Supporting Information

Facile synthesis of 2-iodo-spiro[indene-1,1'-isobenzofuran]-3'-ones *via* an iodine-promoted cascade cyclization

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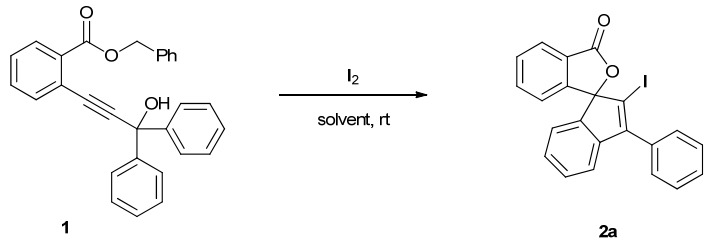
General Remarks

Column chromatography was carried out on silica gel. ^{1}H NMR spectra were recorded on 300/400 MHz in $CDCl_3$ and ^{13}C NMR spectra were recorded on 75/100 MHz in $CDCl_3$. IR spectra were recorded on a FT-IR spectrometer and only major peaks are reported in cm^{-1}. All compounds were further characterized by high resolution mass spectra (HRMS); copies of their ^{1}H NMR and ^{13}C NMR spectra are provided in the Supporting Information. Room temperature is 23–25°C. THF were distilled over Na/benzophenone, 1,2-dichloroethane, dichloromethane, CH_3CN, CH_3NO_2 and DMF were distilled over CaH_2, other solvents were used without further purification.

Table S1 Optimization of reaction conditions for the formation of **2a**[a]

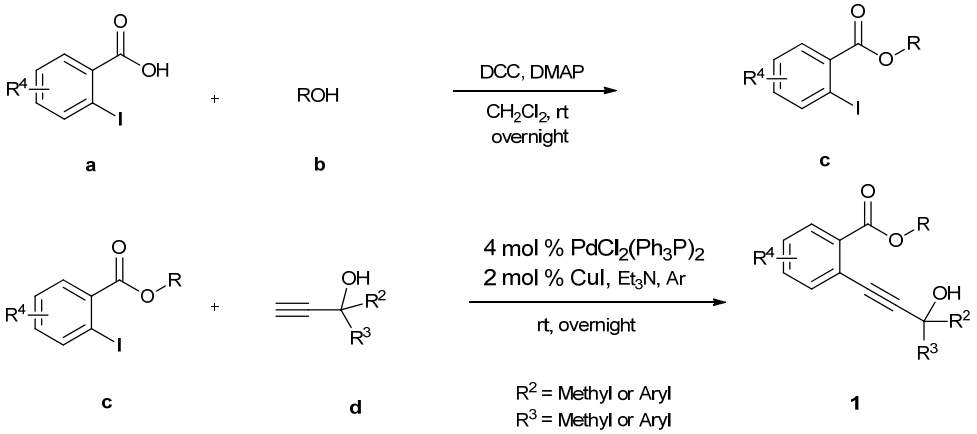


1 **2a**

Entry	Solvent	I_2 (equiv.)	Temperature (°C)	Yield[b] (%) / **2a**
1	$ClCH_2CH_2Cl$	1.5	rt	81
2	**$ClCH_2CH_2Cl$**	**2.0**	**rt**	**88**
3	$ClCH_2CH_2Cl$	3.0	rt	87
4	$ClCH_2CH_2Cl$	2.0	80	80
5	$ClCH_2CH_2Cl$	2.0	0	67
6	CH_2Cl_2	2.0	rt	78
7	CH_3CN	2.0	rt	81
8	CH_3NO_2	2.0	rt	28

[a] All reactions were run under the following conditions, unless otherwise indicated: 0.2 mmol of **1** with I_2 in 4 mL anhydrous solvent at room temperature. [b] Isolated yield.

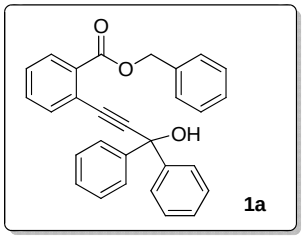
General Procedure A: Synthesis of 2-(3-hydroxy-3,3-diarylprop-1-yn-1-yl)benzoate derivatives



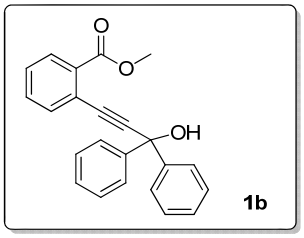
To a stirred solution of 2-iodobenzoic acids **a** (10 mmol) in CH_2Cl_2, was added DCC (dicyclohexylcarbodiimide, 11 mmol), DMAP (Dimethylaminopyridine, 2 mmol) and alcohols **b** in sequence. The resulting solution was stirred overnight at room temperature then filtered through a sand core funnel and washed with diethyl ether (2 x 40mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography to obtain the pure product **c** in moderate to good yields.

To a soluton of 2-iodobenzoates **c** in Et_3N (5 mL) was added $PdCl_2(PPh_3)_2$ (4 mol %) and CuI (2 mol %) and the reaction vial was flushed with Ar and the reaction mixture was stirred for 5 minutes. A solution of aryl propargyl alcohols **d** in Et_3N (5 mL) were then added dropwise through a syringe for 5 minutes. The resulting solution was stirred at room temperature overnight. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched by addition of saturated aqueous ammonium chloride (10 mL) and extracted with ethyl ether (3 x 40 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography to give **1**.

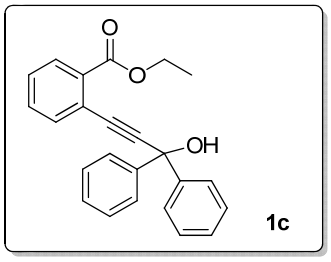
Characterization Data of 1a-1zc



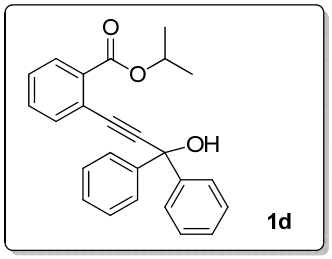
Benzyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1a** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.97 (d, *J* = 0.8 Hz, 1H), 7.96-7.66 (m, 4H), 7.56 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.42 (td, *J* = 7.2, 1.2 Hz, 1H), 7.36-7.22 (m, 12H), 5.25 (s, 2H), 3.29 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 144.9, 135.7, 134.1, 131.8, 131.7, 130.5, 128.5, 128.3, 128.2, 128.1, 127.5, 126.1, 123.1, 96.9, 85.7, 74.8, 66.9. IR (neat, cm^{-1}): 3426, 3061, 1715, 1251, 755, 698. HRMS (ESI) Calcd for $C_{29}H_{23}O_3$: M+H = 419.1642. Found: 419.1648.



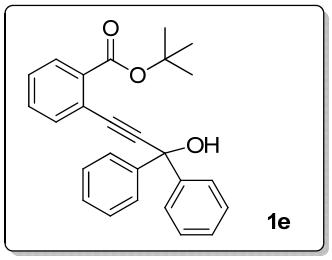
Methyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1b** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.92 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.70 (dd, *J* = 3.2, 1.2 Hz, 4H), 7.56 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.36-7.26 (m, 5H), 7.24-7.22 (m, 2H), 3.75 (s, 3H), 3.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.6, 145.1, 134.0, 131.9, 131.6, 130.4, 128.1, 127.6, 126.1, 122.9, 96.8, 85.7, 74.9, 52.1. IR (neat, cm^{-1}): 3426, 3061, 1718, 1285, 756, 699. HRMS (ESI) Calcd for $C_{23}H_{19}O_3$: M+H = 343.1329. Found: 343.1335.



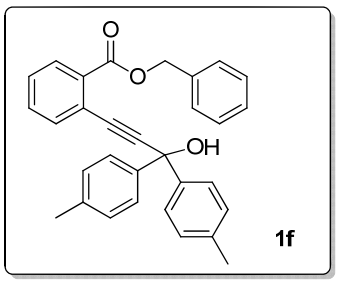
Ethyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1c** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.93 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 4H), 7.57 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.43 (td, *J* = 7.6, 1.2 Hz, 1H), 7.38-7.26 (m, 5H), 7.25-7.22 (m, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.55 (s, 1H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.1, 145.0, 134.0, 132.3, 131.5, 130.2, 128.2, 127.5, 126.1, 122.8, 96.7, 85.8, 74.9, 61.3, 14.1. IR (neat, cm^{-1}): 3423, 3062, 1713, 1283, 756, 699. HRMS (ESI) Calcd for $C_{24}H_{21}O_3$: M+H = 357.1485. Found: 357.1484.



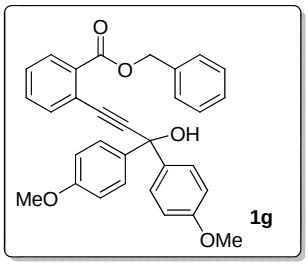
Isopropyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1d** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.89 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 4H), 7.55 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.40 (td, *J* = 7.6, 1.2 Hz, 1H), 7.35-7.26 (m, 5H), 7.24-7.21 (m, 2H), 3.52 (s, 1H), 1.51 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.5, 145.1, 134.1, 132.6, 131.3, 130.1, 128.1, 128.0, 127.4, 126.1, 122.8, 96.8, 85.7, 74.9, 68.9, 21.7. IR (neat, cm^{-1}): 3417, 2982, 1702, 1485, 1290, 758. HRMS (ESI) Calcd for $C_{25}H_{23}O_3$: M+H = 371.1642. Found: 371.1643.



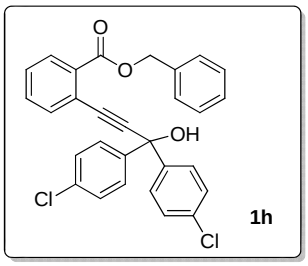
tert-Butyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1e** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.81 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.73 (q, *J* = 1.6 Hz, 4H), 7.55 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.39 (td, *J* = 7.6, 1.2 Hz, 1H), 7.35-7.29 (m, 5H), 7.25-7.22 (m, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 3.55 (s, 1H), 1.25 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.5, 145.1, 134.2, 133.9, 130.9, 129.9, 128.1, 128.0, 127.5, 126.2, 122.4, 96.3, 85.8, 81.7, 74.9, 28.0. IR (neat, cm^{-1}): 3421, 2976, 1708, 1307, 1136, 758, 700. HRMS (ESI) Calcd for $C_{26}H_{25}O_3$: M+H = 385.1798. Found: 385.1799.



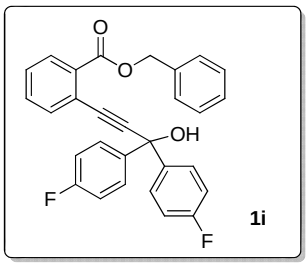
Benzyl-2-(3-hydroxy-3,3-di-*p*-tolylprop-1-yn-1-yl)benzoate **1f** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.95 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.57-7.53 (m, 5H), 7.41 (td, *J* = 7.2, 1.2 Hz, 1H), 7.35-7.31 (m, 3H), 7.30-7.28 (m, 3H), 7.10 (d, *J* = 8.0 Hz, 4H), 5.26 (s, 2H), 3.08 (s, 1H), 2.30 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 142.3, 137.1, 135.8, 134.1, 131.8, 131.7, 130.5, 128.8, 128.5, 128.3, 128.2, 128.0, 126.0, 123.2, 97.3, 85.4, 74.6, 66.8, 21.0. IR (neat, cm^{-1}): 3433, 2922, 1716, 1250, 1079, 756. HRMS (ESI) Calcd for $C_{31}H_{27}O_3$: M+H = 447.1955. Found: 447.1959.



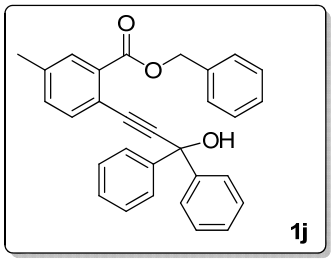
Benzyl-2-(3-hydroxy-3,3-bis(4-methoxyphenyl)prop-1-yn-1-yl)benzoate **1g** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.96 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.58-7.55 (m, 5H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.36-7.23 (m, 6H), 6.82 (d, *J* = 8.6 Hz, 4H), 5.28 (s, 2H), 3.76 (s, 6H), 3.15 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 158.9, 137.5, 135.8, 134.1, 132.2, 131.7, 130.5, 128.5, 128.2, 128.1, 128.0, 127.5, 123.2, 113.4, 97.3, 85.3, 74.2, 66.8, 55.2. IR (neat, cm^{-1}): 3438, 2955, 1719, 1507, 1250, 833. HRMS (ESI) Calcd for $C_{31}H_{27}O_5$: M+H = 479.1853. Found: 479.1855.



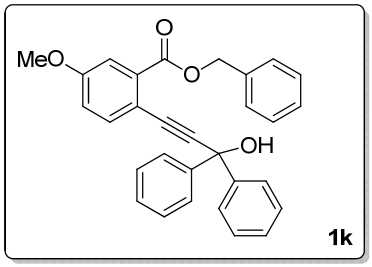
Benzyl-2-(3,3-bis(4-chlorophenyl)-3-hydroxyprop-1-yn-1-yl)benzoate **1h** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.98 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.58-7.53 (m, 4H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.43 (td, *J* = 7.6, 1.2 Hz, 1H), 7.37 (d, *J* = 0.8 Hz, 1H), 7.36-7.29 (m, 5H), 7.23 (d, *J* = 5.6 Hz, 4H), 5.24 (s, 2H), 3.73 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.5, 143.2, 135.6, 134.2, 133.6, 131.9, 131.5, 130.6, 128.6, 128.5, 128.4, 128.3, 128.2, 127.6, 122.8, 95.8, 86.2, 73.9, 66.9. IR (neat, cm^{-1}): 3412, 3065, 1717, 1486, 1273, 752. HRMS (ESI) Calcd for $C_{29}H_{21}Cl_2O_3$: M+H = 487.0862. Found: 487.0860.



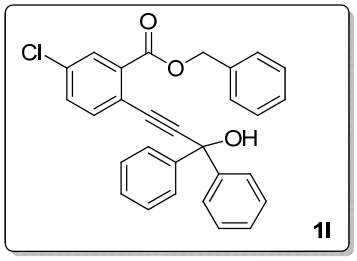
Benzyl-2-(3,3-bis(4-fluorophenyl)-3-hydroxyprop-1-yn-1-yl)benzoate **1i** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.97 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.63-7.59 (m, 4H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.42 (td, *J* = 7.6, 1.2 Hz, 1H), 7.36-7.28 (m, 6H), 6.98-6.94 (m, 4H), 5.24 (s, 2H), 3.77 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.6, 163.4, 160.9, 140.8, 140.7, 135.6, 134.2, 131.9, 131.5, 130.6, 128.5, 128.3, 128.2, 128.1, 128.0, 127.9, 122.9, 115.1, 114.8, 96.4, 85.9, 73.9, 66.9. IR (neat, cm^{-1}): 3416, 3067, 1716, 1504, 1252, 837. HRMS (ESI) Calcd for $C_{29}H_{21}F_2O_3$: M+H = 455.1453. Found: 455.1460.



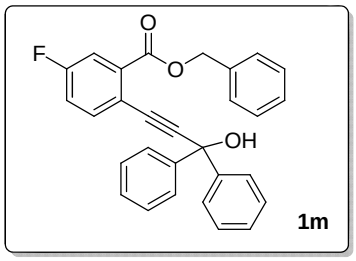
Benzyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)-5-methylbenzoate **1j** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.76 (dd, *J* = 0.8 Hz, 1H), 7.67 (q, *J* = 1.6 Hz, 4H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.33-7.21 (m, 12H), 5.24 (s, 2H), 3.22 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.1, 145.1, 138.5, 135.8, 134.0, 132.5, 131.6, 131.0, 128.5, 128.3, 128.2, 128.1, 127.5, 126.2, 120.1, 96.0, 85.8, 74.8, 66.8, 21.2. IR (neat, cm^{-1}): 3428, 3060, 1715, 1201, 748, 698. HRMS (ESI) Calcd for $C_{30}H_{25}O_3$: M+H = 433.1798. Found: 433.1801.



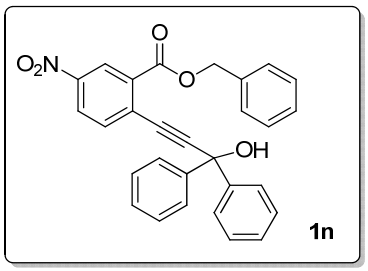
Benzyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)-5-methoxybenzoate **1k** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.57 (d, *J* = 7.6 Hz, 4H), 7.44-7.32 (m, 2H), 7.23-7.12 (m, 11H), 6.87 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.14 (s, 2H), 3.69 (s, 3H), 3.12 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 159.2, 145.2, 135.7, 135.5, 133.2, 128.5, 128.3, 128.2, 128.1, 127.5, 126.1, 126.0, 118.0, 115.3, 115.1, 95.1, 85.6, 74.8, 66.9, 55.5. IR (neat, cm^{-1}): 3433, 1751, 1603, 1495, 1221, 699. HRMS (ESI) Calcd for $C_{30}H_{25}O_4$: M+H = 449.1747. Found: 449.1748.



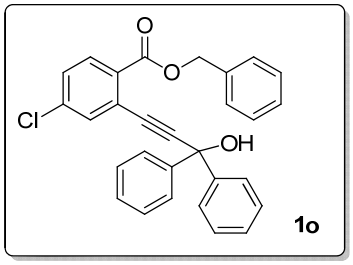
Benzyl-5-chloro-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1l** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.92 (d, *J* = 3.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 4H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.36 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.32-7.21 (m, 11H), 5.22 (s, 2H), 3.43 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 164.6, 144.8, 135.4, 135.3, 134.2, 133.0, 131.9, 130.5, 128.6, 128.4, 128.3, 128.2, 127.6, 126.1, 121.6, 97.9, 84.6, 74.8, 67.3. IR (neat, cm^{-1}): 3435, 1720, 1483, 1289, 1238, 698. HRMS (ESI) Calcd for $C_{29}H_{22}ClO_3$: M+H = 453.1252. Found: 453.1252.



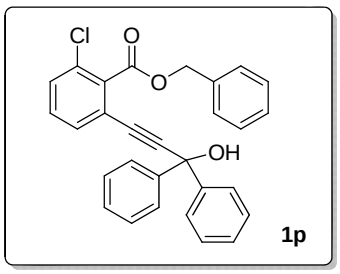
Benzyl-5-fluoro-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1m** Solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 7.65-7.61 (m, 5H), 7.50 (dd, *J* = 5.4, 2.4 Hz, 1H), 7.30-7.18 (m, 11H), 7.13-7.07 (m, 1H), 5.25 (s, 2H), 3.26 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm 164.6, 163.4, 160.0, 144.9, 136.1, 136.0, 135.4, 133.8, 133.7, 128.4, 128.2, 127.6, 126.1, 119.4, 119.3, 119.2, 119.1, 117.8, 117.4, 96.7, 84.7, 74.8, 67.2. IR (neat, cm^{-1}): 3436, 3062, 1720, 1491, 1192, 699. HRMS (ESI) Calcd for $C_{29}H_{22}FO_3$: M+H = 437.1547. Found: 437.1550.



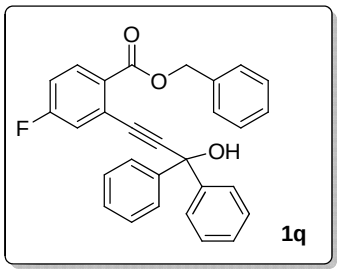
Benzyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)-5-nitrobenzoate **1n** Solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 8.69-8.68 (m, 1H), 8.12 (dd, *J* = 8.7, 2.7 Hz, 1H), 7.57-7.54 (m, 5H), 7.25-7.12 (m, 11H), 5.19 (s, 2H), 3.40 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm 163.8, 146.6, 144.2, 135.2, 134.9, 132.8, 129.5, 128.7, 128.6, 128.5, 128.3, 127.9, 127.8, 126.0, 125.9, 125.6, 102.8, 84.1, 74.9, 67.7. IR (neat, cm^{-1}): 3438, 1725, 1523, 1347, 1267, 752. HRMS (ESI) Calcd for $C_{29}H_{22}NO_5$: M+H = 464.1492. Found: 464.1498.



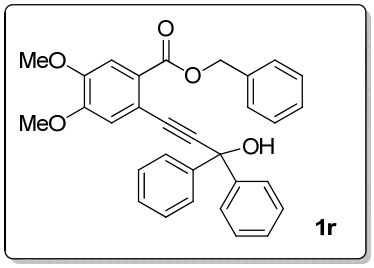
Benzyl-4-chloro-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1o** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.88 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 4H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.32-7.20 (m, 12H), 5.21 (s, 2H), 3.52 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 164.9, 144.7, 138.1, 135.5, 133.8, 131.9, 129.9, 128.5, 128.4, 128.3, 128.2, 127.6, 126.1, 124.9, 98.4, 84.5, 74.8, 67.1. IR (neat, cm^{-1}): 3428, 1718, 1273, 1103, 753, 698. HRMS (ESI) Calcd for $C_{29}H_{22}ClO_3$: M+H = 453.1252. Found: 453.1254.



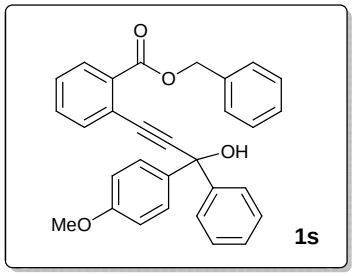
Benzyl-2-chloro-6-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1p** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.59-7.57 (m, 4H), 7.37 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.33-7.20 (m, 13H), 5.17 (s, 2H), 2.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 144.4, 136.0, 134.9, 130.9, 130.5, 130.2, 129.7, 128.4, 128.3, 128.2, 127.8, 126.0, 121.8, 96.4, 83.1, 74.7, 67.7. IR (neat, cm^{-1}): 3448, 1731, 1450, 1272, 1113, 698. HRMS (ESI) Calcd for $C_{29}H_{22}ClO_3$: M+H = 453.1252. Found: 453.1249.



Benzyl-4-fluoro-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)benzoate **1q** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.98 (dd, *J* = 8.8, 6.0 Hz, 1H), 7.66-7.64 (m, 4H), 7.32-7.21 (m, 12H), 7.04-6.99 (m, 1H), 5.22 (s, 2H), 3.45 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.5, 164.8, 162.9, 144.7, 135.6, 133.2, 133.1, 128.5, 128.4, 128.3, 128.2, 127.9, 127.8, 127.6, 126.1, 125.9, 125.8, 120.9, 120.7, 115.7, 115.5, 98.3, 84.6, 74.8, 66.9. IR (neat, cm^{-1}): 3428, 1718, 1256, 1125, 743, 698. HRMS (ESI) Calcd for $C_{29}H_{22}FO_3$: M+H = 437.1547. Found: 437.1548.

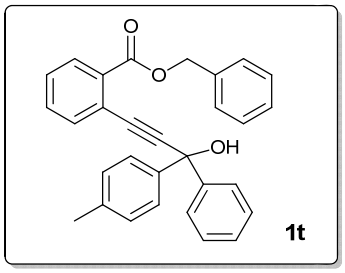


Benzyl-2-(3-hydroxy-3,3-diphenylprop-1-yn-1-yl)-4,5-dimethoxybenzoate **1r** Solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 7.60-7.57 (m, 4H), 7.37 (s, 1H), 7.22-7.10 (m, 11H), 6.85 (s, 1H), 5.13 (s, 2H), 3.76 (s, 3H), 3.71 (s, 3H), 3.39 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm 165.5, 151.5, 148.6, 145.1, 135.9, 128.4, 128.2, 128.1, 127.4, 126.1, 124.3, 116.8, 115.8, 112.8, 95.5, 85.8, 74.8, 66.6, 56.0, 55.9. IR (neat, cm^{-1}): 3425, 2937, 1708, 1517, 1165, 700. HRMS (ESI) Calcd for $C_{31}H_{27}O_5$: M+H = 479.1853. Found: 479.1857.



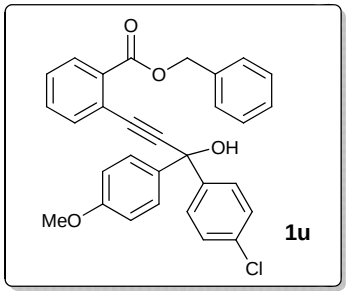
1s

Benzyl-2-(3-hydroxy-3-(4-methoxyphenyl)-3-phenylprop-1-yn-1-yl)benzoate **1s** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.95 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 2H), 7.59-7.53 (m, 3H), 7.39 (td, *J* = 7.6, 1.2 Hz, 1H), 7.33-7.28 (m, 8H), 7.26-7.20 (m, 1H), 6.81 (d, *J* = 6.8 Hz, 2H), 5.25 (s, 2H), 3.73 (s, 3H), 3.44 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 158.9, 145.2, 137.3, 135.7, 134.1, 131.7, 131.6, 130.5, 128.5, 128.2, 128.1, 128.0, 127.5, 127.4, 126.1, 123.1, 113.4, 97.2, 85.5, 74.5, 66.8, 55.2. HRMS (ESI) Calcd for $C_{30}H_{25}O_4$: M+H = 449.1747. Found: 449.1752.



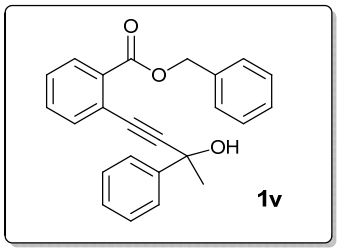
1t

Benzyl-2-(3-hydroxy-3-phenyl-3-(*p*-tolyl)prop-1-yn-1-yl)benzoate **1t** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.94 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.55 (d, *J* = 8.4 Hz, 3H), 7.40 (td, *J* = 7.6, 1.2 Hz, 1H), 7.33-7.19 (m, 9H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.24 (s, 2H), 3.42 (s, 1H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 145.1, 142.2, 137.2, 135.8, 134.1, 131.7, 130.5, 128.8, 128.5, 128.3, 128.2, 128.1, 128.0, 127.4, 126.2, 126.1, 123.2, 97.2, 85.5, 74.7, 66.8, 21.0. HRMS (ESI) Calcd for $C_{30}H_{25}O_3$: M+H = 433.1798. Found: 433.1794.

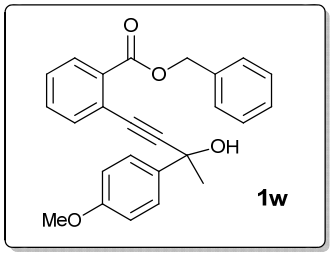


1u

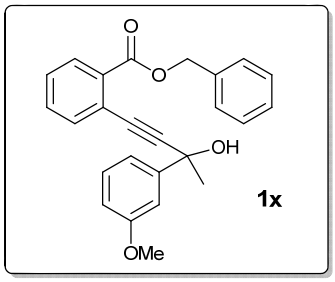
Benzyl-2-(3-(4-chlorophenyl)-3-hydroxy-3-(4-methoxyphenyl)prop-1-yn-1-yl)benzoa te **1u** Solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 7.90 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.52-7.45 (m, 5H), 7.40-7.30 (m, 1H), 7.26-7.15 (m, 8H), 6.74 (dd, *J* = 6.9, 2.1 Hz, 2H), 5.19 (s, 2H), 3.68 (s, 3H), 3.31 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm 165.7, 159.1, 143.8, 136.9, 135.7, 134.1, 133.2, 131.8, 131.6, 130.5, 128.5, 128.2, 127.6, 127.5, 122.9, 113.5, 96.6, 85.8, 74.1, 66.9, 55.2. HRMS (ESI) Calcd for $C_{30}H_{24}ClO_4$: M+H = 483.1385. Found: 483.1386.



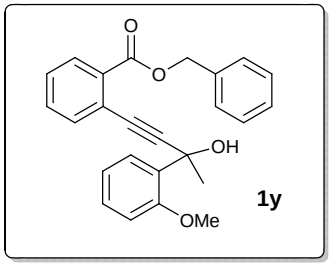
Benzyl-2-(3-hydroxy-3-phenylbut-1-yn-1-yl)benzoate **1v** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.94 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.72 (d, *J* = 7.2 Hz, 2H), 7.53 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.40 (td, *J* = 7.6, 1.2 Hz, 1H), 7.35-7.20 (m, 9H), 5.26 (s, 2H), 3.28 (s, 1H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 145.6, 135.7, 134.1, 131.7, 131.6, 130.5, 128.5, 128.3, 128.2, 128.1, 127.9, 127.5, 125.1, 123.2, 97.8, 83.4, 70.2, 66.8, 33.0. HRMS (ESI) Calcd for $C_{24}H_{21}O_3$: M+H = 357.1485. Found: 357.1488.



Benzyl-2-(3-hydroxy-3-(4-methoxyphenyl)but-1-yn-1-yl)benzoate **1w** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.94 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 (td, *J* = 7.6, 0.8 Hz, 1H), 7.36-7.22 (m, 6H), 6.85 (d, *J* = 8.8 Hz, 2H), 5.27 (s, 2H), 3.76 (s, 3H), 3.21 (s, 1H), 1.79(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 158.9, 137.8, 135.7, 134.1, 131.7, 131.6, 130.4, 128.5, 128.2, 127.9, 126.4, 123.3, 113.4, 98.0, 83.2, 69.8, 66.8, 55.2, 32.9. HRMS (ESI) Calcd for $C_{25}H_{23}O_4$: M+H = 387.1591. Found: 387.1598.

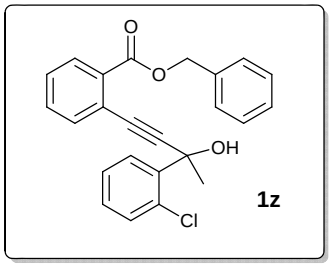


Benzyl-2-(3-hydroxy-3-(3-methoxyphenyl)but-1-yn-1-yl)benzoate **1x** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.95 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.54 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.94 (td, *J* = 7.6, 1.2 Hz, 1H), 7.37-7.29 (m, 8H), 7.28-7.23 (m, 1H), 6.82 (ddd, *J* = 8.0, 2.4, 1.8 Hz, 1H), 5.27 (s, 2H), 3.80 (s, 3H), 3.13 (s, 1H), 1.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 159.5, 147.3, 135.8, 134.1, 131.7, 131.6, 130.5, 129.2, 128.5, 128.2, 127.9, 123.3, 117.5, 113.1, 110.8, 97.7, 83.4, 70.3, 66.8, 55.2, 33.0. HRMS (ESI) Calcd for $C_{25}H_{23}O_4$: M+H = 387.1591. Found: 387.1590.



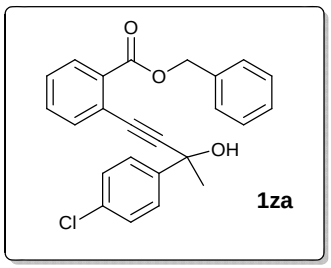
1y

Benzyl-2-(3-hydroxy-3-(2-methoxyphenyl)but-1-yn-1-yl)benzoate **1y** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.92 (d, *J* = 7.6 Hz, 1H), 7.67 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.43-7.39 (m, 3H), 7.35-7.23 (m, 5H), 6.98-6.93 (m, 2H), 5.29 (s, 2H), 4.49 (s, 1H), 3.91 (s, 3H), 1.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 156.8, 135.9, 134.1, 132.4, 132.0, 131.5, 130.3, 128.9, 128.5, 128.2, 128.1, 127.7, 126.6, 123.5, 120.9, 111.6, 97.8, 82.2, 69.7, 66.6, 55.6, 29.6. HRMS (ESI) Calcd for $C_{25}H_{23}O_4$: M+H = 387.1591. Found: 387.1595.



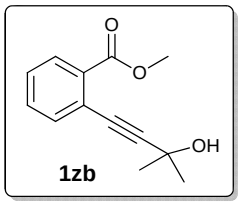
1z

Benzyl-2-(3-(2-chlorophenyl)-3-hydroxybut-1-yn-1-yl)benzoate **1z** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.95 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.86 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.56 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.43 (td, *J* = 7.6, 1.2 Hz, 1H), 7.39-7.30 (m, 7H), 7.29-7.19 (m, 3H), 5.29 (s, 2H), 3.41 (s, 1H), 1.95 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 141.5, 135.8, 133.9, 131.7, 131.6, 131.1, 130.5, 128.8, 128.6, 128.3, 128.2, 127.9, 126.9, 126.8, 123.3, 97.0, 83.2, 69.2, 66.8, 29.4. HRMS (ESI) Calcd for $C_{24}H_{20}ClO_3$: M+H = 391.1095. Found: 391.1096.



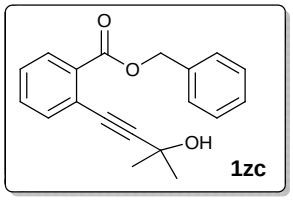
1za

Benzyl-2-(3-(4-chlorophenyl)-3-hydroxybut-1-yn-1-yl)benzoate **1za** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.96 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.65-7.63 (m, 2H), 7.53 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.35-7.23 (m, 8H), 5.27 (s, 2H), 3.41 (s, 1H), 1.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.8, 144.2, 135.7, 134.1, 133.3, 131.8, 131.6, 130.5, 128.5, 128.3, 128.2, 128.1, 126.7, 123.1, 97.3, 83.7, 69.8, 66.9, 33.1. HRMS (ESI) Calcd for $C_{24}H_{20}ClO_3$: M+H = 391.1095. Found: 391.1101.



1zb

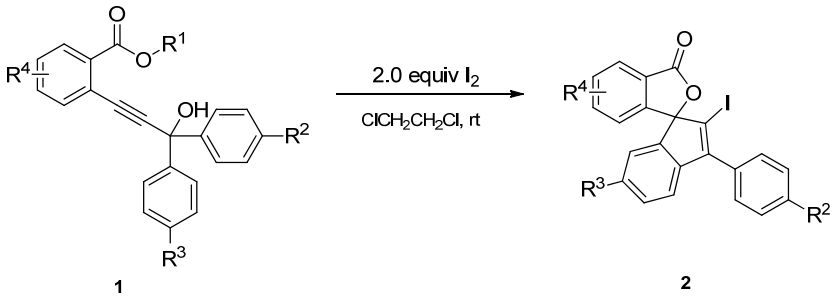
Methyl-2-(3-hydroxy-3-methylbut-1-yn-1-yl)benzoate **1zb** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.49 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.42 (td, *J* = 7.2, 1.2 Hz, 1H), 7.32 (td, *J* = 8.0, 1.2 Hz, 1H), 3.89 (s, 3H), 3.45 (s, 1H), 1.64 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.6, 133.8, 131.8, 131.5, 130.2, 127.7, 123.3, 99.1, 80.6, 65.4, 52.0, 31.2. HRMS (ESI) Calcd for $C_{13}H_{15}O_3$: M+H = 219.1016. Found: 219.1018.



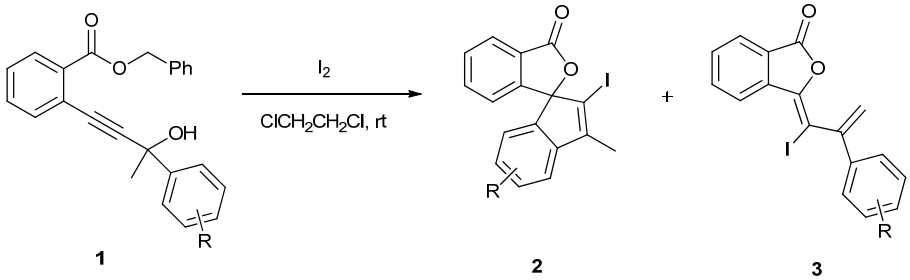
1zc

Benzyl-2-(3-hydroxy-3-methylbut-1-yn-1-yl)benzoate **1zc** Oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.94-7.92 (m, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.43-7.24 (m, 7H), 5.34 (s, 2H), 2.95 (s, 1H), 1.55 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 135.8, 134.0, 131.6, 131.5, 130.4, 128.5, 128.3, 128.2, 127.7, 123.4, 99.2, 80.7, 66.8, 65.3, 31.0. HRMS (ESI) Calcd for $C_{19}H_{19}O_3$: M+H = 295.1329. Found: 295.1333.

General Procedure B: Synthesis of 2-iodo-spiro [indene-1,1'-isobenz-ofuran]-3'-ones and (*E*)-3-(1-iodo-2-allylidene)isobenzofuran-1-ones



1 **2**

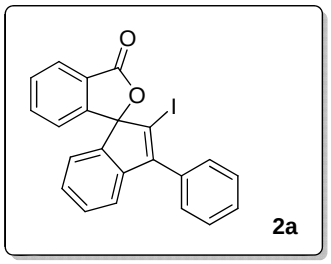


1 **2** **3**

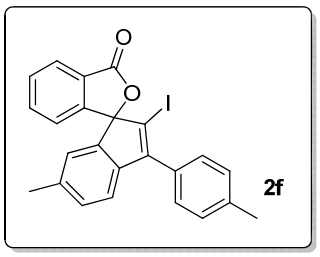
To a solution of 2-(3-hydroxy-3,3-diarylprop-1-yn-1-yl)benzoate derivatives **1** (0.20 mmol) in anhydrous $ClCH_2CH_2Cl$ (4.0 mL) was added I_2 (0.4 mmol, 101.6 mg) at room temperature. When the reaction was considered complete as determined by

TLC analysis, the reaction mixture was quenched by addition of saturated aqueous sodium thiosulfate and diluted with ethyl acetate (3 x 15 mL), washed with water, saturated brine, dried over Na_2SO_4 and evaporated under reduced pressure. The residue was purified by chromatography on silica gel to afford corresponding 2-iodo-spiro[indene-1,1'-isobenzofuran]-3'-one derivatives **2** and (*E*)-3-(1-iodo-2-allylidene)isobenzofuran-1-one derivatives **3**.

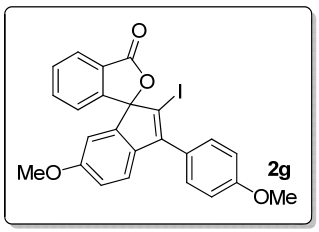
Characterization Data of 2a, 2f-2v, 2z, 3v, 3y-3zc



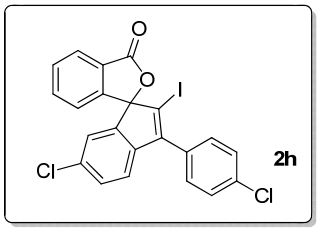
2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2a** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.04-8.02 (m, 1H), 7.64-7.57 (m, 4H), 7.55-7.46 (m, 3H), 7.32-7.25 (m, 2H), 7.17-7.13 (m, 1H), 7.09-7.07 (m, 1H), 7.03 (d, *J* = 6.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.8, 151.5, 148.3, 142.9, 142.6, 134.8, 133.4, 129.9, 129.8, 129.1, 128.7, 128.5, 127.2, 126.9, 125.8, 123.9, 121.7, 120.9, 103.0, 94.7. IR (neat, cm^{-1}): 2920, 1774, 1462, 1383, 1096, 750. HRMS (ESI) Calcd for $C_{22}H_{14}IO_2$: M+H = 437.0033. Found: 437.0029.



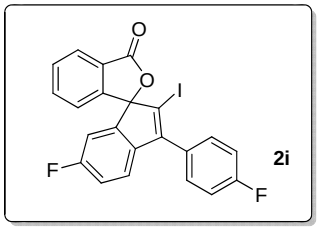
2-iodo-6-methyl-3-(*p*-tolyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2f** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.04-8.02 (m, 1H), 7.64-7.59 (m, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.85 (s, 1H), 2.44 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 151.5, 148.7, 142.8, 140.5, 139.1, 137.4, 134.7, 130.6, 130.1, 129.9, 129.3, 128.5, 127.1, 125.8, 124.8, 121.7, 120.7, 100.9, 94.7, 21.5, 21.2. IR (neat, cm^{-1}): 2919, 1776, 1383, 1096, 1019, 949. HRMS (ESI) Calcd for $C_{24}H_{18}IO_2$: M+H = 465.0346. Found: 465.0345.



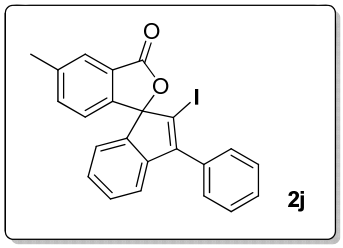
2-iodo-6-methoxy-3-(4-methoxyphenyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2g** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.03-8.01 (m, 1H), 7.64-7.61 (m, 2H), 7.60-7.54 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 1H), 7.08 (dd, *J* = 5.6, 1.6 Hz, 1H), 7.04 (d, *J* = 8.8 Hz, 2H), 6.80-6.60 (m, 1H), 6.59 (s, 1H), 3.88 (s, 3H), 3.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 160.0, 159.4, 150.8, 148.7, 144.5, 135.8, 134.8, 129.9, 129.8, 126.9, 125.8, 121.8, 121.7, 114.2, 113.9, 110.9, 98.1, 94.4, 55.6, 55.3. IR (neat, cm^{-1}): 2921, 1773, 1609, 1249, 1095, 1028. HRMS (ESI) Calcd for $C_{24}H_{18}IO_4$: M+H = 497.0244. Found: 497.0241.



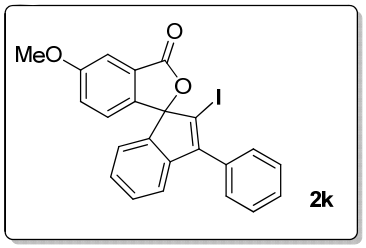
6-chloro-3-(4-chlorophenyl)-2-iodo-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2g** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.06-8.04 (m, 1H), 7.68-7.63 (m, 2H), 7.51 (s, 4H), 7.29 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.09-7.07 (m, 1H), 7.02 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.3, 149.7, 147.4, 144.3, 141.0, 135.3, 135.0, 133.7, 131.4, 130.4, 129.9, 129.8, 129.2, 126.8, 126.1, 124.7, 121.6, 121.5, 103.9, 94.0. IR (neat, cm^{-1}): 2919, 1778, 1383, 1093, 1018, 949. HRMS (ESI) Calcd for $C_{22}H_{12}Cl_2IO_2$: M+H = 504.9254. Found: 504.9259.



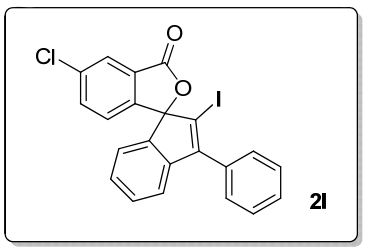
6-chloro-3-(4-chlorophenyl)-2-iodo-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2g** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.06-8.04 (m, 1H), 7.68-7.62 (m, 2H), 7.59-7.55 (m, 2H), 7.25-7.17 (m, 3H), 7.10-7.08 (m, 1H), 7.03-6.98 (m, 1H), 6.79 (dd, *J* = 7.6, 2.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.4, 164.2, 163.5, 161.7, 161.0, 149.8, 147.6, 144.9, 144.8, 138.8, 138.7, 135.0, 130.5, 130.4, 130.3, 129.2, 129.1, 126.9, 126.1, 121.8, 121.7, 121.6, 116.5, 116.3, 116.1, 115.9, 112.6, 112.4, 102.4, 102.3, 93.9. IR (neat, cm^{-1}): 2919, 1779, 1472, 1383, 1228, 1094. HRMS (ESI) Calcd for $C_{22}H_{12}F_2IO_2$: M+H = 472.9845. Found: 472.9841.



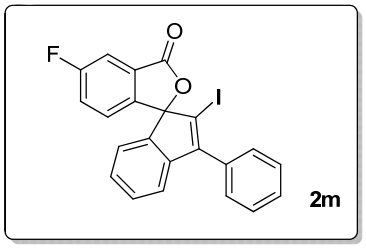
2-iodo-5'-methyl-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2j** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.82 (s, 1H), 7.59-7.57 (m, 2H), 7.53-7.47 (m, 3H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.30-7.23 (m, 2H), 7.14 (td, *J* = 8.4, 0.8 Hz, 1H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 2.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 151.3, 145.5, 142.9, 142.8, 140.4, 135.9, 133.5, 129.7, 129.0, 128.6, 128.5, 127.2, 127.1, 125.8, 123.9, 121.4, 120.9, 103.4, 94.6. IR (neat, cm^{-1}): 2921, 1773, 1383, 1068, 1025, 768. HRMS (ESI) Calcd for $C_{23}H_{16}IO_2$: M+H = 451.0189. Found: 451.0193.



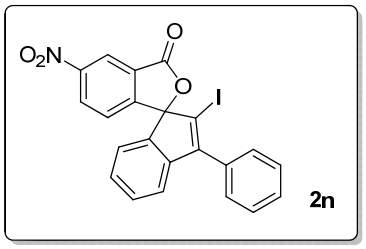
2-iodo-5'-methoxy-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2k** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.51-7.49 (m, 2H), 7.45-7.39 (m, 3H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.22-7.15 (m, 1H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.08-7.05 (m, 2H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 161.3, 151.3, 142.9, 142.6, 140.2, 133.5, 129.7, 129.1, 128.7, 128.6, 128.5, 127.1, 123.9, 123.8, 122.6, 120.1, 107.6, 103.6, 94.6, 55.8. IR (neat, cm^{-1}): 2921, 1774, 1490, 1383, 1283, 1067. HRMS (ESI) Calcd for $C_{23}H_{16}IO_3$: M+H = 467.0139. Found: 467.0139.



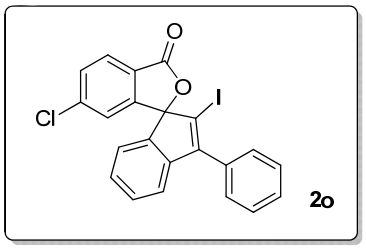
5'-chloro-2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2l** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.99 (d, *J* = 1.6 Hz, 1H), 7.59-7.48 (m, 6H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 6.8 Hz, 1H), 7.18-7.14 (m, 2H), 7.05-7.02 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 168.3, 151.9, 146.6, 142.9, 142.1, 136.3, 135.1, 133.2, 130.0, 129.2, 128.8, 128.7, 128.5, 127.3, 125.7, 123.9, 123.0, 121.1, 102.2, 94.6. IR (neat, cm^{-1}): 2920, 1779, 1463, 1383, 1218, 1107. HRMS (ESI) Calcd for $C_{22}H_{13}ClIO_2$: M+H = 470.9643. Found: 470.9641.



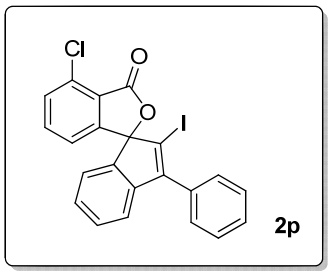
5'-fluoro-2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2m** Solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ ppm 7.59 (d, *J* = 1.8 Hz, 1H), 7.57-7.44 (m, 5H), 7.42-7.16 (m, 3H), 7.11-7.00 (m, 1H), 6.98-6.95 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm 168.6, 165.3, 161.9, 151.8, 143.8, 142.9, 142.1, 130.0, 129.2, 128.7, 128.5, 127.3, 123.9, 123.6, 123.5, 123.0, 122.7, 121.0, 112.4, 112.1, 102.5, 94.6. IR (neat, cm^{-1}): 2921, 1777, 1486, 1382, 1272, 1060. HRMS (ESI) Calcd for $C_{22}H_{13}FIO_2$: M+H = 454.9939. Found: 454.9934.



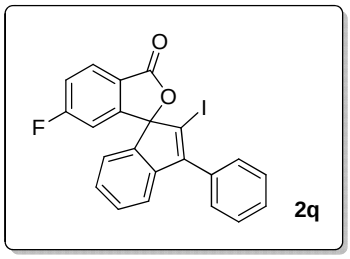
2-iodo-5'-nitro-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2n** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.76 (d, *J* = 1.6 Hz, 1H), 8.39 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.52-7.42 (m, 5H), 7.29-7.17 (m, 4H), 7.11 (td, *J* = 7.6, 0.8 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 167.3, 154.2, 152.8, 149.6, 142.9, 141.4, 132.9, 130.5, 129.7, 129.5, 128.8, 128.7, 128.4, 127.6, 123.9, 123.2, 121.5, 121.4, 100.6, 94.8. IR (neat, cm^{-1}): 2920, 1784, 1535, 1347, 1107, 739. HRMS (ESI) Calcd for $C_{22}H_{13}INO_4$: M+H = 481.9884. Found: 481.9885.



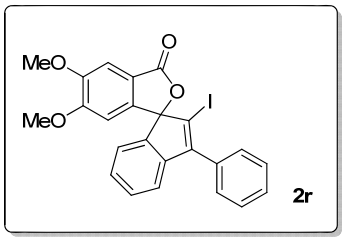
6'-chloro-2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2o** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.96 (d, *J* = 8.4 Hz, 1H), 7.60-7.47 (m, 6H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.18 (td, *J* = 7.6, 1.2 Hz, 1H), 7.06-7.05 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 168.6, 152.0, 150.1, 142.9, 142.1, 141.5, 133.2, 130.8, 130.1, 129.2, 128.7, 128.5, 127.3, 126.9, 125.5, 123.9, 121.9, 121.1, 102.0, 94.2. IR (neat, cm^{-1}): 2920, 1776, 1603, 1382, 1070, 1025. HRMS (ESI) Calcd for $C_{22}H_{13}ClIO_2$: M+H = 470.9643. Found: 470.9643.



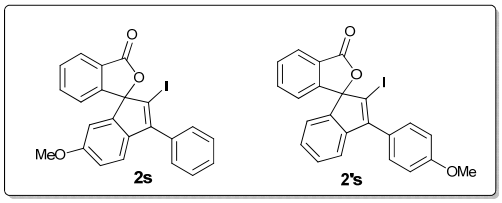
4'-chloro-2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2p** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.58-7.46 (m, 7H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.26-7.24 (m, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.98-6.94 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 166.8, 151.9, 150.8, 142.9, 142.3, 135.7, 133.3, 133.2, 131.4, 129.9, 129.2, 128.7, 128.5, 127.3, 123.9, 123.6, 121.1, 120.2, 102.3, 93.4. IR (neat, cm^{-1}): 2920, 1776, 1594, 1462, 1383, 966. HRMS (ESI) Calcd for $C_{22}H_{13}ClIO_2$: M+H = 470.9643. Found: 470.9645.



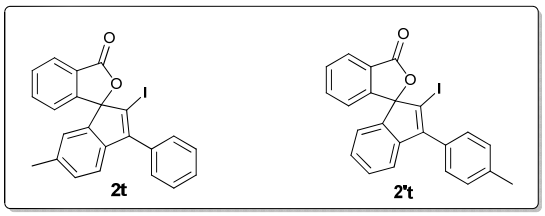
6'-fluoro-2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2q** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.03 (dd, *J* = 8.4, 4.8 Hz, 1H), 7.58 (dd, *J* = 8.4, 1.6 Hz, 2H), 7.55-7.48 (m, 3H), 7.33-7.31 (m, 2H), 7.29-7.25 (m, 1H), 7.17 (td, *J* = 7.6, 1.2 Hz, 1H), 7.06 (d, *J* = 7.2 Hz, 1H), 6.75 (dd, *J* = 7.6, 2.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 168.6, 168.2, 165.6, 151.9, 151.4, 151.3, 142.9, 142.2, 133.2, 130.0, 129.2, 128.7, 128.5, 128.3, 128.2, 127.3, 123.9, 123.2, 123.1, 121.1, 118.5, 118.2, 109.1, 108.8, 102.1, 94.1, 94.0. IR (neat, cm^{-1}): 2921, 1776, 1382, 1279, 1083, 1025. HRMS (ESI) Calcd for $C_{22}H_{13}FIO_2$: M+H = 454.9939. Found: 454.9943.



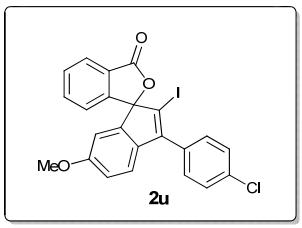
2-iodo-5',6'-dimethoxy-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2r** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.52 (d, *J* = 6.8 Hz, 2H), 7.46-7.37 (m, 3H), 7.33 (s, 1H), 7.24-7.17 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.32 (s, 1H), 3.89 (s, 3H), 3.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 155.4, 151.2, 151.1, 142.9, 142.6, 142.2, 133.4, 129.7, 129.1, 128.6, 128.5, 127.1, 123.9, 120.9, 119.3, 106.1, 103.6, 102.6, 94.2. IR (neat, cm^{-1}): 2920, 1768, 1600, 1383, 1307, 1070. HRMS (ESI) Calcd for $C_{24}H_{18}IO_4$: M+H = 497.0244. Found: 497.0243.



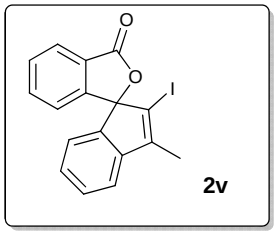
2-iodo-3-(4-methoxyphenyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2s** and 2-iodo-6-methoxy-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2's**, **2s**:**2's** = 2.7:1.0. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.04-8.02 (m, 1.3H), 7.65-7.44 (m, 8.4H), 7.29-7.25 (m, 1.1H), 7.15 (d, *J* = 8.0 Hz, 1.3H), 7.09 (d, *J* = 6.4 Hz, 1.1H), 7.07-7.01 (m, 1.3H), 6.79 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.61 (d, *J* = 2.0 Hz, 1H), 3.88 (s, 1.1H), 3.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 160.1, 159.5, 151.3, 151.1, 148.6, 148.5, 144.4, 143.1, 142.7, 135.7, 134.8, 134.7, 133.6, 130.0, 129.9, 129.7, 129.0, 128.6, 128.5, 127.0, 126.9, 125.8, 125.5, 123.8, 121.7, 121.6, 120.9, 114.3, 114.0, 111.0, 102.1, 99.0, 94.7, 94.4, 55.6, 55.3. IR (neat, cm^{-1}): 2926, 1774, 1476, 1283, 1096, 949. HRMS (ESI) Calcd for $C_{23}H_{15}INaO_3$: M+Na = 488.9958. Found: 488.9973.



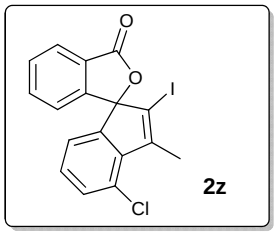
2-iodo-3-(*p*-tolyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2t** and 2-iodo-6-methyl-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2't**, **2t**:**2't** = 3.5:1.0. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.04-8.02 (m, 1.2H), 7.65-7.60 (m, 4.4H), 7.59-7.44 (m, 3.6H), 7.34-7.25 (m, 1.4H), 7.16-7.01 (m, 3.8H), 6.86 (s, 1H), 2.43 (s, 0.8H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 151.5, 148.6, 148.4, 143.0, 142.8, 142.7, 140.3, 139.1, 137.4, 134.7, 133.6, 130.4, 130.2, 129.9, 129.7, 129.4, 129.0, 128.6, 128.5, 128.4, 127.1, 127.0, 125.7, 124.8, 123.8, 121.7, 120.9, 120.7, 102.4, 101.3, 94.7, 21.5, 21.2. IR (neat, cm^{-1}): 2923, 1768, 1472, 1220, 1010, 875. HRMS (ESI) Calcd for $C_{23}H_{15}INaO_2$: M+Na = 473.0009. Found: 473.0027.



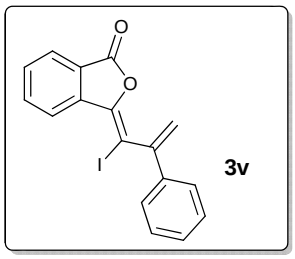
6-chloro-2-iodo-3-(4-methoxyphenyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2u** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.04-8.02 (m, 1H), 7.65-7.59 (m, 2H), 7.54-7.48 (m, 4H), 7.13-7.07 (m, 2H), 6.79 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.61 (d, *J* = 2.4 Hz, 1H), 3.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.8, 159.6, 150.3, 148.4, 144.4, 135.3, 135.0, 134.9, 132.1, 130.0, 129.9, 129.0, 126.9, 125.9, 121.7, 121.5, 114.4, 111.2, 99.8, 94.3, 55.6. IR (neat, cm^{-1}): 2920, 1775, 1606, 1482, 1282, 1094. HRMS (ESI) Calcd for $C_{23}H_{15}ClIO_3$: M+H = 500.9749. Found: 500.9745.



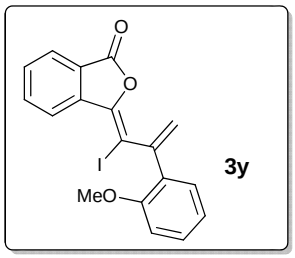
2-iodo-3-methyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2v** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.02-7.98 (m, 1H), 7.60-7.56 (m, 2H), 7.35-7.29 (m, 2H), 7.11 (td, *J* = 7.2, 1.6 Hz, 1H), 6.97-6.94 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.9, 148.8, 148.4, 143.3, 142.6, 134.6, 129.8, 126.9, 125.7, 123.3, 121.6, 119.5, 102.2, 94.4, 15.5. IR (neat, cm^{-1}): 2921, 1774, 1463, 1220, 1087, 754. HRMS (ESI) Calcd for $C_{17}H_{11}INaO_2$: M+Na = 396.9696. Found: 396.9708.



4-chloro-2-iodo-3-methyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2z** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.01-7.99 (m, 1H), 7.62-7.57 (m, 2H), 7.26-7.25 (m, 1H), 7.06-6.98 (m, 2H), 6.82 (dd, *J* = 7.6, 0.8 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 169.5, 148.3, 147.9, 145.3, 139.2, 134.8, 131.6, 130.1, 128.2, 127.1, 126.8, 125.8, 122.1, 121.6, 105.5, 93.7, 19.6. IR (neat, cm^{-1}): 2922, 1777, 1457, 1282, 1088, 948. HRMS (ESI) Calcd for $C_{17}H_{10}ClINaO_2$: M+Na = 430.9306. Found: 430.9319.

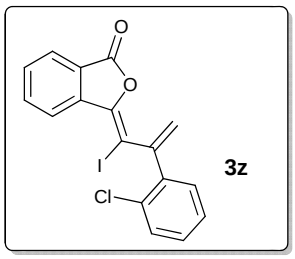


(*E*)-3-(1-iodo-2-phenylallylidene)isobenzofuran-1(3*H*)-one **3v** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.91-7.88 (m, 1H), 7.85-7.83 (m, 1H), 7.54-7.50 (m, 4H), 7.39-7.37 (m, 3H), 5.88 (s, 1H), 5.69 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.6, 148.8, 146.7, 136.3, 135.8, 134.6, 130.3, 129.0, 128.8, 126.6, 126.5, 125.7, 123.5, 117.8, 80.3. IR (neat, cm^{-1}): 2921, 1788, 1466, 1253, 1020, 966. HRMS (ESI) Calcd for $C_{17}H_{11}INaO_2$: M+Na = 396.9696. Found: 396.9708.



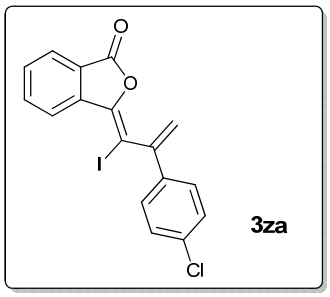
3y

(*E*)-3-(1-iodo-2-(2-methoxyphenyl)allylidene)isobenzofuran-1(3*H*)-one **3y** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.14 (d, *J* = 7.2 Hz, 1H), 7.89-7.88 (m, 1H), 7.58-7.51 (m, 2H), 7.37-7.31 (m, 2H), 6.99-6.92 (m, 2H), 5.79 (s, 2H), 3.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.9, 157.8, 148.1, 144.7, 136.8, 134.1, 130.7, 130.1, 130.0, 126.7, 126.6, 125.4, 124.2, 121.6, 120.6, 111.4, 84.5, 55.4. IR (neat, cm^{-1}): 2930, 1783, 1464, 1252, 1024, 745. HRMS (ESI) Calcd for $C_{18}H_{13}INaO_3$: M+Na = 426.9802. Found: 426.9811.



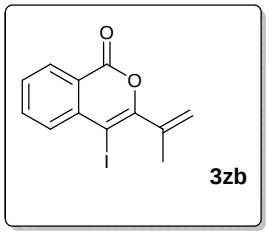
3z

(*E*)-3-(2-(2-chlorophenyl)-1-iodoallylidene)isobenzofuran-1(3*H*)-one **3z** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.27 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.64-7.55 (m, 2H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.36-7.29 (m, 3H), 5.95 (s, 1H), 5.69 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.5, 148.7, 145.3, 137.3, 136.6, 134.3, 133.0, 131.5, 130.4, 130.3, 129.9, 126.9, 126.8, 125.7, 124.0, 123.1, 83.8. IR (neat, cm^{-1}): 2924, 1784, 1467, 1257, 1024, 970. HRMS (ESI) Calcd for $C_{17}H_{10}ClINaO_2$: M+Na = 430.9306. Found: 430.9318.

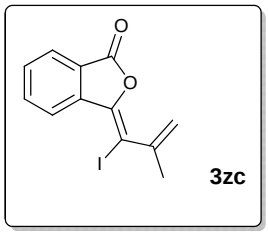


3za

(*E*)-3-(2-(4-chlorophenyl)-1-iodoallylidene)isobenzofuran-1(3*H*)-one **3za** Solid, ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.91-7.89 (m, 1H), 7.80-7.78 (m, 1H), 7.54 (t, *J* = 4.0 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 5.87 (s, 1H), 5.71 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.4, 149.0, 145.7, 136.2, 135.0, 134.7, 134.3, 130.5, 129.1, 127.9, 126.6, 125.8, 123.3, 118.2, 79.4. IR (neat, cm^{-1}): 2923, 1784, 1465, 1255, 1086, 1018. HRMS (ESI) Calcd for $C_{17}H_{10}ClINaO_2$: M+Na = 430.9306. Found: 430.9314.

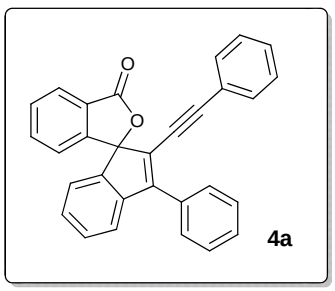


4-iodo-3-(prop-1-en-2-yl)-1*H*-isochromen-1-one **3zb** Solid. The procedure is the same as the general procedure B, except that the reaction temperature is 80 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.26-8.24 (m, 1H), 7.83-7.76 (m, 2H), 7.54 (td, *J* = 8.0, 1.6 Hz, 1H), 5.50-5.47 (m, 2H), 2.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.4, 156.4, 139.5, 138.0, 135.5, 131.5, 129.6, 129.0, 122.7, 120.3, 74.6, 20.7. HRMS (ESI) Calcd for $C_{12}H_9INaO_2$: M+Na = 334.9539. Found: 334.9547.



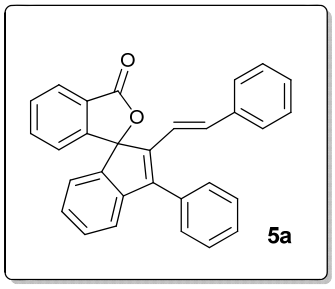
(*E*)-3-(1-iodo-2-methylallylidene)isobenzofuran-1(3*H*)-one **3zc** Solid. The procedure is the same as the general procedure B, except that the reaction temperature is 80 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.99 (d, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.65-7.62 (m, 1H), 7.55 (td, *J* = 7.6, 0.8 Hz, 1H), 5.40 (d, *J* = 0.4 Hz, 1H), 5.31-5.30 (m, 1H), 2.12 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 165.6, 146.5, 143.3, 136.4, 134.5, 130.1, 126.4, 125.6, 123.2, 118.7, 84.3, 21.6. IR (neat, cm^{-1}): 2921, 1779, 1647, 1464, 1029, 684. HRMS (ESI) Calcd for $C_{12}H_9INaO_2$: M+Na = 334.9539. Found: 334.9548.

Typical Procedure for 4a, 5a and 6a Synthesis and Characterization Data of 4a, 5a and 6a

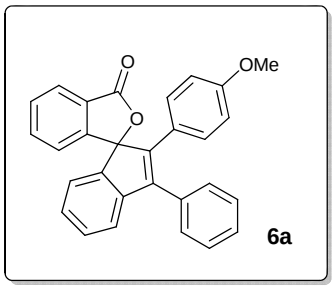


3-phenyl-2-(phenylethynyl)-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one 4a: To a solution of 2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2a** (87.4 mg, 0.20 mmol) in anhydrous CH_3CN (2 mL) was added $PdCl_2(PPh_3)_2$ (5.6 mg, 4 mol%), CuI (0.76 mg, 2 mol%) and K_2CO_3 (55.2 mg, 2.0 equiv.). The reaction vial was flushed with Ar and the reaction mixture was stirred for 5 minutes at room temperature. A solution of ethynylbenzene (30.6 mg, 1.5 equiv.) in anhydrous CH_3CN

(2 mL) were then added dropwise through a syringe. The resulting solution was stirred at room temperature for 36 h. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched by addition of saturated aqueous ammonium chloride (5 mL) and extracted with ethyl ether (3 x 20 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography to give **4a** (yield 74%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.99-7.97 (m, 1H), 7.80 (d, J = 7.2 Hz, 2H), 7.53-7.46 (m, 5H), 7.41 (d, J = 7.6 Hz, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.20-7.16 (m, 2H), 7.14-7.10 (m, 2H), 7.09-7.03 (m, 3H), 6.99 (d, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 170.3, 148.4, 148.3, 142.2, 142.1, 134.6, 132.8, 131.5, 131.4, 130.0, 129.7, 129.3, 128.6, 128.5, 128.2, 128.0, 126.7, 125.6, 125.2, 123.8, 122.5, 122.1, 121.8, 99.4, 93.6, 82.9. IR (neat, cm^{-1}): 2920, 2851, 1773, 1605, 1382, 1075, 1022, 757. HRMS (ESI) Calcd for $C_{30}H_{19}O_2$: M+H = 411.1380. Found: 411.1378.

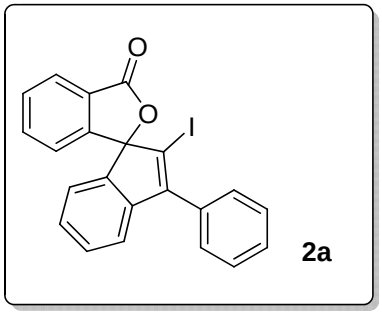


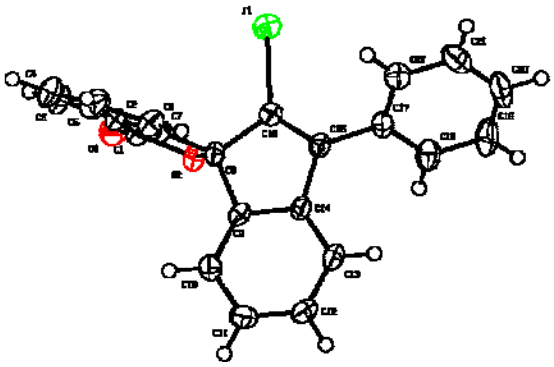
(*E*)-3-phenyl-2-styryl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one 5a: To a solution of 2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2a** (87.4 mg, 0.20 mmol) in DMF (2 mL) was added K_2CO_3 (138.0 mg, 5.0 equiv), tetrabutylammonium bromide (128.8 mg, 2.0 equiv.), $Pd(OAc)_2$ (1.34 mg, 3 mol%). The reaction vial was flushed with Ar and the reaction mixture was stirred for 5 minutes at room temperature. A solution of styrene (208 mg, 10 equiv.) in DMF (2 mL) were then added dropwise through a syringe. The resulting solution was stirred at 100 °C for 12 h. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched slowly by addition of aqueous 1M HCl (5 mL) and extracted with ethyl ether (3 x 20 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography to give **5a** (yield 96%) as a solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.02 (s, 1H), 7.49 (s, 6H), 7.42 (d, J = 2.8 Hz, 1H), 7.21 (s, 2H), 7.08-7.03 (m, 5H), 6.98 (d, J = 7.2 Hz, 2H), 6.86-6.82 (m, 2H), 5.90 (d, J = 16.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 170.6, 150.5, 145.6, 143.4, 142.7, 137.8, 136.9, 134.9, 133.1, 130.9, 129.7, 129.6, 129.4, 128.8, 128.7, 128.4, 127.8, 127.5, 126.4, 126.2, 125.9, 122.6, 121.7, 121.4, 119.8, 93.4. IR (neat, cm^{-1}): 2920, 1769, 1624, 1426, 1383, 1072, 756, 696. HRMS (ESI) Calcd for $C_{30}H_{21}O_2$: M+H = 413.1536. Found: 413.1536.



2-(4-methoxyphenyl)-3-phenyl-3'H-spiro[indene-1,1'-isobenzofuran]-3'-one 6a: To a solution of 2-iodo-3-phenyl-3'*H*-spiro[indene-1,1'-isobenzofuran]-3'-one **2a** (87.4 mg, 0.20 mmol) in DMF : H_2O (1 mL : 0.25 mL) was added (4-methoxyphenyl)boronic acid (39.5 mg, 1.3 equiv), Na_2CO_3 (63.6 mg, 3.0 equiv), $Pd(OAc)_2$ (0.90 mg, 2 mol%). The reaction vial was flushed with Ar and the reaction mixture was stirred for 20 h at 40°C. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched slowly by addition of aqueous 1M HCl (5 mL) and extracted with ethyl ether (3 x 20 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography to give **6a** (yield 99%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.80 (d, J = 7.6 Hz, 1H), 7.46-7.43 (m, 1H), 7.39-7.31 (m, 1H), 7.29-7.21 (m, 7H), 7.10-7.05 (m, 2H), 6.88 (d, J = 7.2 Hz, 1H), 6.73 (d, J = 8.8 Hz, 2H), 6.45 (d, J = 8.8 Hz, 2H), 3.54 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 170.6, 158.9, 149.3, 143.4, 142.8, 142.6, 141.1, 134.5, 133.6, 130.1, 129.6, 129.3, 129.2, 128.5, 128.1, 127.0, 126.6, 125.8, 125.0, 122.9, 121.6, 121.2, 113.6, 94.9, 54.9. IR (neat, cm^{-1}): 2921, 1770, 1605, 1510, 1383, 1250, 1091, 753. HRMS (ESI) Calcd for $C_{29}H_{21}O_3$: M+H = 417.1485. Found: 417.1485.

Crystallographic data





structure of 2a

Datablock:

Bond precision: C-C = 0.0053 A Wavelength=0.71073

Cell: a=9.369(2) b=9.971(2) c=10.815(4)
alpha=98.526(3) beta=93.088(3) gamma=117.892(2)

Temperature: 293 K

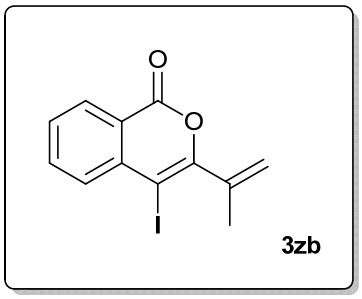
	Calculated	Reported
Volume	874.3(4)	874.3(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C22 H13 I O2	?
Sum formula	C22 H13 I O2	C22 H13 I O2
Mr	436.22	436.22
Dx,g cm-3	1.657	1.657
Z	2	2
Mu (mm-1)	1.843	1.843
F000	428.0	428.0
F000'	427.22	
h,k,lmax	11,12,13	11,12,13
Nref	3247	3182
Tmin,Tmax	0.661,0.705	0.677,0.721
Tmin'	0.648	

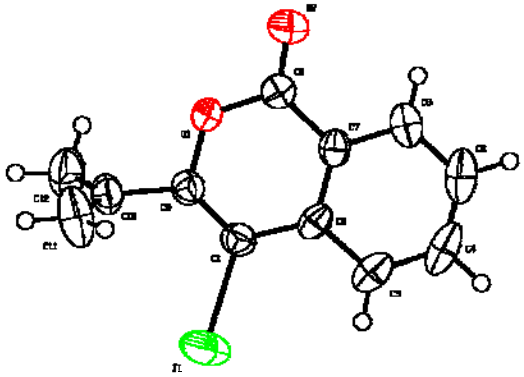
Correction method= MULTI-SCAN

Data completeness= 0.980 Theta(max)= 25.500

R(reflections)= 0.0278(2771) wR2(reflections)= 0.0624(3182)

S = 1.045 Npar= 226





structure of 3zb

Datablock:

Bond precision: C-C = 0.0073 A Wavelength=0.71073

Cell: a=7.714(4) b=18.219(10) c=8.198(5)
alpha=90 beta=97.004(5) gamma=90

Temperature: 569 K

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Volume	1143.6(11)	1143.5(11)
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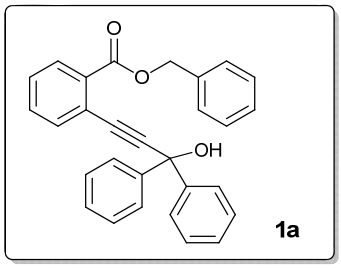
Hall group	-P 2yab	-P 2yab
Moiety formula	C12 H9 I O2	C12 H9 I O2
Sum formula	C12 H9 I O2	C12 H9 I O2
Mr	312.09	312.09
Dx,g cm-3	1.813	1.813
Z	4	4
Mu (mm-1)	2.777	2.777
F000	600.0	600.0
F000'	598.35	
h,k,lmax	9,22,9	9,22,9
Nref	2129	2120
Tmin,Tmax	0.536,0.678	0.379,0.746
Tmin'	0.523	

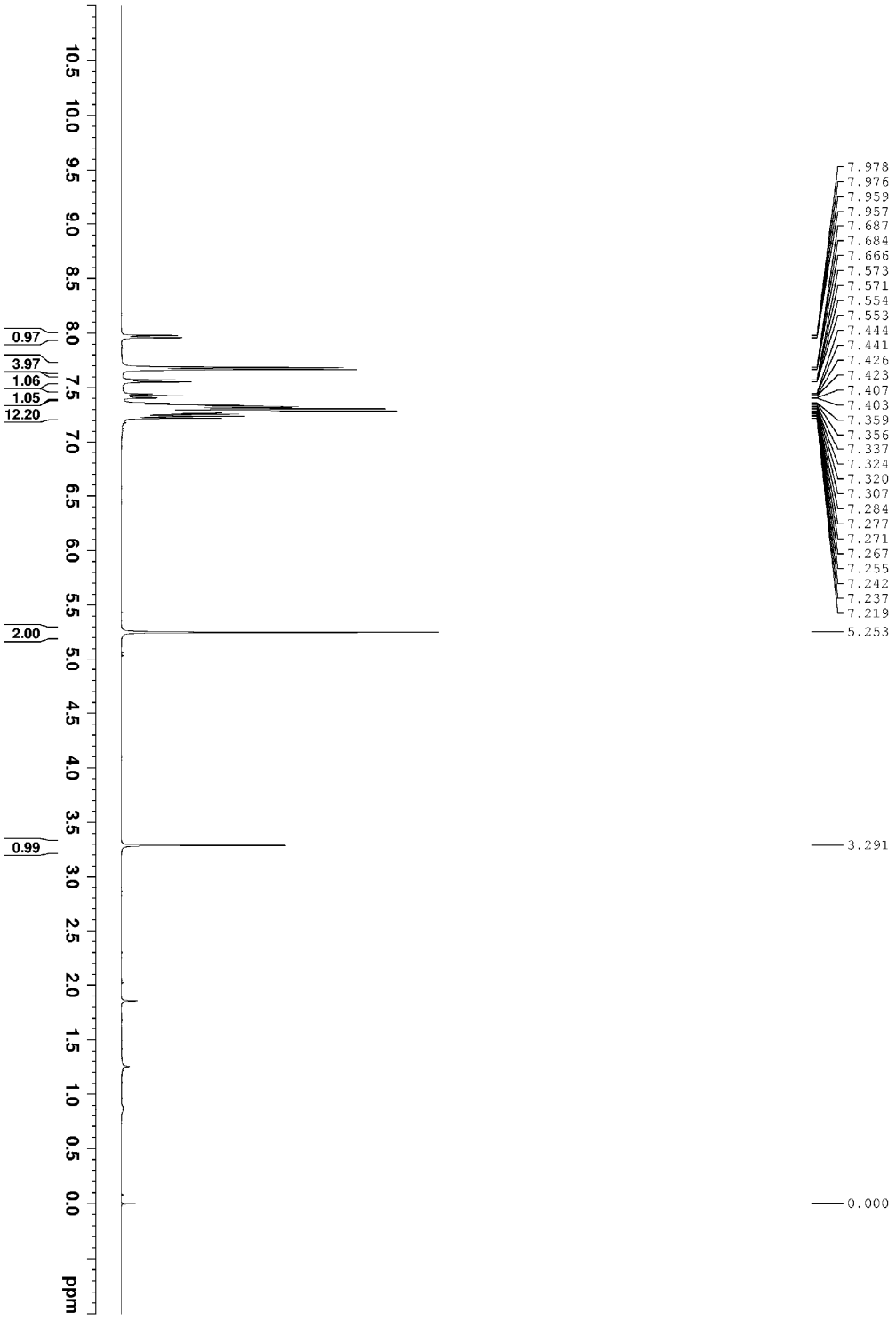
Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.500

R(reflections)= 0.0410(1603) wR2(reflections)= 0.0972(2120)

S = 1.060 Npar= 138


O
O
OH
1a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1.05
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7.573
7.571
7.554
7.553
7.444
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7.407
7.403
7.359
7.356
7.337
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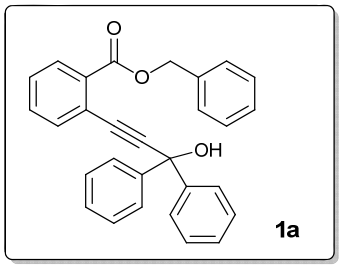
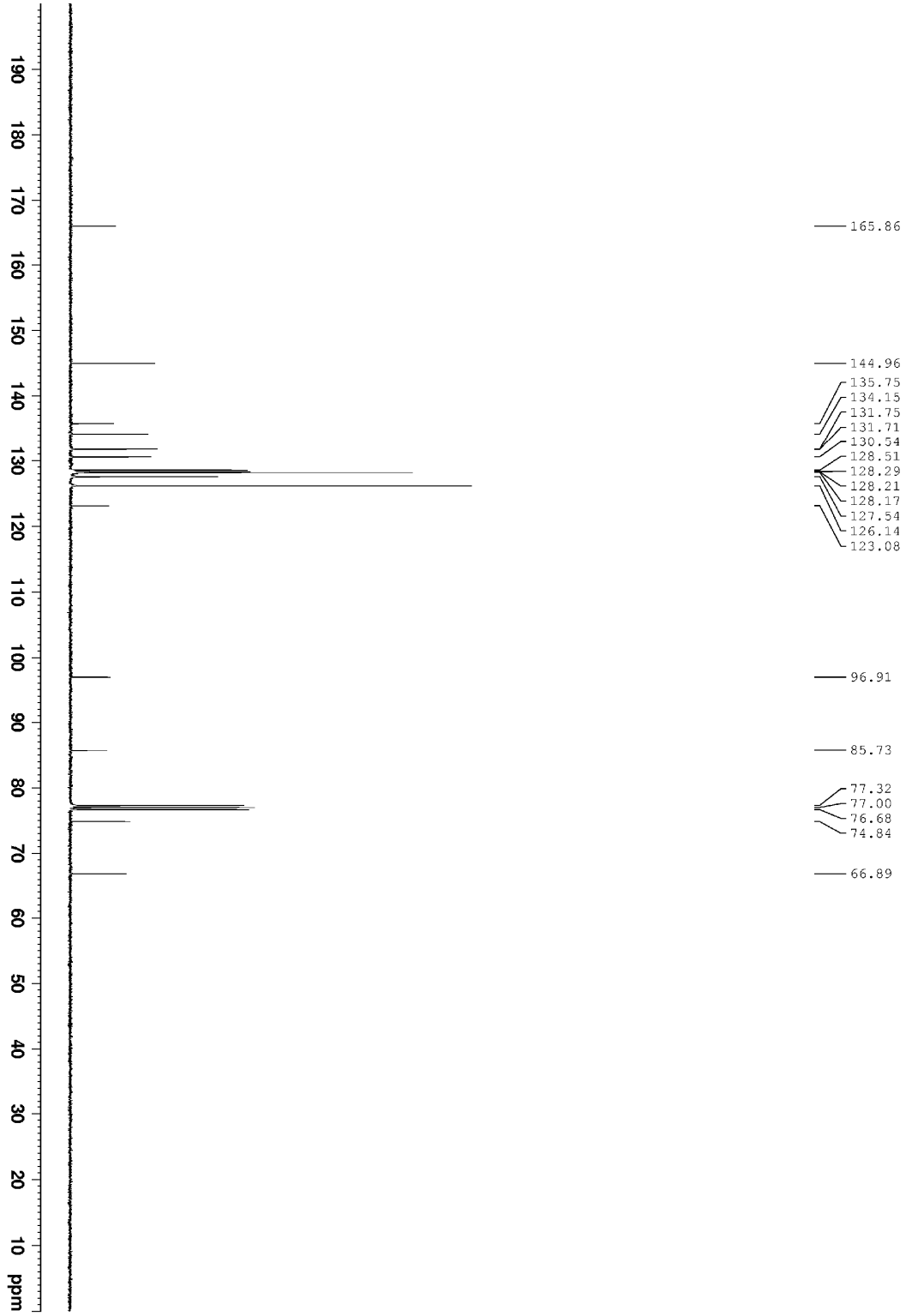
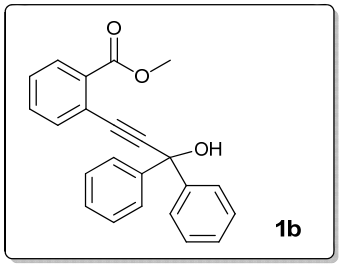
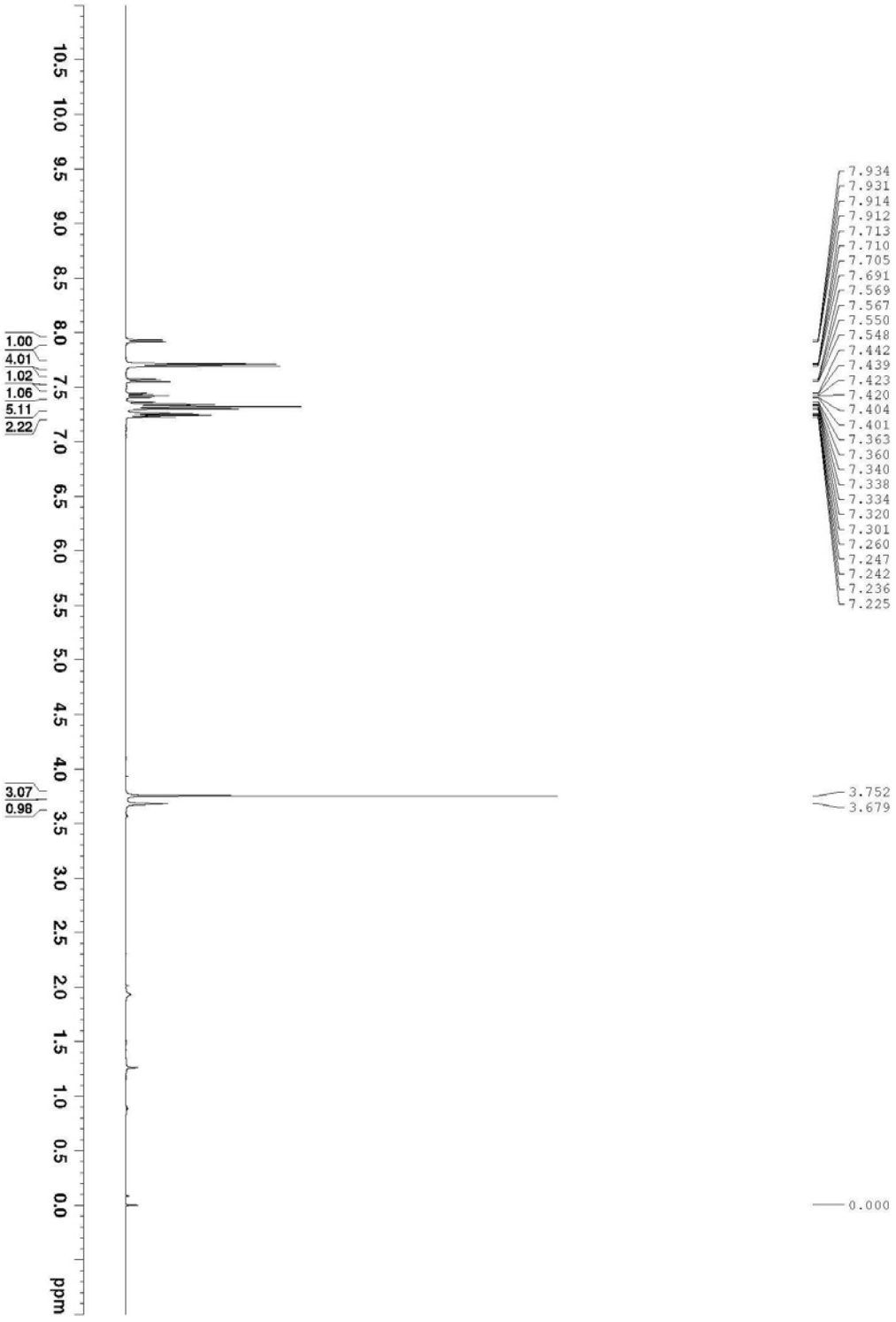





O
O
OH
1b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2.22
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7.931
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7.912
7.713
7.710
7.705
7.691
7.569
7.567
7.550
7.548
7.442
7.439
7.423
7.420
7.404
7.401
7.363
7.360
7.340
7.338
7.334
7.320
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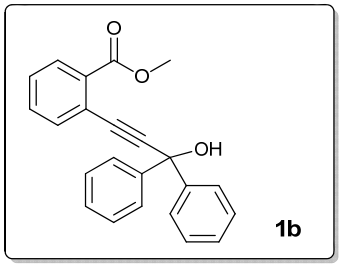
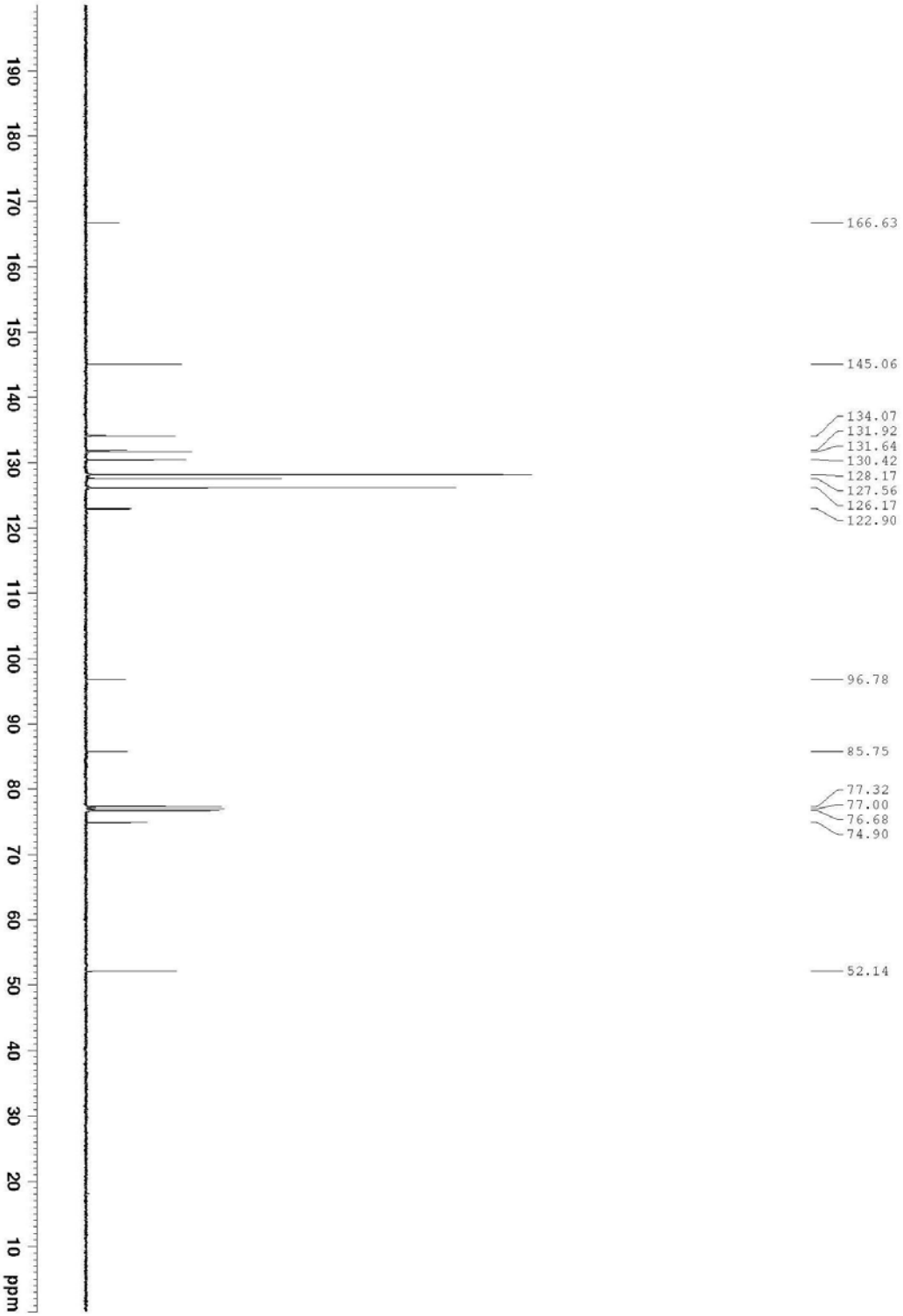
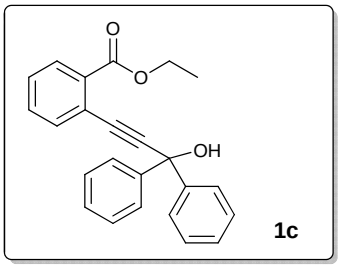
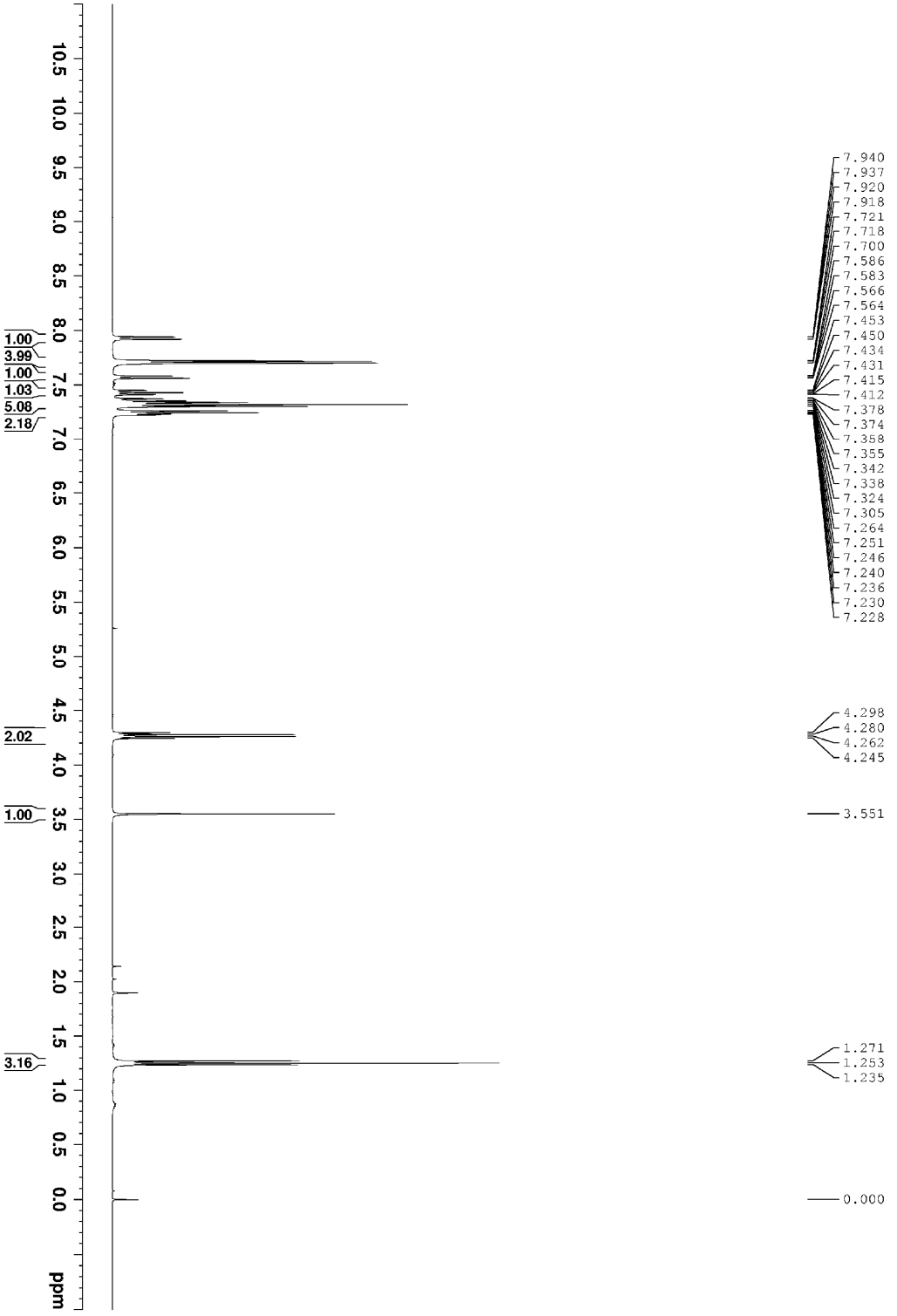
7.260
7.247
7.242
7.236
7.225
3.752
3.679
0.000






O
O
OH

1c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2.02
1.00
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7.718
7.700
7.586
7.583
7.566
7.564
7.453
7.450
7.434
7.431
7.415
7.412
7.378
7.374
7.358
7.355
7.342
7.338
7.324
7.305
7.264
7.251
7.246
7.240
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7.230
7.228
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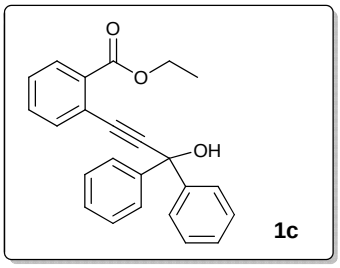
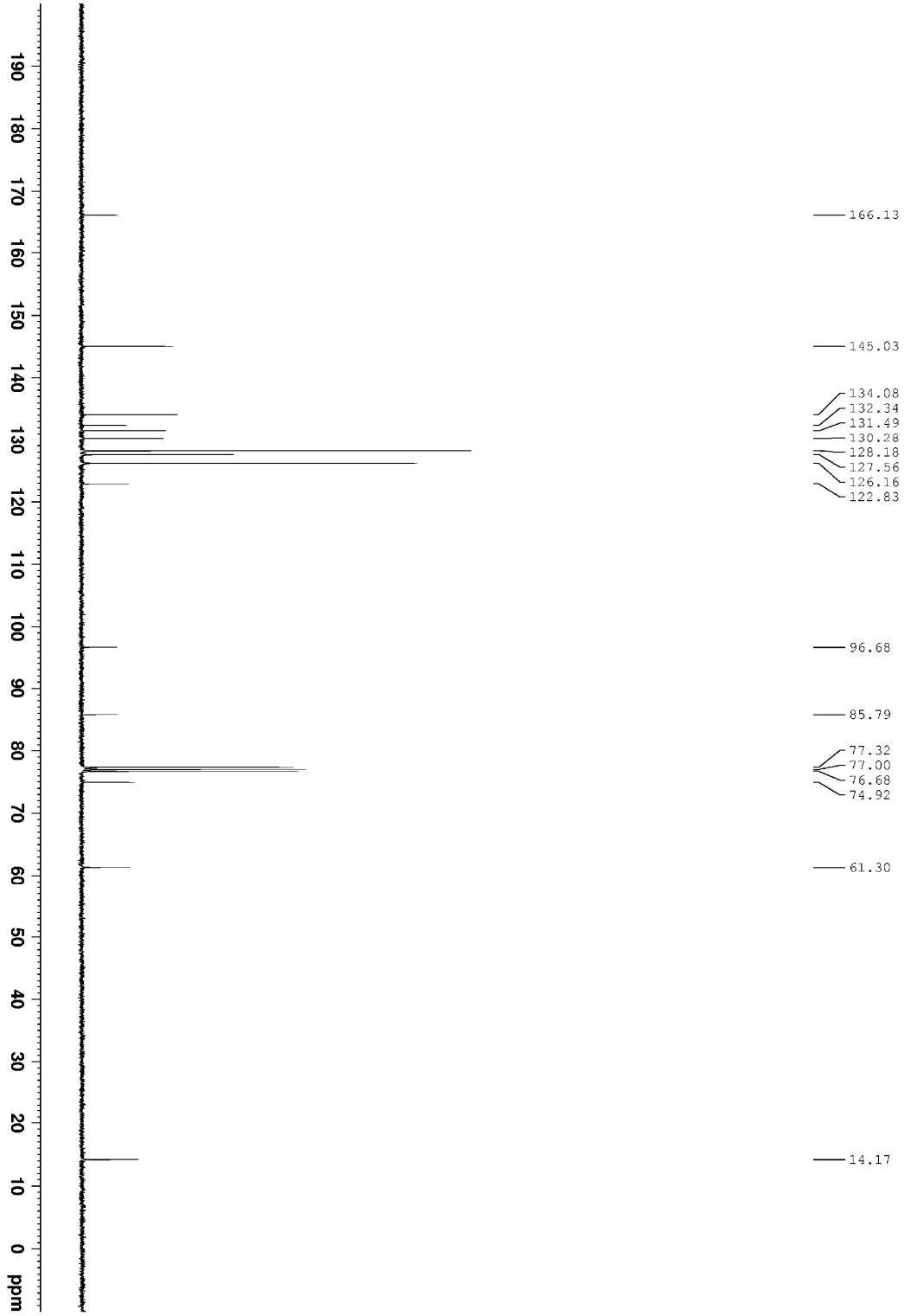
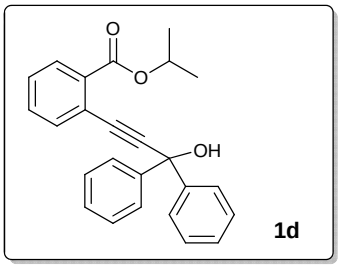
1.253
1.235
0.000

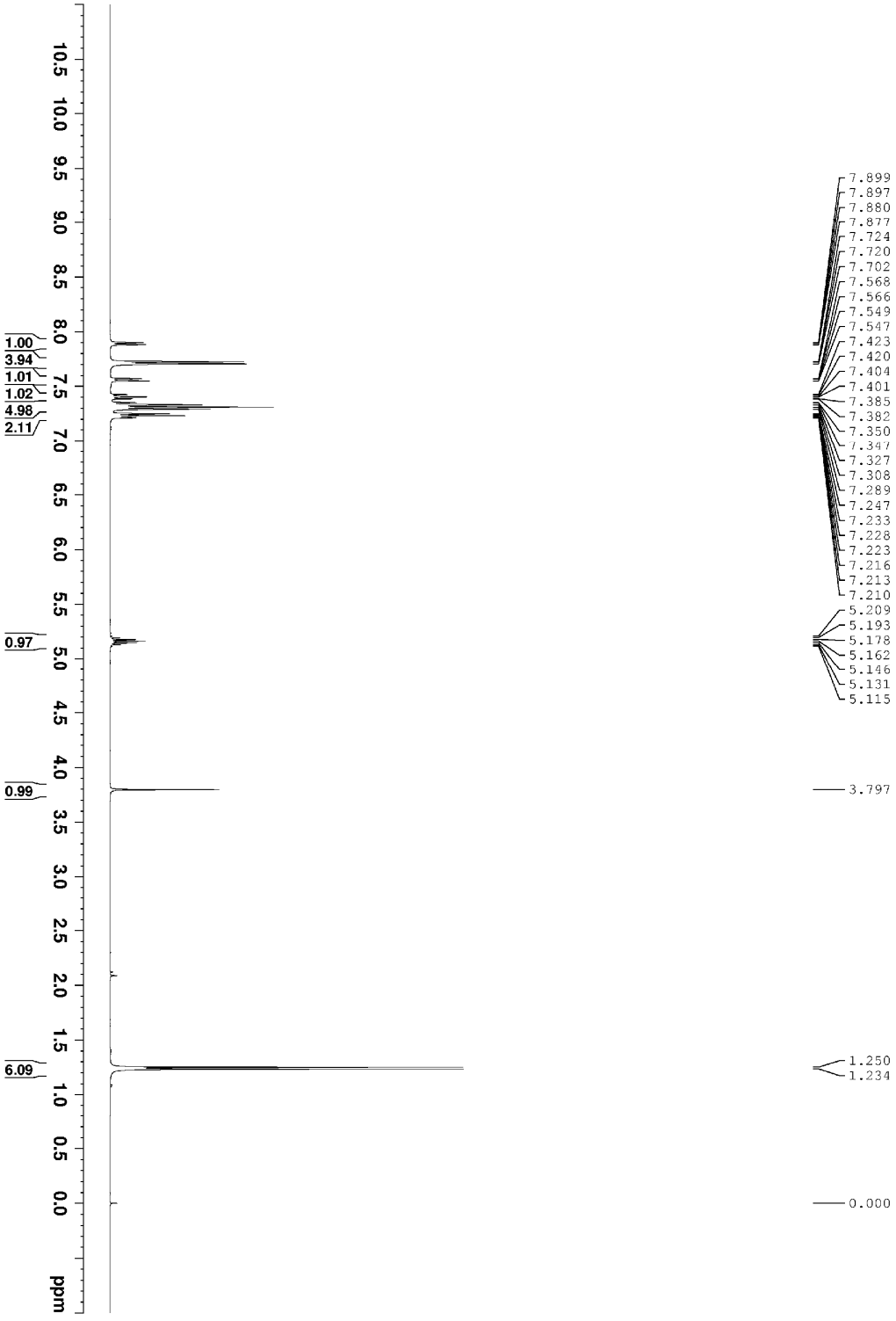


1c




O
O
OH

1d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0.99
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ppm
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7.880
7.877
7.724
7.720
7.702
7.568
7.566
7.549
7.547
7.423
7.420
7.404
7.401
7.385
7.382
7.350
7.347
7.327
7.308
7.289
7.247
7.233
7.228
7.223
7.216
7.213
7.210
5.209
5.193
5.178
5.162
5.146
5.131
5.115
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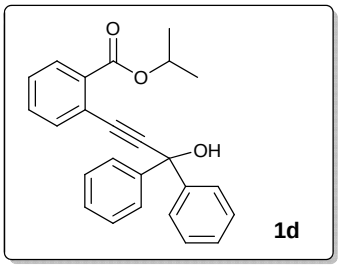
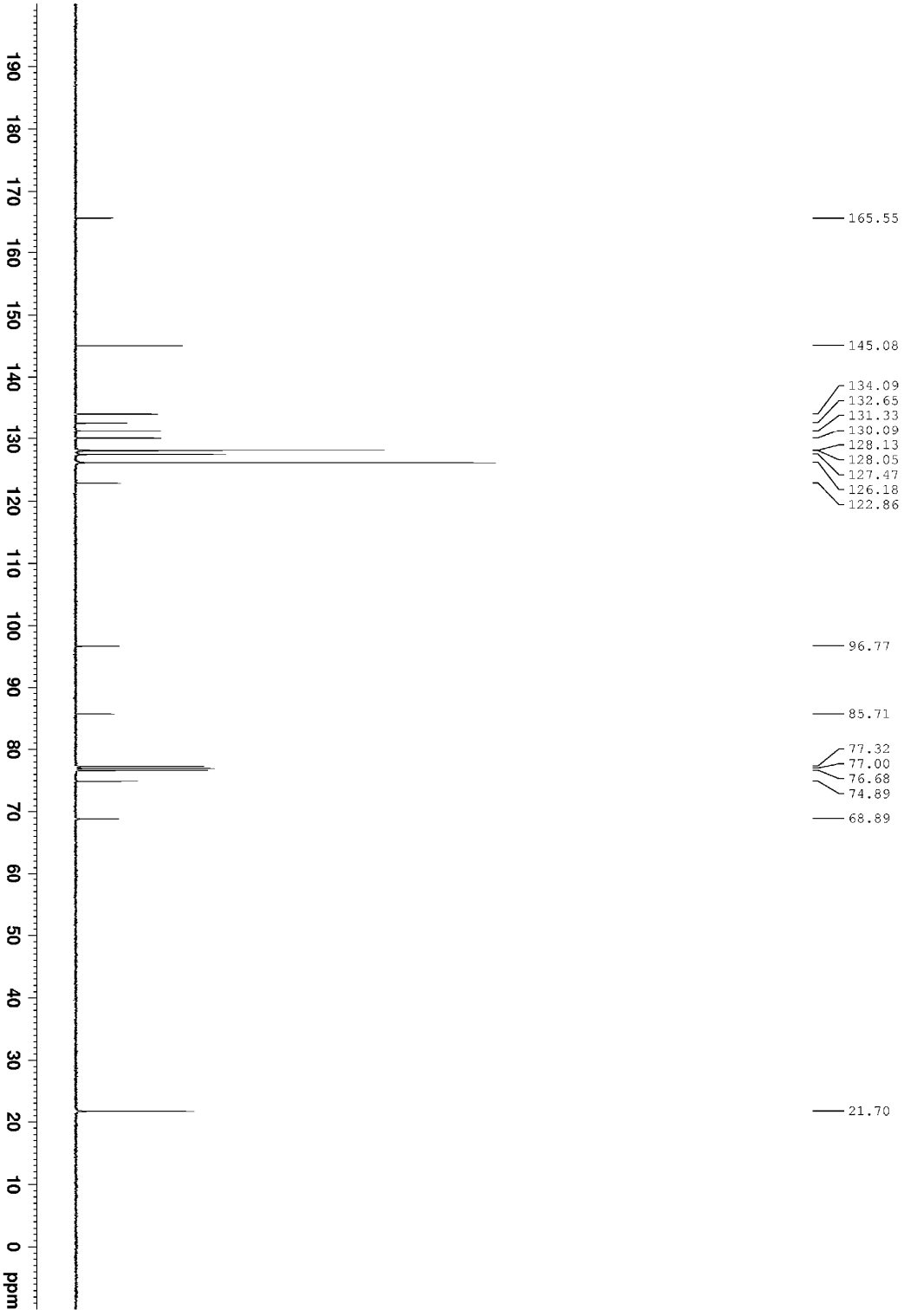
1.250
1.234
0.000


O
O
OH

1d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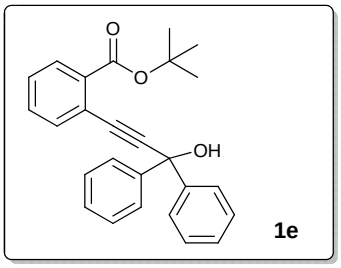
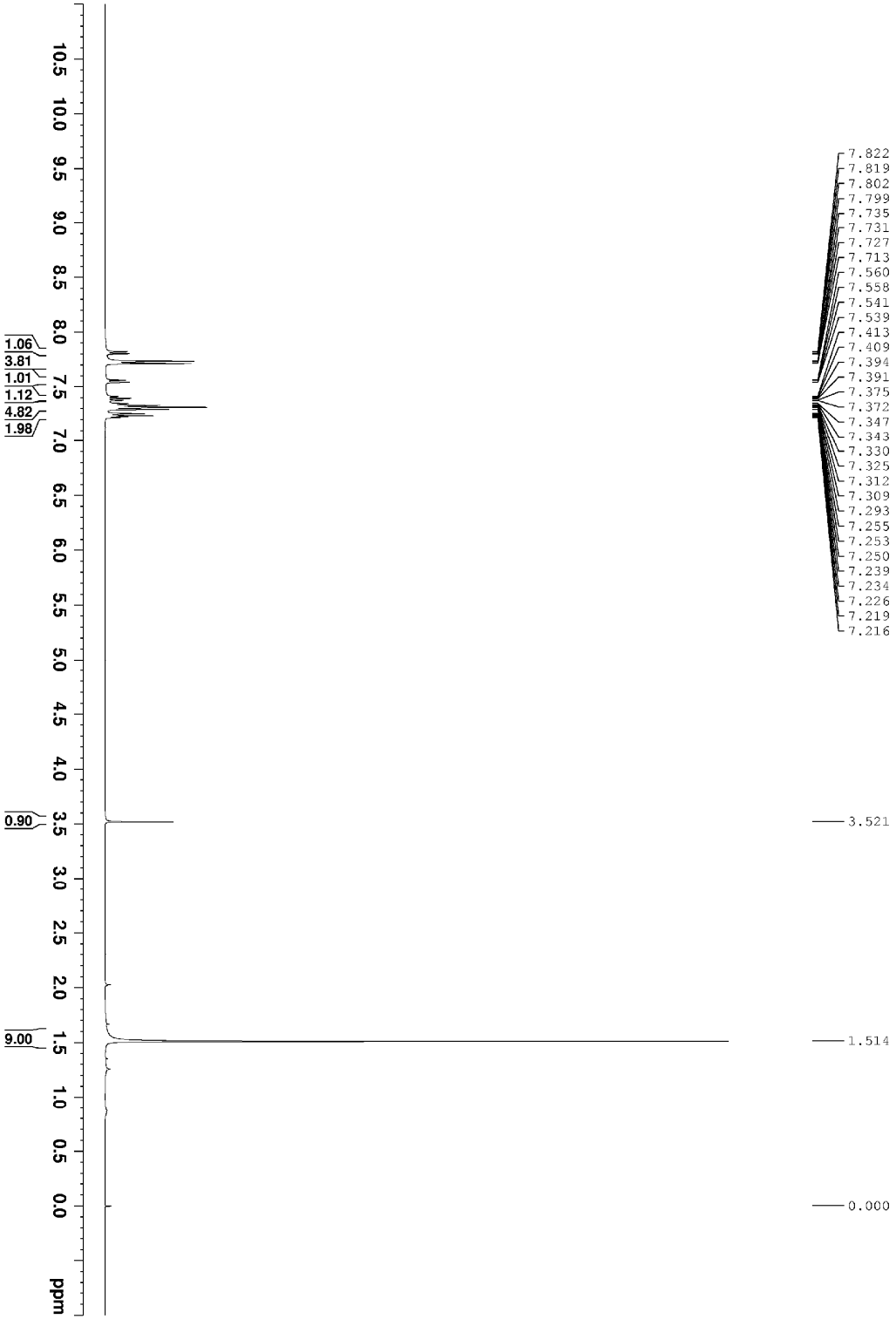
145.08
134.09
132.65
131.33
130.09
128.13
128.05
127.47
126.18
122.86
96.77
85.71
77.32
77.00
76.68
74.89
68.89
21.70
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


O
O
OH

1e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1.01
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1.98
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9.00
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7.819
7.802
7.799
7.735
7.731
7.727
7.713
7.560
7.558
7.541
7.539
7.413
7.409
7.394
7.391
7.375
7.372
7.347
7.343
7.330
7.325
7.312
7.309
7.293
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7.253
7.250
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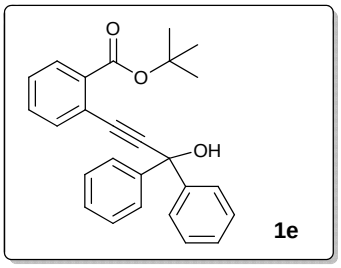
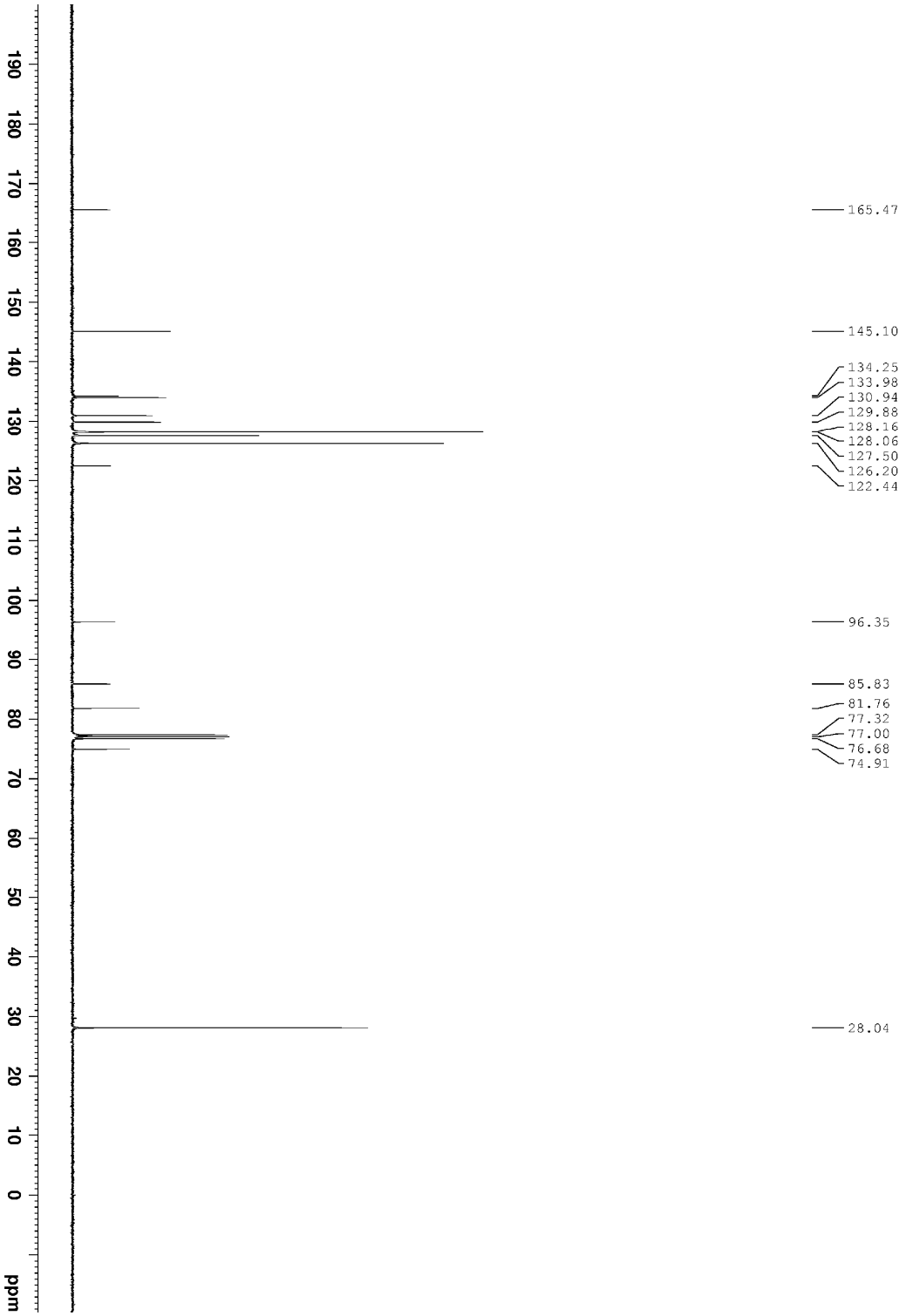
7.234
7.226
7.219
7.216
3.521
1.514
0.000


O
O
OH
1e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180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
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145.10
134.25
133.98
130.94
129.88
128.16
128.06
127.50
126.20
122.44
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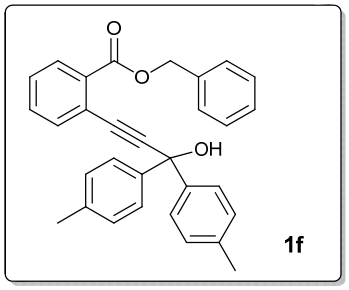
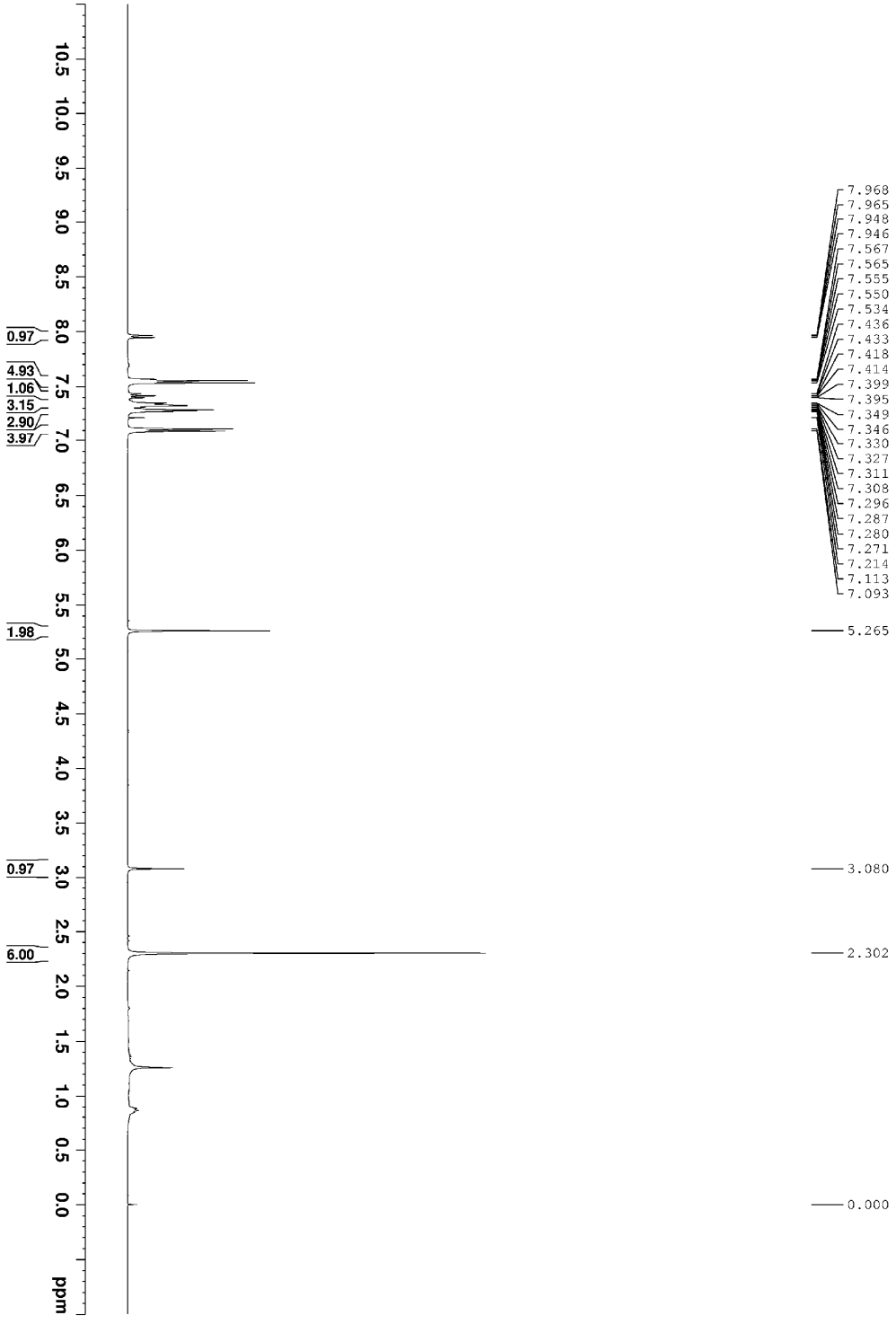
85.83
81.76
77.32
77.00
76.68
74.91
28.04


O
O
OH
1f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1.98
0.97
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7.948
7.946
7.567
7.565
7.555
7.550
7.534
7.436
7.433
7.418
7.414
7.399
7.395
7.349
7.346
7.330
7.327
7.311
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7.271
7.214
7.113
7.093
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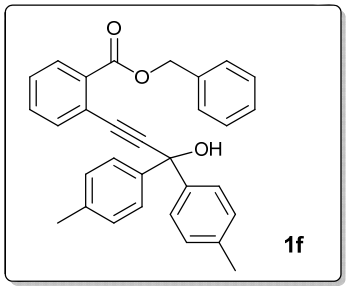
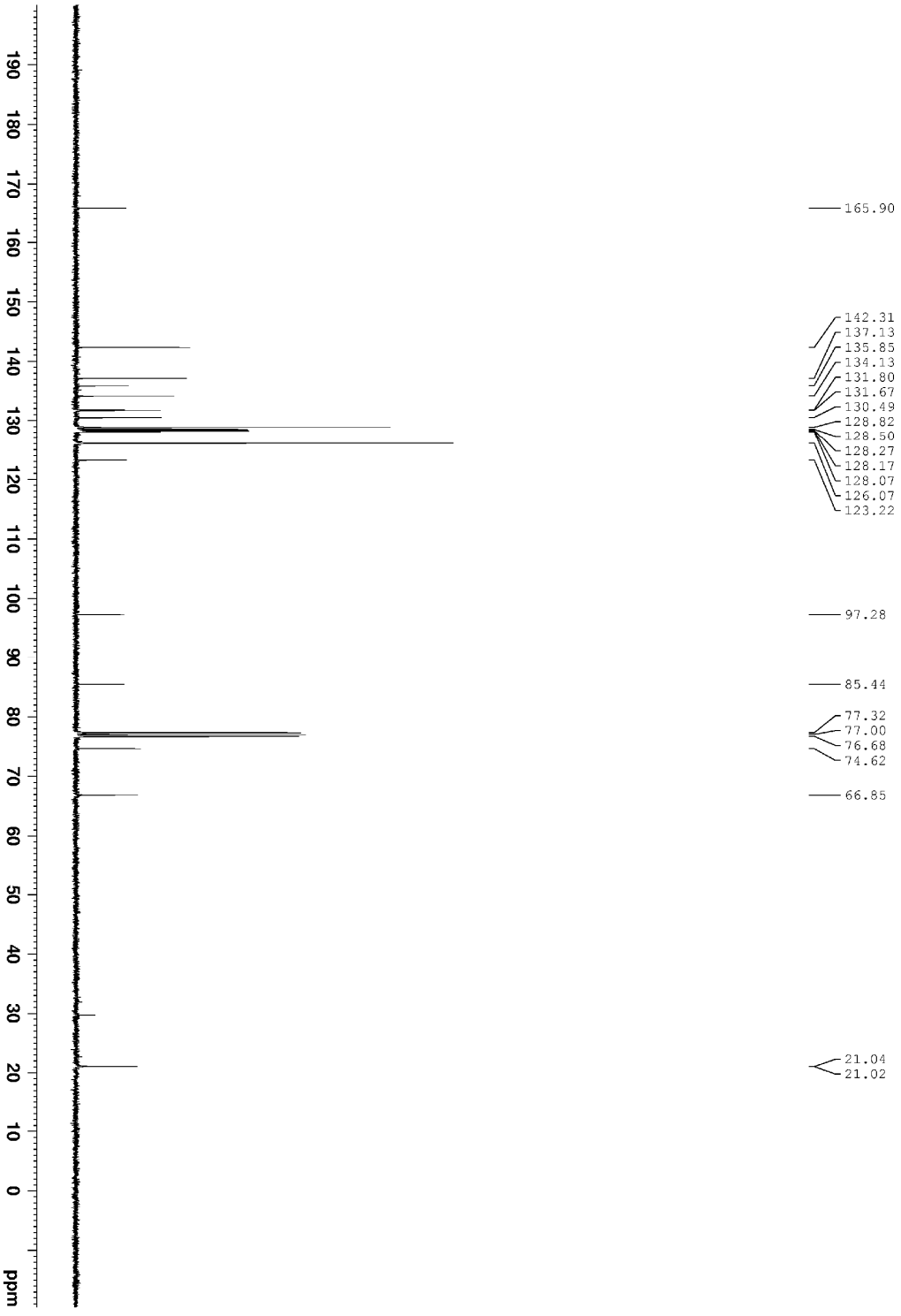
2.302
0.000


O
O
OH
1f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160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
165.90
142.31
137.13
135.85
134.13
131.80
131.67
130.49
128.82
128.50
128.27
128.17
128.07
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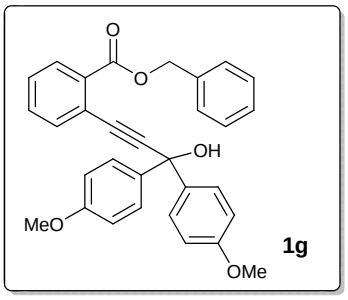
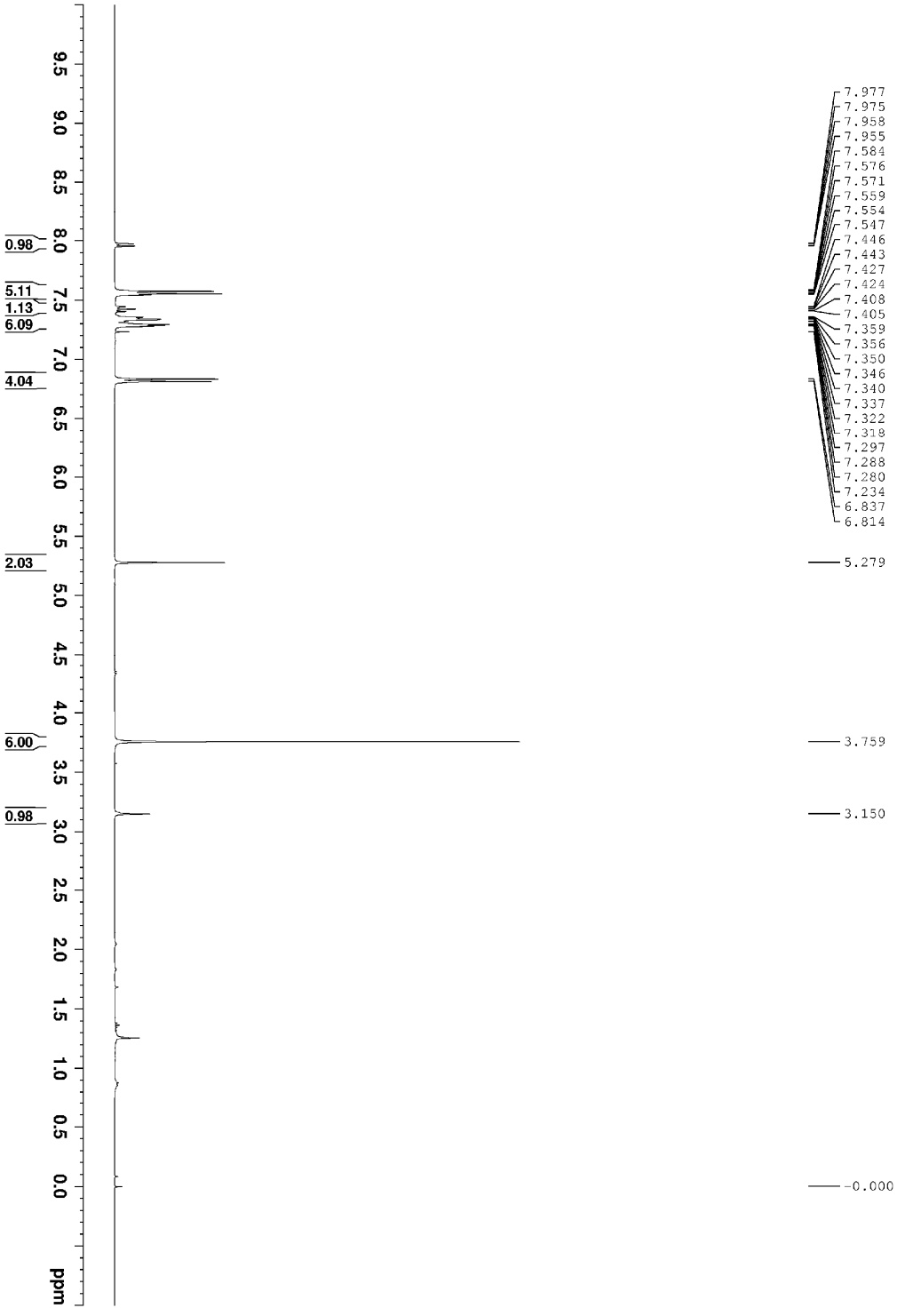
77.00
76.68
74.62
66.85
21.04
21.02


O
O
OH
MeO
OMe
1g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4.04
2.03
6.00
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7.571
7.559
7.554
7.547
7.446
7.443
7.427
7.424
7.408
7.405
7.359
7.356
7.350
7.346
7.340
7.337
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7.280
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6.814
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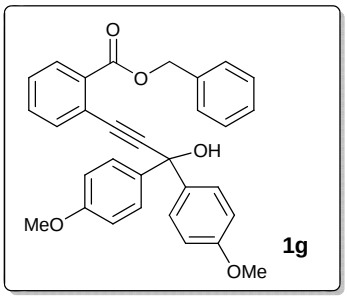
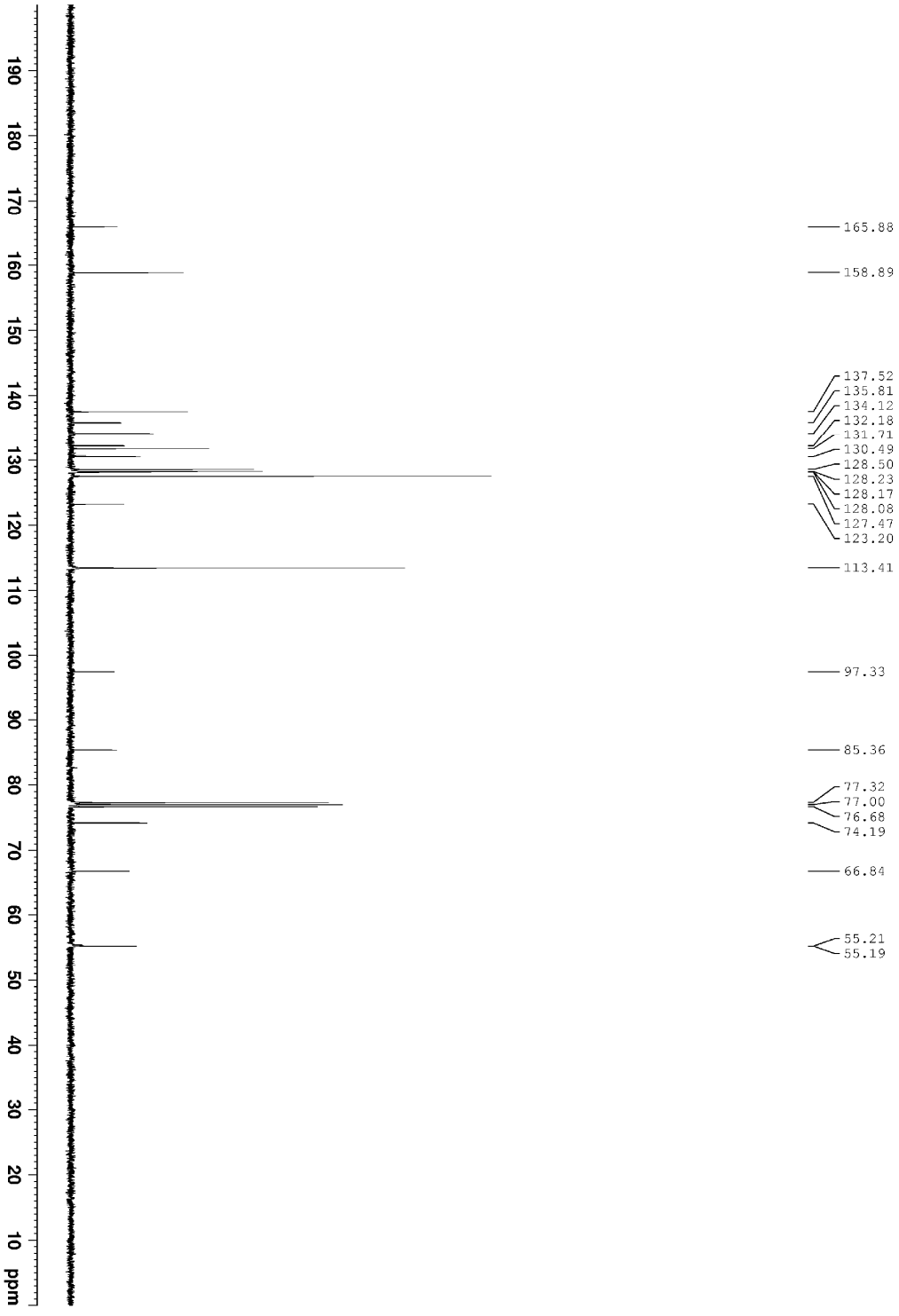
3.150
-0.000


O
O
OH
MeO
OMe

1g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150
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130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
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158.89
137.52
135.81
134.12
132.18
131.71
130.49
128.50
128.23
128.17
128.08
127.47
123.20
113.41
97.33
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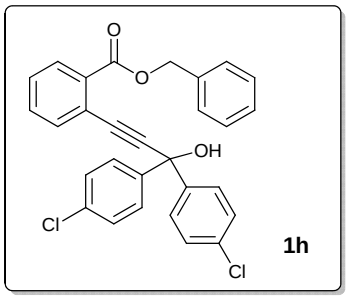
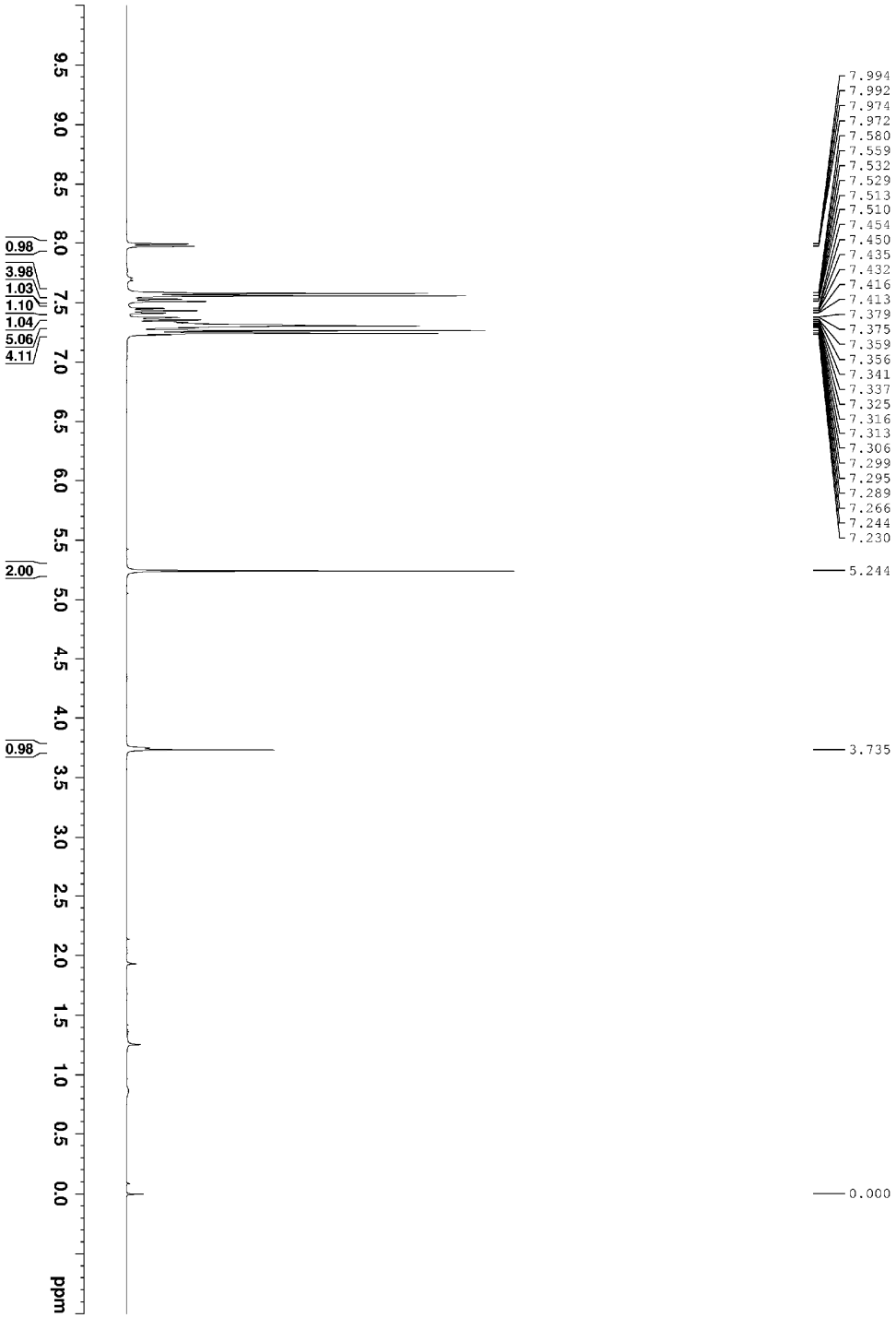
77.32
77.00
76.68
74.19
66.84
55.21
55.19


O
O
OH
Cl
Cl

1h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4.11
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0.98
ppm
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7.580
7.559
7.532
7.529
7.513
7.510
7.454
7.450
7.435
7.432
7.416
7.413
7.379
7.375
7.359
7.356
7.341
7.337
7.325
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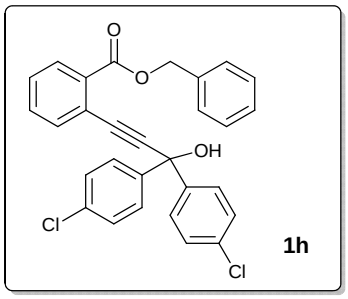
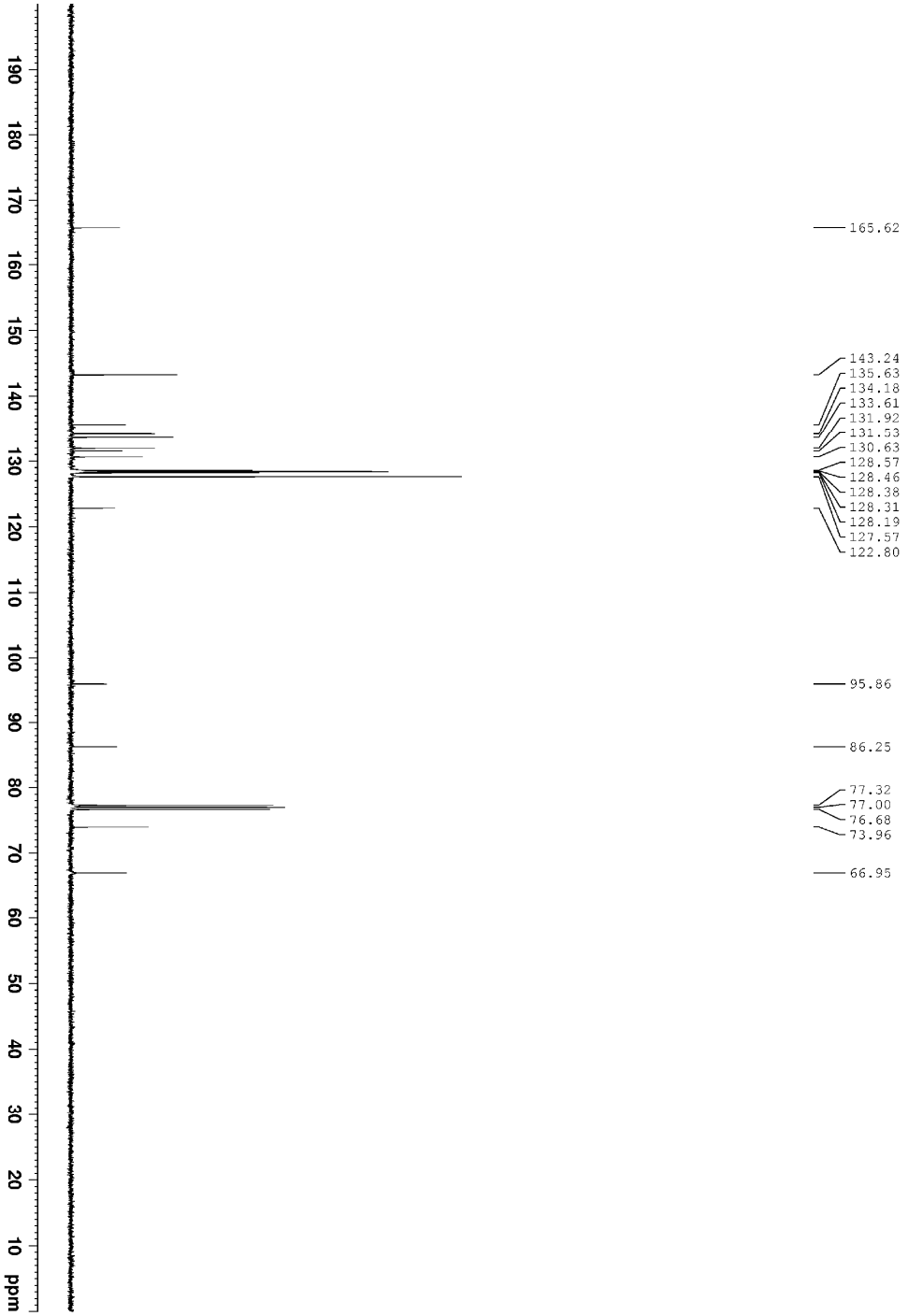
0.000


O
O
OH
Cl
Cl

1h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70
60
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40
30
20
10
ppm
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143.24
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134.18
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131.53
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128.57
128.46
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127.57
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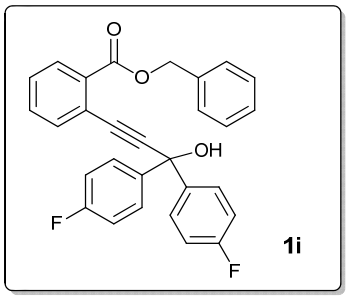
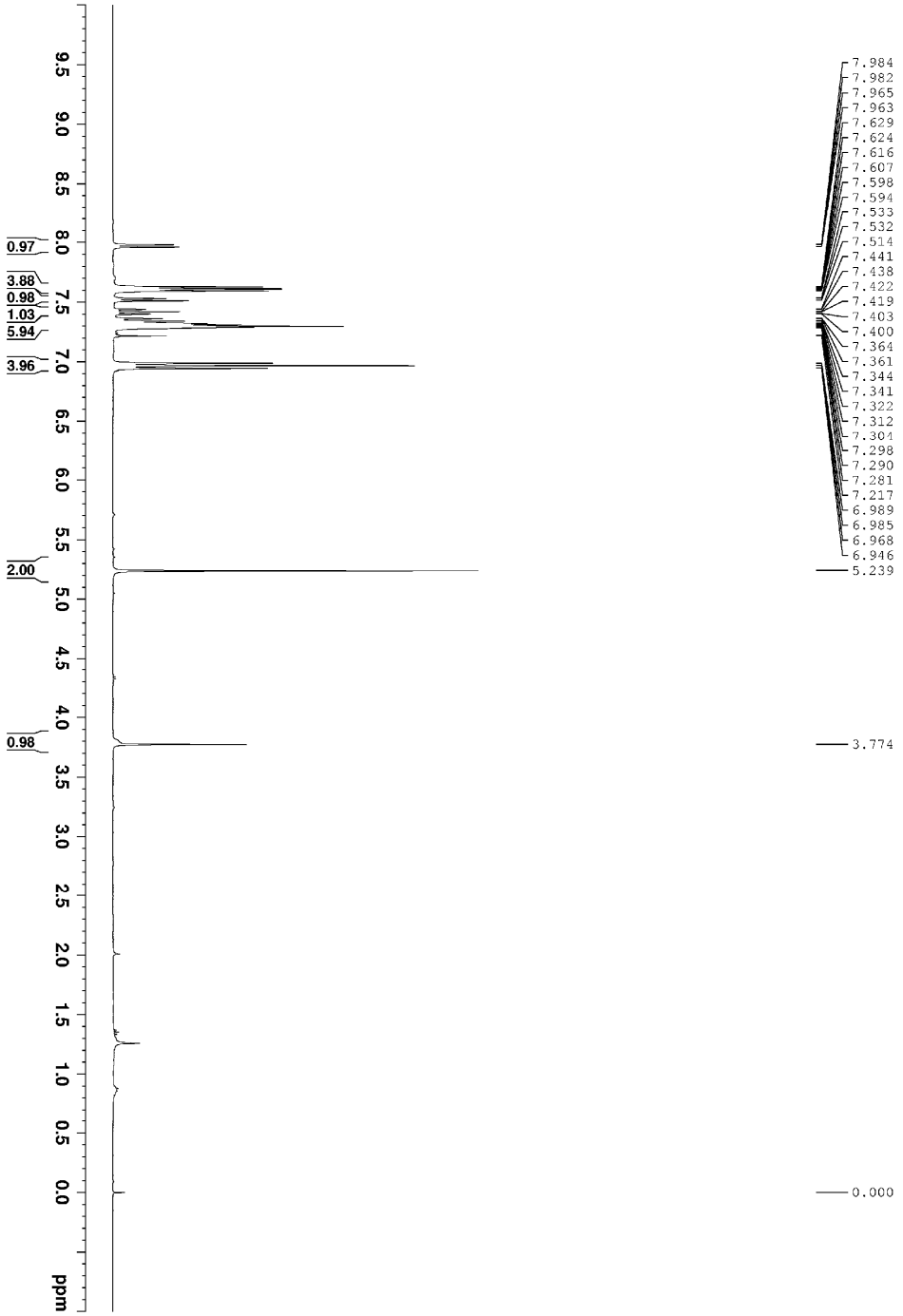
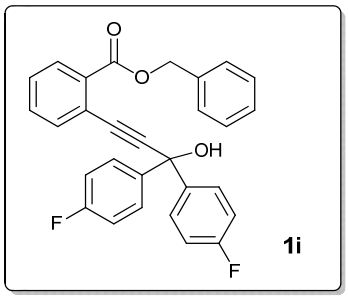
76.68
73.96
66.95



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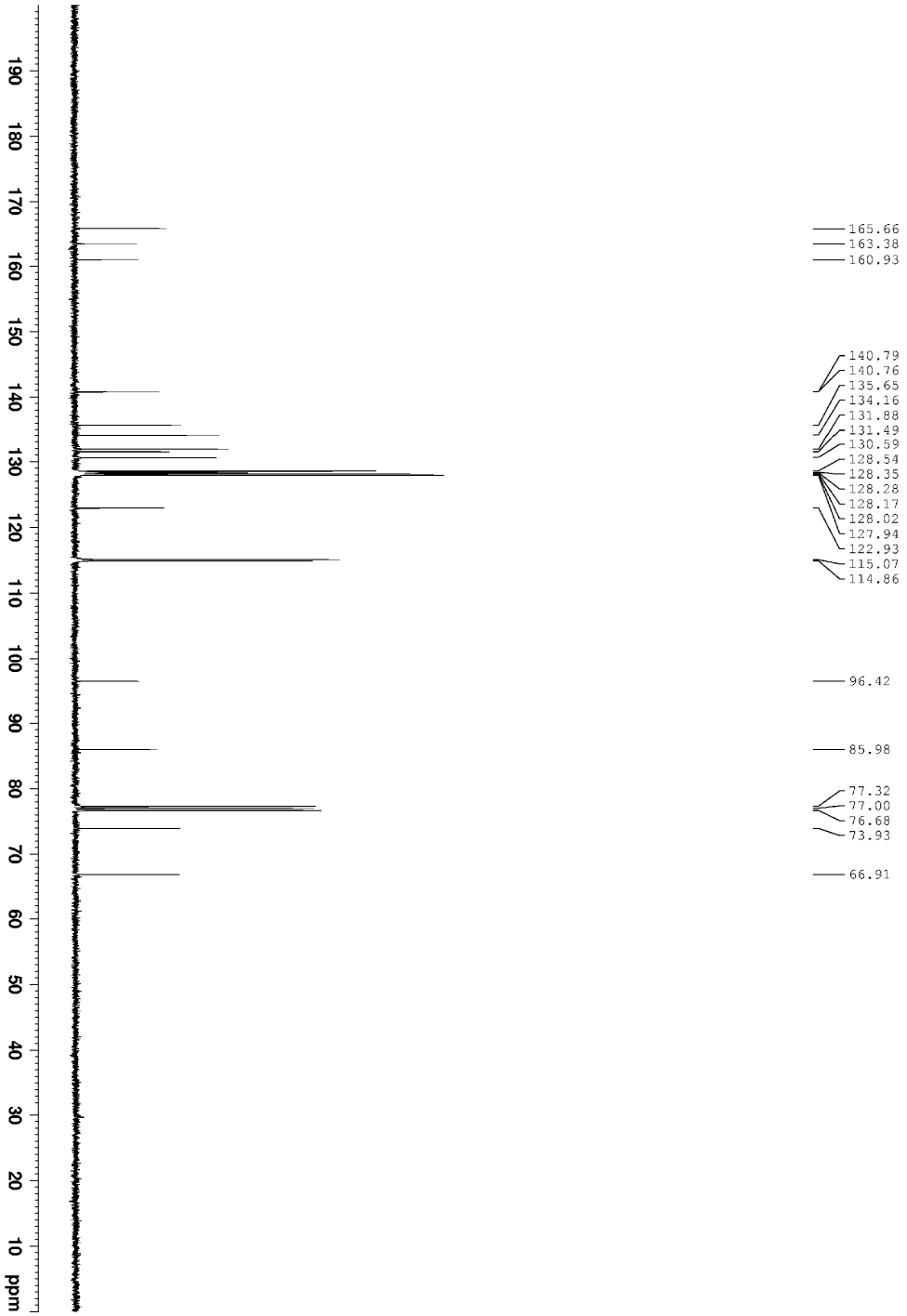
O
OH
F
F

1i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40
30
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10
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165.66
163.38
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140.79
140.76
135.65
134.16
131.88
131.49
130.59
128.54
128.35
128.28
128.17
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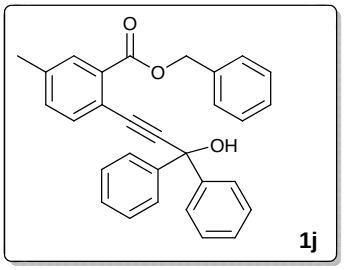
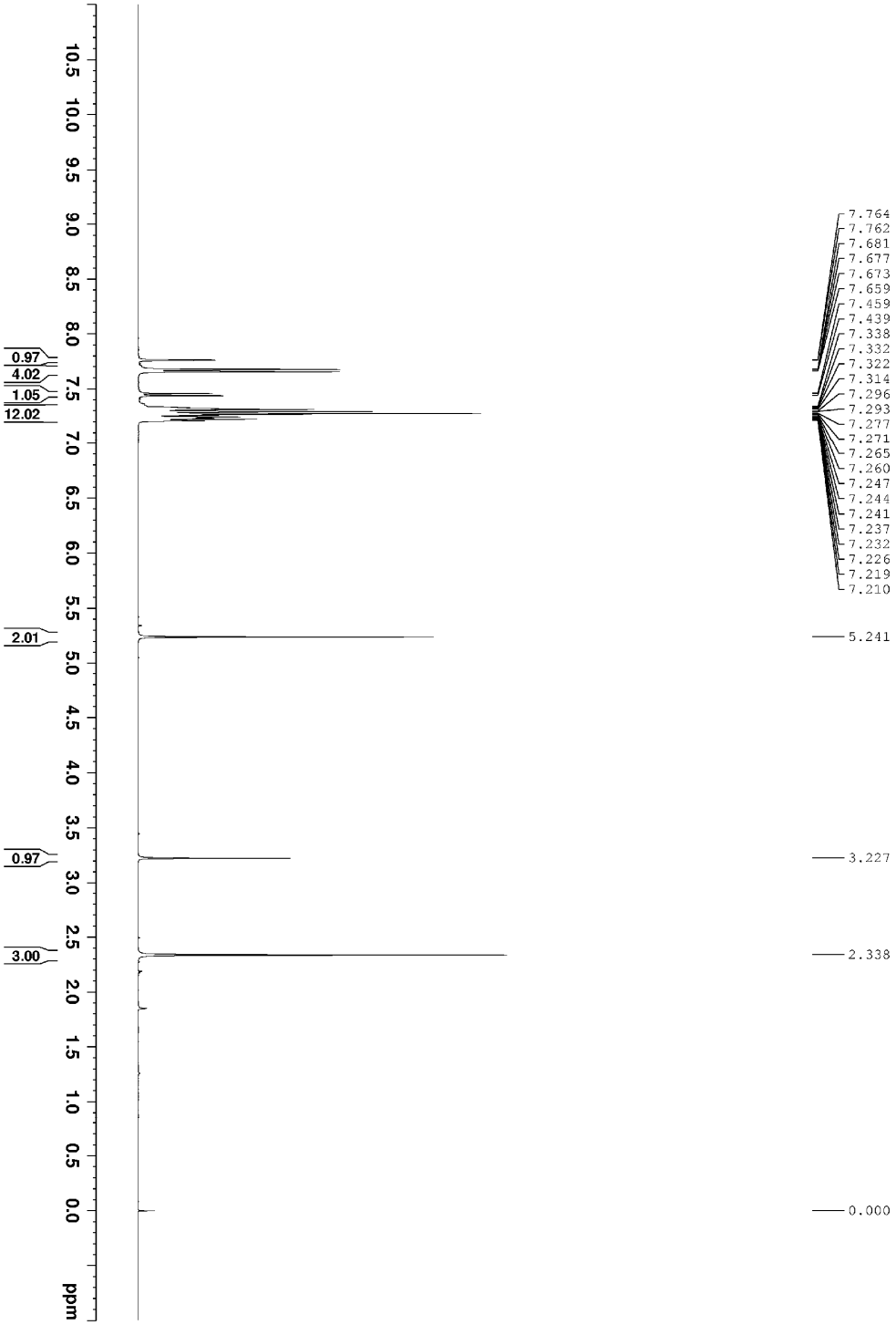
85.98
77.32
77.00
76.68
73.93
66.91


O
O
OH
1j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7.439
7.338
7.332
7.322
7.314
7.296
7.293
7.277
7.271
7.265
7.260
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7.237
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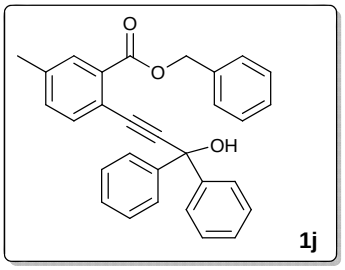
0.000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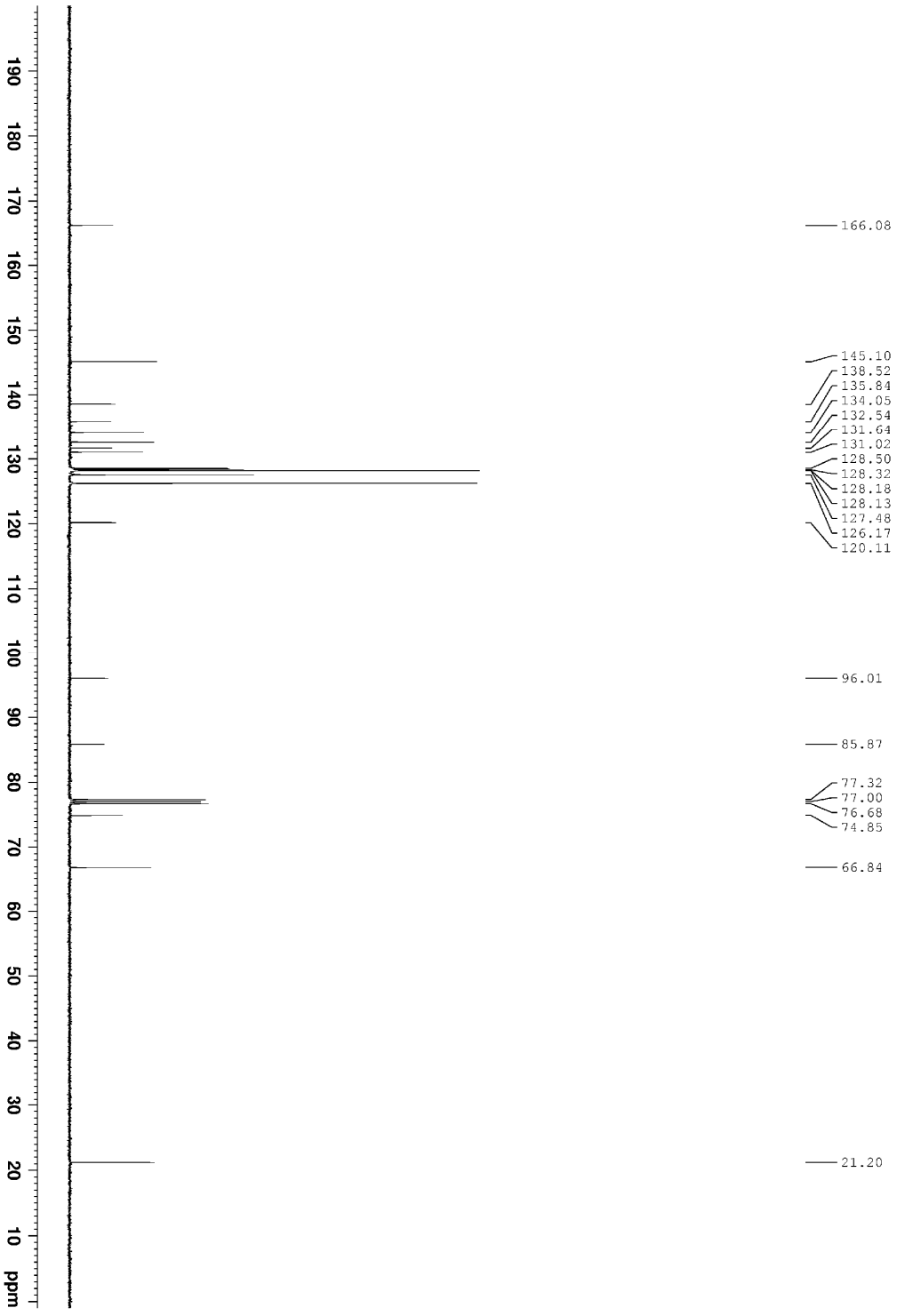
O
OH
1j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140
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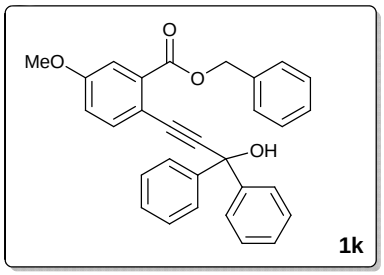
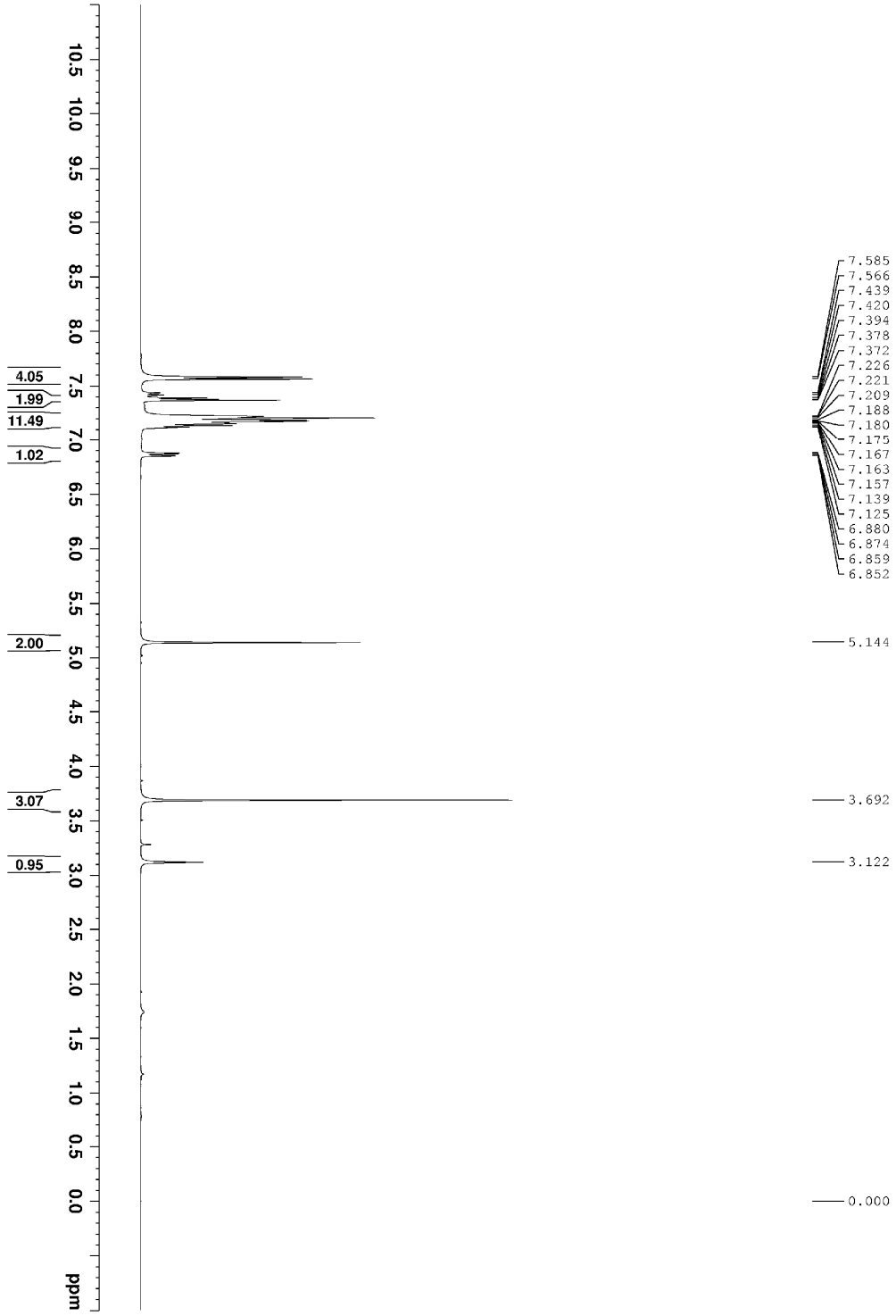
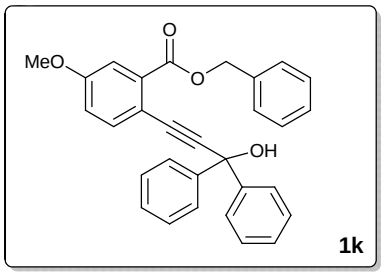
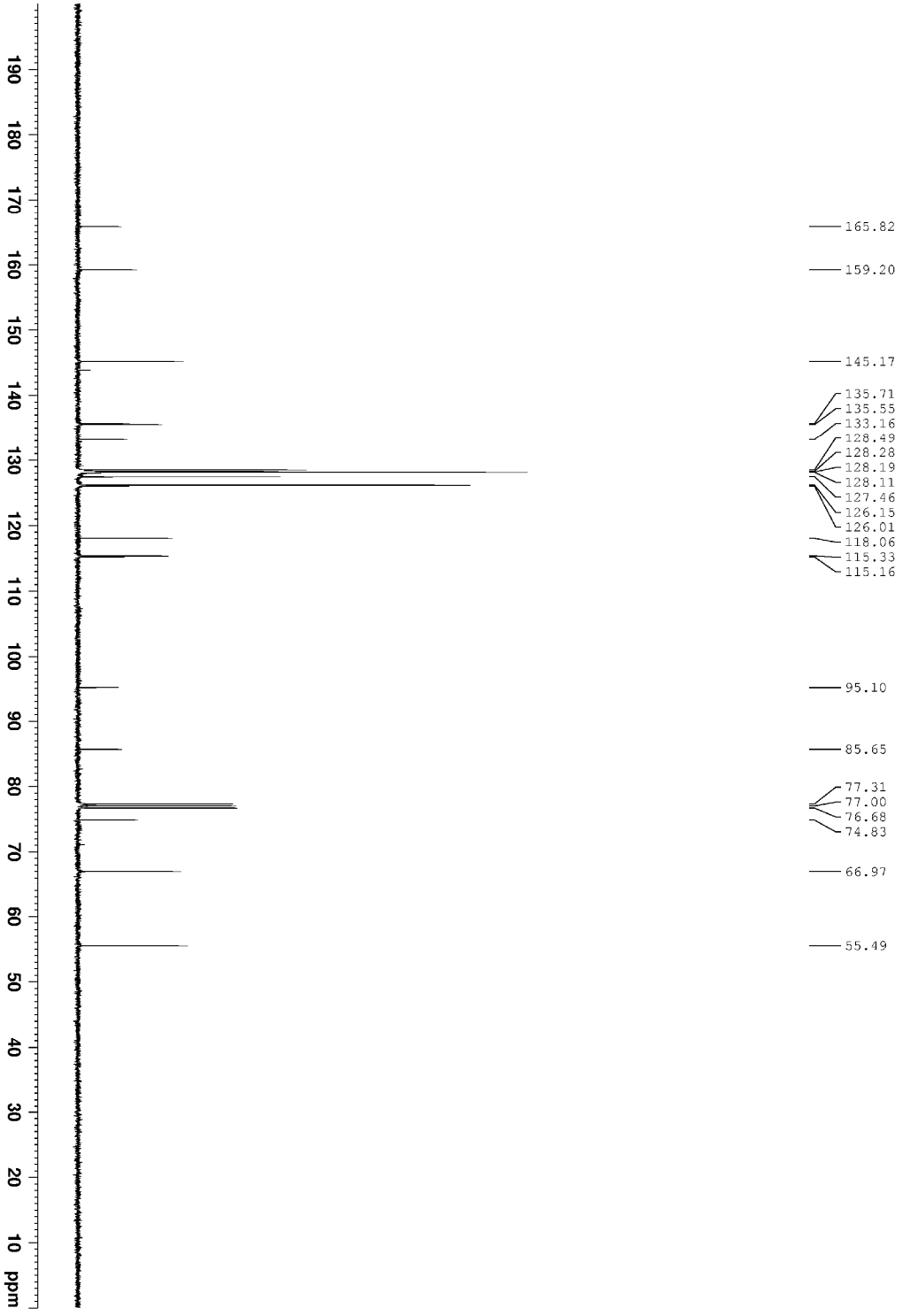
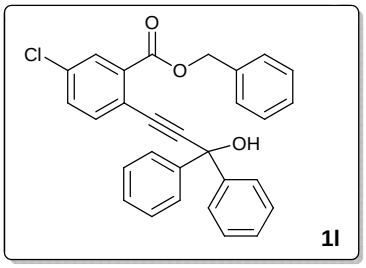
120
110
100
90
80
70
60
50
40
30
20
10
ppm
166.08
145.10
138.52
135.84
134.05
132.54
131.64
131.02
128.50
128.32
128.18
128.13
127.48
126.17
120.11
96.01
85.87
77.32
77.00
76.68
74.85
66.84
21.20

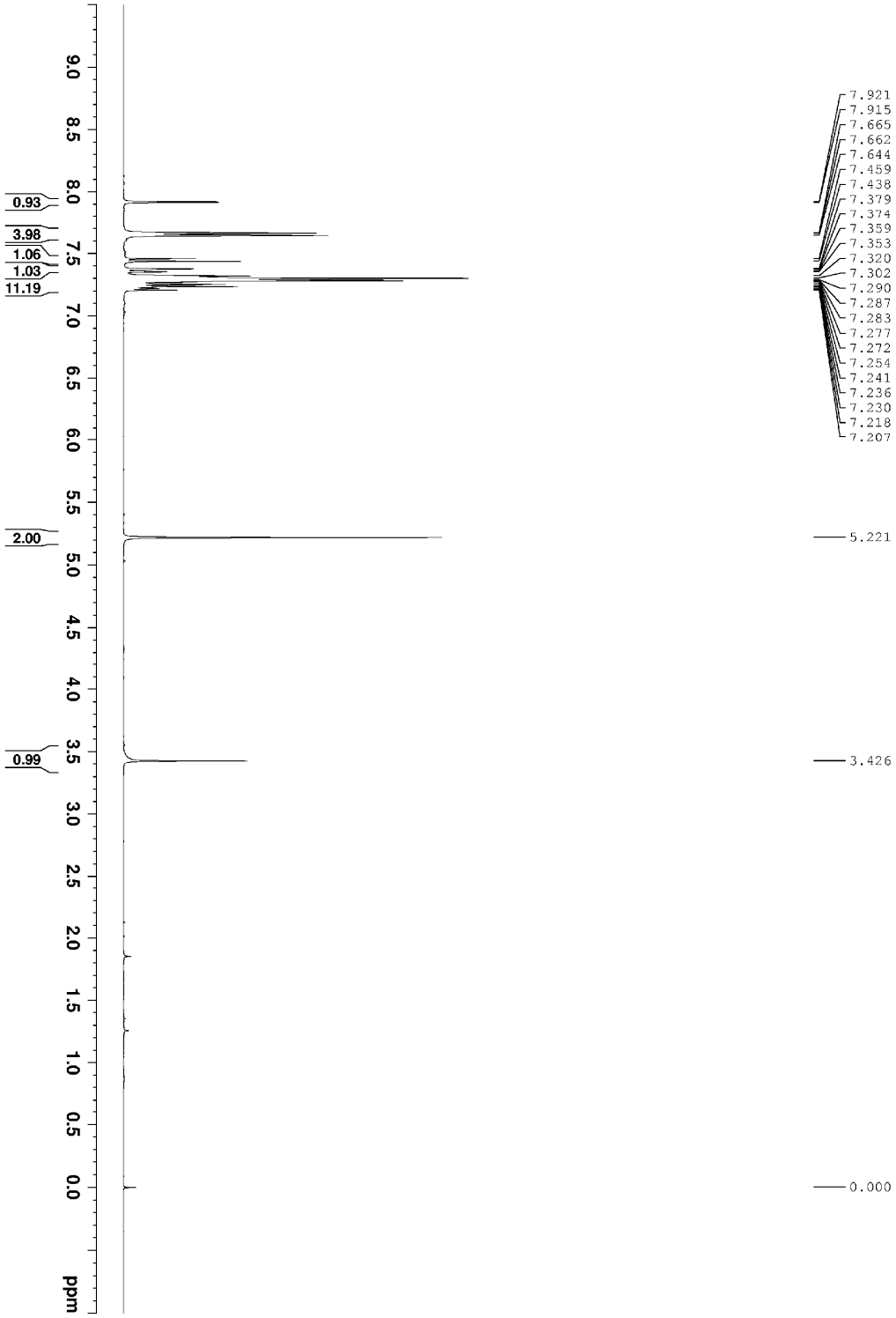









Cl
O
O
OH
1l


0.93
3.98
1.06
1.03
11.19
2.00
0.99
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
ppm
7.921
7.915
7.665
7.662
7.644
7.459
7.438
7.379
7.374
7.359
7.353
7.320
7.302
7.290
7.287
7.283
7.277
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7.254
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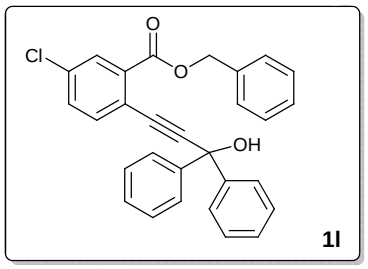
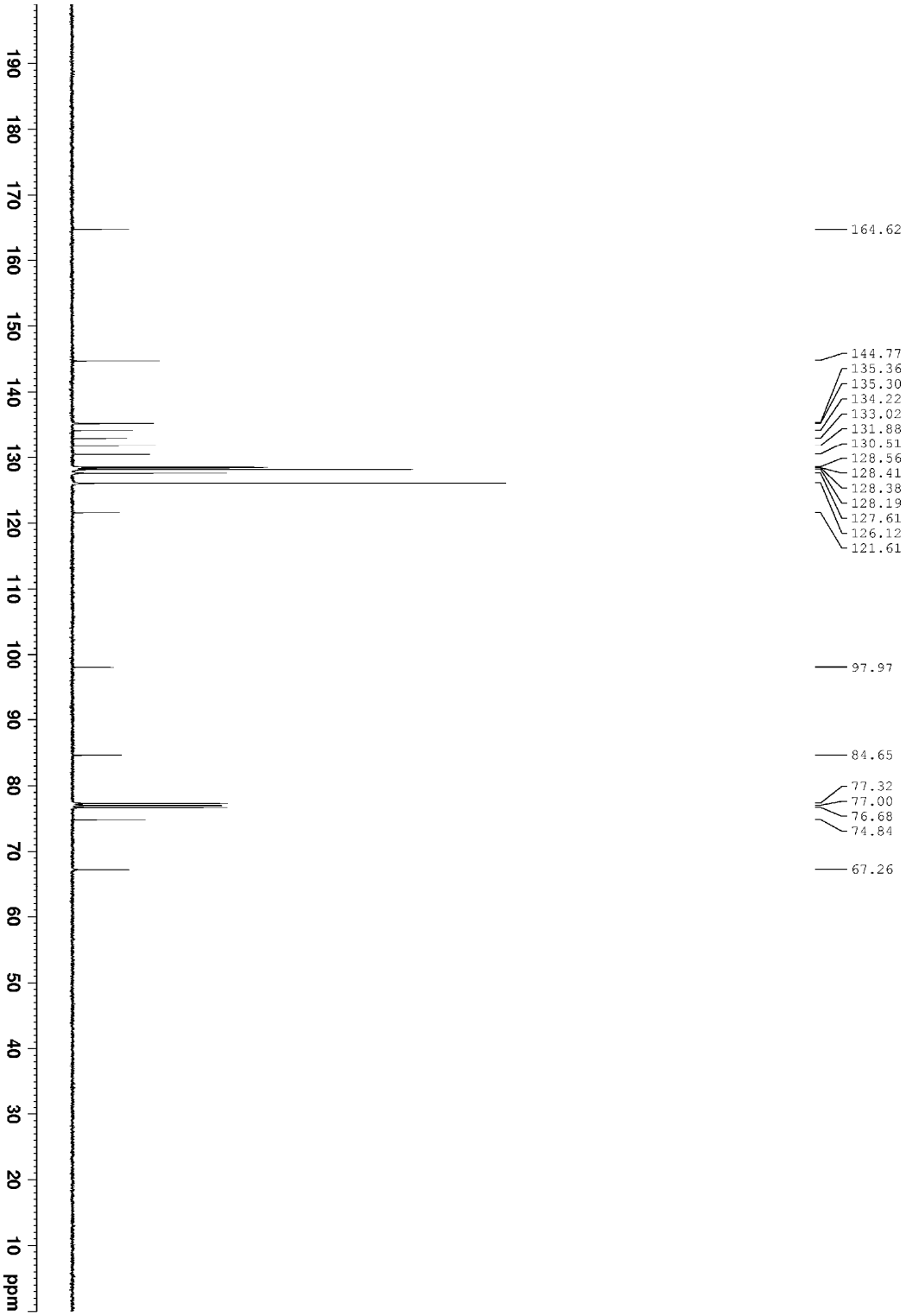
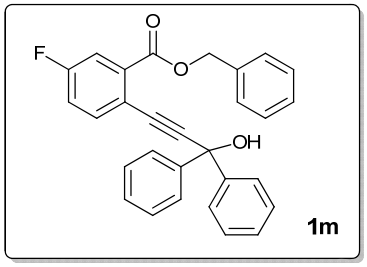
7.236
7.230
7.218
7.207
5.221
3.426
0.000

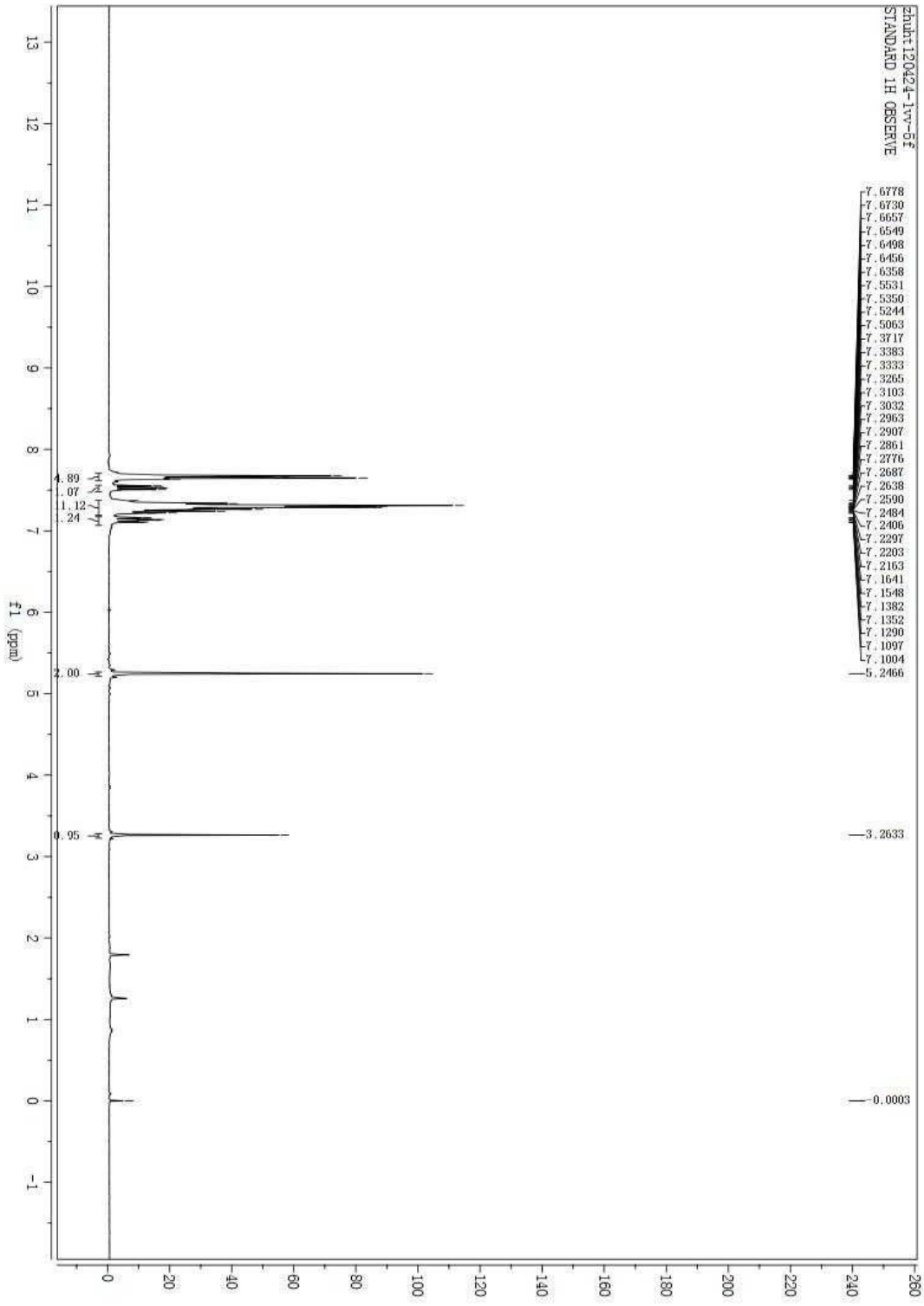

Cl
O
O
OH

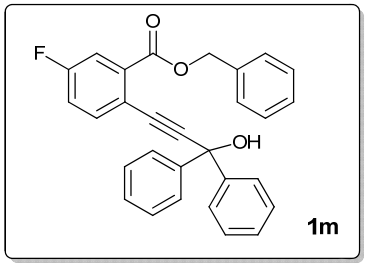
1l


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
164.62
144.77
135.36
135.30
134.22
133.02
131.88
130.51
128.56
128.41
128.38
128.19
127.61
126.12
121.61
97.97
84.65
77.32
77.00
76.68
74.84
67.26

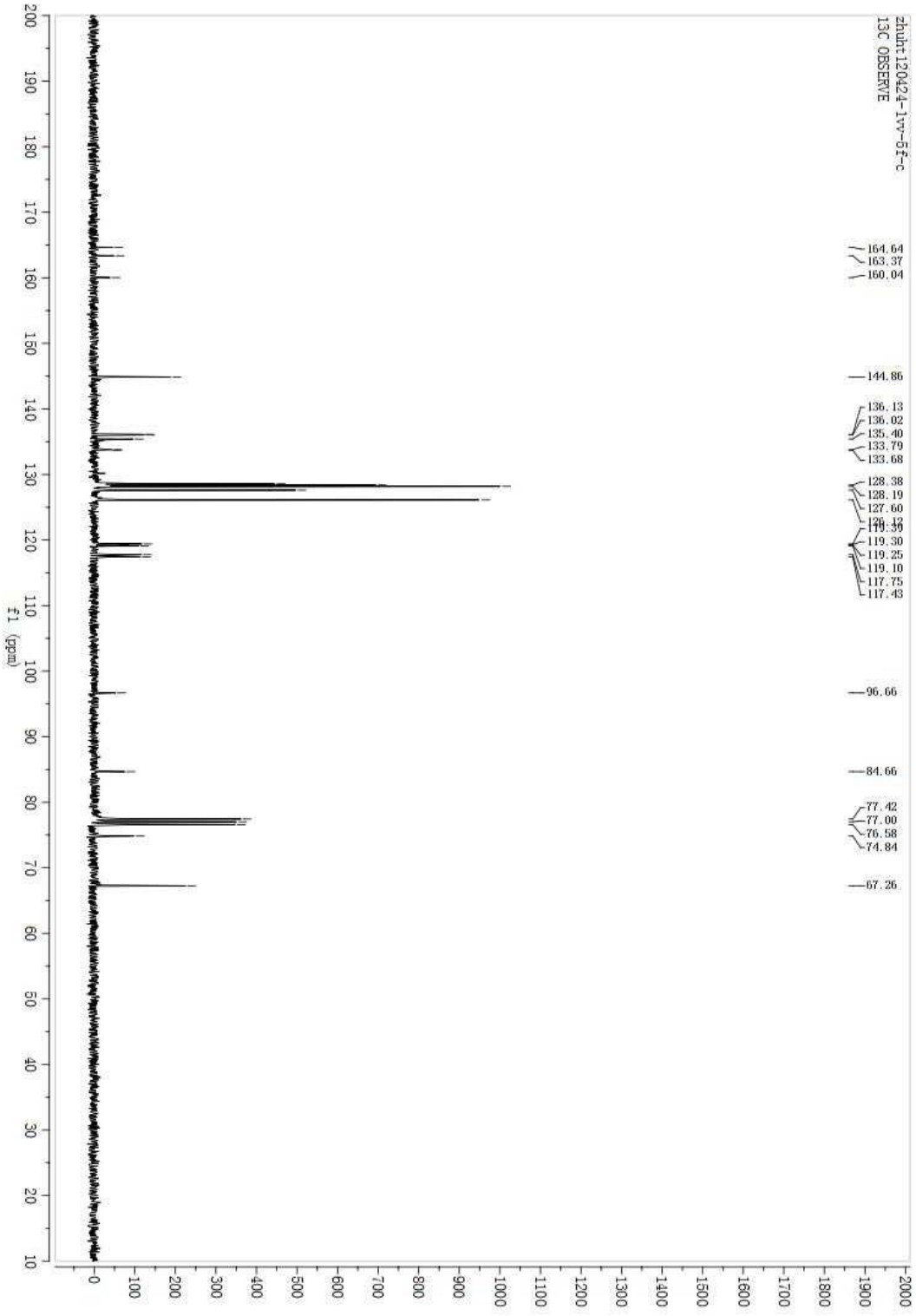

F
O
O
OH

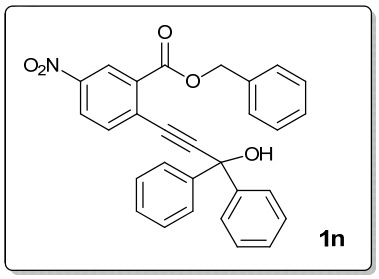
1m


zhuht120424-1vv-6f
STANDARD 1H OBSERVE
7.6778
7.6730
7.6657
7.6549
7.6498
7.6456
7.6358
7.5531
7.5350
7.5244
7.5063
7.3717
7.3383
7.3333
7.3265
7.3103
7.3032
7.2963
7.2907
7.2861
7.2776
7.2687
7.2638
7.2590
7.2484
7.2406
7.2297
7.2203
7.2163
7.1641
7.1548
7.1382
7.1352
7.1290
7.1097
7.1004
5.2466
3.2633
0.0003
4.89
1.07
1.12
1.24
2.00
0.95
f1 (ppm)

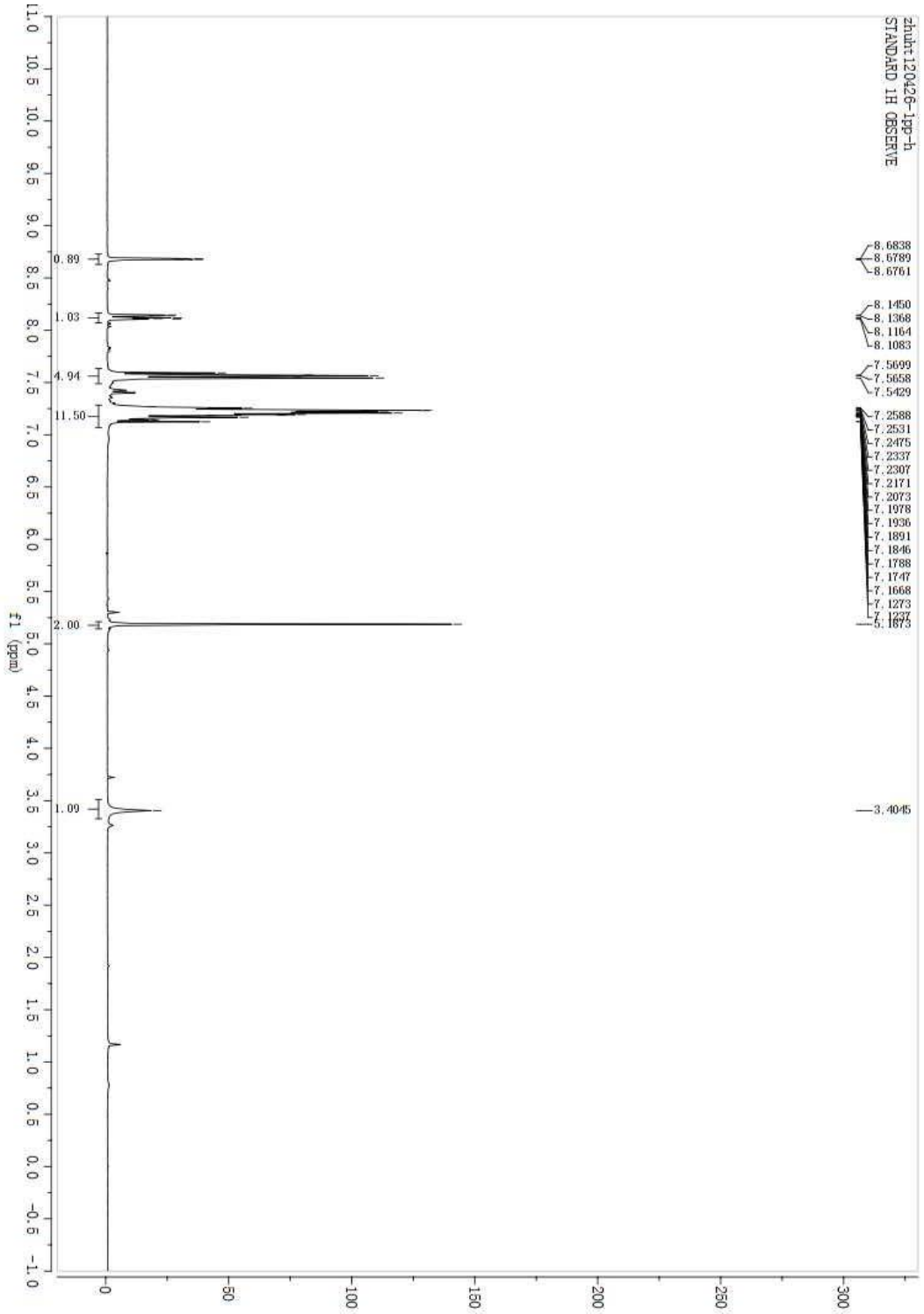

F
O
O
OH

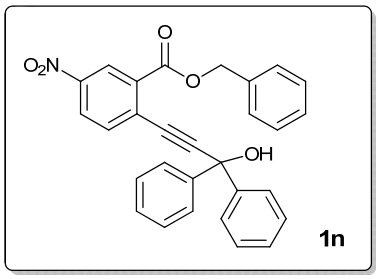
1m


zhuht120424-1w-5f-c
13C OBSERVE
164.64
163.37
160.04
144.86
136.13
136.02
135.40
133.79
133.68
128.38
128.19
127.60
119.30
119.25
119.10
117.75
117.43
96.66
84.66
77.42
77.00
76.58
74.84
67.26
f1 (ppm)

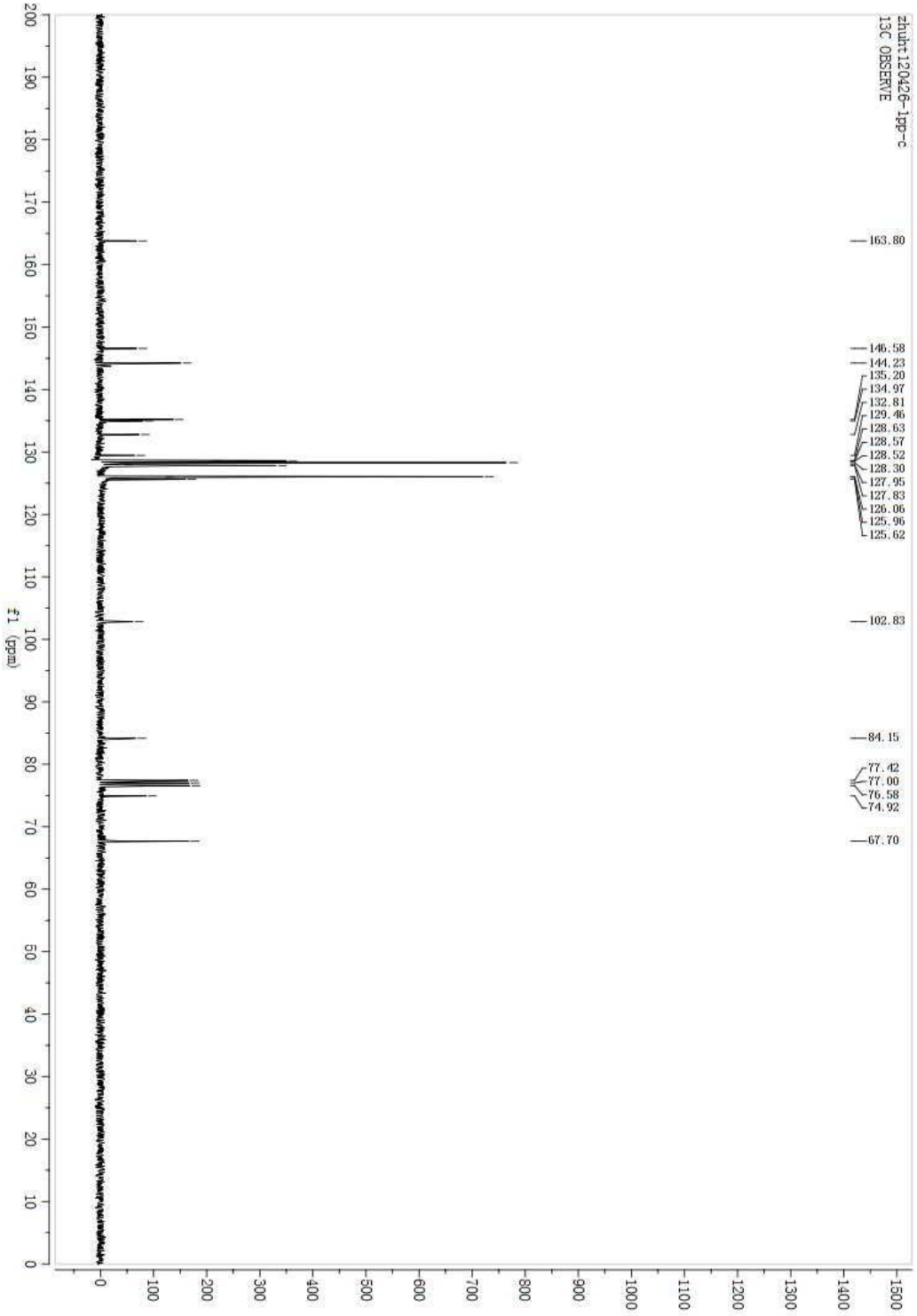

O
O2N
O
OH

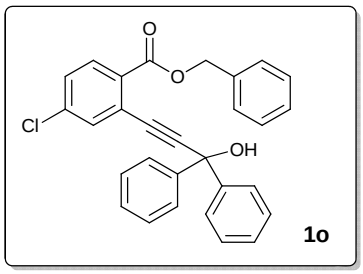
1n


zhuht120426-1pp-h
STANDARD 1H OBSERVE
0.89
1.03
4.94
11.50
2.00
1.09
f1 (ppm)
8.6838
8.6789
8.6761
8.1450
8.1368
8.1164
8.1083
7.5699
7.5658
7.5429
7.2588
7.2531
7.2475
7.2337
7.2307
7.2171
7.2073
7.1978
7.1936
7.1891
7.1846
7.1788
7.1747
7.1668
7.1273
7.1237
5.1873
3.4045

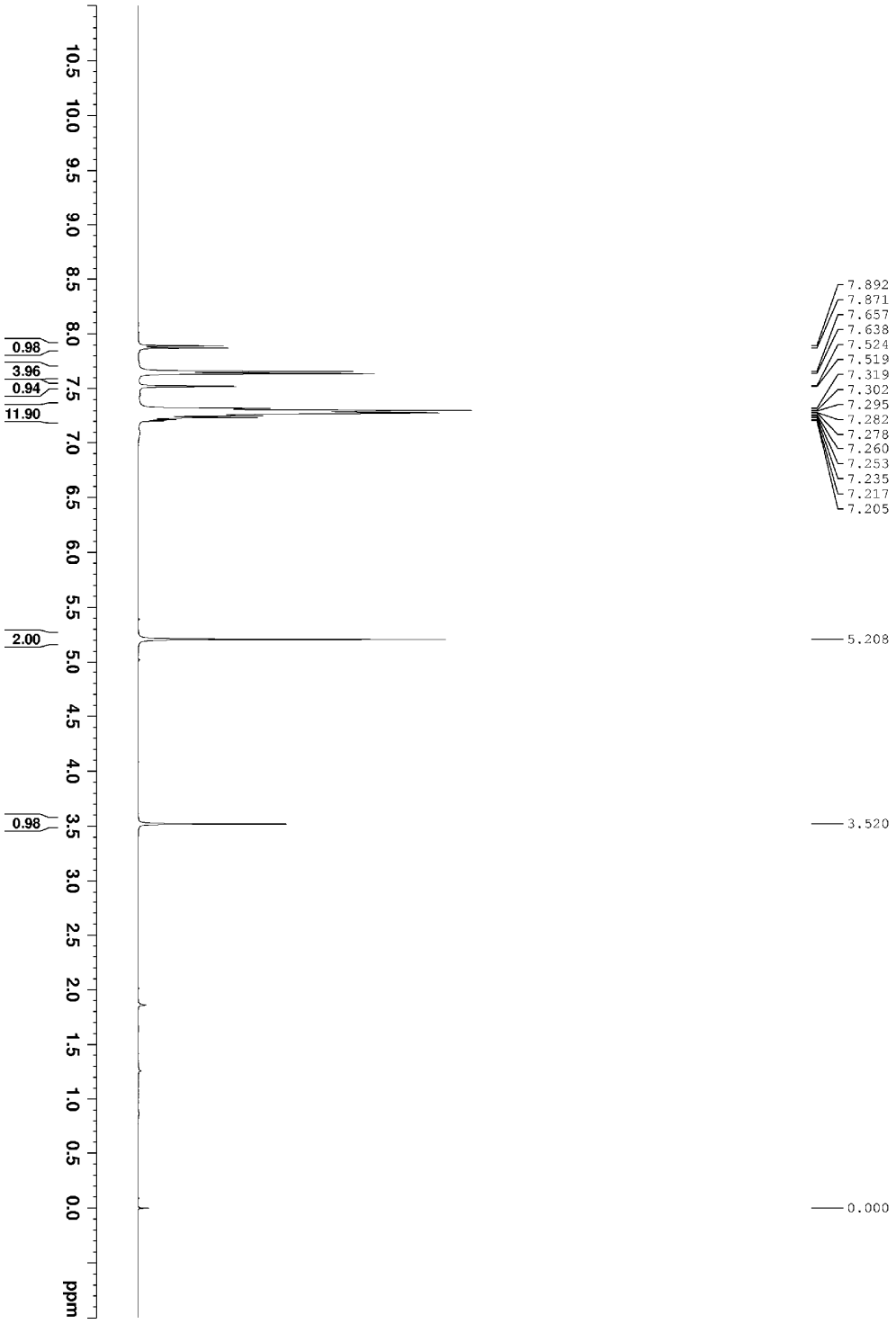

O
O2N
O
OH

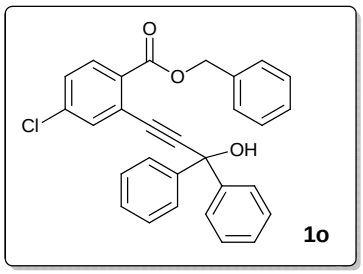
1n


zhubt120426-1pp-c
13C OBSERVE
163.80
146.58
144.23
135.20
134.97
132.81
129.46
128.63
128.57
128.52
128.30
127.95
127.83
126.06
125.96
125.62
102.83
84.15
77.42
77.00
76.58
74.92
67.70
f1 (ppm)

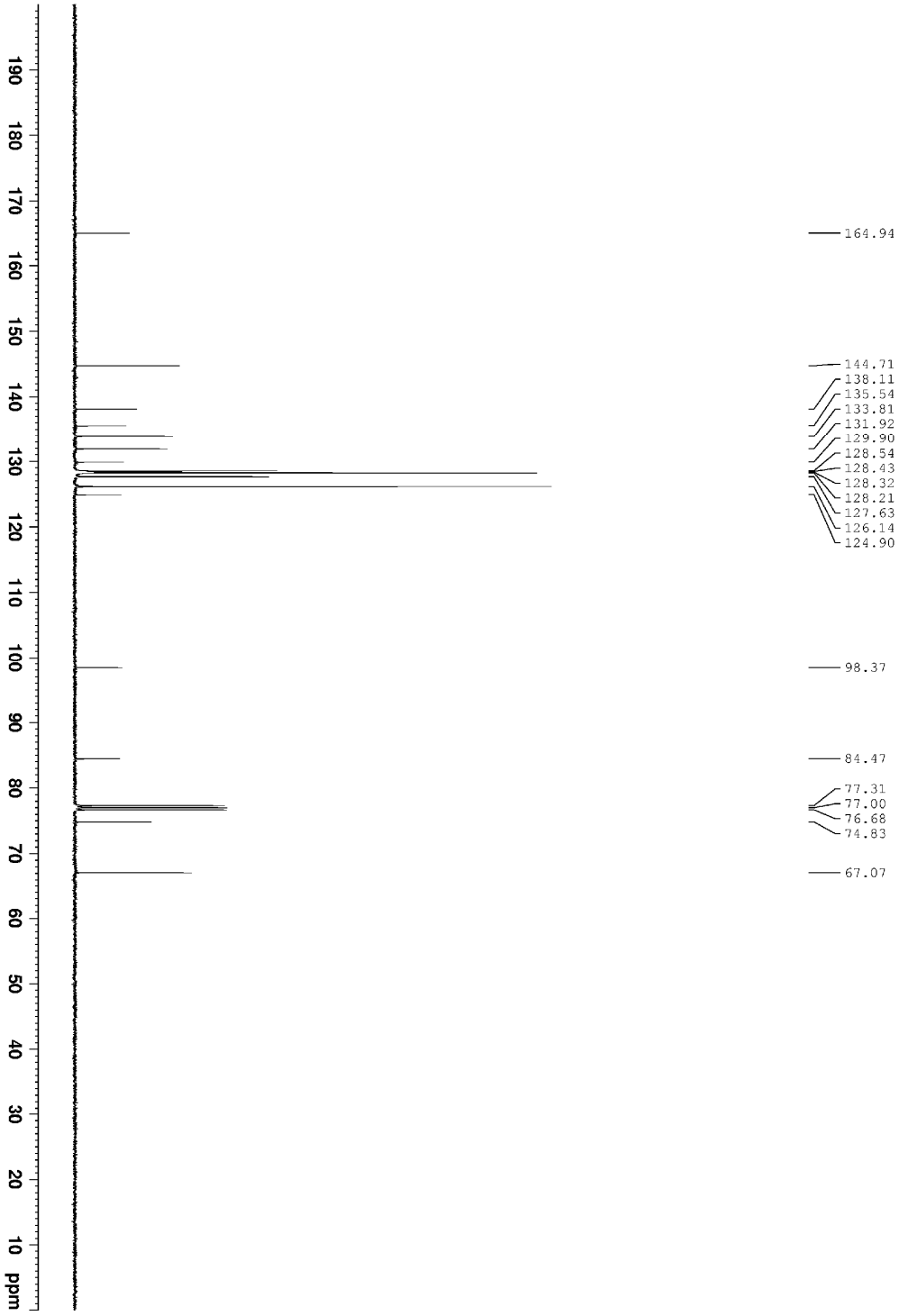

O
O
Cl
OH

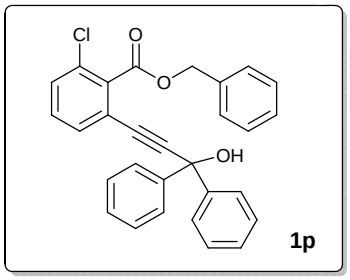
1o


0.98
3.96
0.94
11.90
2.00
0.98
7.892
7.871
7.657
7.638
7.524
7.519
7.319
7.302
7.295
7.282
7.278
7.260
7.253
7.235
7.217
7.205
5.208
3.520
0.000
ppm

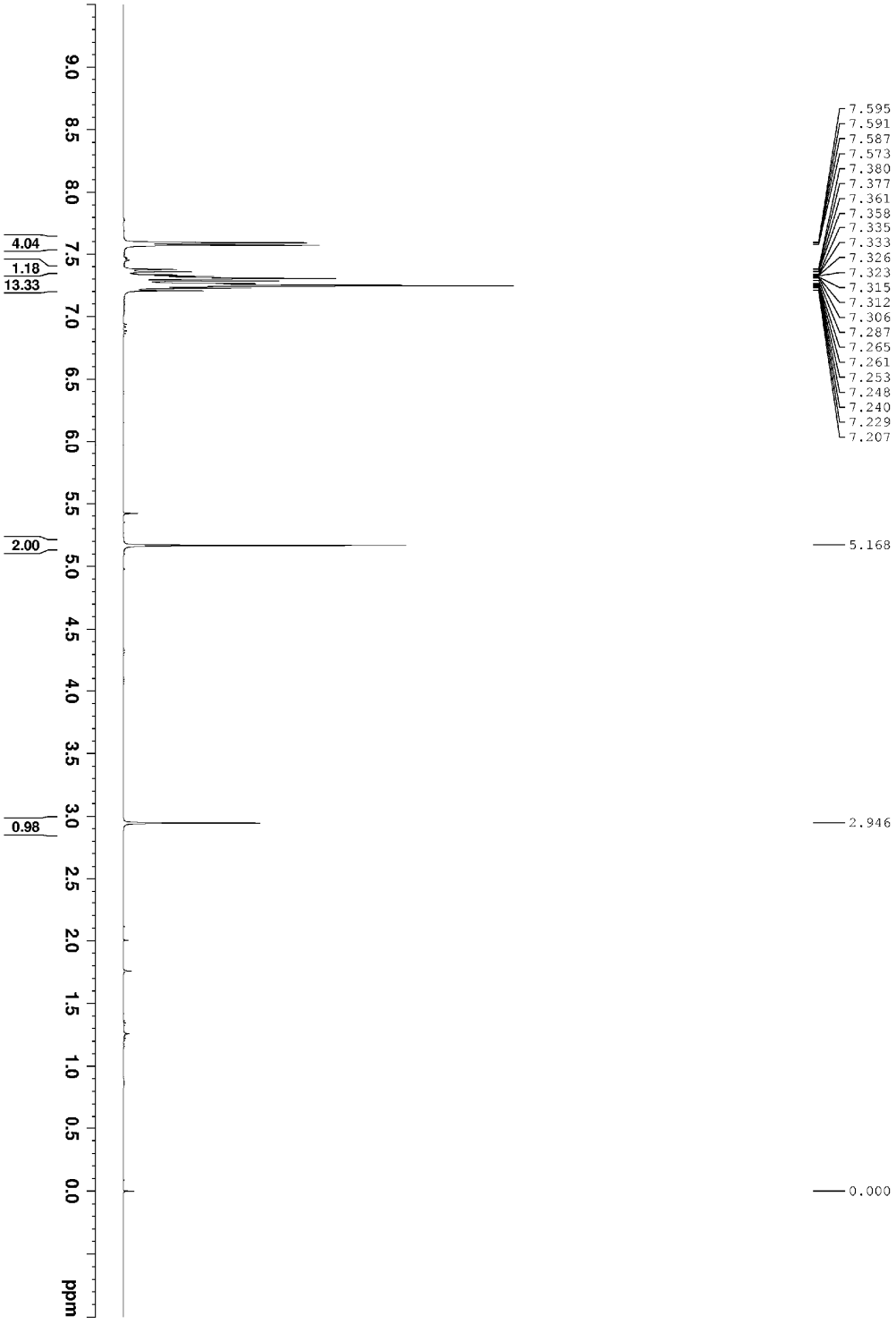

O
O
Cl
OH

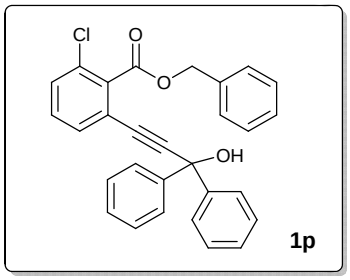
1o


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
164.94
144.71
138.11
135.54
133.81
131.92
129.90
128.54
128.43
128.32
128.21
127.63
126.14
124.90
98.37
84.47
77.31
77.00
76.68
74.83
67.07

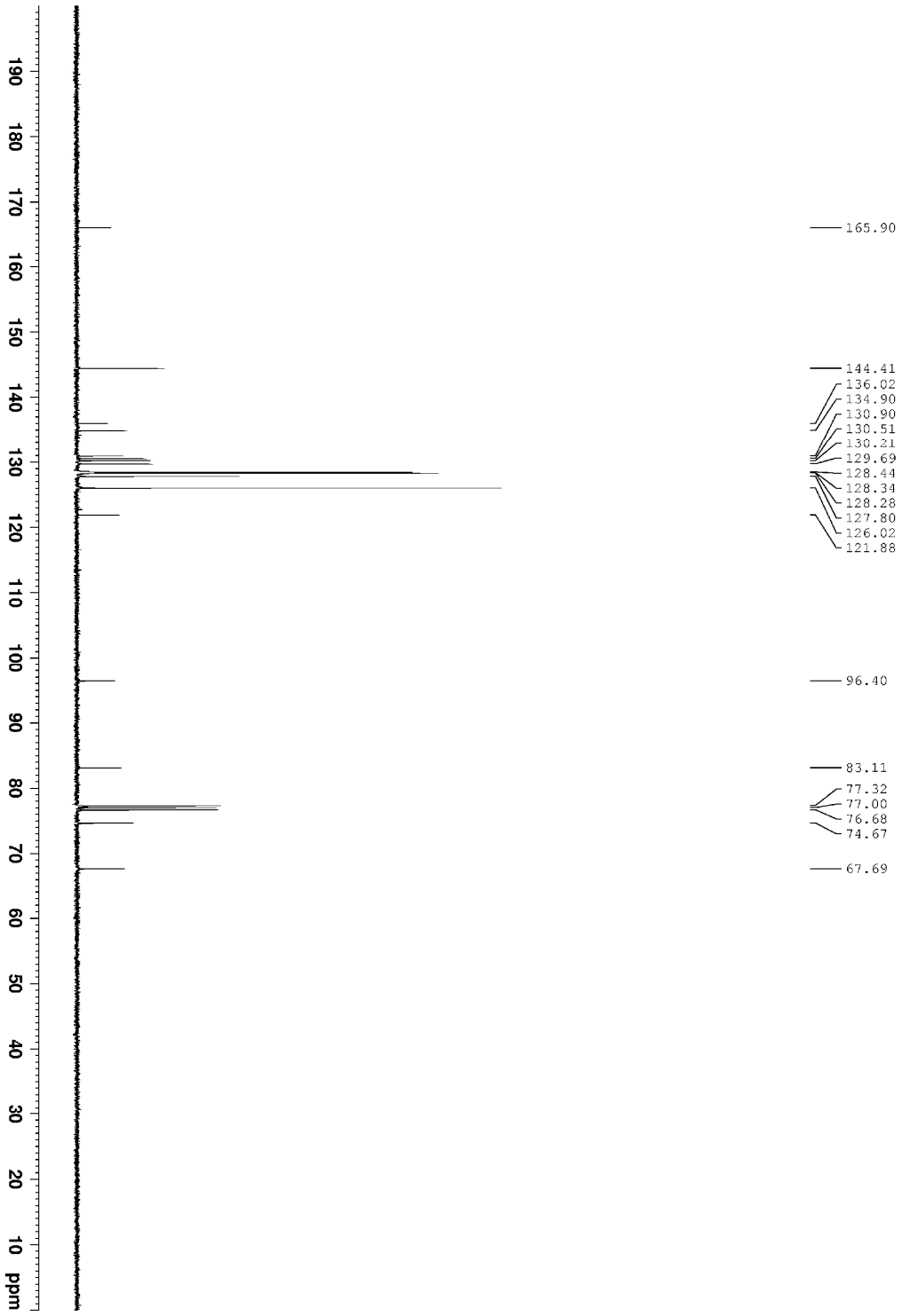

Cl
O
O
OH

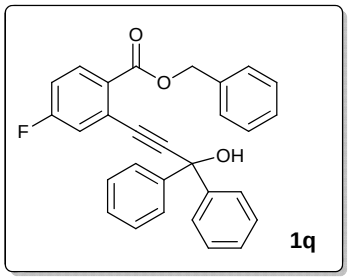
1p


4.04
1.18
13.33
2.00
0.98
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
ppm
7.595
7.591
7.587
7.573
7.380
7.377
7.361
7.358
7.335
7.333
7.326
7.323
7.315
7.312
7.306
7.287
7.265
7.261
7.253
7.248
7.240
7.229
7.207
5.168
2.946
0.000

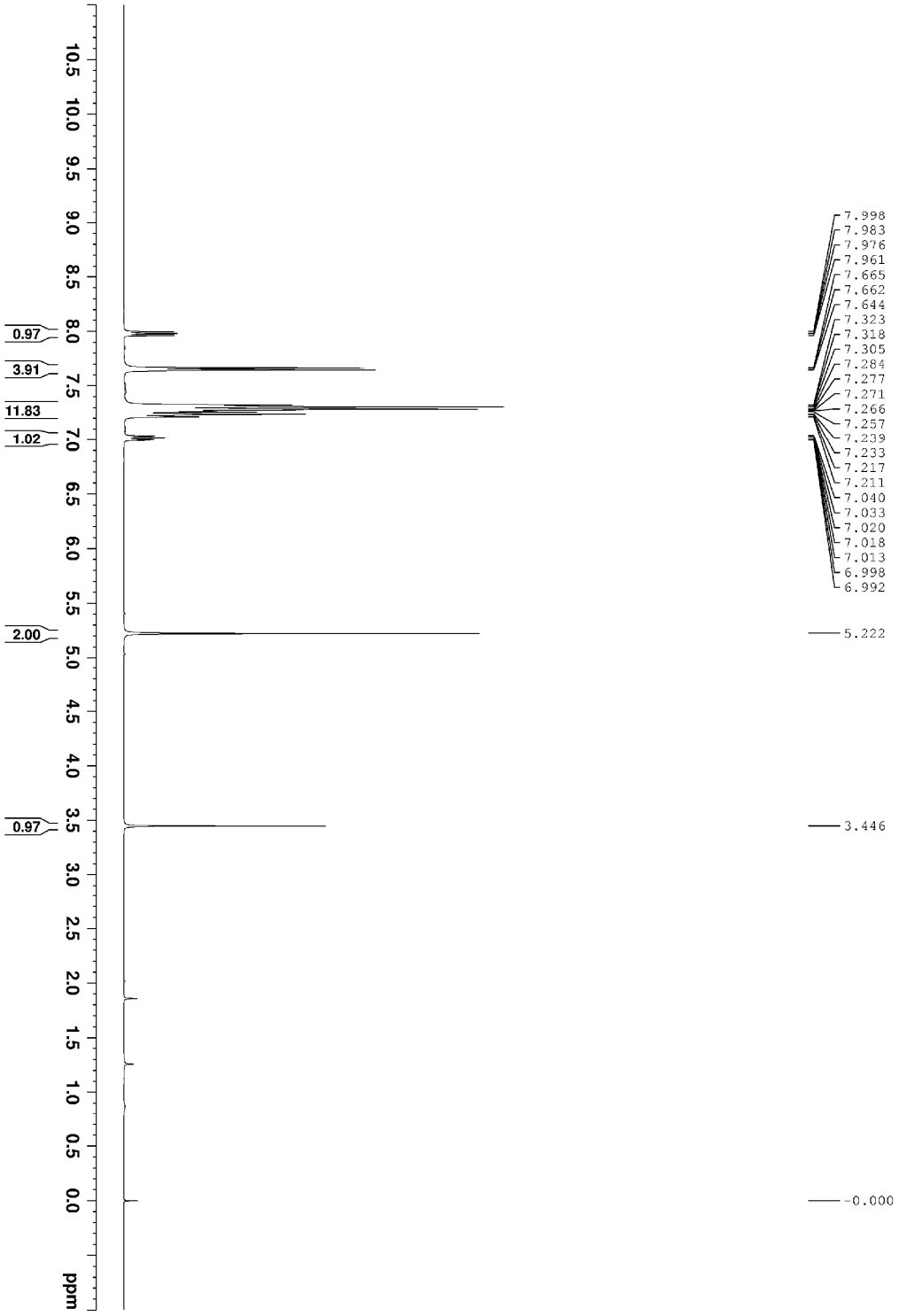


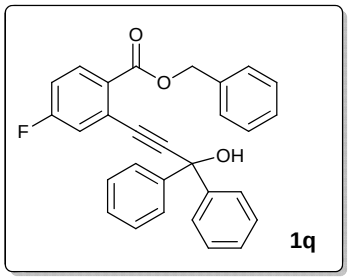
1p



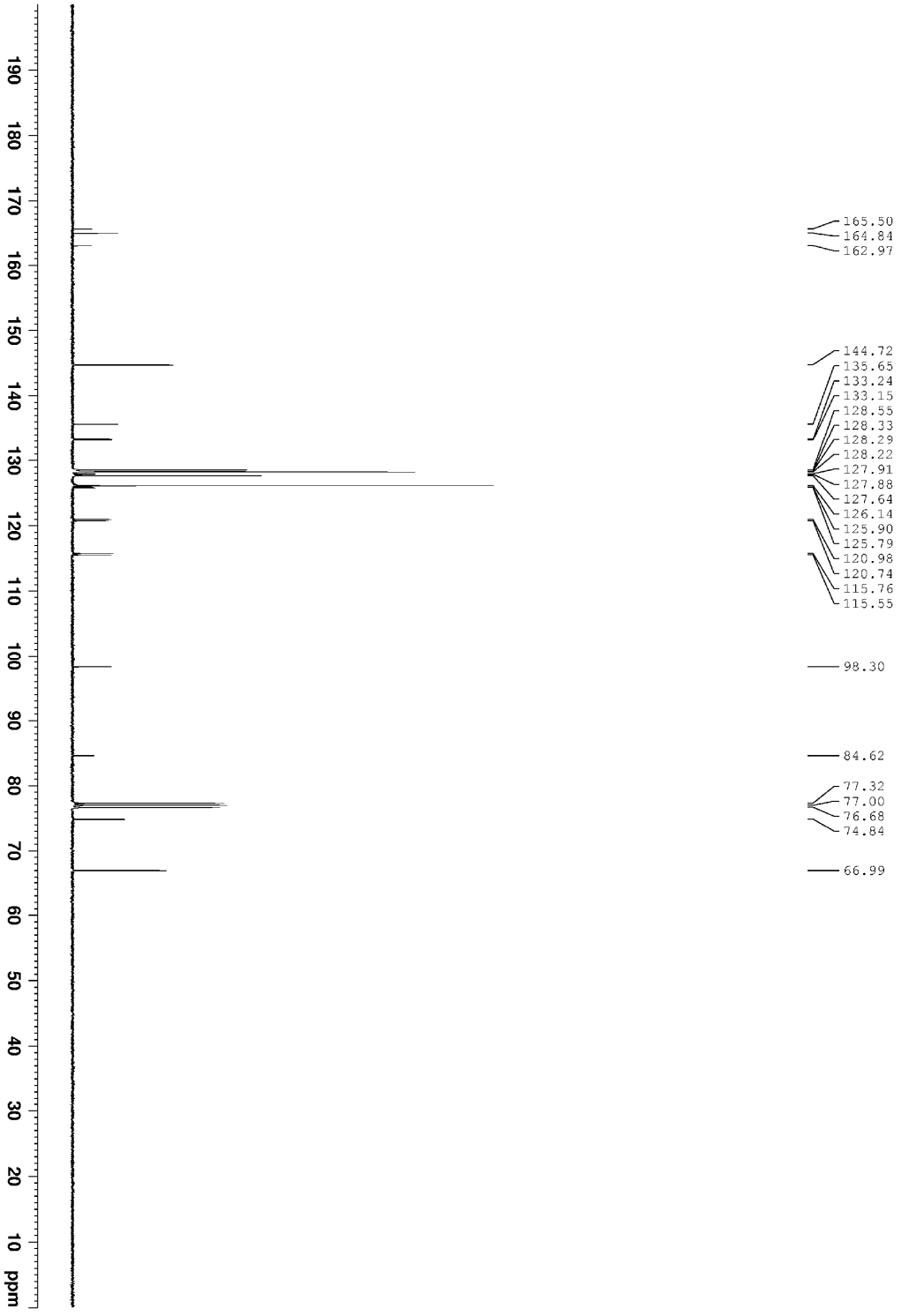

O
O
F
OH

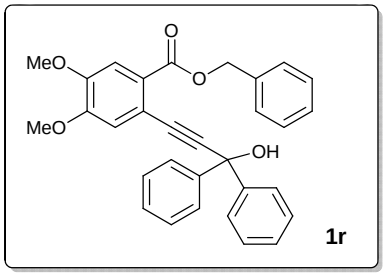
1q


0.97
3.91
11.83
1.02
2.00
0.97
7.998
7.983
7.976
7.961
7.665
7.662
7.644
7.323
7.318
7.305
7.284
7.277
7.271
7.266
7.257
7.239
7.233
7.217
7.211
7.040
7.033
7.020
7.018
7.013
6.998
6.992
5.222
3.446
-0.000
ppm

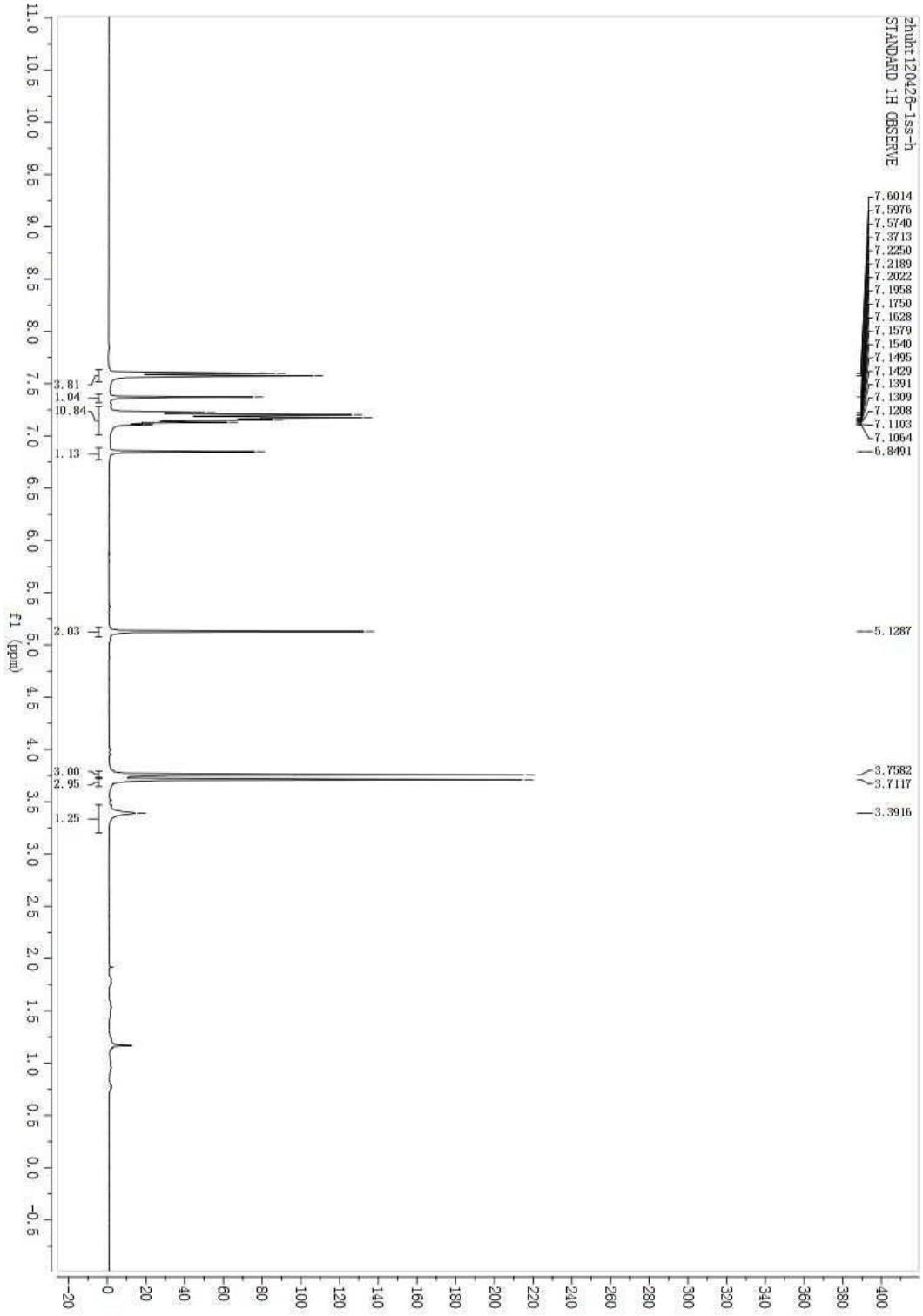

O
O
F
OH

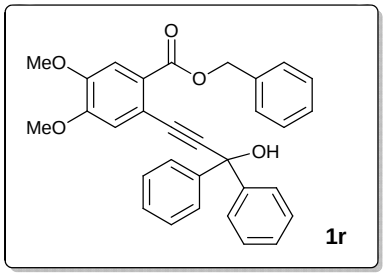
1q


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
165.50
164.84
162.97
144.72
135.65
133.24
133.15
128.55
128.33
128.29
128.22
127.91
127.88
127.64
126.14
125.90
125.79
120.98
120.74
115.76
115.55
98.30
84.62
77.32
77.00
76.68
74.84
66.99

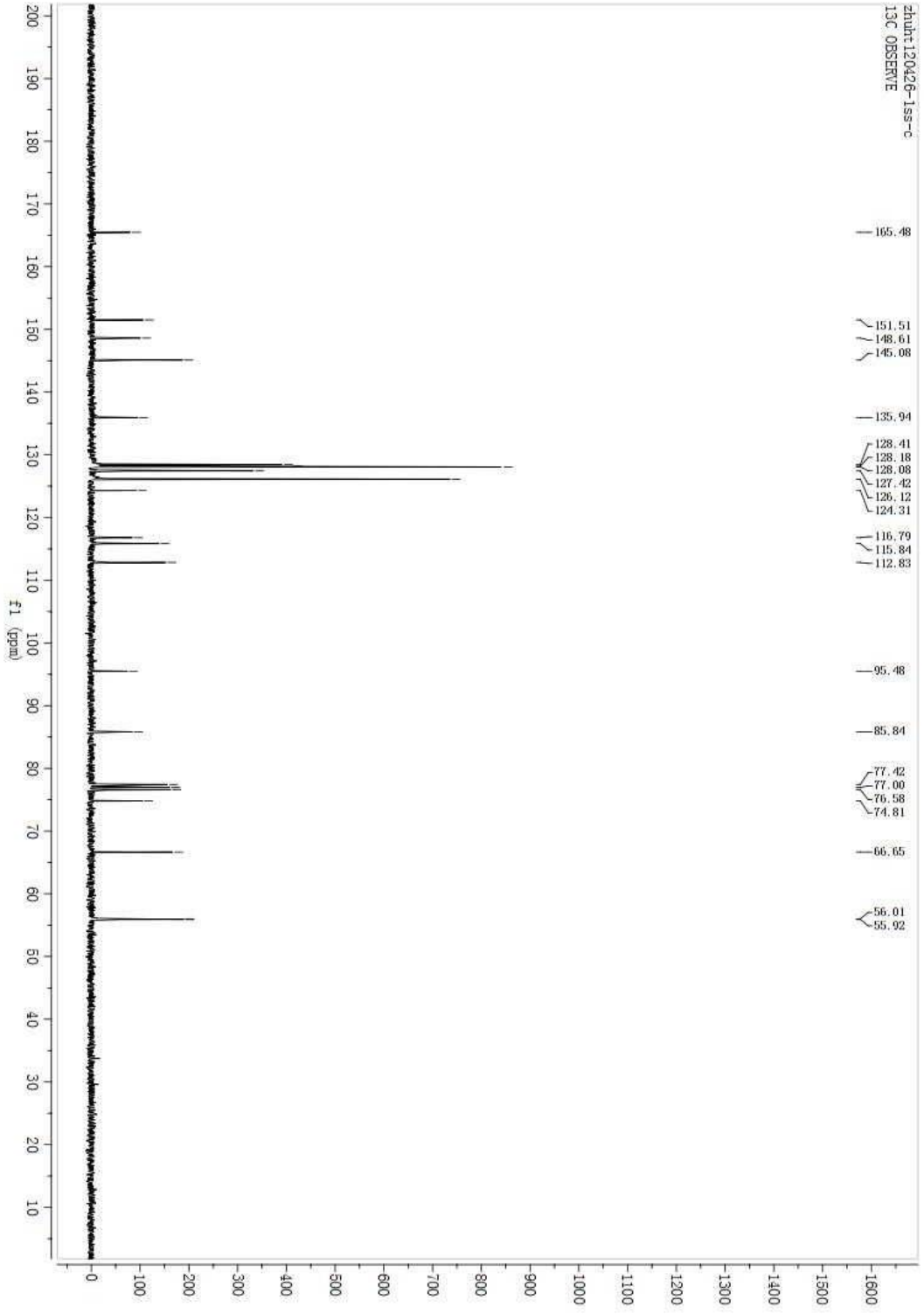

MeO
MeO
O
O
OH

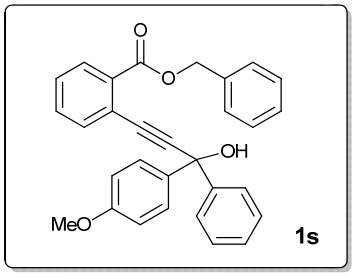
1r


zhubt120426-1ss-h
STANDARD 1H OBSERVE
7.6014
7.5976
7.5740
7.3713
7.2250
7.2189
7.2022
7.1958
7.1750
7.1628
7.1579
7.1540
7.1495
7.1429
7.1391
7.1309
7.1208
7.1103
7.1064
6.8491
5.1287
3.7582
3.7117
3.3916
3.81
1.04
10.84
1.13
2.03
3.00
2.95
1.25
f1 (ppm)

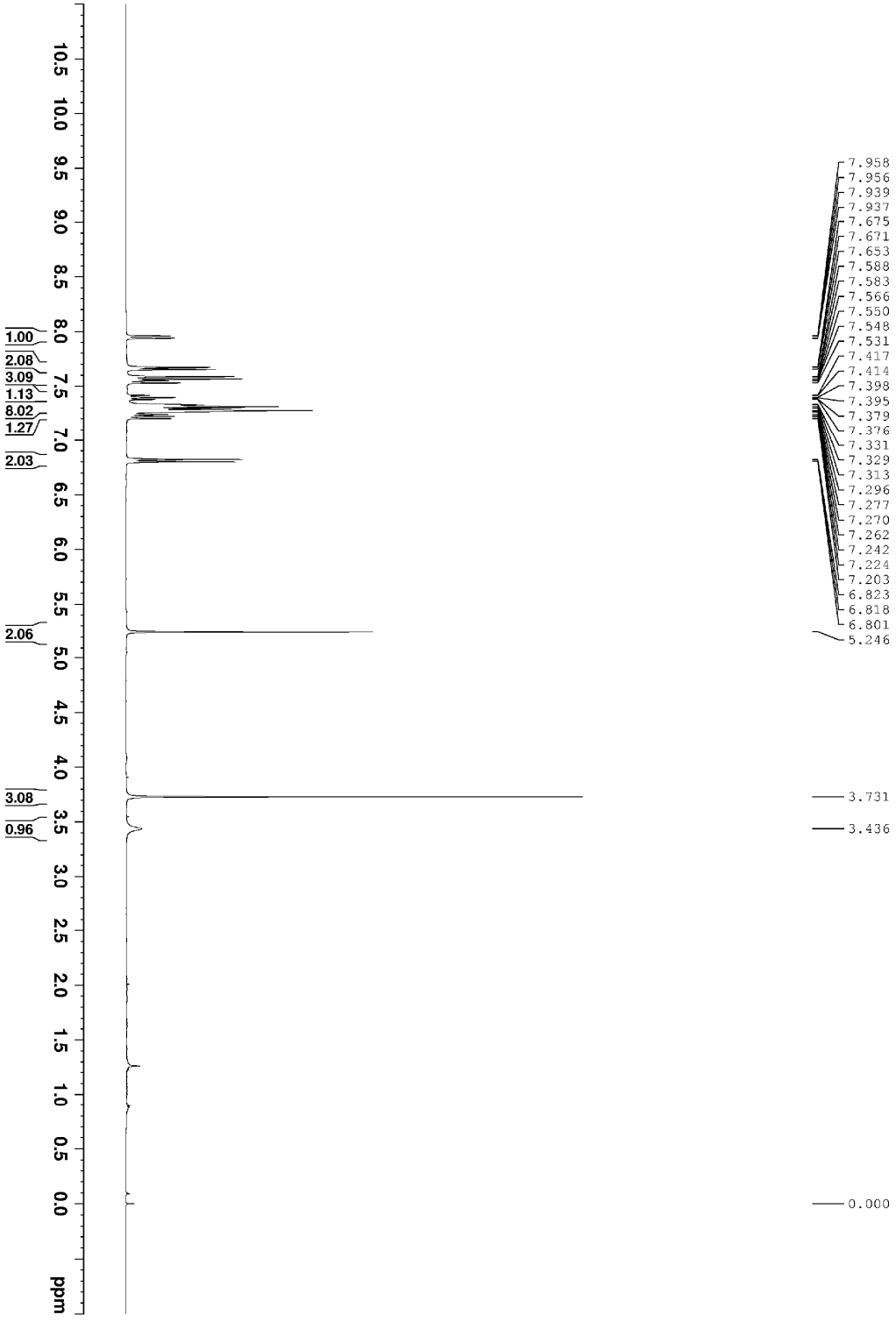

MeO
MeO
O
O
OH

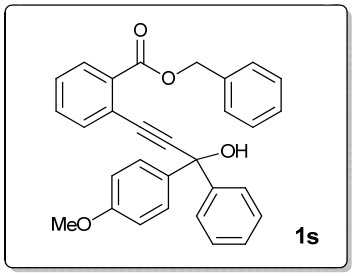
1r


zhuht120426-1ss-c
13C OBSERVE
165.48
151.51
148.61
145.08
135.94
128.41
128.18
128.08
127.42
126.12
124.31
116.79
115.84
112.83
95.48
85.84
77.42
77.00
76.58
74.81
66.65
56.01
55.92
f1 (ppm)

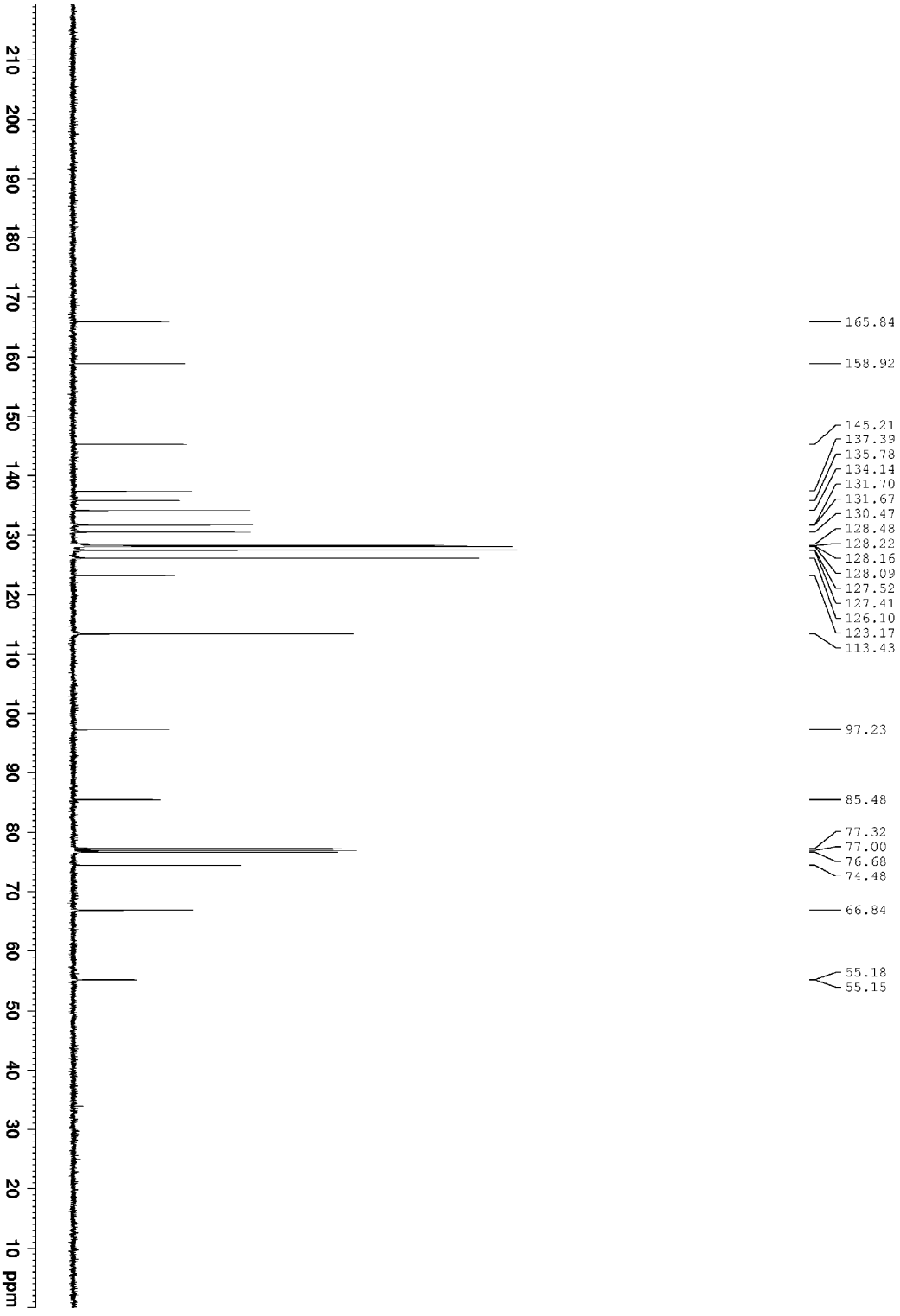

O
O
OH
MeO

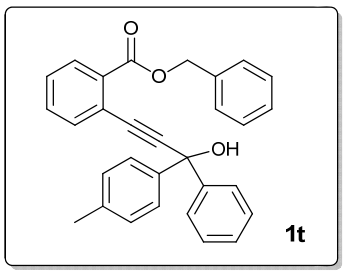
1s

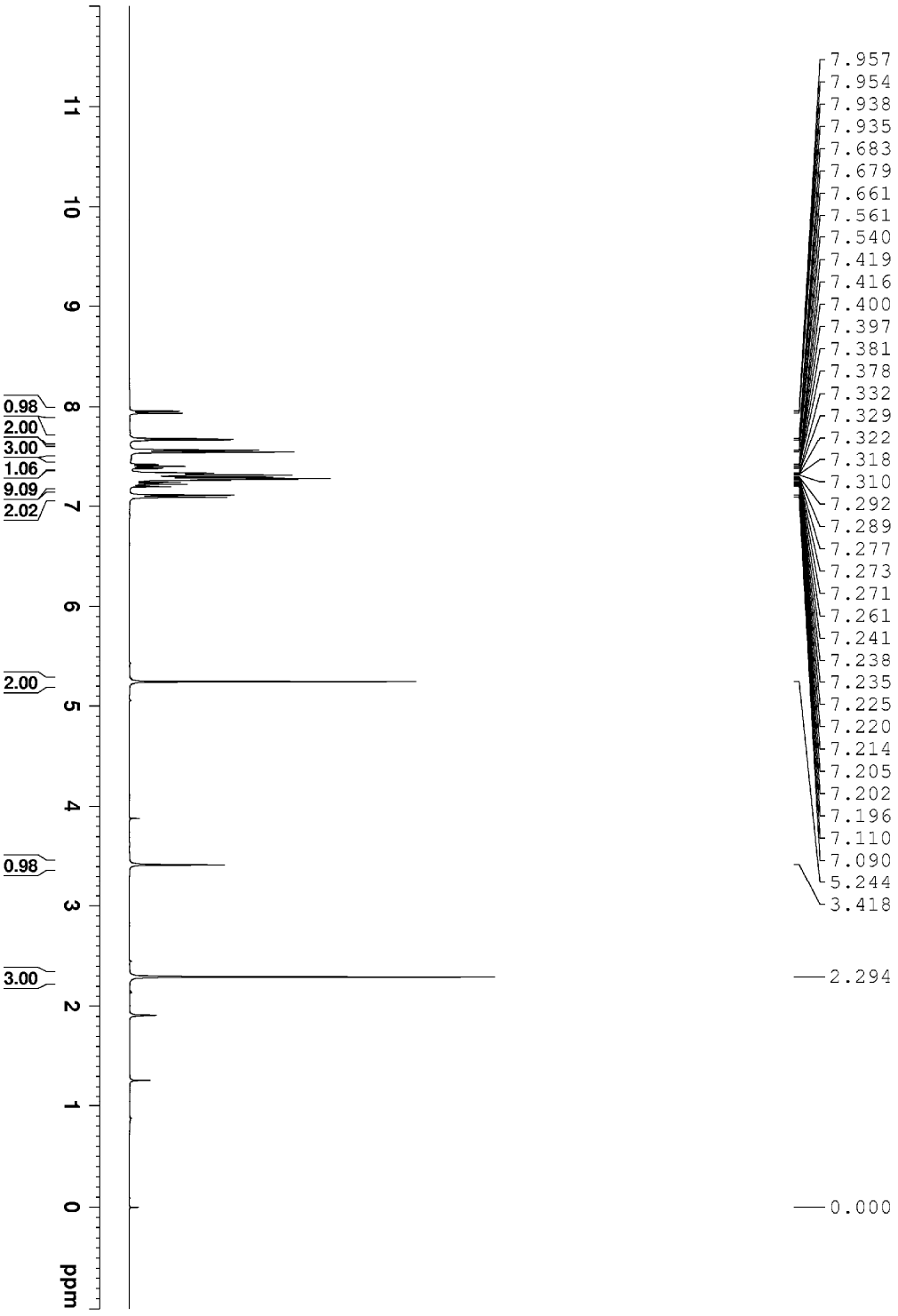

1.00
2.08
3.09
1.13
8.02
1.27
2.03
2.06
3.08
0.96
ppm
7.958
7.956
7.939
7.937
7.675
7.671
7.653
7.588
7.583
7.566
7.550
7.548
7.531
7.417
7.414
7.398
7.395
7.379
7.376
7.331
7.329
7.313
7.296
7.277
7.270
7.262
7.242
7.224
7.203
6.823
6.818
6.801
5.246
3.731
3.436
0.000

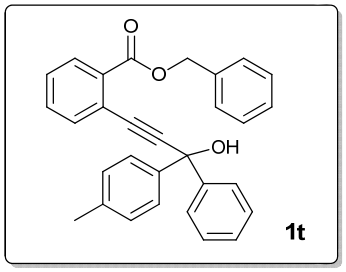

O
O
OH
MeO

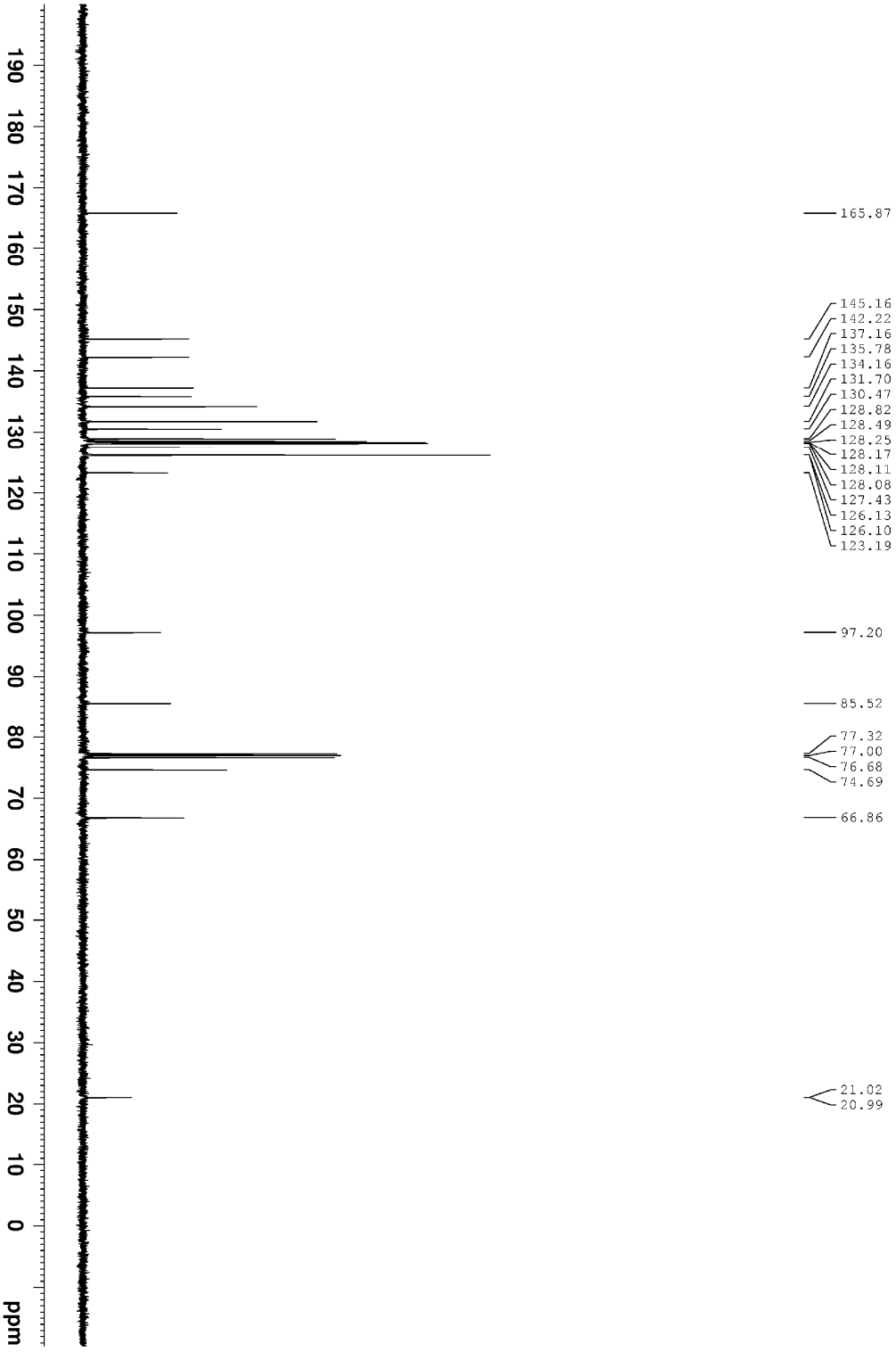
1s

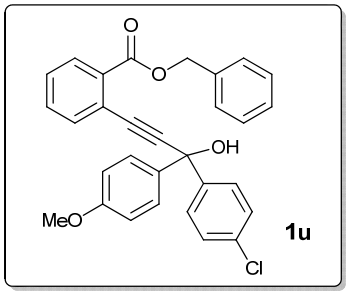

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
165.84
158.92
145.21
137.39
135.78
134.14
131.70
131.67
130.47
128.48
128.22
128.16
128.09
127.52
127.41
126.10
123.17
113.43
97.23
85.48
77.32
77.00
76.68
74.48
66.84
55.18
55.15


O
O
OH
1t

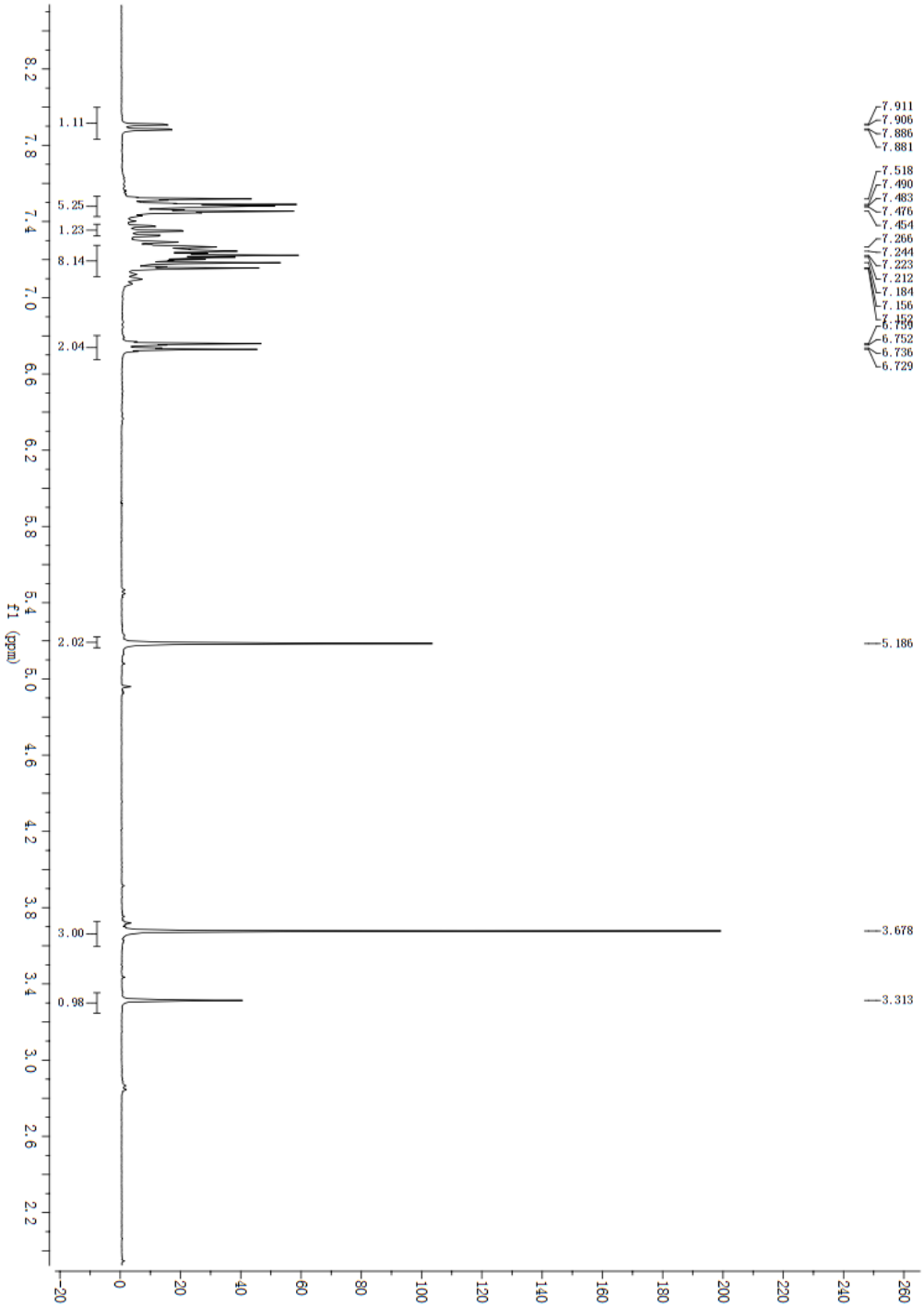

0.98
2.00
3.00
1.06
9.09
2.02
2.00
0.98
3.00
ppm
7.957
7.954
7.938
7.935
7.683
7.679
7.661
7.561
7.540
7.419
7.416
7.400
7.397
7.381
7.378
7.332
7.329
7.322
7.318
7.310
7.292
7.289
7.277
7.273
7.271
7.261
7.241
7.238
7.235
7.225
7.220
7.214
7.205
7.202
7.196
7.110
7.090
5.244
3.418
2.294
0.000






O
O
OH
MeO
Cl

1u


1.11
5.25
1.23
8.14
2.04
2.02
3.00
0.98
7.911
7.906
7.886
7.881
7.518
7.490
7.483
7.476
7.454
7.266
7.244
7.223
7.212
7.184
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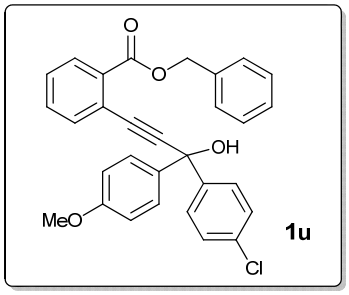
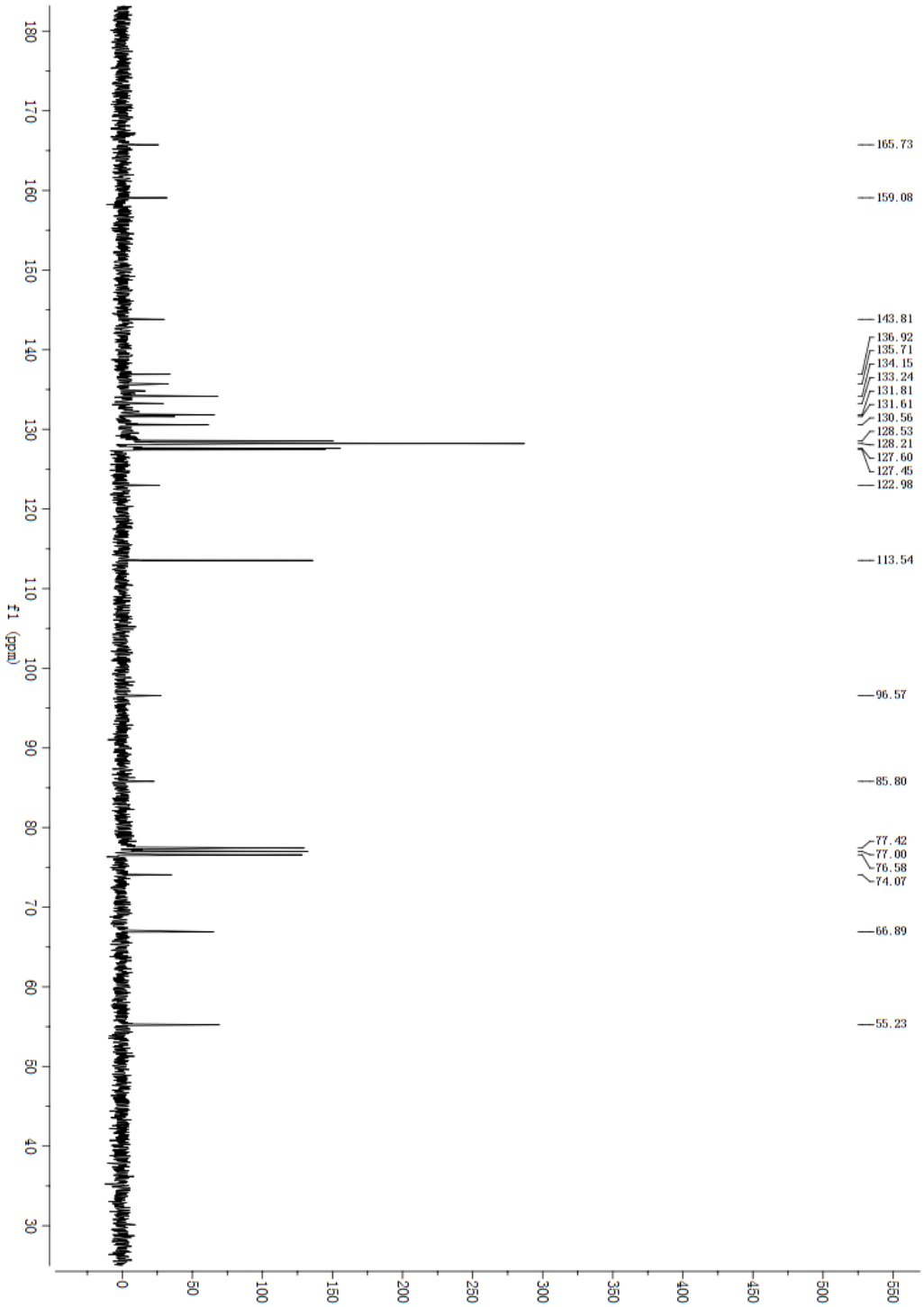
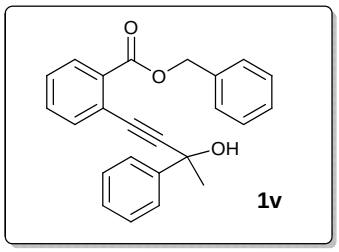
7.152
6.759
6.752
6.736
6.729
5.186
3.678
3.313
f1 (ppm)

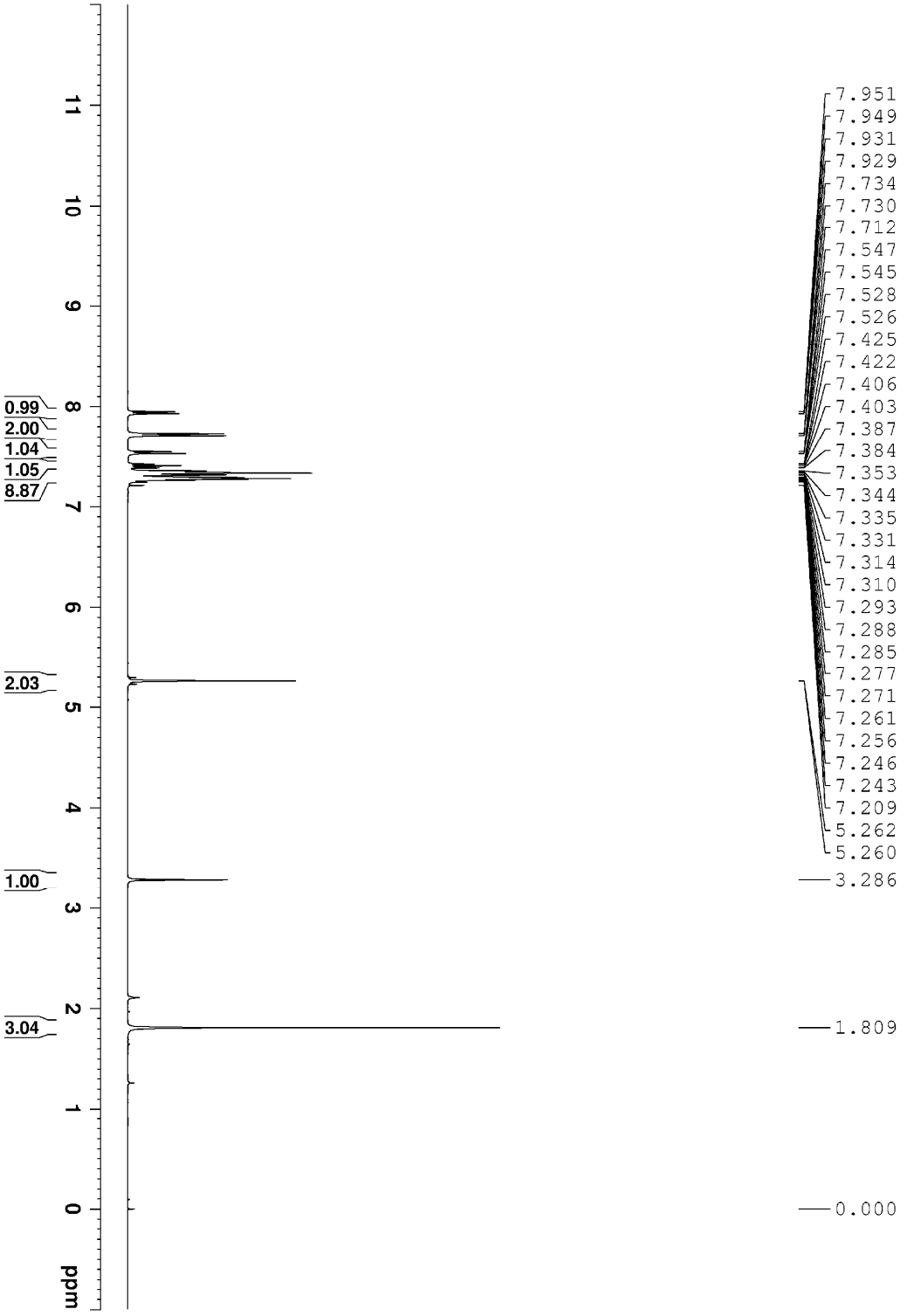

O
O
OH
MeO
Cl

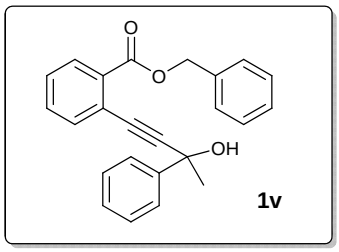
1u


165.73
159.08
143.81
136.92
135.71
134.15
133.24
131.81
131.61
130.56
128.53
128.21
127.60
127.45
122.98
113.54
96.57
85.80
77.42
77.00
76.58
74.07
66.89
55.23
f1 (ppm)

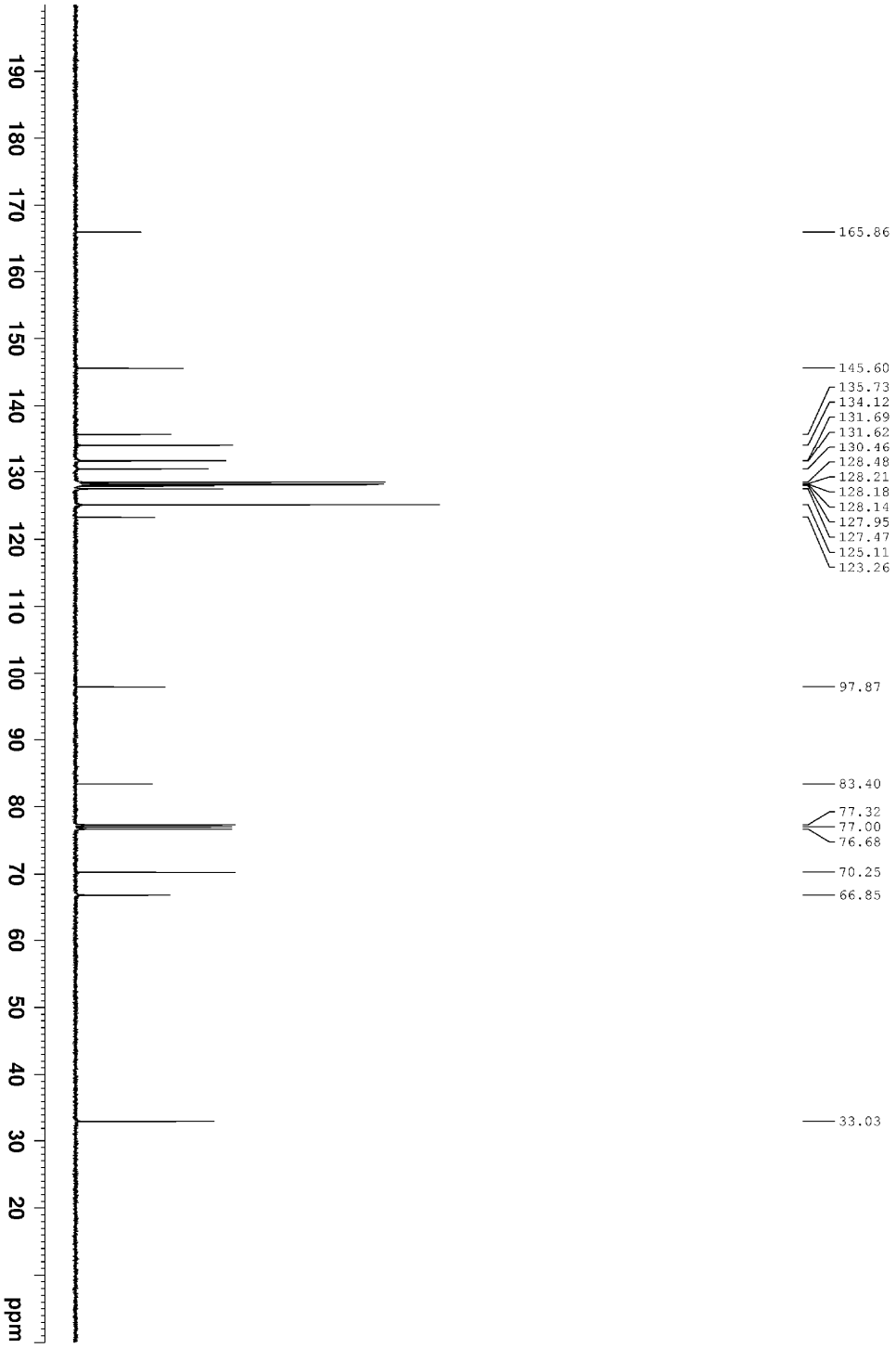

O
O
OH

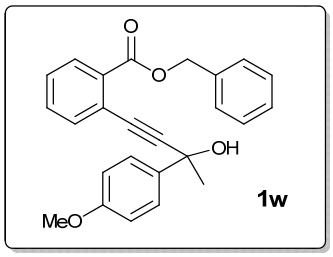
1v

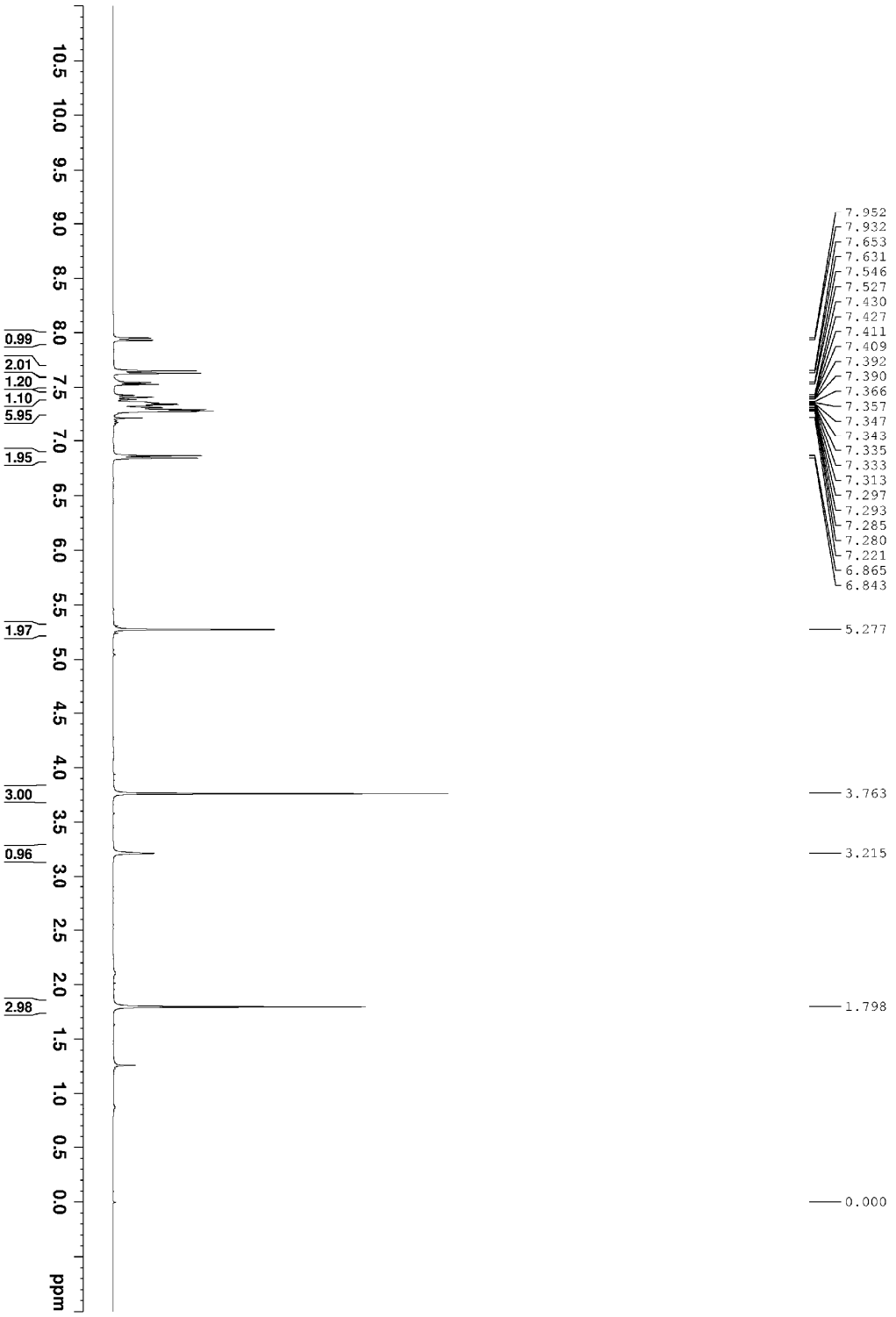

0.99
2.00
1.04
1.05
8.87
2.03
1.00
3.04
ppm
7.951
7.949
7.931
7.929
7.734
7.730
7.712
7.547
7.545
7.528
7.526
7.425
7.422
7.406
7.403
7.387
7.384
7.353
7.344
7.335
7.331
7.314
7.310
7.293
7.288
7.285
7.277
7.271
7.261
7.256
7.246
7.243
7.209
5.262
5.260
3.286
1.809
0.000

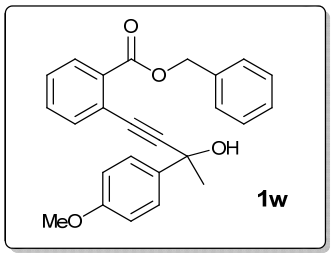


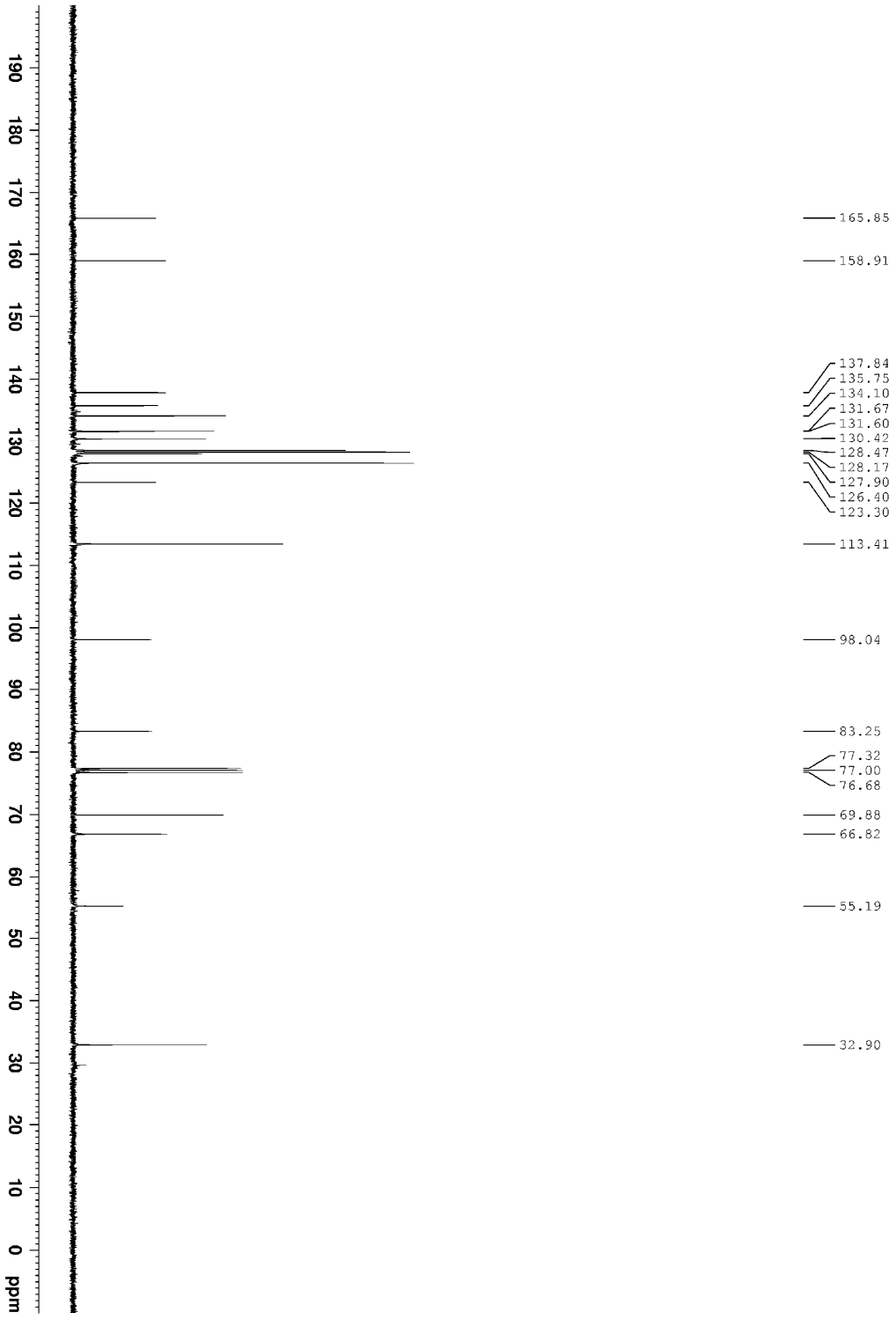
1v




O
O
OH
MeO
1w


0.99
2.01
1.20
1.10
5.95
1.95
1.97
3.00
0.96
2.98
ppm
7.952
7.932
7.653
7.631
7.546
7.527
7.430
7.427
7.411
7.409
7.392
7.390
7.366
7.357
7.347
7.343
7.335
7.333
7.313
7.297
7.293
7.285
7.280
7.221
6.865
6.843
5.277
3.763
3.215
1.798
0.000


O
O
OH
MeO
1w


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
165.85
158.91
137.84
135.75
134.10
131.67
131.60
130.42
128.47
128.17
127.90
126.40
123.30
113.41
98.04
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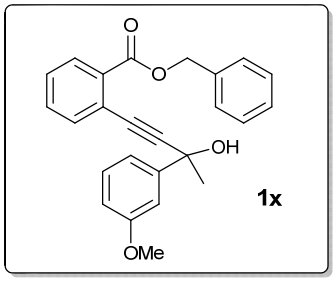
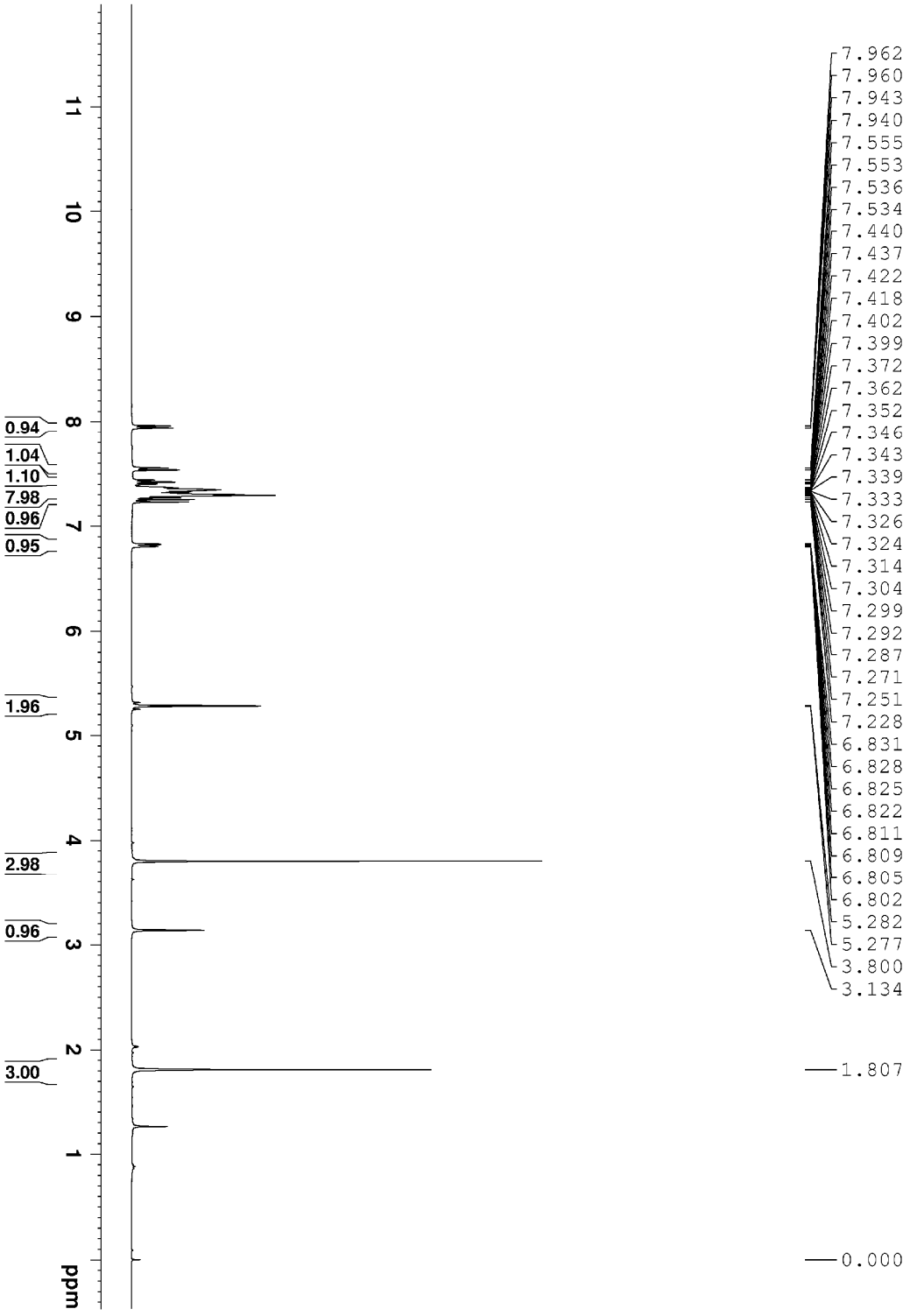
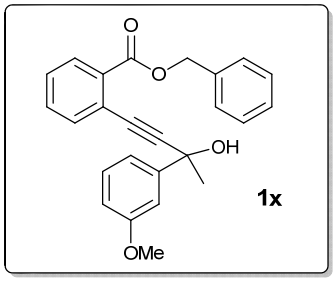
77.32
77.00
76.68
69.88
66.82
55.19
32.90

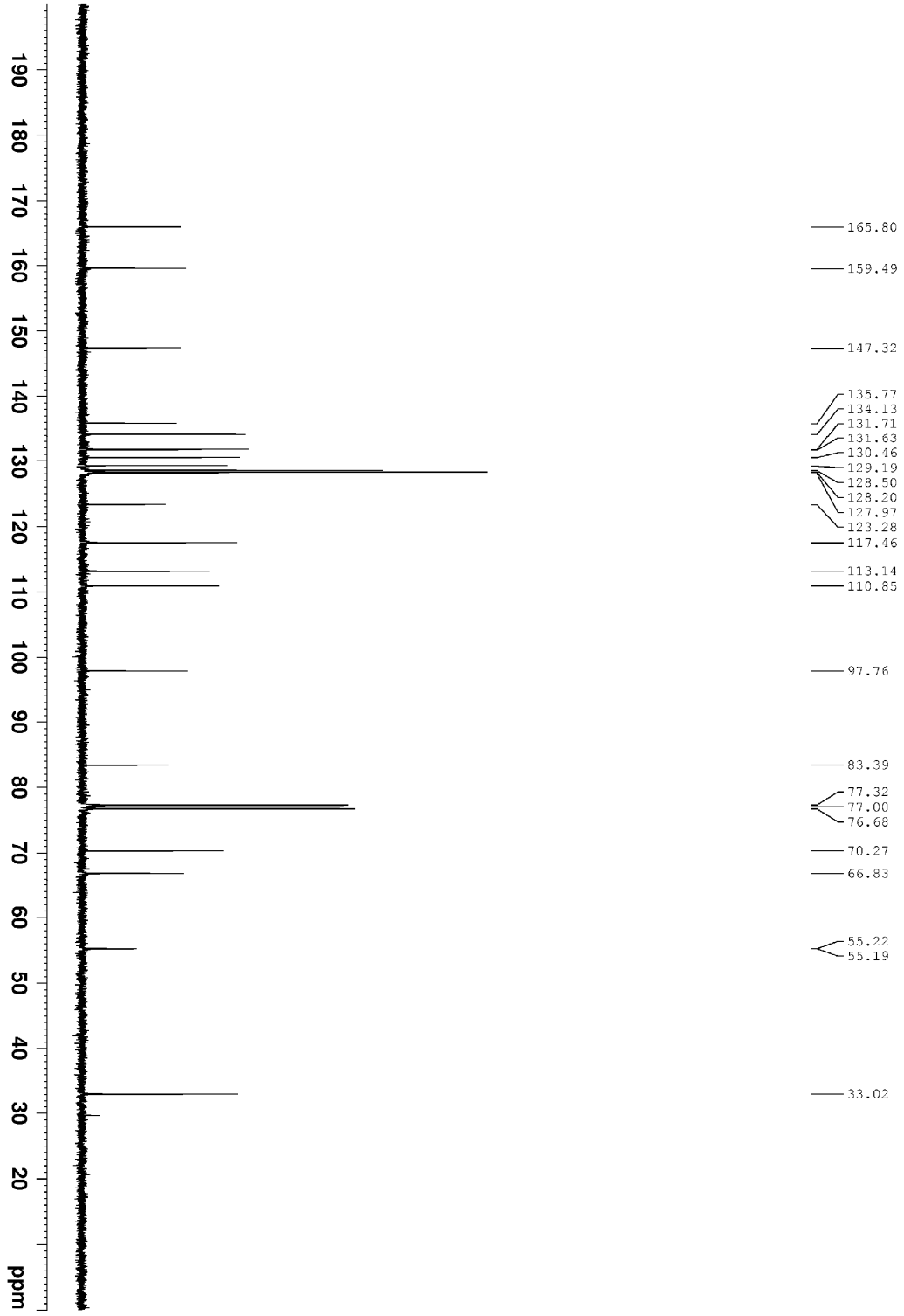

O
O
OH
OMe

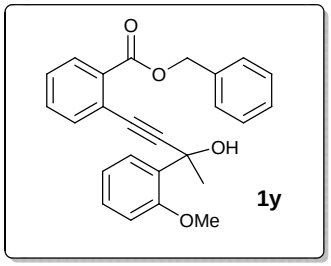
1x


0.94
1.04
1.10
7.98
0.96
0.95
1.96
2.98
0.96
3.00
11
10
9
8
7
6
5
4
3
2
1
ppm
7.962
7.960
7.943
7.940
7.555
7.553
7.536
7.534
7.440
7.437
7.422
7.418
7.402
7.399
7.372
7.362
7.352
7.346
7.343
7.339
7.333
7.326
7.324
7.314
7.304
7.299
7.292
7.287
7.271
7.251
7.228
6.831
6.828
6.825
6.822
6.811
6.809
6.805
6.802
5.282
5.277
3.800
3.134
1.807
0.000

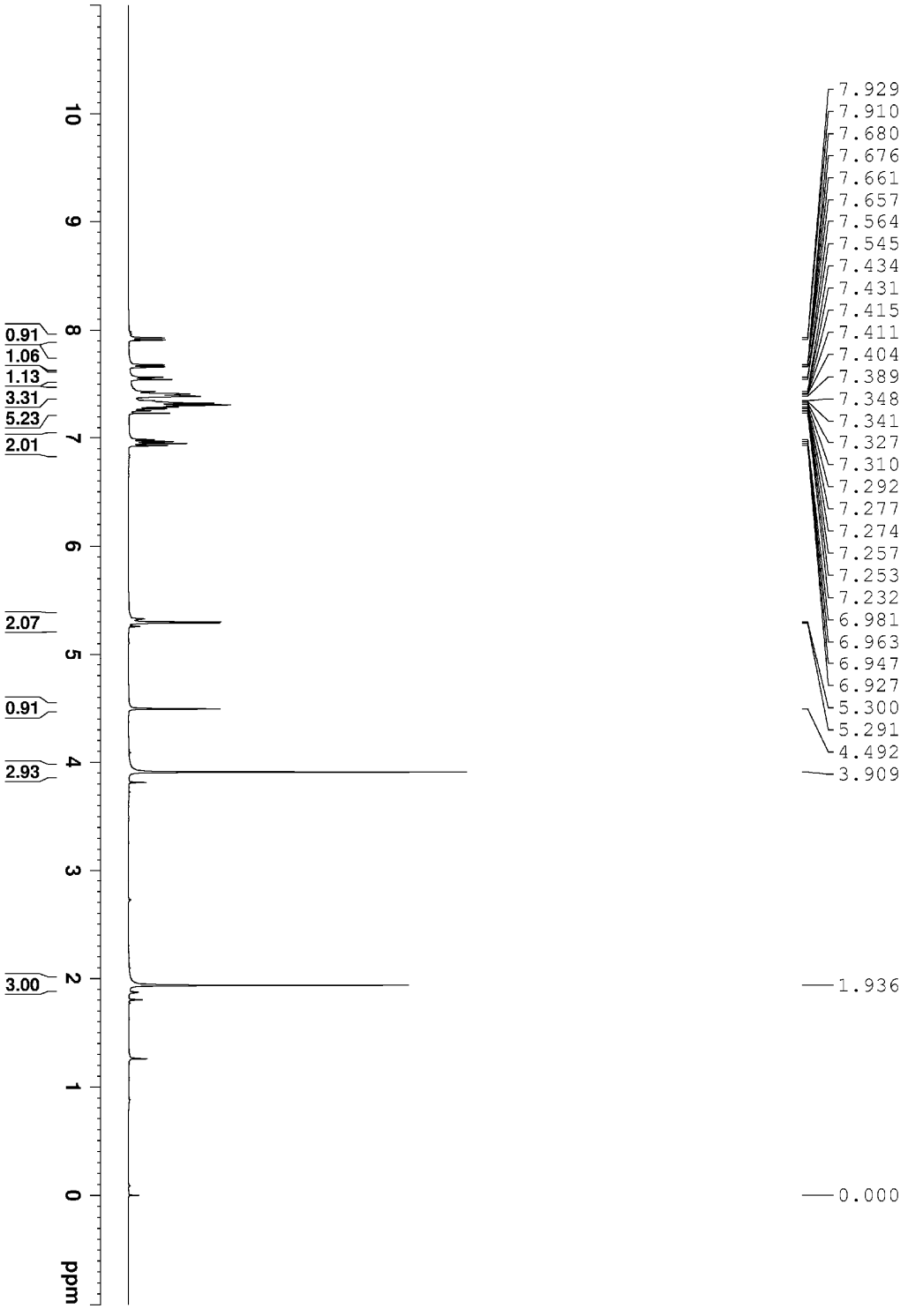

O
O
OH
OMe

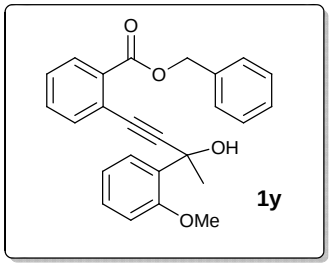
1x


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
165.80
159.49
147.32
135.77
134.13
131.71
131.63
130.46
129.19
128.50
128.20
127.97
123.28
117.46
113.14
110.85
97.76
83.39
77.32
77.00
76.68
70.27
66.83
55.22
55.19
33.02

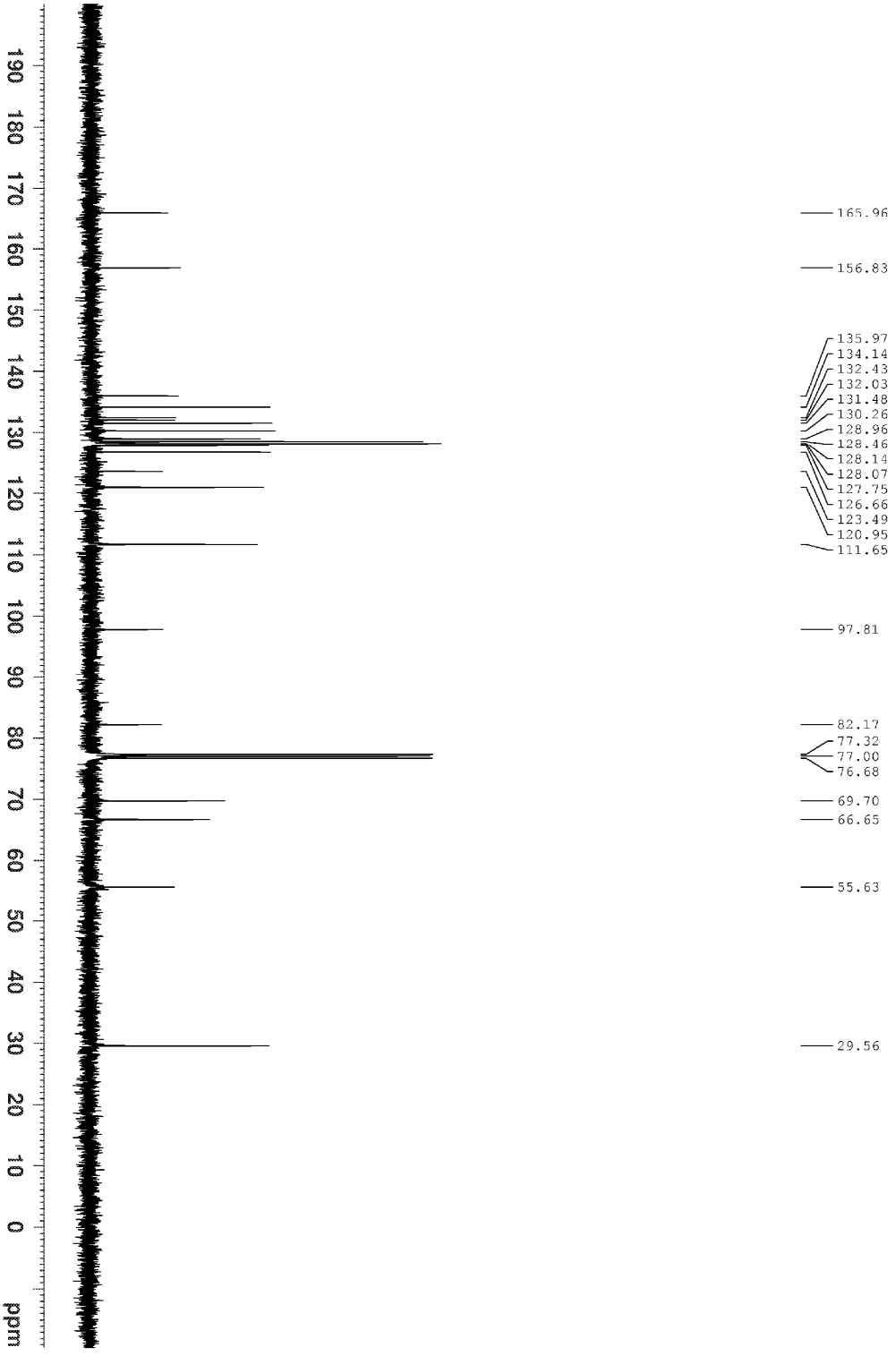


1y




O
O
OH
OMe

1y


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
165.96
156.83
135.97
134.14
132.43
132.03
131.48
130.26
128.96
128.46
128.14
128.07
127.75
126.66
123.49
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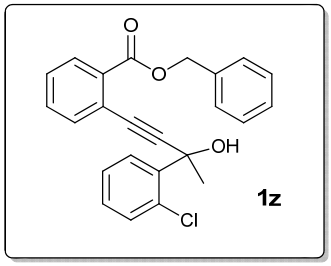
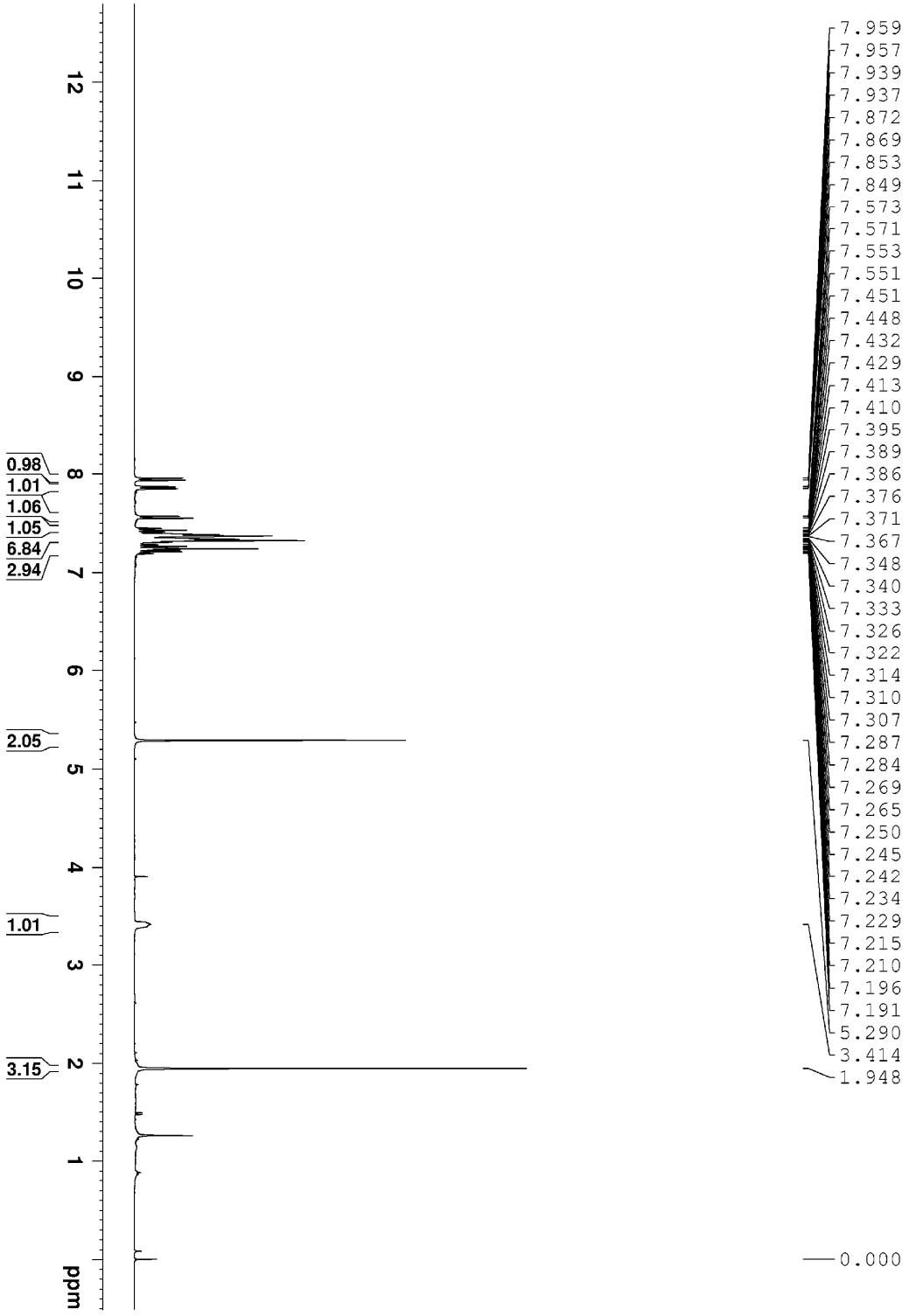
77.00
76.68
69.70
66.65
55.63
29.56


O
O
OH
Cl
1z


0.98
1.01
1.06
1.05
6.84
2.94
2.05
1.01
3.15
12
11
10
9
8
7
6
5
4
3
2
1
ppm
7.959
7.957
7.939
7.937
7.872
7.869
7.853
7.849
7.573
7.571
7.553
7.551
7.451
7.448
7.432
7.429
7.413
7.410
7.395
7.389
7.386
7.376
7.371
7.367
7.348
7.340
7.333
7.326
7.322
7.314
7.310
7.307
7.287
7.284
7.269
7.265
7.250
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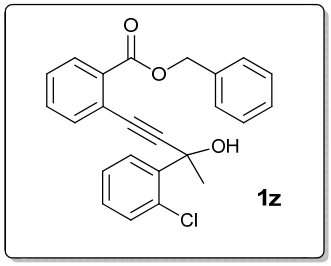
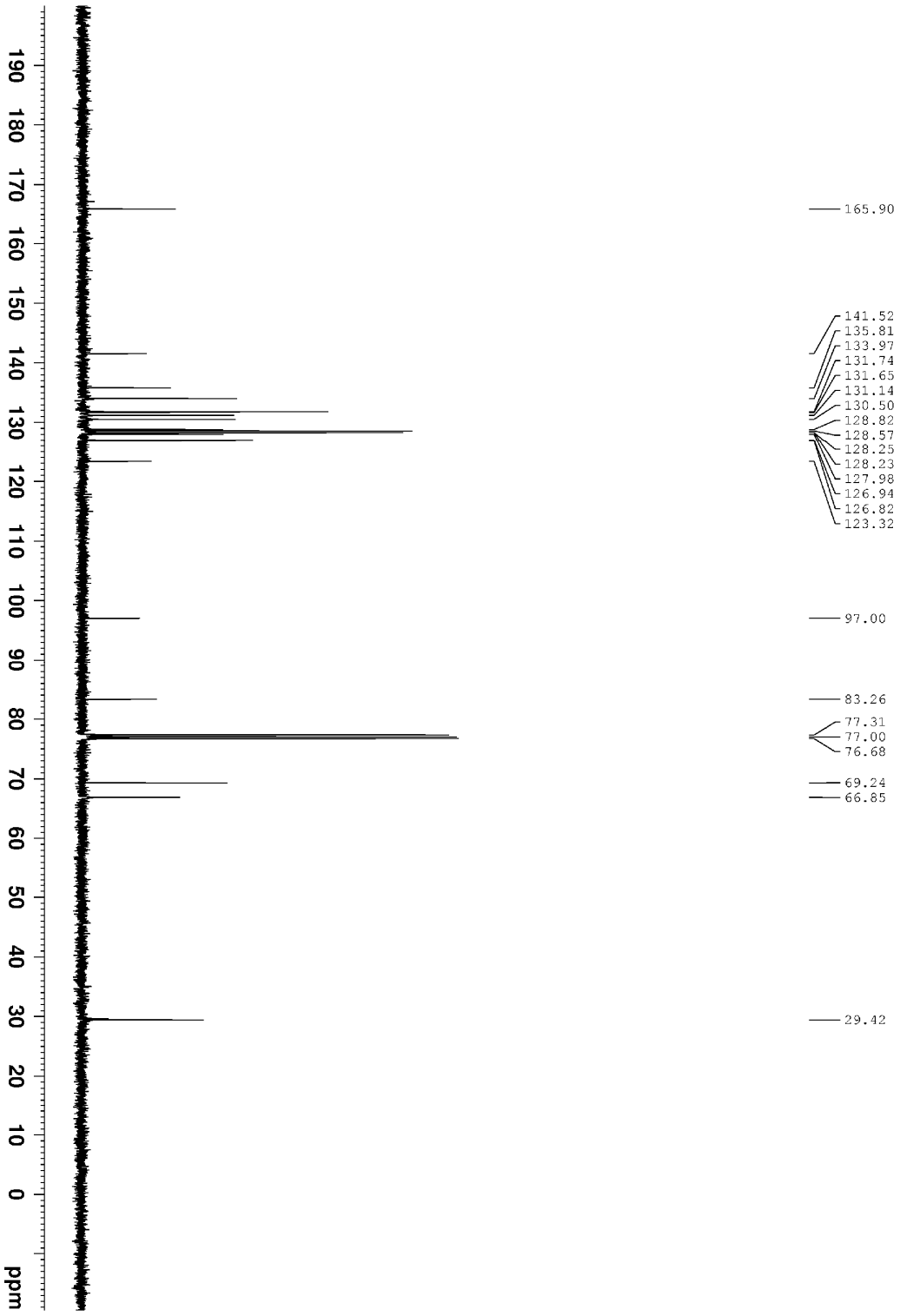
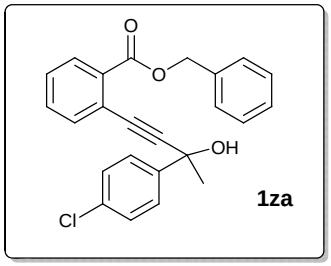
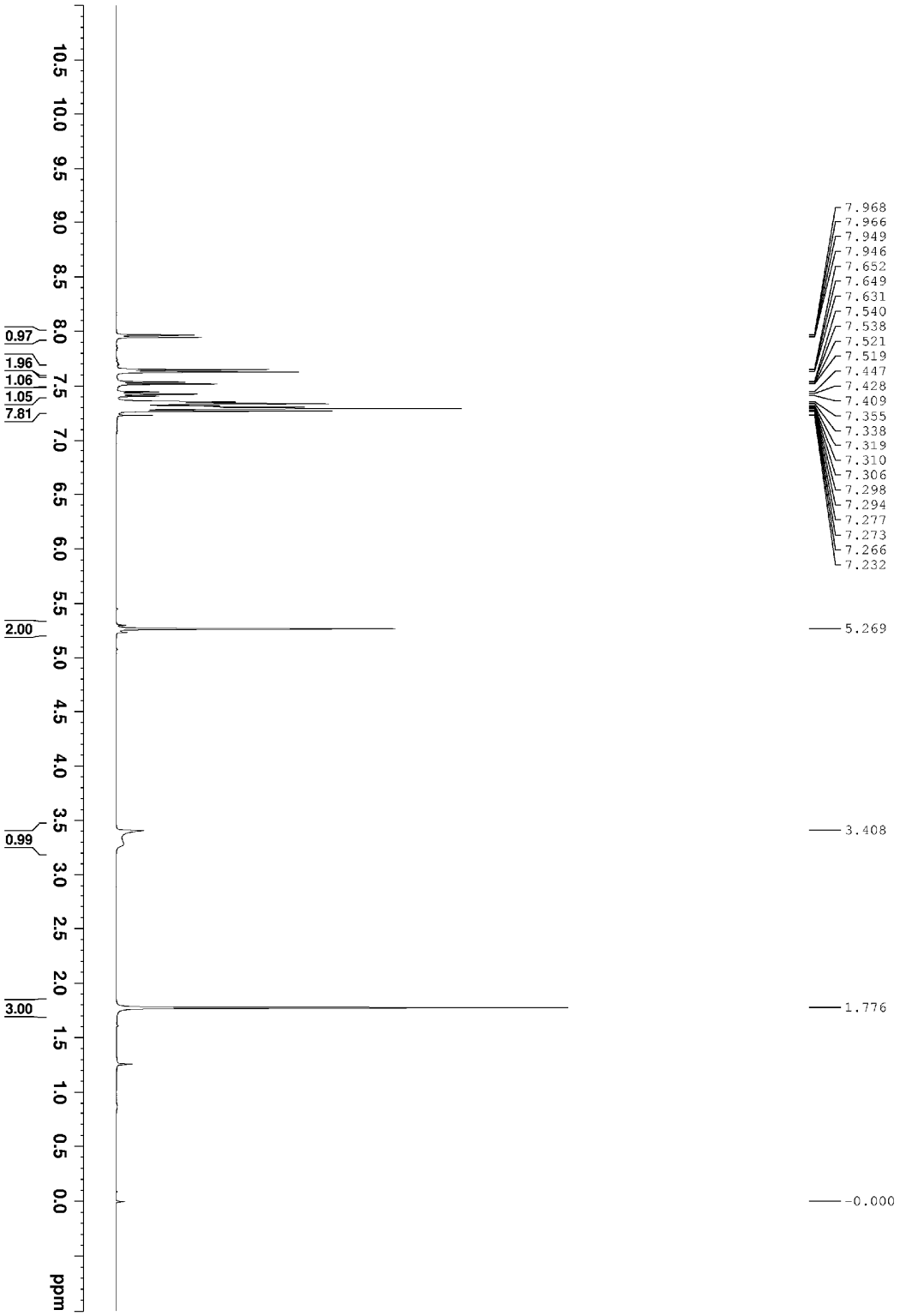
7.191
5.290
3.414
1.948
0.000

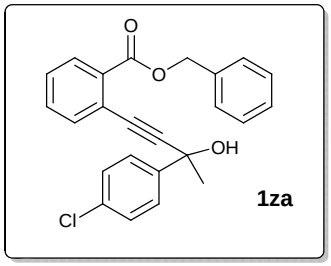




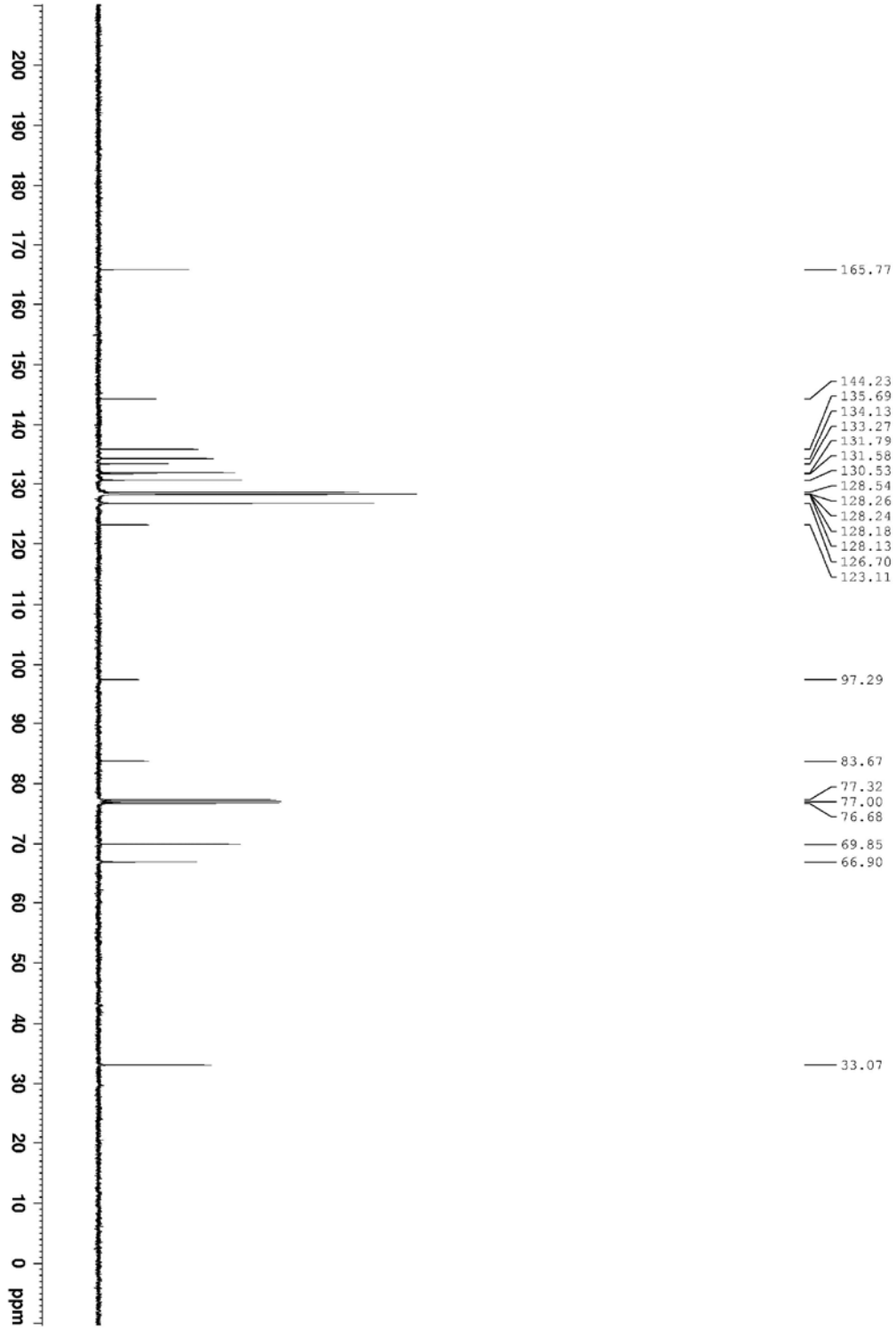

O
O
OH
Cl

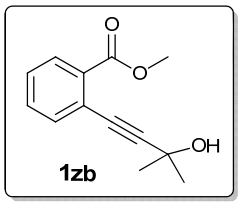
1za

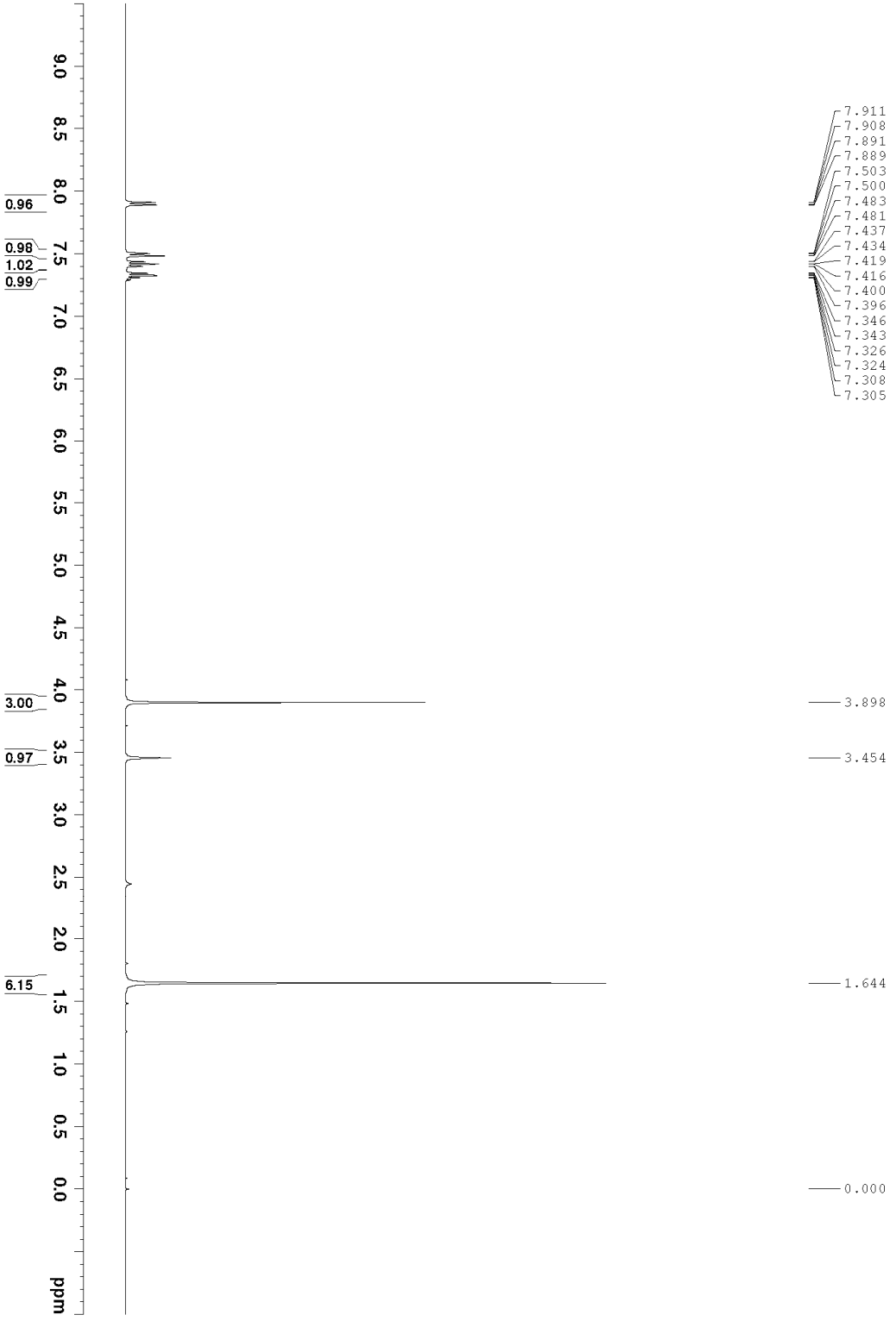

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.97
1.96
1.06
1.05
7.81
2.00
0.99
3.00
7.968
7.966
7.949
7.946
7.652
7.649
7.631
7.540
7.538
7.521
7.519
7.447
7.428
7.409
7.355
7.338
7.319
7.310
7.306
7.298
7.294
7.277
7.273
7.266
7.232
5.269
3.408
1.776
-0.000


O
O
OH
Cl

1za


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
165.77
144.23
135.69
134.13
133.27
131.79
131.58
130.53
128.54
128.26
128.24
128.18
128.13
126.70
123.11
97.29
83.67
77.32
77.00
76.68
69.85
66.90
33.07


O
O
OH
1zb


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
ppm
0.96
0.98
1.02
0.99
3.00
0.97
6.15
7.911
7.908
7.891
7.889
7.503
7.500
7.483
7.481
7.437
7.434
7.419
7.416
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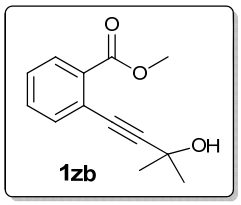
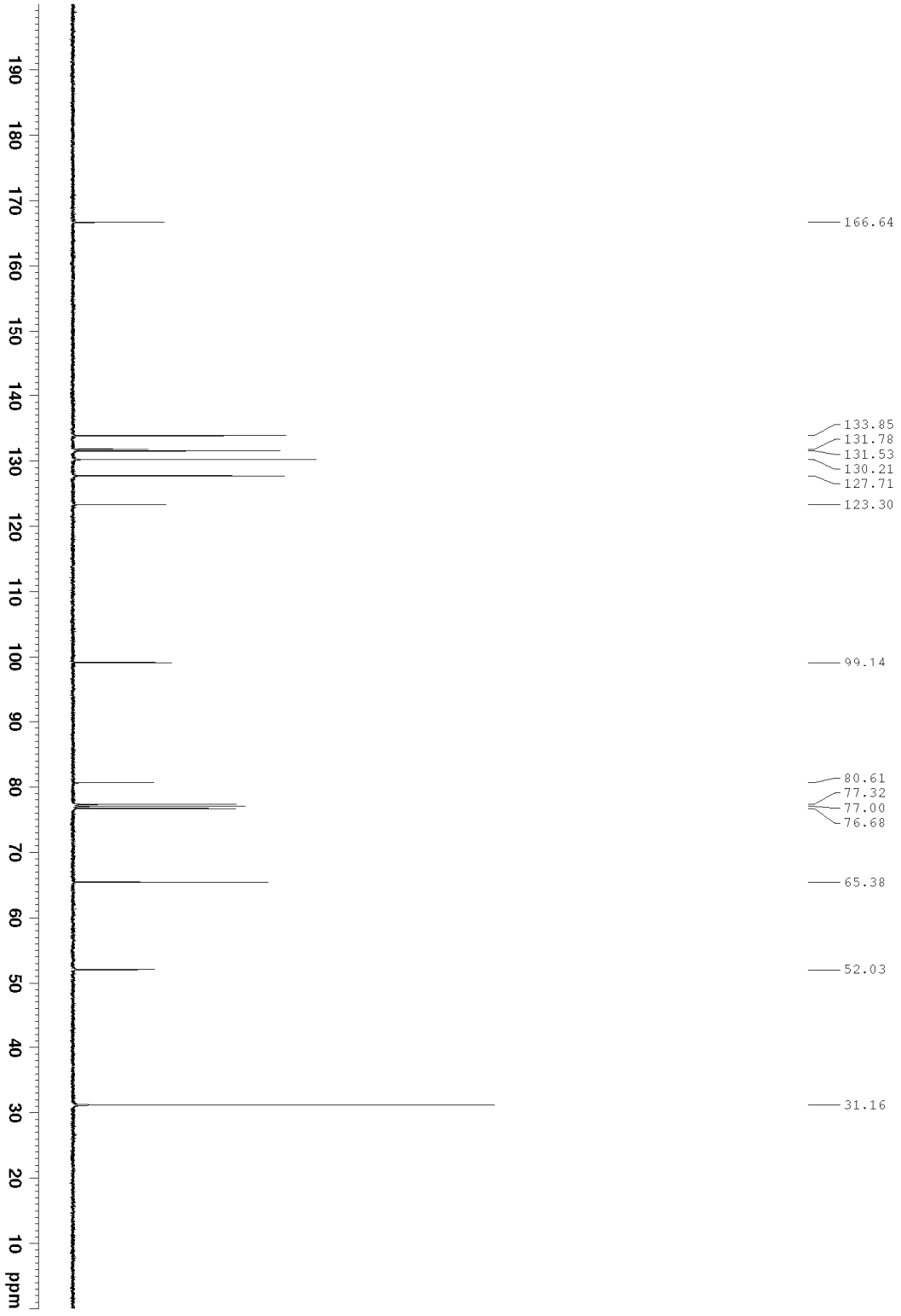
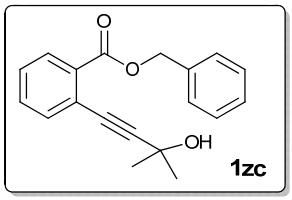
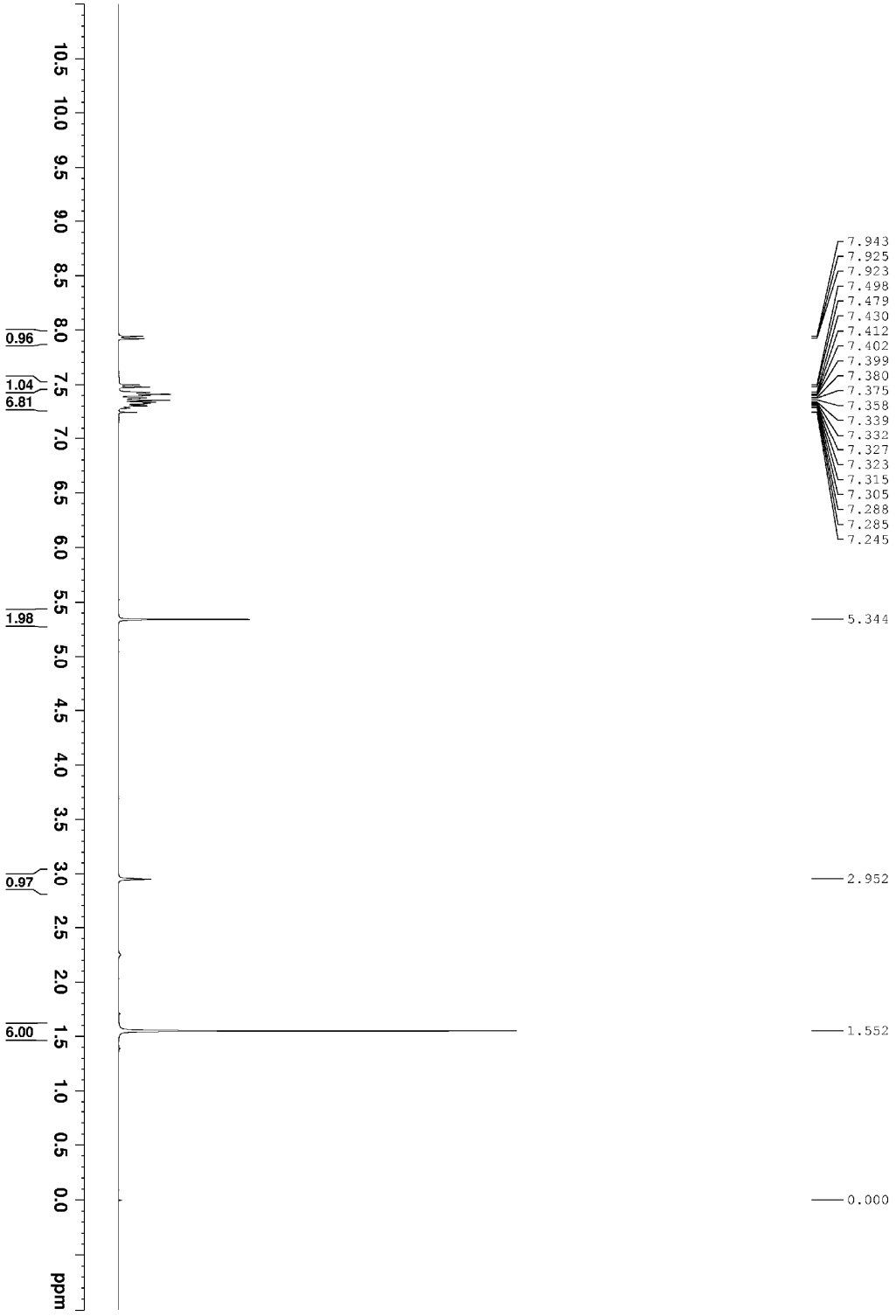
7.308
7.305
3.898
3.454
1.644
0.000

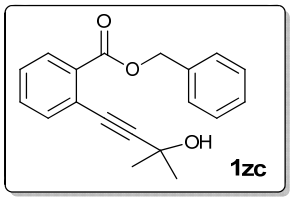

O
O
OH

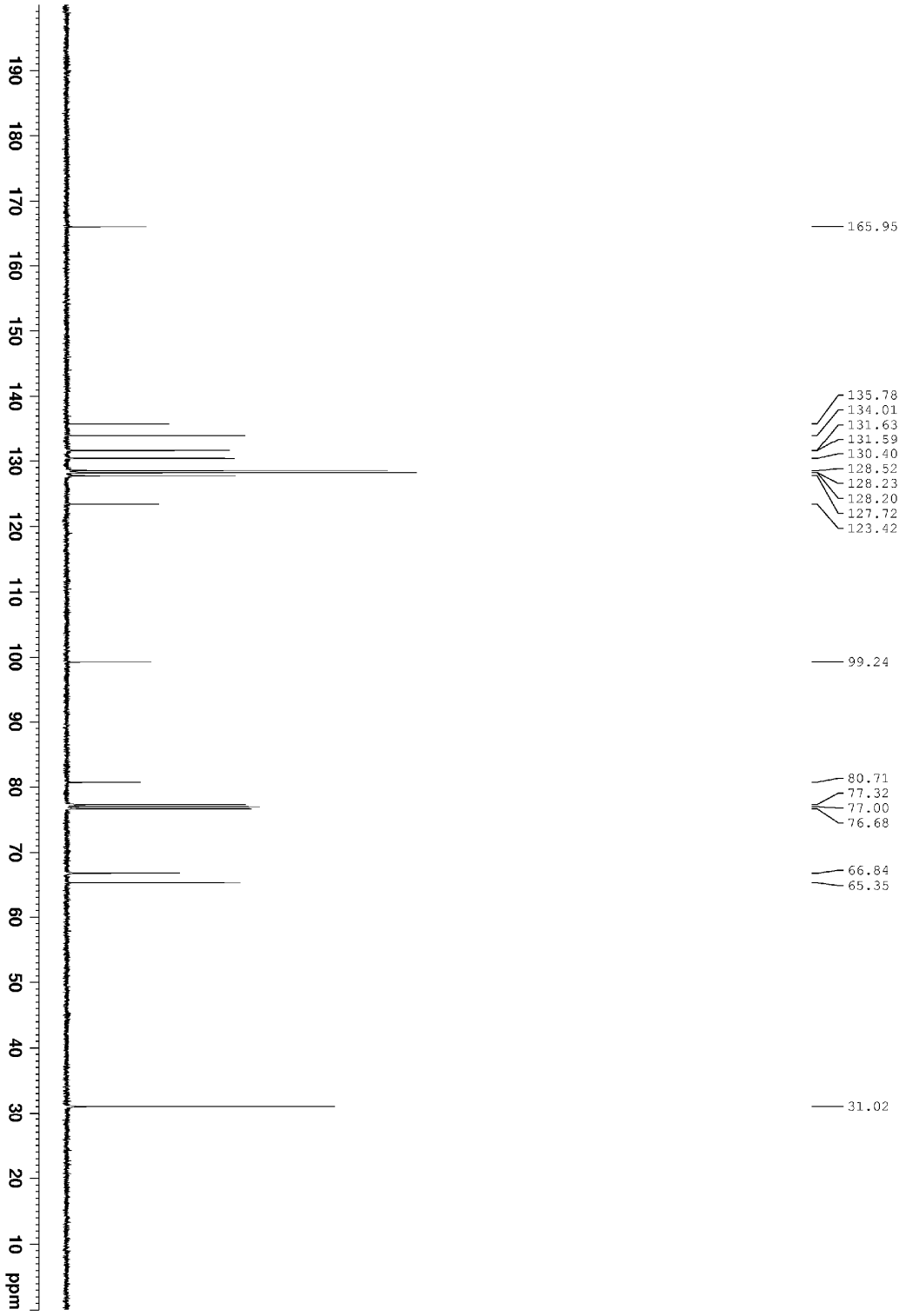
1zb

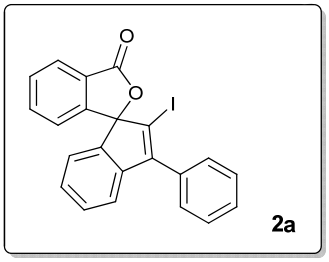

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
166.64
133.85
131.78
131.53
130.21
127.71
123.30
99.14
80.61
77.32
77.00
76.68
65.38
52.03
31.16


O
O
OH
1zc


0.96
1.04
6.81
1.98
0.97
6.00
7.943
7.925
7.923
7.498
7.479
7.430
7.412
7.402
7.399
7.380
7.375
7.358
7.339
7.332
7.327
7.323
7.315
7.305
7.288
7.285
7.245
5.344
2.952
1.552
0.000
ppm



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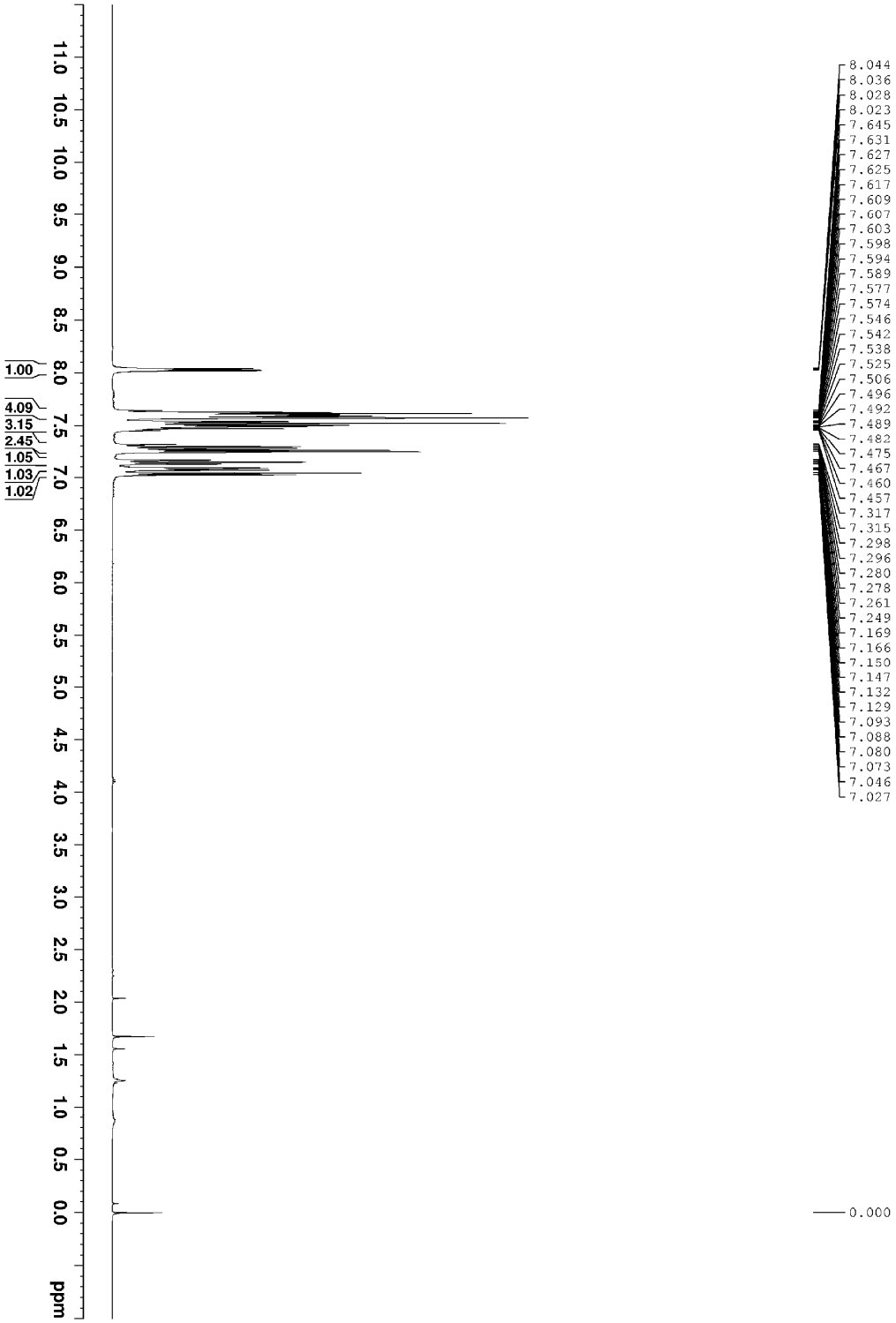
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0.0
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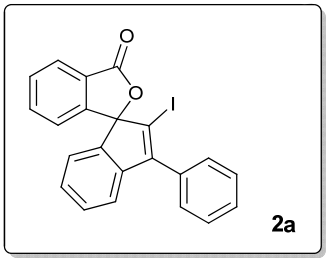
7.027
0.000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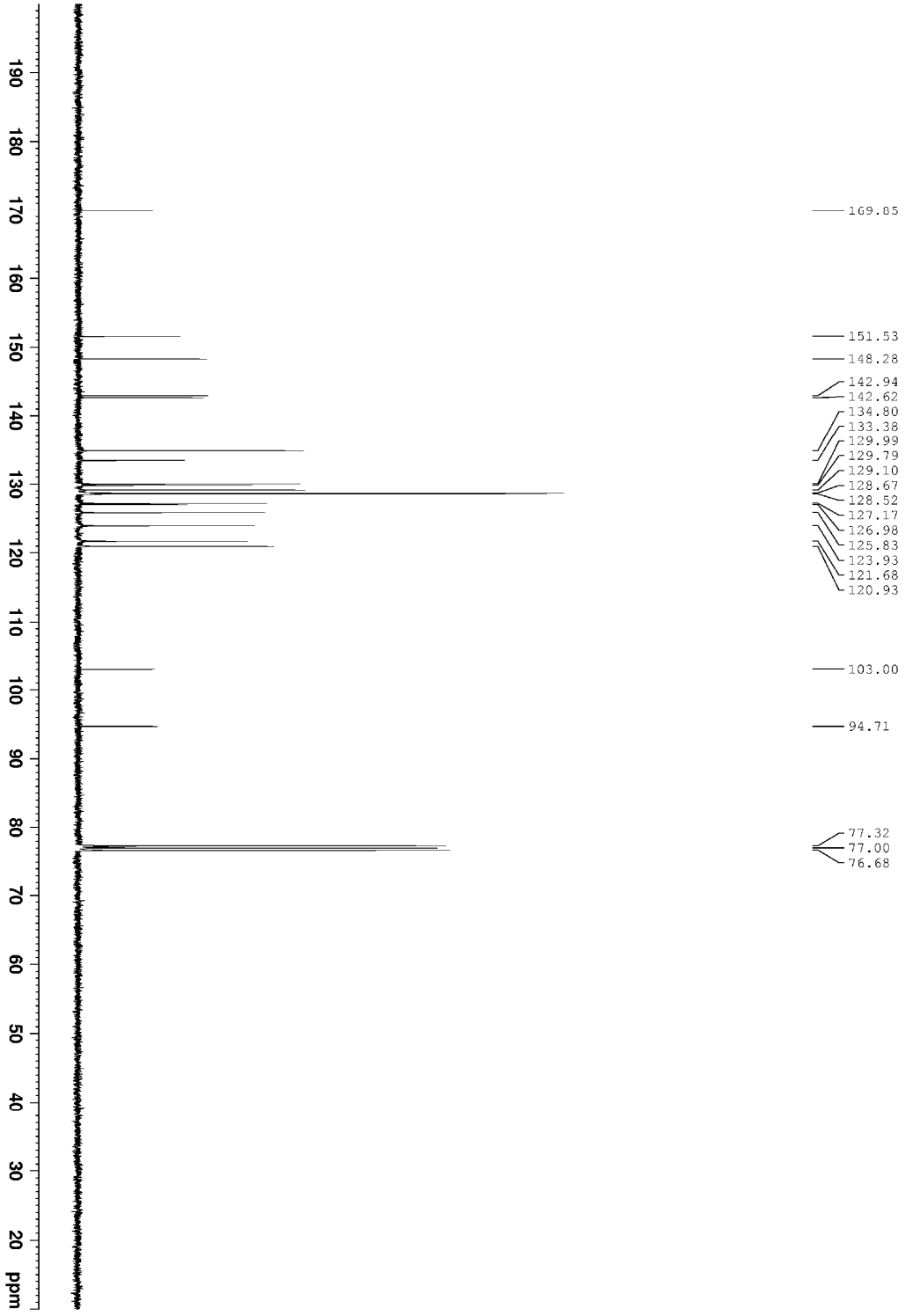
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129.10
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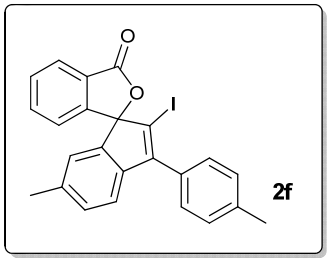
77.00
76.68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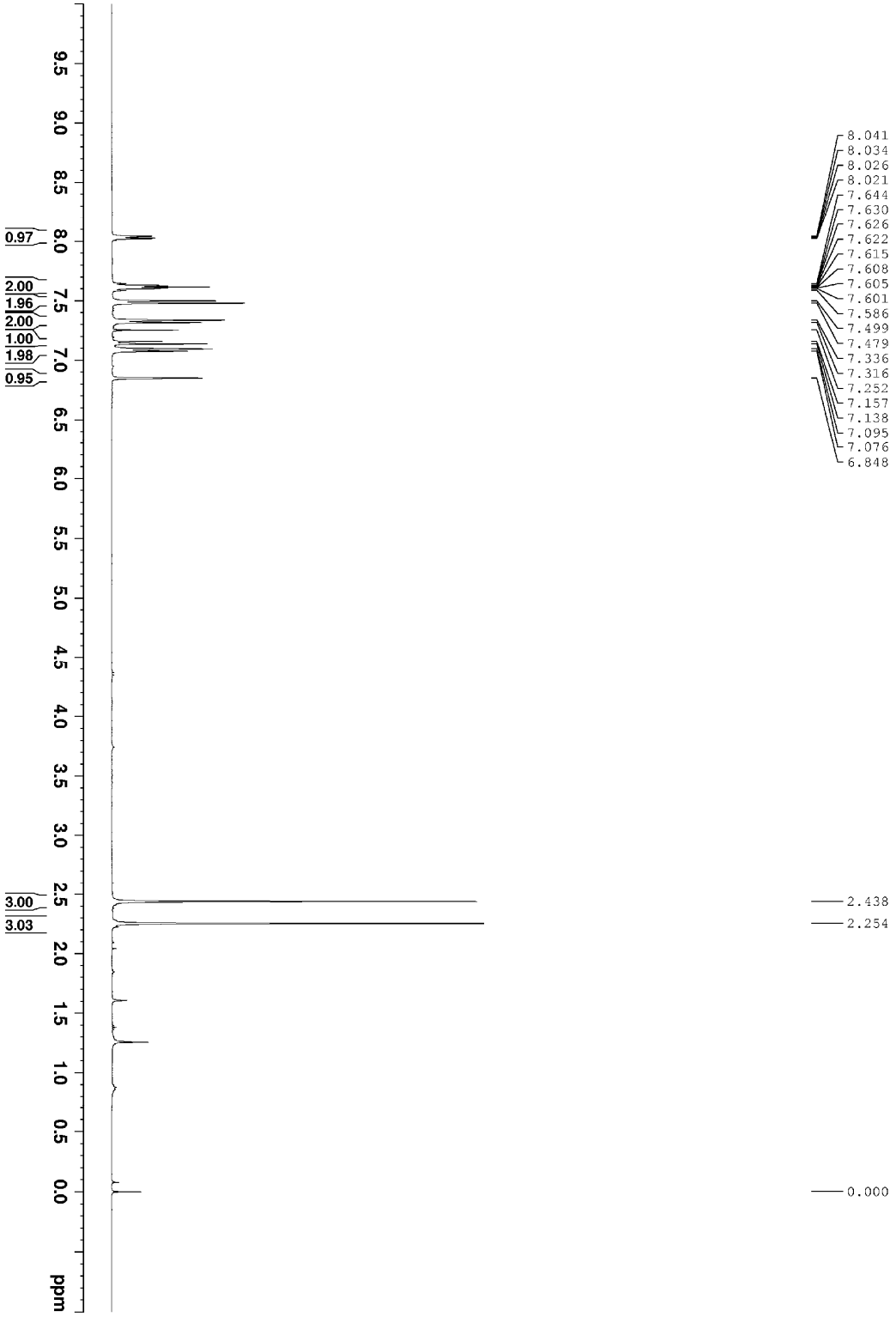
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
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8.034
8.026
8.021
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7.630
7.626
7.622
7.615
7.608
7.605
7.601
7.586
7.499
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7.138
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7.076
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2.254
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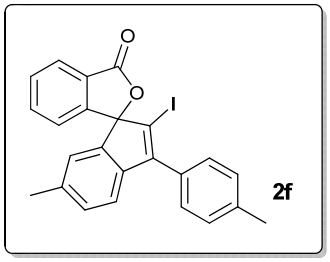
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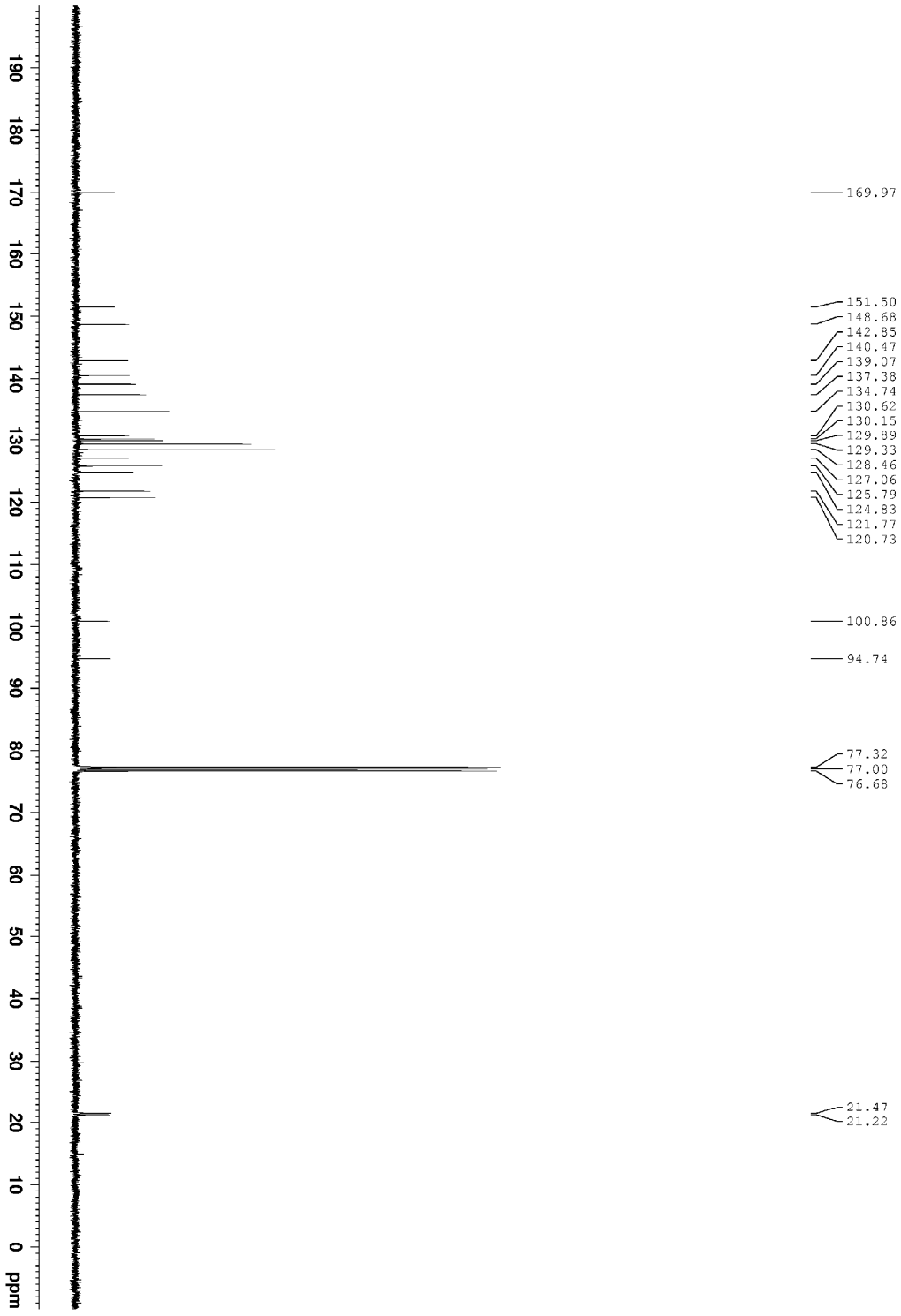
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130.15
129.89
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128.46
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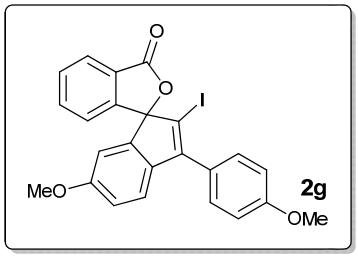
76.68
21.47
21.22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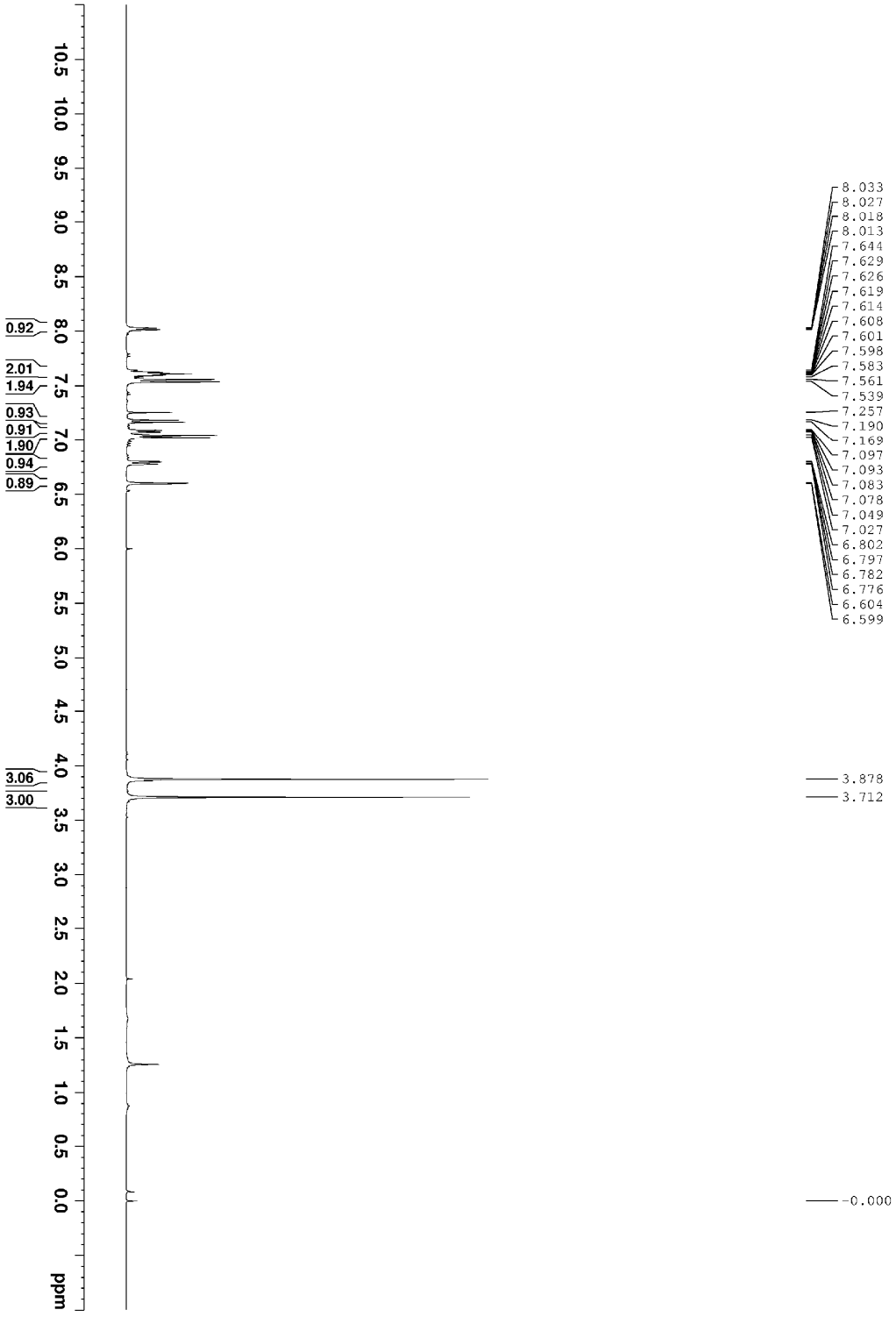
O
I
MeO
OMe
2g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7.608
7.601
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7.257
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7.093
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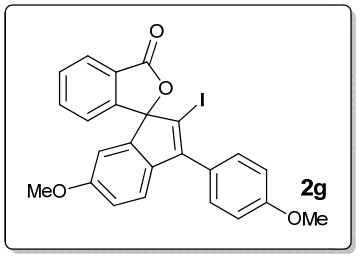
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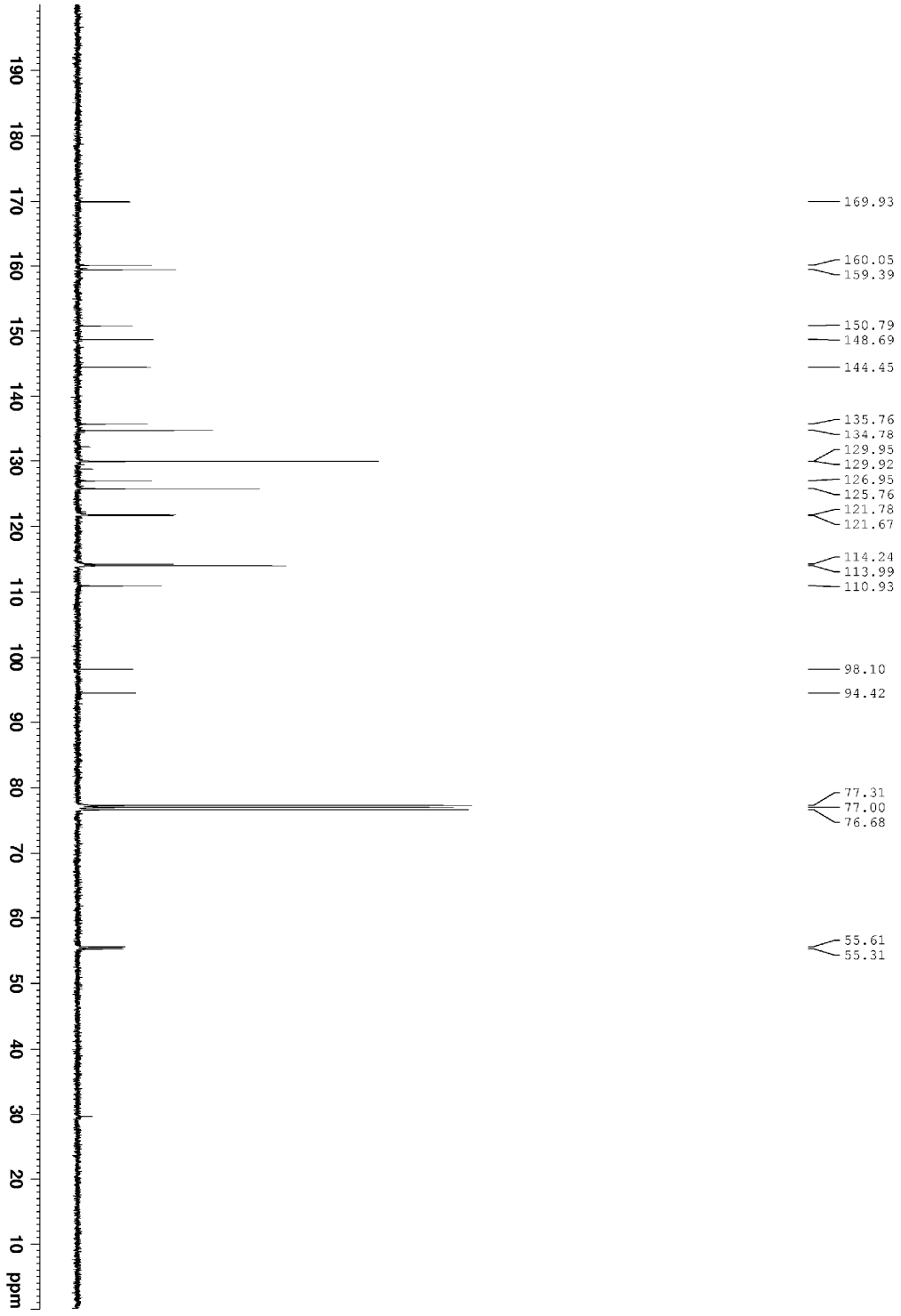
I
MeO
OMe
2g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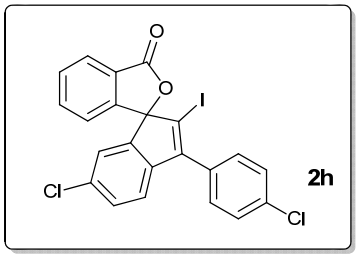
55.31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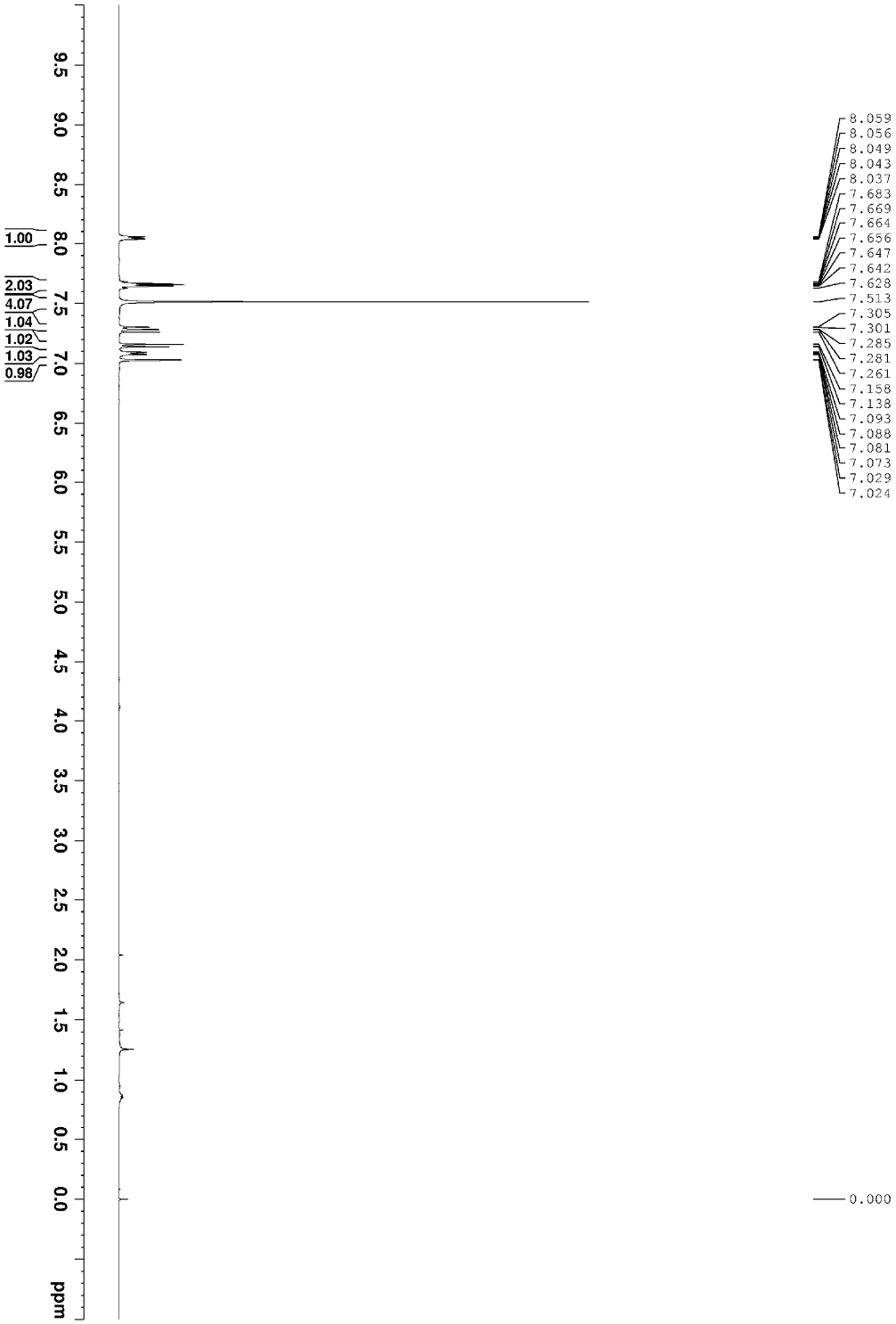
I
Cl
Cl
2h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6.0
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5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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0.0
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8.049
8.043
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7.513
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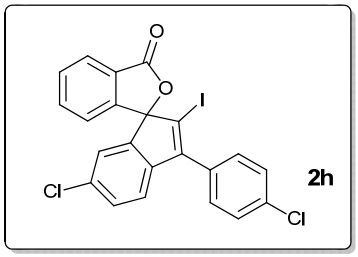
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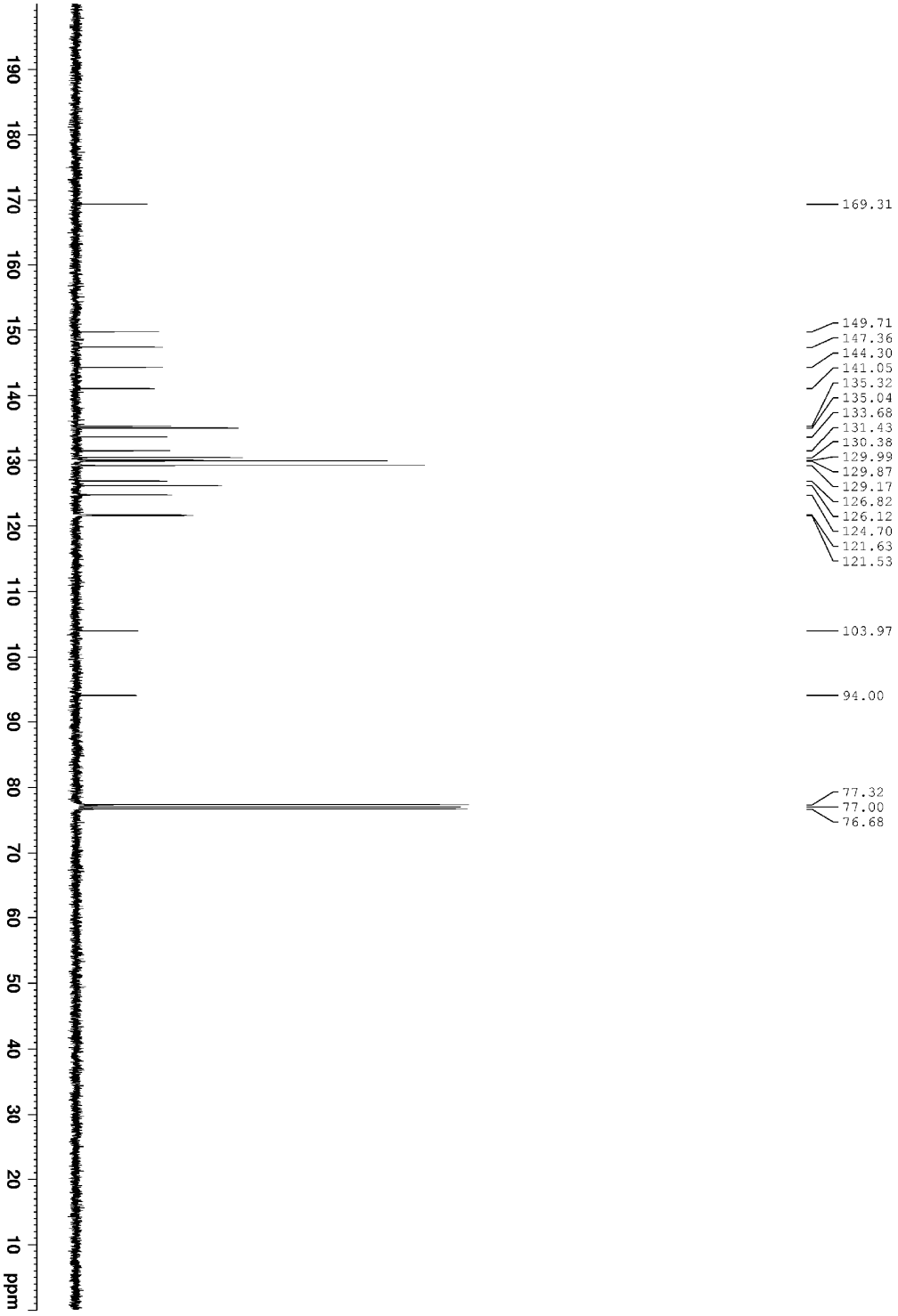
I
Cl
Cl
2h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10
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135.04
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129.99
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121.53
103.97
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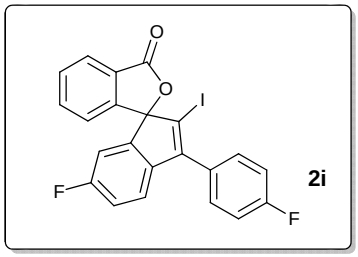
77.32
77.00
76.68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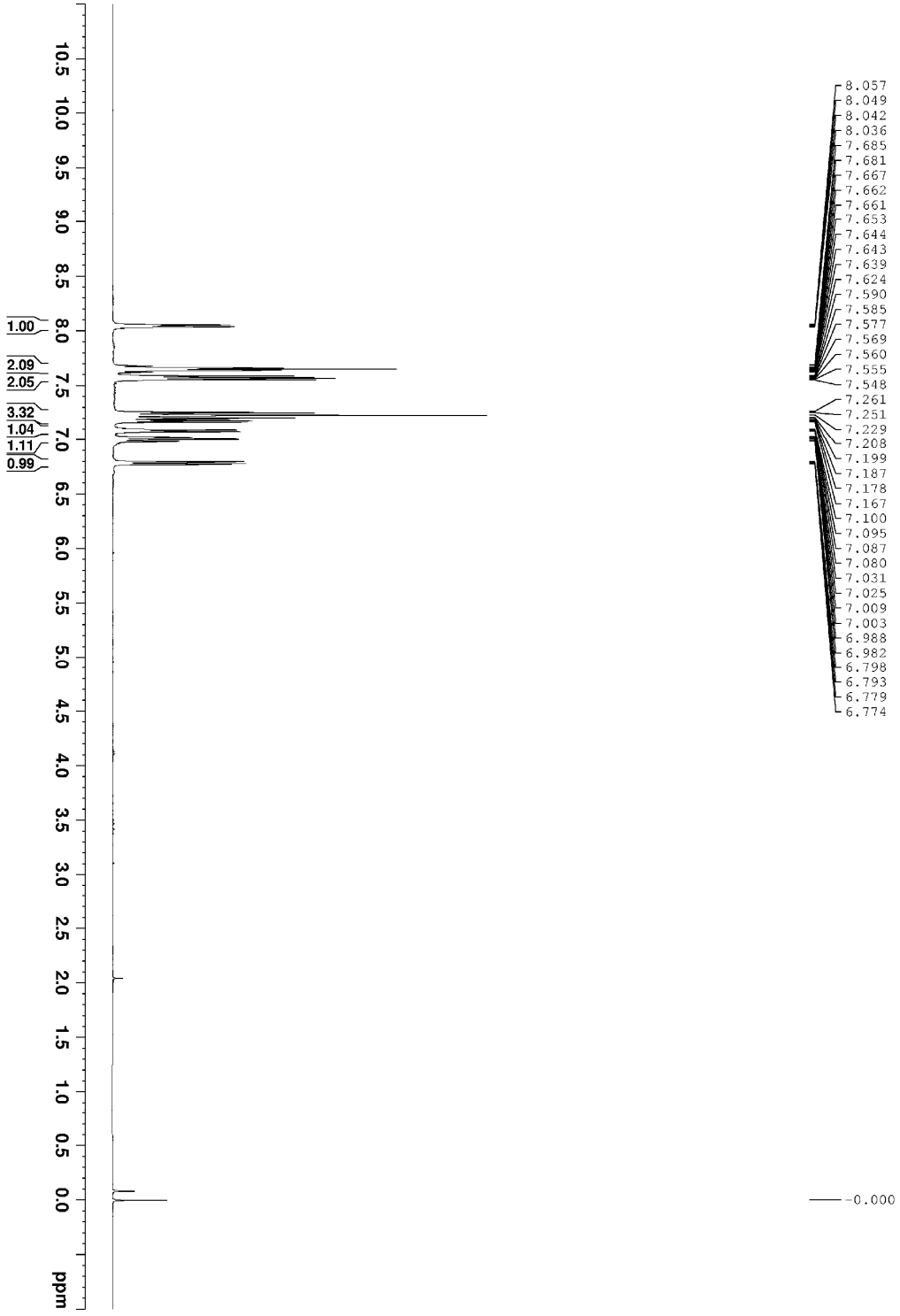
O
I
F
F
2i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1.04
1.11
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6.5
6.0
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7.087
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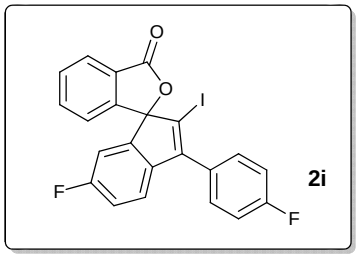
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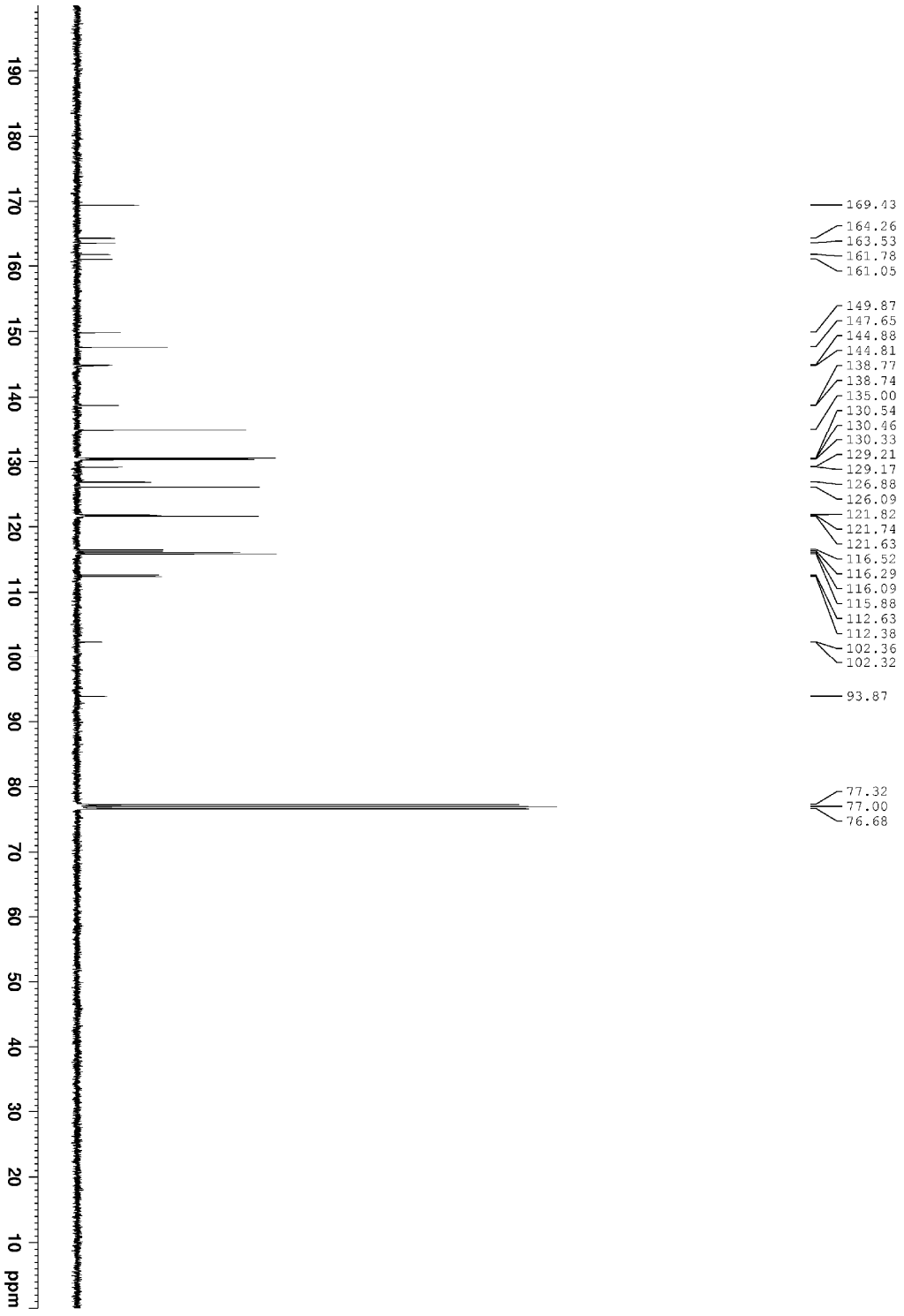
I
F
F
2i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138.74
135.00
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130.33
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129.17
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121.63
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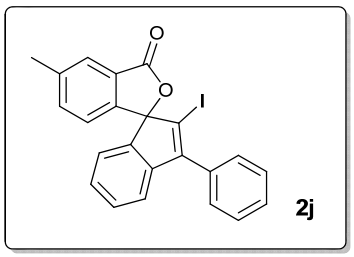
77.00
76.68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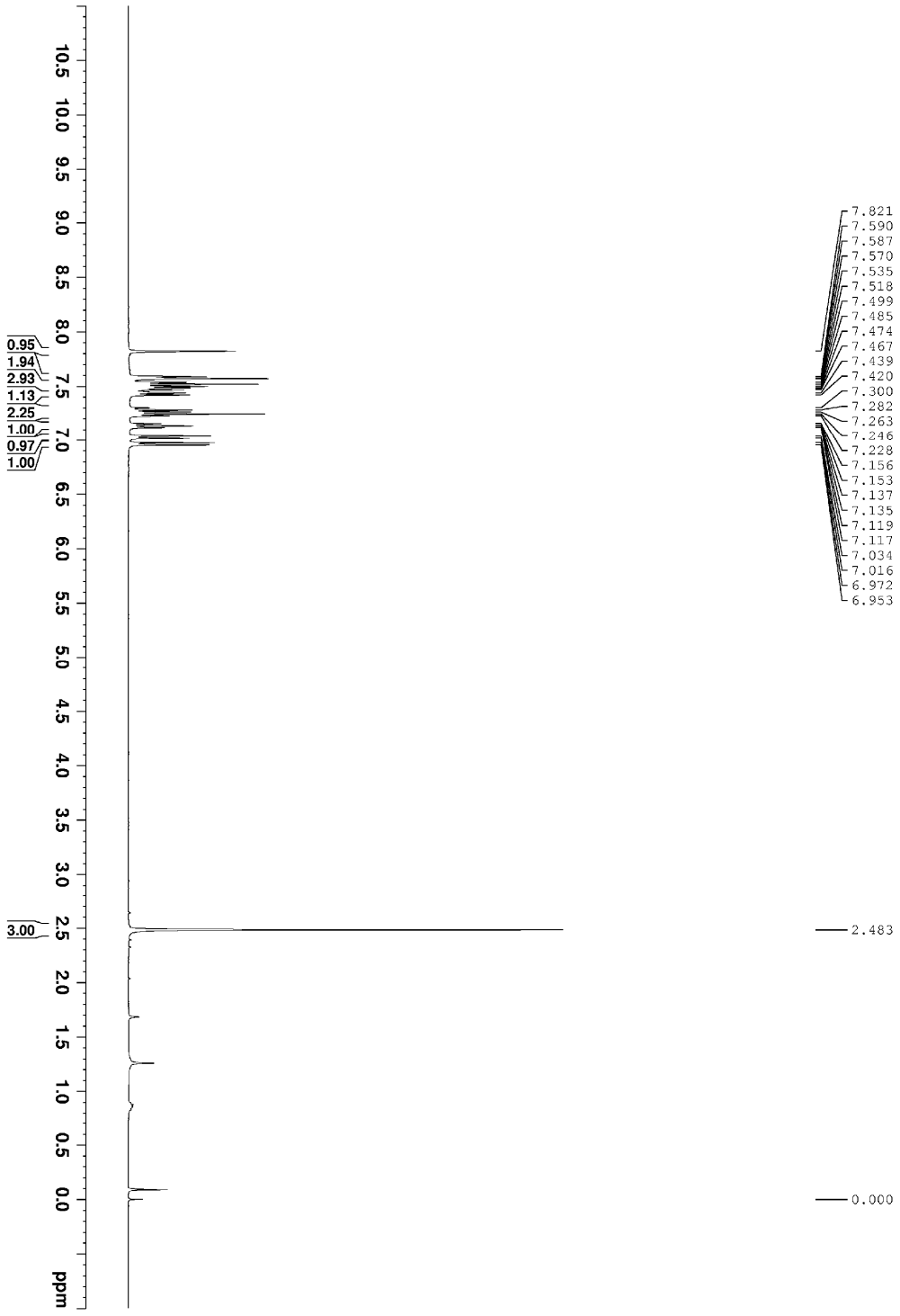
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7.570
7.535
7.518
7.499
7.485
7.474
7.467
7.439
7.420
7.300
7.282
7.263
7.246
7.228
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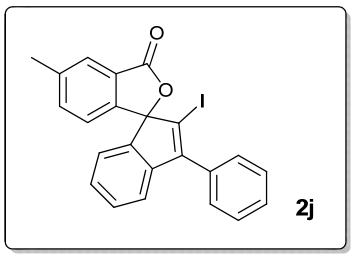
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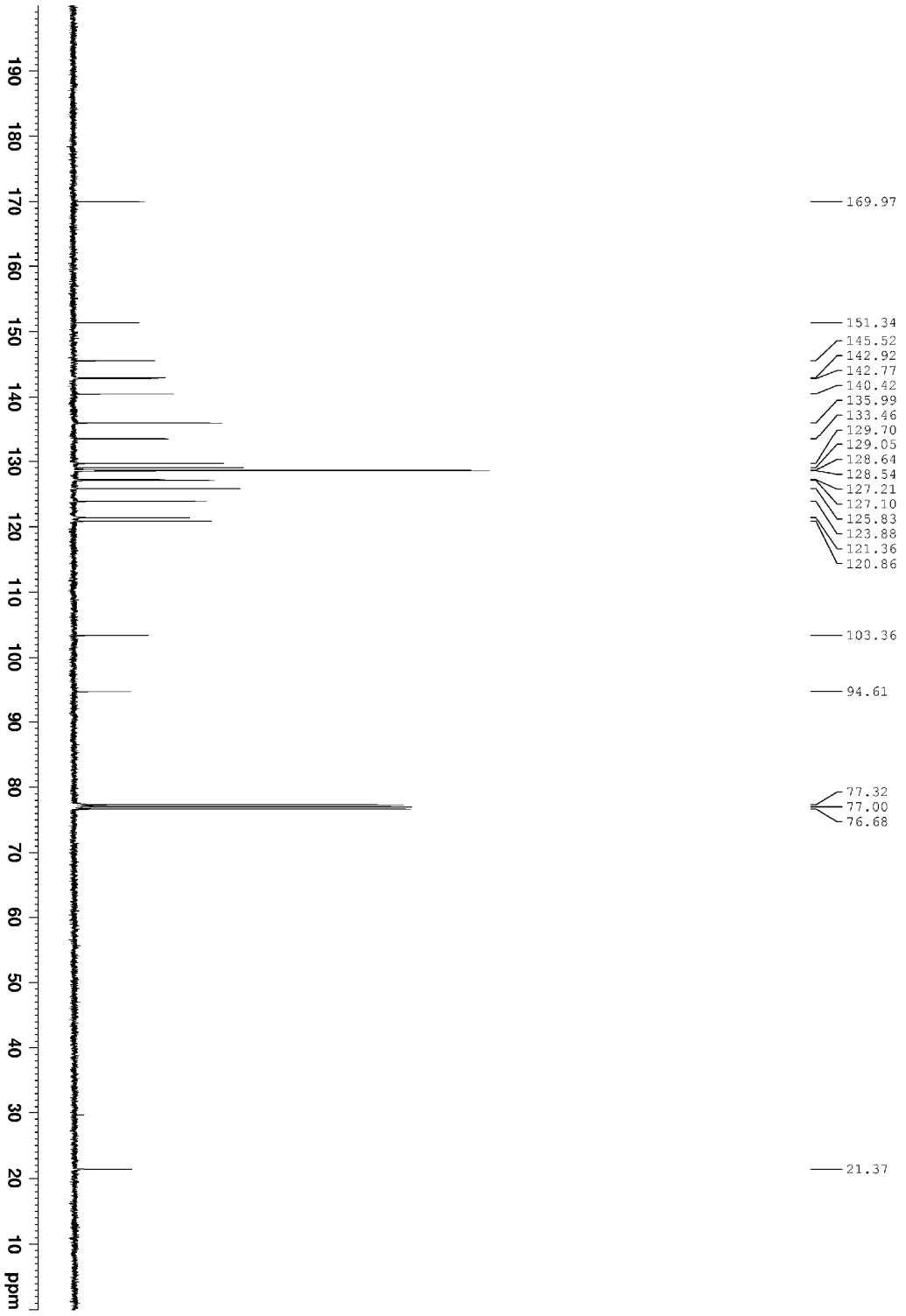
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129.70
129.05
128.64
128.54
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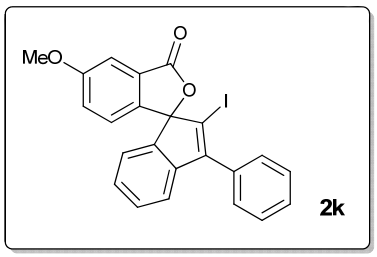
MeO
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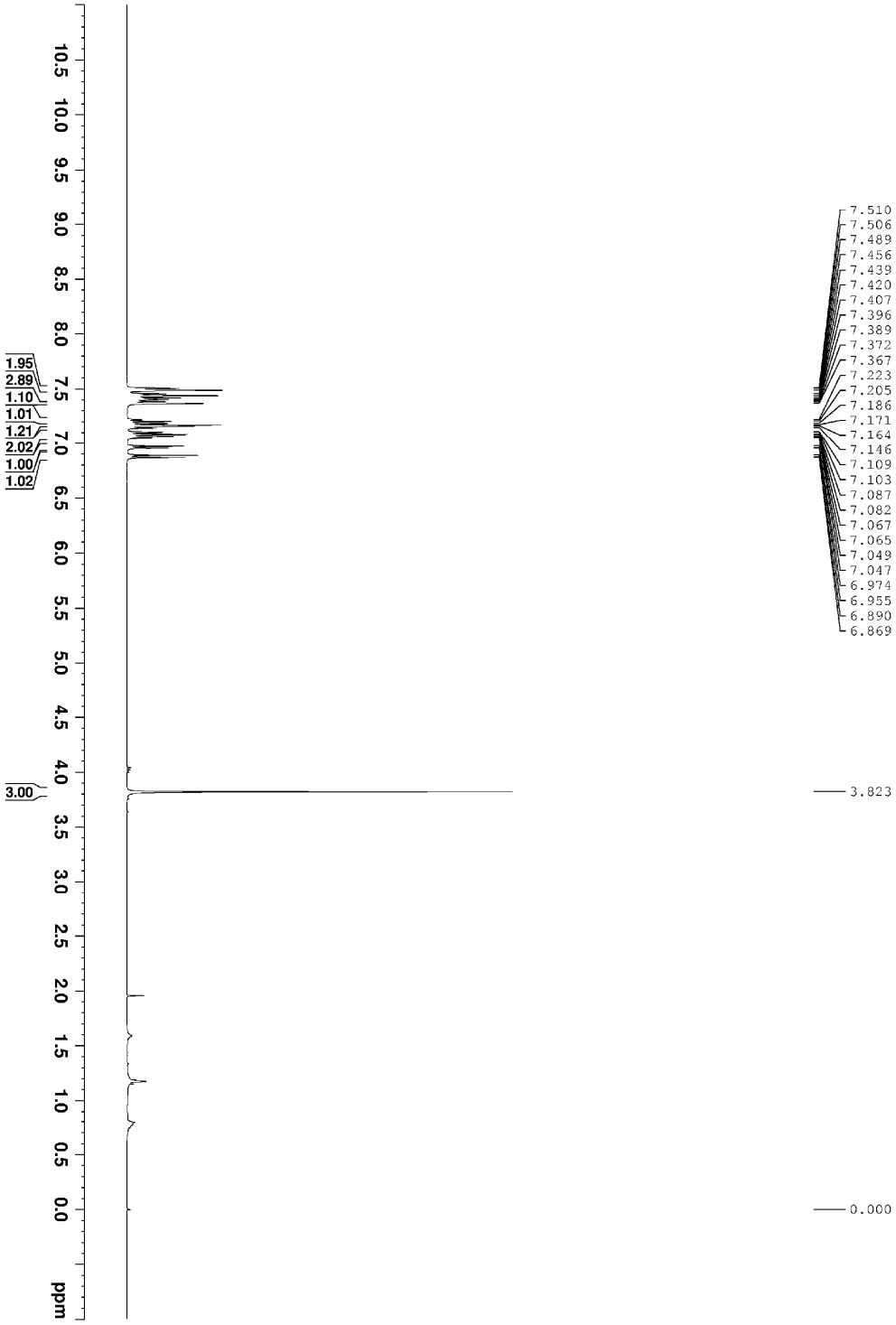
O
I
2k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1.02
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7.439
7.420
7.407
7.396
7.389
7.372
7.367
7.223
7.205
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7.171
7.164
7.146
7.109
7.103
7.087
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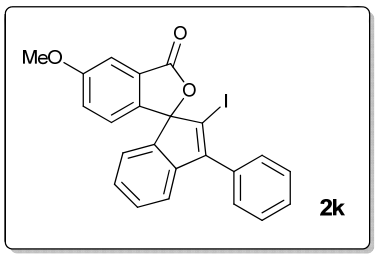
ppm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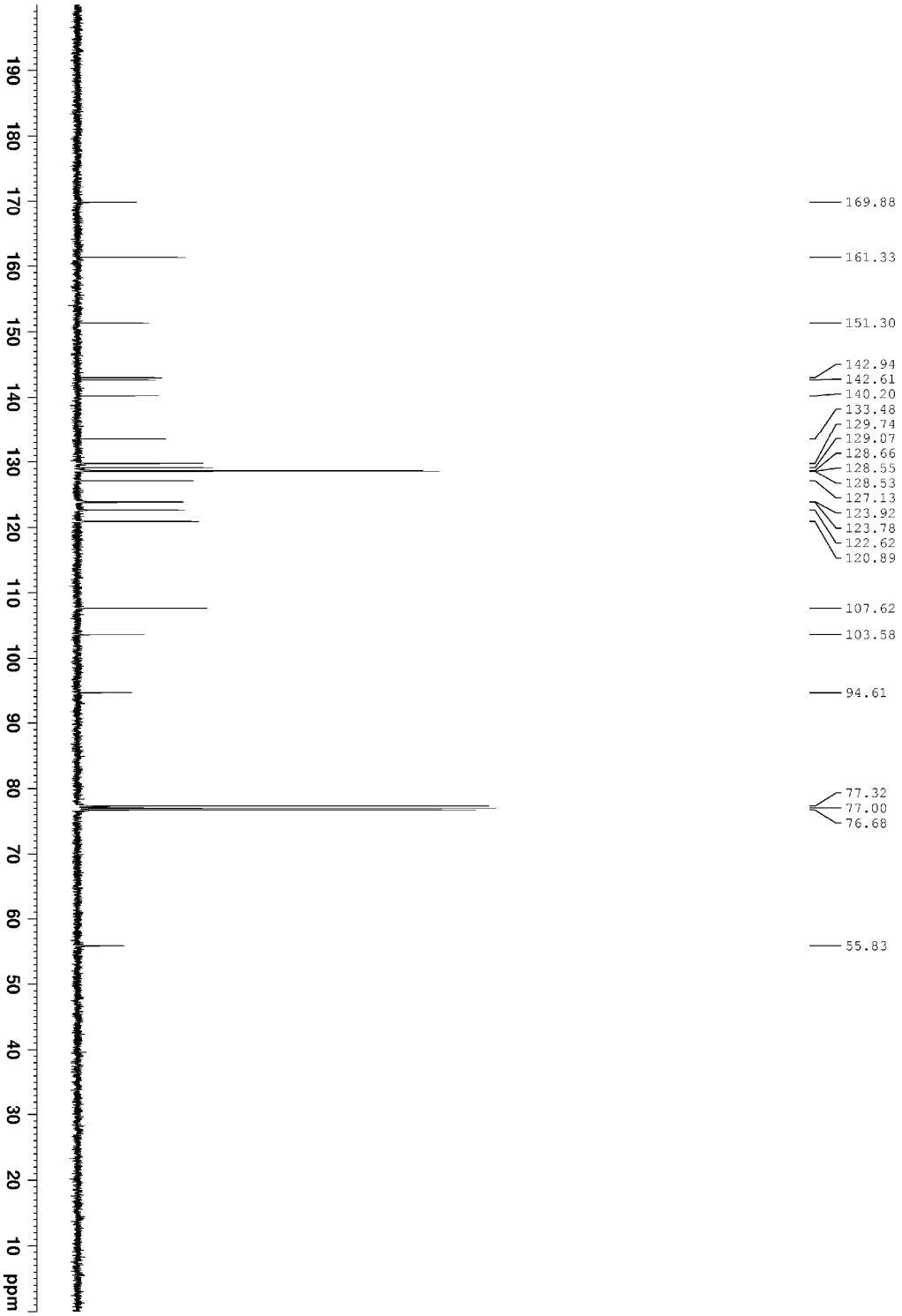
2k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77.00
76.68
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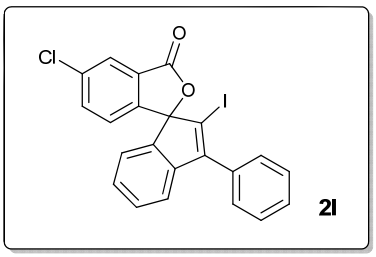
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O
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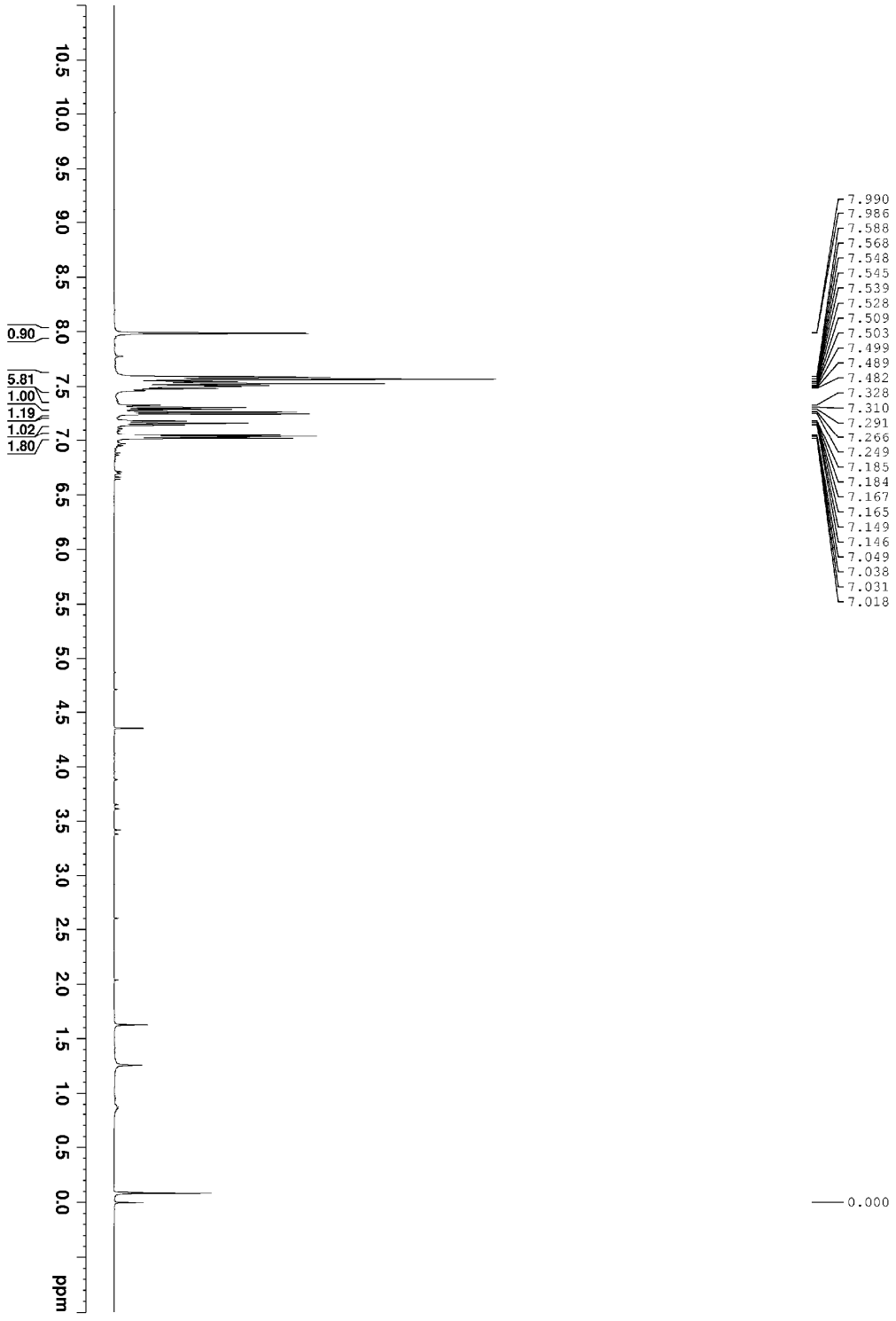
I

2l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7.503
7.499
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7.482
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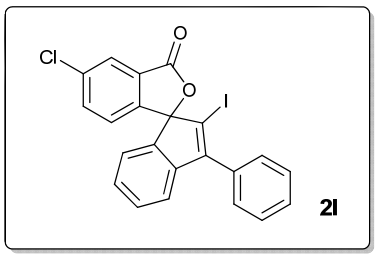
0.000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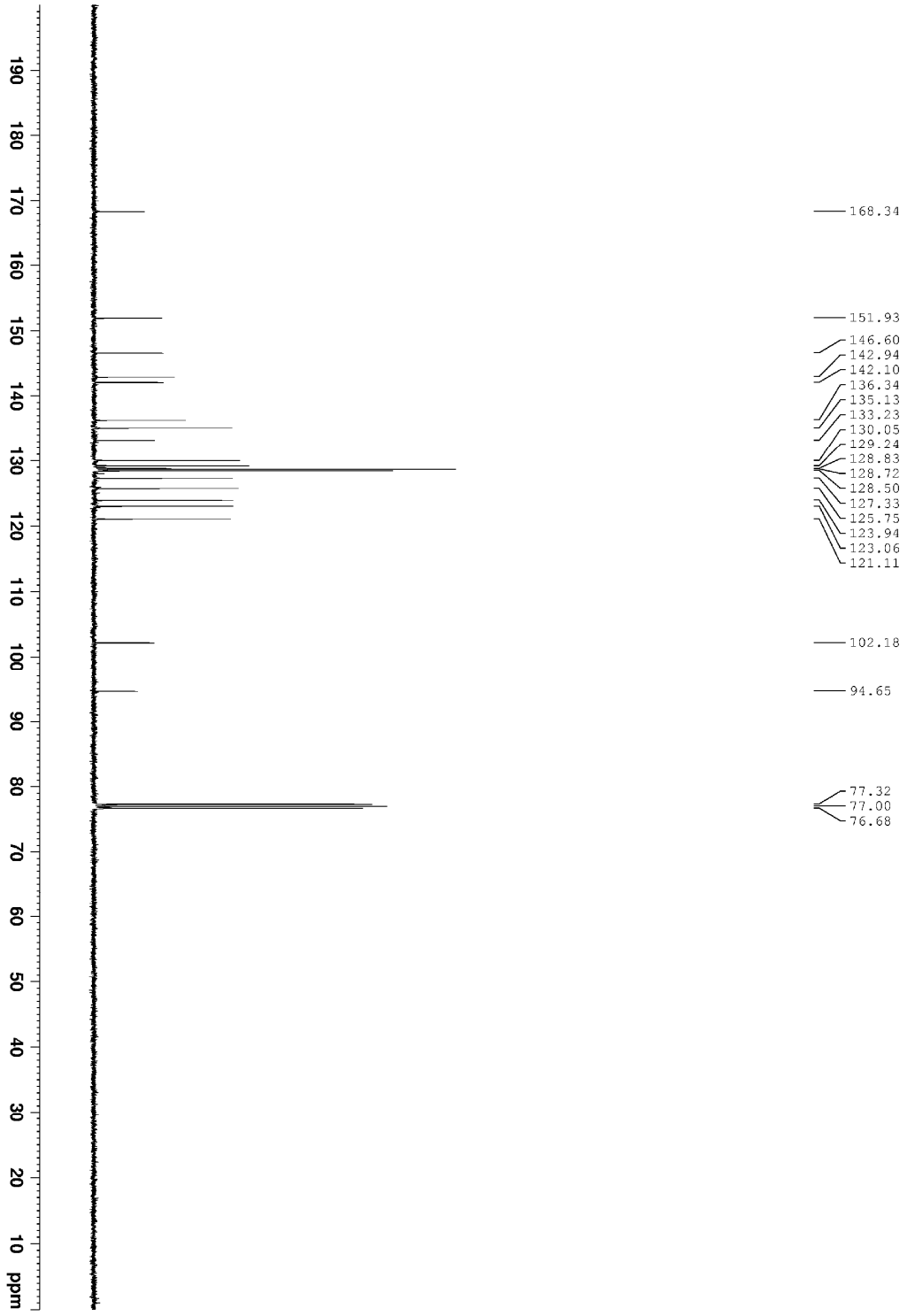
I

2l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ppm
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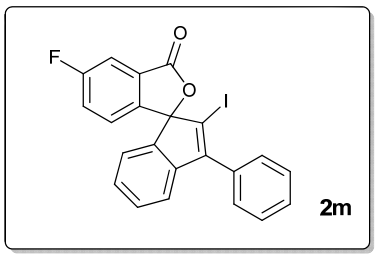
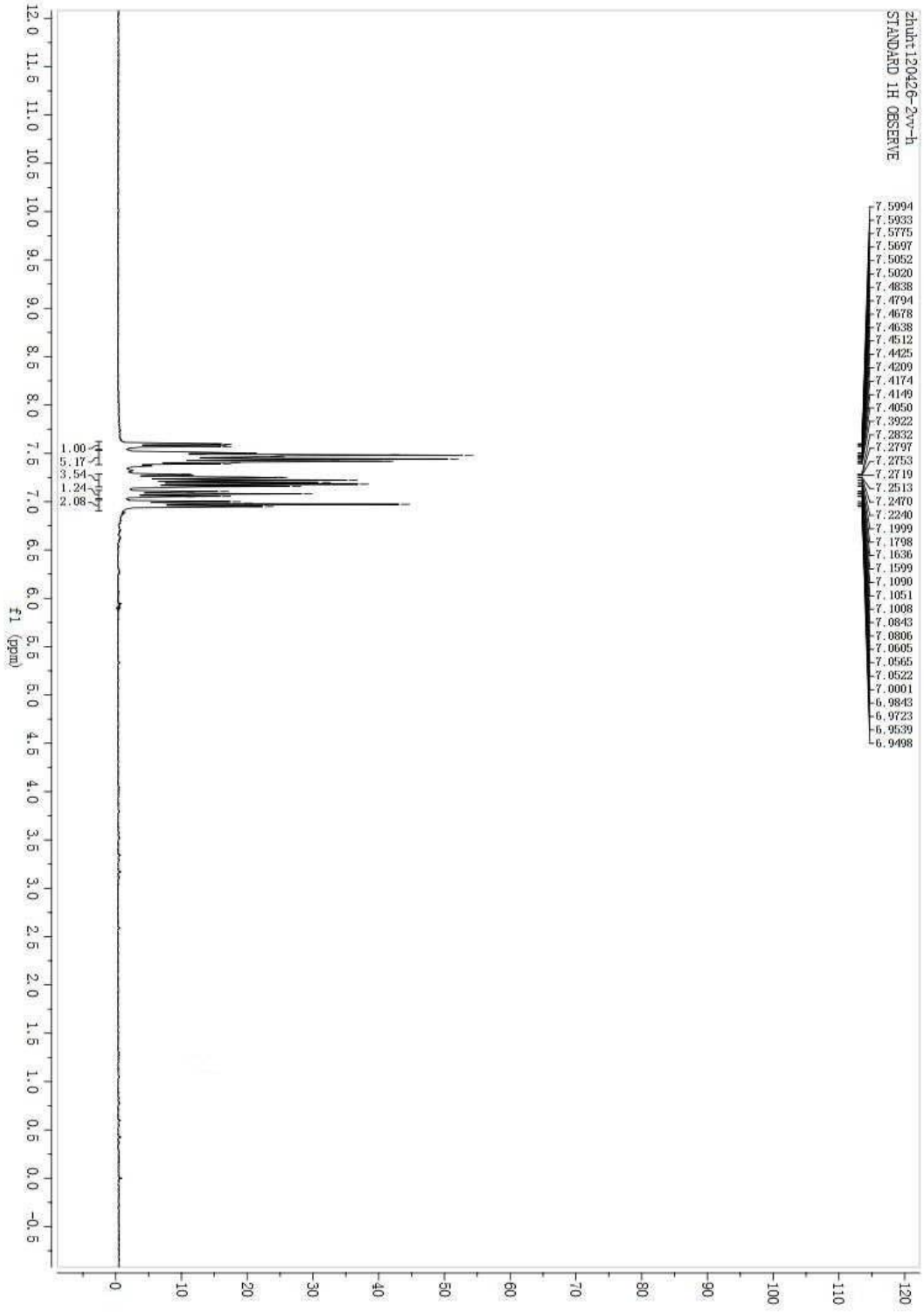
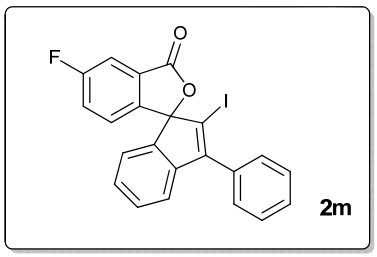
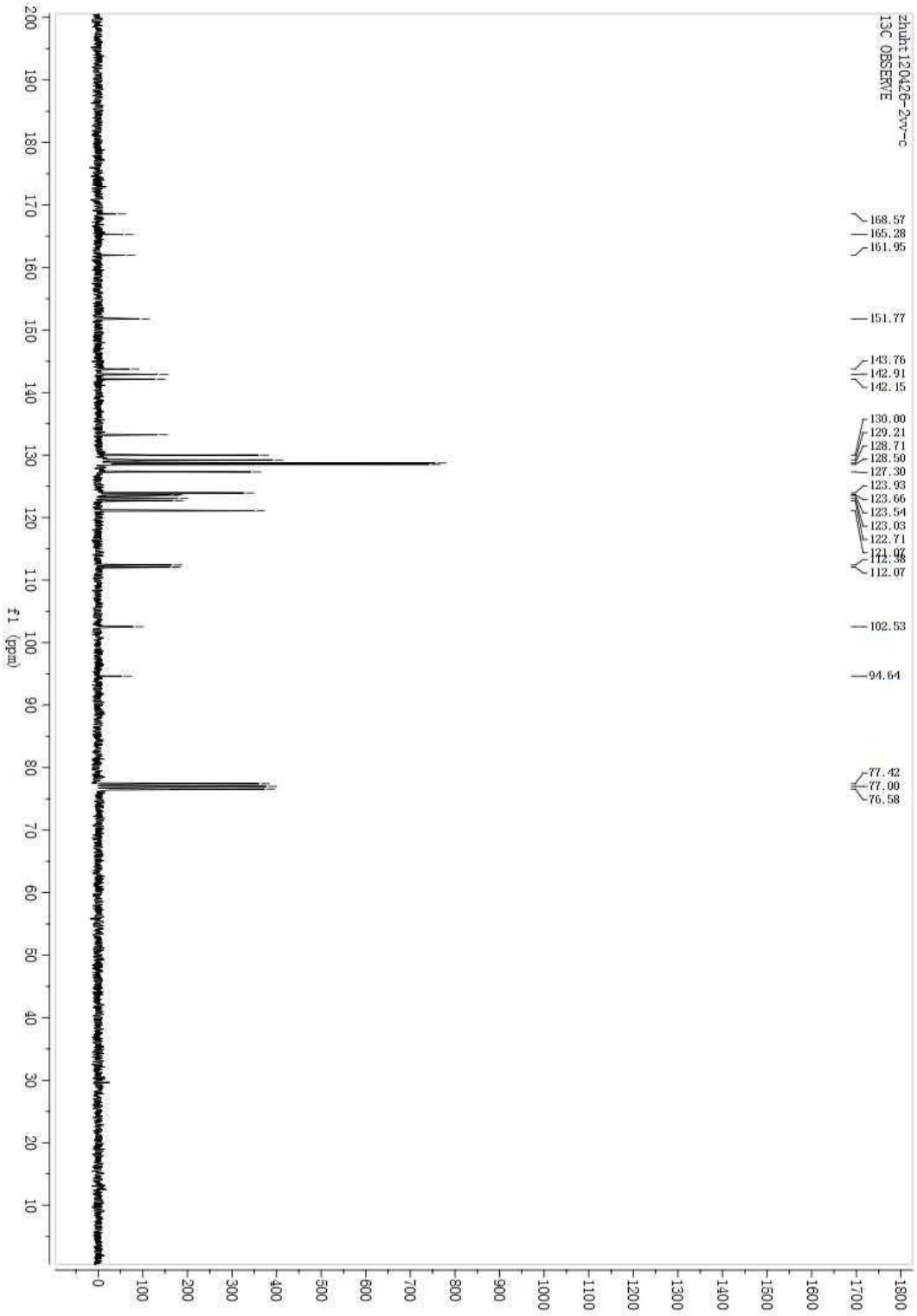
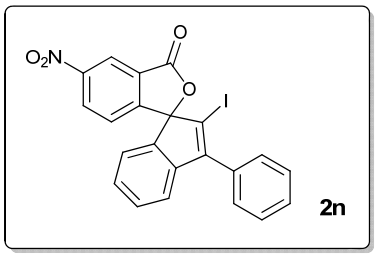
130.05
129.24
128.83
128.72
128.50
127.33
125.75
123.94
123.06
121.11
102.18
94.65
77.32
77.00
76.68

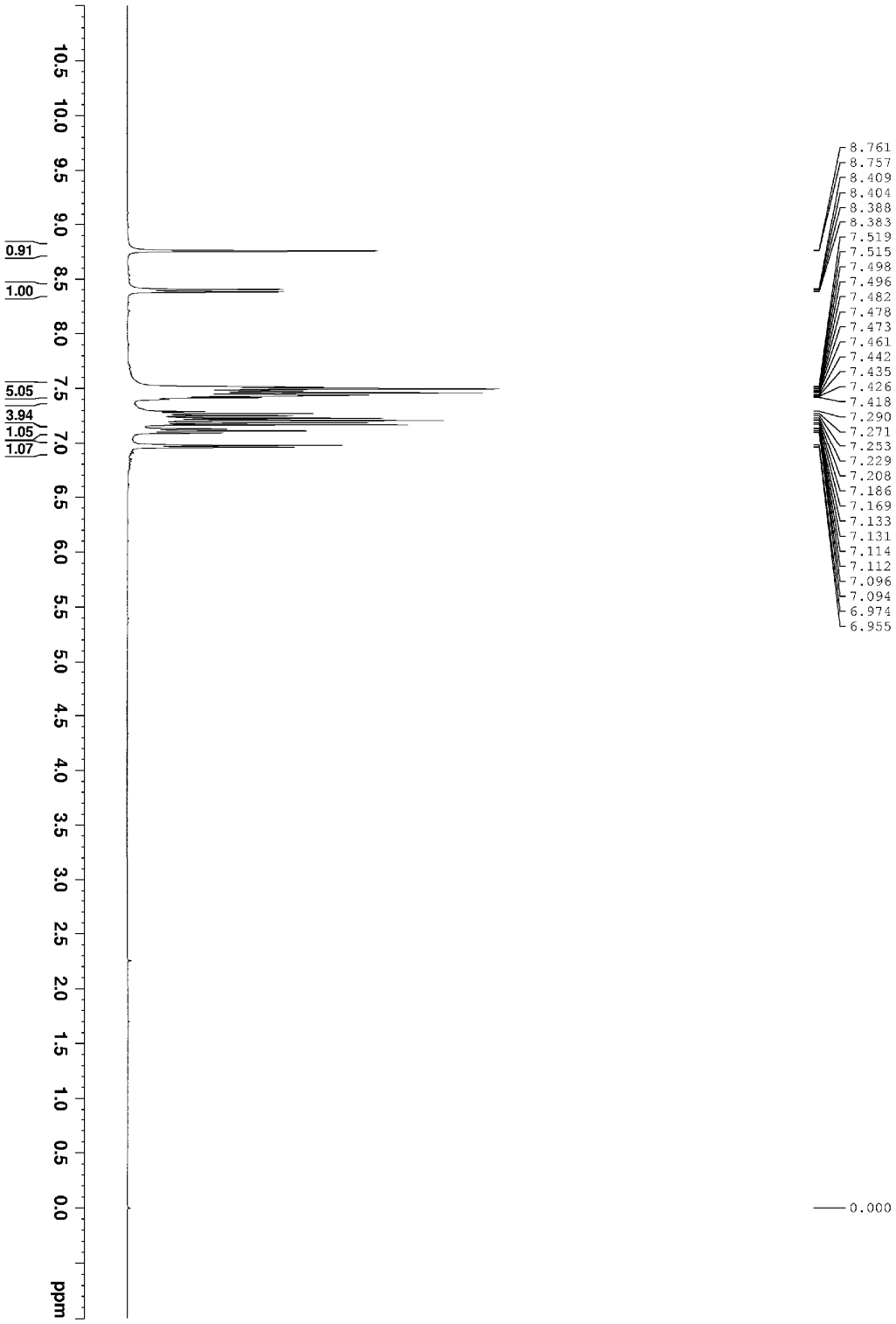

F
O
O
I
2m

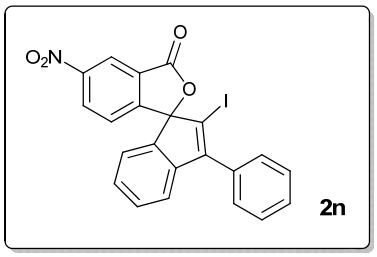

zhuht120426-2vv-h
STANDARD 1H OBSERVE
7.5994
7.5933
7.5775
7.5697
7.5052
7.5020
7.4838
7.4794
7.4678
7.4638
7.4512
7.4425
7.4209
7.4174
7.4149
7.4050
7.3922
7.2832
7.2797
7.2753
7.2719
7.2513
7.2470
7.2240
7.1999
7.1798
7.1636
7.1599
7.1090
7.1051
7.1008
7.0843
7.0806
7.0605
7.0565
7.0522
7.0001
6.9843
6.9723
6.9539
6.9498
1.00
5.17
3.54
1.24
2.08
f1 (ppm)

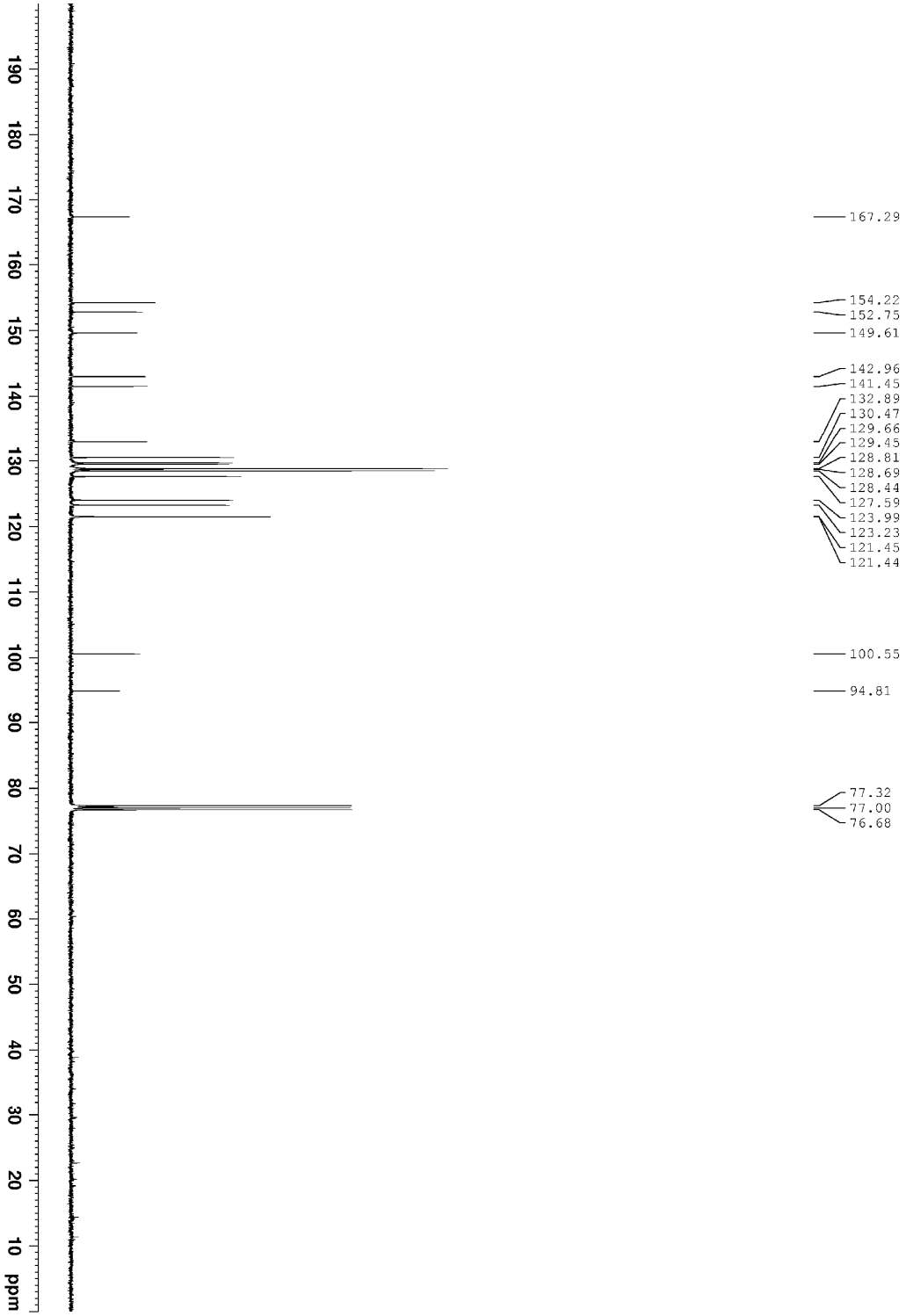

F
O
O
I
2m

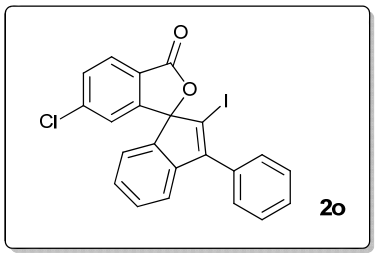

zhuht120426-2vv-c
13C OBSERVE
168.57
165.28
161.95
151.77
143.76
142.91
142.15
130.00
129.21
128.71
128.50
127.30
123.93
123.66
123.54
123.03
122.71
112.07
102.53
94.64
77.42
77.00
76.58
f1 (ppm)

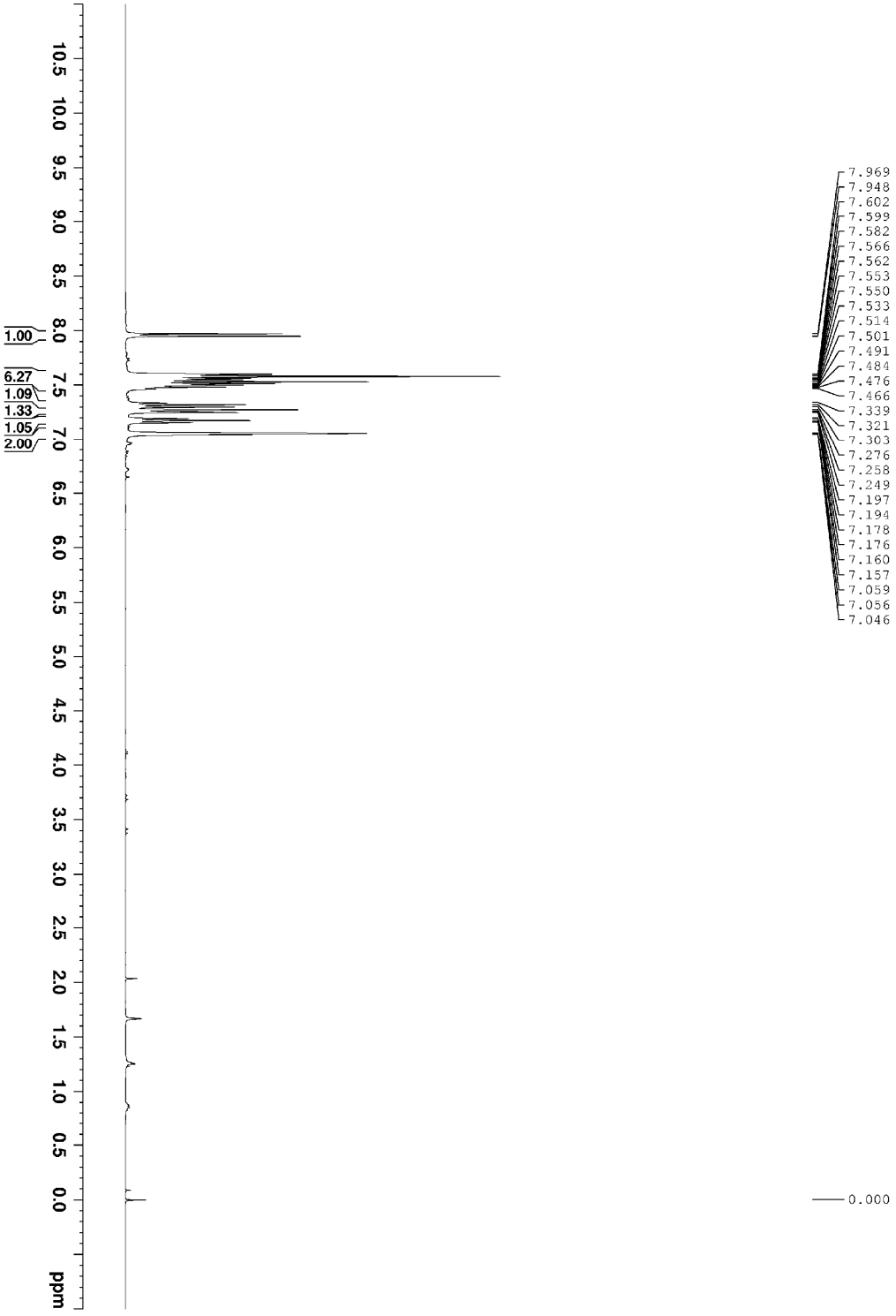

O2N
O
O
I
2n

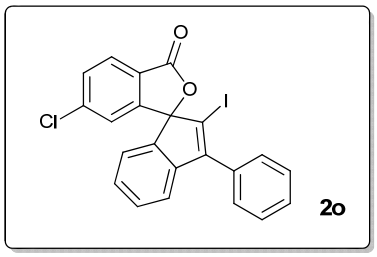

0.91
1.00
5.05
3.94
1.05
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm
8.761
8.757
8.409
8.404
8.388
8.383
7.519
7.515
7.498
7.496
7.482
7.478
7.473
7.461
7.442
7.435
7.426
7.418
7.290
7.271
7.253
7.229
7.208
7.186
7.169
7.133
7.131
7.114
7.112
7.096
7.094
6.974
6.955
0.000

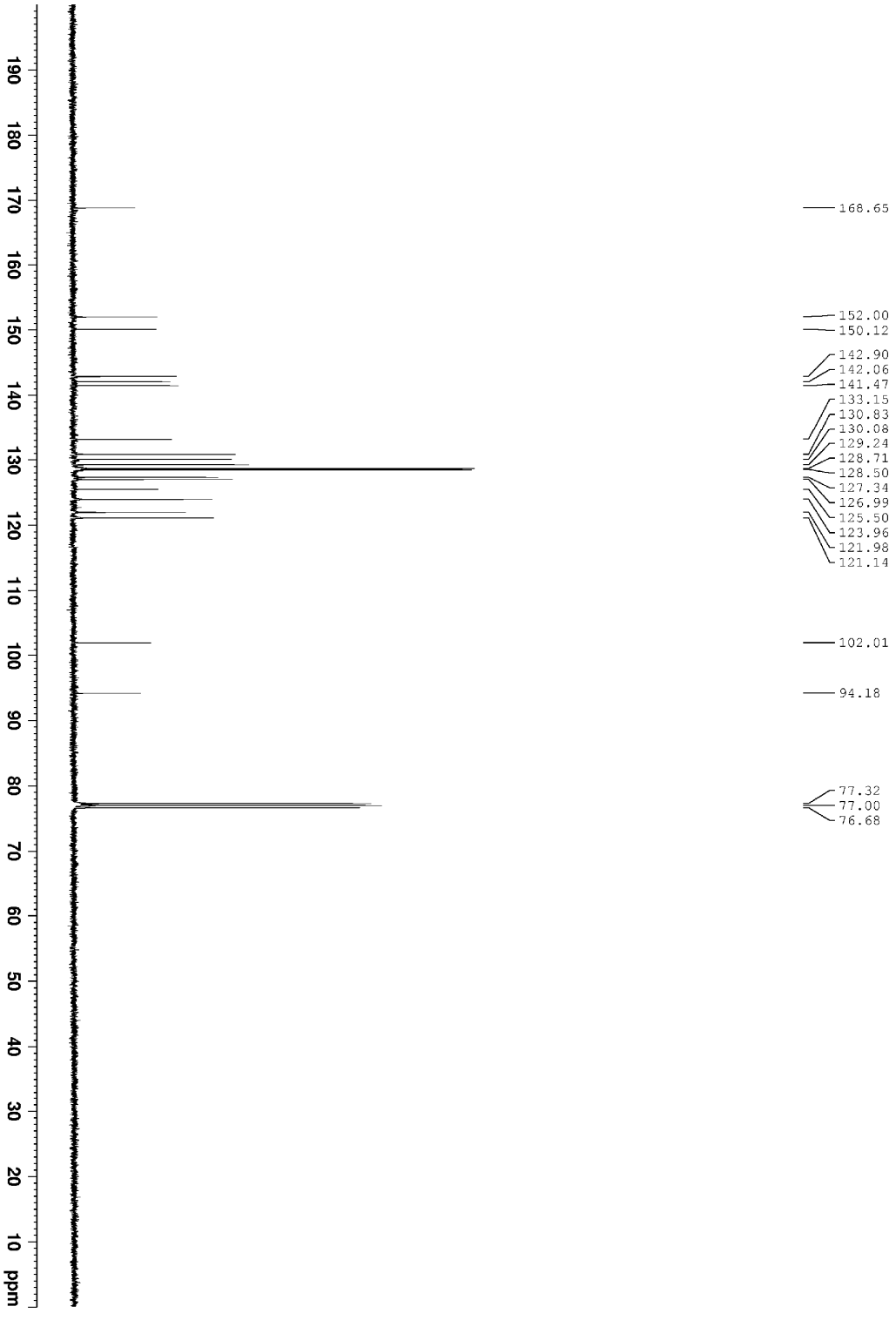

O2N
O
O
I
2n

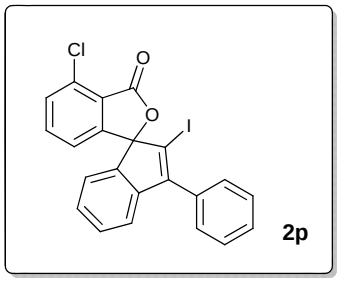

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
167.29
154.22
152.75
149.61
142.96
141.45
132.89
130.47
129.66
129.45
128.81
128.69
128.44
127.59
123.99
123.23
121.45
121.44
100.55
94.81
77.32
77.00
76.68

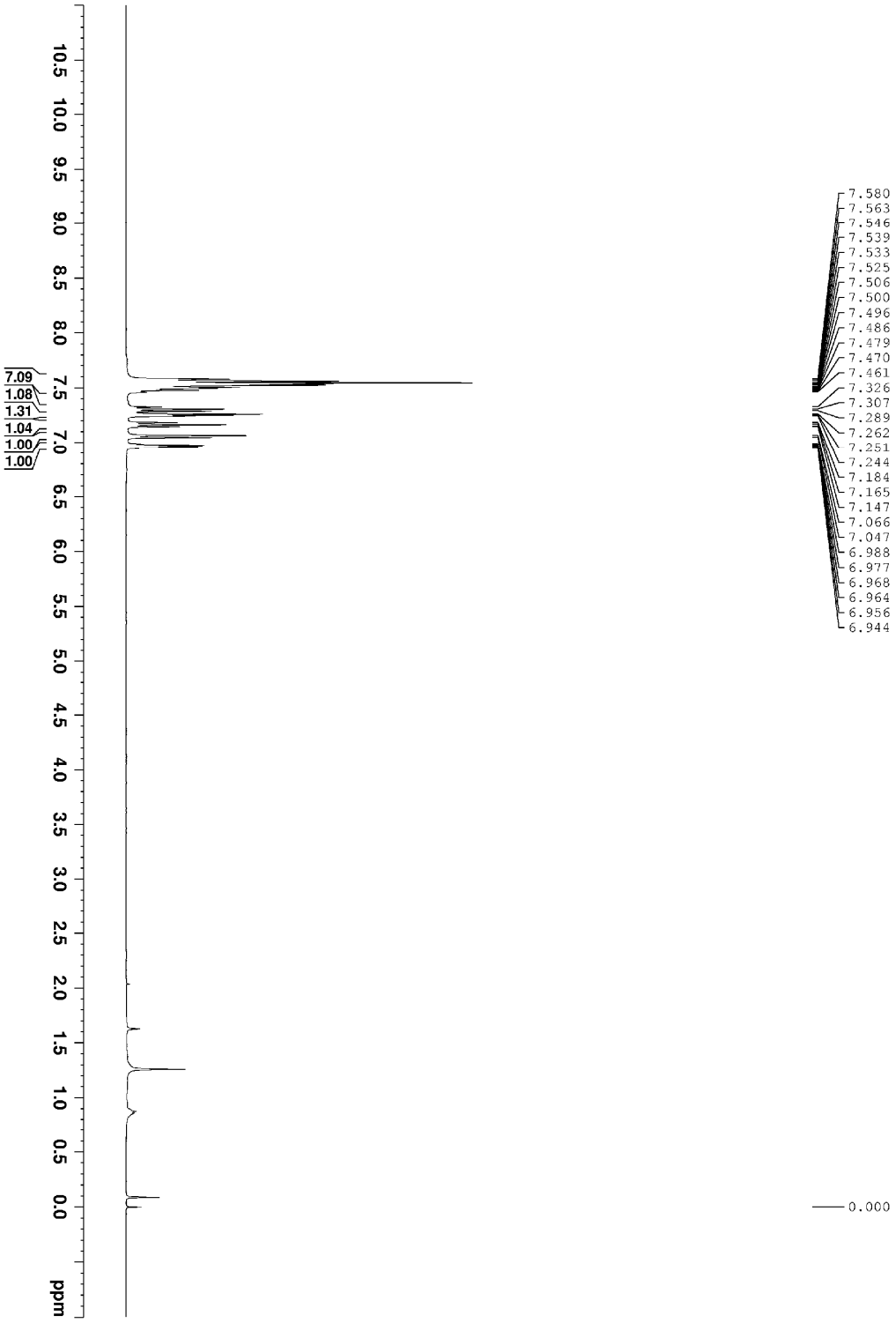

O
O
Cl
I
2o

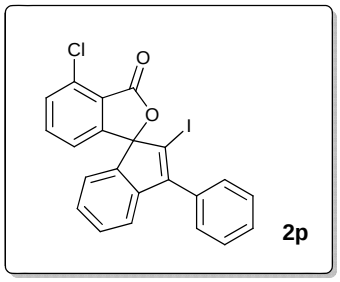

1.00
6.27
1.09
1.33
1.05
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
7.969
7.948
7.602
7.599
7.582
7.566
7.562
7.553
7.550
7.533
7.514
7.501
7.491
7.484
7.476
7.466
7.339
7.321
7.303
7.276
7.258
7.249
7.197
7.194
7.178
7.176
7.160
7.157
7.059
7.056
7.046
0.000

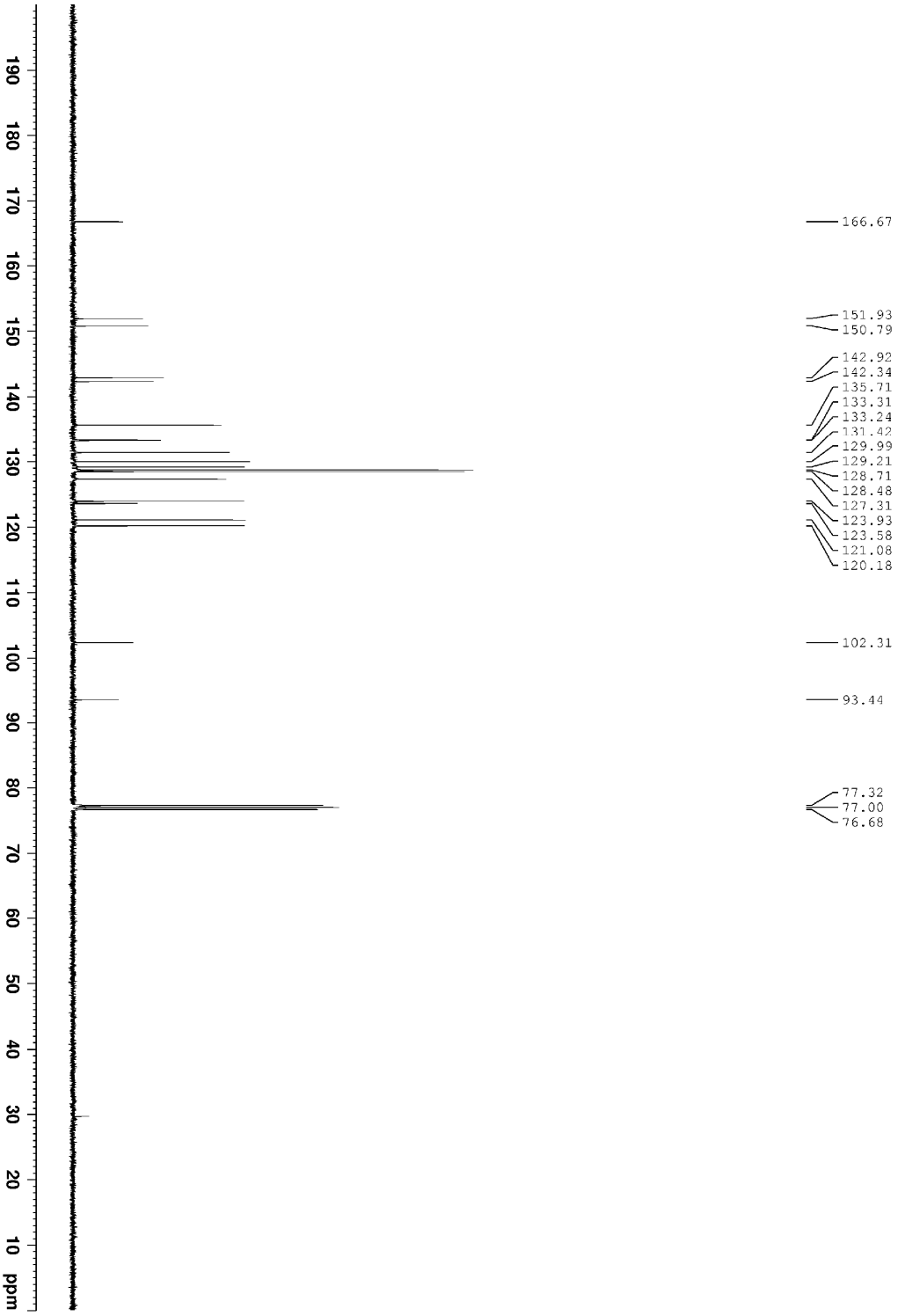

O
O
Cl
I
2o

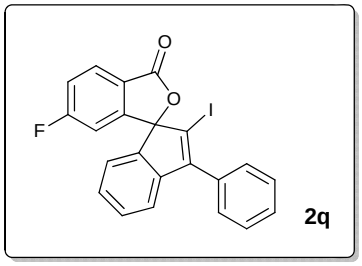

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
168.65
152.00
150.12
142.90
142.06
141.47
133.15
130.83
130.08
129.24
128.71
128.50
127.34
126.99
125.50
123.96
121.98
121.14
102.01
94.18
77.32
77.00
76.68


Cl
O
O
I
2p

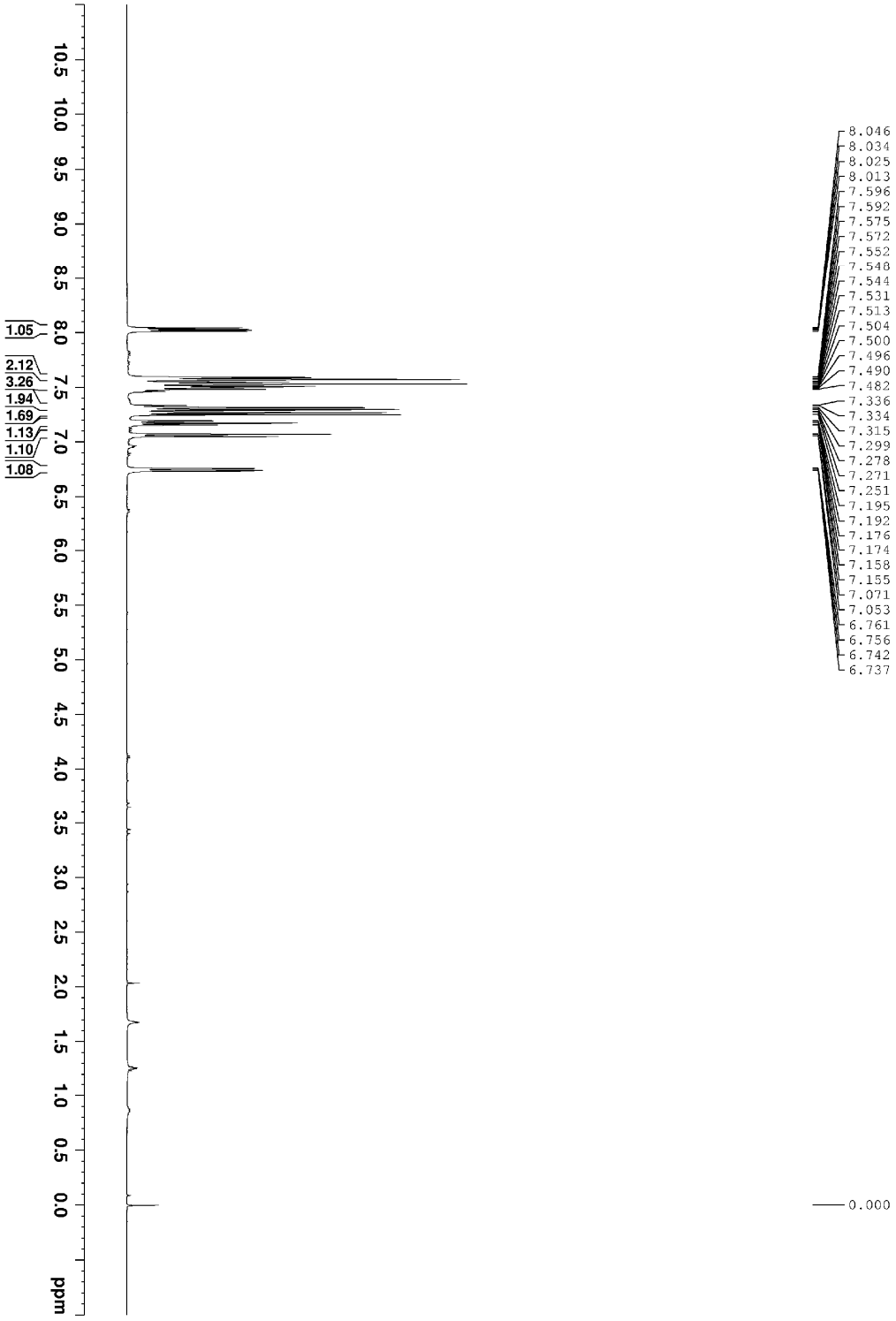

7.09
1.08
1.31
1.04
1.00
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
7.580
7.563
7.546
7.539
7.533
7.525
7.506
7.500
7.496
7.486
7.479
7.470
7.461
7.326
7.307
7.289
7.262
7.251
7.244
7.184
7.165
7.147
7.066
7.047
6.988
6.977
6.968
6.964
6.956
6.944
0.000

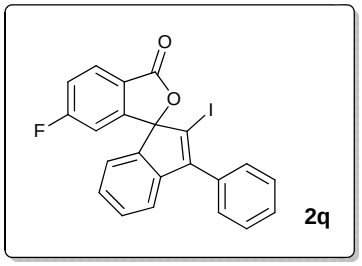

Cl
O
O
I
2p

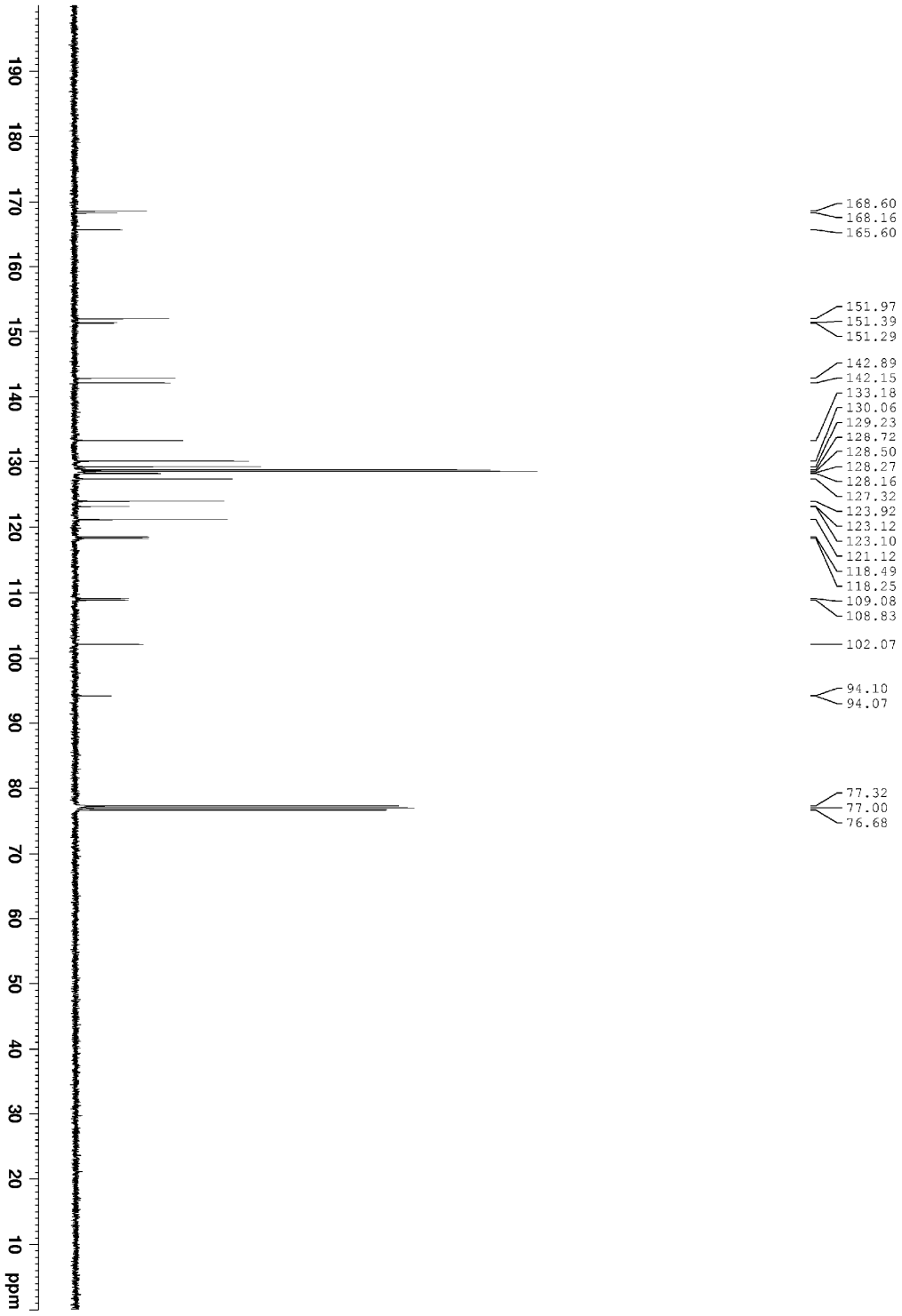

166.67
151.93
150.79
142.92
142.34
135.71
133.31
133.24
131.42
129.99
129.21
128.71
128.48
127.31
123.93
123.58
121.08
120.18
102.31
93.44
77.32
77.00
76.68
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

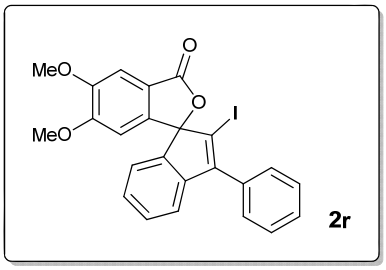

O
O
I
F

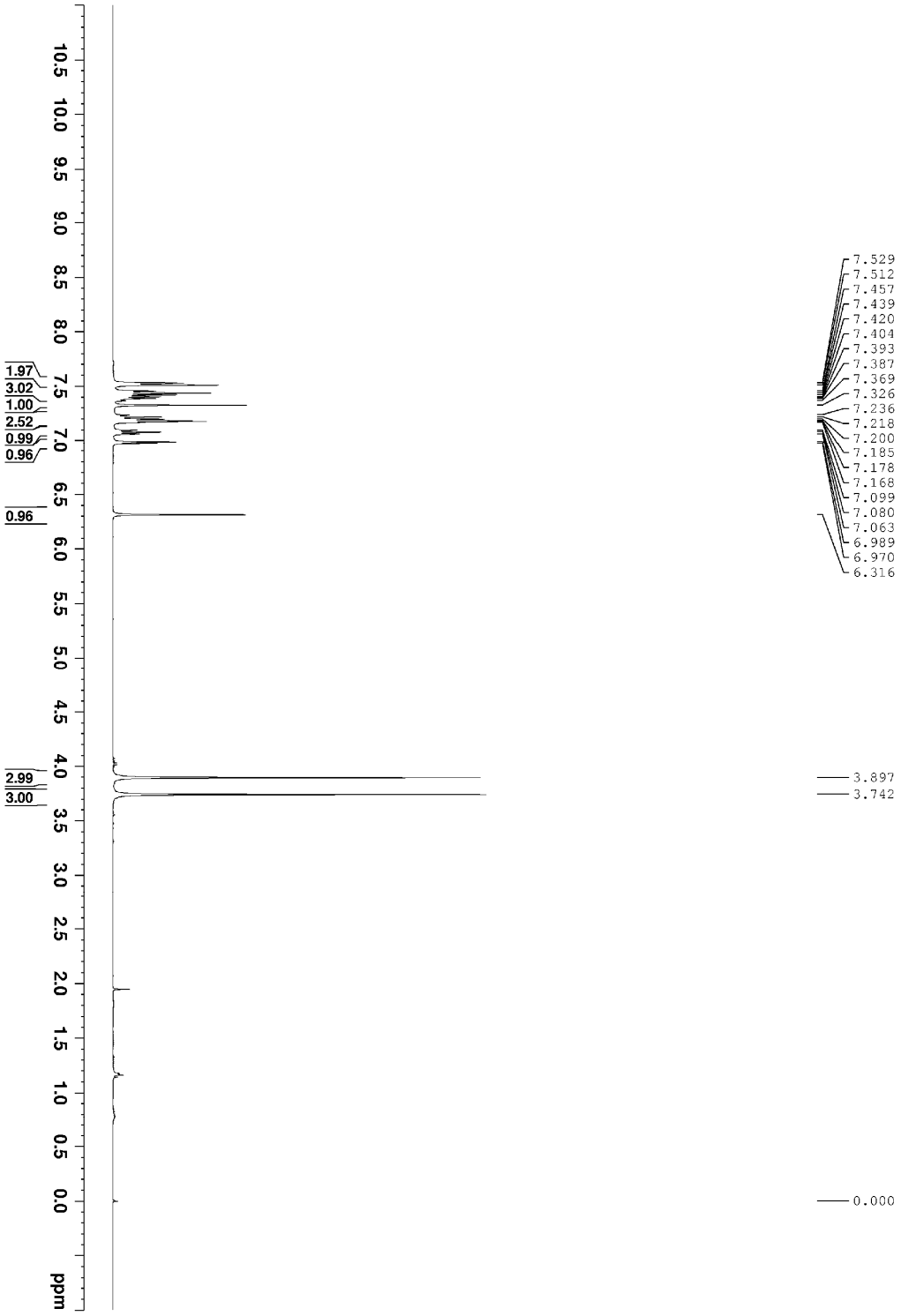
2q

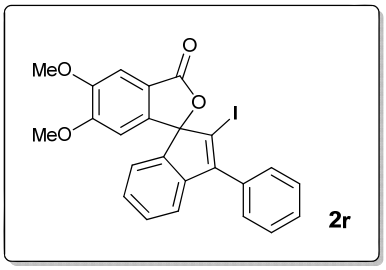

1.05
2.12
3.26
1.94
1.69
1.13
1.10
1.08
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
8.046
8.034
8.025
8.013
7.596
7.592
7.575
7.572
7.552
7.548
7.544
7.531
7.513
7.504
7.500
7.496
7.490
7.482
7.336
7.334
7.315
7.299
7.278
7.271
7.251
7.195
7.192
7.176
7.174
7.158
7.155
7.071
7.053
6.761
6.756
6.742
6.737
0.000

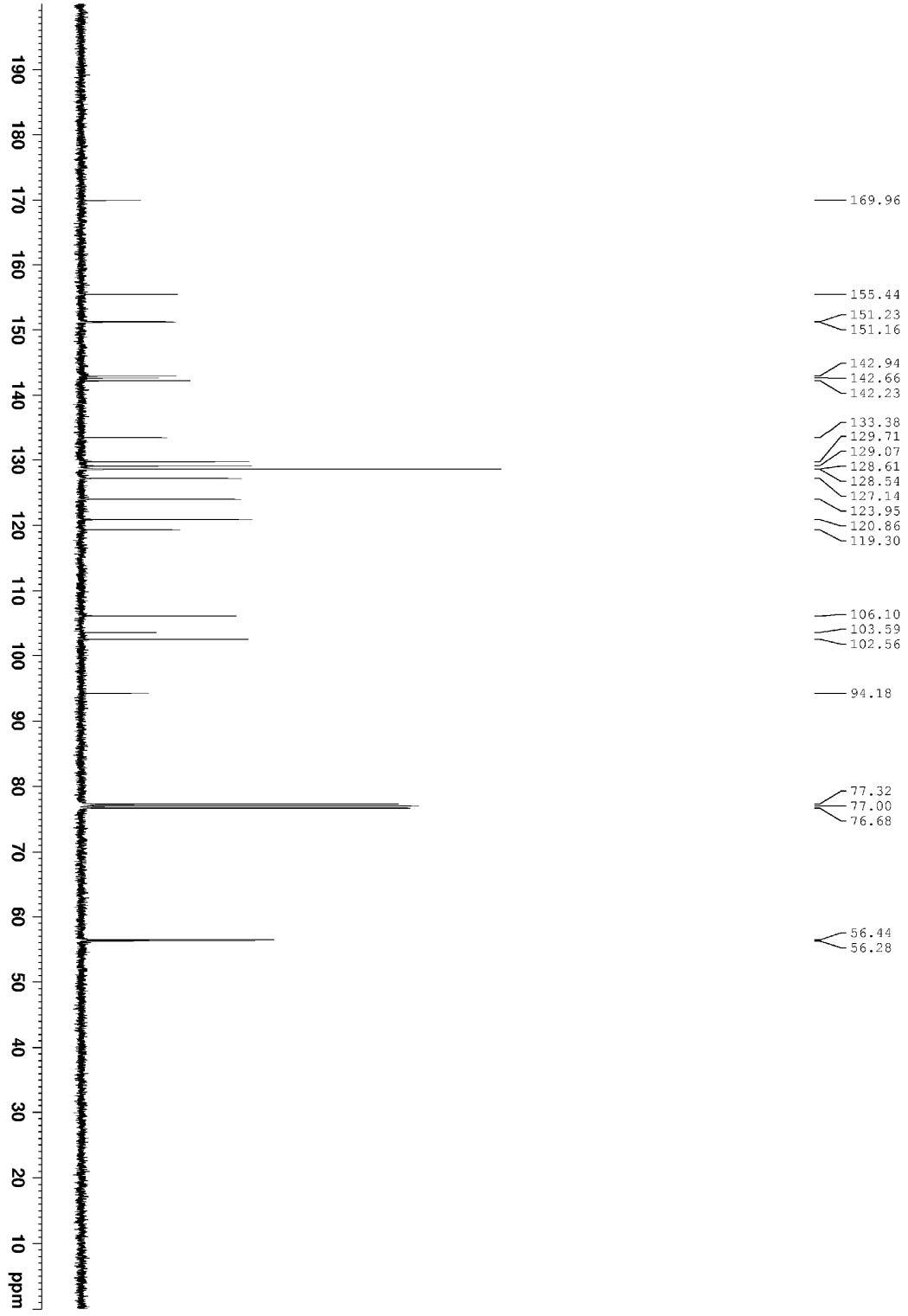

O
O
I
F
2q

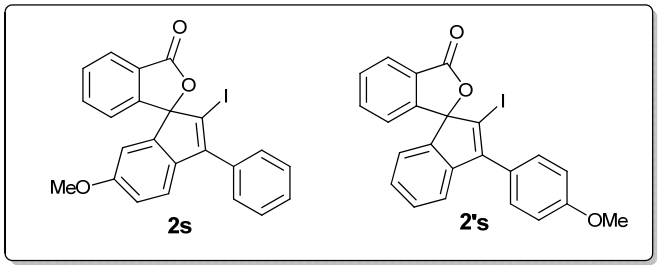

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
168.60
168.16
165.60
151.97
151.39
151.29
142.89
142.15
133.18
130.06
129.23
128.72
128.50
128.27
128.16
127.32
123.92
123.12
123.10
121.12
118.49
118.25
109.08
108.83
102.07
94.10
94.07
77.32
77.00
76.68

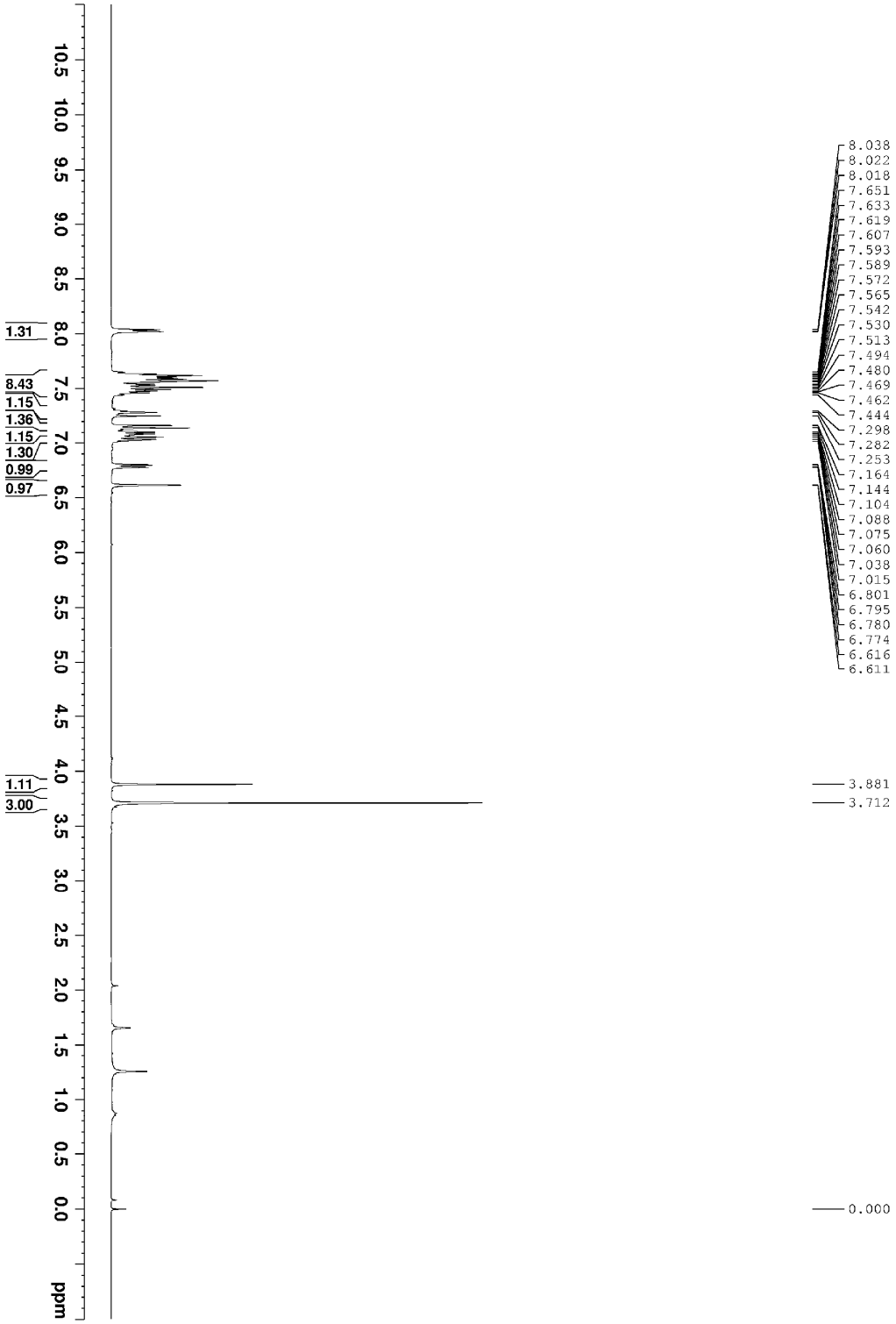

MeO
MeO
O
O
I
2r

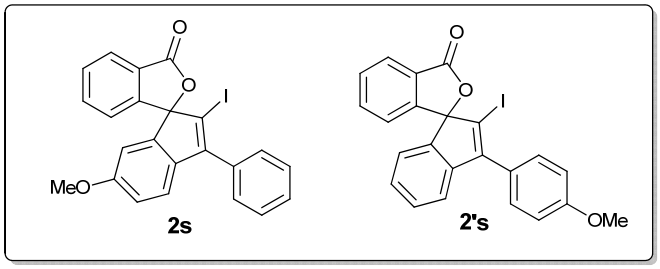

1.97
3.02
1.00
2.52
0.99
0.96
0.96
2.99
3.00
7.529
7.512
7.457
7.439
7.420
7.404
7.393
7.387
7.369
7.326
7.236
7.218
7.200
7.185
7.178
7.168
7.099
7.080
7.063
6.989
6.970
6.316
3.897
3.742
0.000
ppm

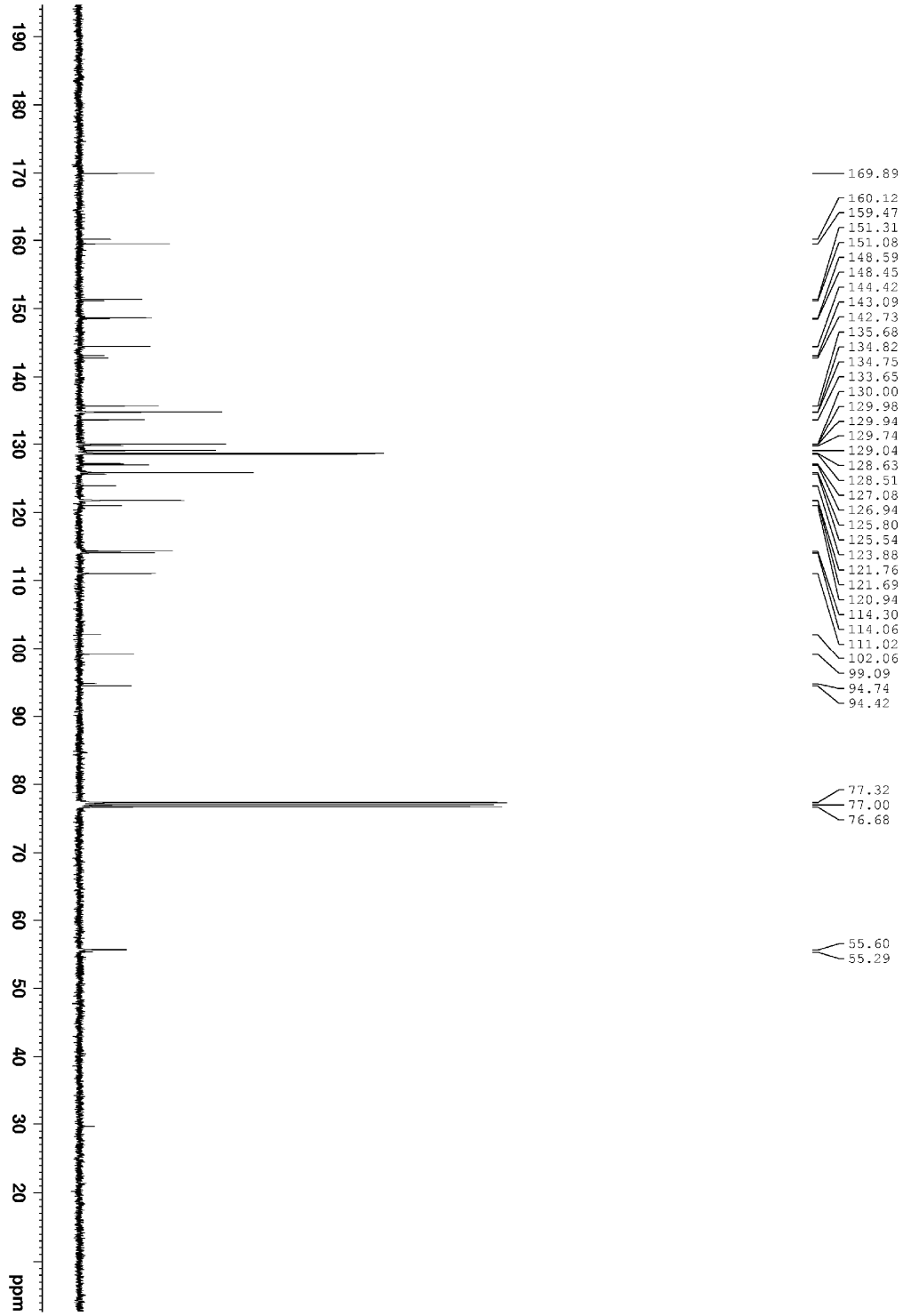

MeO
MeO
O
O
I
2r

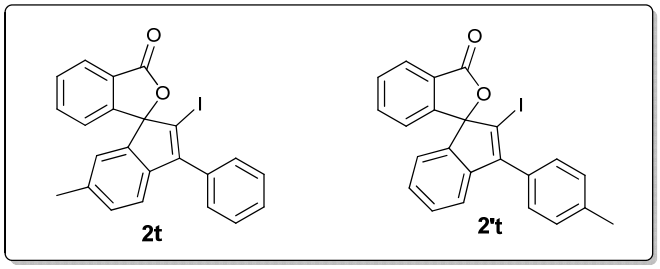

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
169.96
155.44
151.23
151.16
142.94
142.66
142.23
133.38
129.71
129.07
128.61
128.54
127.14
123.95
120.86
119.30
106.10
103.59
102.56
94.18
77.32
77.00
76.68
56.44
56.28

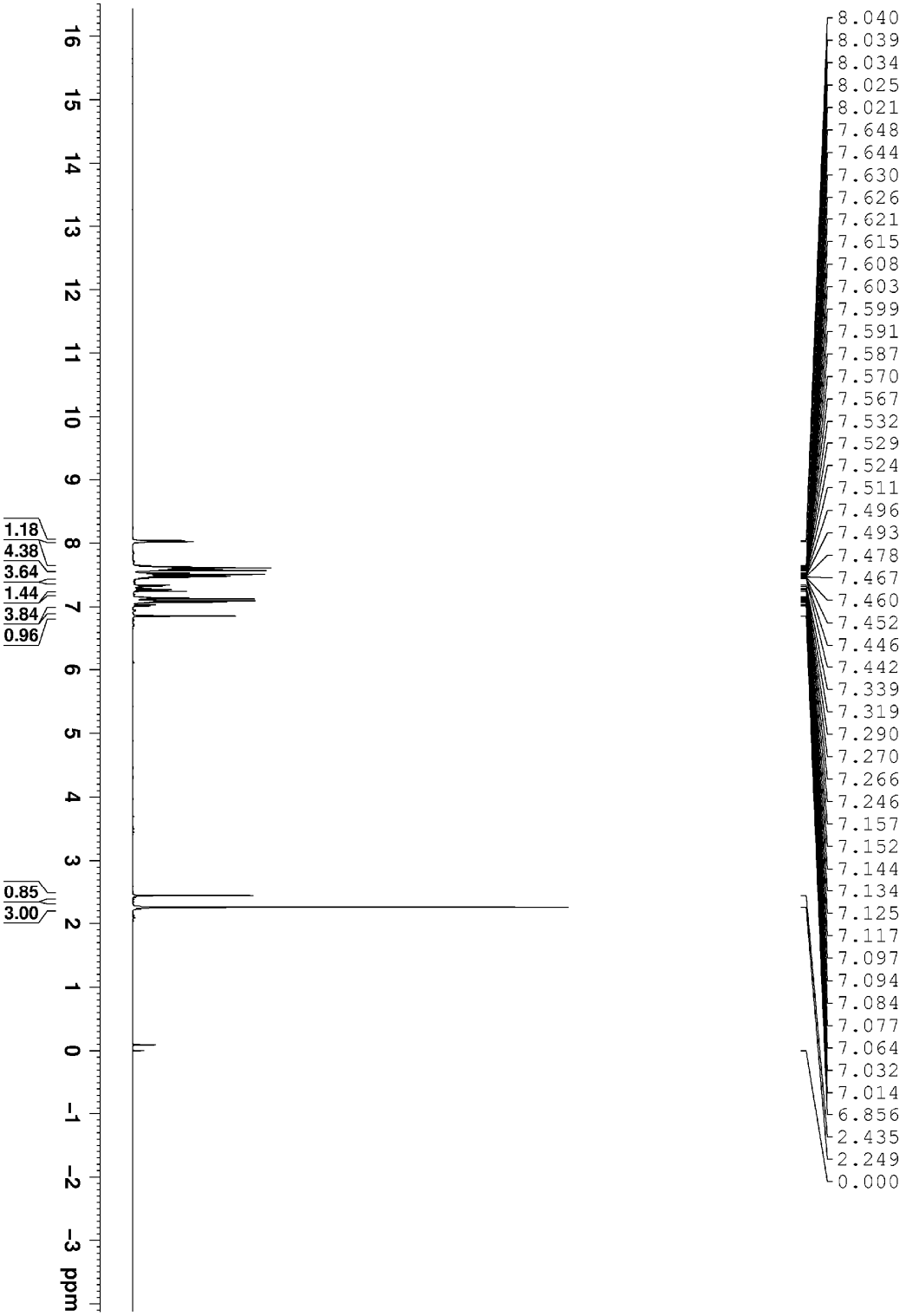

O
O
I
MeO
2s
O
O
I
OMe
2's

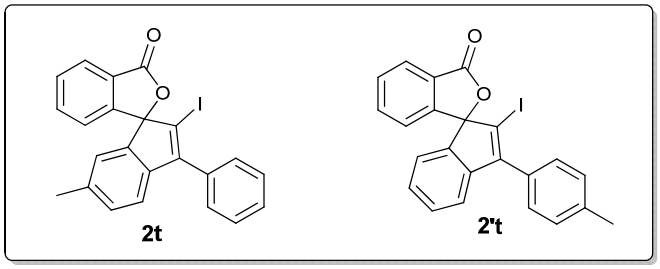

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.31
8.43
1.15
1.36
1.15
1.30
0.99
0.97
1.11
3.00
8.038
8.022
8.018
7.651
7.633
7.619
7.607
7.593
7.589
7.572
7.565
7.542
7.530
7.513
7.494
7.480
7.469
7.462
7.444
7.298
7.282
7.253
7.164
7.144
7.104
7.088
7.075
7.060
7.038
7.015
6.801
6.795
6.780
6.774
6.616
6.611
3.881
3.712
0.000

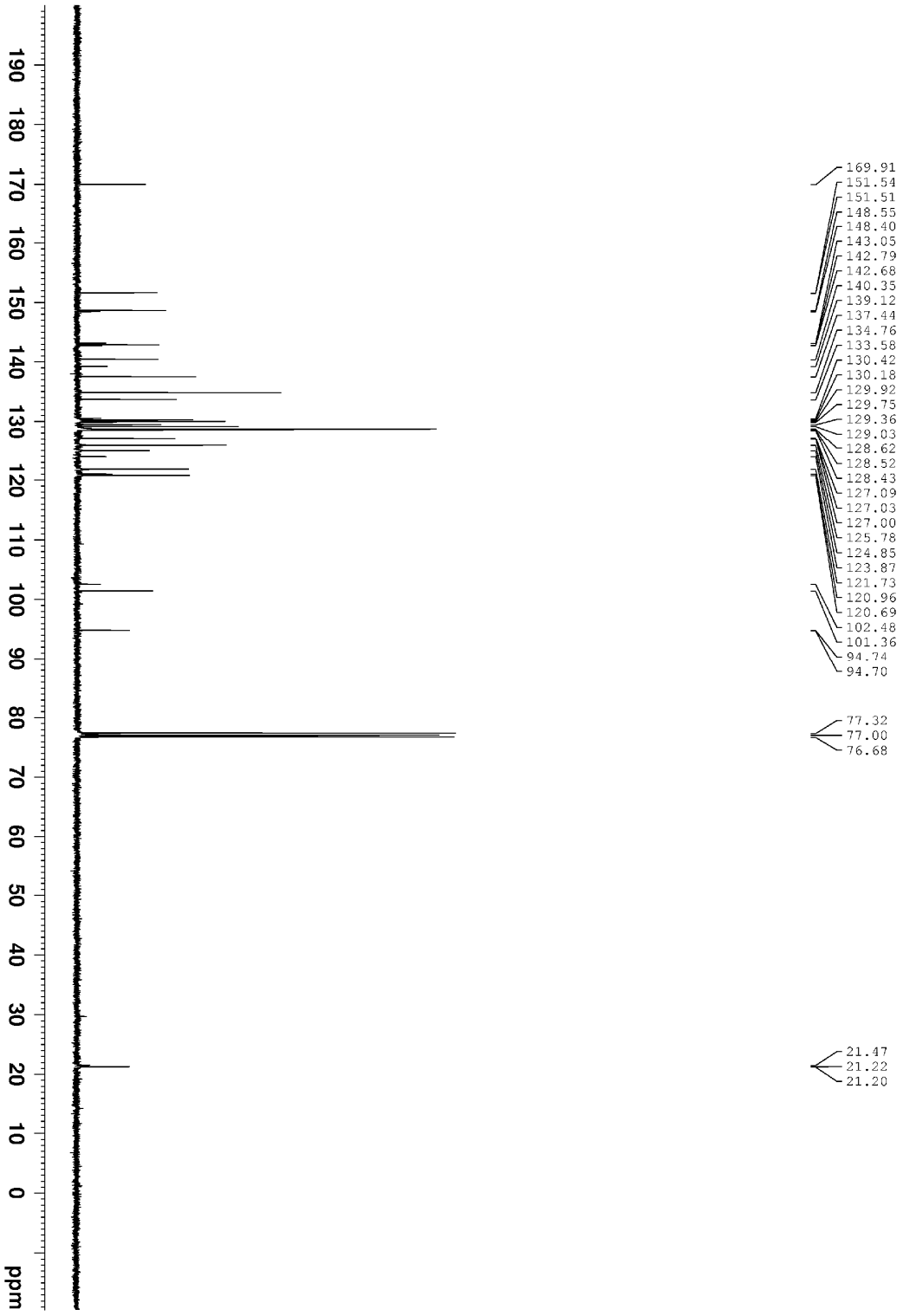

O
O
I
MeO
2s
O
O
I
OMe
2's


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
169.89
160.12
159.47
151.31
151.08
148.59
148.45
144.42
143.09
142.73
135.68
134.82
134.75
133.65
130.00
129.98
129.94
129.74
129.04
128.63
128.51
127.08
126.94
125.80
125.54
123.88
121.76
121.69
120.94
114.30
114.06
111.02
102.06
99.09
94.74
94.42
77.32
77.00
76.68
55.60
55.29


2t
2't


1.18
4.38
3.64
1.44
3.84
0.96
0.85
3.00
ppm
8.040
8.039
8.034
8.025
8.021
7.648
7.644
7.630
7.626
7.621
7.615
7.608
7.603
7.599
7.591
7.587
7.570
7.567
7.532
7.529
7.524
7.511
7.496
7.493
7.478
7.467
7.460
7.452
7.446
7.442
7.339
7.319
7.290
7.270
7.266
7.246
7.157
7.152
7.144
7.134
7.125
7.117
7.097
7.094
7.084
7.077
7.064
7.032
7.014
6.856
2.435
2.249
0.000


2t
2't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142.68
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139.12
137.44
134.76
133.58
130.42
130.18
129.92
129.75
129.36
129.03
128.62
128.52
128.43
127.09
127.03
127.00
125.78
124.85
123.87
121.73
120.96
120.69
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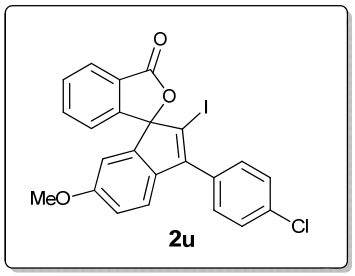
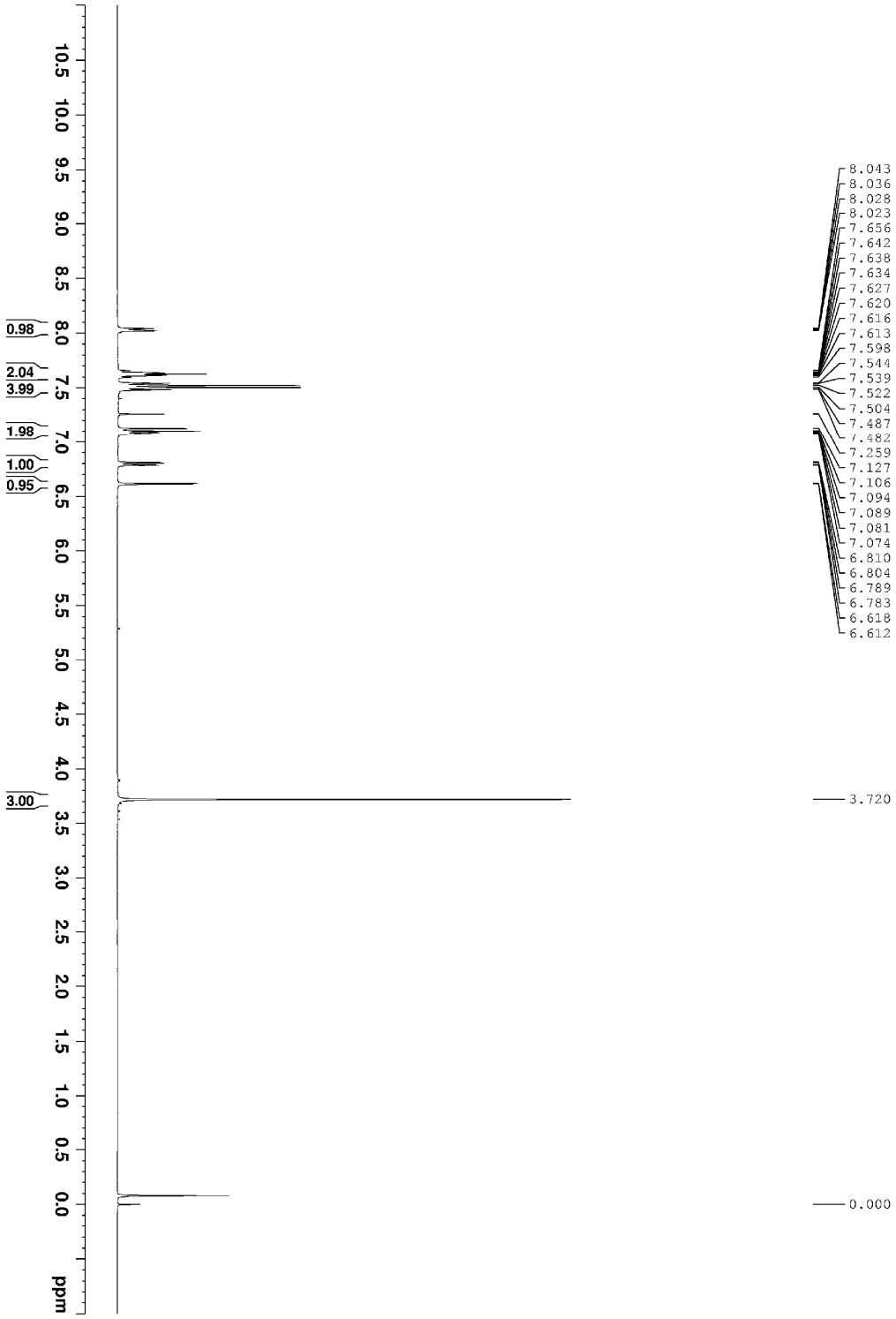
101.36
94.74
94.70
77.32
77.00
76.68
21.47
21.22
21.20
ppm


O
O
I
MeO
Cl

2u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0.95
3.00
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8.028
8.023
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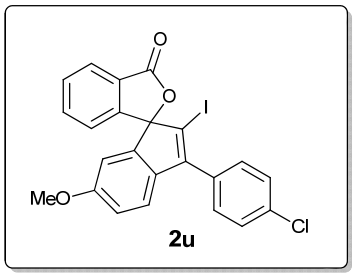
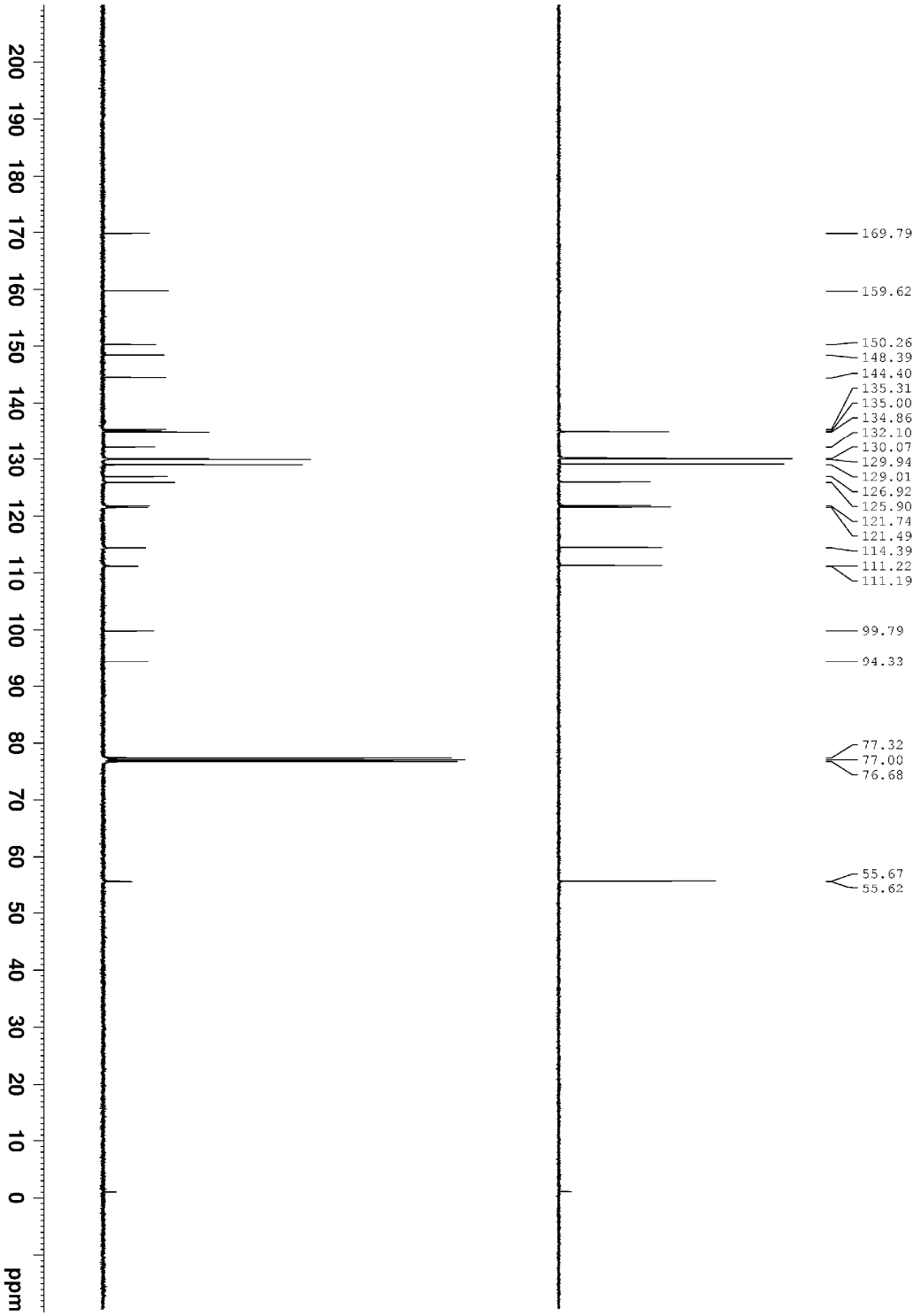
7.642
7.638
7.634
7.627
7.620
7.616
7.613
7.598
7.544
7.539
7.522
7.504
7.487
7.482
7.259
7.127
7.106
7.094
7.089
7.081
7.074
6.810
6.804
6.789
6.783
6.618
6.612
3.720
0.000


O
O
I
MeO
Cl

2u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190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
169.79
159.62
150.26
148.39
144.40
135.31
135.00
134.86
132.10
130.07
129.94
129.01
126.92
125.90
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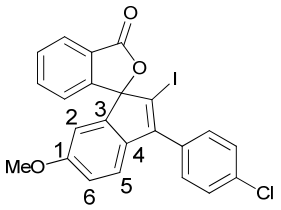
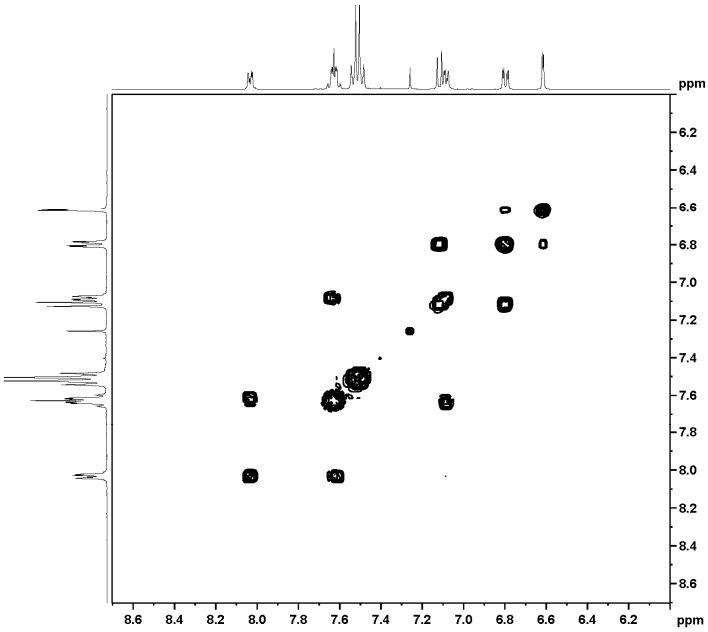
94.33
77.32
77.00
76.68
55.67
55.62

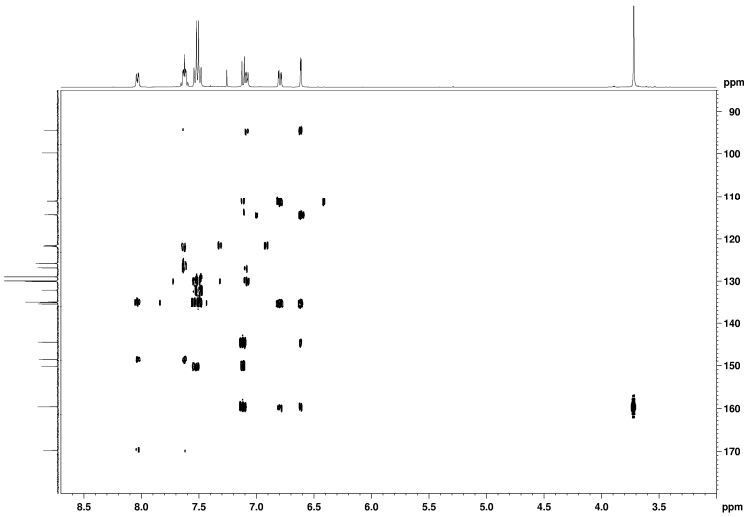


2u

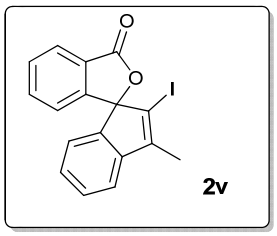
The ^{1}H–^{1}H COSY spectrum and HMBC correlations from δ_H 3.72 (3H, s) to δ_C 159.6 (C-1) and from δ_H 7.11 (1H, d, J = 8.4 Hz, H_5), 6.79 (1H, dd, J = 8.4, 2.4 Hz, H_6) and 6.61 (1H, d, J = 2.4 Hz, H_2) to δ_C 159.6 (C-1) confirmed the structure of **2u**.

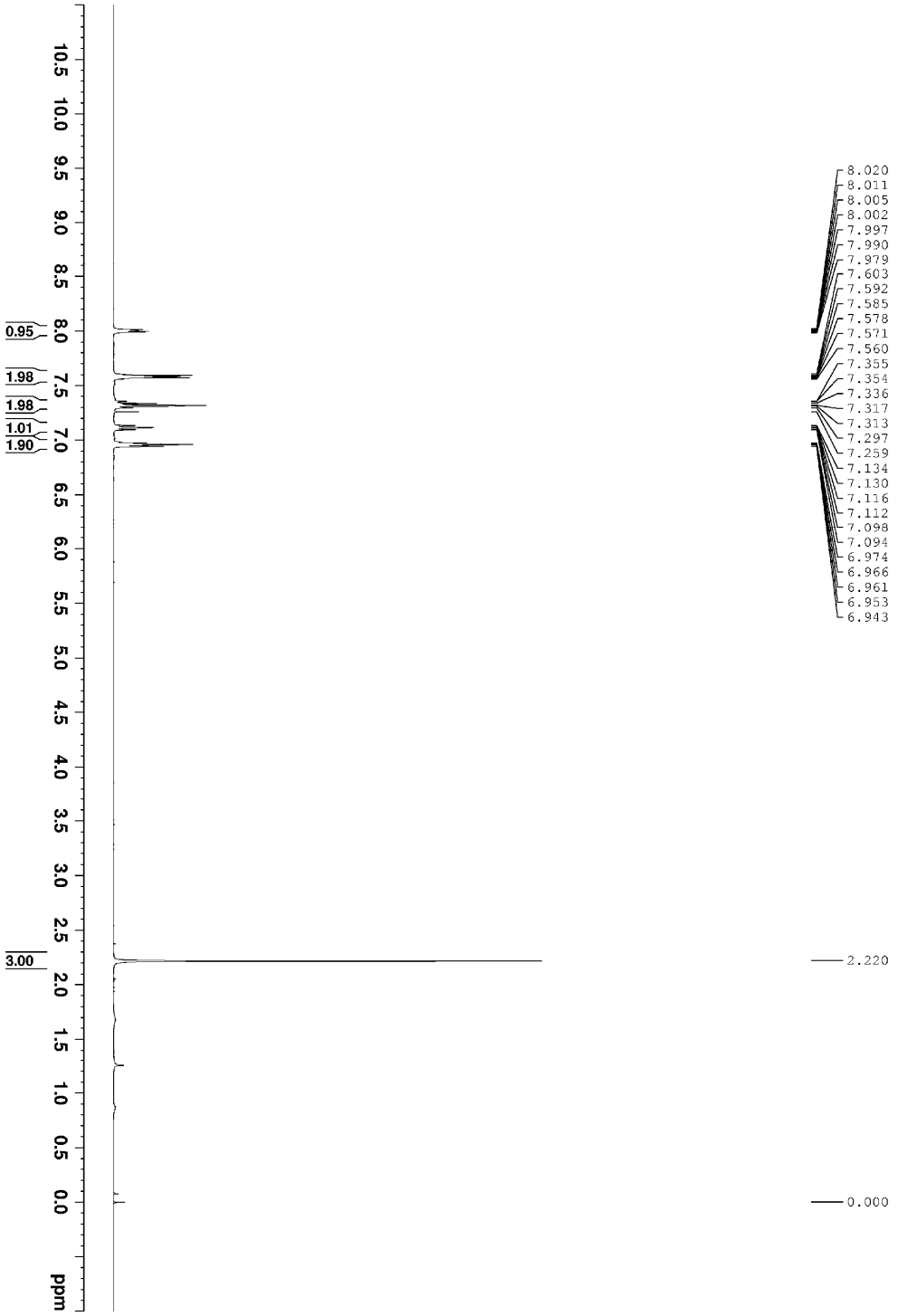


^{1}H-^{1}H COSY spectrum of 2u in $CDCl_3$



HMBC spectrum of 2u in $CDCl_3$


O
O
I
2v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1.90
3.00
ppm
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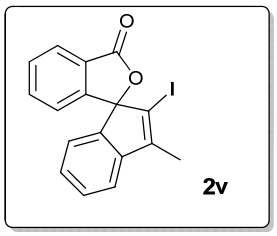
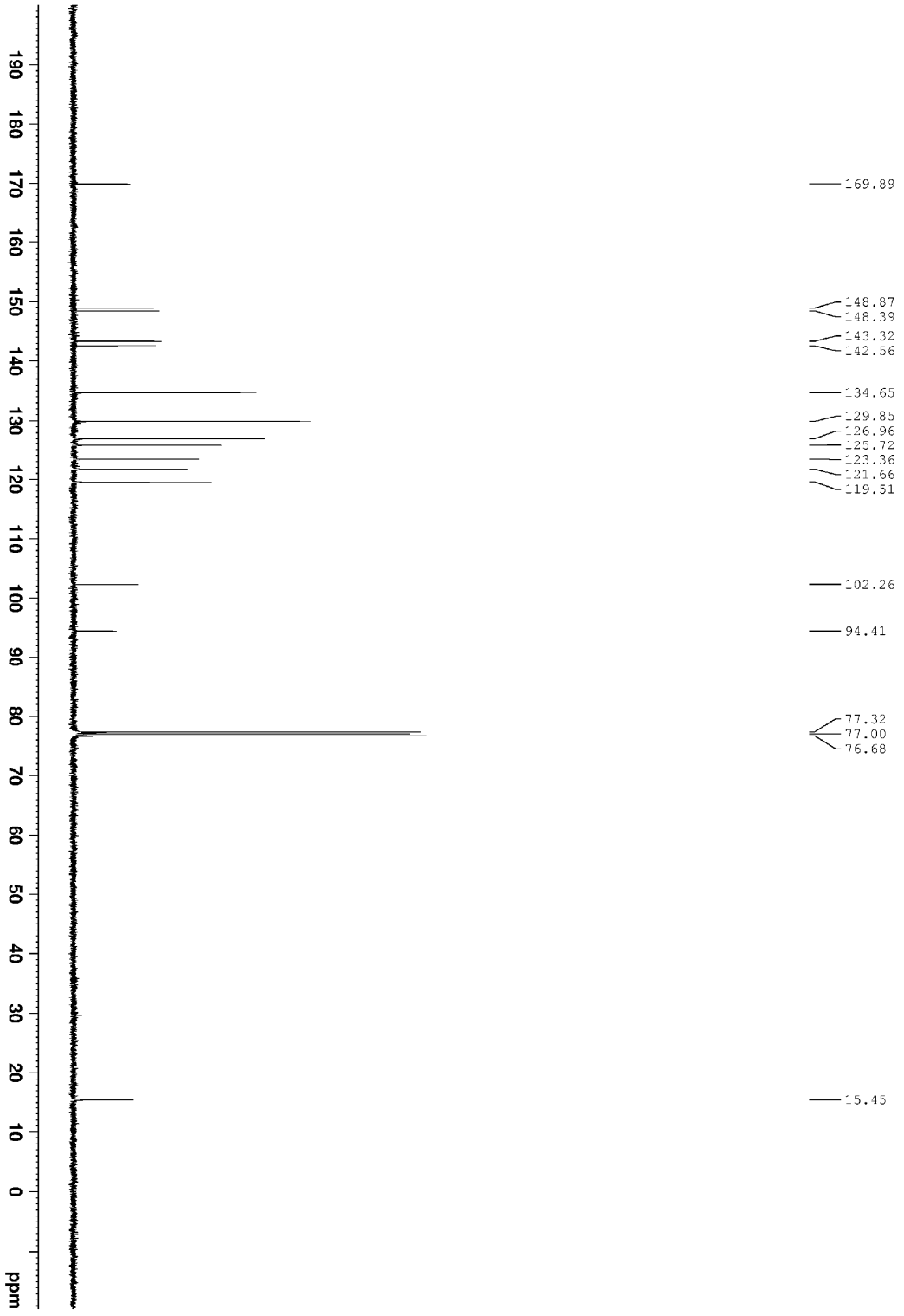
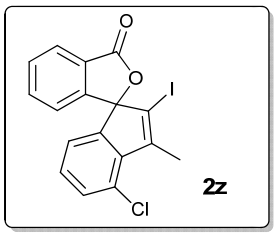
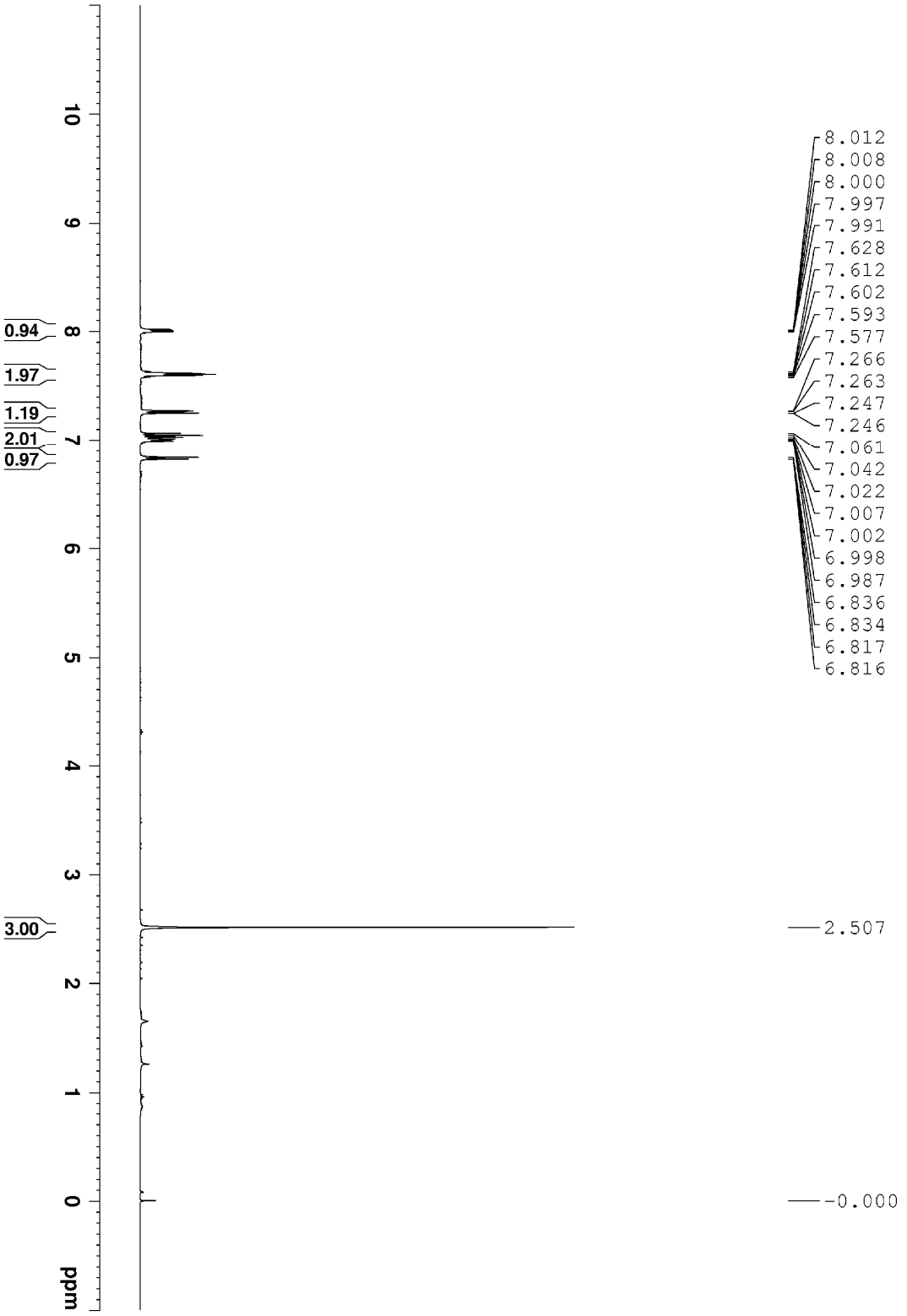
8.011
8.005
8.002
7.997
7.990
7.979
7.603
7.592
7.585
7.578
7.571
7.560
7.355
7.354
7.336
7.317
7.313
7.297
7.259
7.134
7.130
7.116
7.112
7.098
7.094
6.974
6.966
6.961
6.953
6.943
2.220
0.000






O
O
I
Cl

2z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0.97
3.00
10
9
8
7
6
5
4
3
2
1
0
ppm
8.012
8.008
8.000
7.997
7.991
7.628
7.612
7.602
7.593
7.577
7.266
7.263
7.247
7.246
7.061
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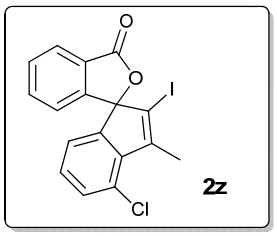
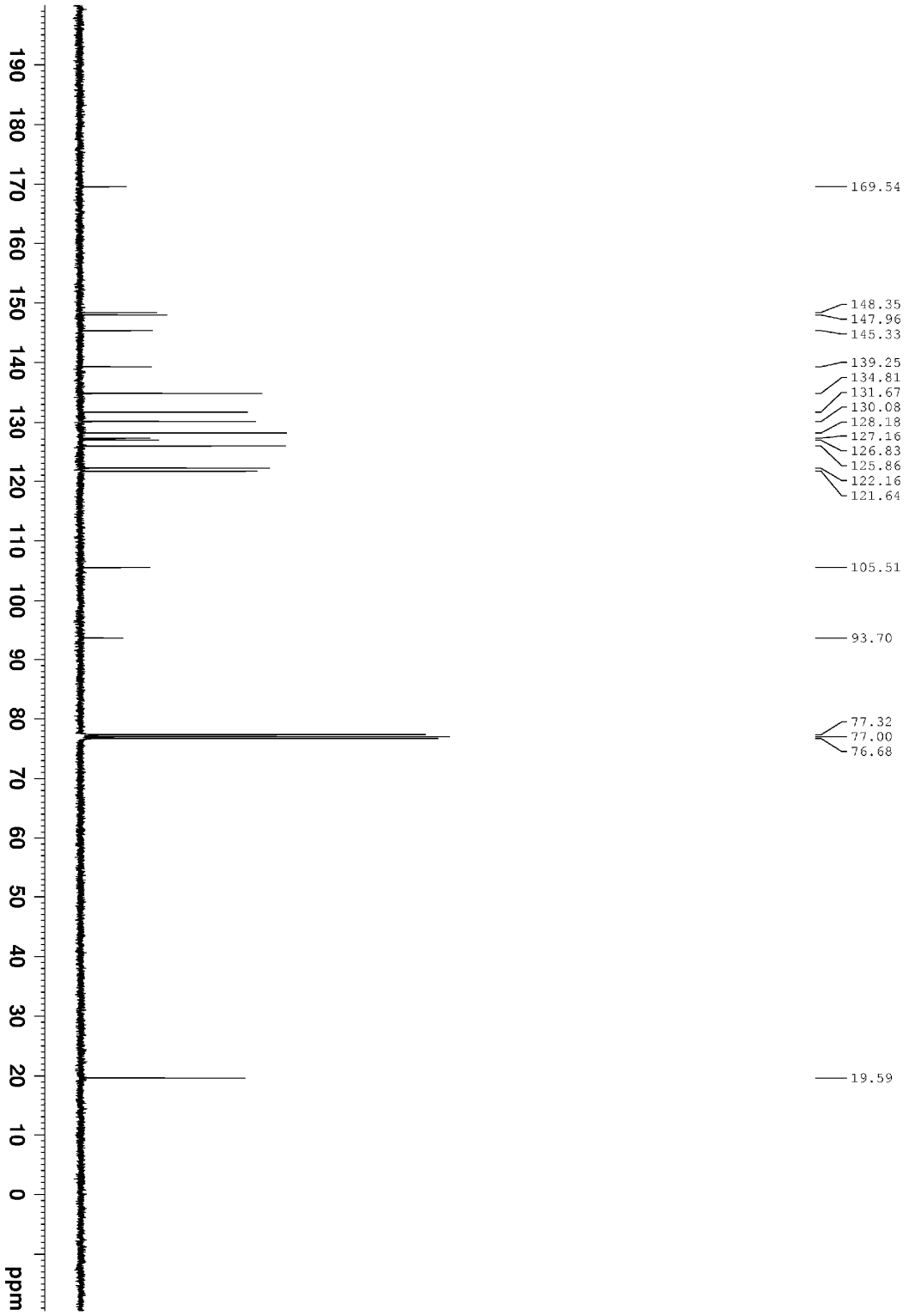
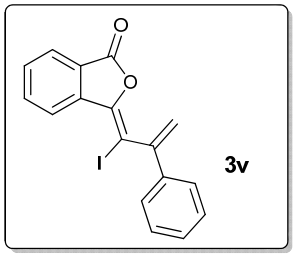
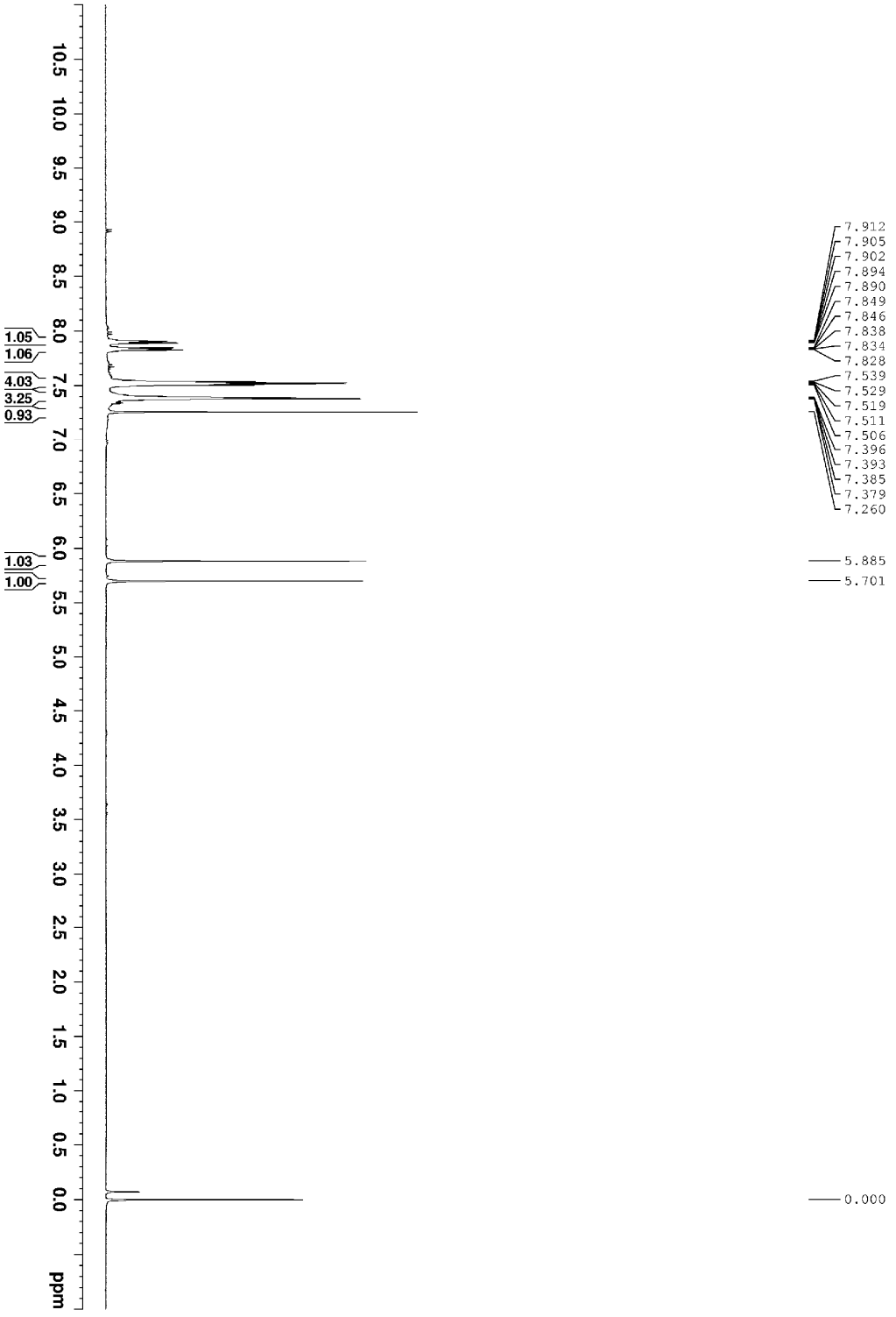
6.834
6.817
6.816
2.507
-0.000






O
O
I
3v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7.849
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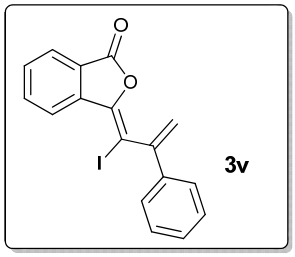
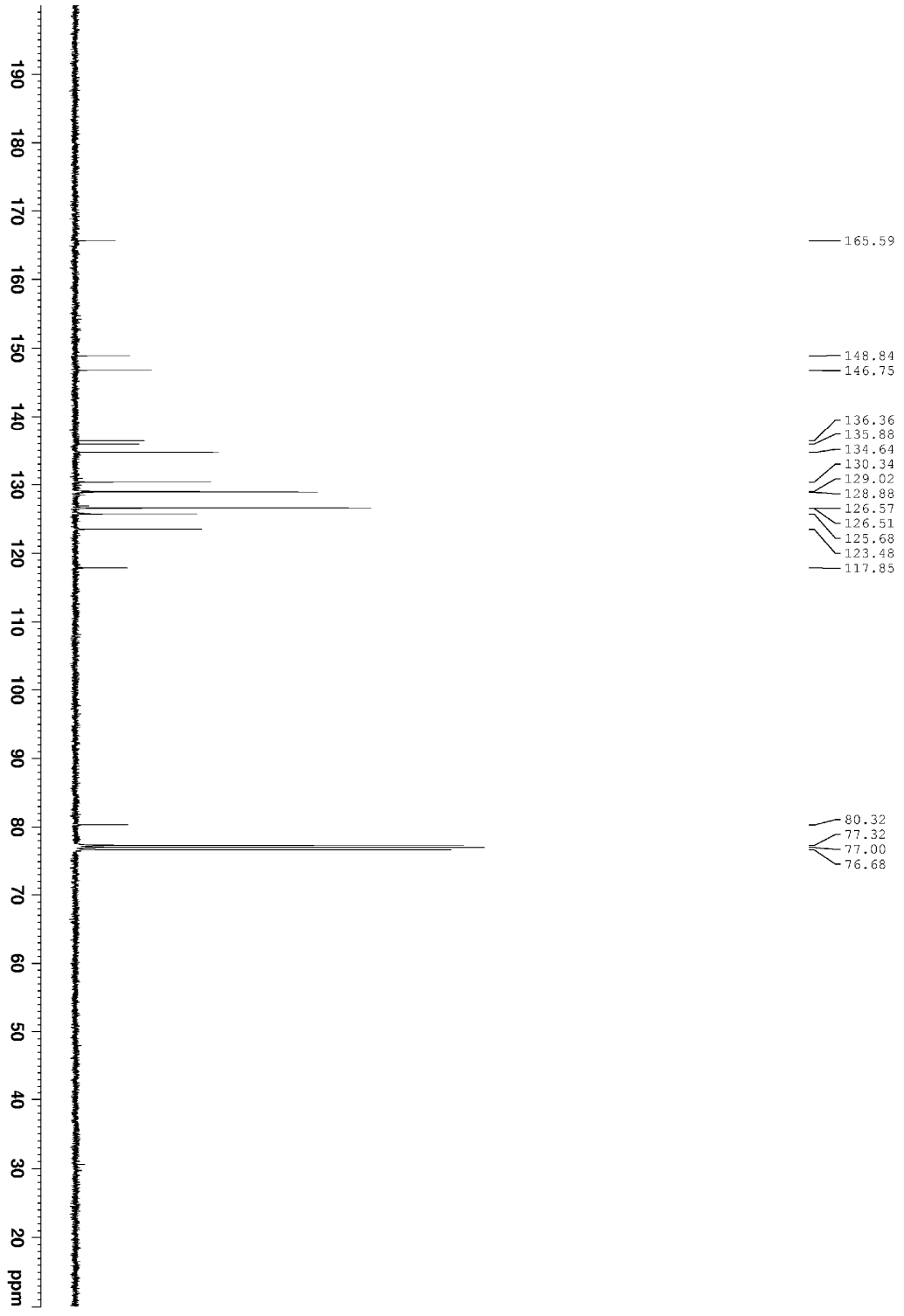
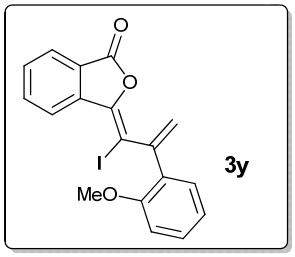
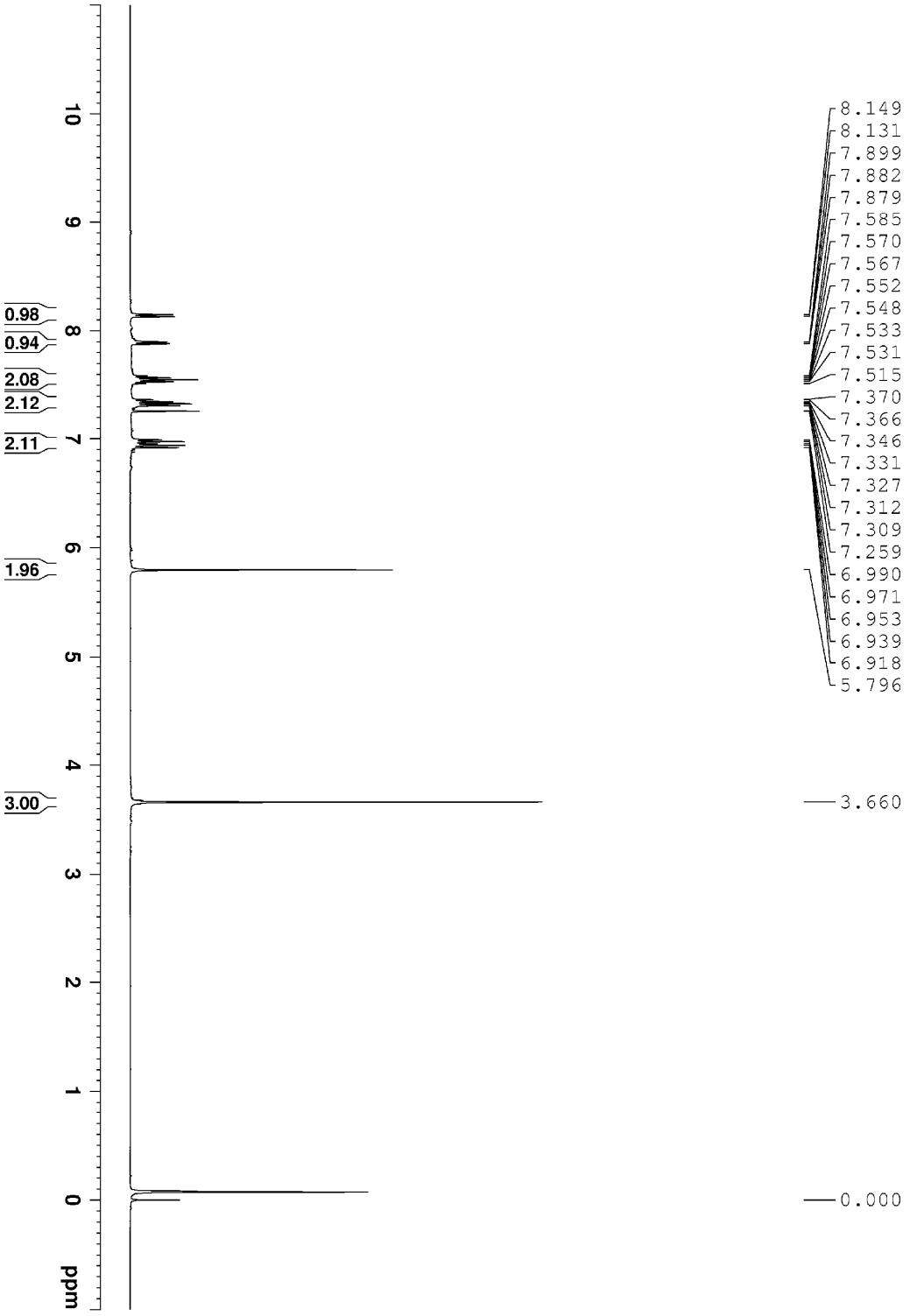
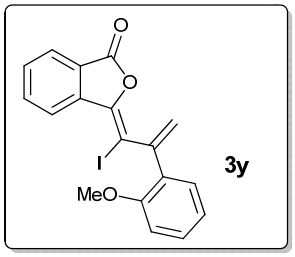
7.838
7.834
7.828
7.539
7.529
7.519
7.511
7.506
7.396
7.393
7.385
7.379
7.260
5.885
5.701
0.000



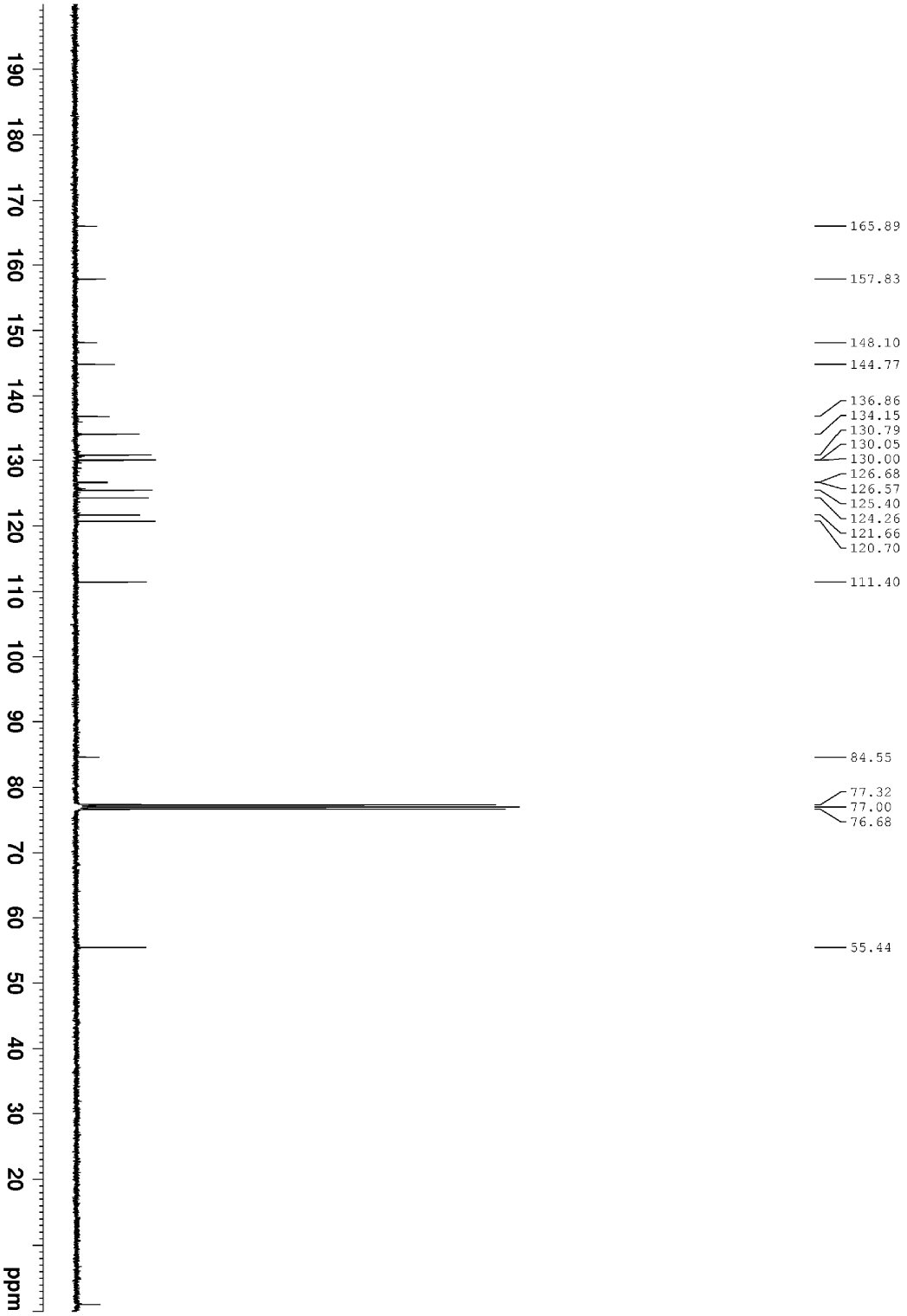







O
O
I
MeO

3y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150
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120
110
100
90
80
70
60
50
40
30
20
ppm
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157.83
148.10
144.77
136.86
134.15
130.79
130.05
130.00
126.68
126.57
125.40
124.26
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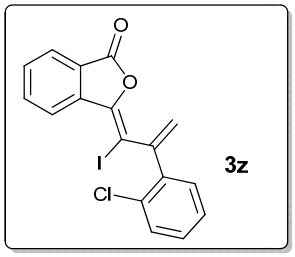
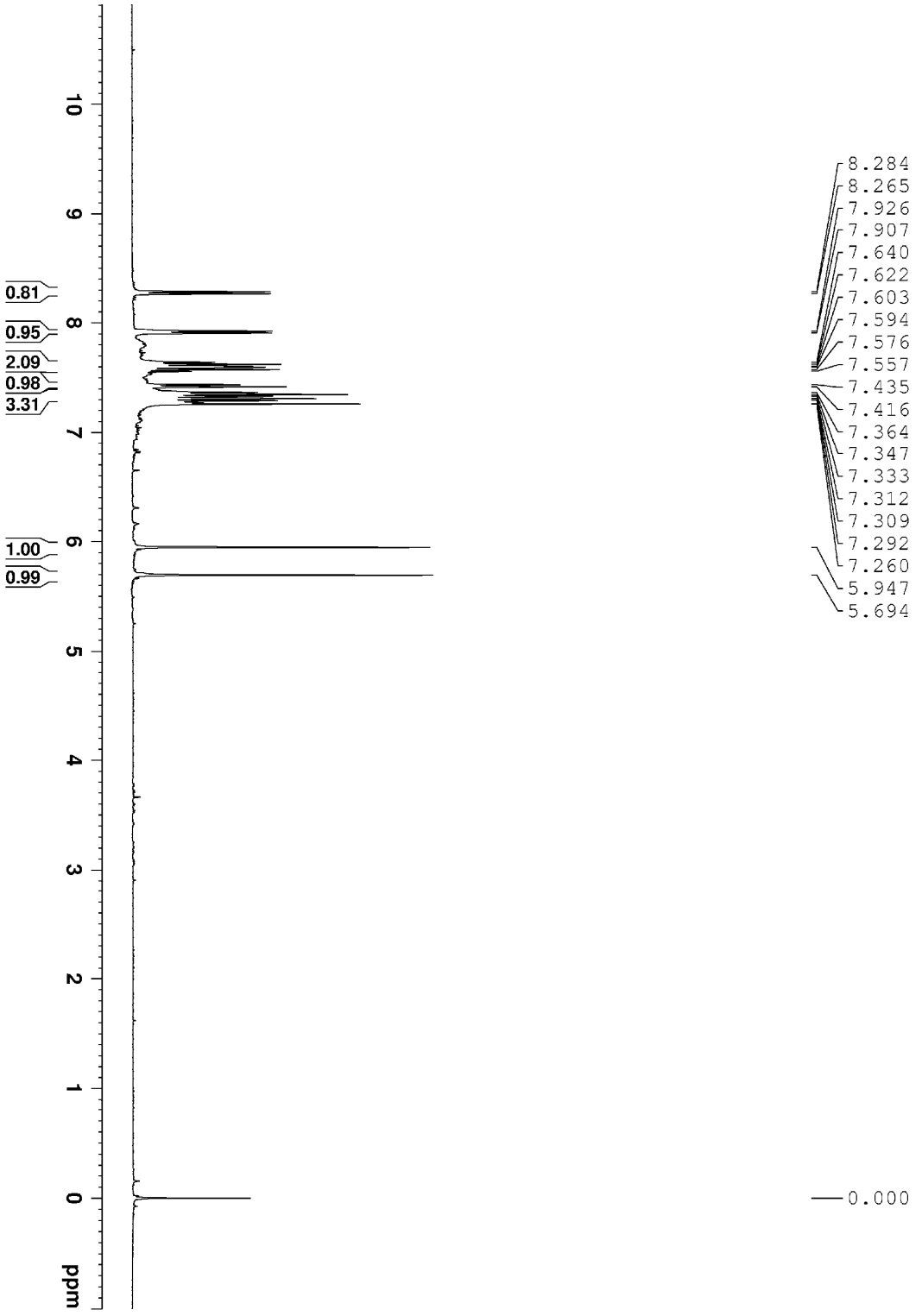
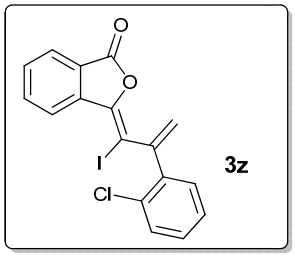
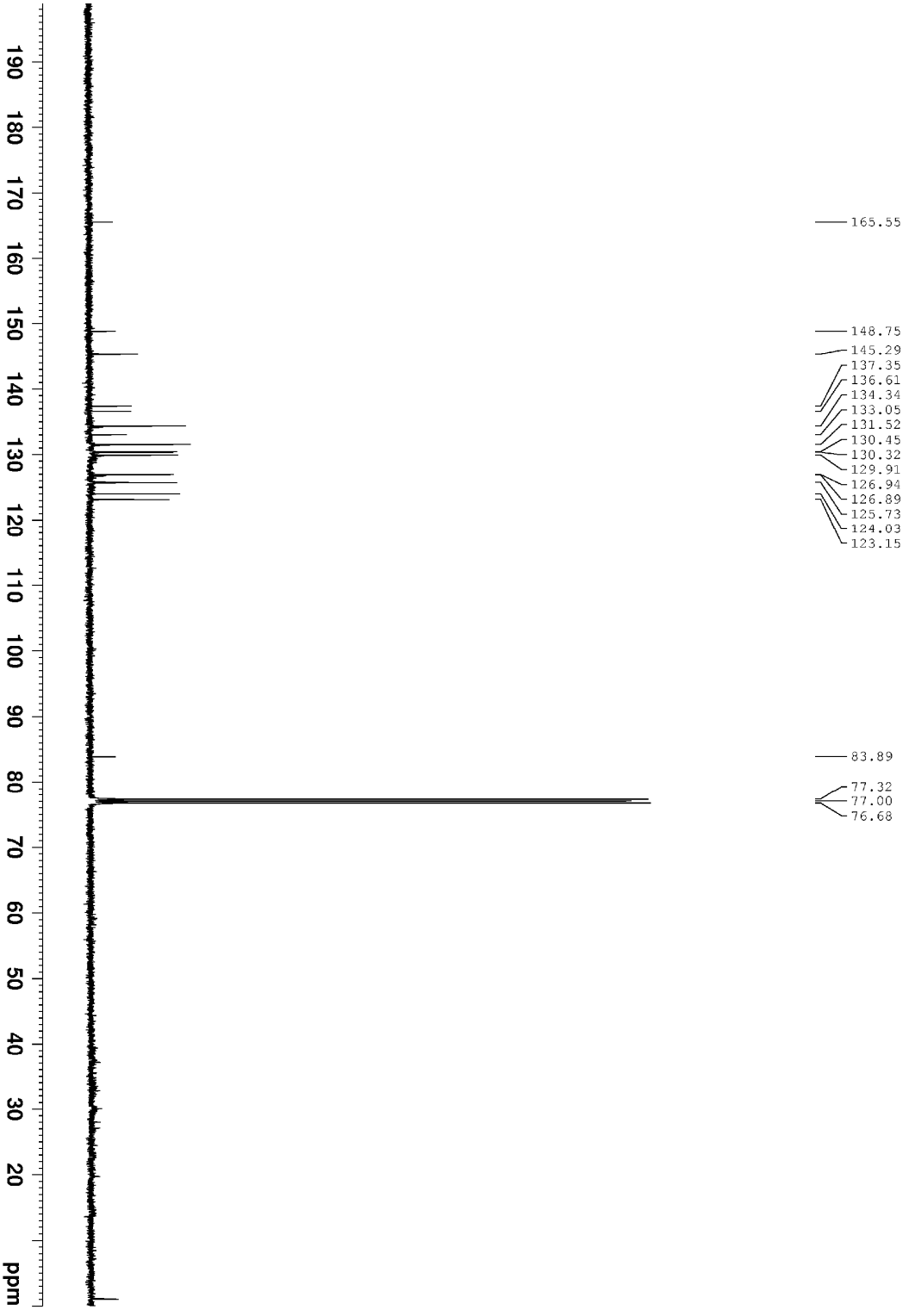
111.40
84.55
77.32
77.00
76.68
55.44






O
O
I
Cl
3z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70
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40
30
20
ppm
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148.75
145.29
137.35
136.61
134.34
133.05
131.52
130.45
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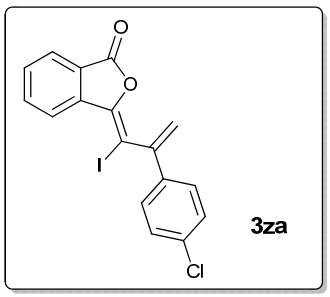
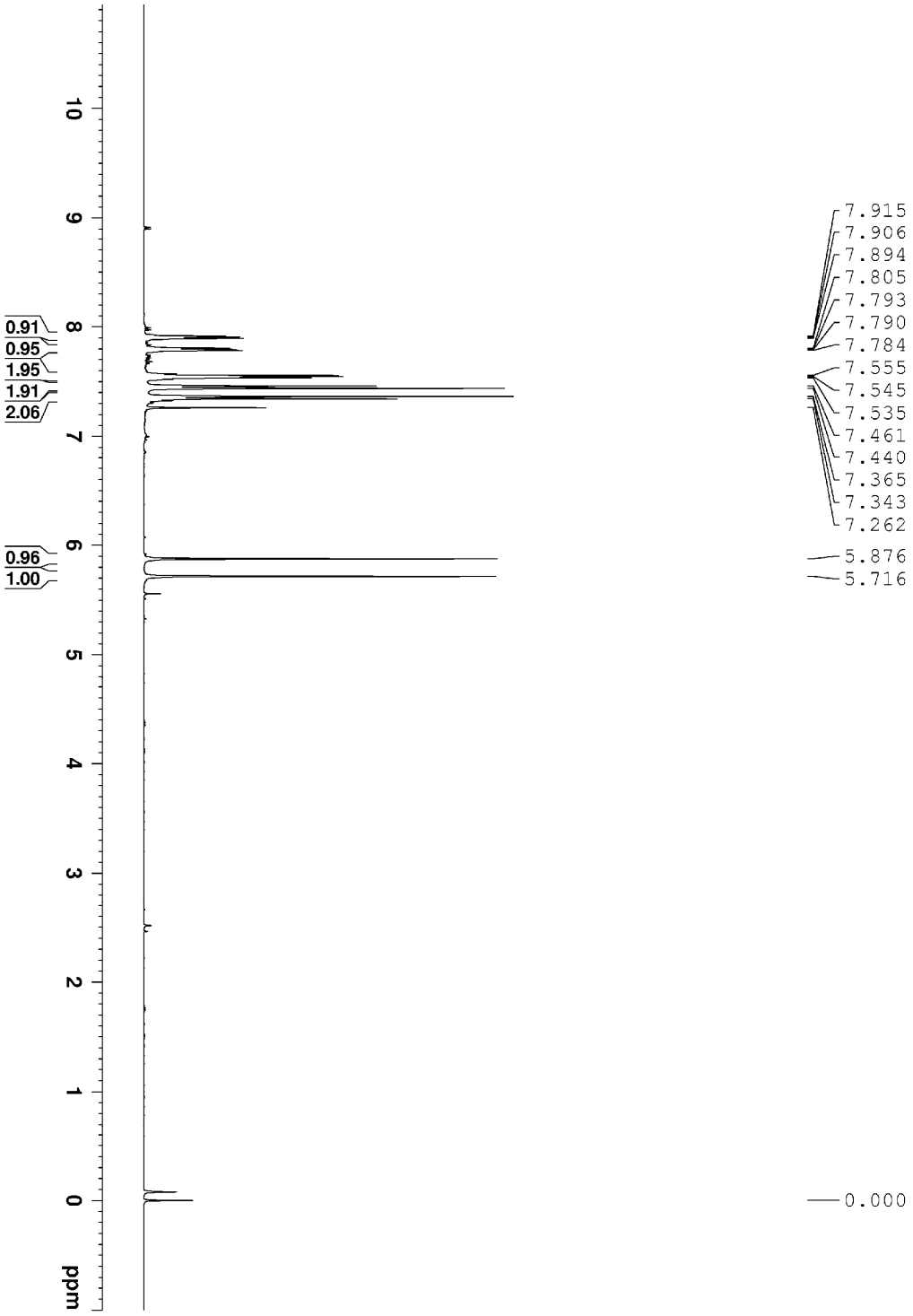
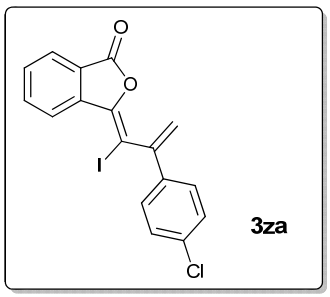
126.94
126.89
125.73
124.03
123.15
83.89
77.32
77.00
76.68

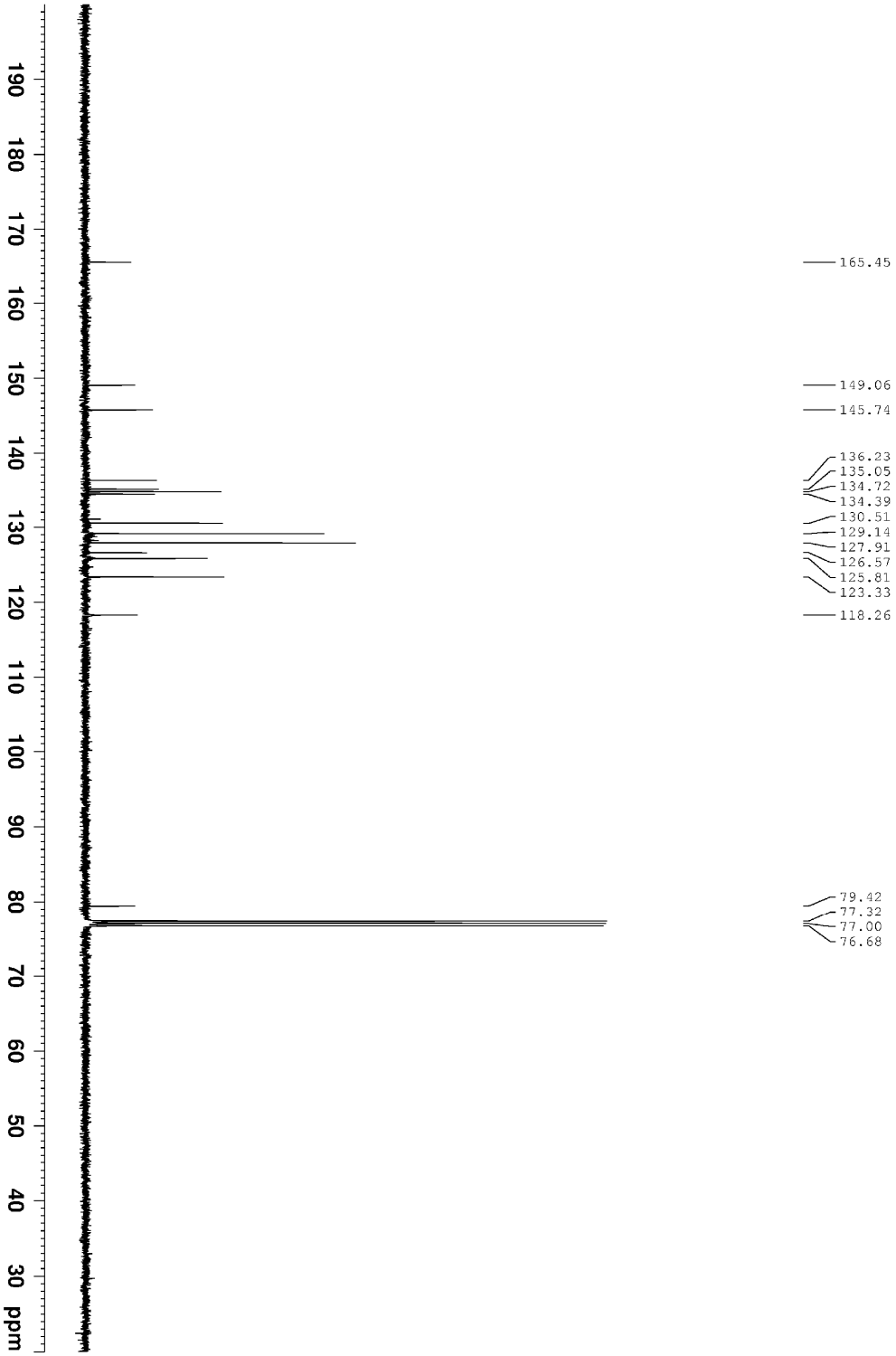


3za




O
O
I
Cl

3za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150
140
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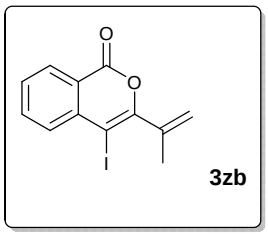
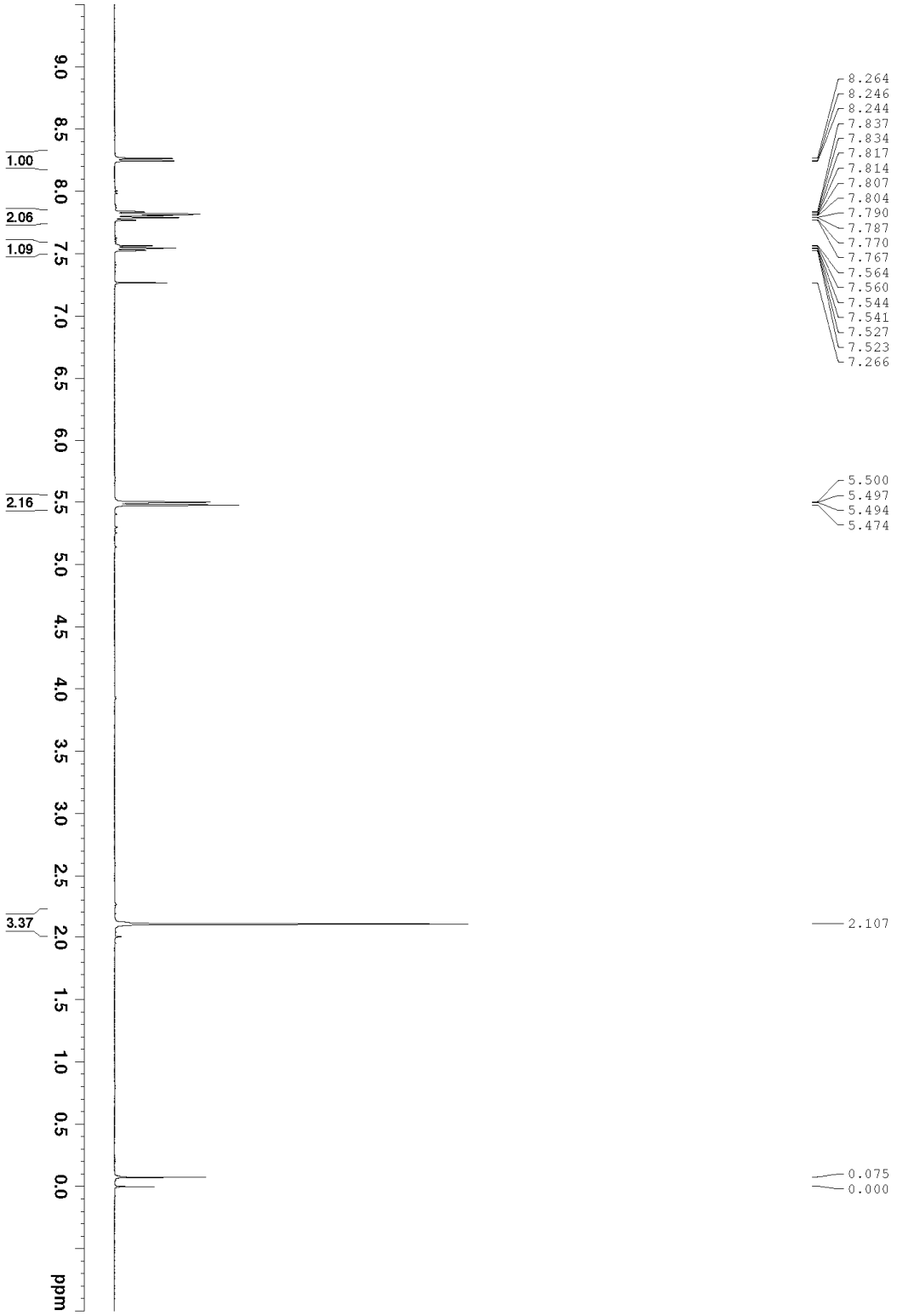
120
110
100
90
80
70
60
50
40
30
ppm
165.45
149.06
145.74
136.23
135.05
134.72
134.39
130.51
129.14
127.91
126.57
125.81
123.33
118.26
79.42
77.32
77.00
76.68


O
O
I
3zb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1.09
2.16
3.37
8.264
8.246
8.244
7.837
7.834
7.817
7.814
7.807
7.804
7.790
7.787
7.770
7.767
7.564
7.560
7.544
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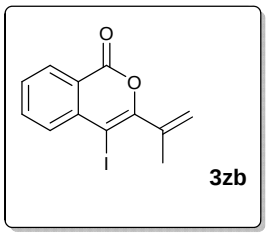
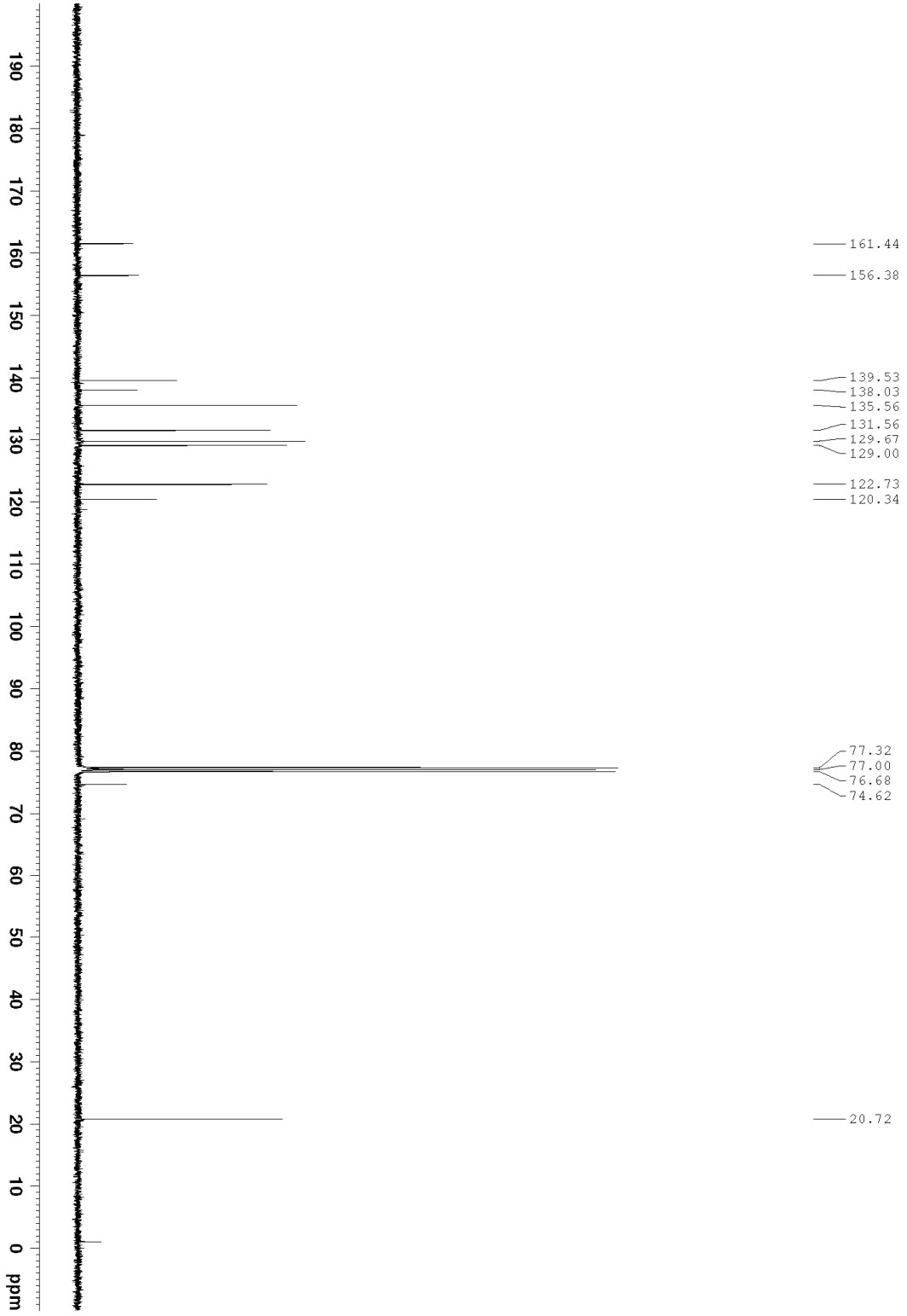
5.494
5.474
2.107
0.075
0.000
ppm


O
O
I

3zb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120
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100
90
80
70
60
50
40
30
20
10
0
ppm
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156.38
139.53
138.03
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129.67
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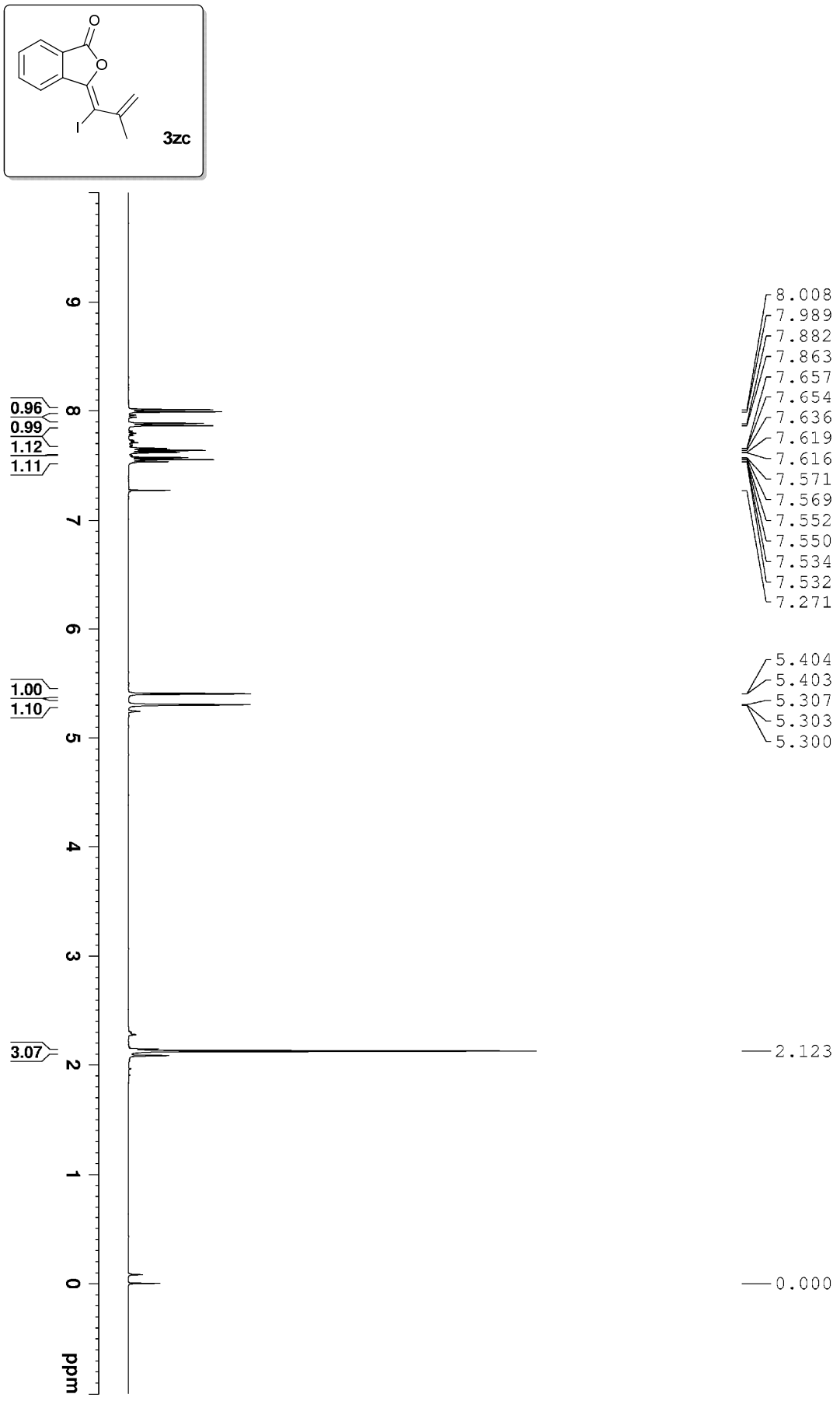
122.73
120.34
77.32
77.00
76.68
74.62
20.72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7.636
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7.616
7.571
7.569
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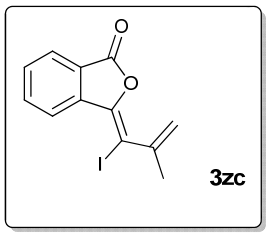
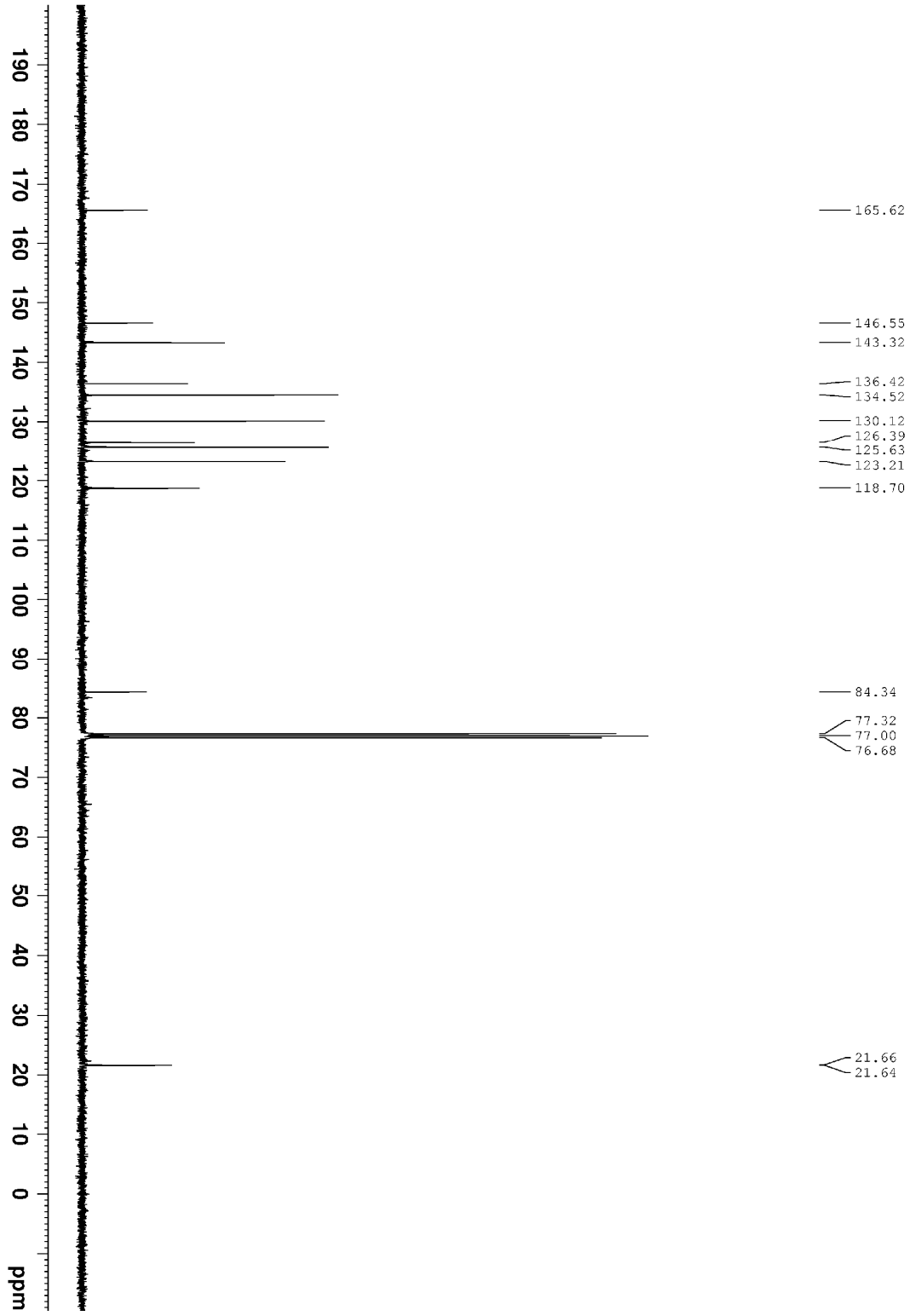
7.550
7.534
7.532
7.271
5.404
5.403
5.307
5.303
5.300
2.123
0.000
0.96
0.99
1.12
1.11
1.00
1.10
3.07
ppm


O
O
I

3zc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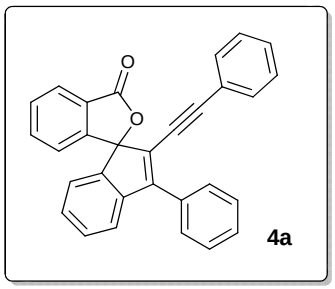
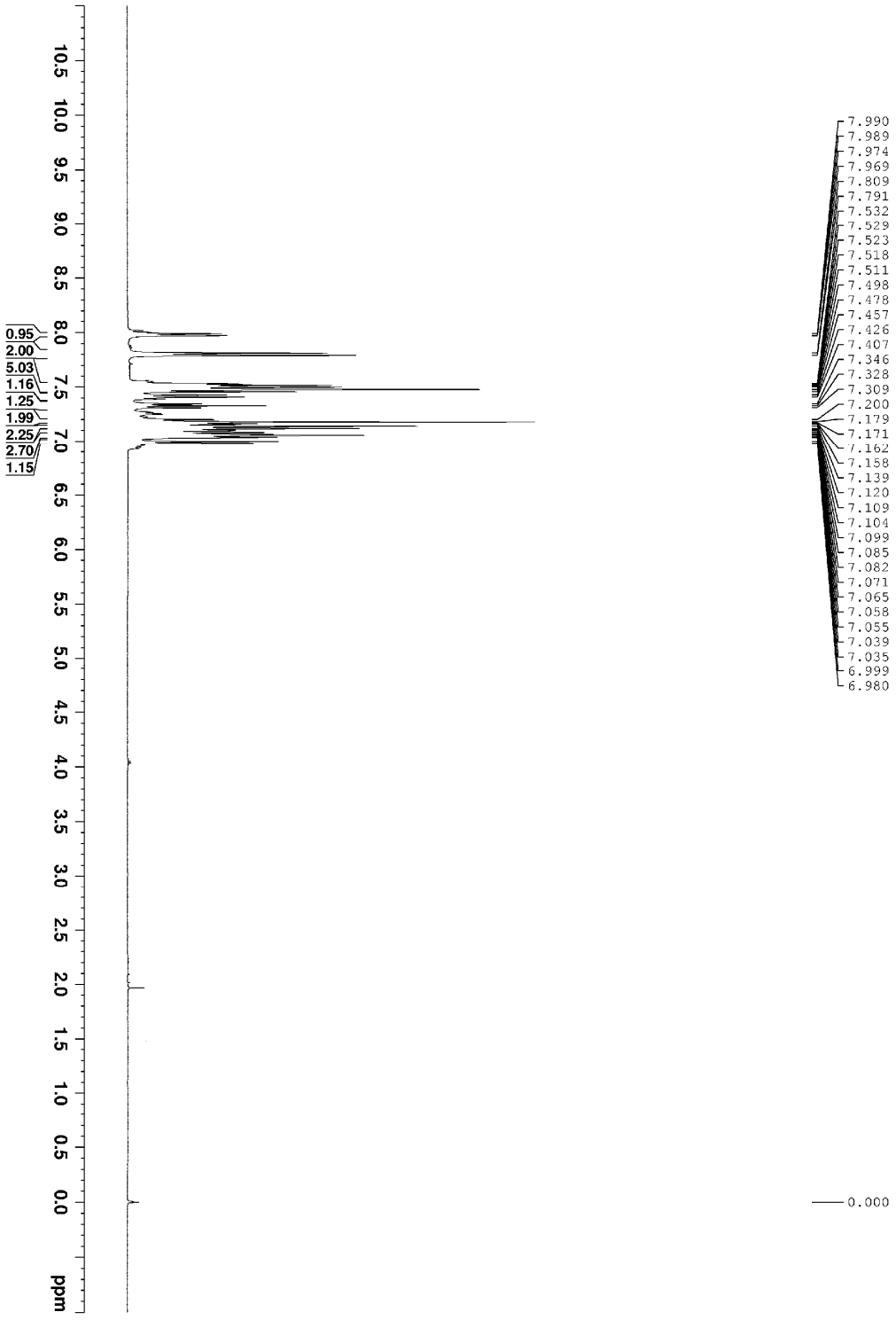
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
165.62
146.55
143.32
136.42
134.52
130.12
126.39
125.63
123.21
118.70
84.34
77.32
77.00
76.68
21.66
21.64


O
O
4a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1.25
1.99
2.25
2.70
1.15
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
ppm
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7.989
7.974
7.969
7.809
7.791
7.532
7.529
7.523
7.518
7.511
7.498
7.478
7.457
7.426
7.407
7.346
7.328
7.309
7.200
7.179
7.171
7.162
7.158
7.139
7.120
7.109
7.104
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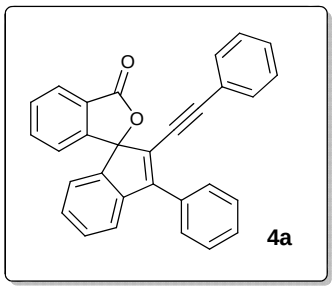
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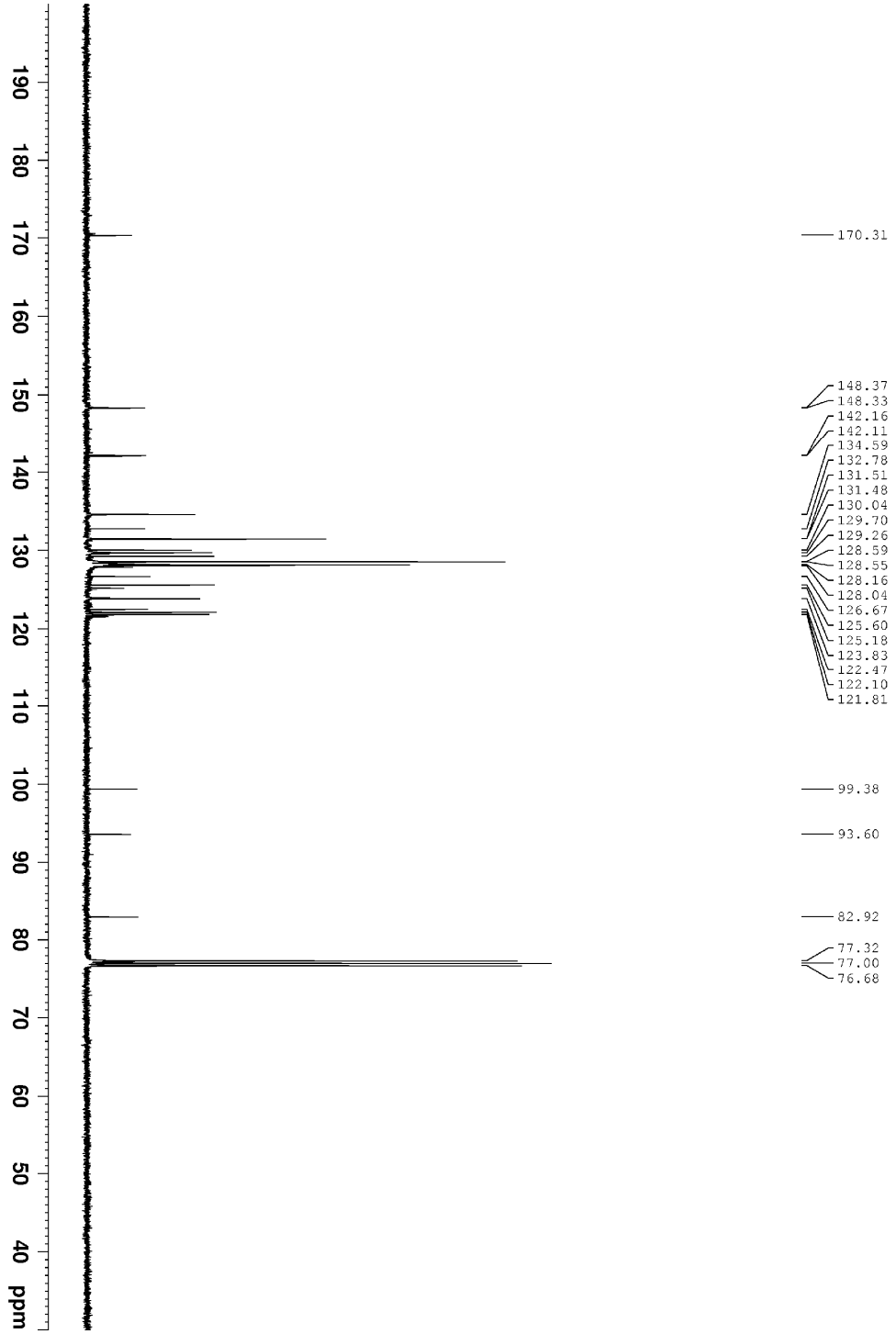
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180
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140
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120
110
100
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70
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40
ppm
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148.33
142.16
142.11
134.59
132.78
131.51
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130.04
129.70
129.26
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128.16
128.04
126.67
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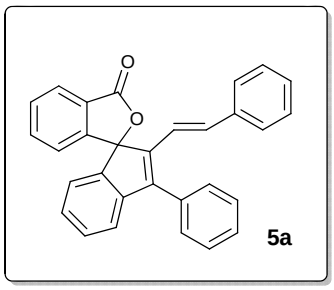
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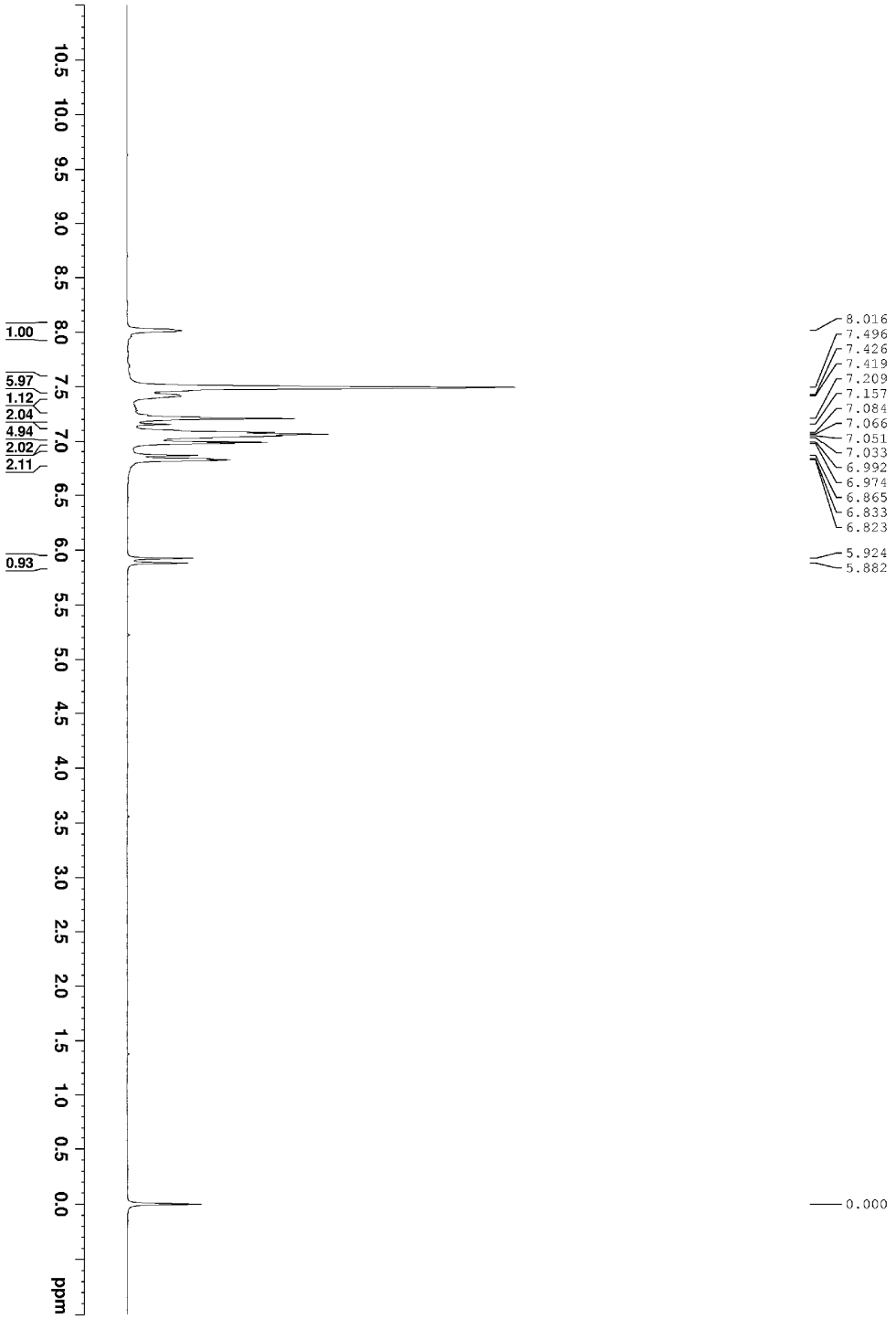
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0.93
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7.157
7.084
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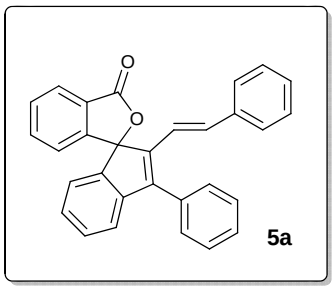
ppm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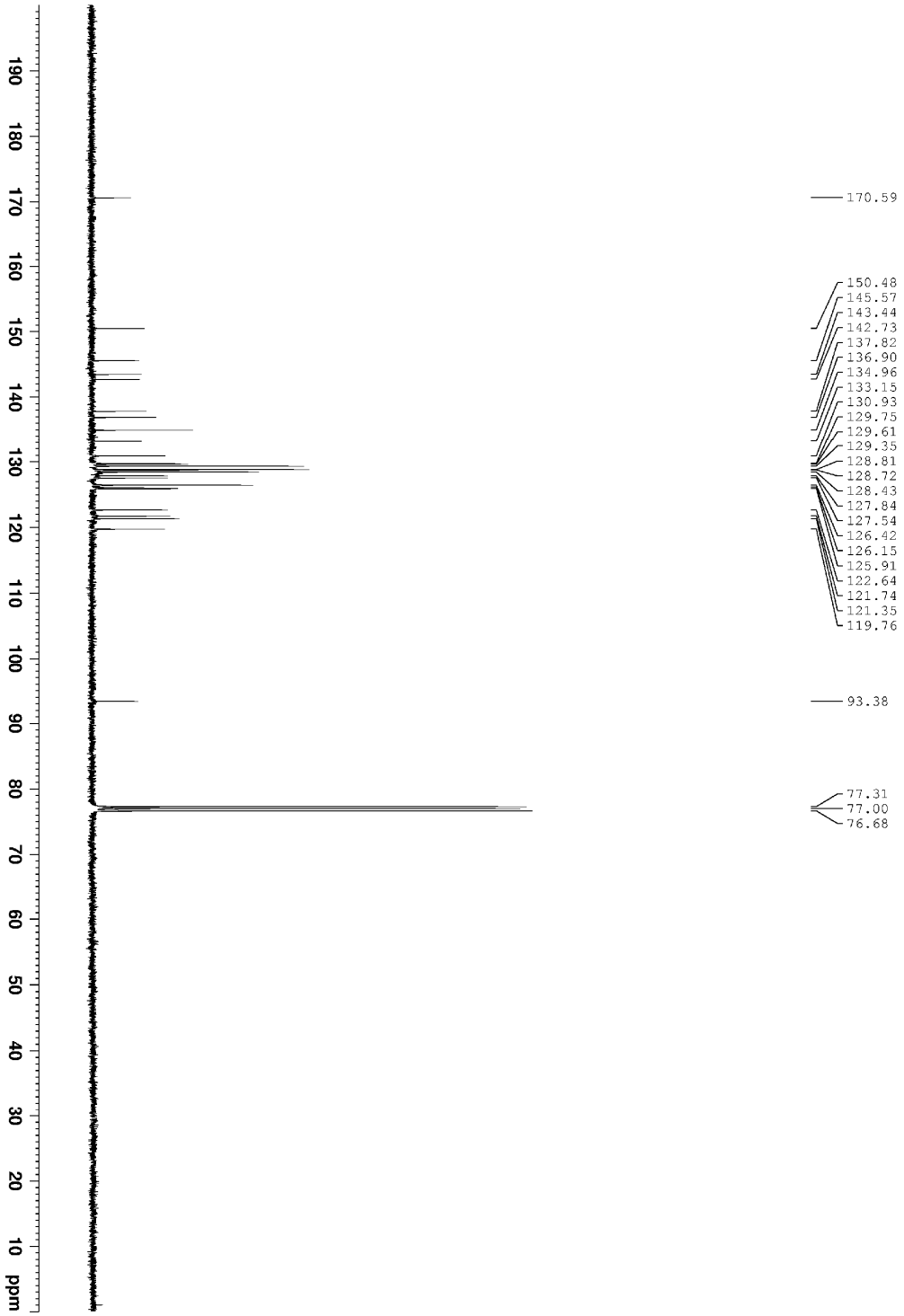
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180
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160
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30
20
10
ppm
170.59
150.48
145.57
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142.73
137.82
136.90
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133.15
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128.81
128.72
128.43
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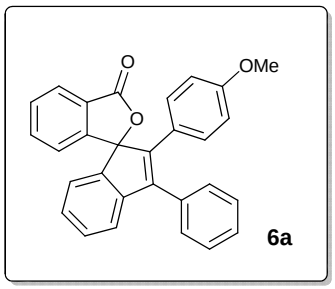
76.68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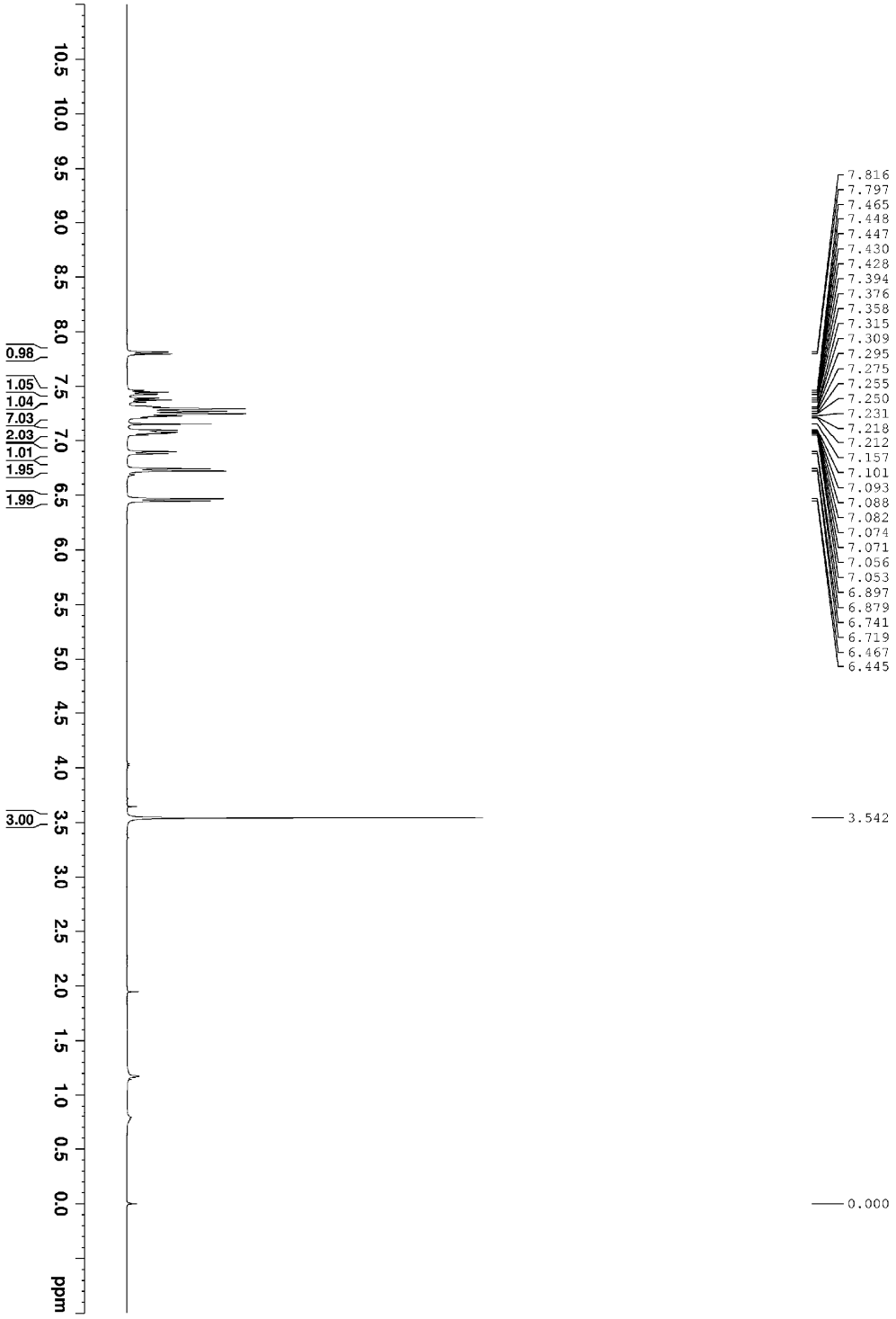
6a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7.03
2.03
1.01
1.95
1.99
3.00
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ppm
7.816
7.797
7.465
7.448
7.447
7.430
7.428
7.394
7.376
7.358
7.315
7.309
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7.275
7.255
7.250
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7.212
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7.101
7.093
7.088
7.082
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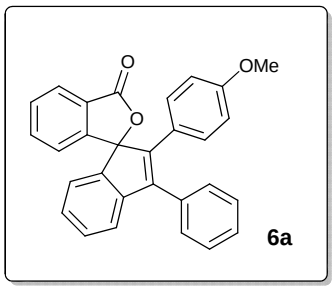

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