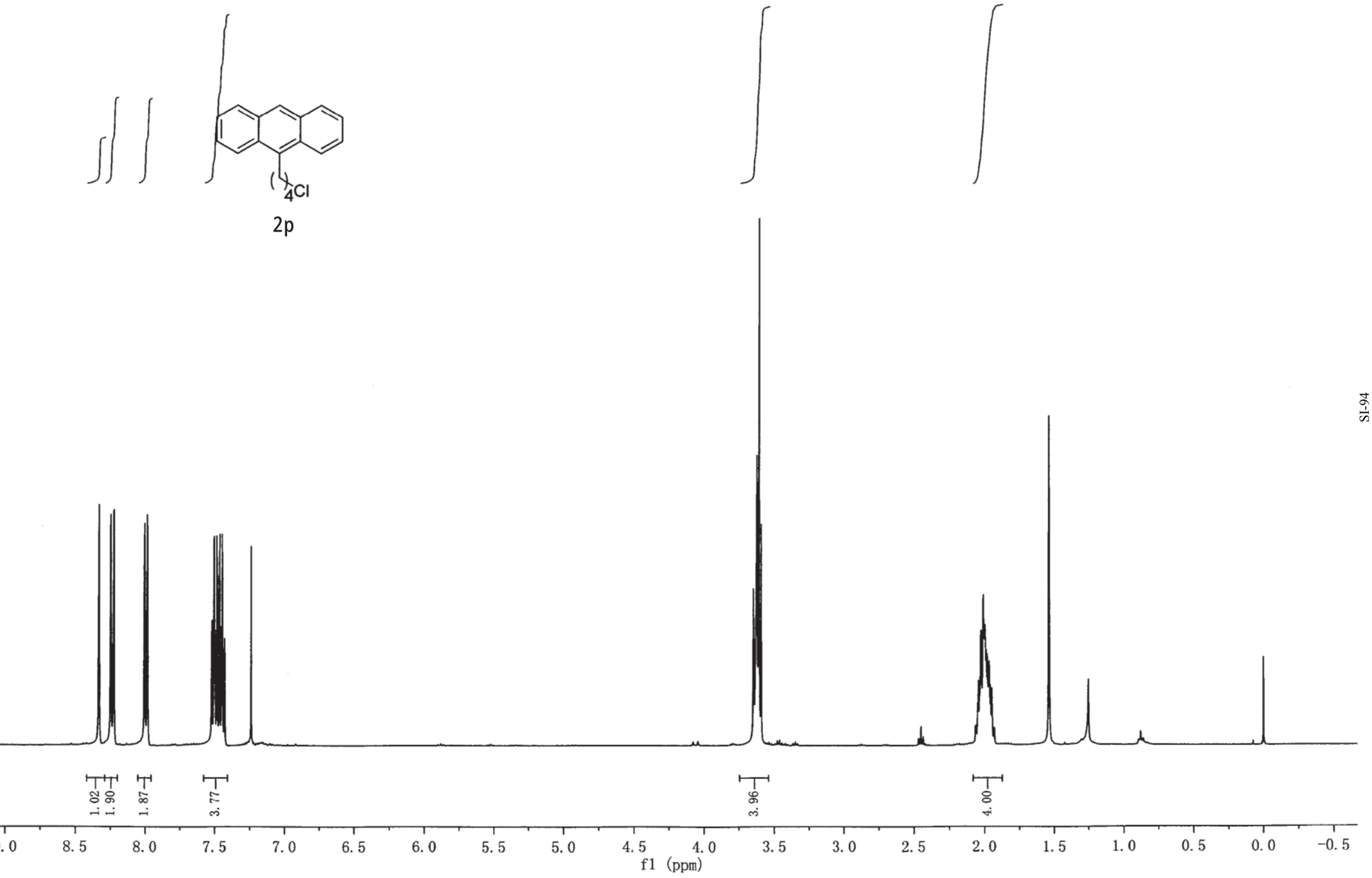

1.00
1.97
1.94
3.92
2.00
1.05
5.14
3.57
2.23
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

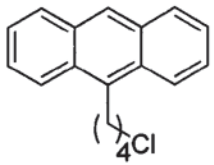
2o



2o

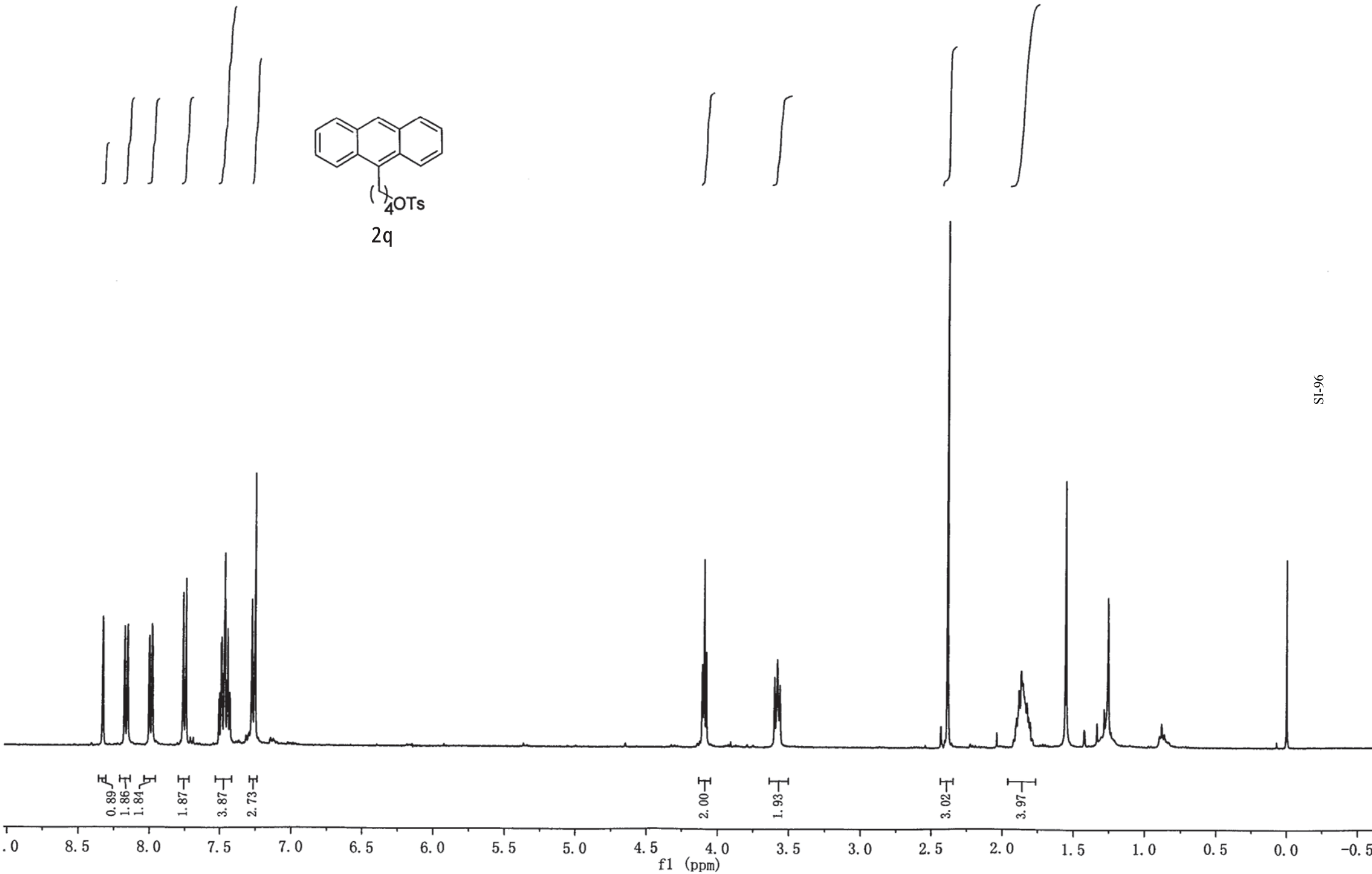

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Cl
4
2p
1.02
1.90
1.87
3.77
3.96
4.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)


4Cl

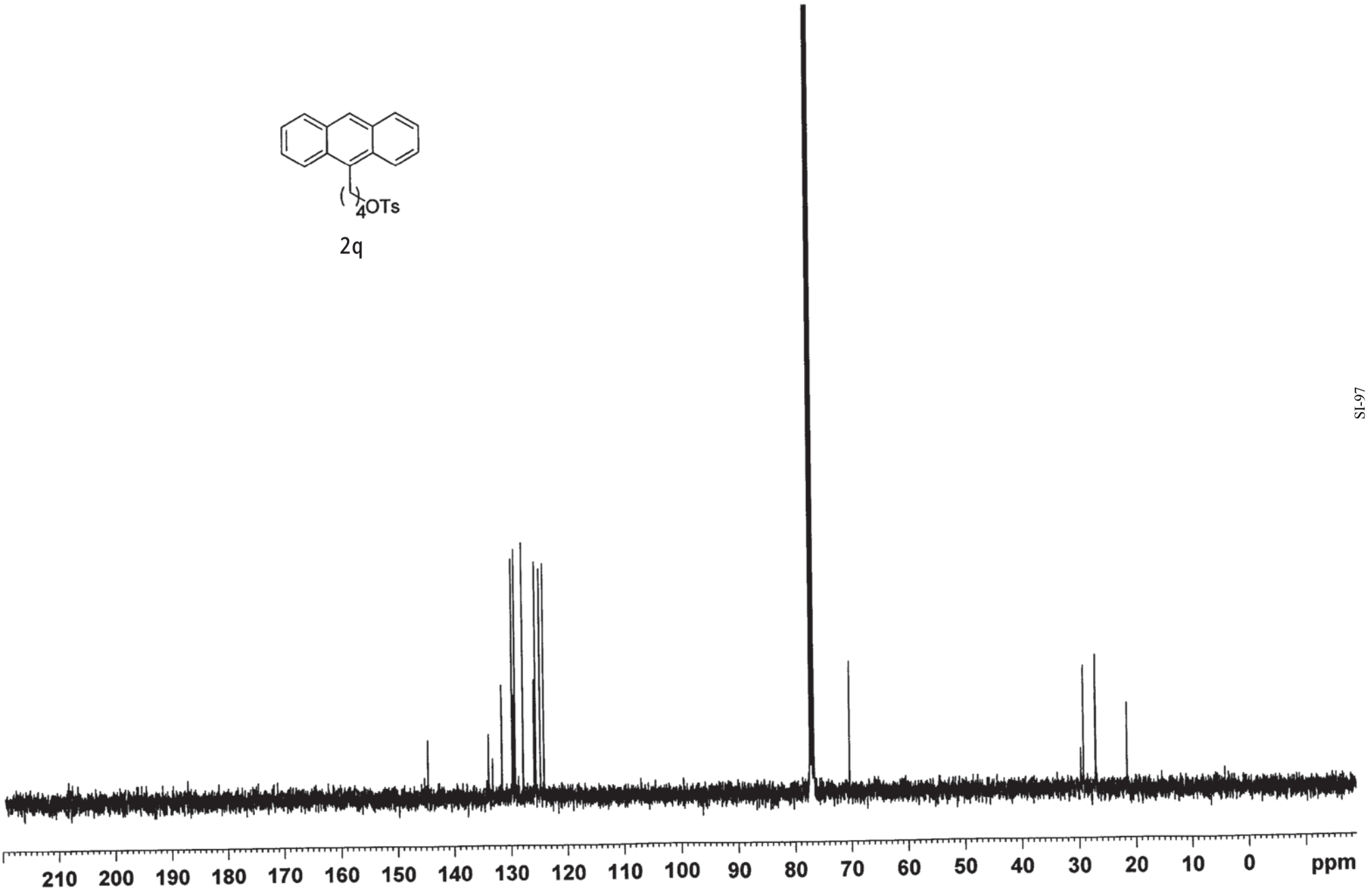
2p

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OTs
4
2q
0.89
1.86
1.84
1.87
3.87
2.73
2.00
1.93
3.02
3.97
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

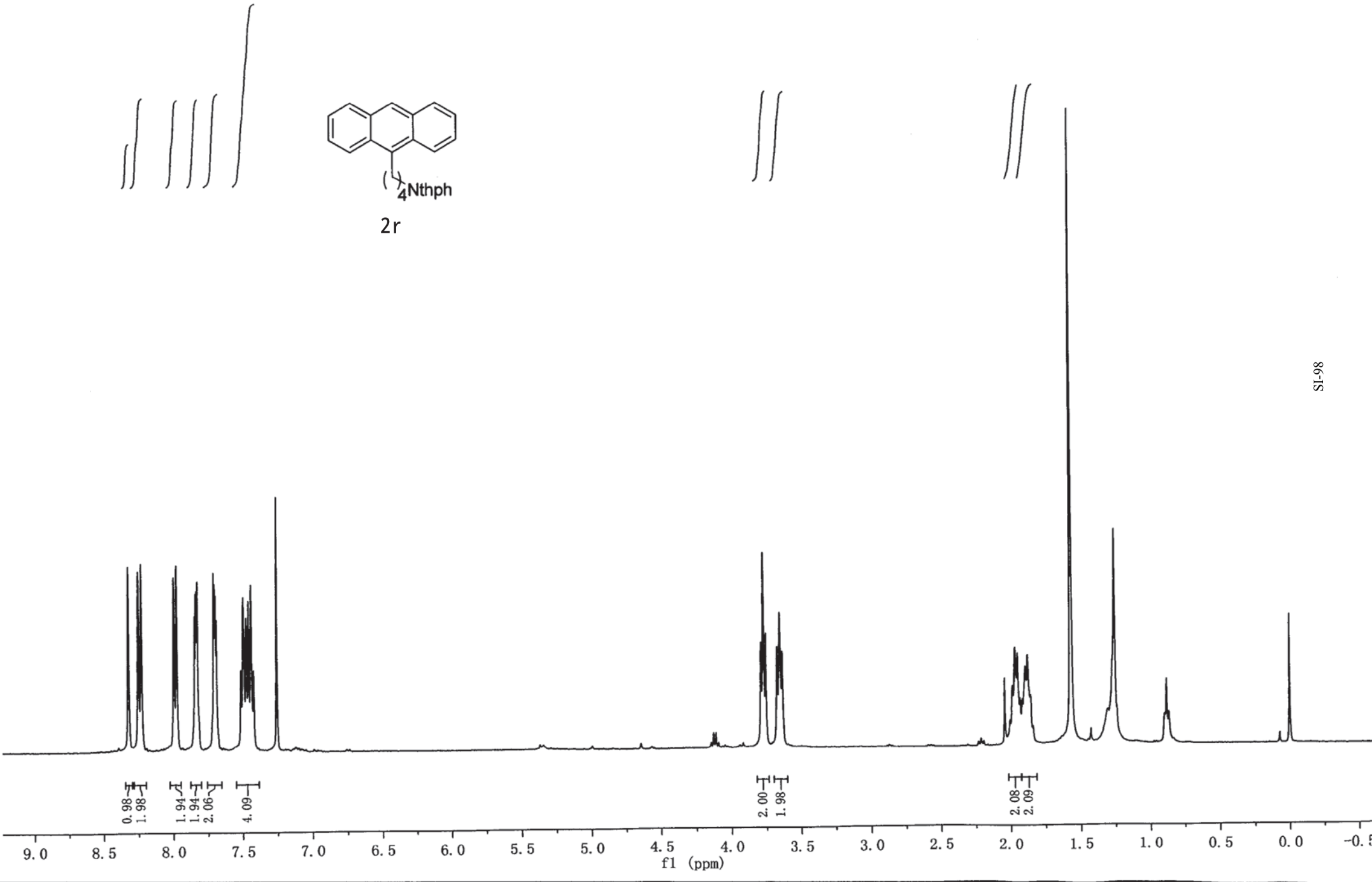
4
OTs

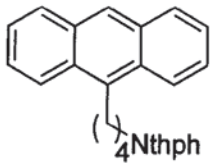
2q


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

4Nthph

2r

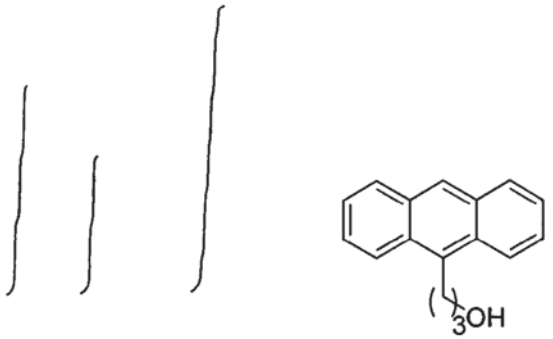

0.98
1.98
1.94
1.94
2.06
4.09
2.00
1.98
2.08
2.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



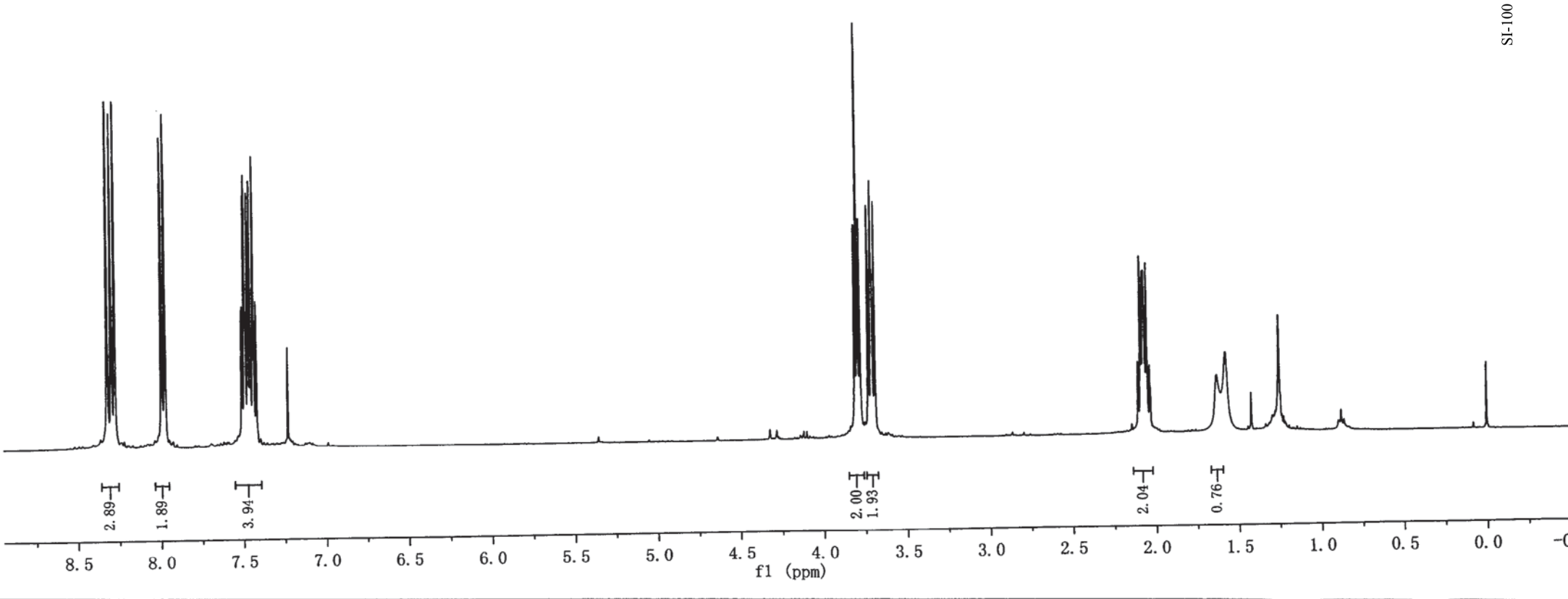
2r

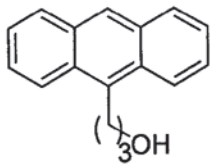
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10

f1 (ppm)

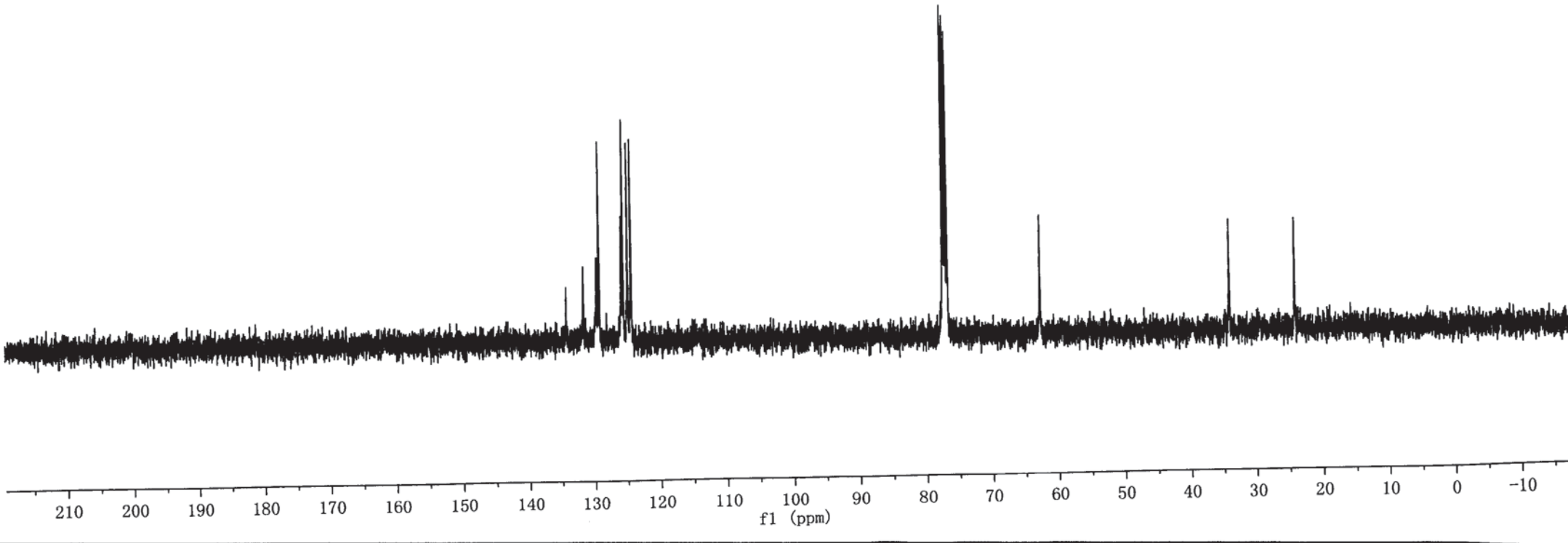

3OH

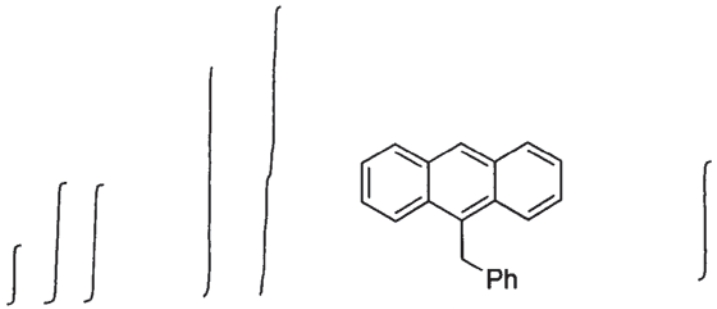
2s


SI-100
2.89
1.89
3.94
2.00
1.93
2.04
0.76
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

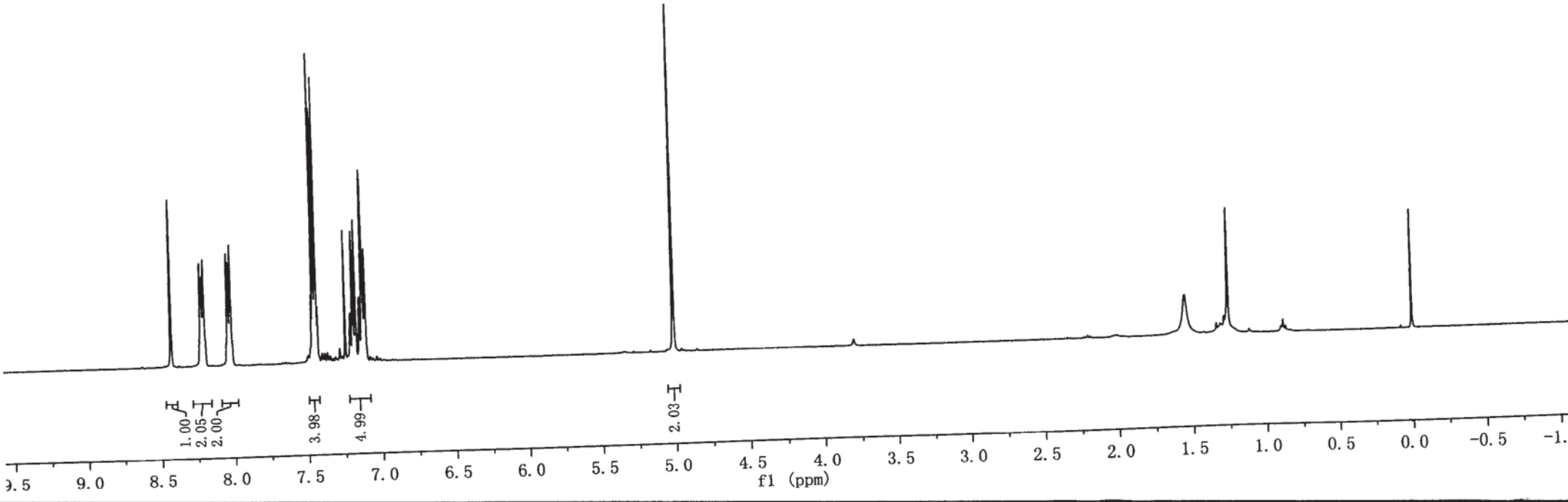

OH

2s


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

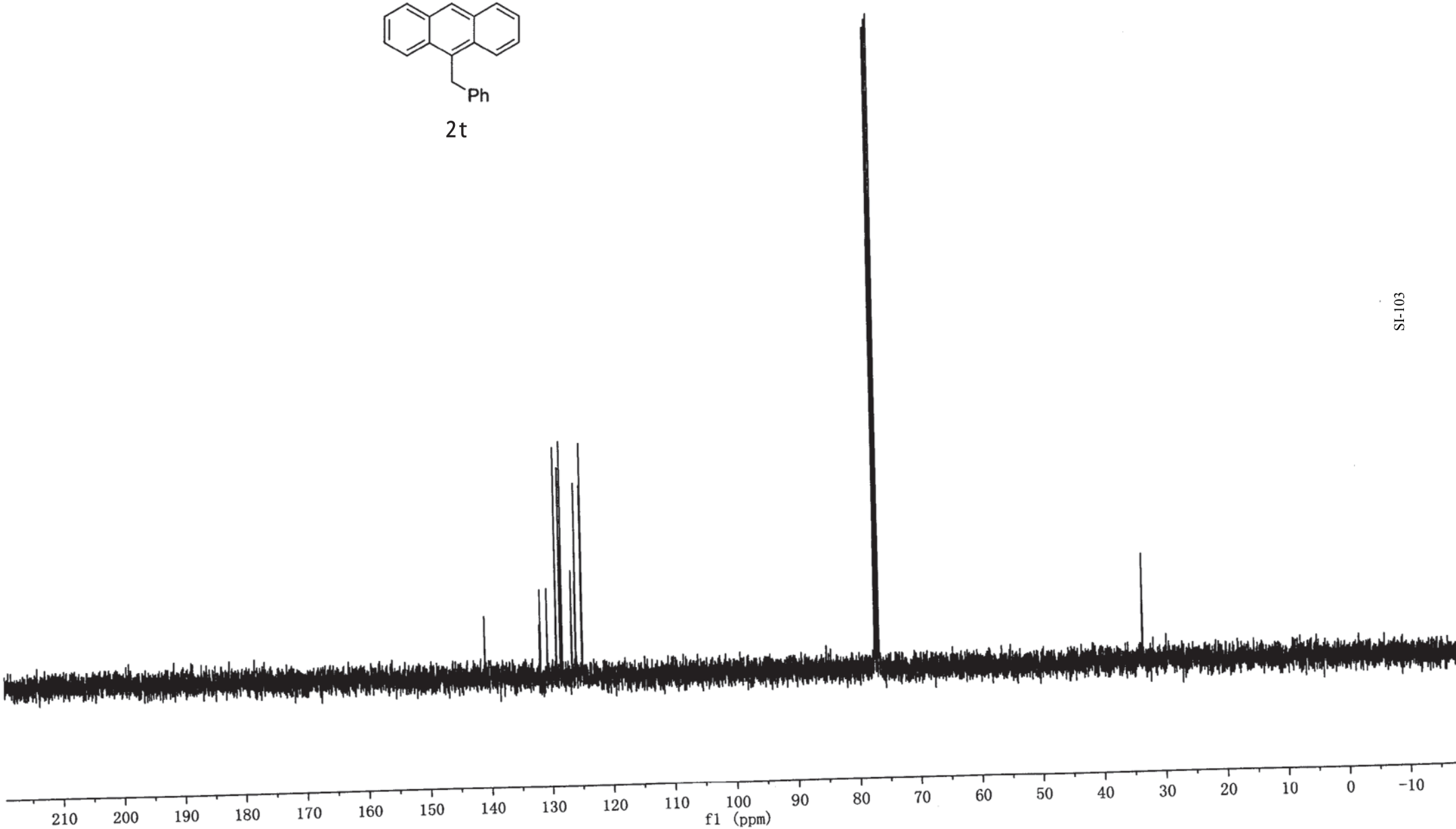

Ph

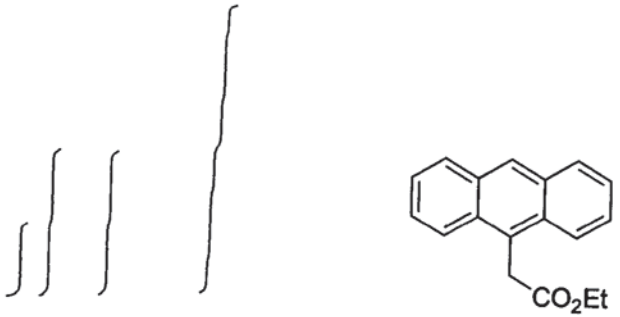
2t


1.00
2.05
2.00
3.98
4.99
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

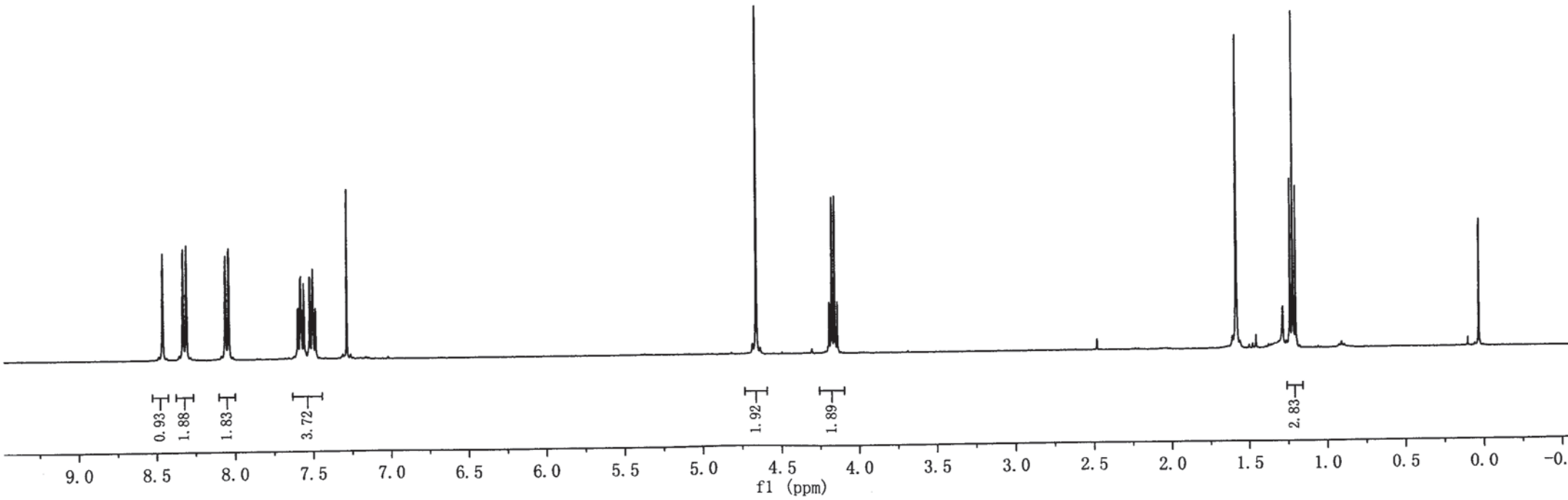
Ph

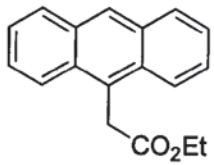
2t


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CO2Et

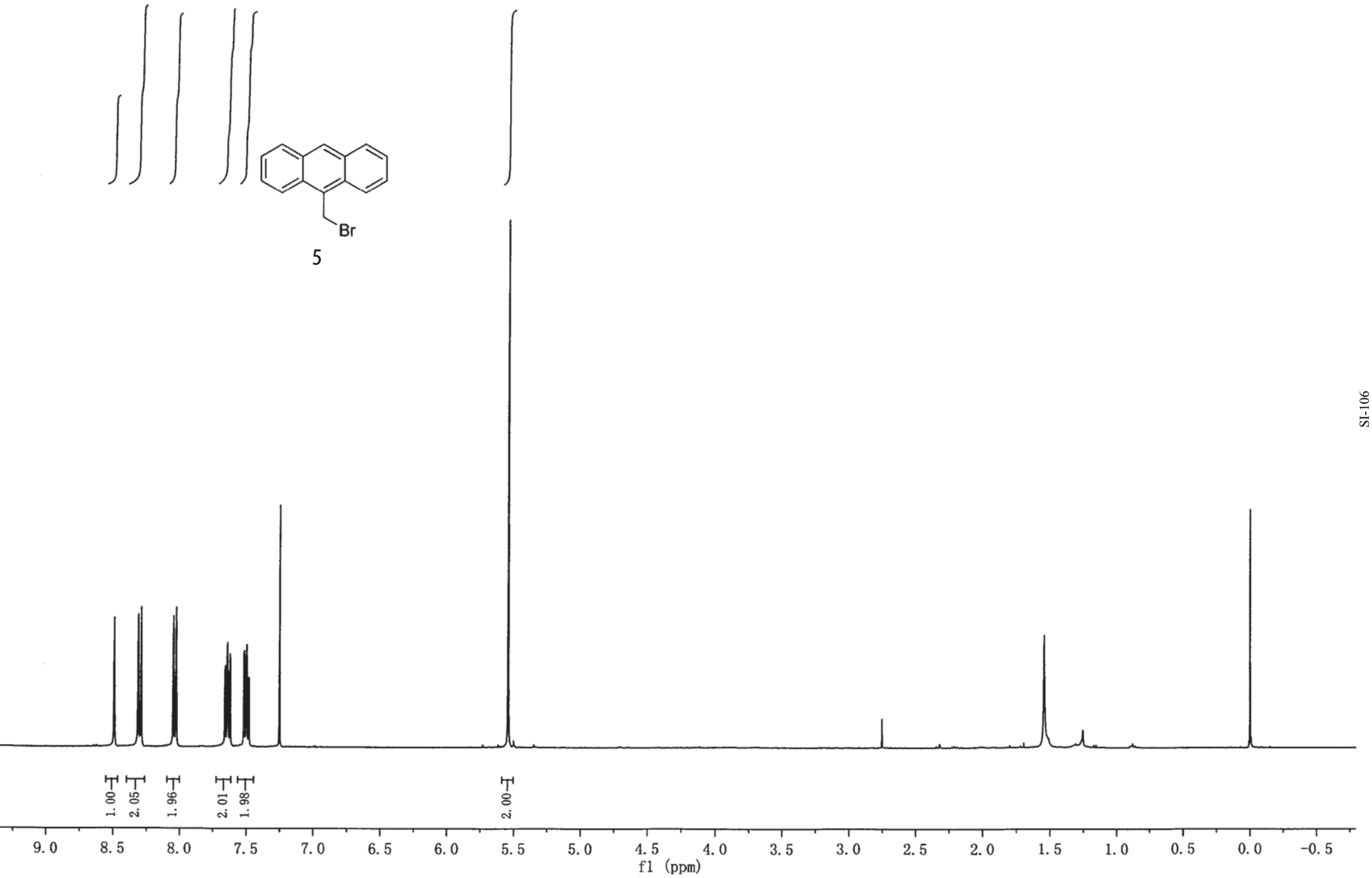
2u

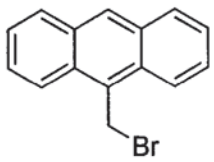

0.93
1.88
1.83
3.72
1.92
1.89
2.83
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CO2Et

2u

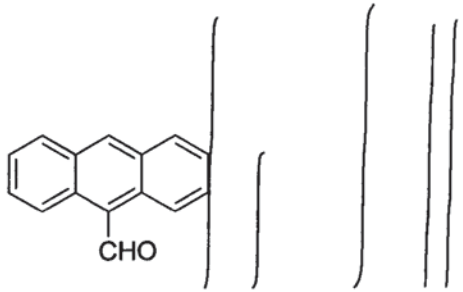
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Br
5
1.00
2.05
1.96
2.01
1.98
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



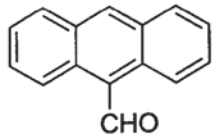
5

f1 (ppm)


CHO

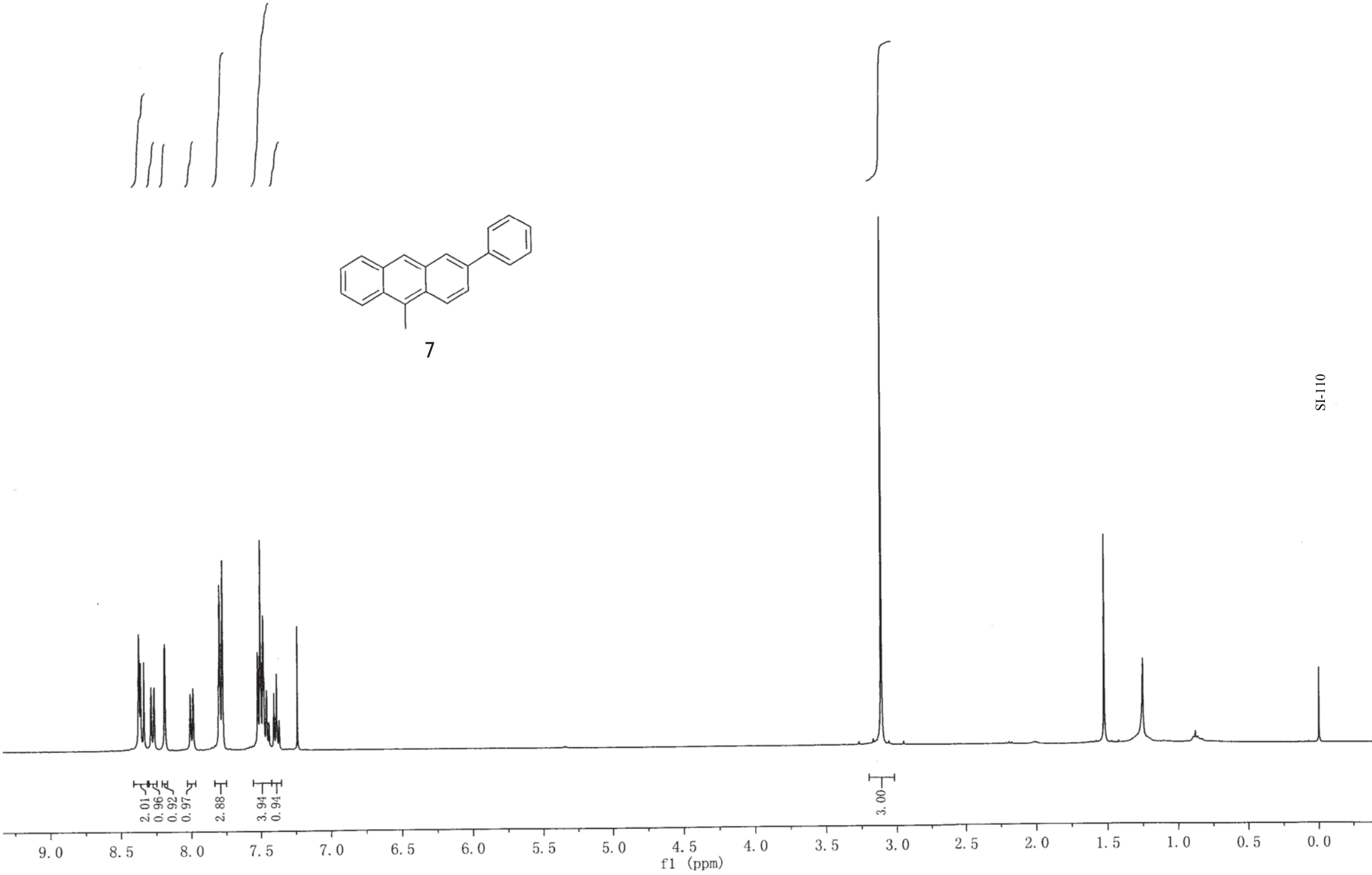
6

1.03
2.02
1.00
2.11
1.96
2.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

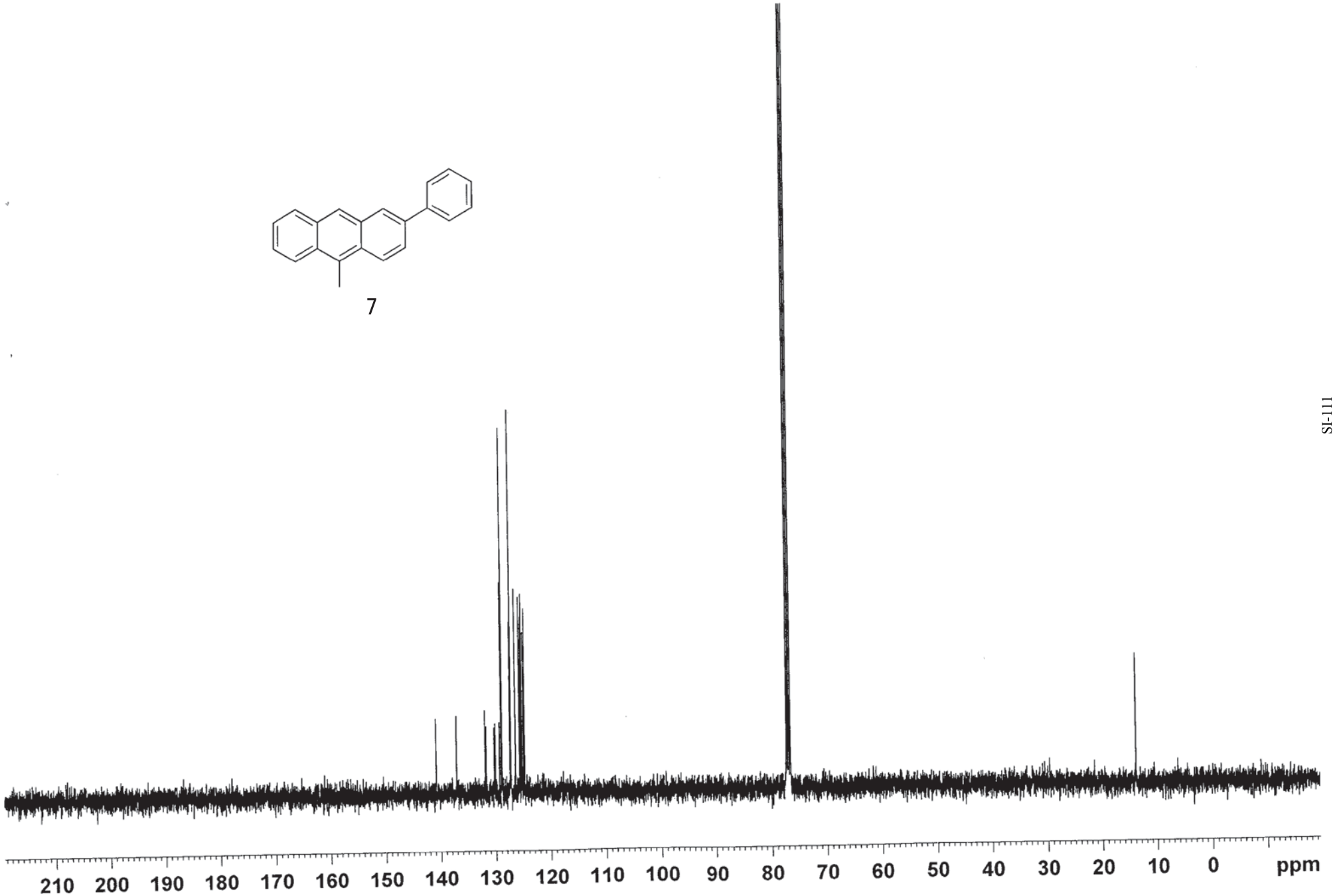

CHO

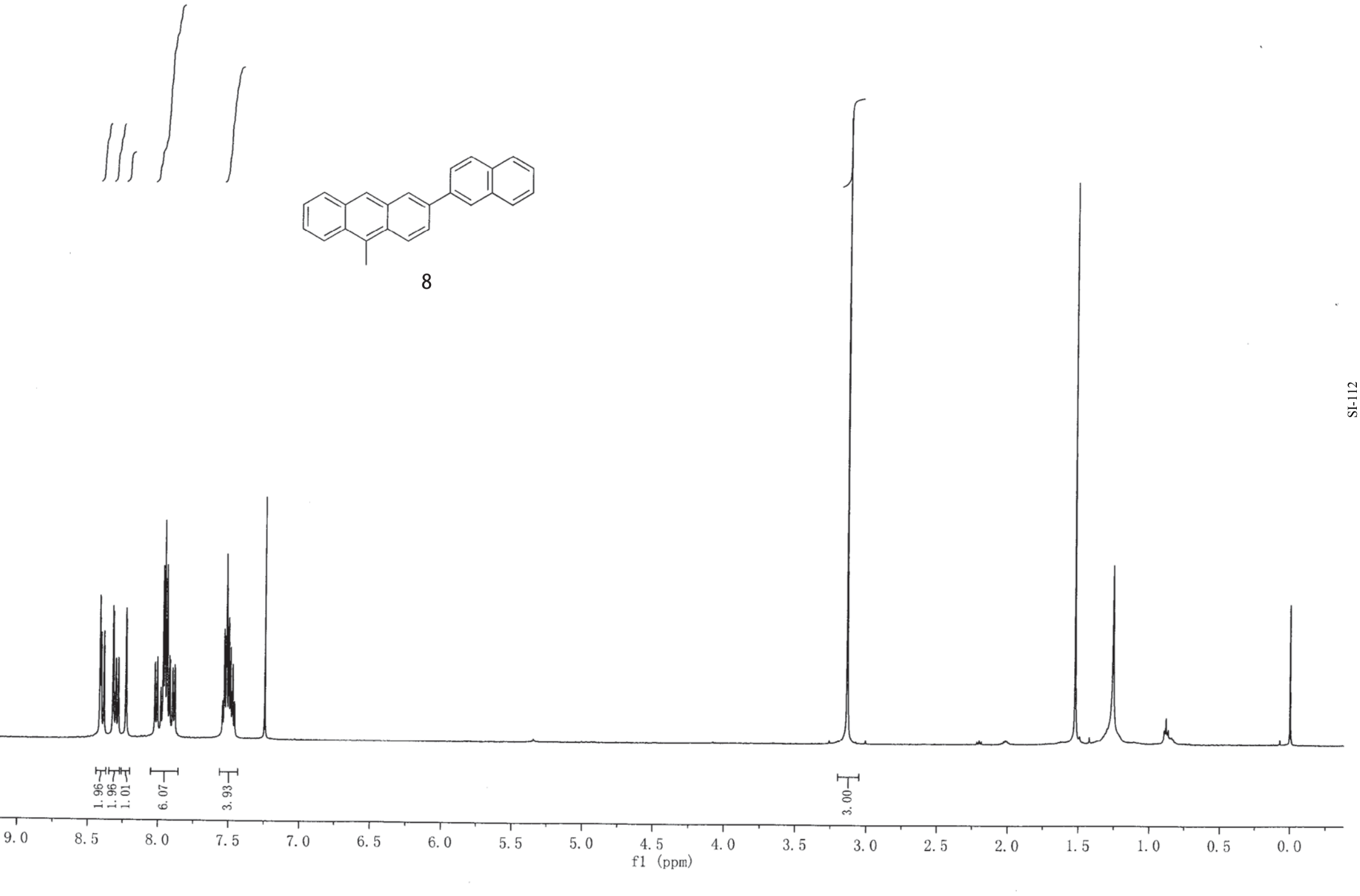
6

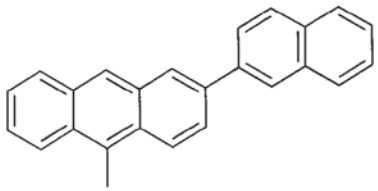
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7
SI-110
2.01
0.96
0.92
0.97
2.88
3.94
0.94
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

7


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8
1.96
1.96
1.01
6.07
3.93
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
SI-112



8

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm