Supplementary Material (ESI) for Chemical Communications

Supporting Information For

Gold-catalyzed reaction of enynols by a dimerization-fragmentation process: An expeditious assembly of enyne molecular architecture

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General Information

The materials for preparation of substrates **1a-1o,** as well as AuCl were used as purchased, and the solvent CH_3CN was dried and freshly distilled over P_2O_5 before use. All reactions under standard conditions were monitored by thin-layer chromatography (TLC) on gel F254 plates. The silica gel (200-300 meshes) is used for column chromatography, and the distillation range of petroleun is 60-90℃. ^1H and ^{13}C NMR spectra were recorded on the 300 MHz or 400 MHz instruments, and spectral data are reported in *ppm* relative to tetramethylsilane (TMS) as internal standard. MS (EI) were measured on spectrometer by direct inleet at 70 ev, and signals were given in *m/z* with relative intensity (%) in brackets. MS (ESI) were measured on Bruker Esquire6000 mass spectrometer. HRMS data were measured with ESI or EI techniques. MALDI-TOF MS were conducted on a Bruker BIFLEX Ⅲ time-of-flight (TOF) mass spectrometer (Bruker Daltonics, Billerica, MA, USA). Fluorescence spectra measuements performed on a Hitachi F-4500 spectrofluorimeter.

General Procedure for Homocoupling Reaction of Enynols 1:

To a solution of 1,3,5-triaryls-enynols **1** (0.5 mmol) in 2 mL CH_3CN was added 5 mmol% AuCl under Ar atmosphere. The mixture was stirred at room temperature for 5 min until the starting material disappeared completely by inspection of TLC. The solvent was removed *in vacu*o and the residue was purified by flash chromatography on Et_3N-treated silica gel (petroleum/ethyl acetate = 25/1) to furnish the expected products as amorphous solids.

Experimental Procedure for Tandem Reaction of 1m:

To a solution of 1,5-diphenyl-3-(α- thienyl) pent-2-en-4-yn-1-ol **1m** (158 mg, 0.5 mmol) in 2 mL CH_3CN was added AuCl(6 mg, 0.025 mmol) under Ar atmosphere. The mixture was stirred at room temperature for about 16 hours until the coupling product disappeared completely by inspection of TLC. The solvent was removed *in vacuo* and the residue was purified by flash chromatography on silica gel (petroleum/ethyl acetate = 30/1) to furnish product **3m** as an amorphous solid in 64% yield.

Experimental Procedure for Tandem Reaction of 1n:

To a solution of 1,5-di(β - thienyl)-3-(α - thienyl) pent-2-en-4-yn-1-ol **1n** (164mg, 0.5 mmol) in 2 mL CH_3CN was added AuCl(6 mg, 0.025 mmol) under Ar atmosphere. The mixture was stirred at room temperature for about 4 hours. The solvent was removed *in vacuo* and the residue was purified by flash chromatography on silica gel (petroleum/dichloromethane = 5/1) to furnish product **3n** as an amorphous solid in 40% yield.

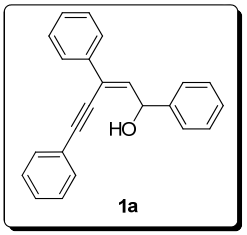
Experimental Procedure for Base-Promoted Thermocyclization of 2a:

To a solution of dienyne **2a** (496 mg, 1mmol) in 10 mL DME was added KOH (90 mg, 1.6 mmol) under Ar atmosphere. The mixture was stirred at reflux temperature for about 20 min until the starting material disappeared completely by inspection of TLC. The reaction mixture was diluted by addition of 10 mL Et_2O followed by addition of 10 mL water. The organic layer was seperated and the aqueous phase was re-extracted with Et_2O (2 × 20 mL) . The combined extracts was washed with water and brine, dried over Na_2SO_4, concentrated under reduced pressure, and purified by chromatography on silica gel eluting with petroleum to yield the product **4a** in 62% yield.

Experimental Procedure for Heterocoupling Reaction of 1o with 1a:

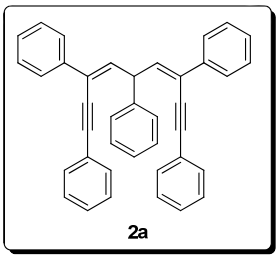
To a mixture of **1o** (135.5 mg, 0.25 mmol, 1.0 eq) and **1a** (620 mg, 2.0 mmol, 8.0 eq) in 8 mL CH_3CN was added AuCl (26 mg, 0.11 mmol, 0.45 eq) under Ar atmosphere. The mixture was stirred at room temperature for 5 min until substrate **1o** disappeared completely by inspection of TLC. The solvent was removed *in vacuo* and the residue was purified by flash chromatography (petroleum/ethyl acetate = 25/1) on Et_3N-treated silica gel to furnish the product **2ao** as an amorphous solid in 74% yield based on **1o**.

Spectroscopic Data for Substrates and Products



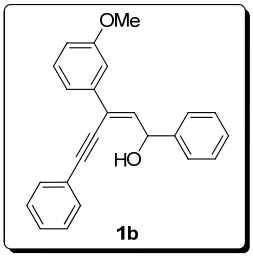
1a

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.72 (m, 2H), 7.60-7.58 (m, 4H), 7.44-7.31 (m, 9H), 6.62 (d, J = 8.4 Hz, 1H), 6.14 (d, J = 8.4 Hz, 1H), 2.52 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.5, 138.2, 137.0, 131.6, 128.7, 128.6, 128.4, 128.39, 128.3, 127.7, 126.3, 125.9, 124.1, 122.8, 96.5, 85.9, 73.0 ppm; MS (EI) *m/z* (%): 310 (M^+, 8), 281 (8), 233 (12), 205 (63), 105 (100), 77 (71).



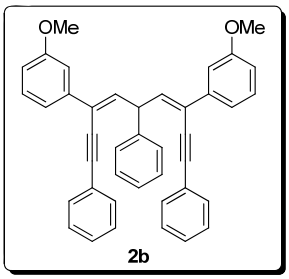
2a

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80-7.78 (m, 4H), 7.56-7.54 (m, 2H), 7.47-7.40 (m, 10H), 7.39-7.32 (m, 2H), 7.31-7.25 (m, 3H), 7.21-7.17 (m, 4H), 6.74 (d, J = 9.6 Hz, 2H), 5.92 (t，J = 9.6 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6, 137.9, 137.2, 131.7, 128.8, 128.4, 128.2, 127.9, 127.6, 126.7, 126.3, 124.6, 123.1, 95.9, 86.7, 48.6 ppm; MS (EI) *m/z* (%): 496 (M^+, 57), 417 (29), 215 (90), 191 (100), 165 (46), 105 (80); HRMS (EI): calculated for $C_{39}H_{28}$ $[M]^+$: 496.2186; found: 496.2191.

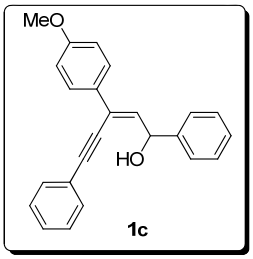


1b

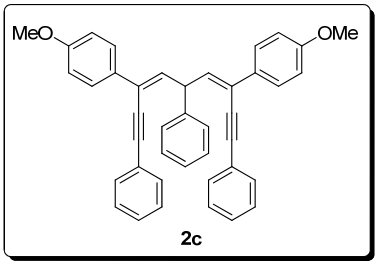
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59-7.57 (m, 4H), 7.43-7.33 (m, 5H), 7.31-7.25 (m, 4H), 6.90-6.88 (m, 1H), 6.62 (dd, J = 8.7 Hz, J = 1.2 Hz, 1H), 6.12 (d, J = 8.7 Hz, 1H), 3.84 (s, 3H), 2.56 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.6, 142.5, 138.5, 138.46, 138.4, 131.5, 129.3, 128.6, 128.5, 128.4, 127.6, 125.9, 124.0, 122.8, 118.7, 113.8, 112.0, 96.4, 85.8, 72.9, 55.2 ppm; MS (EI) *m/z* (%): 340 (M^+, 5), 311 (3), 263 (4), 221 (42), 105 (74), 77 (100).



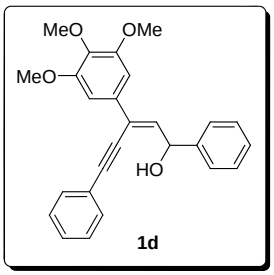
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, J = 8.0 Hz, 2H), 7.47-7.27 (m, 15H), 7.21-7.18 (m, 4H), 6.93-6.90 (m, 2H), 6.75 (d, J = 9.6 Hz, 2H), 5.92 (t, J = 9.6 Hz, 1H), 3.88 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 142.5, 139.4, 137.3, 131.7, 129.3, 128.8, 128.1, 127.6, 126.7, 124.5, 123.1, 118.7, 113.4, 112.2, 95.9, 86.6, 55.2, 48.5 ppm; MS (EI) *m/z* (%): 556 (M^+,78), 465 (23), 273 (92), 165 (54), 149 (90), 44 (100); HRMS (ESI): calculated for $C_{41}H_{33}O_2$ $[M+H]^+$: 557.2475; found: 557.2475.



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66-7.64 (m, 2H), 7.59-7.57 (m, 4H), 7.42-7.34 (m, 6H), 6.91 (d, J = 8.7 Hz, 2H), 6.51 (d, J =9.0 Hz, 1H), 6.11(d, J = 8.7 Hz, 1H), 3.83(s, 3H), 2.55(brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.7, 142.7, 136.3, 131.6, 129.5, 128.6, 128.5, 128.4, 127.6, 127.5, 125.9, 123.6, 122.8, 113.7, 96.3, 86.1, 73.0, 55.2 ppm; MS (EI) *m/z* (%): 340 (M^+, 27), 311 (10), 263 (17), 221 (88), 105 (86), 77 (100).

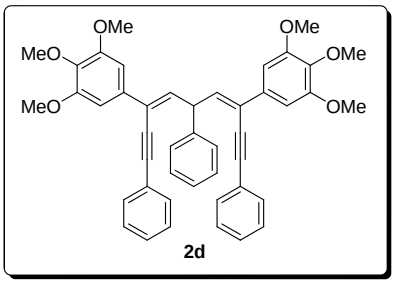


^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.69 (m, 4H), 7.53-7.37 (m, 8H), 7.29-7.25 (m, 3H), 7.19-7.15 (m, 4H), 6.95-6.93 (m, 4H), 6.61 (d, J = 9.6 Hz, 2H), 5.86 (t, J = 9.6 Hz, 1H), 3.84 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 143.0, 135.6, 131.7, 130.6, 128.7, 128.1, 127.6, 127.5, 126.5, 123.8, 123.2, 113.7, 95.6, 87.0, 55.3, 48.5 ppm; MS (EI) *m/z* (%) 556 (M^+, 17), 209 (15), 149 (64), 131 (35), 111 (42), 44 (100); HRMS (ESI): calculated for $C_{41}H_{33}O_2$ $[M+H]^+$: 557.2475; found: 557.2478.



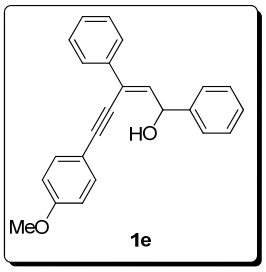
1d

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59-7.53 (m, 4H), 7.41-7.26 (m, 6H), 6.94 (s, 2H), 6.54 (d, J = 8.7 Hz, 1H), 6.10 (d, J = 8.7 Hz, 1H), 3.89 (s, 6H), 3.88 (s, 3H), 2.73 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.0, 142.6, 138.3, 137.8, 132.7, 131.4, 128.7, 128.5, 128.4, 127.6, 125.8, 123.8, 122.7, 103.6, 96.5, 85.9, 72.9, 60.8, 56.0 ppm; MS (EI) *m/z* (%): 400 (M^+,16), 295 (32), 281 (40), 105 (100), 91 (29), 77 (80).



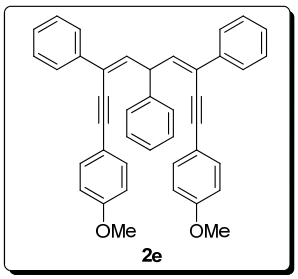
2d

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.38 (m, 8H), 7.30-7.17 (m, 7H), 6.99 (s, 4H), 6.64 (d, J = 10 Hz, 2H), 5.85 (t, J = 9.6 Hz, 1H), 3.92 (s, 12H), 3.88 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.1, 142.5, 138.2, 136.6, 133.6, 131.6, 128.8, 128.3, 128.2, 127.6, 126.7, 124.5, 123.0, 103.8, 96.0, 86.6, 60.8, 56.2, 48.6 ppm; MS (EI) *m/z* (%): 676 (M^+, 2), 564 (80), 527 (23), 438 (45), 339 (28), 44 (100); HRMS (ESI): calculated for $C_{45}H_{41}O_6$ $[M+H]^+$: 677.2898; found: 677.2909.



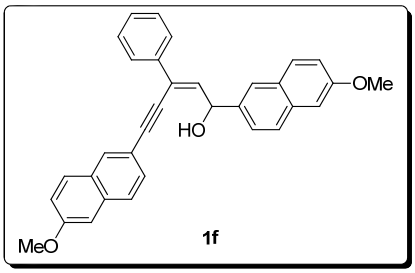
1e

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73-7.70 (m, 2H), 7.59-7.51 (m, 4H), 7.42-7.32 (m, 6H), 6.92(dd, J = 6.8 Hz, J = 2.0 Hz, 2H), 6.58(d, J = 8.4 Hz, 1H), 6.12 (d, J = 8.8 Hz, 1H), 3.84 (s, 3H), 2.56 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 142.7, 137.6, 137.2, 133.1, 128.5, 128.4, 128.2, 127.6, 126.3, 125.9, 124.4, 114.9, 114.1, 96.7, 84.7, 73.0, 55.3 ppm; MS(EI) *m/z* (%) 340 (M^+,42), 235 (100), 221 (95), 203 (45), 105 (29),77 (20).



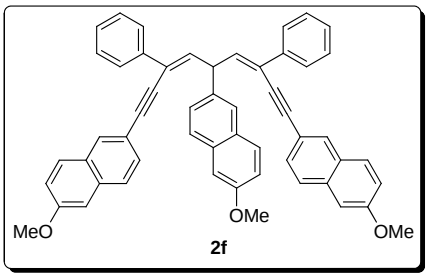
2e

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.0 Hz, 2H), 7.49-7.23 (m, 15H), 6.66-6.62 (m, 6H), 5.85 (t, J = 9.6 Hz, 1H), 3.75 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 142.9, 138.2, 136.6, 133.2, 128.7, 128.4, 127.8, 127.6, 126.6, 126.3, 124.7, 115.4, 113.8, 95.8, 85.5, 55.2, 48.5 ppm; MS (EI) *m/z* (%): 556 (M^+,6), 391 (97), 315 (77), 203 (94), 105 (100), 91 (64); HRMS (ESI): calculated for $C_{41}H_{33}O_2$ $[M+H]^+$: 557.2475; found: 557.2468.



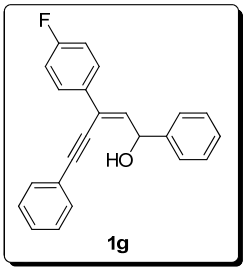
1f

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.98 (d, J = 12.3 Hz, 2H), 7.76-7.57 (m, 9H), 7.41-7.14 (m, 6H), 6.69 (d, J = 8.1 Hz, 1H), 6.29 (d, J = 8.7 Hz, 1H), 3.93 (s, 3H), 3.92 (s, 3H), 2.55 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.7, 158.0, 138.3, 138.1, 137.5, 135.5, 134.6, 134.4, 131.7, 129.8, 129.7, 129.14, 129.1, 128.7, 128.6, 127.6, 127.3, 126.7, 125.3, 125.1, 124.7, 119.9, 119.2, 118.0, 106.1, 105.9, 97.7, 86.0, 73.5, 55.6, 55.5 ppm; MS (EI) *m/z* (%) 470 (M^+,10), 271 (52), 239 (40), 185 (100), 115 (80), 57 (73).



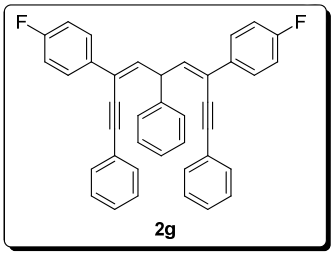
2f

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.85-7.66 (m, 9H), 7.43-7.13 (m, 15H), 6.93-6.77 (m, 6H), 6.11 (t, J = 9.6 Hz, 1H), 3.91 (s, 3H), 3.87 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.0, 157.4, 138.0, 137.9, 136.9, 133.9, 133.4, 131.2, 129.3, 129.2, 129.1, 129.0, 128.4, 128.2, 127.9, 127.3, 126.9, 126.5, 126.4, 125.6, 124.7, 118.9, 117.9, 105.5, 105.4, 96.5, 86.4, 55.3, 55.2, 48.5 ppm; MS (ESI), *m/z*: 737.4 $[M+H]^+$.



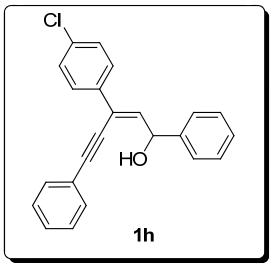
1g

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.69-7.65 (m, 2H), 7.60-7.57 (m, 4H), 7.43-7.32 (m, 6H), 7.06 (t, J = 8.7 Hz, 2H), 6.54 (d, J = 9.0 Hz, 1H), 6.10 (d, J = 8.7 Hz, 1H), 2.57 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 164.4, 161.1, 142.5, 138.0, 133.2, 133.1, 131.6, 128.8, 128.6, 128.5, 128.1, 128.0, 127.7, 125.9, 123.1, 122.7, 115.4, 115.1, 96.7, 85.7, 73.0 ppm; MS (EI) *m/z* (%): 328 (M^+,5), 299 (5), 251 (8), 223 (31), 105 (100), 77 (70).



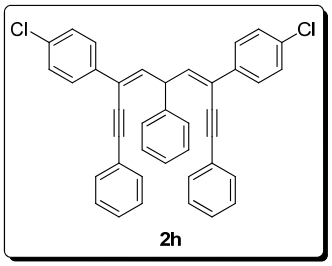
2g

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.69 (m, 4H), 7.50-7.37 (m, 8H), 7.32-7.25 (m, 3H), 7.18-7.15 (m, 4H), 7.09-7.05 (m, 4H), 6.62 (dd, J = 9.4 Hz, J = 3.4 Hz, 2H), 5.82 (t, J = 10.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9, 161.4, 142.5, 136.9, 134.0, 131.7, 128.9, 128.3, 128.2, 128.0, 127.9, 127.6, 126.8, 126.3, 123.6, 123.0, 115.4, 115.2, 96.2, 86.4, 48.7 ppm; MS (EI) *m/z* (%): 532 (M^+,5),496 (100), 394 (71), 317 (64), 215 (44), 44 (39); HRMS (EI): calculated for $C_{39}H_{26}F_2$ $[M]^+$: 532.1997; found: 532.1998.



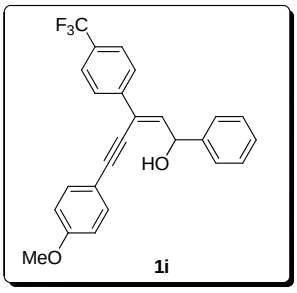
1h

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.63-7.57 (m, 6H), 7.45-7.31 (m, 8H), 6.59 (d, J = 9.0 Hz, 1H), 6.11 (d, J = 8.7 Hz, 1H), 2.81 (brs, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.3, 138.5, 135.4, 134.0, 131.6, 128.8, 128.6, 128.5, 128.4, 127.8, 127.5, 125.9, 122.9, 122.5, 96.8, 85.4, 73.0 ppm; MS (EI) *m/z* (%): 344 (M^+,6), 315 (3), 267 (7), 225 (35), 105 (100), 77 (62).



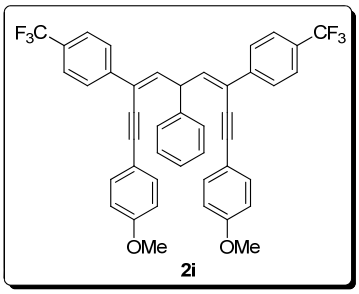
2h

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66 (d, J = 8.7 Hz, 4H), 7.48-7.14 (m, 19H), 6.66 (d, J = 9.9 Hz, 2H), 5.82 (t, J = 9.3 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.2, 137.2, 136.3, 133.7, 131.7, 128.9, 128.5, 128.4, 128.2, 127.5, 127.2, 126.8, 123.6, 122.8, 96.3, 86.1, 48.7 ppm; MS (EI) *m/z* (%): 564 (M^+, 4), 379 (22), 165 (24), 130 (78), 57 (70), 44 (100); HRMS (EI): calculated for $C_{39}H_{26}Cl_2$ $[M]^+$: 564.1406; found: 564.1402.



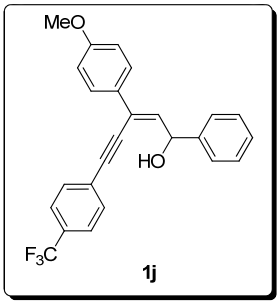
1i

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 2H), 7.61-7.48 (m, 6H), 7.41-7.29 (m, 3H), 6.92-6.90 (m, 2H), 6.61 (d, J = 8.4 Hz, 1H), 6.08 (d, J = 8.4 Hz, 1H), 3.84 (s, 3H), 2.42 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.2, 142.4, 140.8, 139.4, 133.2, 130.3, 128.7, 127.9, 126.7, 125.9, 125.4, 123.4, 122.7, 114.6, 114.2, 97.4, 84.0, 73.1, 55.3 ppm; MS (EI) *m/z* (%): 408 (M^+,57), 303 (56), 289 (100), 235 (26), 105 (67), 77 (24).



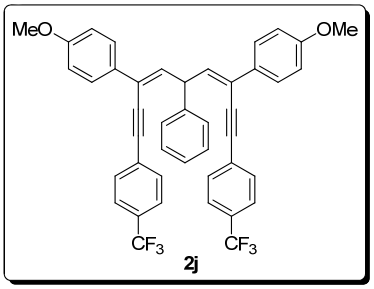
2i

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 8.0 Hz, 4H), 7.60 (d, J = 8.4 Hz, 4H), 7.46-7.28 (m, 9H), 6.71-6.66 (m, 6H), 5.83 (t, J = 9.6 Hz, 1H), 3.78 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 141.6, 138.0, 133.2, 130.0, 128.9, 127.6, 126.9, 126.6, 125.3, 124.0, 114.9, 113.9, 96.8, 84.7, 55.2, 48.8 ppm; MS (EI) *m/z* (%): 692 (M^+, 2), 527 (2), 239 (8), 176 (40), 149 (65), 43 (100); HRMS (ESI): calculated for $C_{43}H_{31}O_2F_6$ $[M+H]^+$: 693.2223; found: 693.2227.



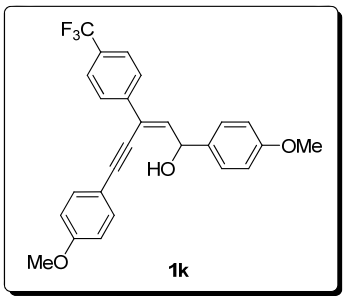
1j

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66-7.60 (m, 6H), 7.56-7.51 (m, 2H), 7.41-7.29 (m, 3H), 6.92-6.89 (m, 2H), 6.54 (d, J = 8.8 Hz, 1H), 6.23 (d, J = 8.8 Hz, 1H), 3.81 (s, 3H), 2.40 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 142.6, 137.4, 131.8, 131.7, 129.2, 128.7, 127.8, 127.5, 126.7, 126.4, 125.9, 125.4, 123.3, 113.9, 94.7, 88.4, 73.1, 55.3 ppm; MS (EI) *m/z* (%): 408 (M^+, 52), 303 (42), 289 (100), 235 (40), 105 (72), 77 (32).



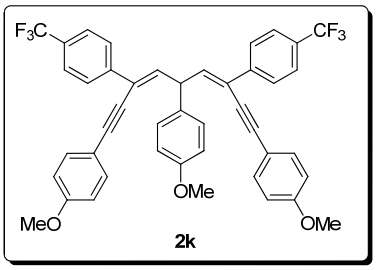
2j

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.81(d, J = 7.5 Hz, 4H), 7.61 (d, J = 9.0 Hz, 4H), 7.47-7.27 (m, 9H), 6.72-6.66 (m, 6H), 5.84 (t, J = 9.5 Hz, 1H), 3.78 (s, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.7, 142.5, 136.3, 131.7, 129.9, 128.9, 127.5, 127.4, 126.8, 125.0, 123.5, 113.9, 94.0, 89.3, 55.3, 48.7 ppm; MS *m/z* (%): 692 (M^+, 2), 540 (7), 420 (11), 201 (30), 130 (68), 43 (100); HRMS (EI): calculated for $C_{43}H_{30}O_2F_6$ $[M]^+$: 692.2145; found: 692.2140.

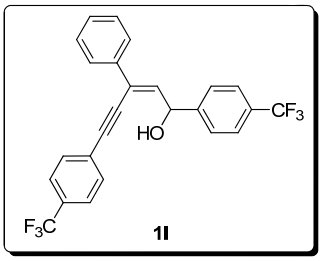


1k

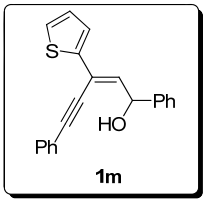
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.8 Hz, 4H), 6.94 (d, J = 8.4 Hz, 4H), 6.69 (d, J = 8.4 Hz, 1H), 6.11 (d, J = 8.4 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 2.08 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 159.1, 140.7, 139.7, 134.6, 133.0, 127.2, 126.5, 126.46, 125.2, 125.14, 125.10, 122.5, 114.5, 114.1, 113.9, 97.3, 84.0, 72.6, 55.1, 55.0 ppm; MS (EI) *m/z* (%): 438 (M^+, 41), 330 (26), 289 (60), 135 (100), 121 (26), 71 (16).



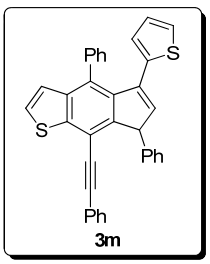
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 8.0 Hz, 4H), 7.60 (d, J = 8.4 Hz, 4H), 7.37-7.31 (m, 6H), 6.90 (d, J = 8.8 Hz, 2H), 6.67 (d, J = 9.2 Hz, 6H), 5.78 (t, J = 9.4 Hz, 1H), 3.79 (s, 3H), 3.78 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.8, 158.6, 141.6, 138.3, 134.2, 133.2, 130.0, 129.6, 128.5, 126.6, 125.3, 123.7, 114.9, 114.4, 113.9, 96.7, 84.7, 55.3, 55.2, 47.9 ppm; MS (EI) *m/z* (%) 722 (M^+, 0.4), 692 (9), 560 (5), 176 (28), 149 (31), 44 (100); HRMS (ESI): calculated for $C_{44}H_{33}O_3F_6$ $[M+H]^+$: 723.2328; found: 723.2325.



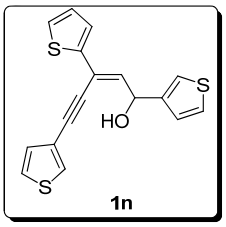
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72-7.63 (m, 10H), 7.42-7.36 (m, 3H), 6.58 (d, J = 8.8 Hz, 1H), 6.15 (d, J = 9.2 Hz, 1H), 2.60 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.1, 138.2, 136.4, 131.9, 128.8, 128.6, 126.3, 126.2, 125.6, 125.5, 125.2, 124.7, 95.3, 87.9, 72.5 ppm.



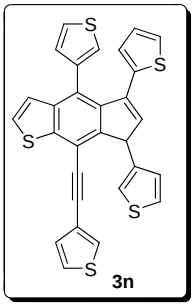
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.65-7.58 (m, 4H), 7.51-7.40 (m, 6H), 7.38-7.24 (m, 2H), 7.05-7.03 (m, 1H), 6.55 (d, J = 9.0 Hz, 1H), 6.08 (d, J = 8.7 Hz, 1H), 2.62 (brs, 1H) ppm; ^{13}CNMR(75 MHz, $CDCl_3$):δ 142.3, 141.9, 135.9, 131.6, 128.8, 128.6, 128.4, 127.7, 127.4, 125.9, 125.7, 125.3, 122.4, 118.4, 95.6, 84.8, 72.7 ppm; MS (EI) *m/z* (%): 316 (M^+,8), 287 (16), 211 (35), 105 (91), 77 (100), 51 (39).



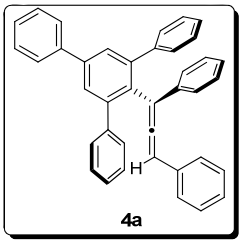
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.39-7.26 (m, 12H), 7.24-7.07 (m, 5H), 6.98-6.96 (m,1H), 6.64 (d, J = 0.6 Hz, 1H), 6.57-6.54 (m, 1H), 6.26 (dd, J = 3.6 Hz, J = 1.2 Hz, 1H), 5.00(d, J = 2.1 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 147.6, 142.2, 140.6, 139.2, 138.0, 137.8, 137.7, 137.3, 131.7, 131.5, 129.9, 128.6, 128.4, 128.2, 127.3, 126.9, 126.8, 126.6, 126.55, 125.9, 124.5, 123.8, 122.9, 113.3, 98.2, 85.0, 54.6 ppm; MS (EI) *m/z* (%): 506 (M^+, 100), 429 (31), 395 (14), 325 (22), 71 (28), 57 (38); HRMS (EI): calculated for $C_{35}H_{22}S_2$ $[M]^+$: 506.1157; found: 506.1151.



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, J = 2.0 Hz, 1H), 7.35-7.33 (m, 4H), 7.27-7.20 (m, 3H), 7.02 (t, J = 4.4 Hz, 1H), 6.49 (d, J = 8.8 Hz, 1H), 6.06 (d, J = 8.8 Hz, 1H), 2.27 (brs, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.5, 141.8, 135.1, 129.7, 129.4, 127.4, 126.3, 125.9, 125.8, 125.7, 125.4, 121.4, 121.0, 118.7, 91.0, 84.1, 69.7 ppm; MS (EI) *m/z* (%): 328 (M^+, 4), 299 (23), 217 (35), 159 (51), 111 (80), 44 (100).

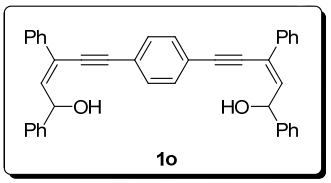


^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, J = 2Hz, 1H), 7.38 (d, J = 5.2Hz, 1H), 7.31-7.29 (m, 1H), 7.25-7.22 (m, 3H), 7.11-7.08 (m, 2H), 7.05-7.02 (m, 2H), 6.92 (s, 1H), 6.85-6.84 (m, 1H), 6.70-6.68 (m, 1H), 6.60 (d, J = 2.4Hz, 1H), 6.40 (d, J = 2.8 Hz, 1H), 5.11 (d, J = 2.0 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.1, 140.5, 139.6, 138.0, 137.8, 137.6, 137.5, 137.4, 129.9, 129.4, 129.1, 127.4, 126.8, 126.4, 126.0, 125.4, 125.2, 124.5, 124.2, 124.1, 124.06, 122.4, 122.0, 113.3, 93.5, 84.4, 49.7ppm; MS (EI) *m/z* (%): 524 (M^+, 3), 354 (17), 309 (38), 159 (25), 149(100), 111 (63), 83 (83); HRMS (APCI): calculated for $C_{29}H_{16}S_5$ $[M+H]^+$: 524.9928; found: 524.9935.



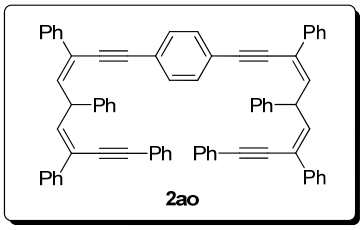
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79-7.76 (m, 4H), 7.54-7.43 (m, 7H), 7.36-7.34 (m, 6H), 7.24-7.19 (m, 8H), 6.91-6.88 (m, 2H), 6.18 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 208.7, 141.9, 140.4, 140.2, 137.3, 133.8, 132.0, 129.3, 128.8, 128.5, 128.3,

128.0, 127.7, 127.6, 127.2, 127.1, 126.9, 126.7, 126.69, 126.6, 109.8, 97.2 ppm; MS (EI) *m/z* (%): 496 (M^+,56), 417 (15), 341 (44), 239 (12), 178 (31), 77 (100); HRMS (EI): calculated for $C_{39}H_{28}$ $[M]^+$: 496.2186; found: 496.2183.



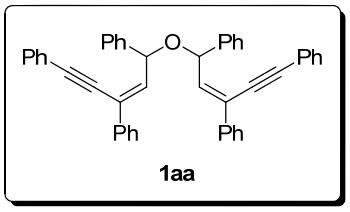
1o

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74-7.70 (m, 4H), 7.63-7.32 (m, 20H), 6.67 (d, J = 8.7 Hz, 2H), 6.14 (d, J = 8.1 Hz, 2H), 2.93 (brs, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 142.8, 139.2, 137.2, 132.8, 132.0, 129.0, 128.8, 128.7, 128.1, 126.7, 126.3, 124.3, 123.4, 96.4, 88.4, 73.4 ppm; MS (EI) *m/z* (%): 542 (M^+,3), 423 (6), 262 (40), 183 (43), 105 (94), 44(100).



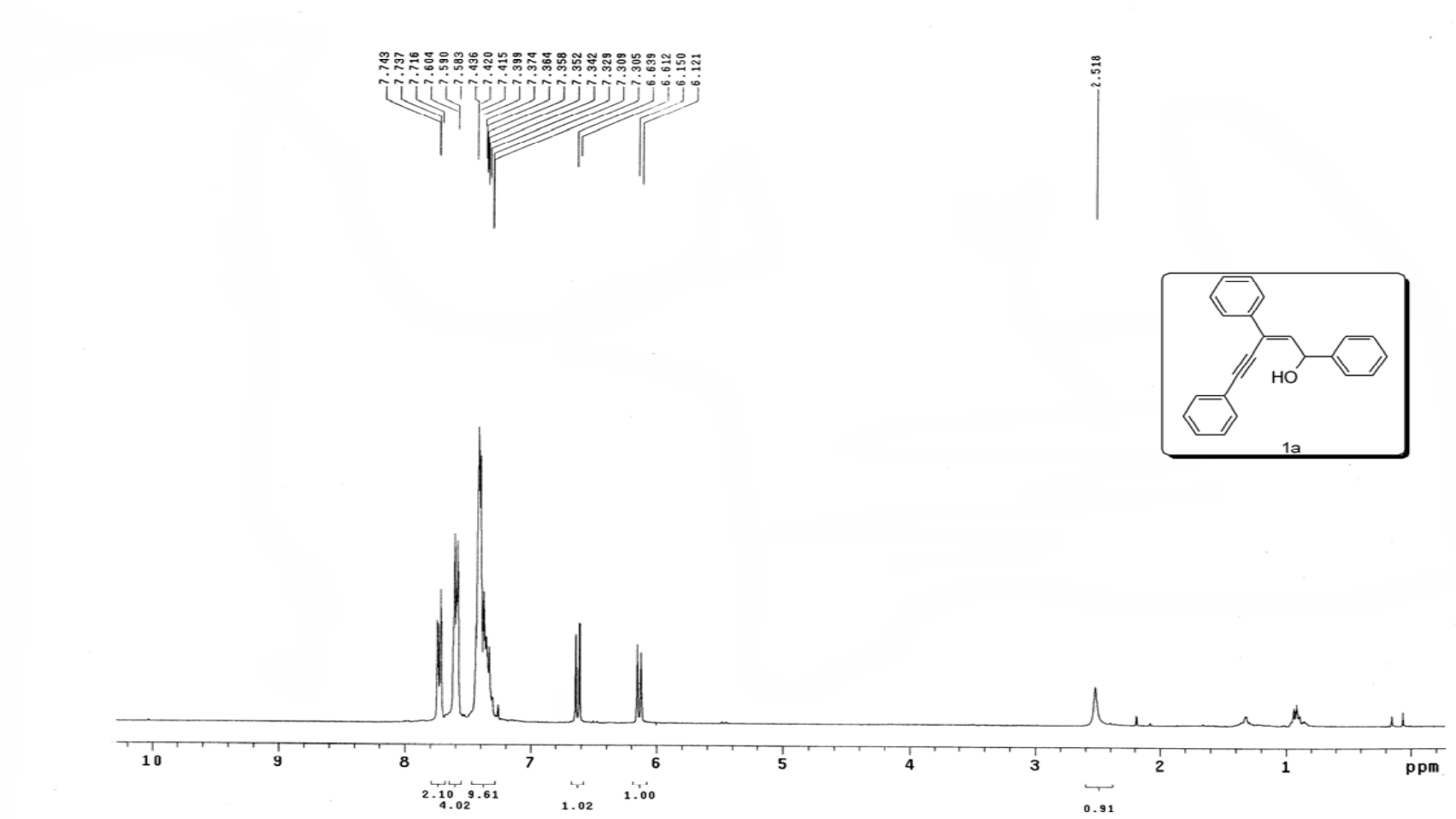
2ao

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73-7.70 (m, 8H), 7.48 (d, J = 7.6 Hz, 4H), 7.40-7.20 (m, 23H), 7.11-7.05 (m, 9H), 6.68 (t, J = 9.6 Hz, 4H), 5.84 (t, J = 9.6 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.5, 137.9, 137.7, 137.6, 136.9, 131.6, 131.4, 128.8, 128.44, 128.42, 128.4, 128.2, 128.02, 128.0, 127.6, 126.8, 126.3, 126.29, 124.7, 124.5, 122.9, 122.8, 95.9, 95.5, 88.5, 86.6, 48.6 ppm; MALDI-TOF MS, *m/z*: 915.7 $[M+H]^+$; 937.6 $[M+Na]^+$.



1aa

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.64-7.62 (d, 7H), 7.41-7.36 (t, 8H), 7.31-7.24 (m, 13H), 7.22-7.15 (m, 2H), 6.64 (d, J = 9.0 Hz, 2H), 6.07 (d, J = 9.3 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.3, 137.1, 136.9, 131.6, 128.6, 128.3, 128.2, 128.1, 128.06, 127.6, 126.7, 126.5, 126.3, 125.4, 122.9, 96.5, 86.1, 77.6 ppm; MS (ESI), *m/z*: 603.0 $[M+H]^+$.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7.329
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7.305
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6.612
6.150
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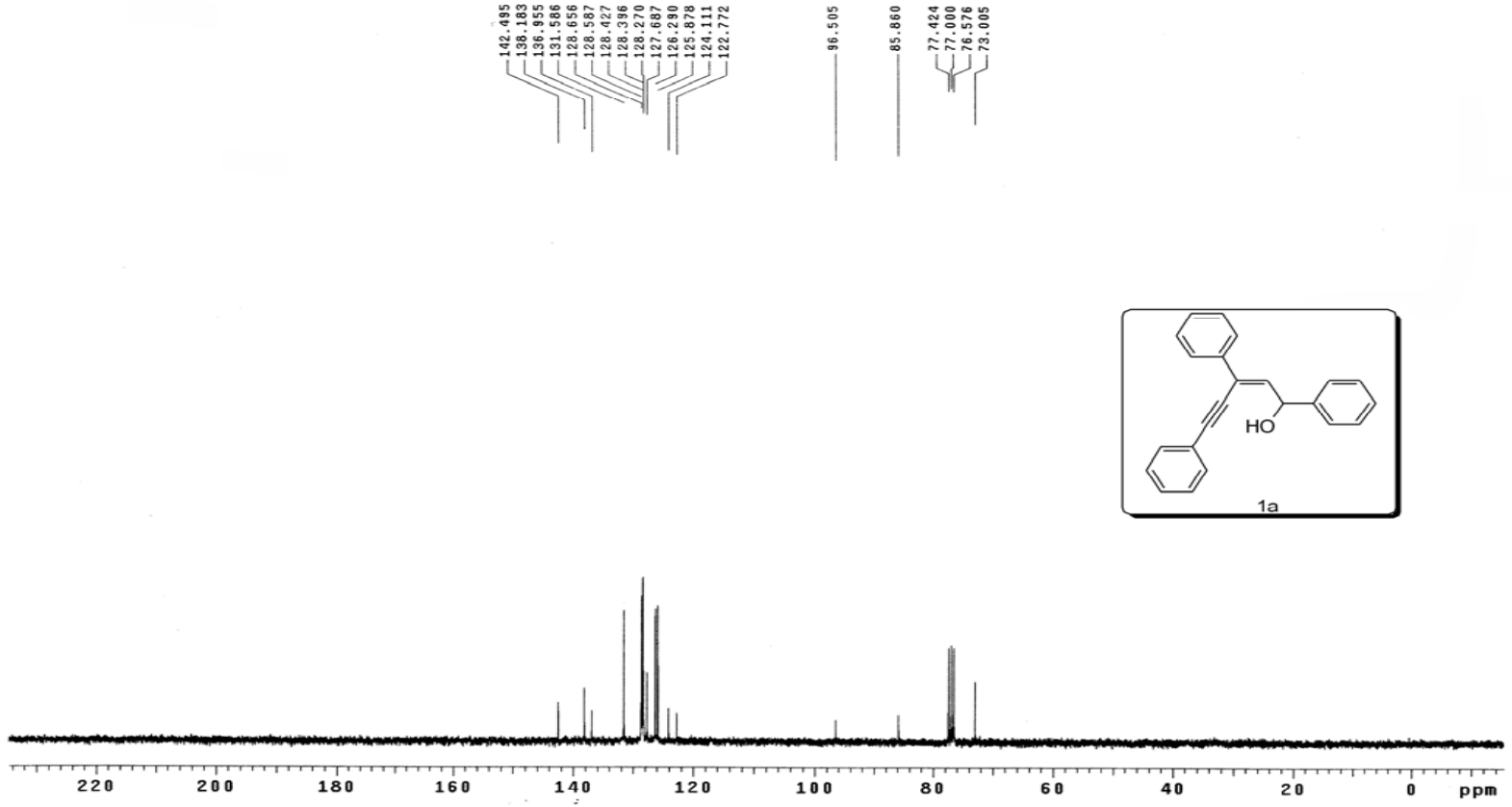
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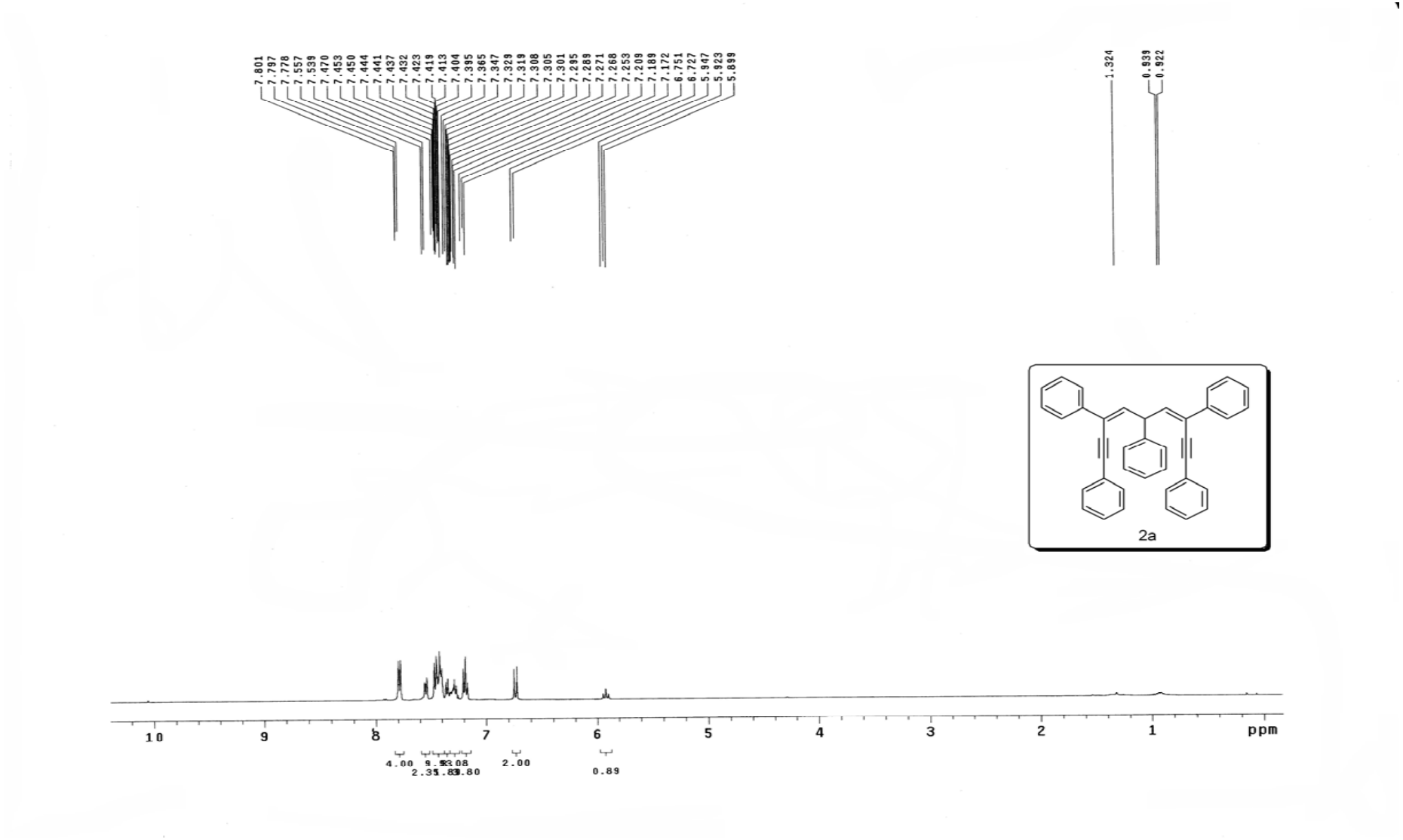
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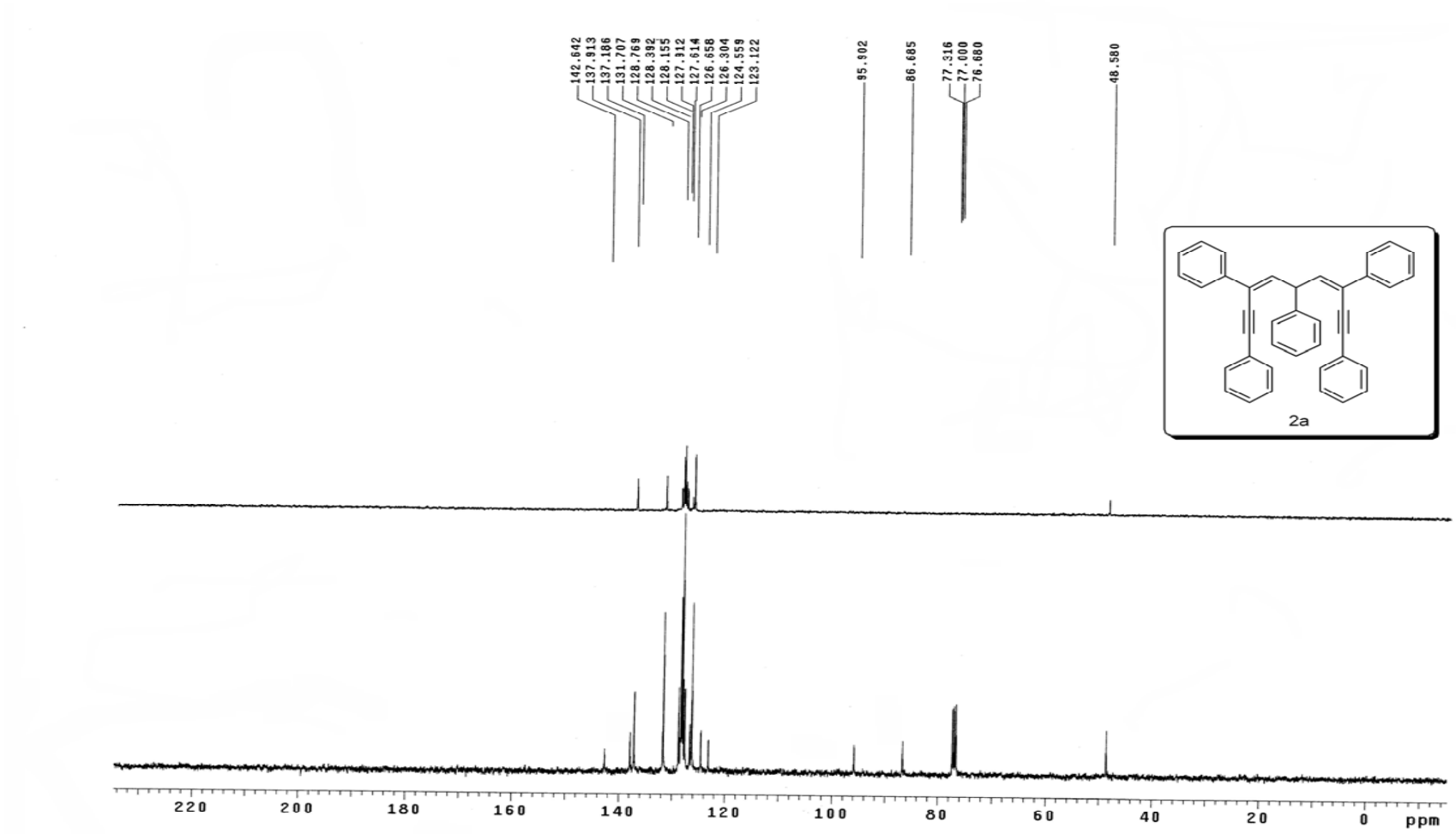
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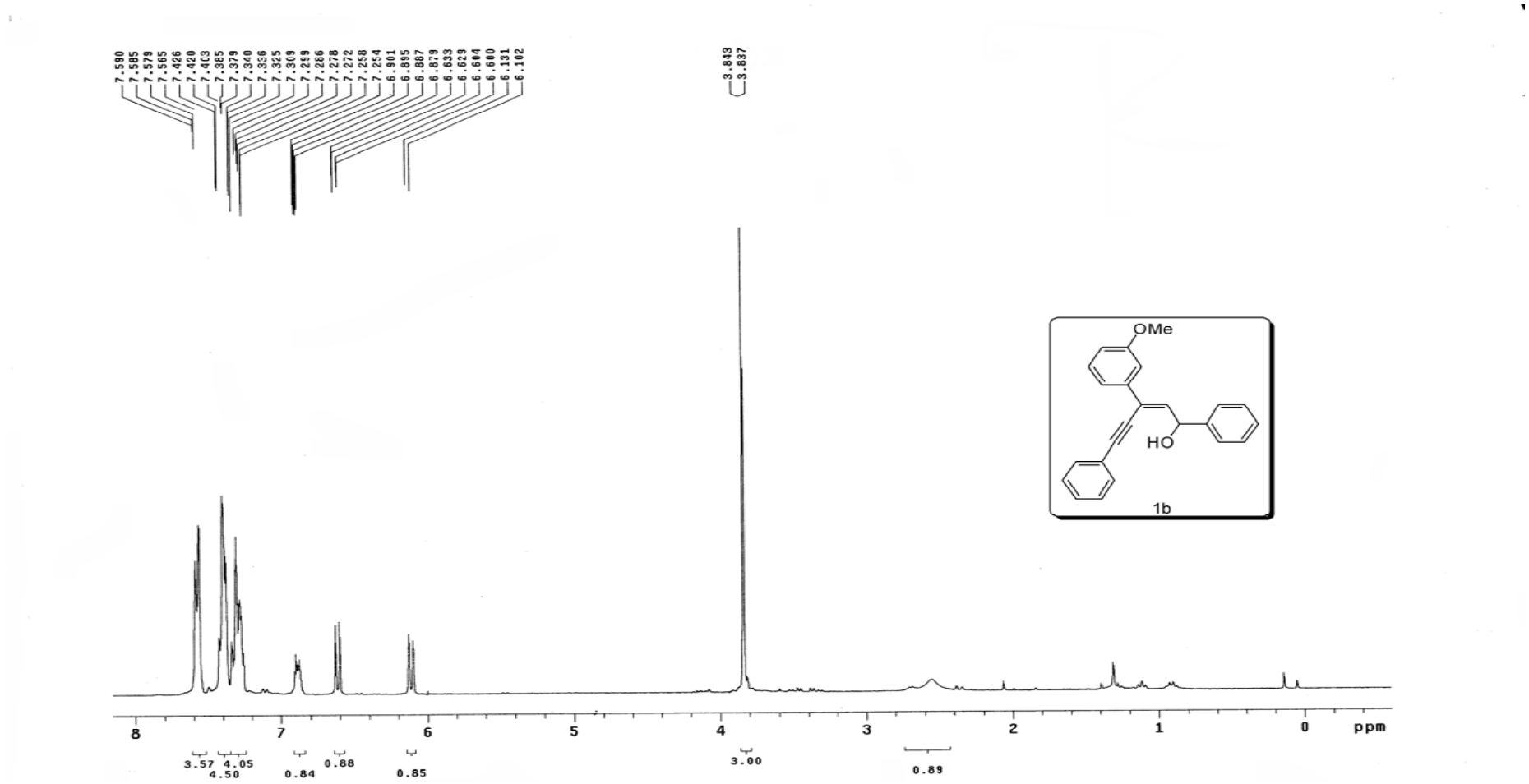
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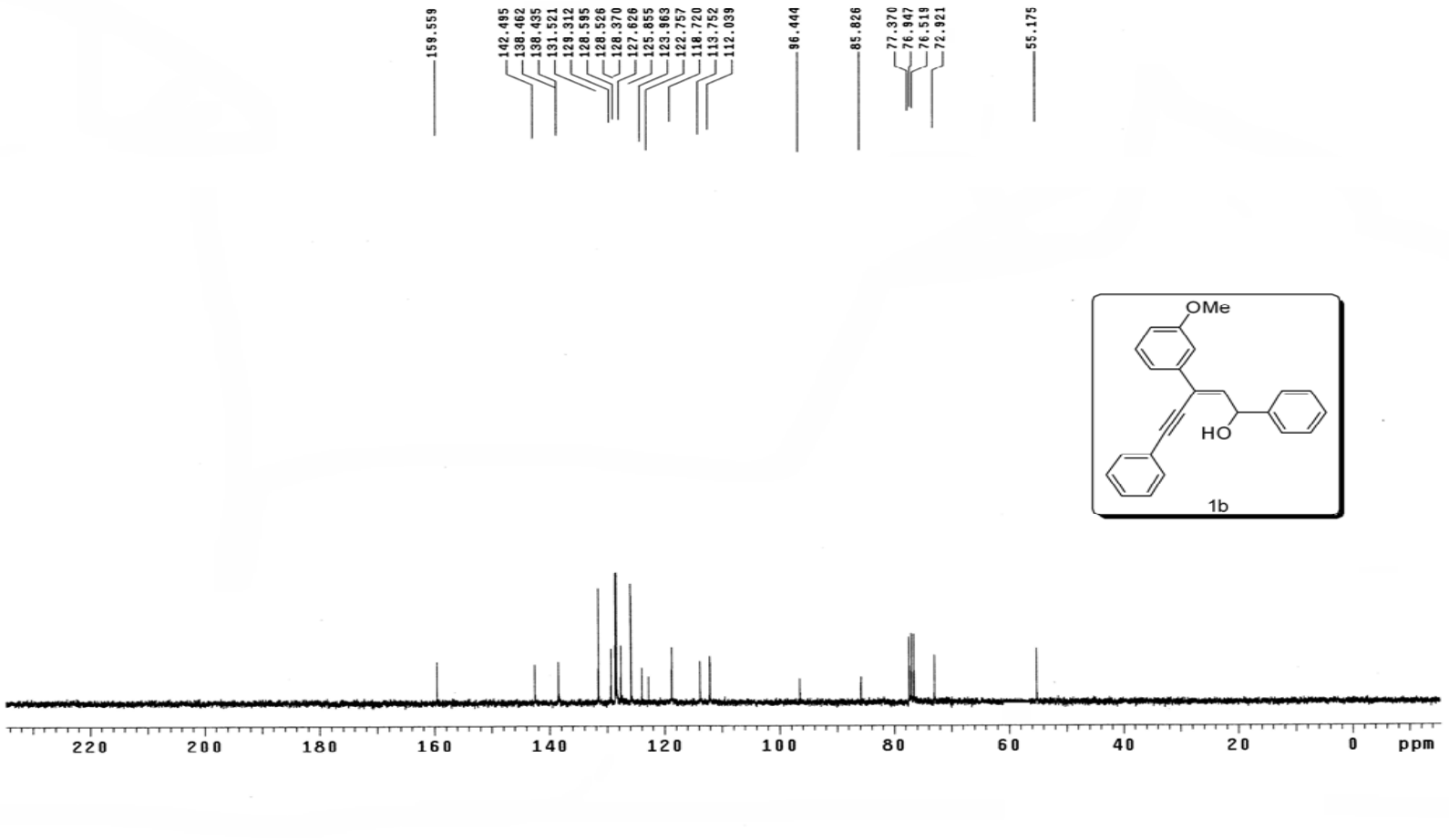
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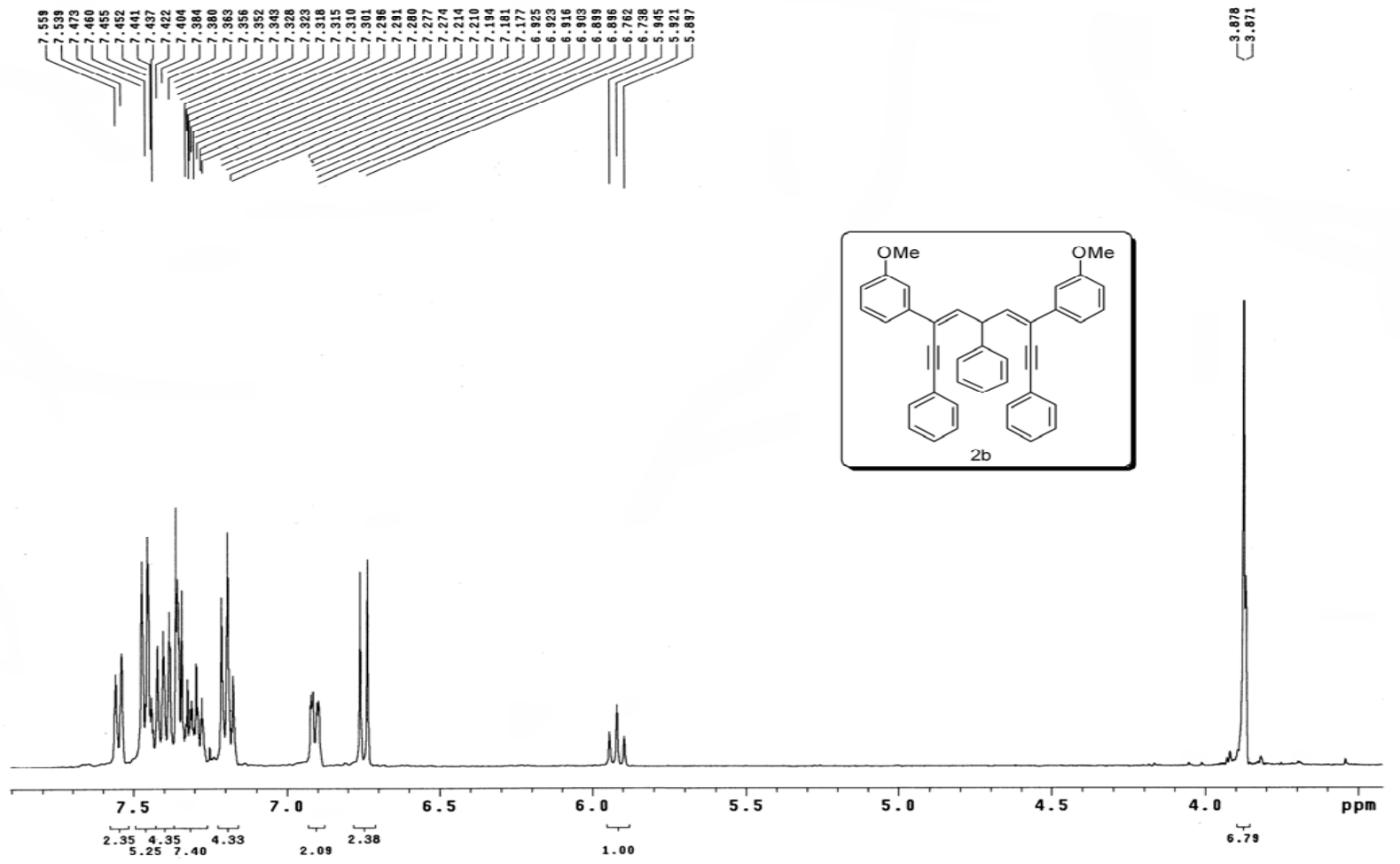
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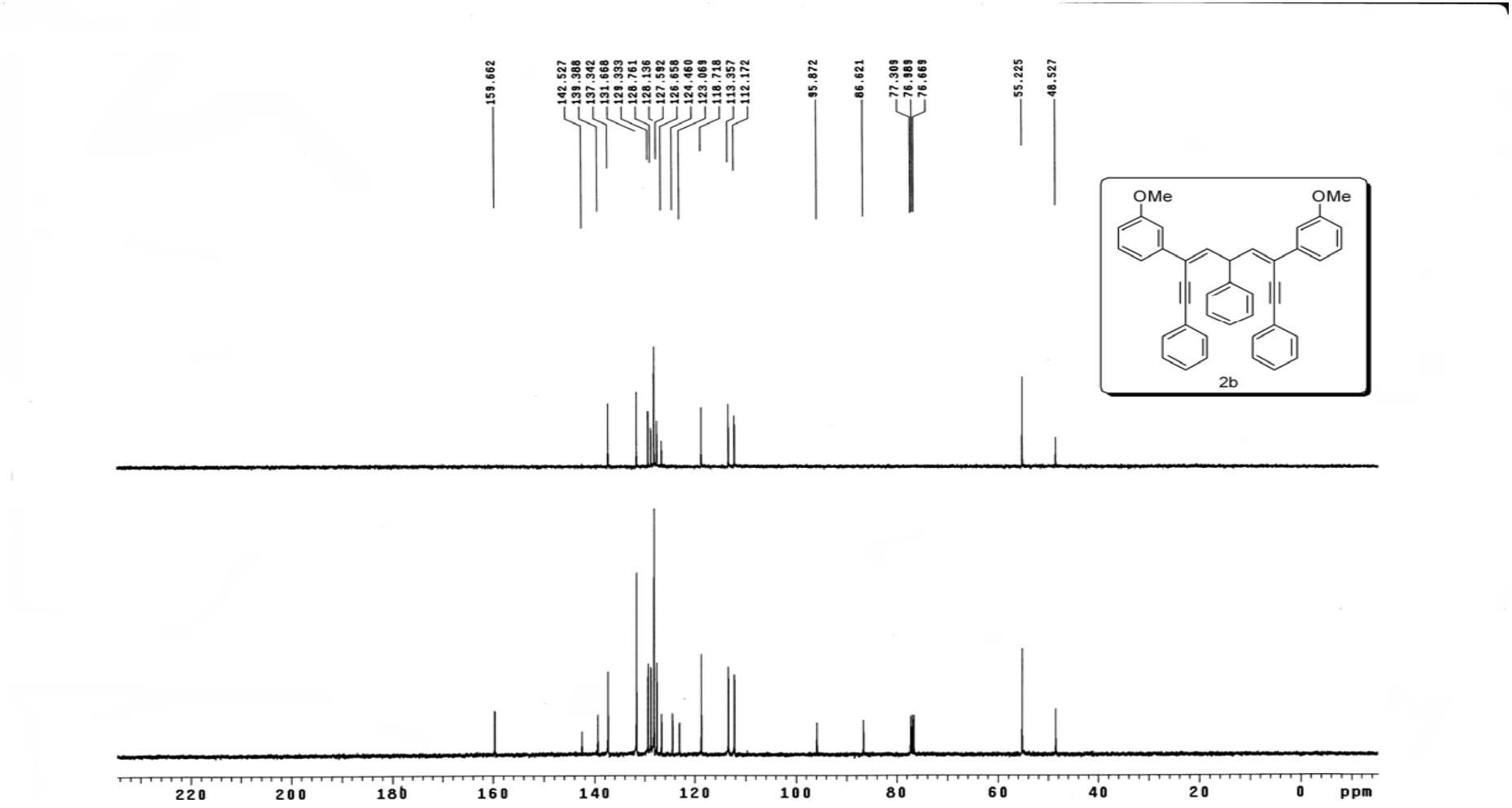
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OMe
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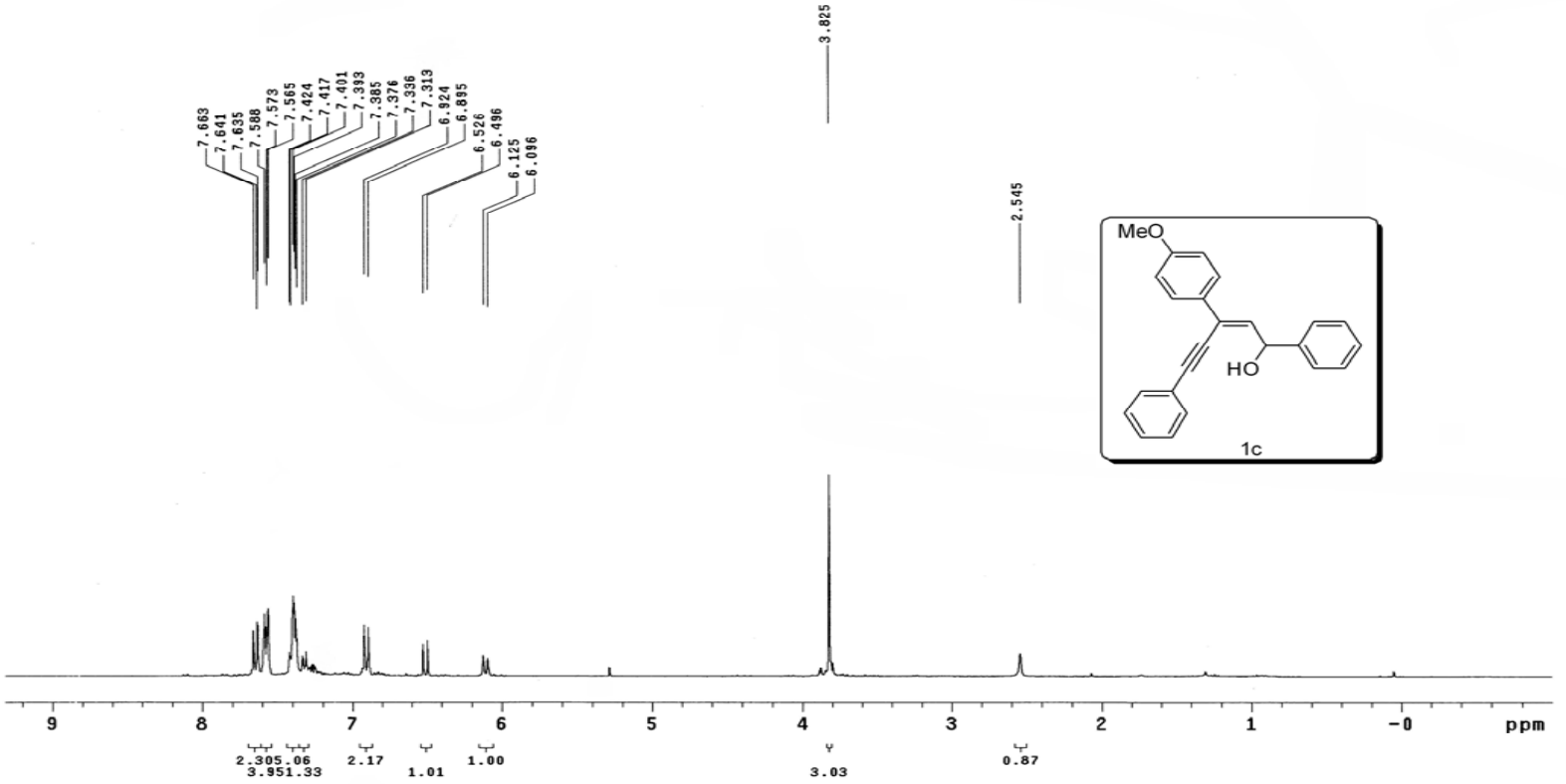
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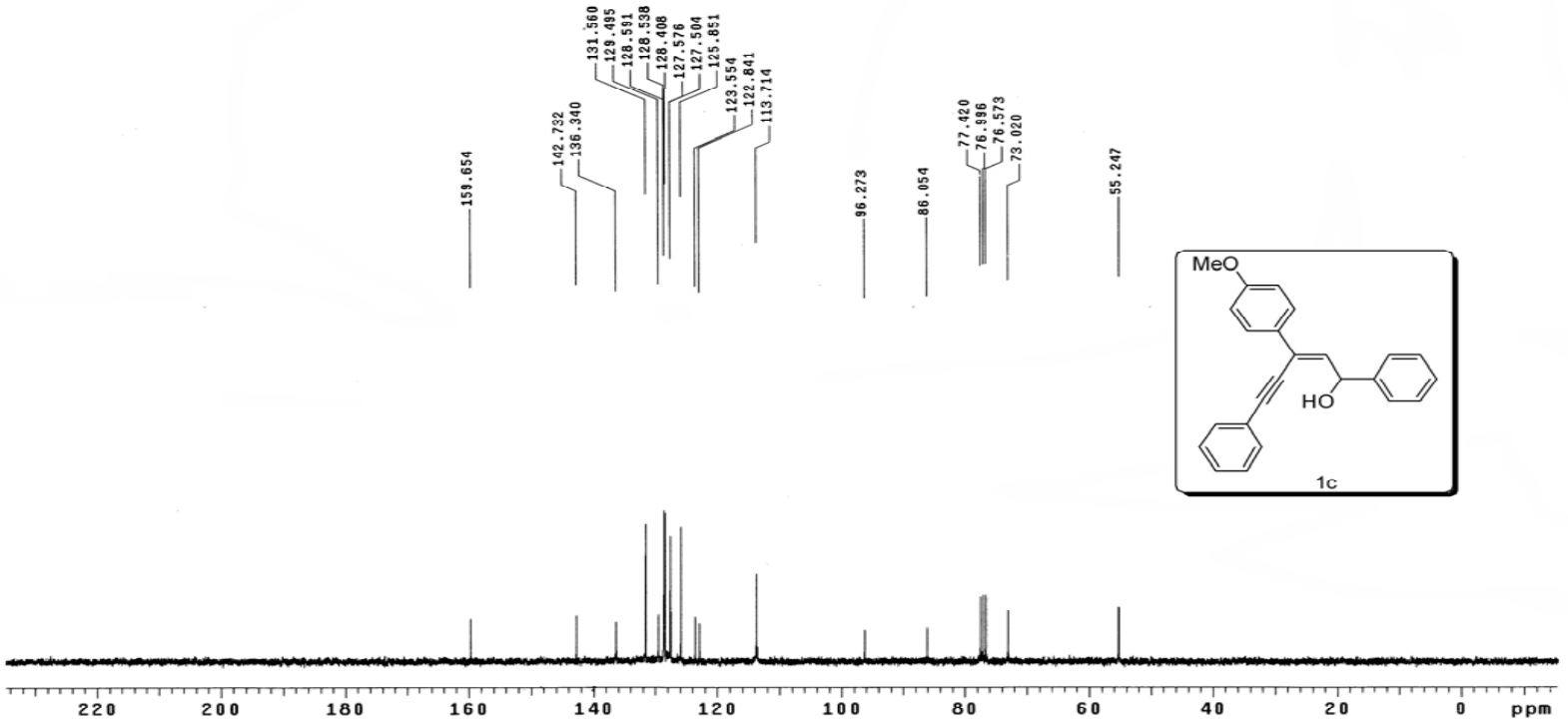
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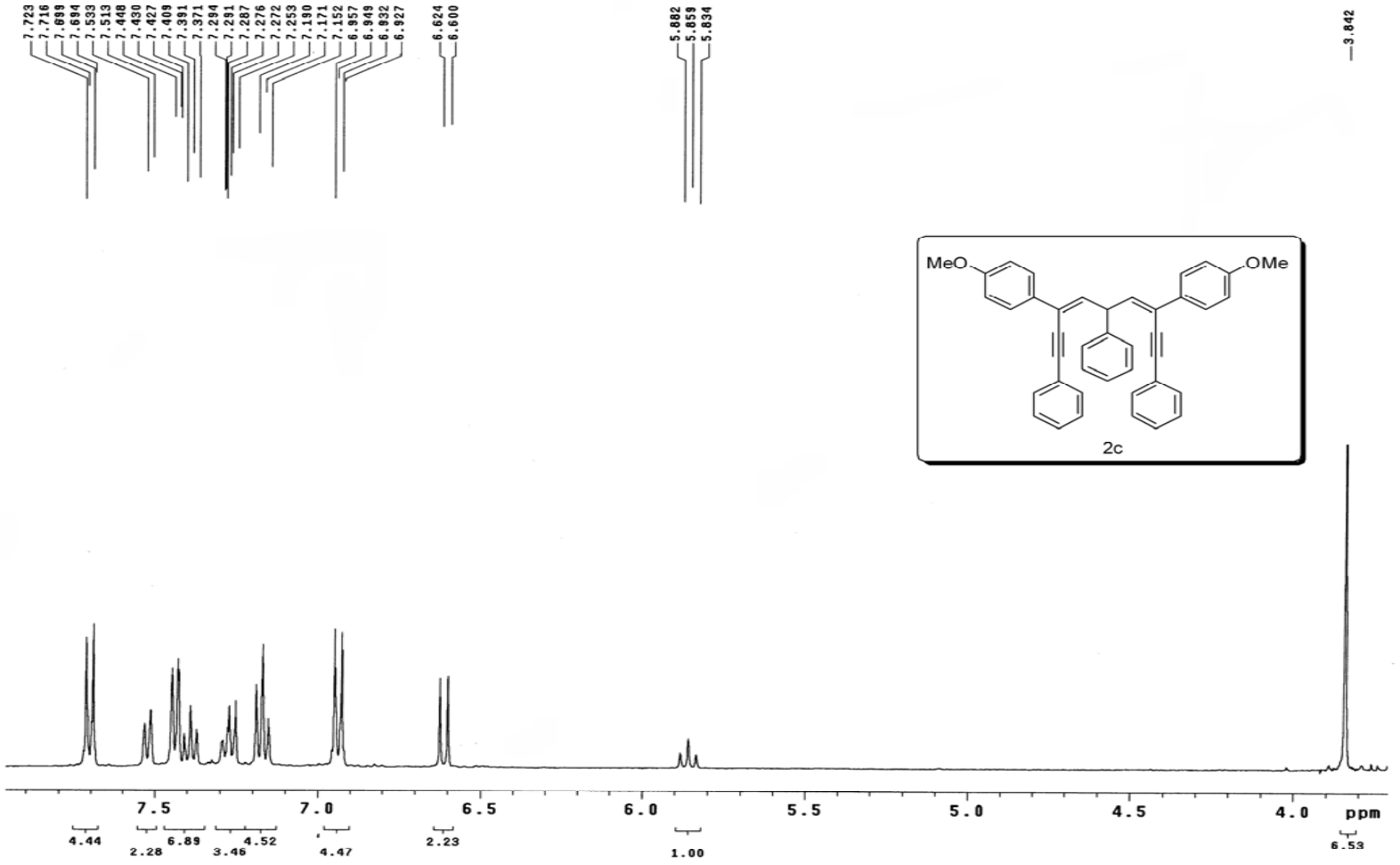
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MeO
OMe
2c
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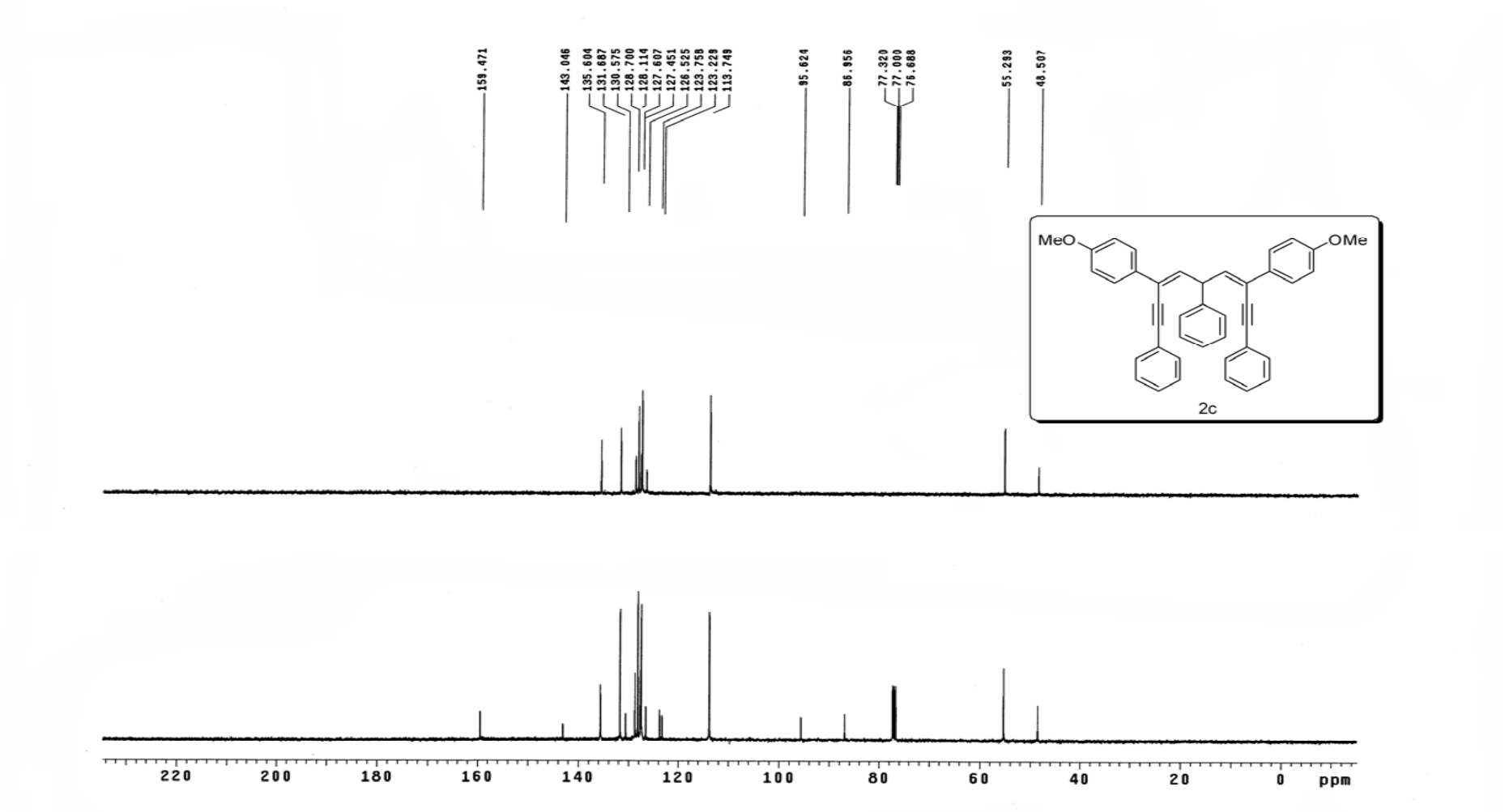
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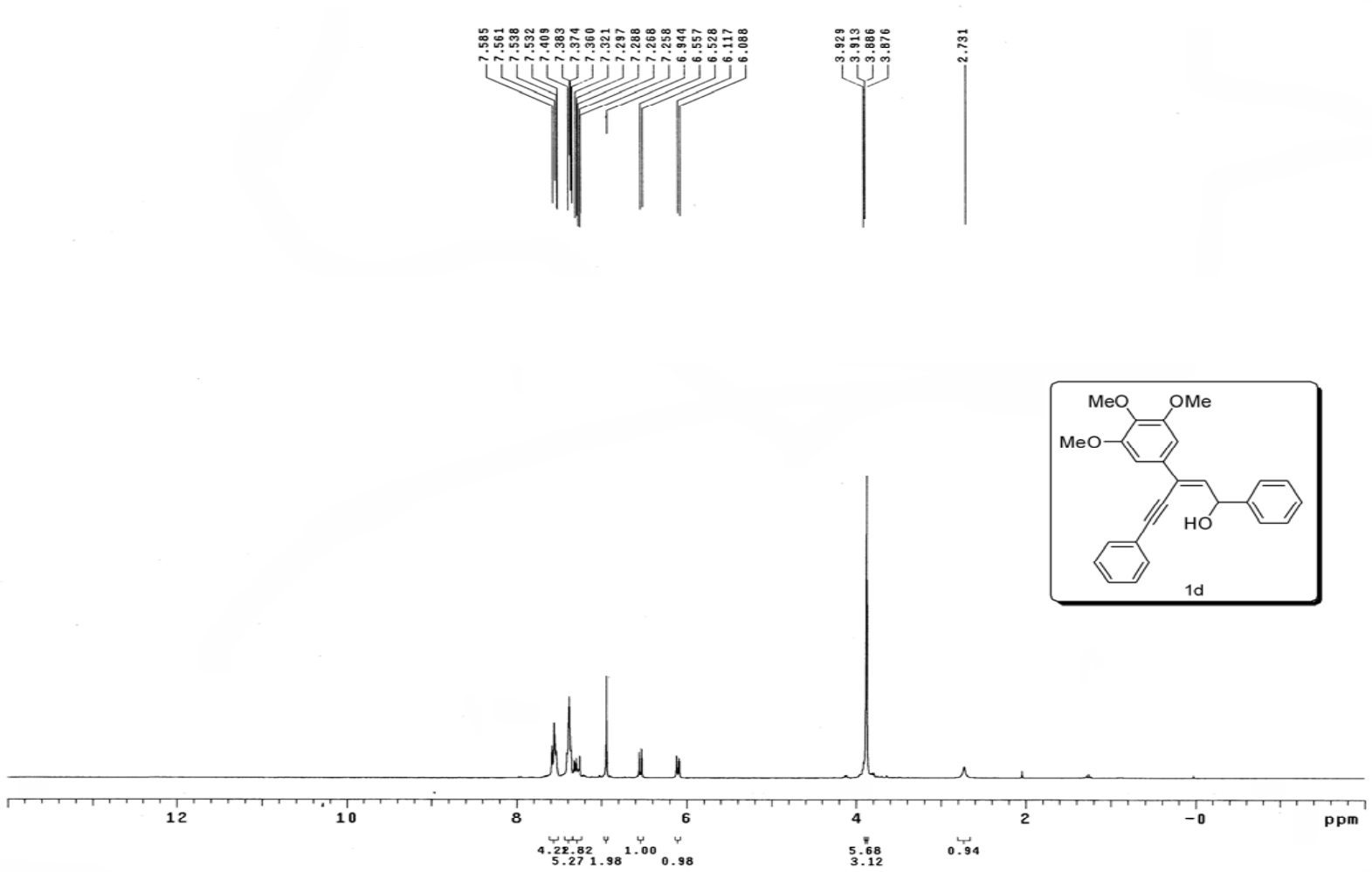
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2.731
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OMe
MeO
HO
1d
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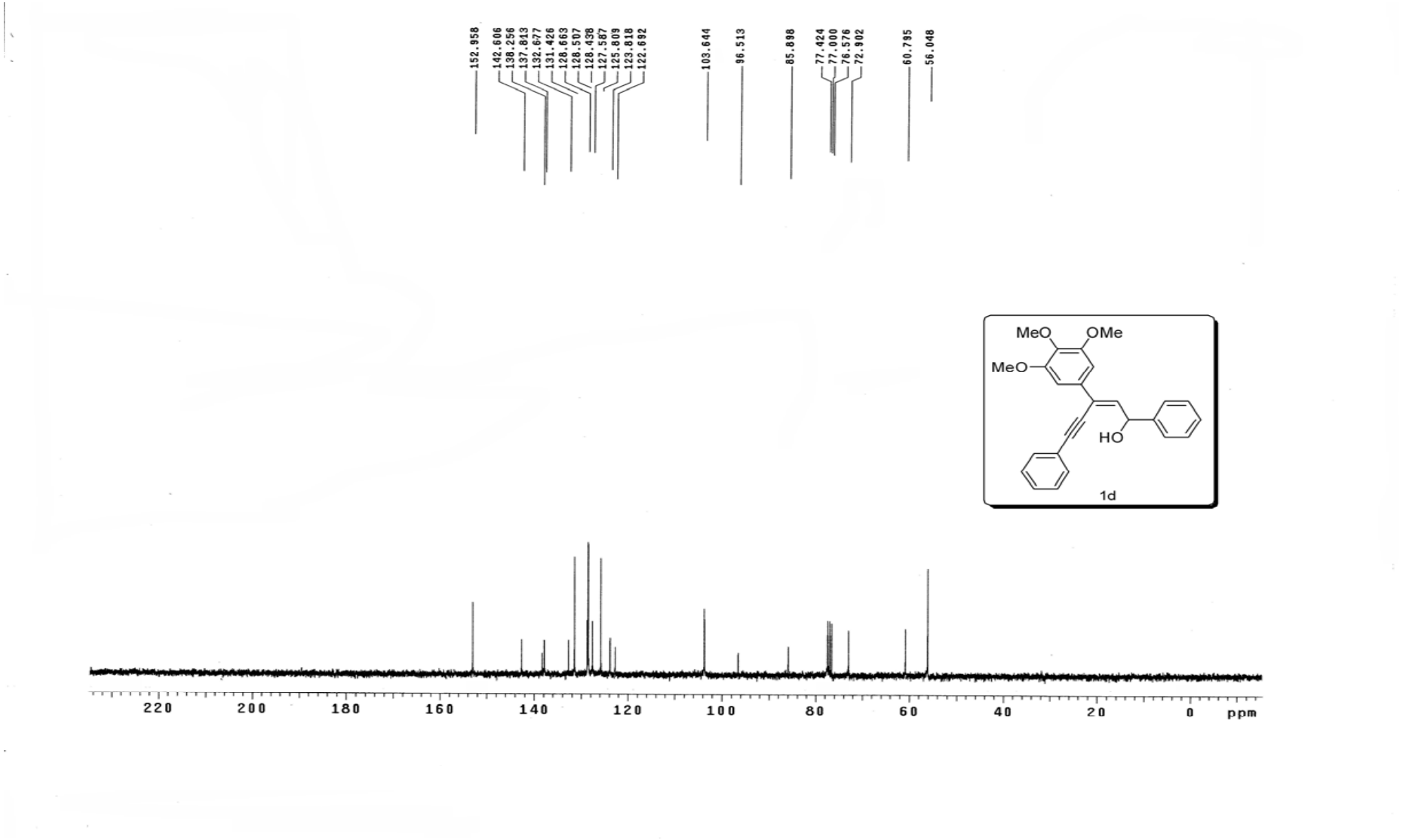
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HO
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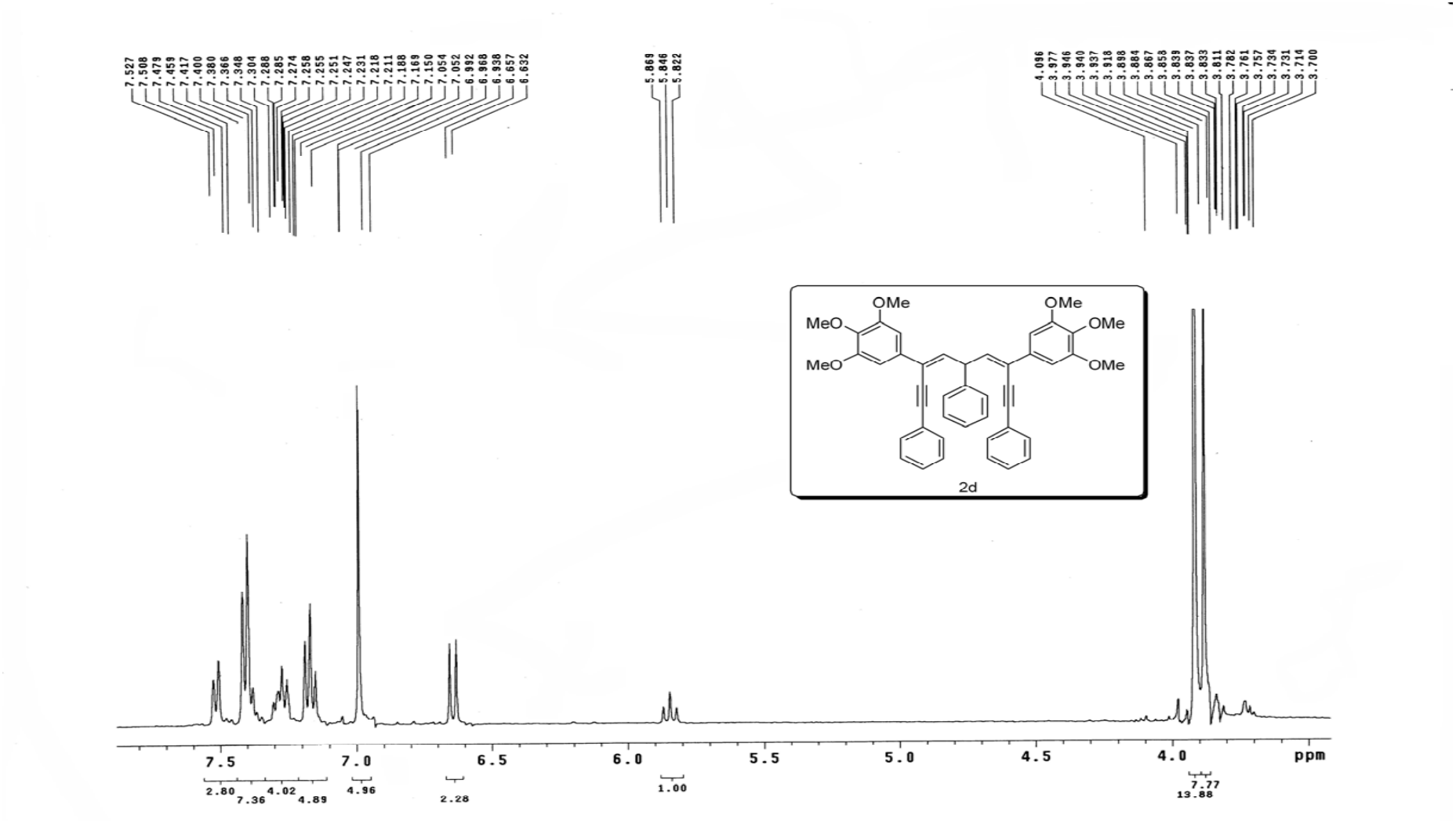
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7.150
7.054
7.052
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3.937
3.918
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3.757
3.734
3.731
3.714
3.700
OMe
MeO
MeO
OMe
OMe
OMe
2d
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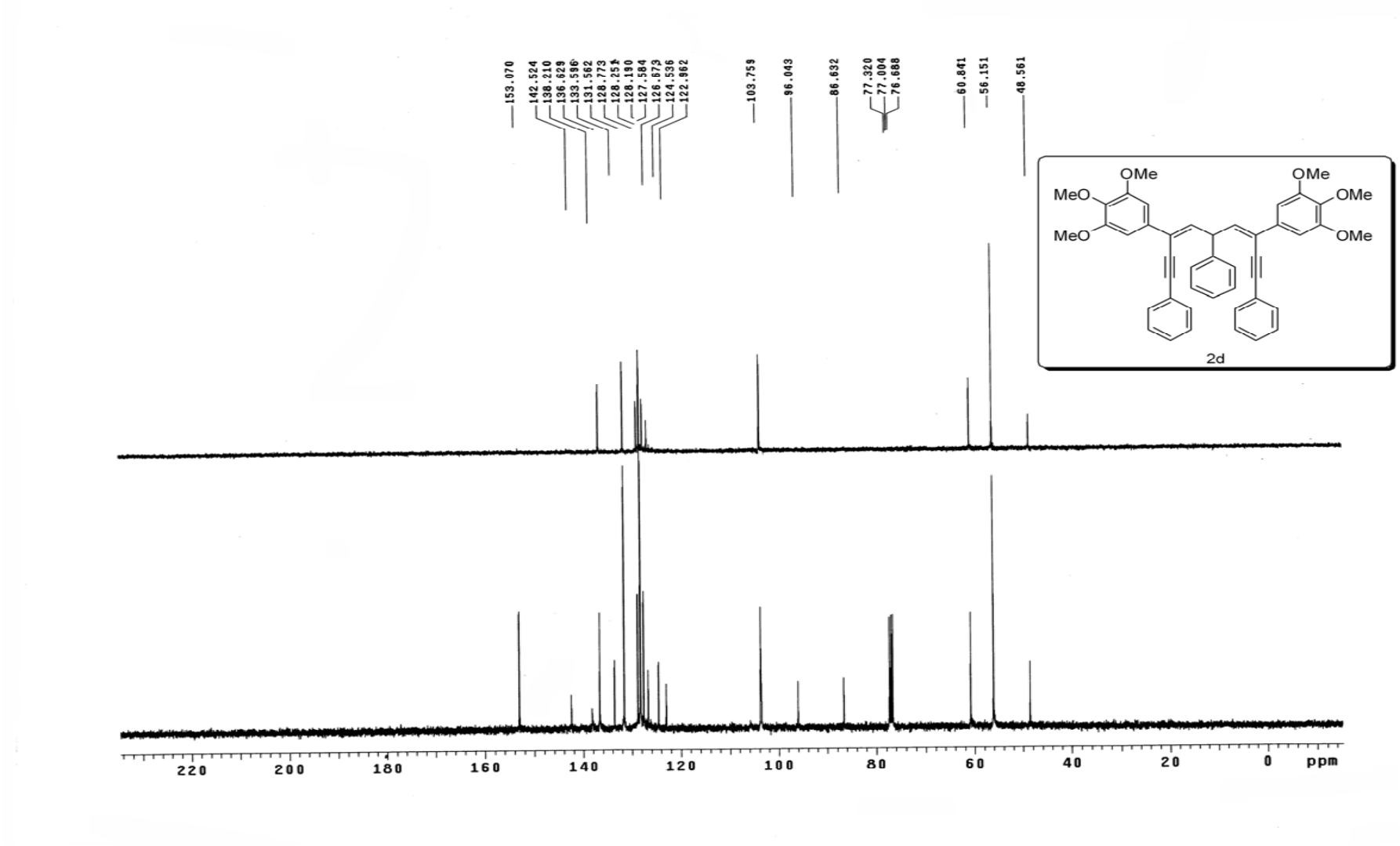
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OMe
MeO
MeO
OMe
OMe
OMe
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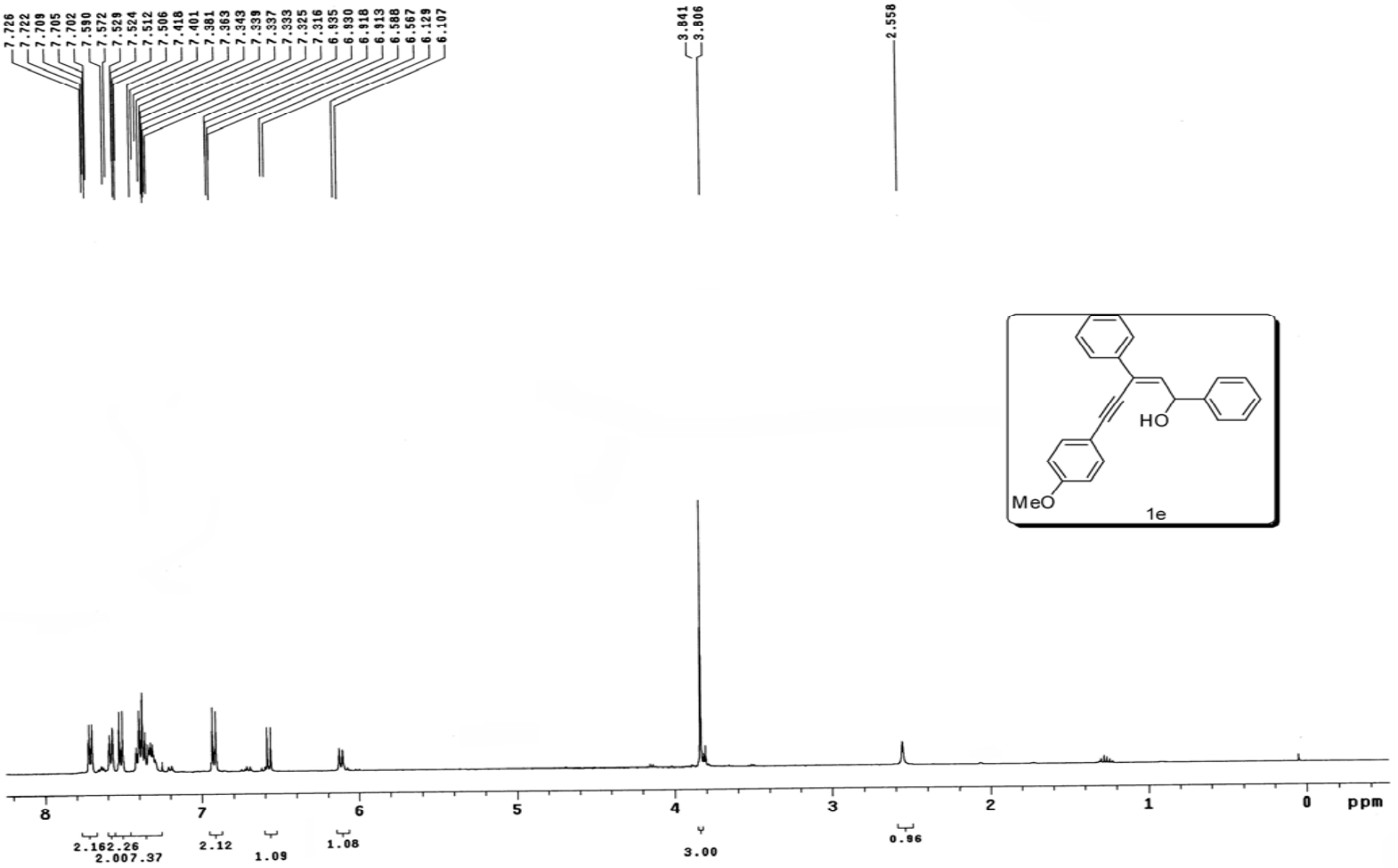
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MeO
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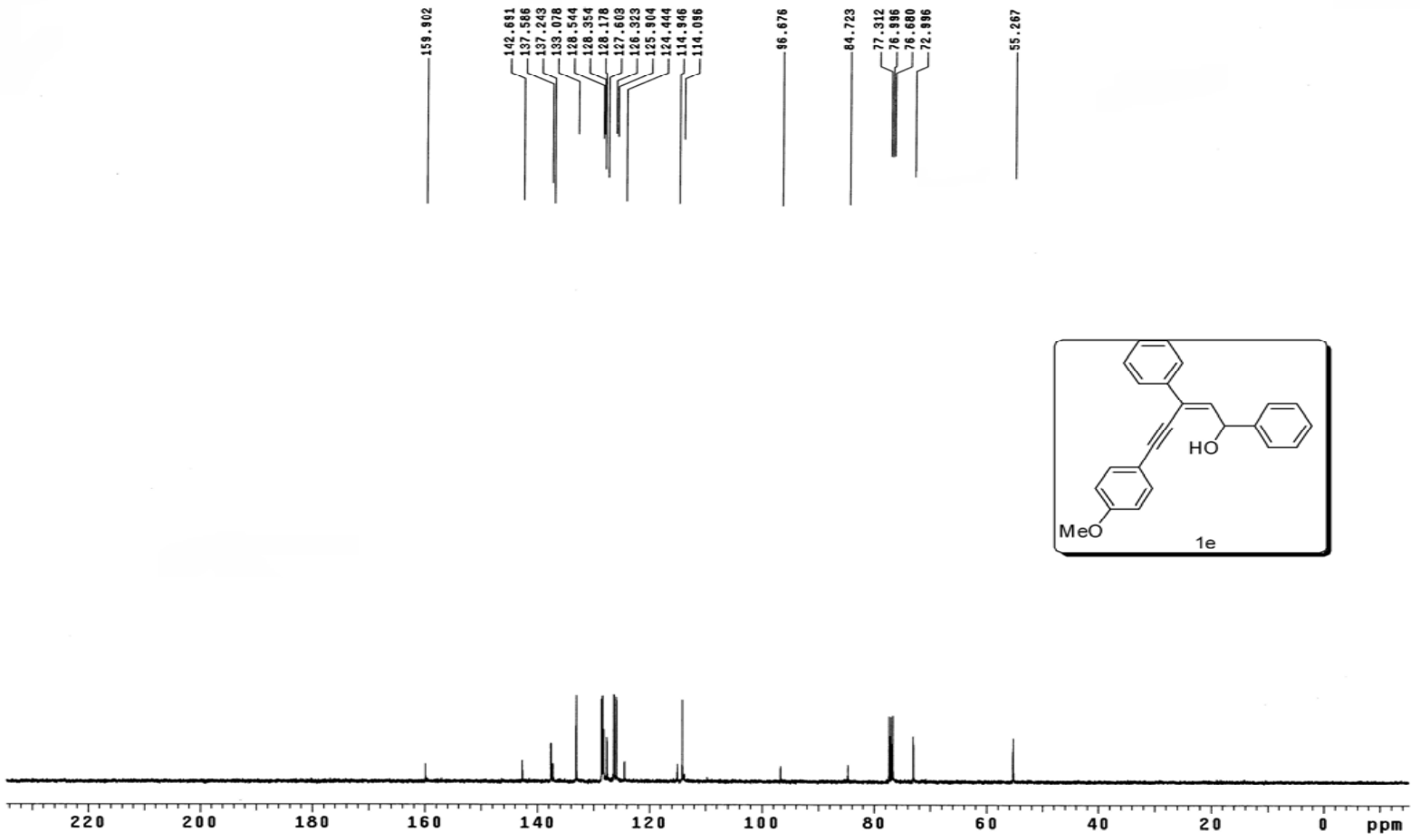
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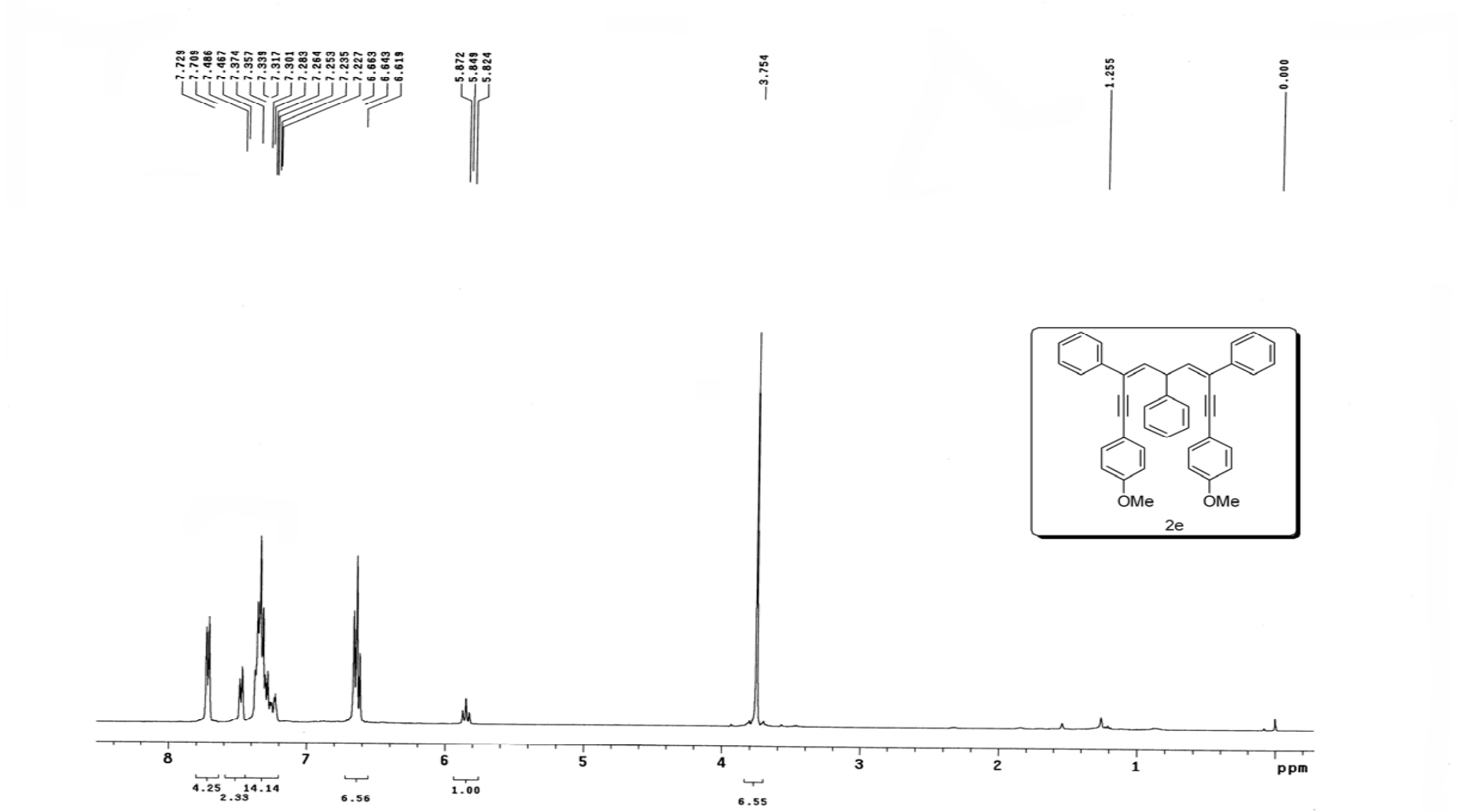
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OMe
OMe
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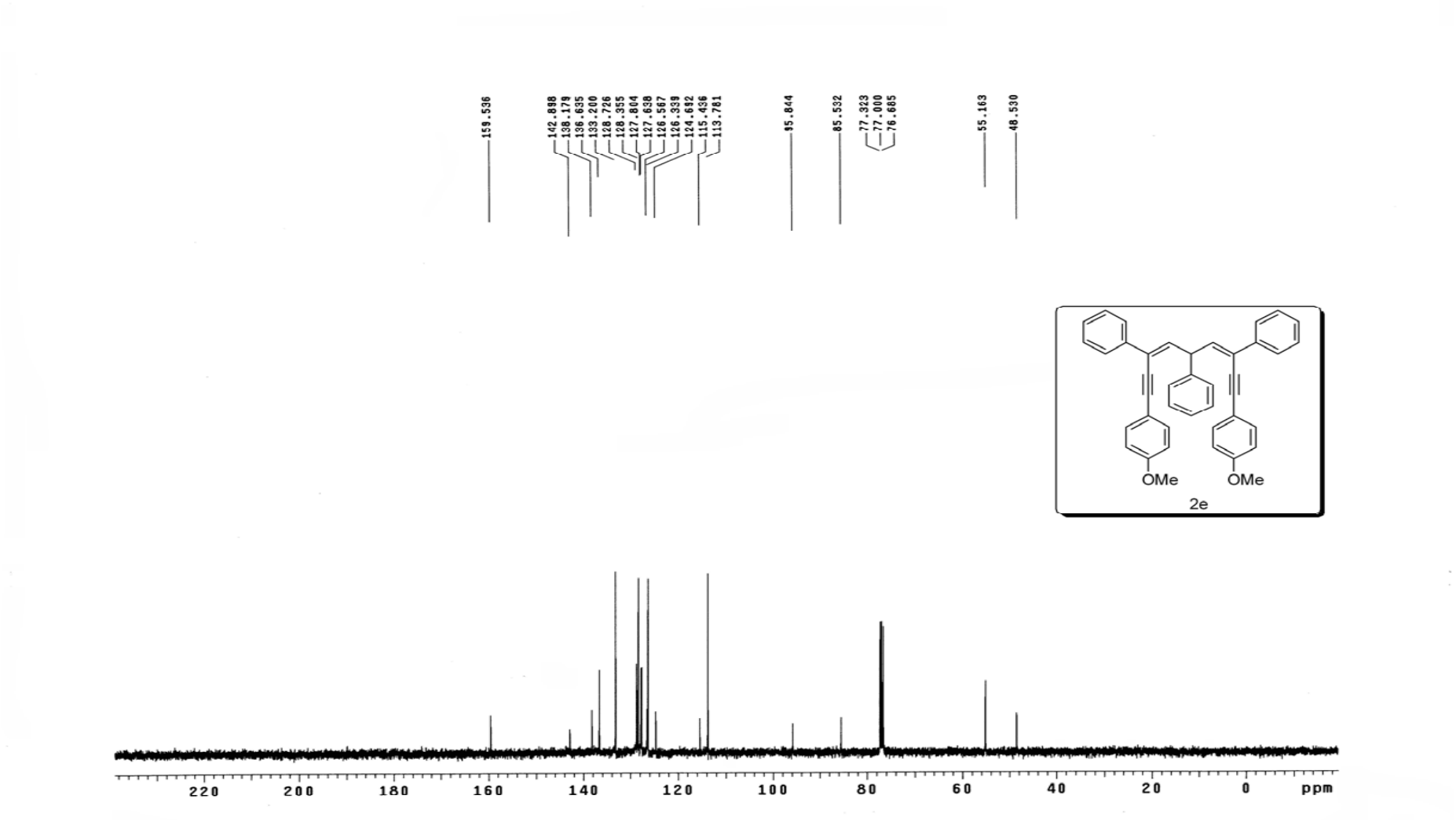
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OMe
2e
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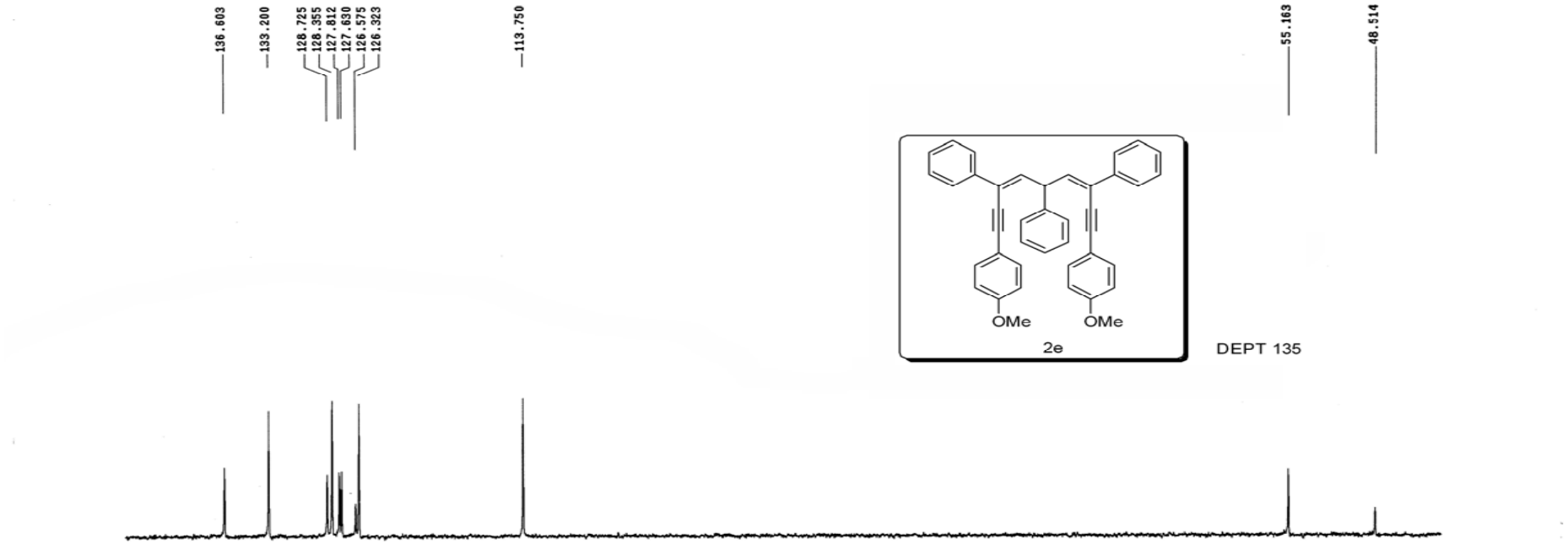
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OMe
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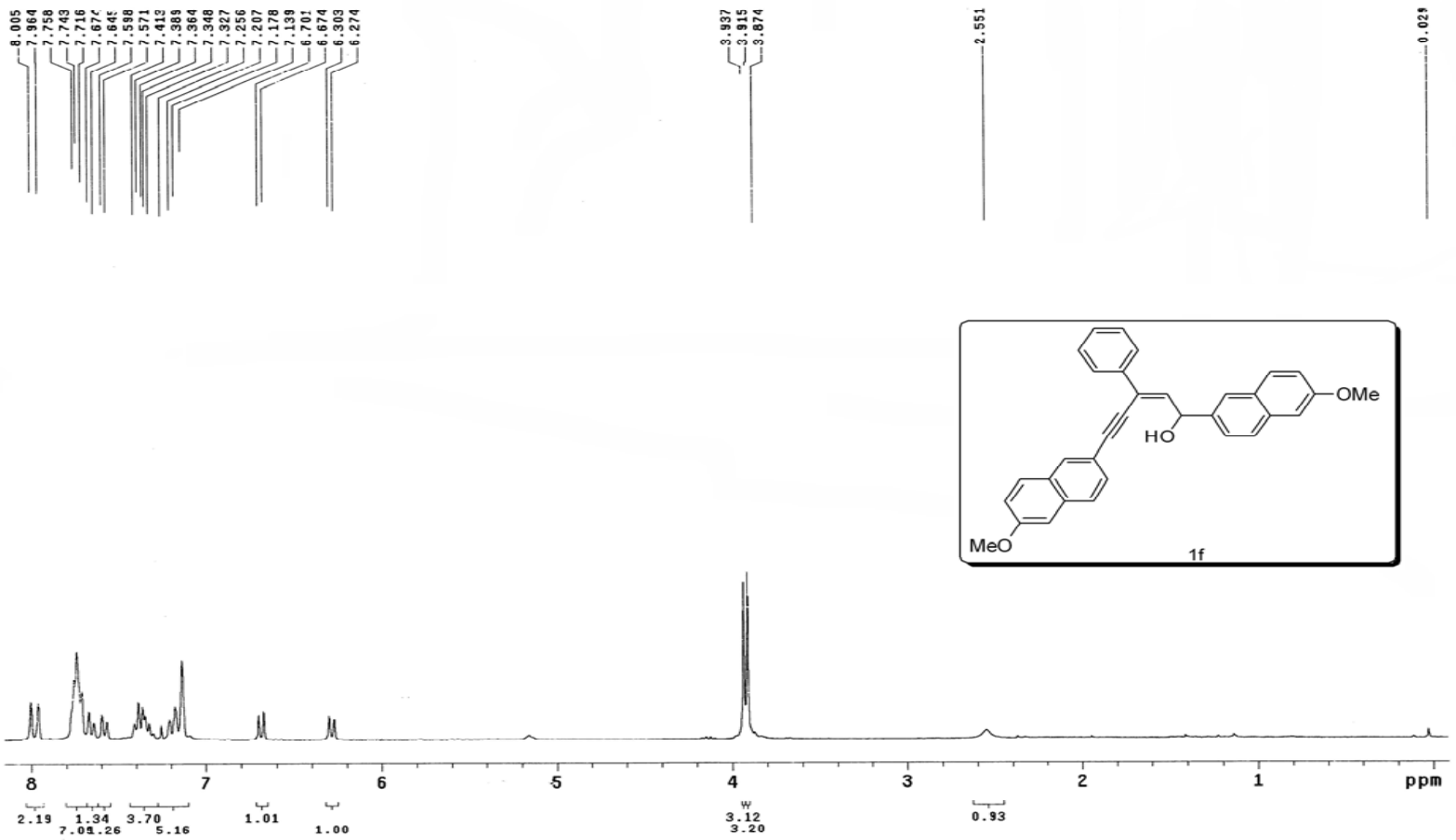
DEPT 135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HO
MeO
1f
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7
6
5
4
3
2
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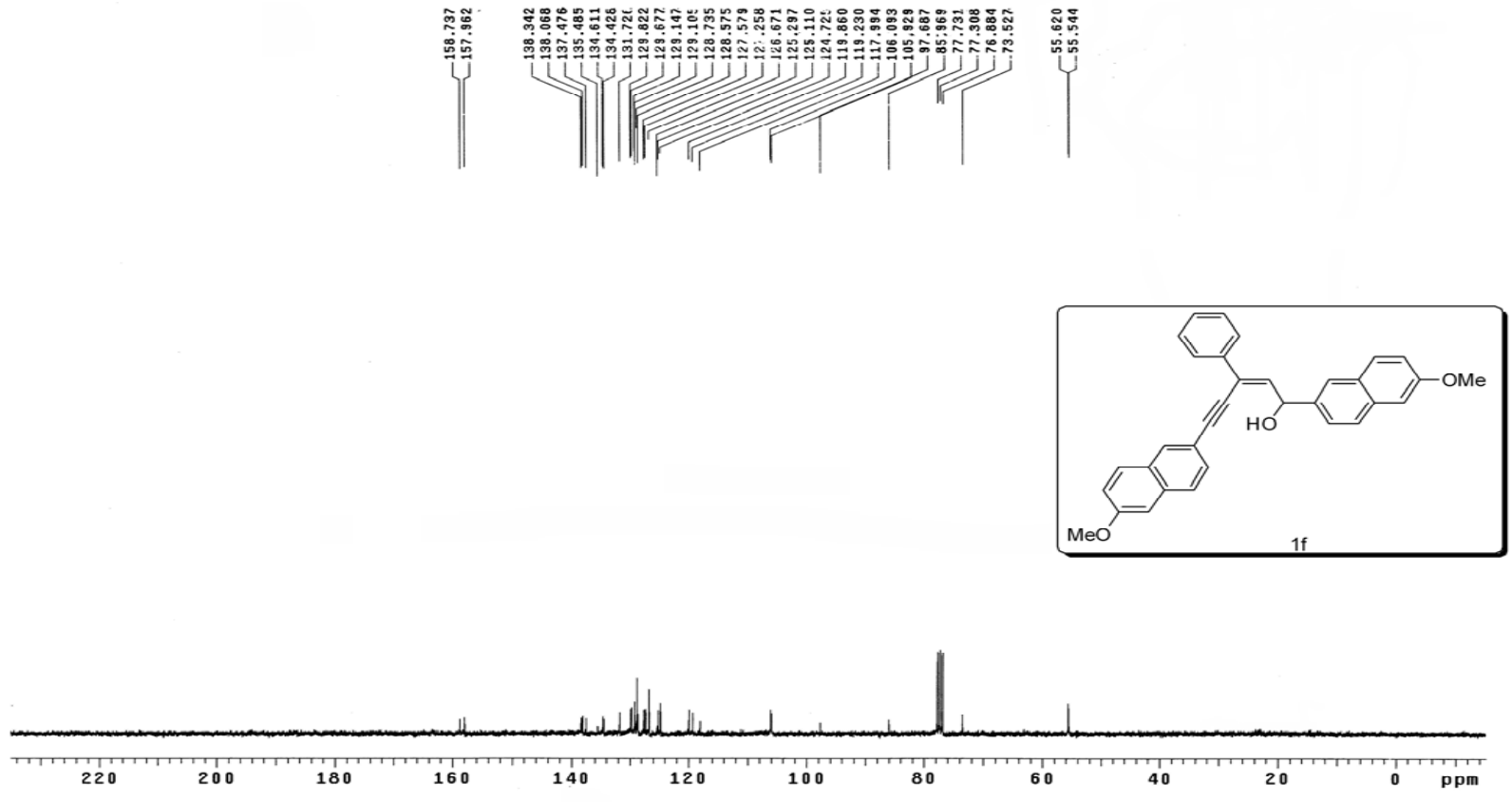
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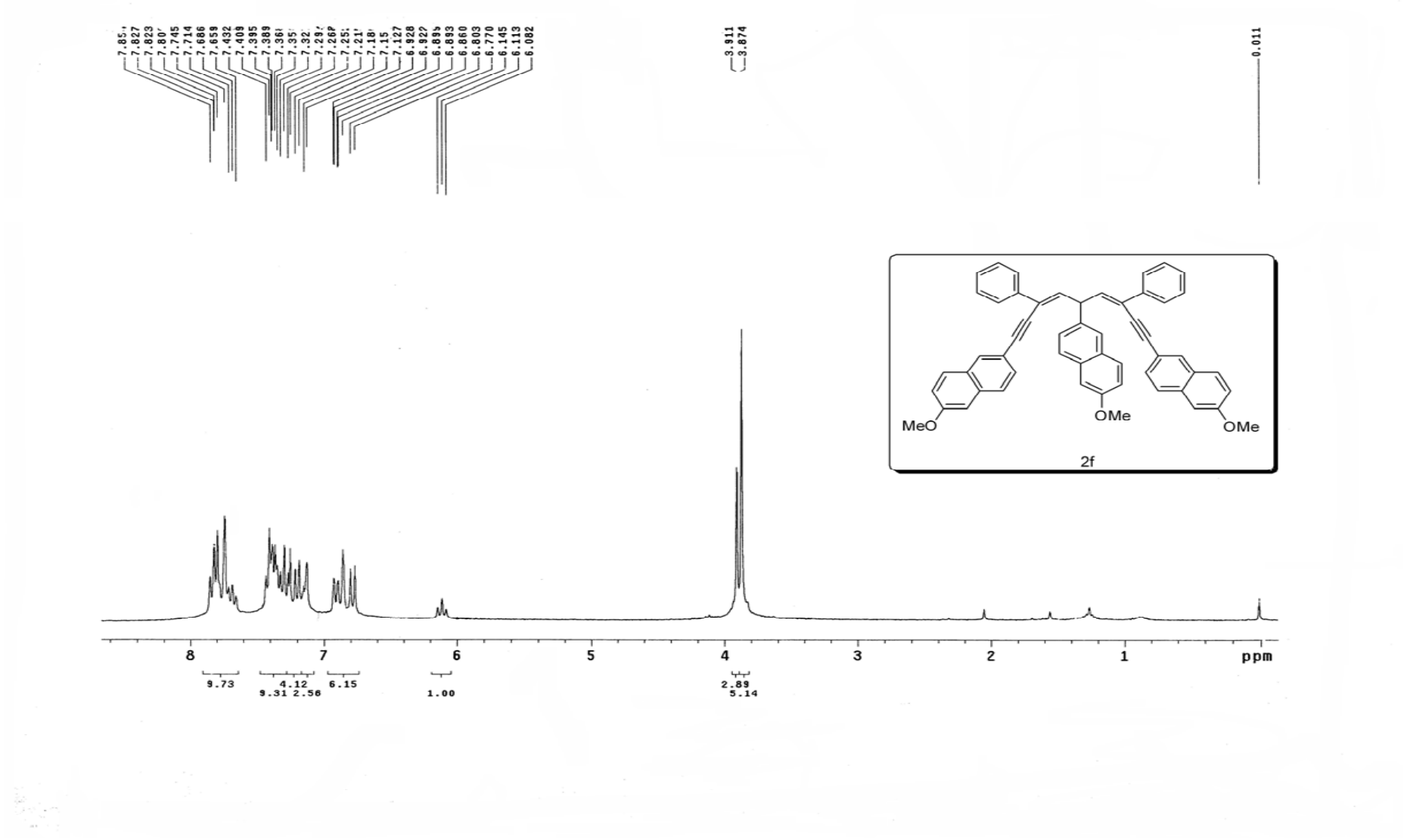
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OMe
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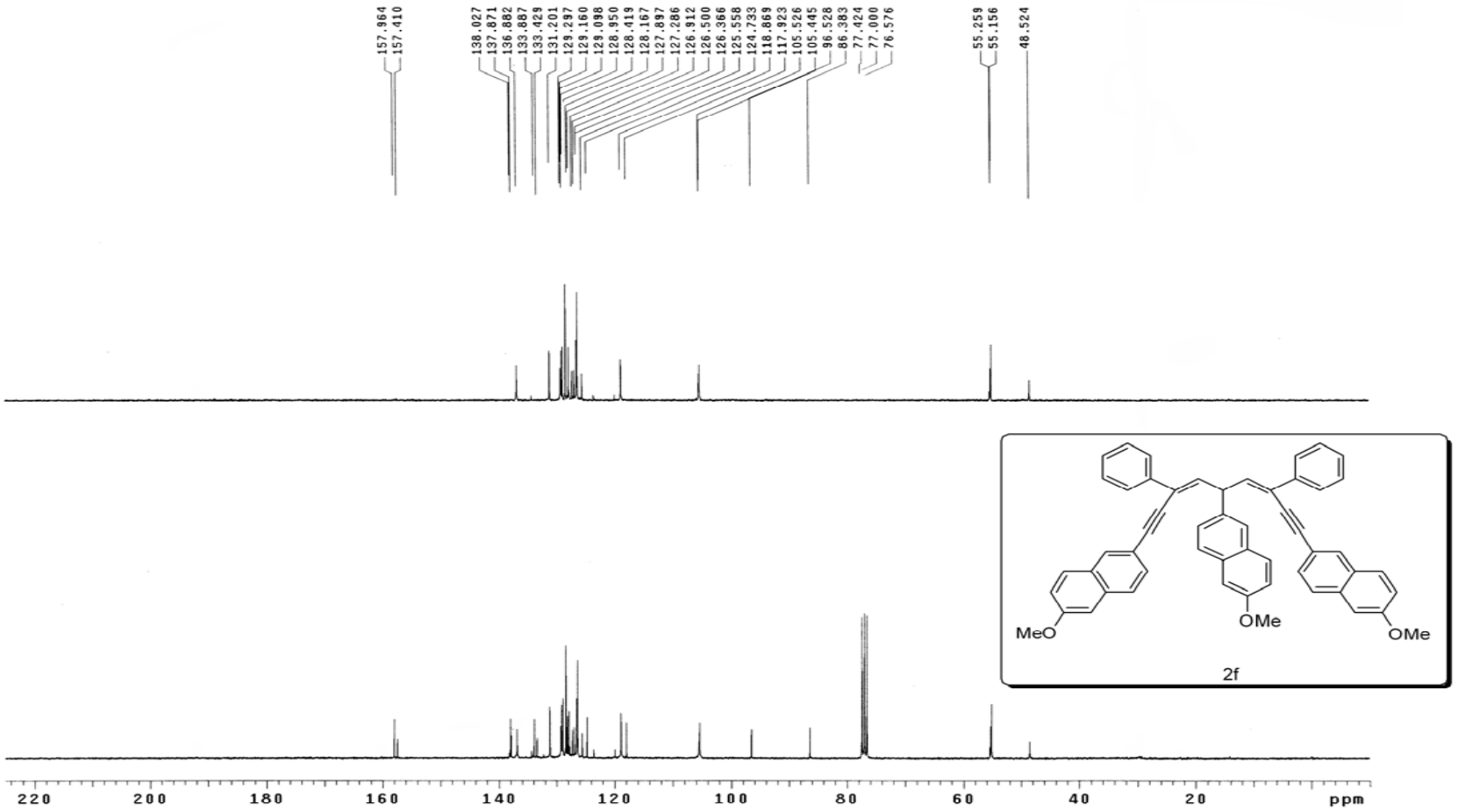
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OMe
OMe
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20
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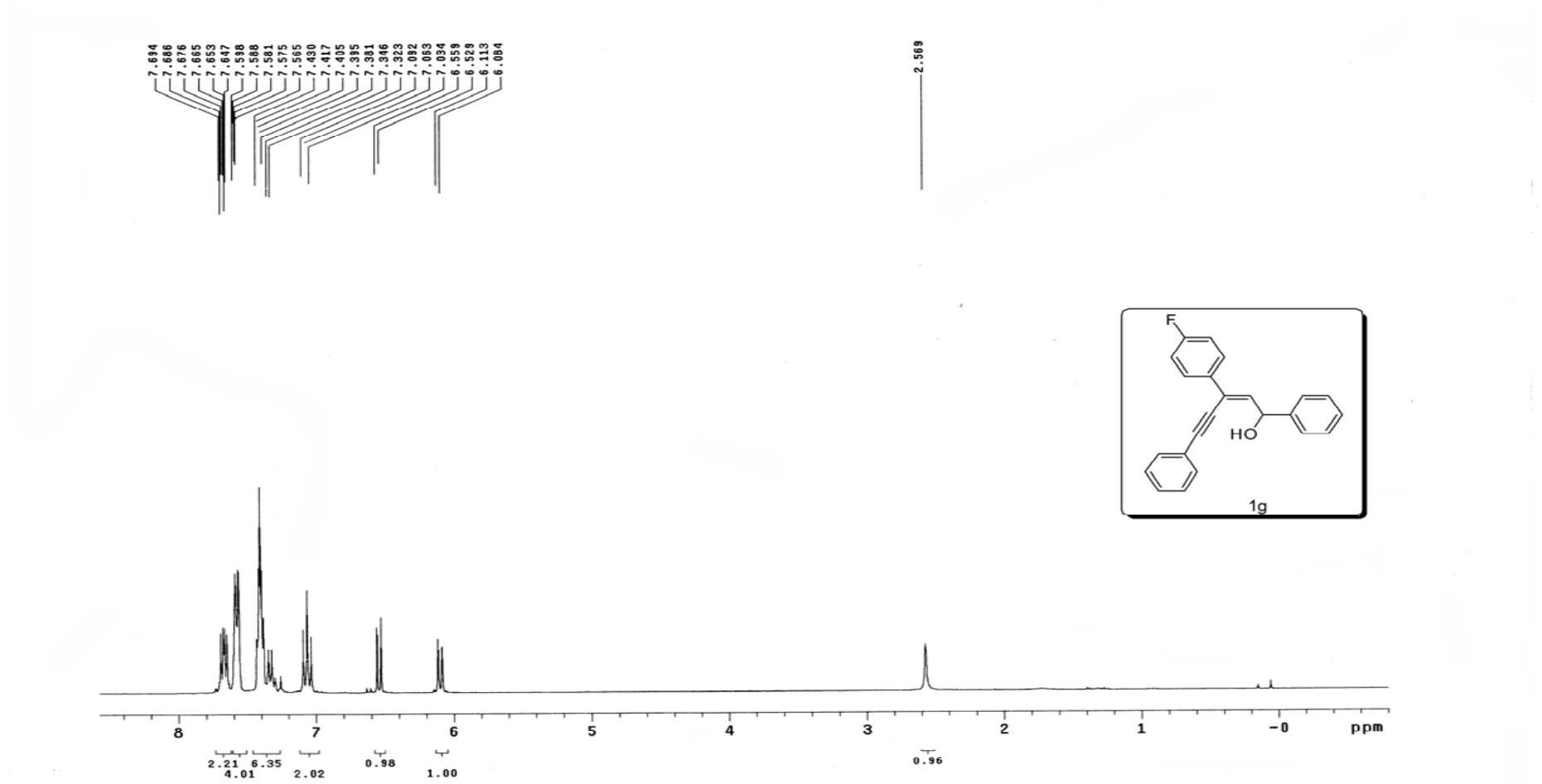
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1g
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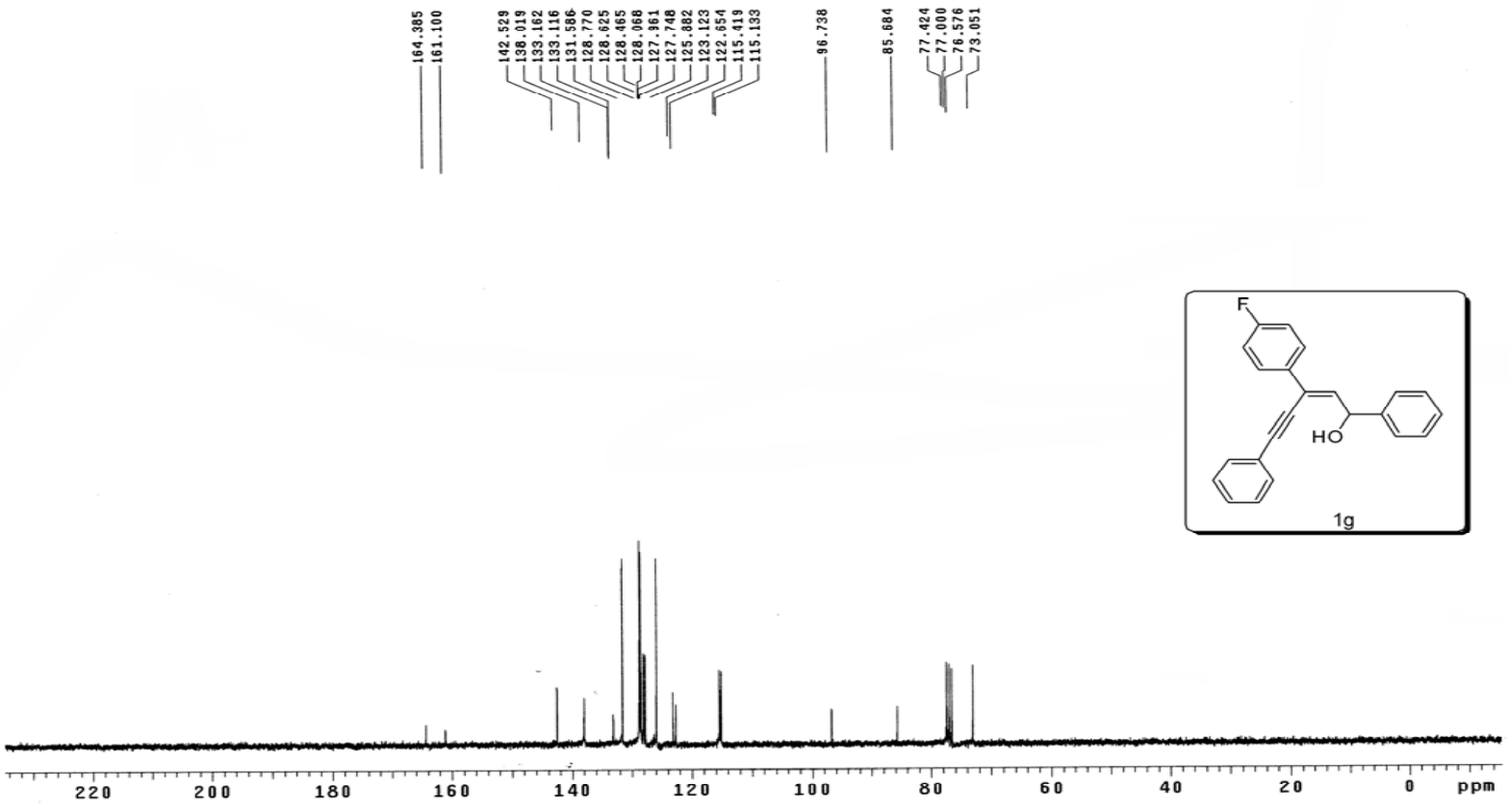
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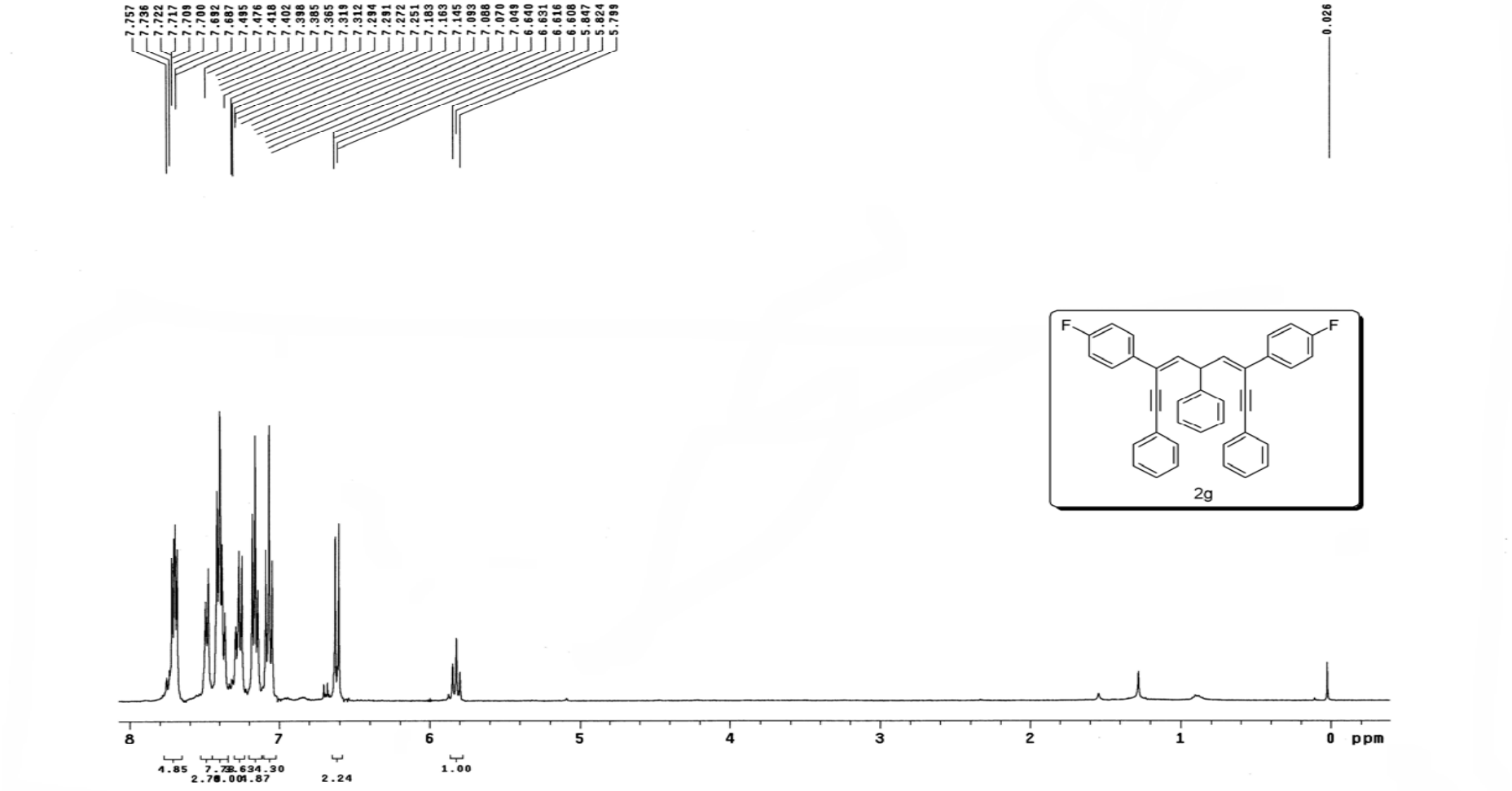
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6.631
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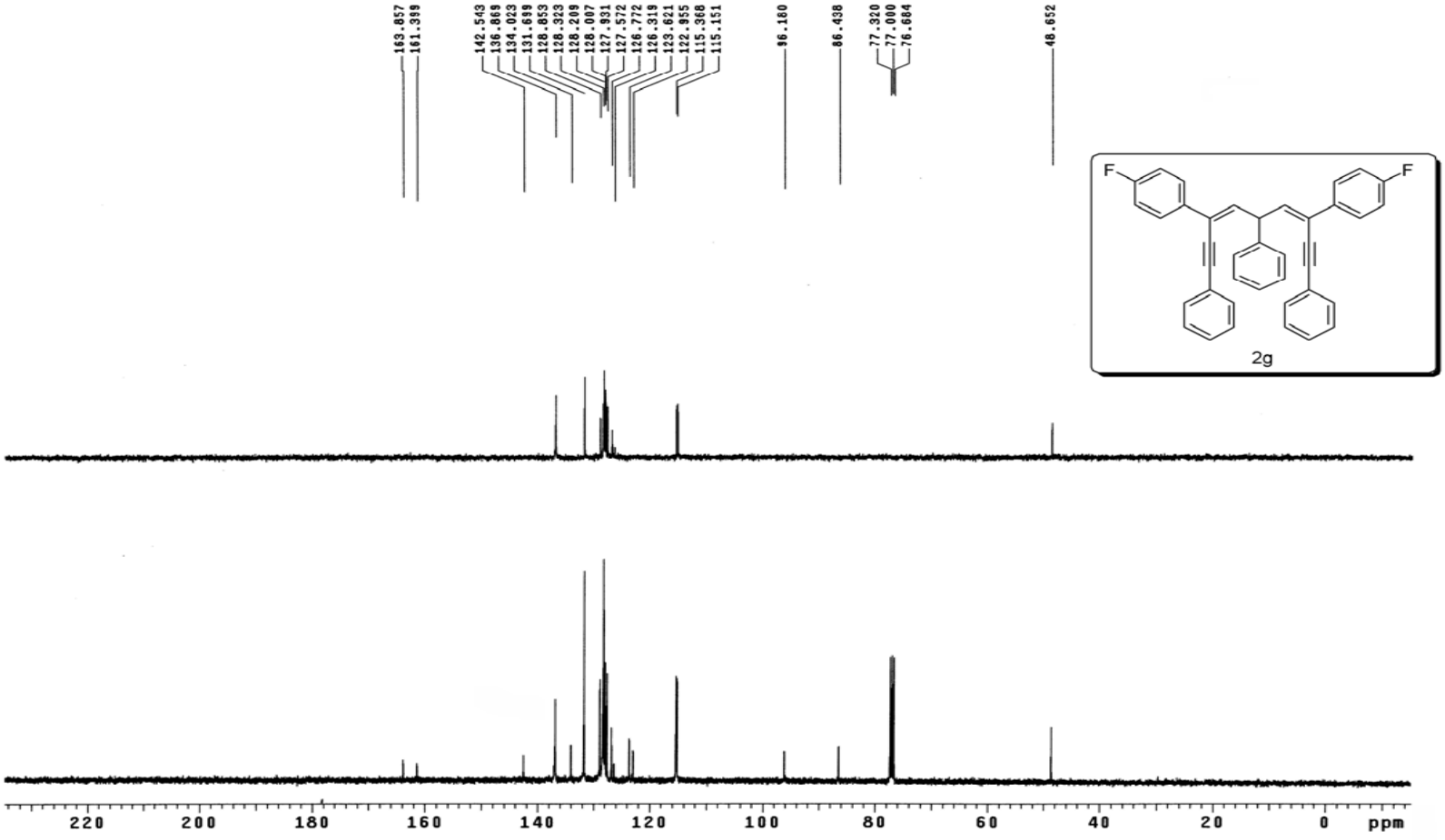
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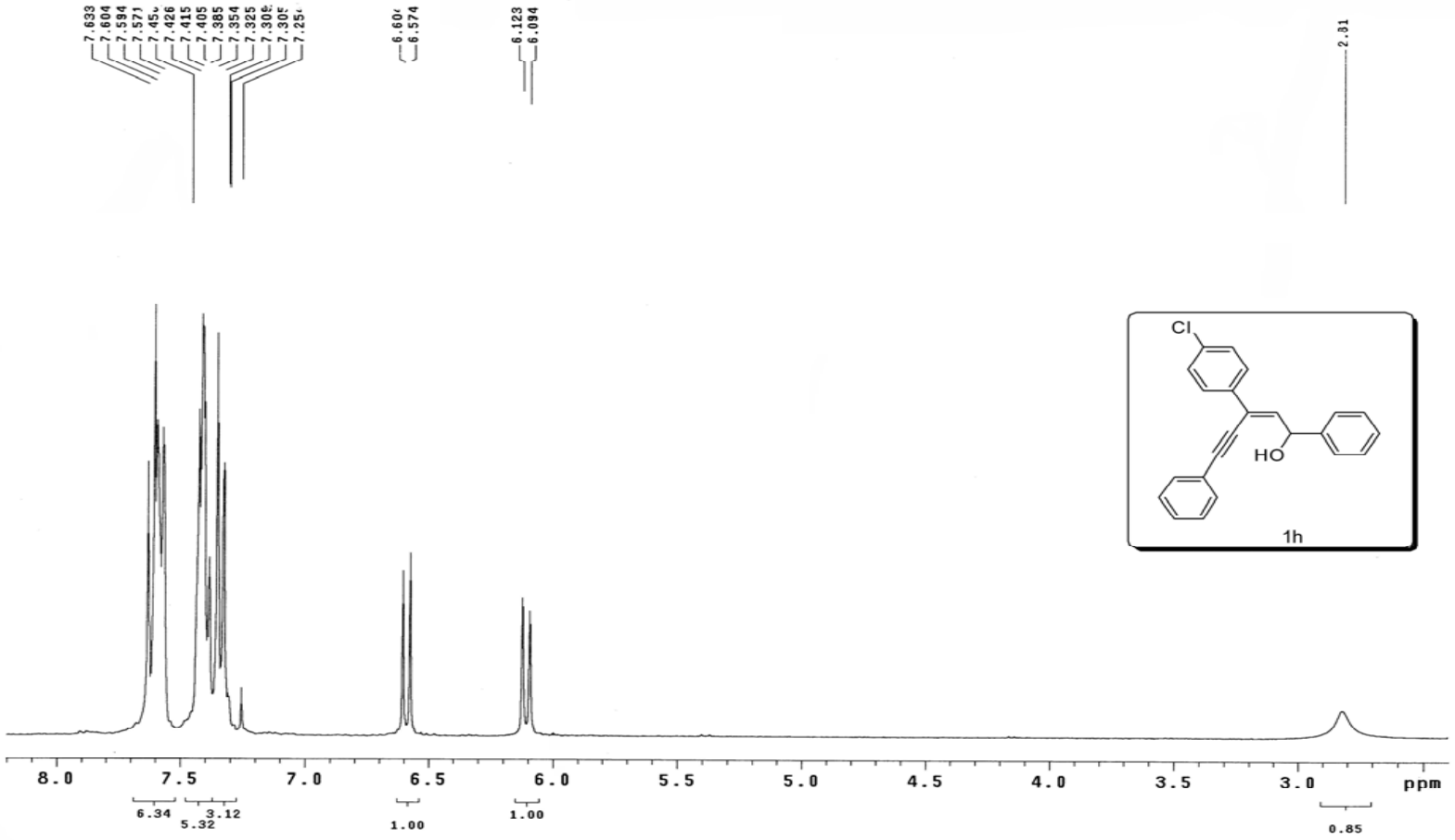
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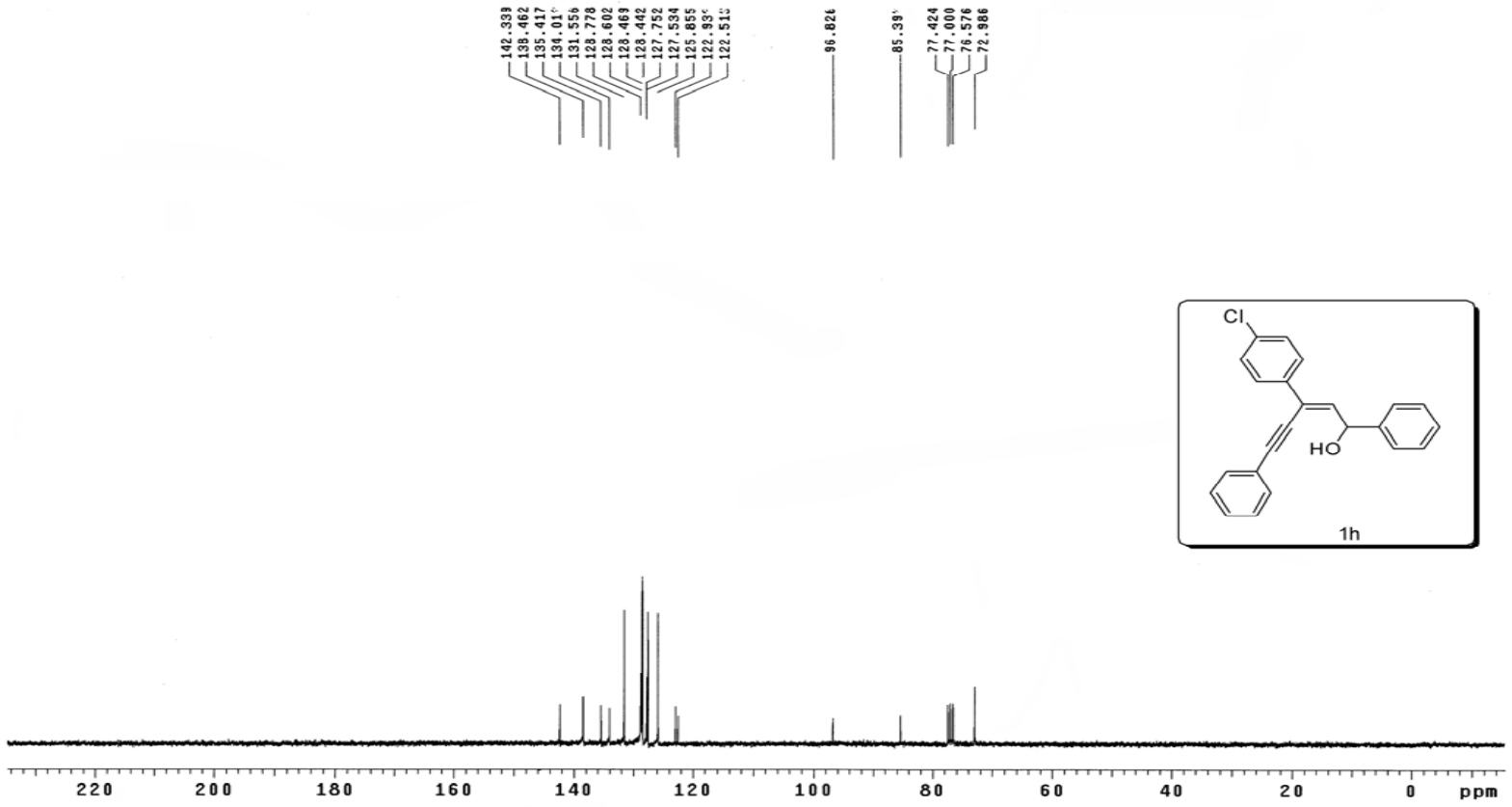
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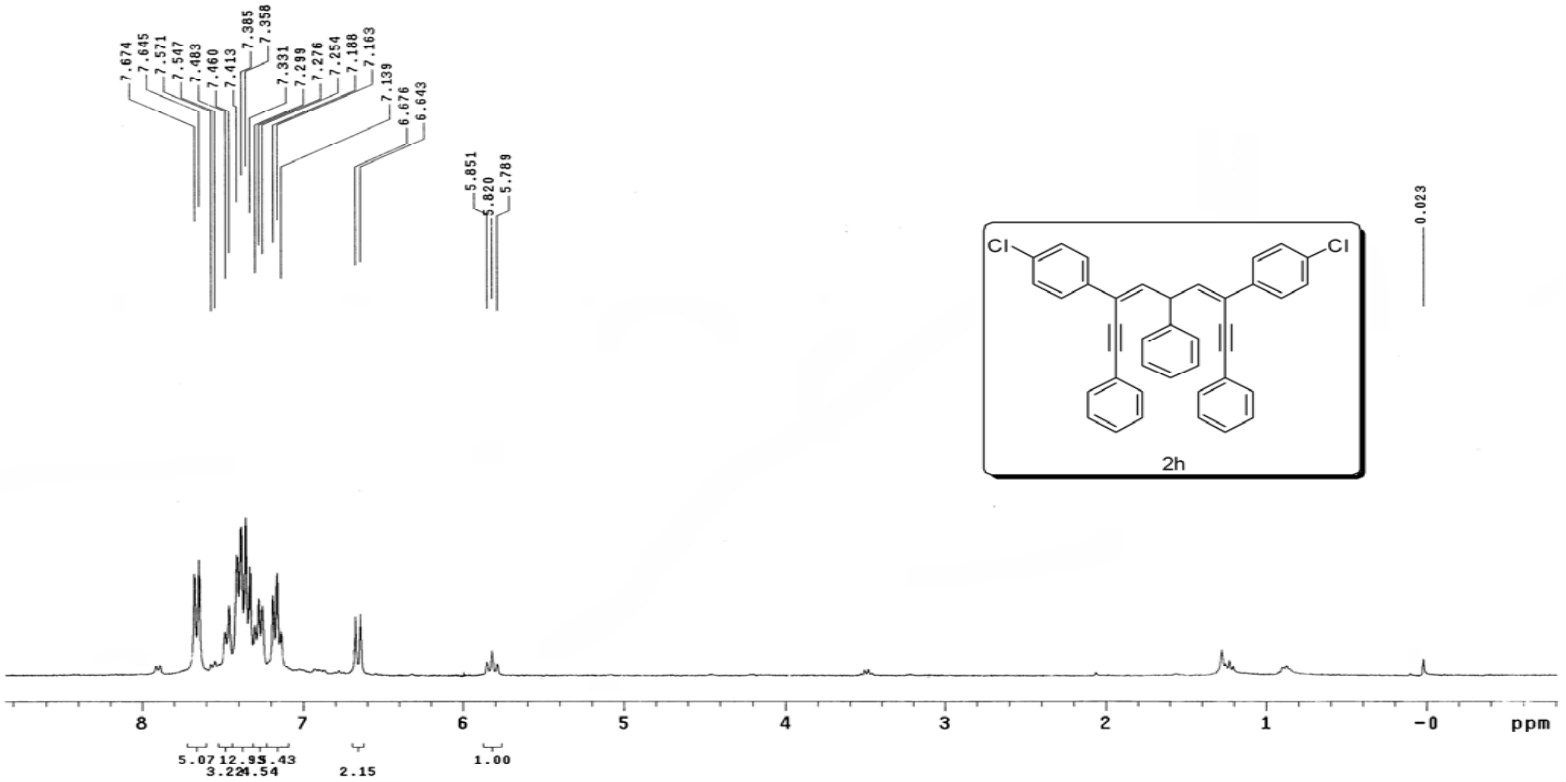
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Cl
Cl
2h
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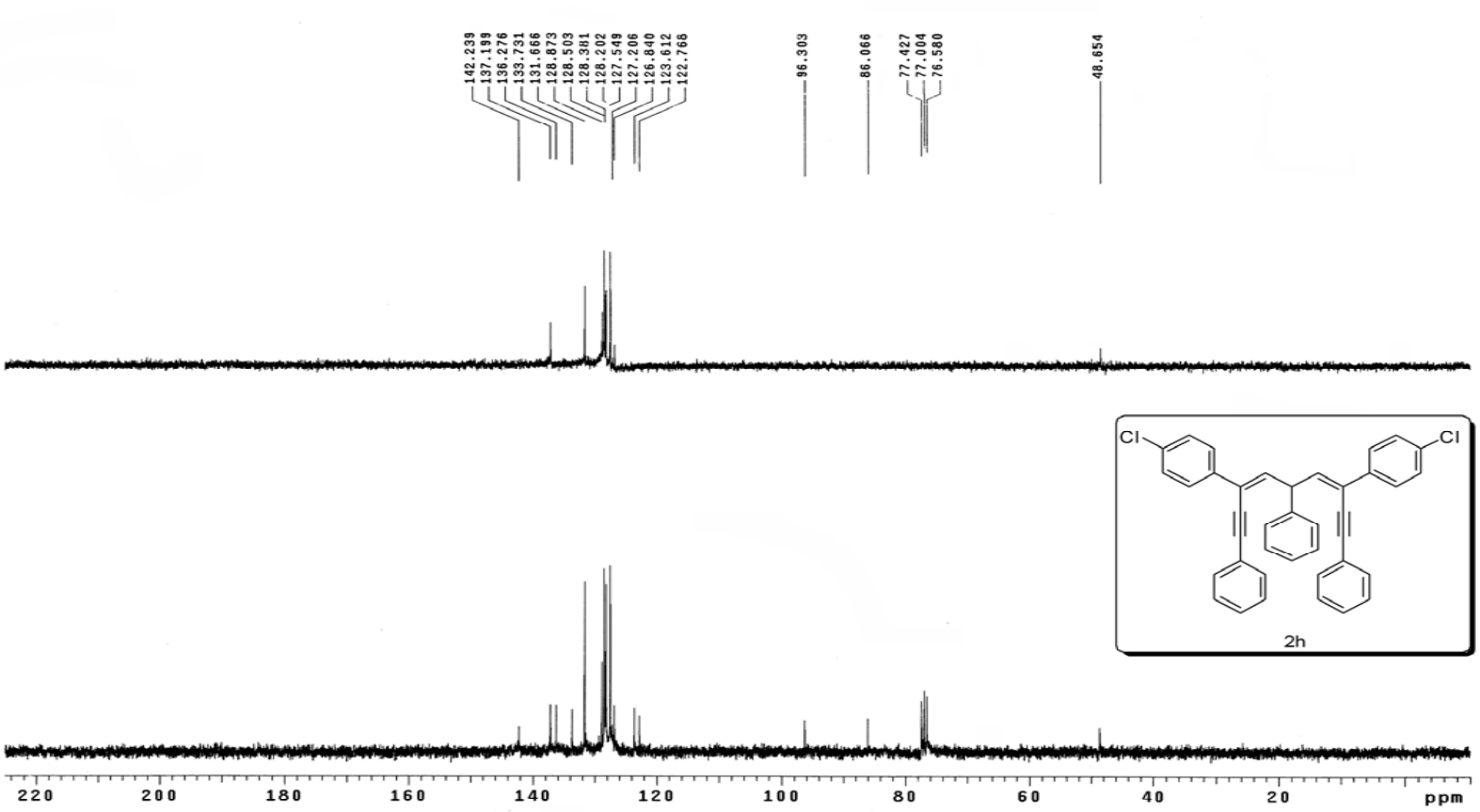
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Cl
Cl
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180
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100
80
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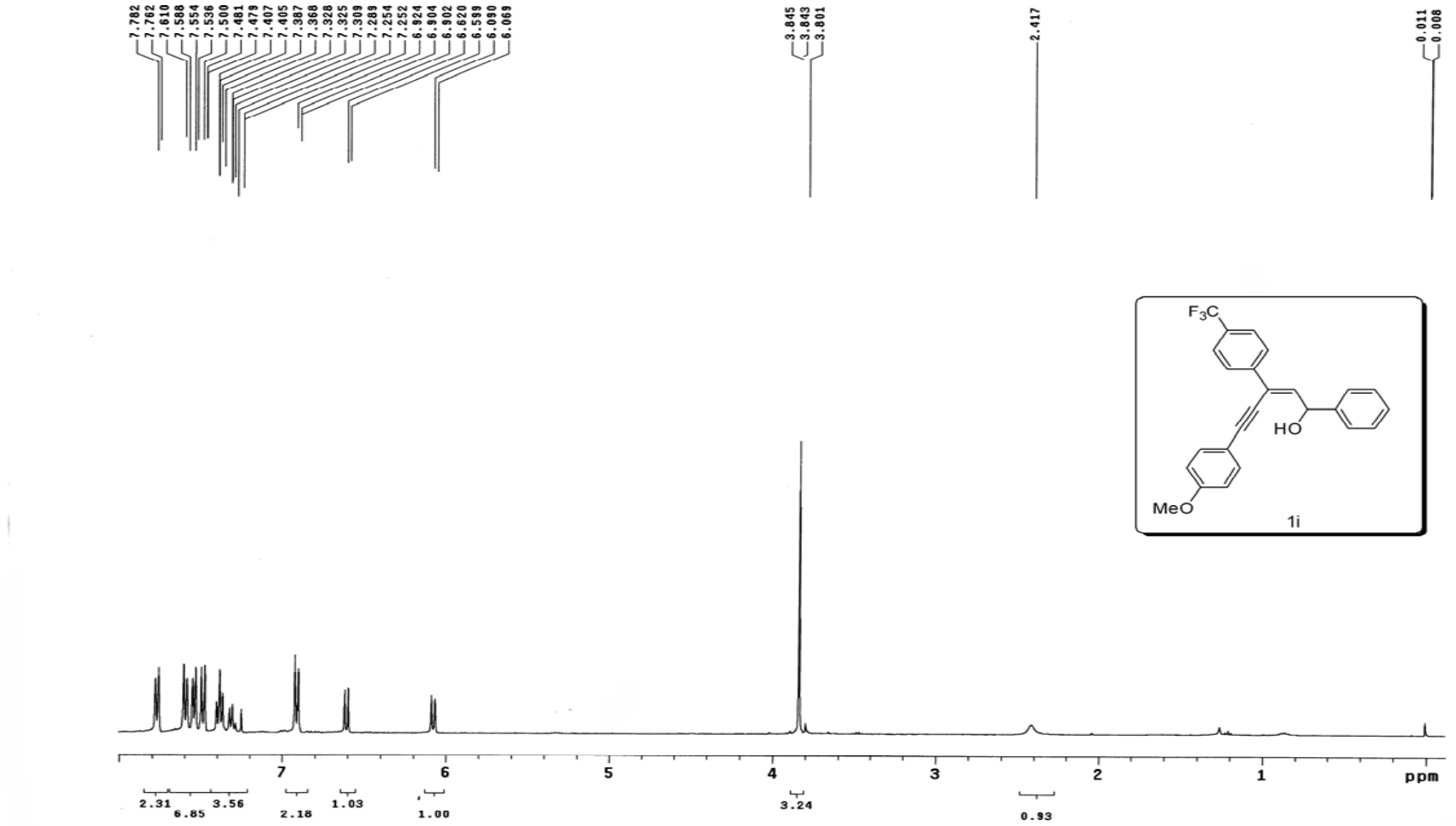
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7.554
7.536
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7.481
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7.407
7.405
7.387
7.368
7.328
7.325
7.309
7.289
7.254
7.252
6.924
6.904
6.902
6.620
6.599
6.090
6.069
3.845
3.843
3.801
2.417
0.011
0.008
F3C
HO
MeO
1i
7
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2
1
ppm
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6.85
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2.18
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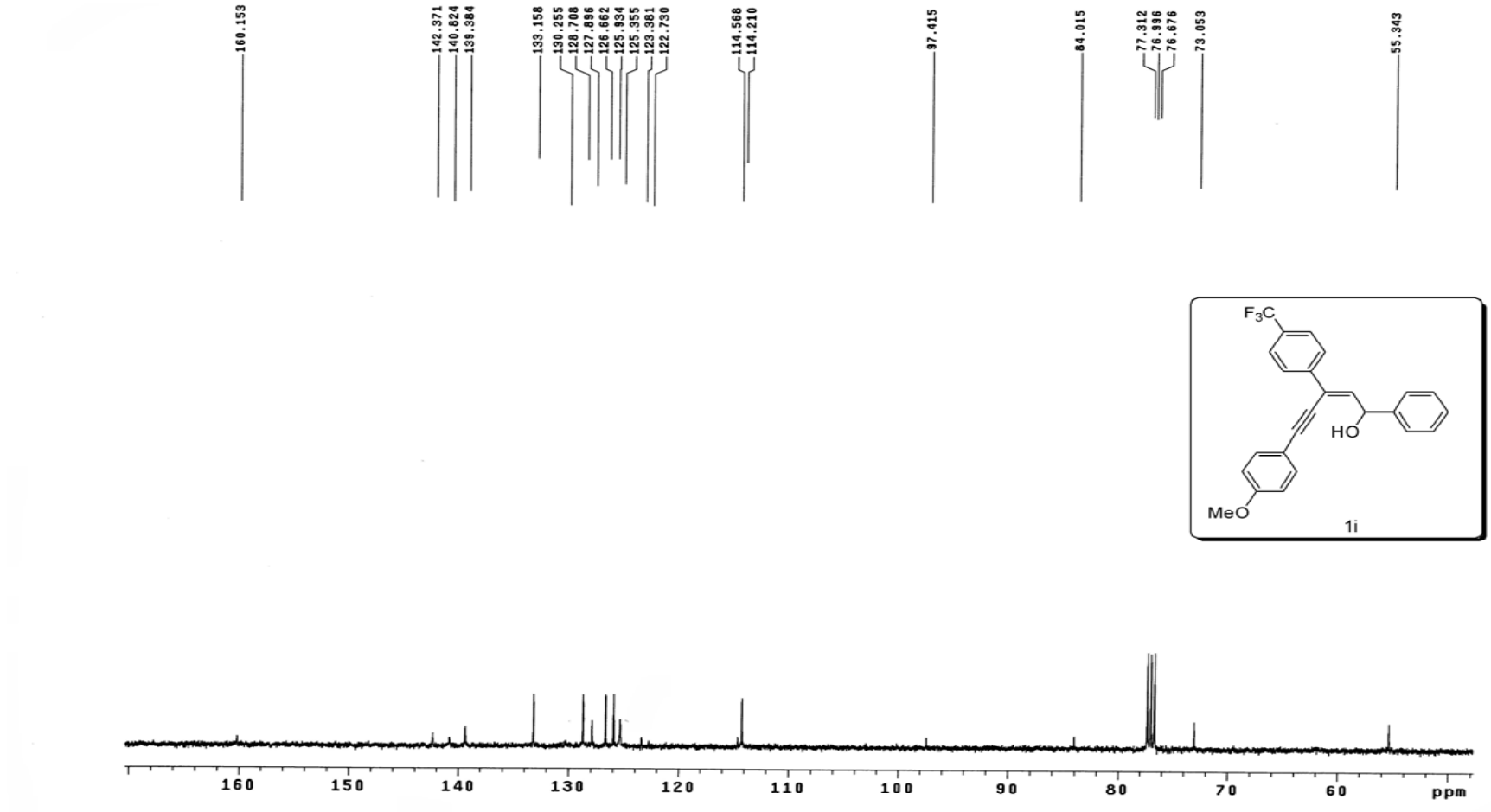
3.24
0.93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125.355
123.381
122.730
114.568
114.210
97.415
84.015
77.312
76.996
76.676
73.053
55.343
F3C
HO
MeO
1i
160
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120
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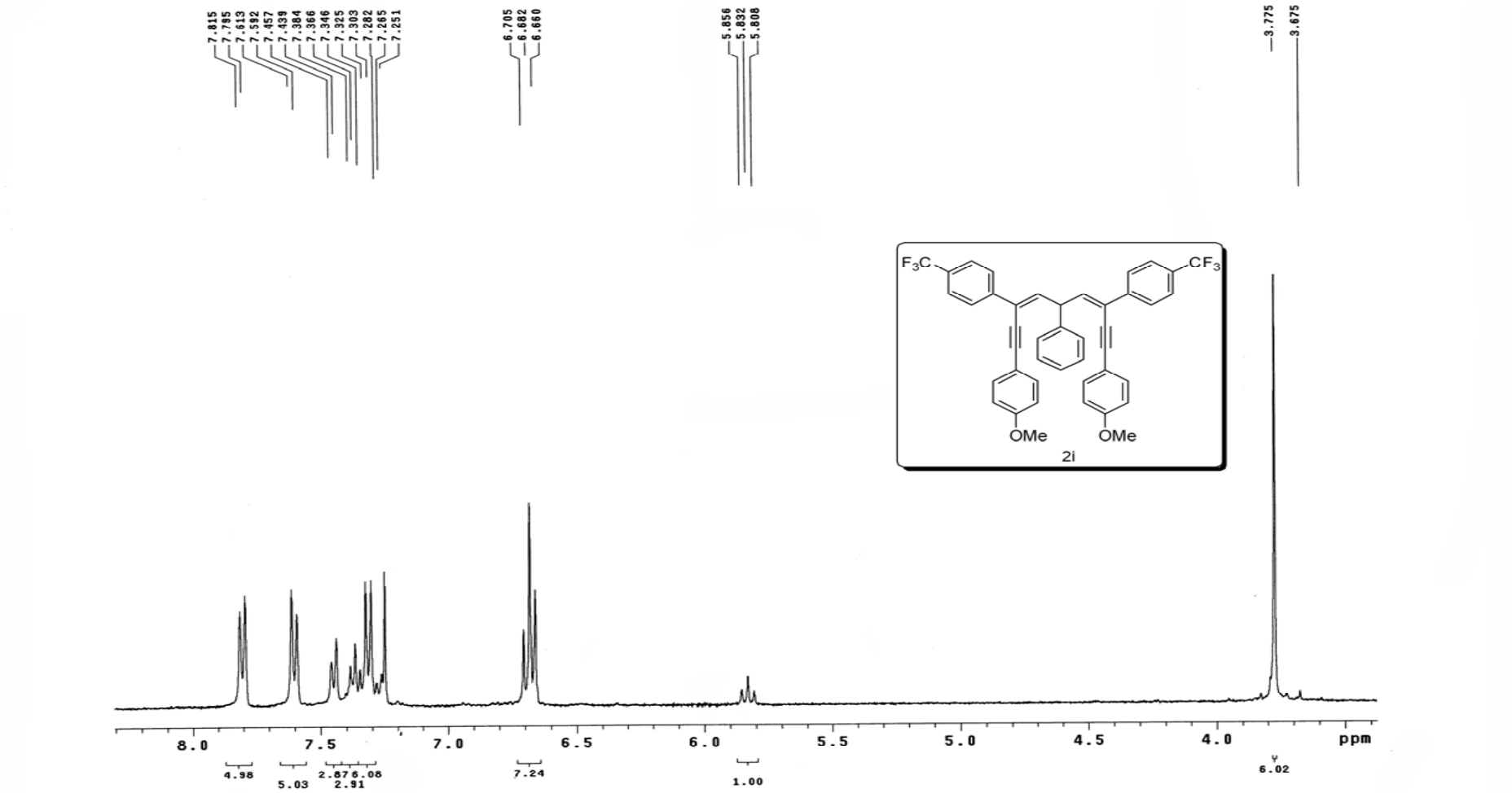
80
70
60
ppm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7.592
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7.439
7.384
7.366
7.346
7.325
7.303
7.282
7.265
7.251
6.705
6.682
6.660
5.856
5.832
5.808
3.775
3.675
F3C
CF3
OMe
OMe
2i
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
ppm
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6.08
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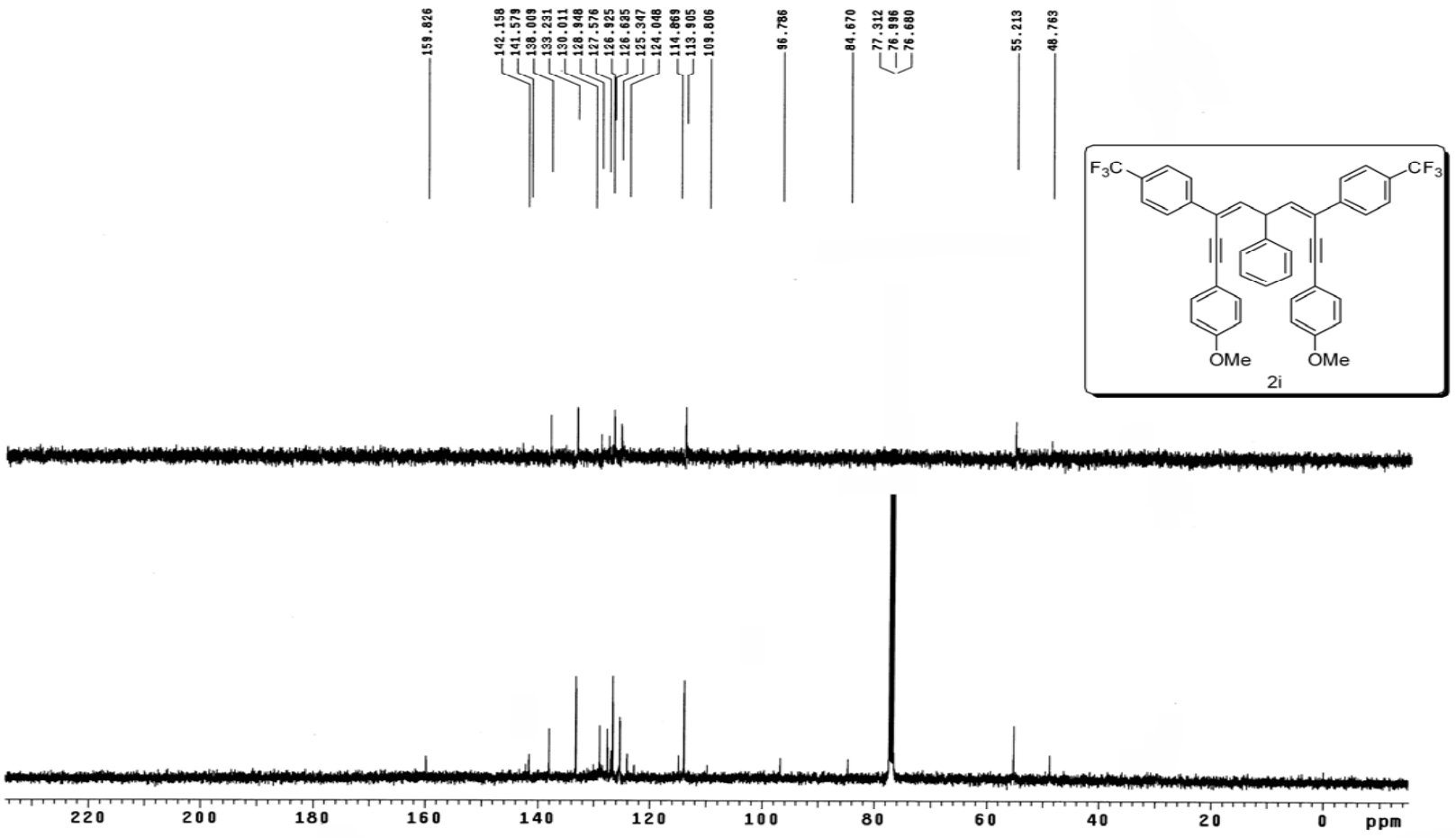
1.00
6.02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138.009
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127.576
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125.347
124.048
114.869
113.905
109.806
96.786
84.670
77.312
76.996
76.680
55.213
48.763
F3C
CF3
OMe
OMe
2i
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200
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160
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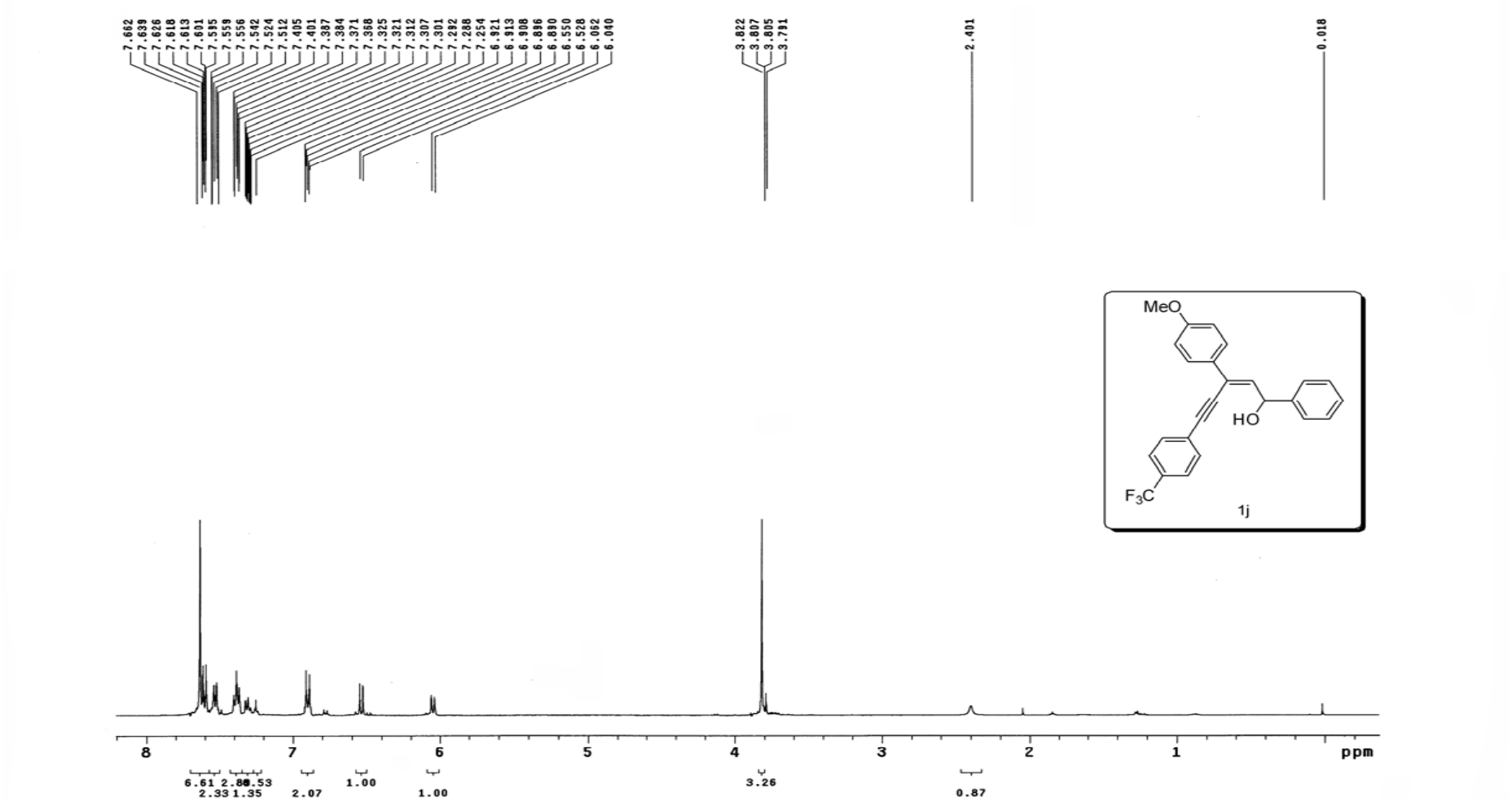
120
100
80
60
40
20
0
ppm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7.613
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7.595
7.559
7.556
7.542
7.524
7.512
7.405
7.401
7.387
7.384
7.371
7.368
7.325
7.321
7.312
7.307
7.301
7.292
7.288
7.254
6.921
6.913
6.908
6.886
6.880
6.550
6.528
6.062
6.040
3.822
3.807
3.805
3.791
2.401
0.018
MeO
HO
F3C
1j
8
7
6
5
4
3
2
1
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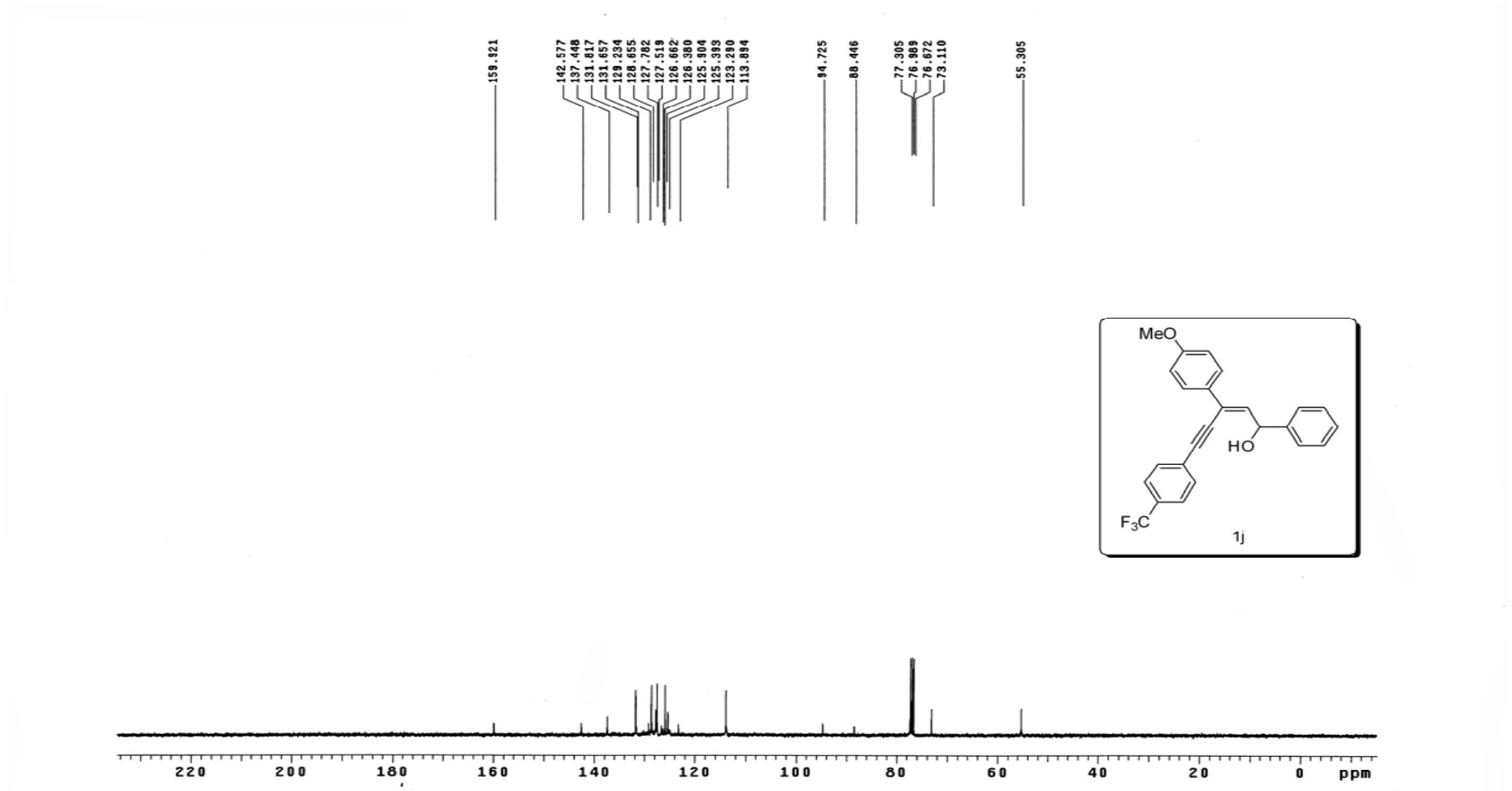
0.87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126.380
125.904
125.393
123.290
113.894
94.725
88.446
77.305
76.989
76.672
73.110
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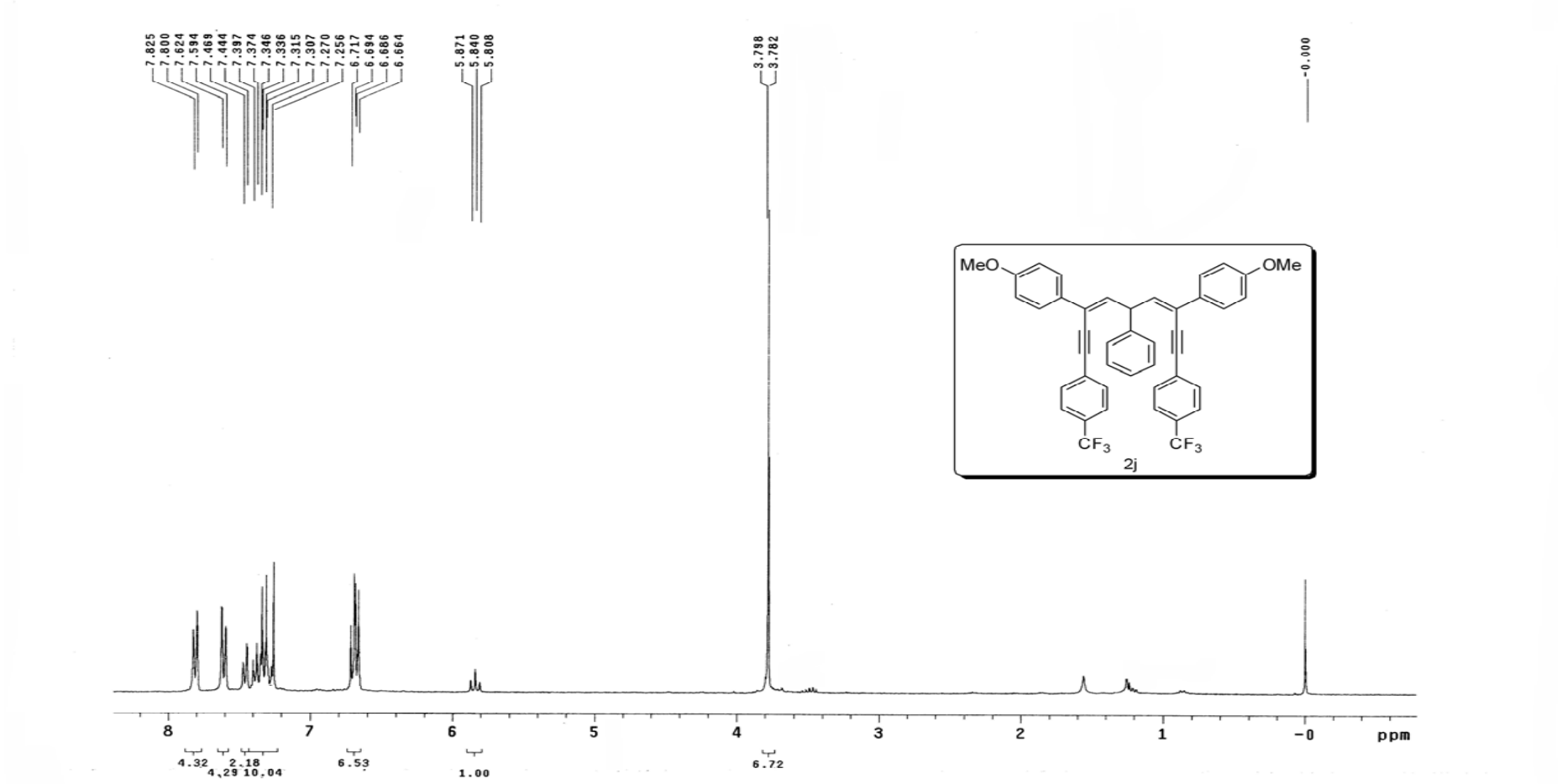
MeO
HO
F3C
1j
220
200
180
160
140
120
100
80
60
40
20
0
ppm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7.594
7.469
7.444
7.397
7.374
7.346
7.336
7.315
7.307
7.270
7.256
6.717
6.694
6.686
6.664
5.871
5.840
5.808
3.798
3.782
-0.000
MeO
OMe
CF3
CF3
2j
8
7
6
5
4
3
2
1
-0
ppm
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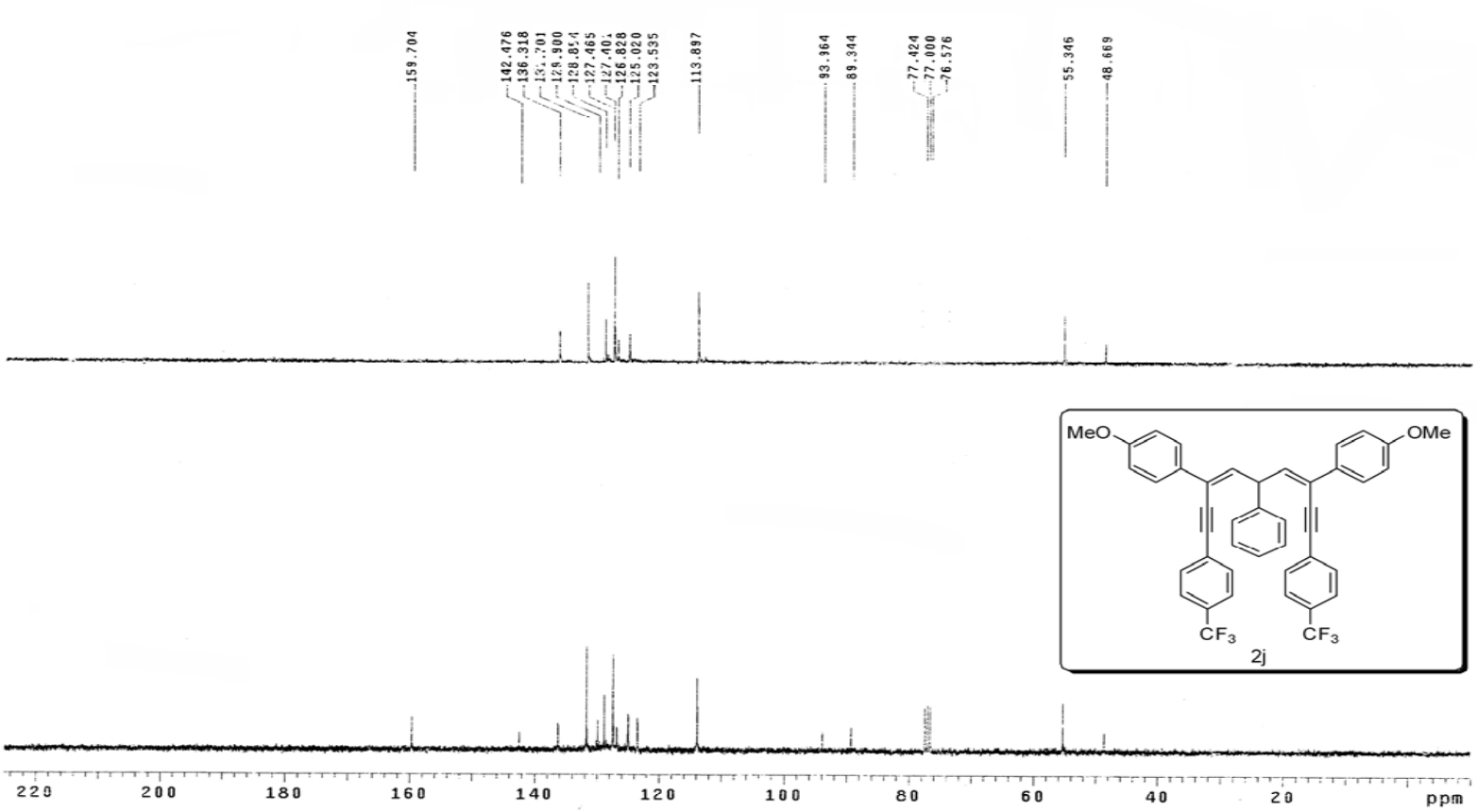
2.18
4.29
10.04
6.53
1.00
6.72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89.344
77.424
77.000
76.576
55.346
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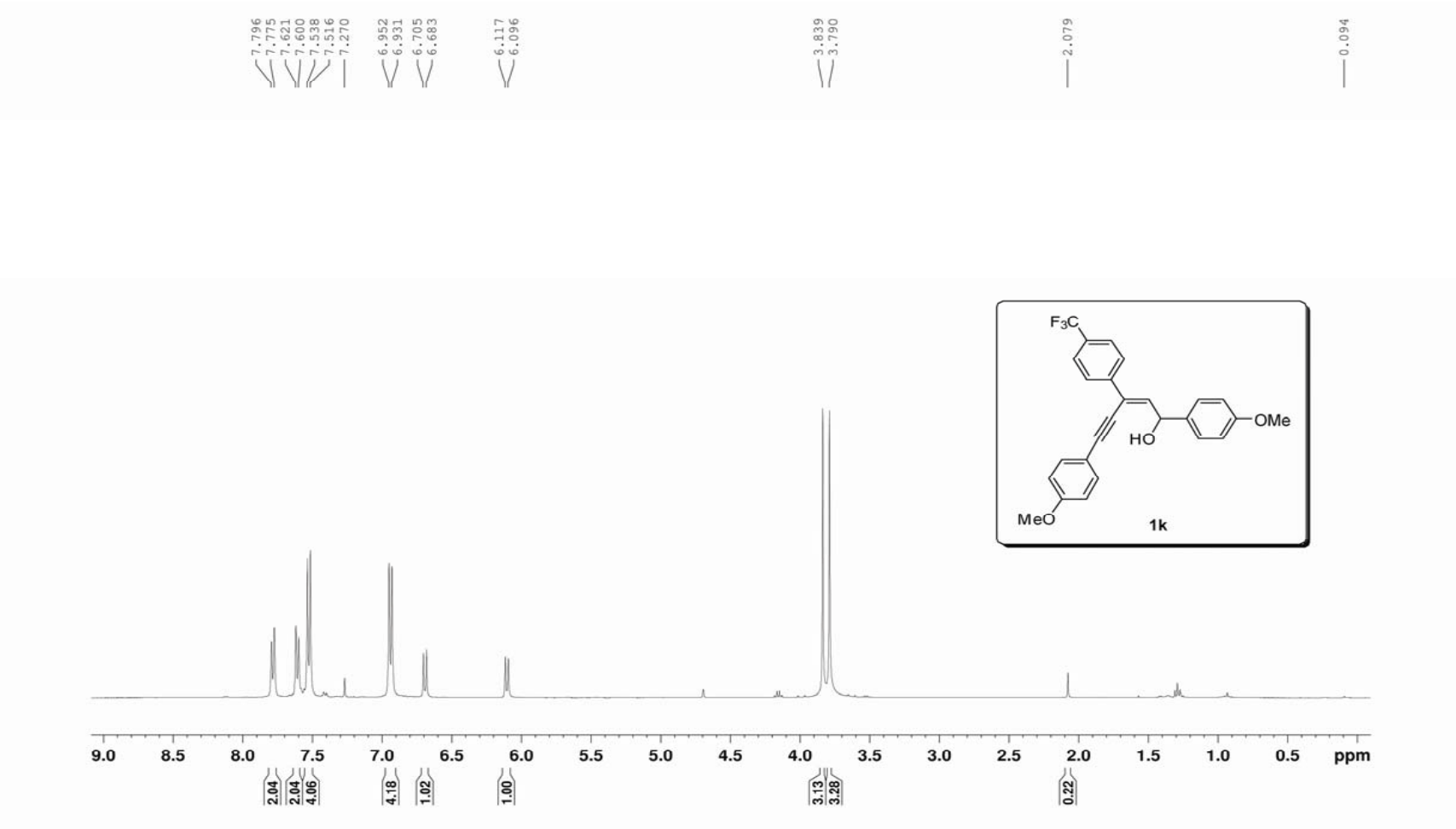
MeO
OMe
CF3
CF3
2j
220
200
180
160
140
120
100
80
60
40
20
ppm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7.538
7.516
7.270
6.952
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6.705
6.683
6.117
6.096
3.839
3.790
2.079
0.094
F3C
OMe
HO
MeO
1k
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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ppm
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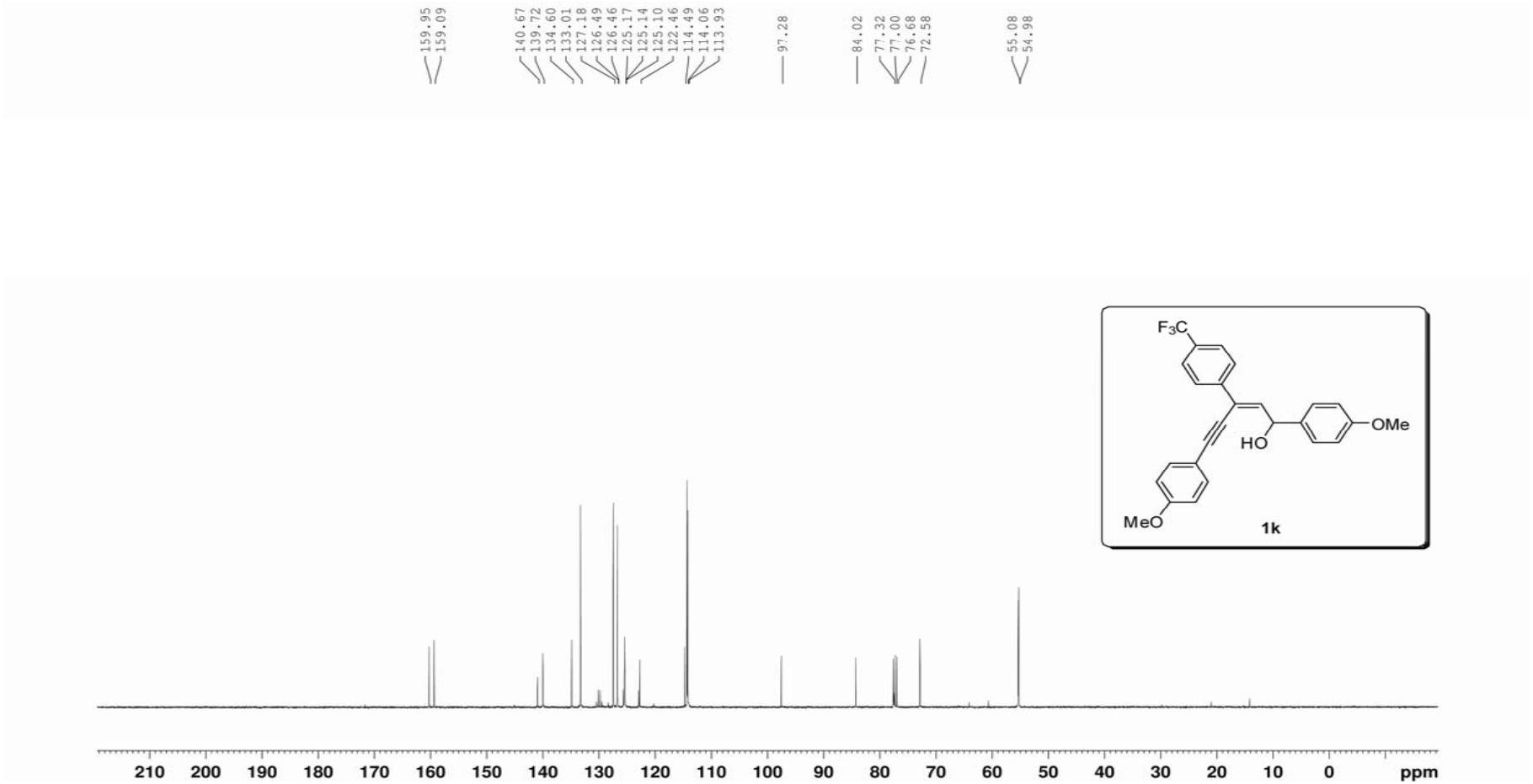
2.04
4.06
4.18
1.02
1.00
3.13
3.28
0.22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133.01
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126.49
126.46
125.17
125.14
125.10
122.46
114.49
114.06
113.93
97.28
84.02
77.32
77.00
76.68
72.58
55.08
54.98
F3C
OMe
HO
MeO
1k
210
200
190
180
170
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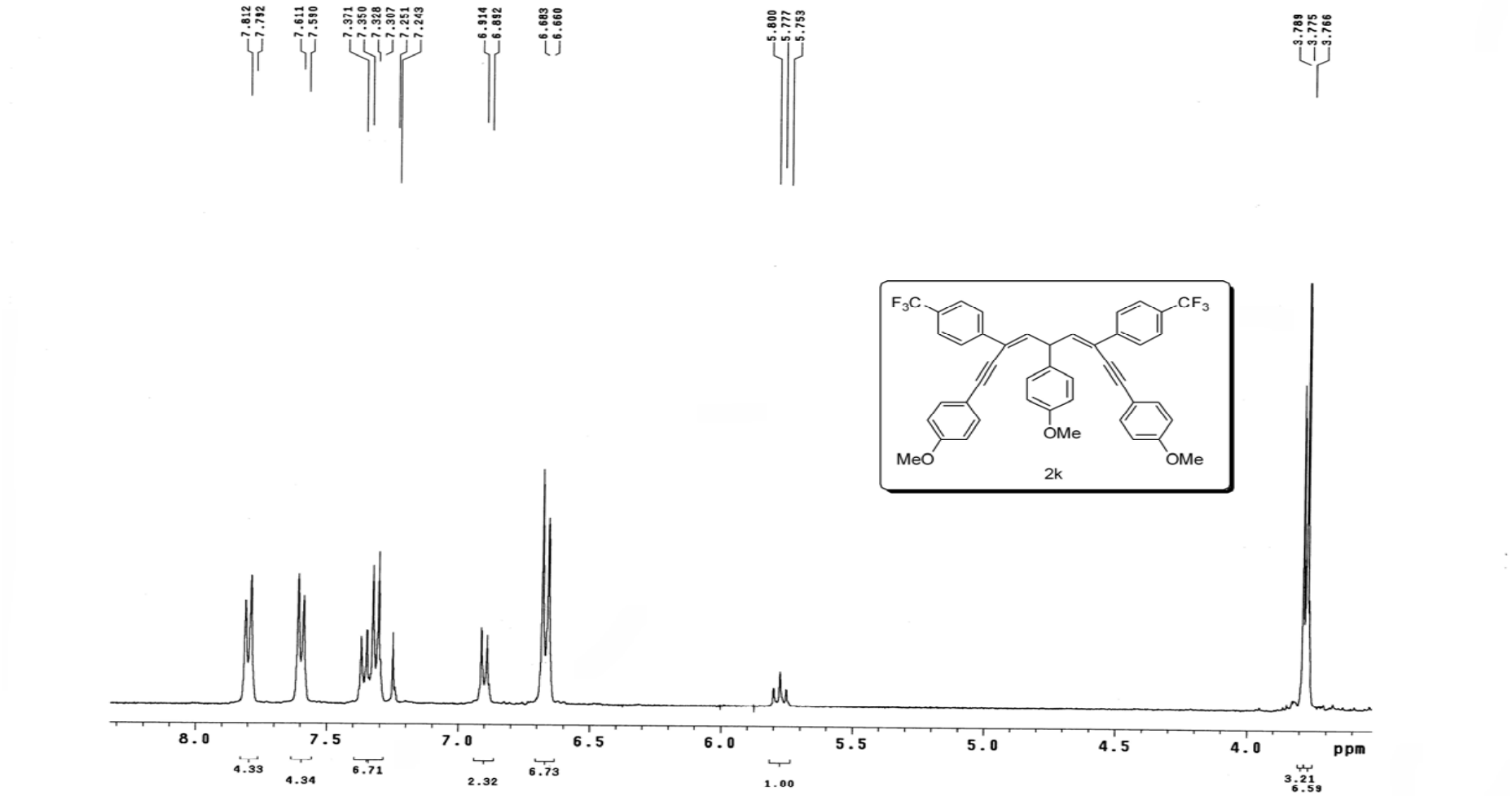
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.611
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7.350
7.328
7.307
7.251
7.243
6.914
6.892
6.683
6.660
5.800
5.777
5.753
3.789
3.775
3.766
F3C
CF3
OMe
MeO
OMe
2k
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
ppm
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4.34
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2.32
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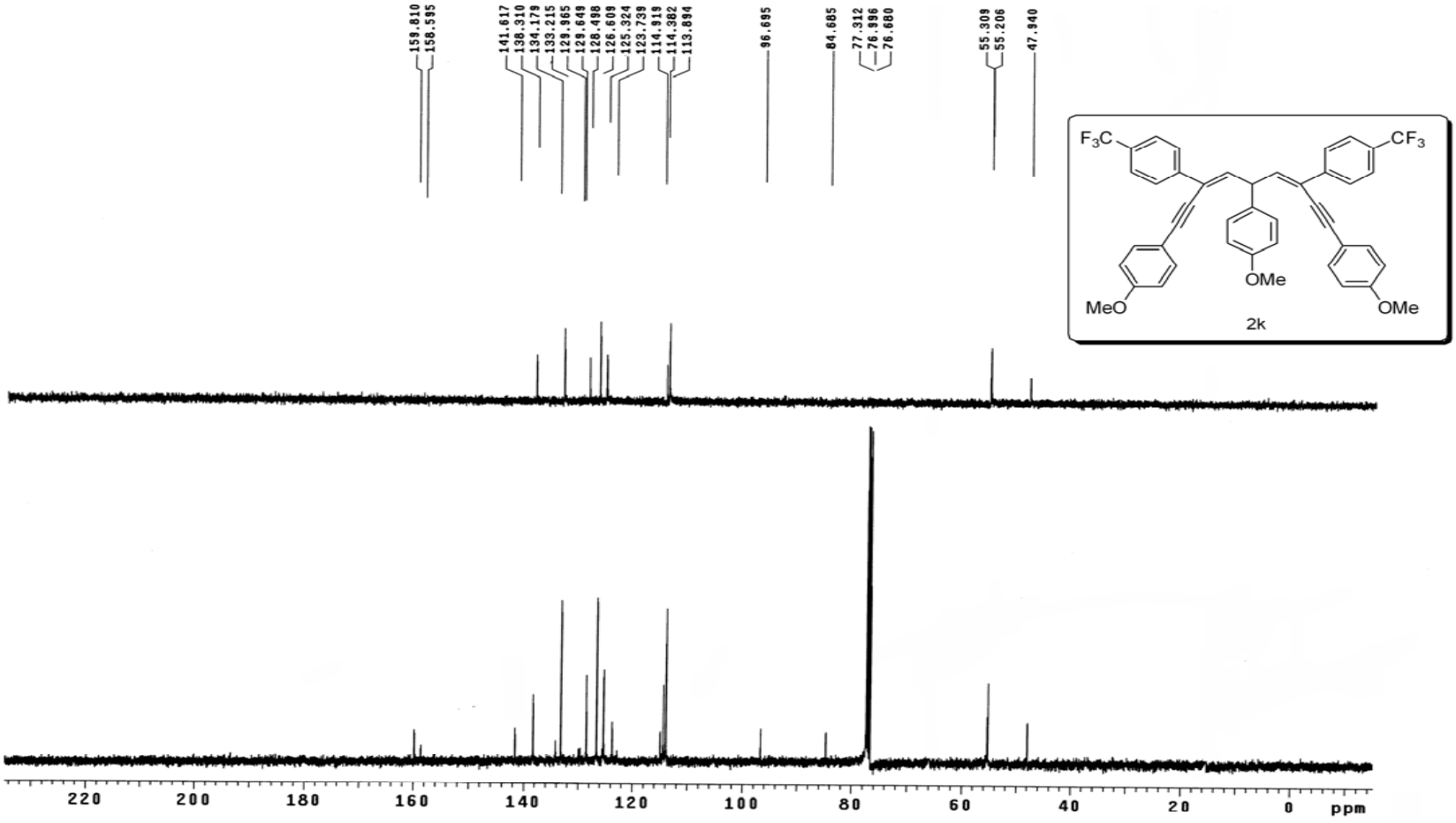
6.59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133.215
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129.649
128.498
126.609
125.324
123.739
114.919
114.382
113.894
96.695
84.685
77.312
76.996
76.680
55.309
55.206
47.940
F3C
CF3
OMe
MeO
OMe
2k
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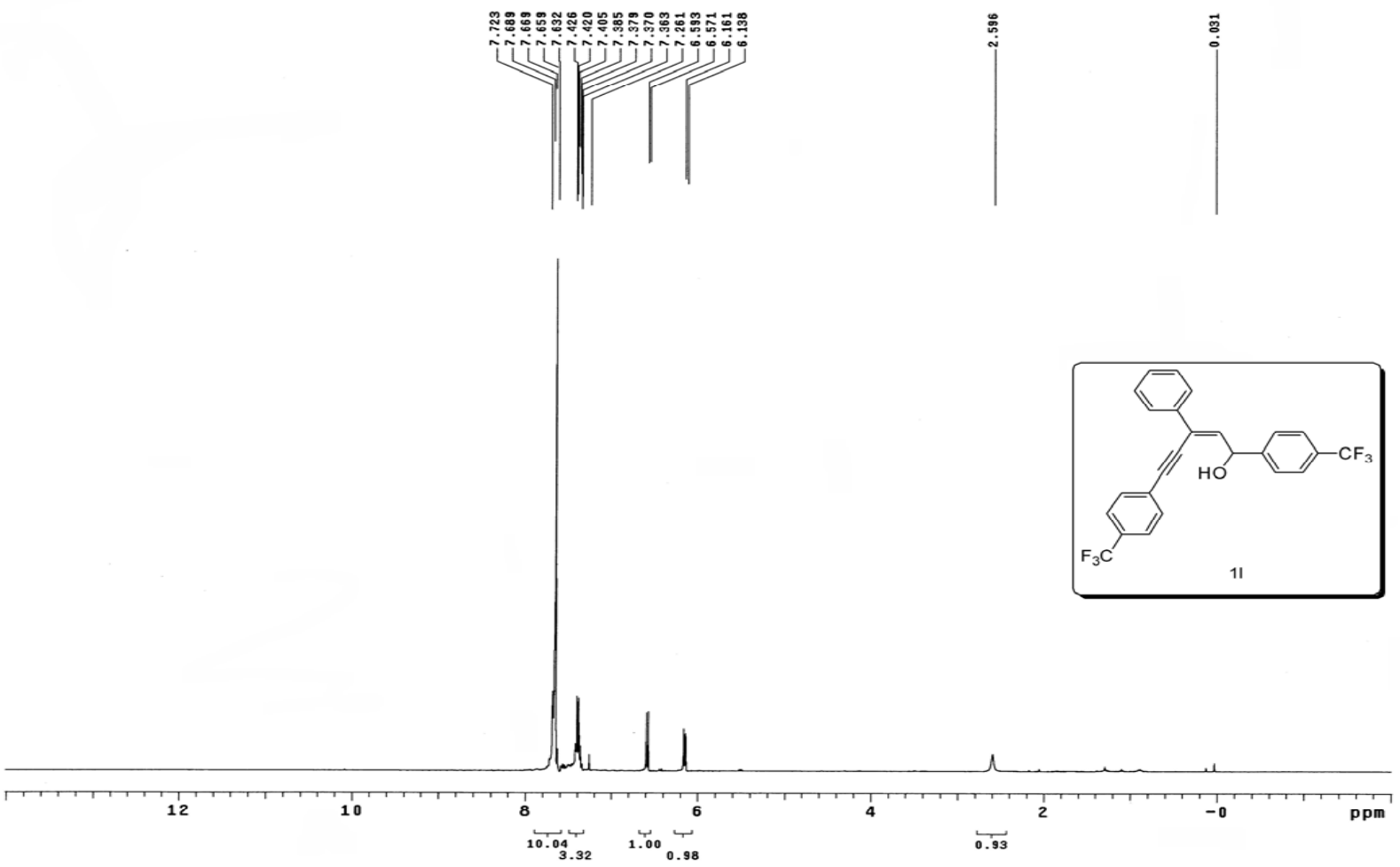
140
120
100
80
60
40
20
0
ppm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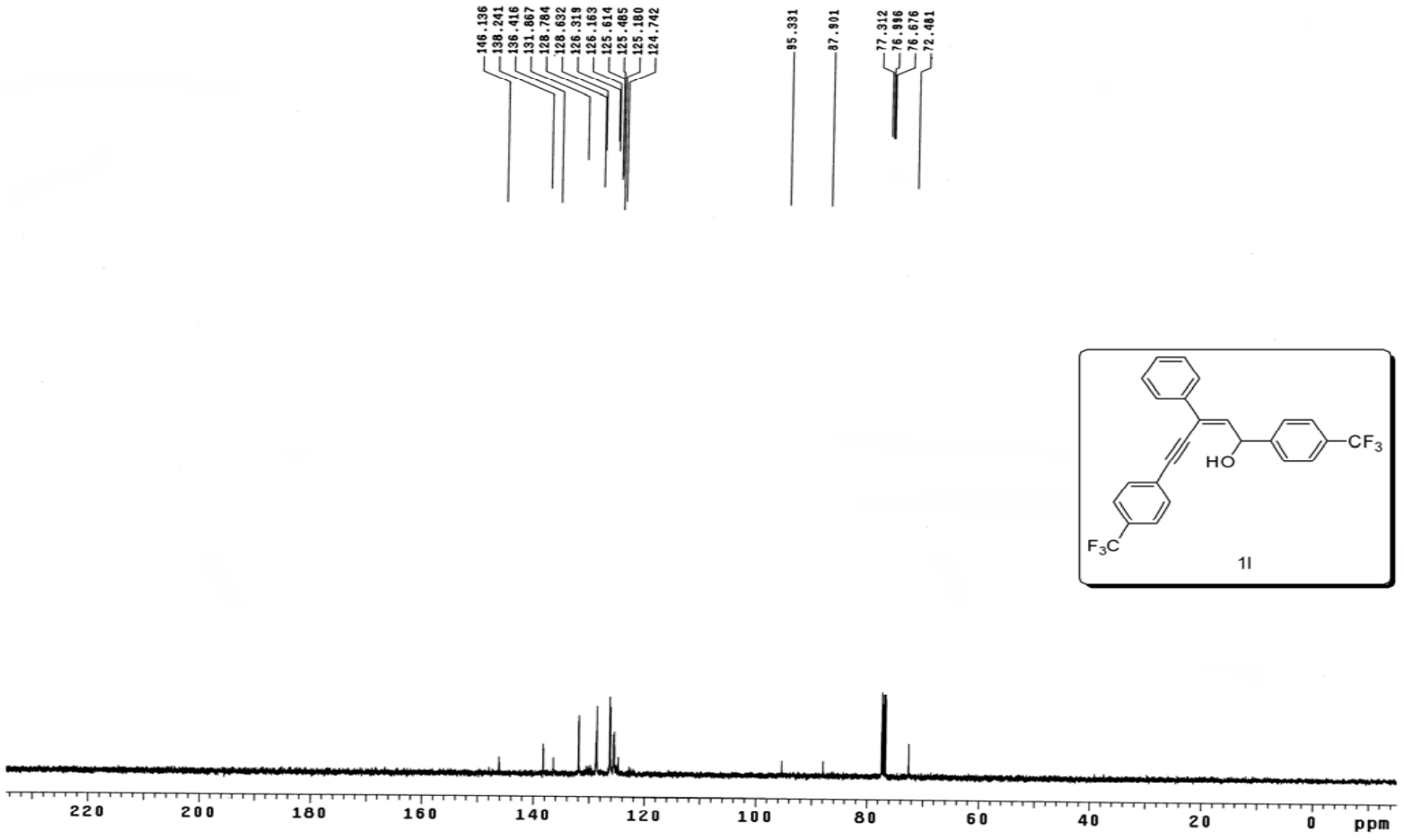
7.659
7.632
7.426
7.420
7.405
7.385
7.379
7.370
7.363
7.261
6.593
6.571
6.161
6.138
2.596
0.031
HO
CF3
F3C
1l
12
10
8
6
4
2
-0
ppm
10.04
3.32
1.00
0.98
0.93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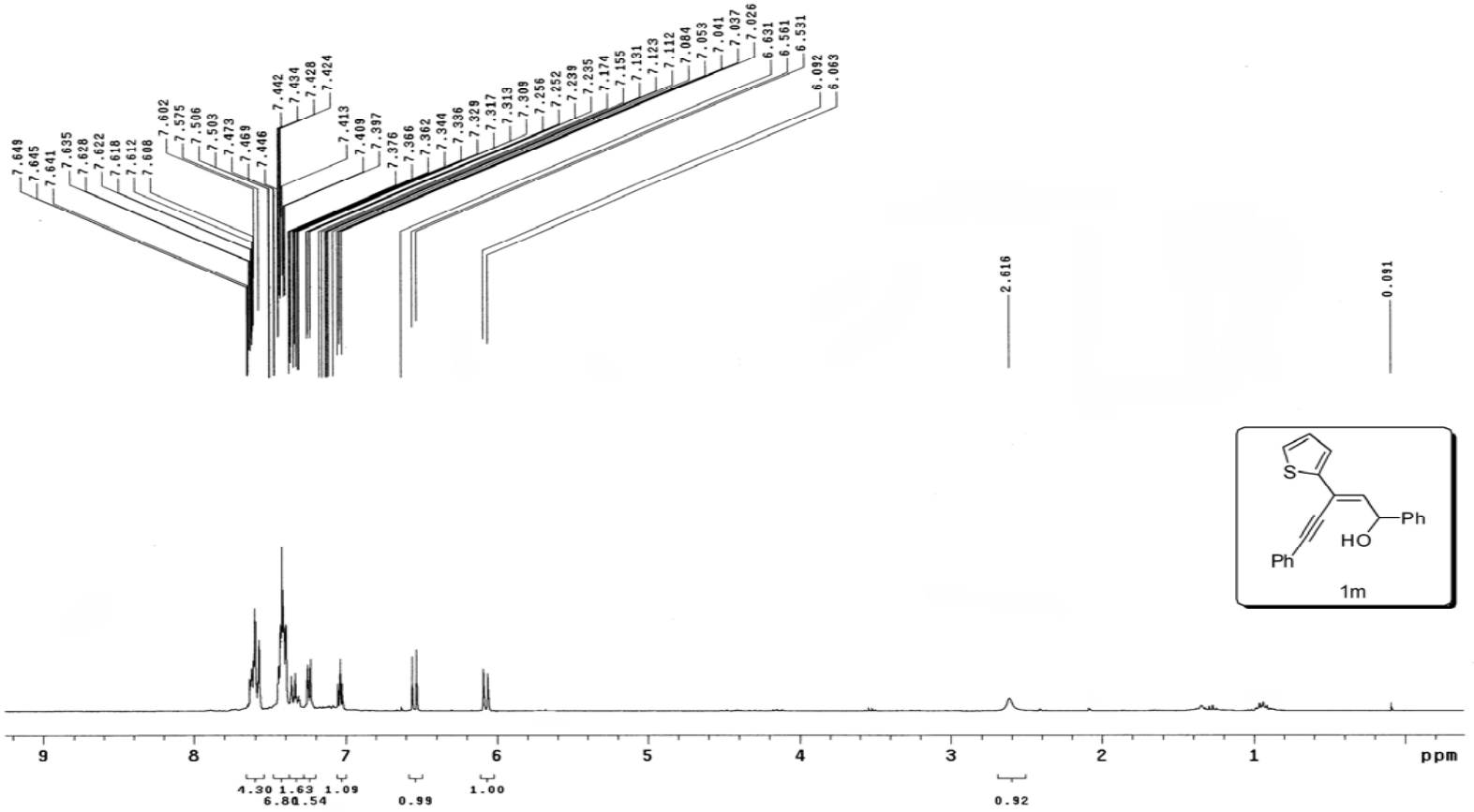
126.319
126.163
125.614
125.485
125.180
124.742
95.331
87.901
77.312
76.996
76.676
72.481
CF3
HO
F3C
1l
220
200
180
160
140
120
100
80
60
40
20
0
ppm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7.618
7.612
7.608
7.602
7.575
7.506
7.503
7.473
7.469
7.446
7.442
7.434
7.428
7.424
7.413
7.409
7.397
7.376
7.366
7.362
7.344
7.336
7.329
7.317
7.313
7.308
7.256
7.252
7.239
7.235
7.174
7.155
7.131
7.123
7.112
7.084
7.053
7.041
7.037
7.026
6.631
6.561
6.531
6.092
6.063
2.616
0.091
S
Ph
HO
Ph
1m
9
8
7
6
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4
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2
1
ppm
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1.09
0.99
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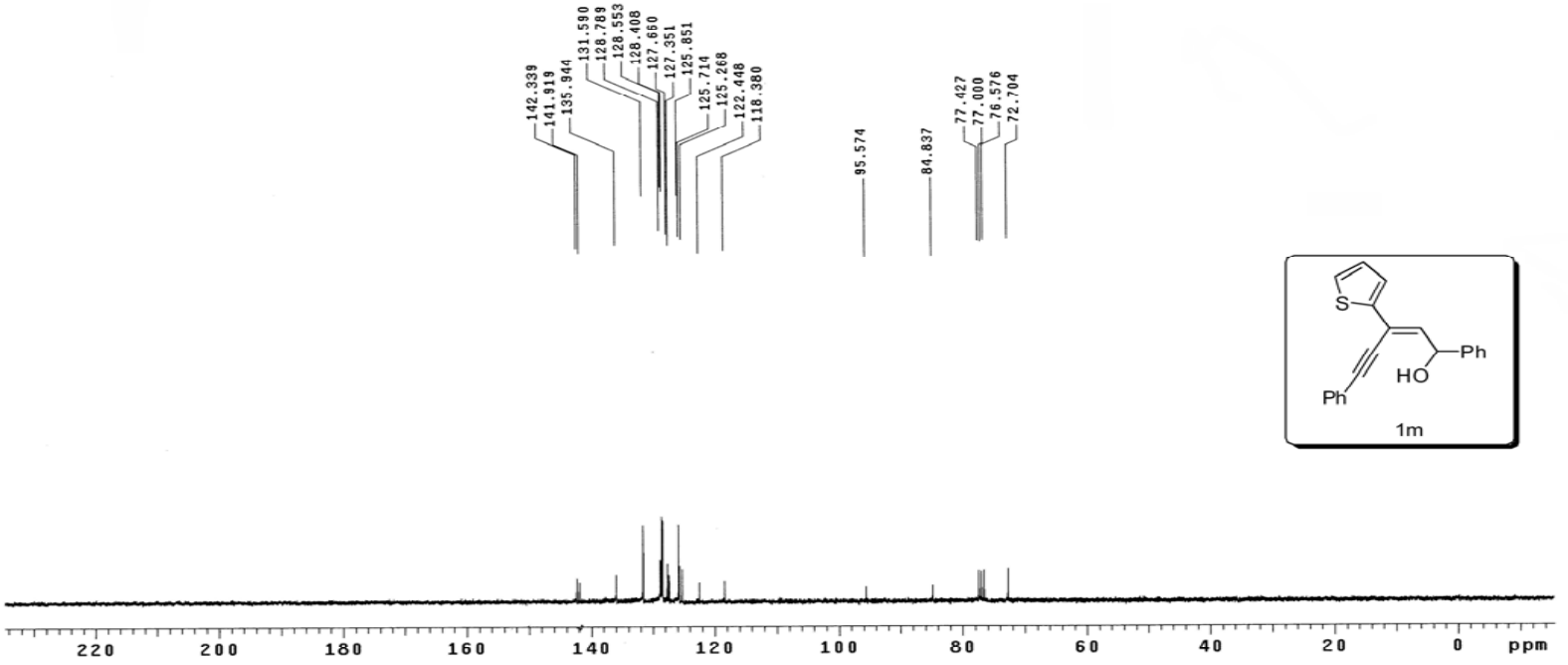
1.54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127.351
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125.714
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122.448
118.380
95.574
84.837
77.427
77.000
76.576
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S
Ph
HO
Ph
1m
220
200
180
160
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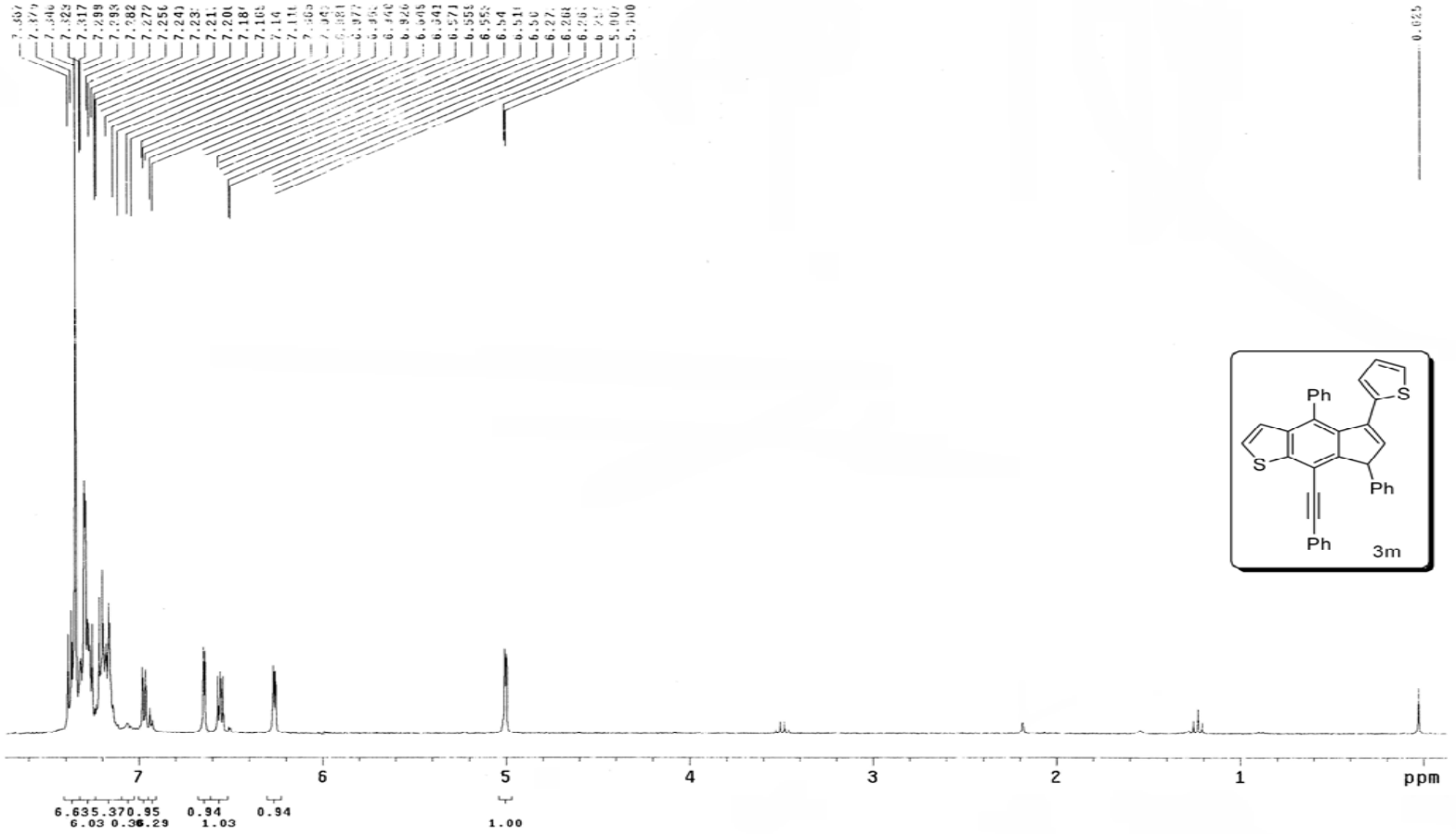
120
100
80
60
40
20
0
ppm


Ph
S
S
Ph
Ph
3m
7
6
5
4
3
2
1
ppm
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5.37
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0.36
6.29
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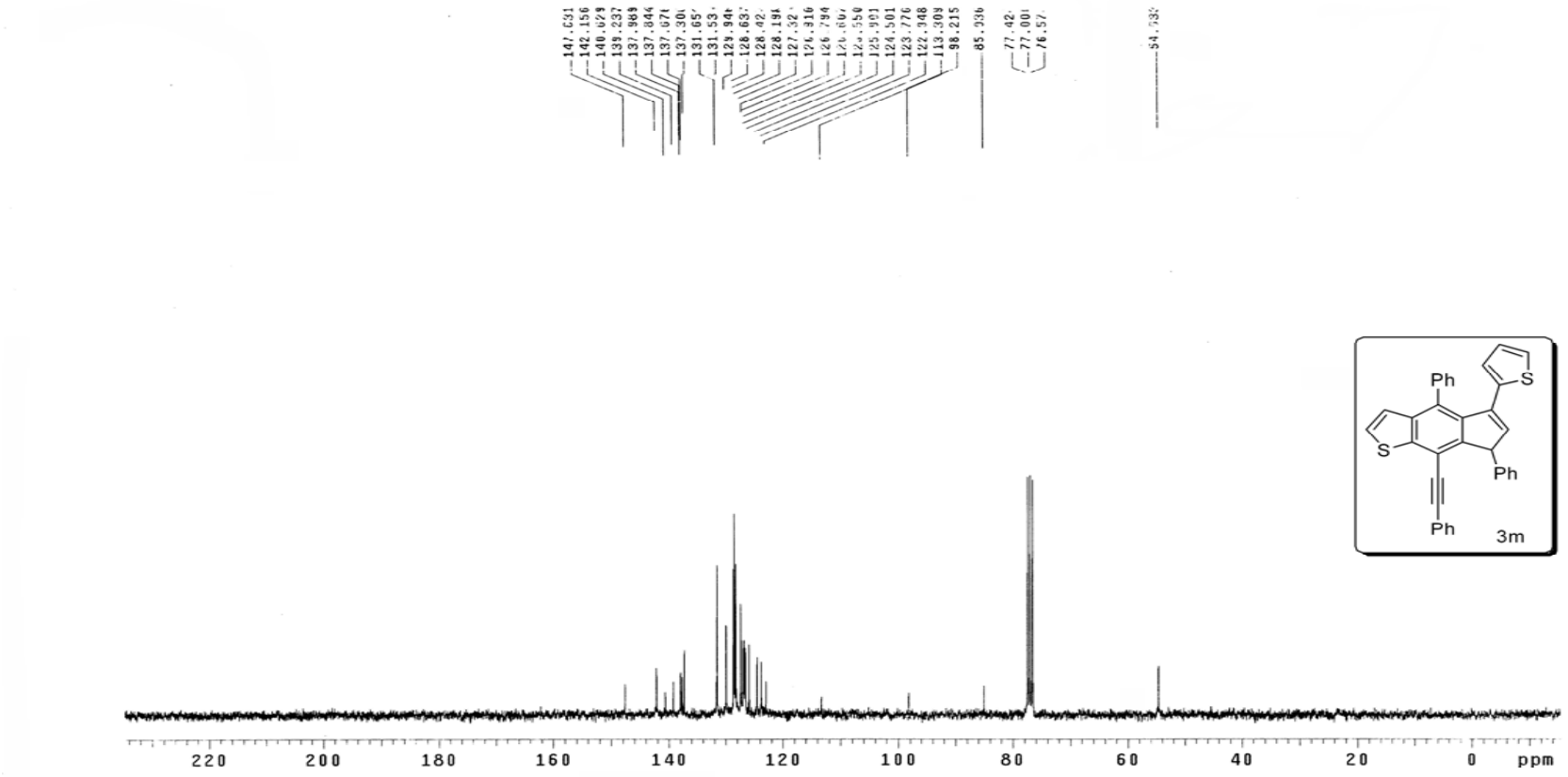
1.03
0.94
1.00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137.306
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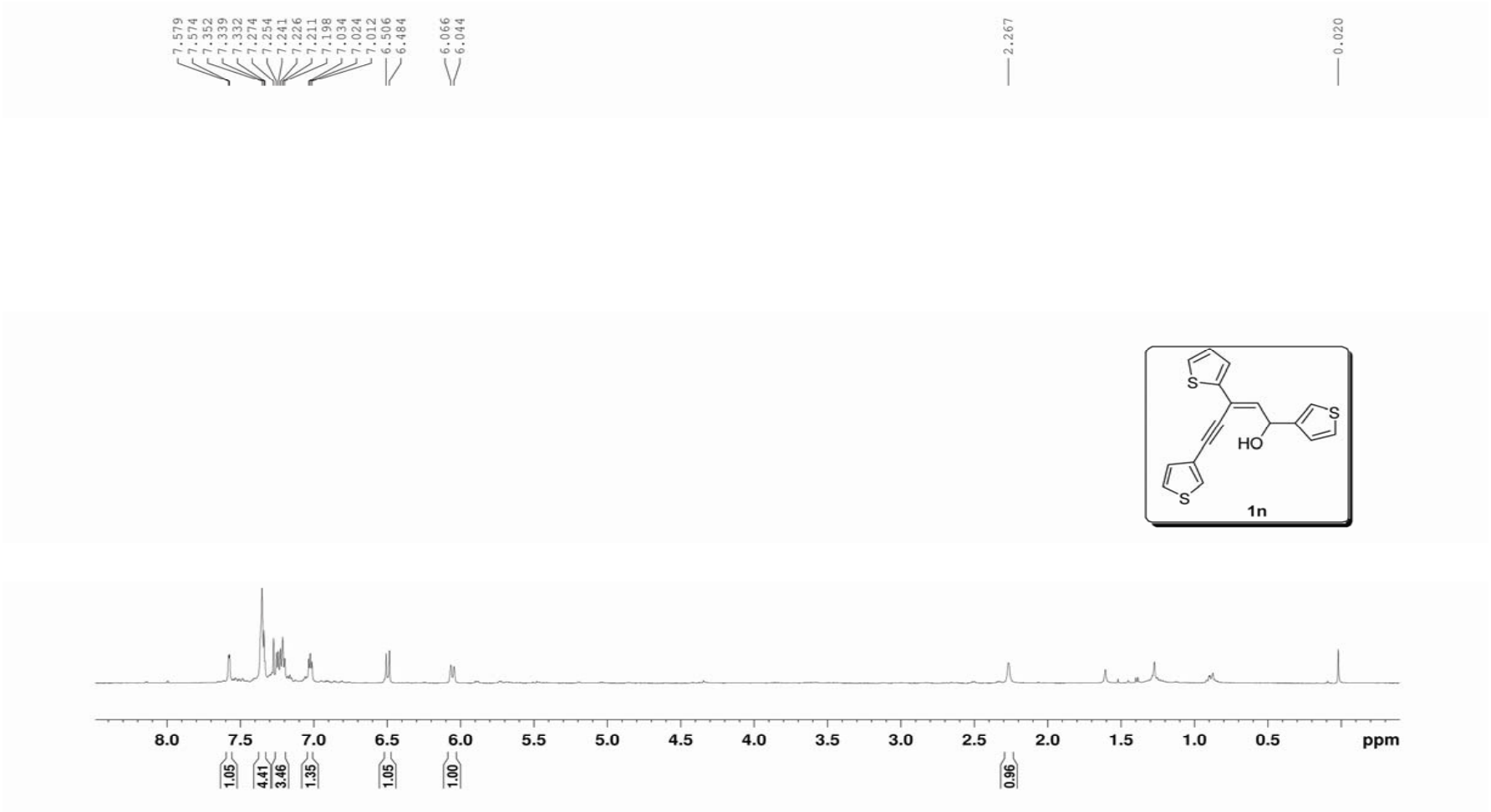
131.53
129.94
128.63
128.49
128.194
127.32
126.316
126.794
125.901
124.501
123.776
122.348
113.309
98.215
85.936
77.42
77.001
76.57
54.532
Ph
S
S
Ph
Ph
3m
220
200
180
160
140
120
100
80
60
40
20
0
ppm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7.339
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7.254
7.241
7.226
7.211
7.198
7.034
7.024
7.012
6.506
6.484
6.066
6.044
2.267
0.020
S
S
HO
S
1n
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
ppm
1.05
4.41
3.46
1.35
1.05
1.00
0.96


143.49
141.82
135.12
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129.40
127.43
126.29
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125.79
125.71
125.39
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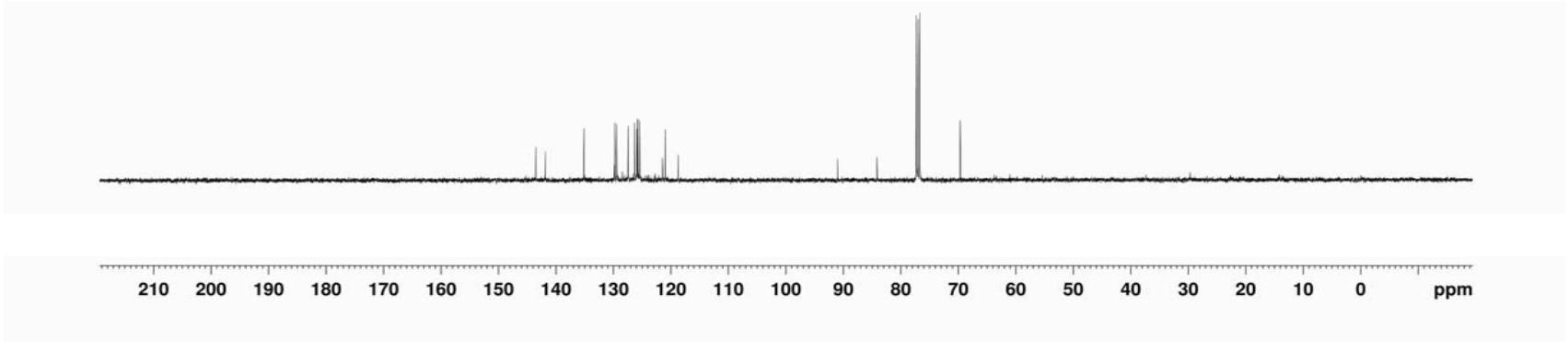
90.99
84.12
77.32
77.00
76.68
69.65


S
S
HO
S
1n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200
190
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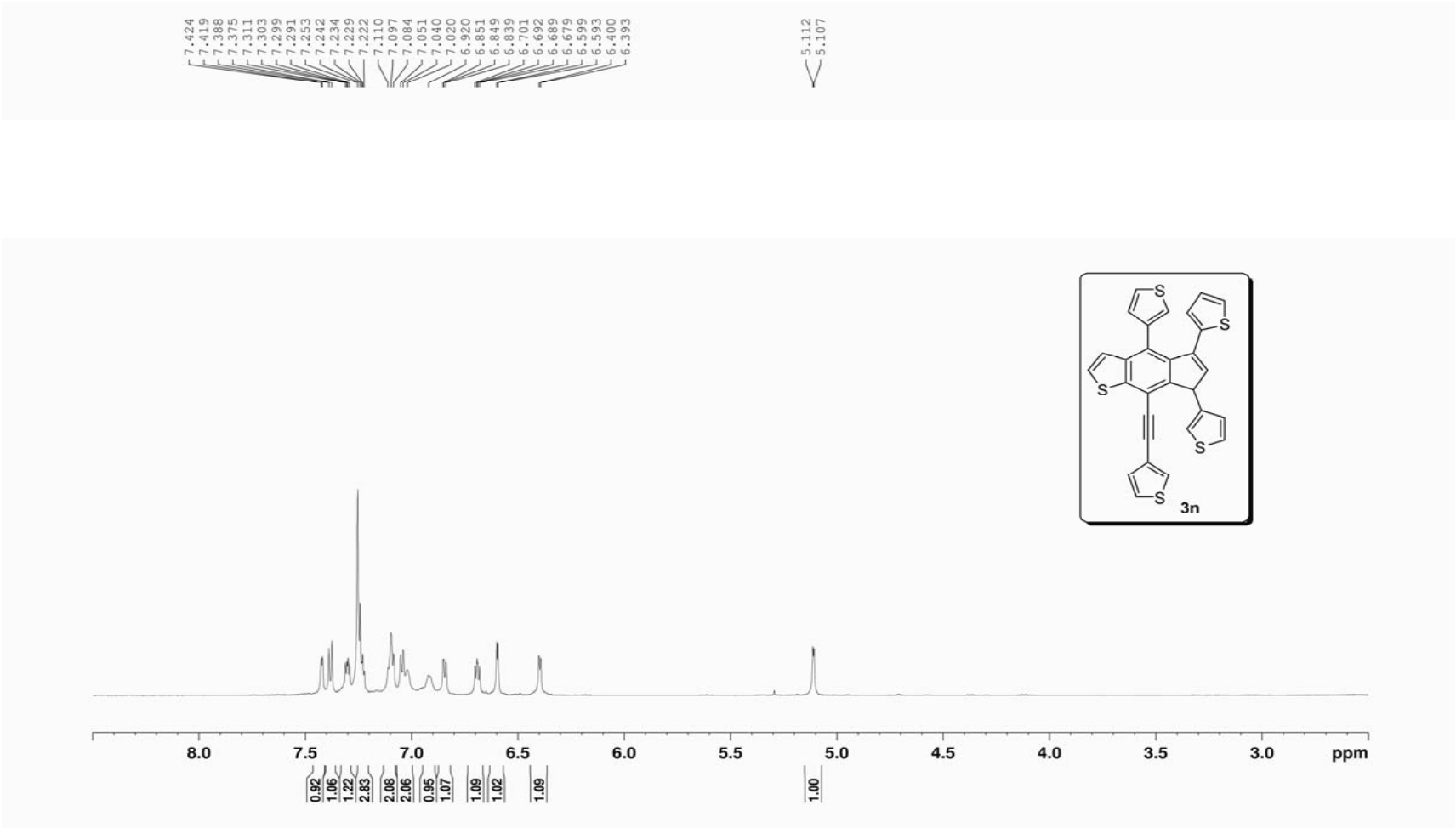
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.303
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7.291
7.253
7.242
7.234
7.229
7.222
7.110
7.097
7.084
7.051
7.040
7.020
6.920
6.851
6.849
6.839
6.701
6.692
6.689
6.679
6.599
6.593
6.400
6.393
5.112
5.107
3n
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm
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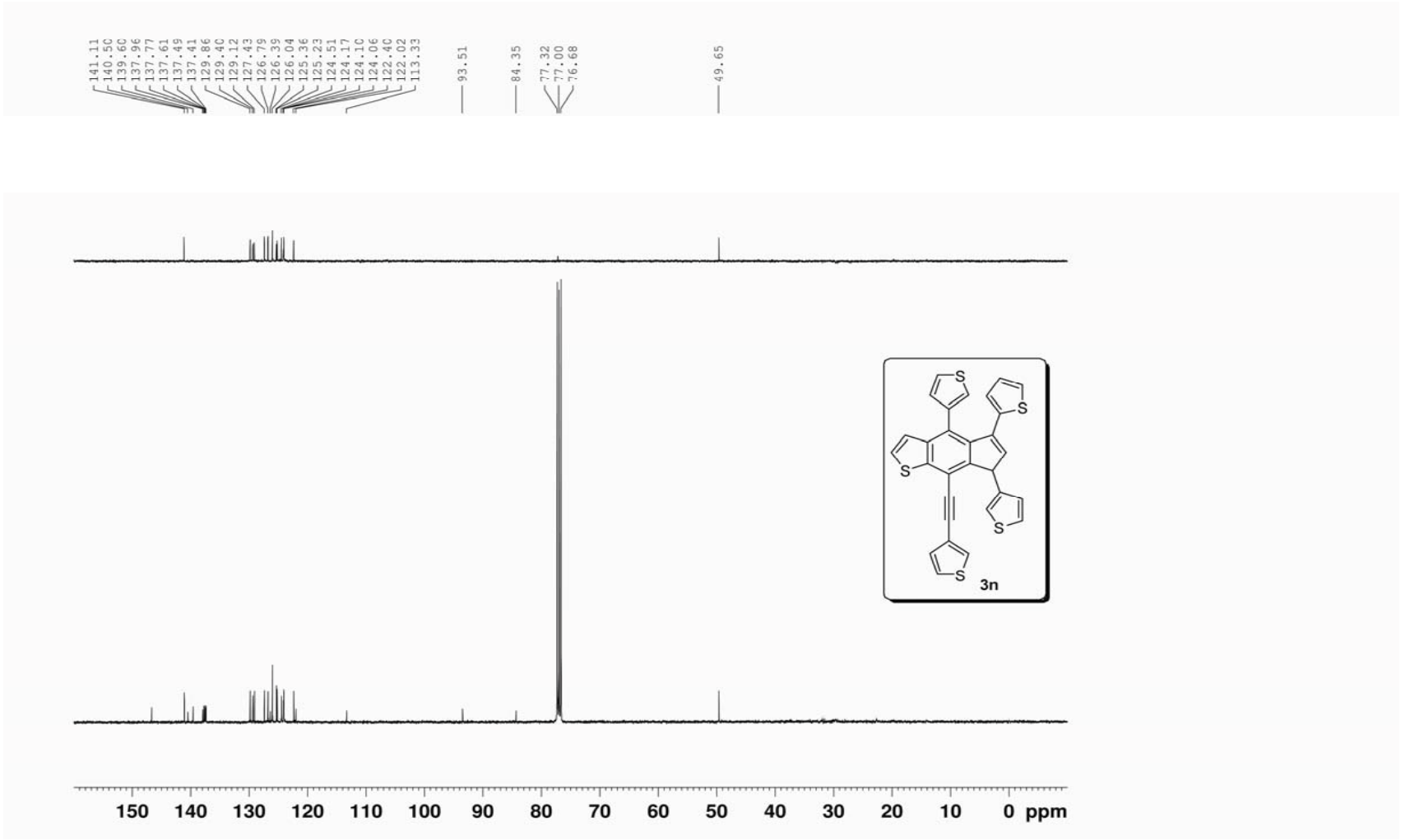
2.06
0.95
1.07
1.09
1.02
1.09
1.00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137.49
137.41
129.86
129.40
129.12
127.43
126.79
126.39
126.04
125.36
125.23
124.51
124.17
124.10
124.06
122.40
122.02
113.33
93.51
84.35
77.32
77.00
76.68
49.65
S
S
S
S
S
3n
150
140
130
120
110
100
90
80
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60
50
40
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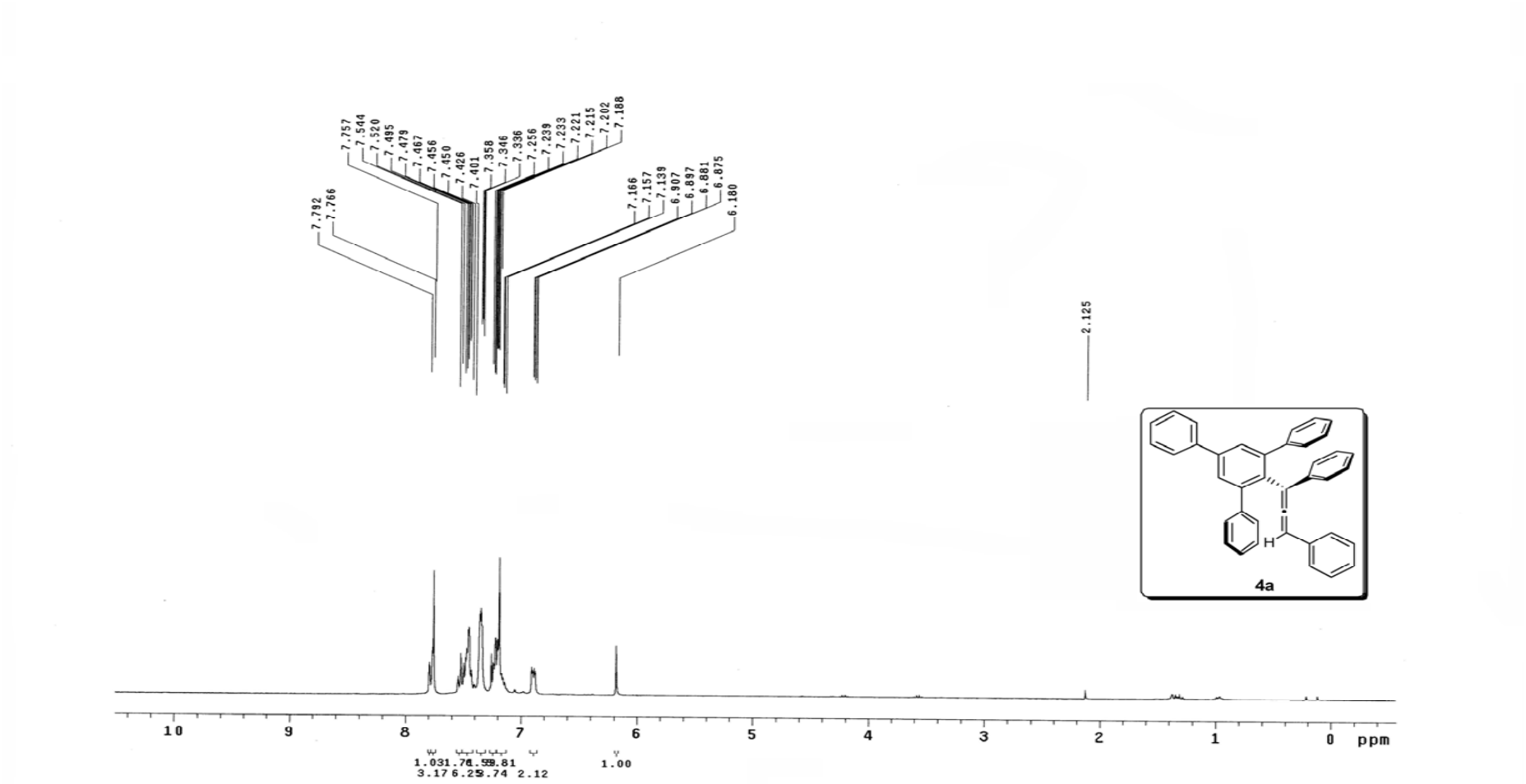
20
10
0 ppm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7.467
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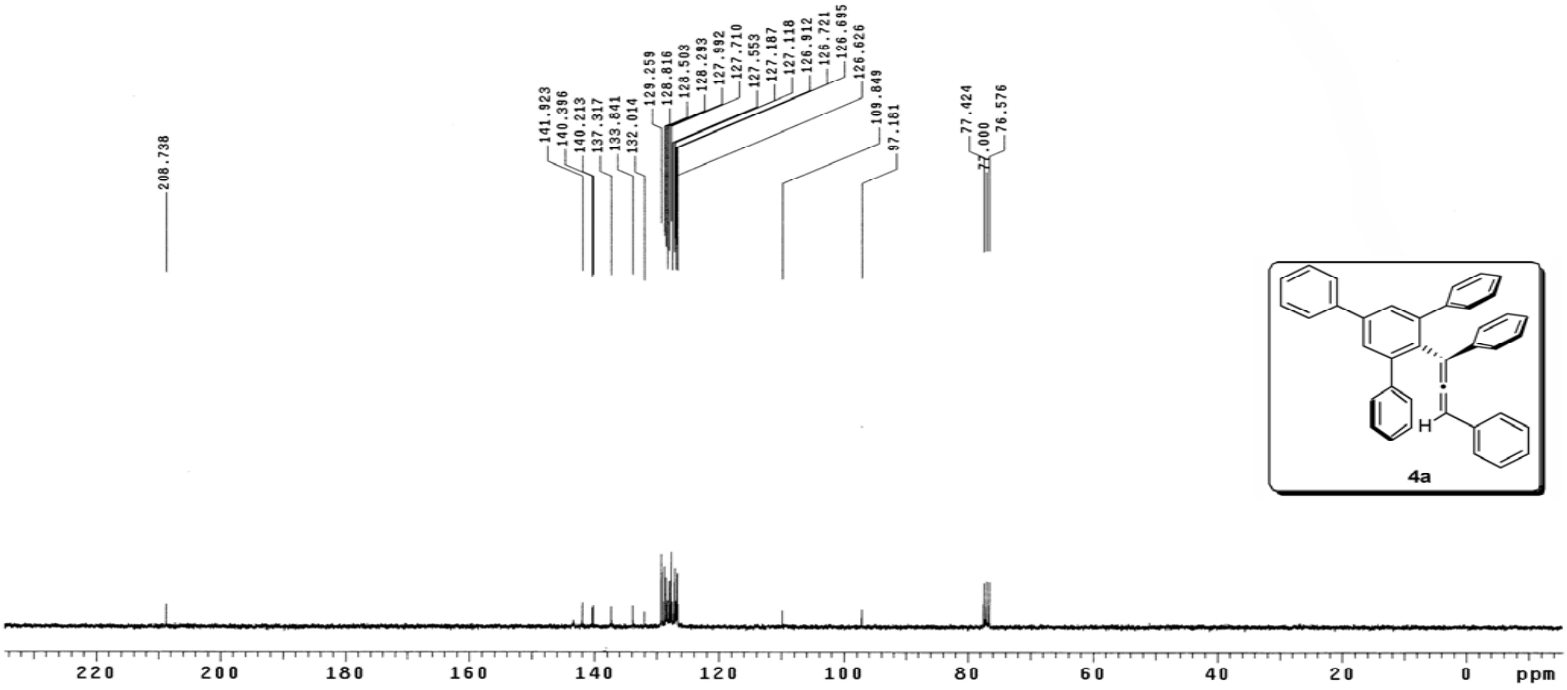
7.450
7.426
7.401
7.358
7.346
7.336
7.256
7.239
7.233
7.221
7.215
7.202
7.188
7.166
7.157
7.139
6.907
6.897
6.881
6.875
6.180
2.125
H
4a
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03 1.76 1.59 3.81
3.17 6.25 3.74 2.12
1.00


208.738
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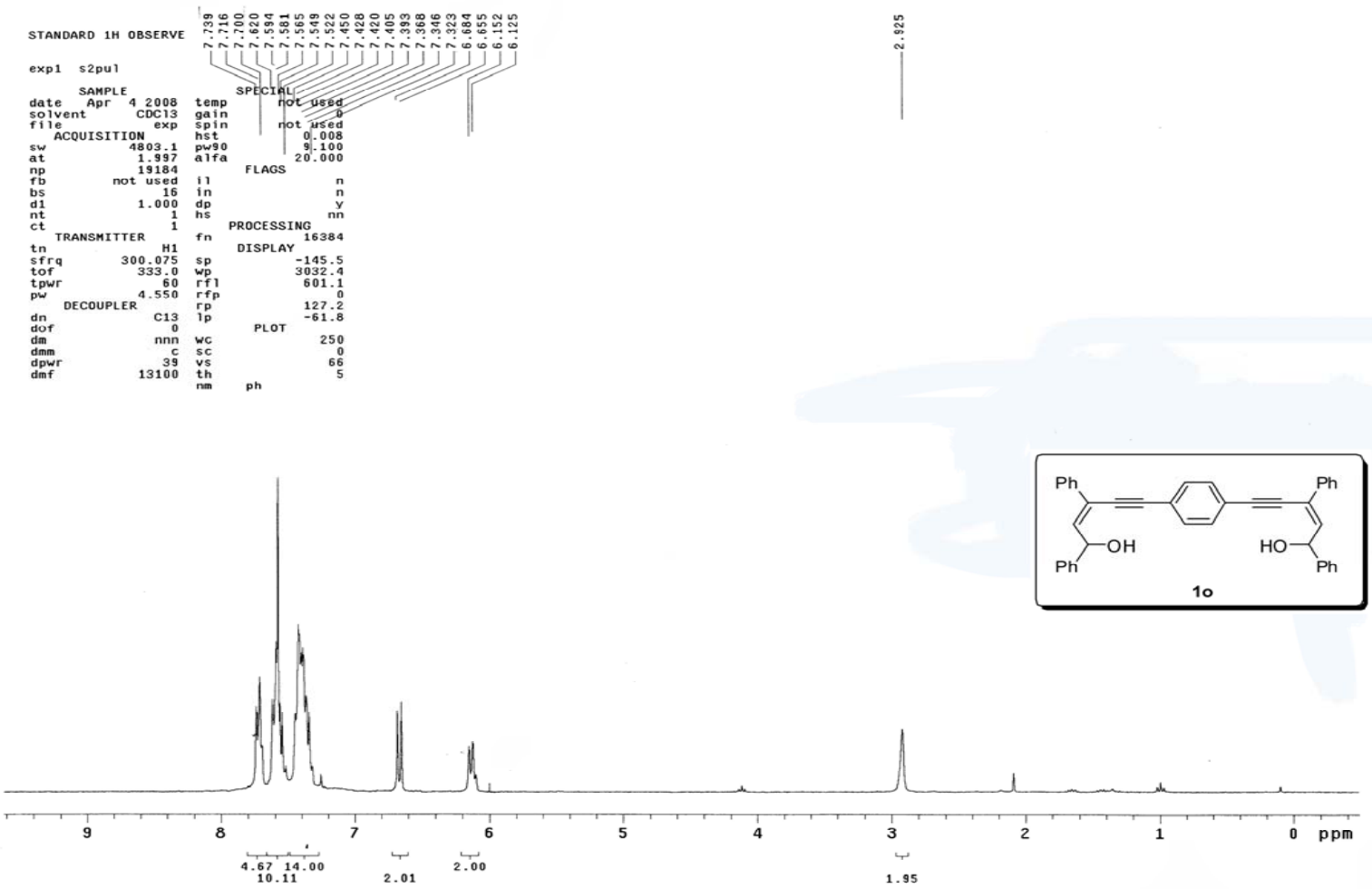
132.014
129.259
128.816
128.503
128.293
127.992
127.710
127.553
127.187
127.118
126.912
126.721
126.695
126.626
109.849
97.161
77.424
77.000
76.576
H
4a
220
200
180
160
140
120
100
80
60
40
20
0
ppm


STANDARD 1H OBSERVE
exp1 s2pul
SAMPLE
date Apr 4 2008
solvent CDCl3
file exp
ACQUISITION
sw 4803.1
at 1.997
np 19184
fb not used
bs 16
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nt 1
ct 1
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tn H1
sfrq 300.075
tof 333.0
tpwr 60
pw 4.550
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 39
dmf 13100
SPECIAL
temp not used
gain 0
spin not used
hst 0.008
pw90 9.100
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
fn 16384
DISPLAY
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wp 3032.4
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rp 127.2
lp -61.8
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sc 0
vs 66
th 5
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7.700
7.620
7.594
7.581
7.565
7.549
7.522
7.450
7.428
7.420
7.405
7.393
7.368
7.346
7.323
6.684
6.655
6.152
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Ph
HO
Ph
Ph
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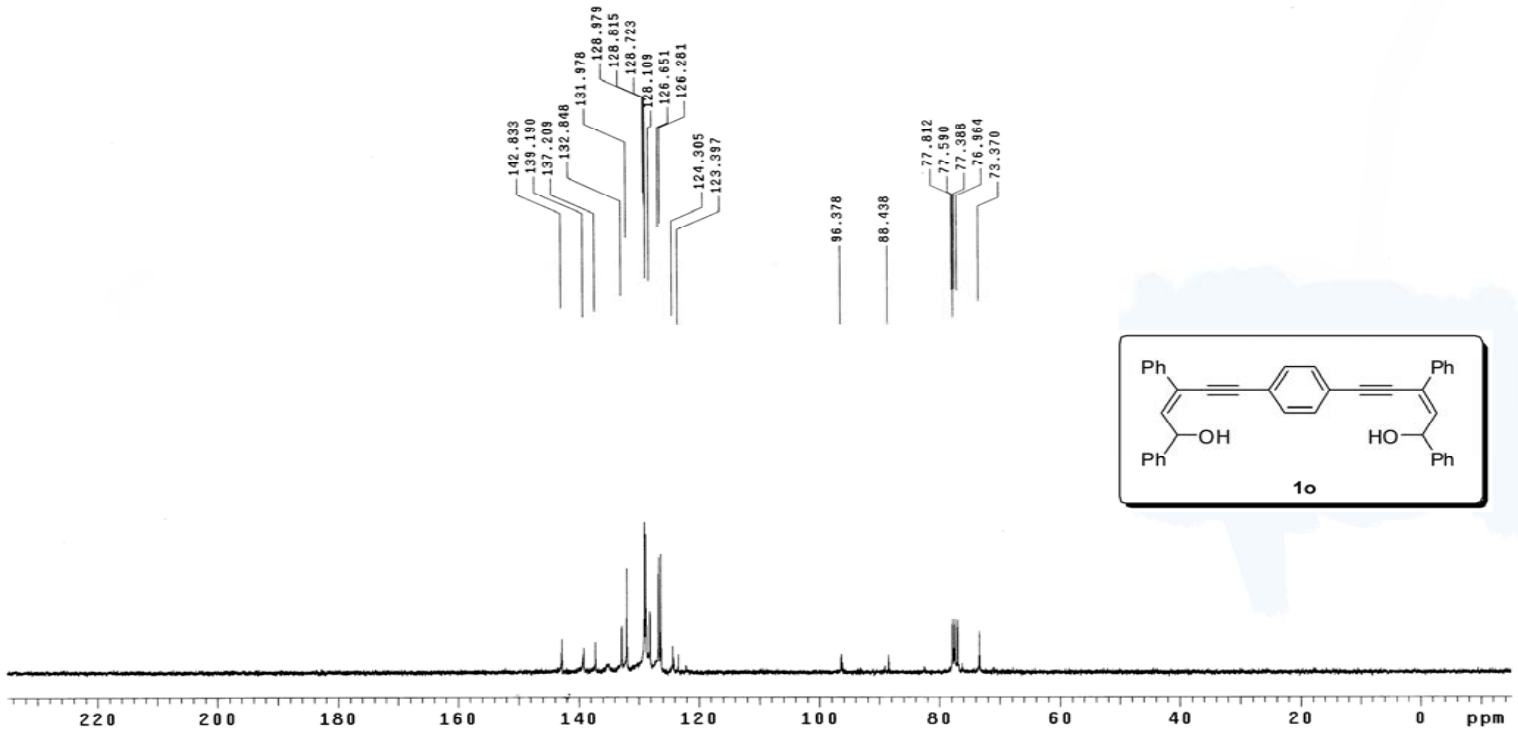
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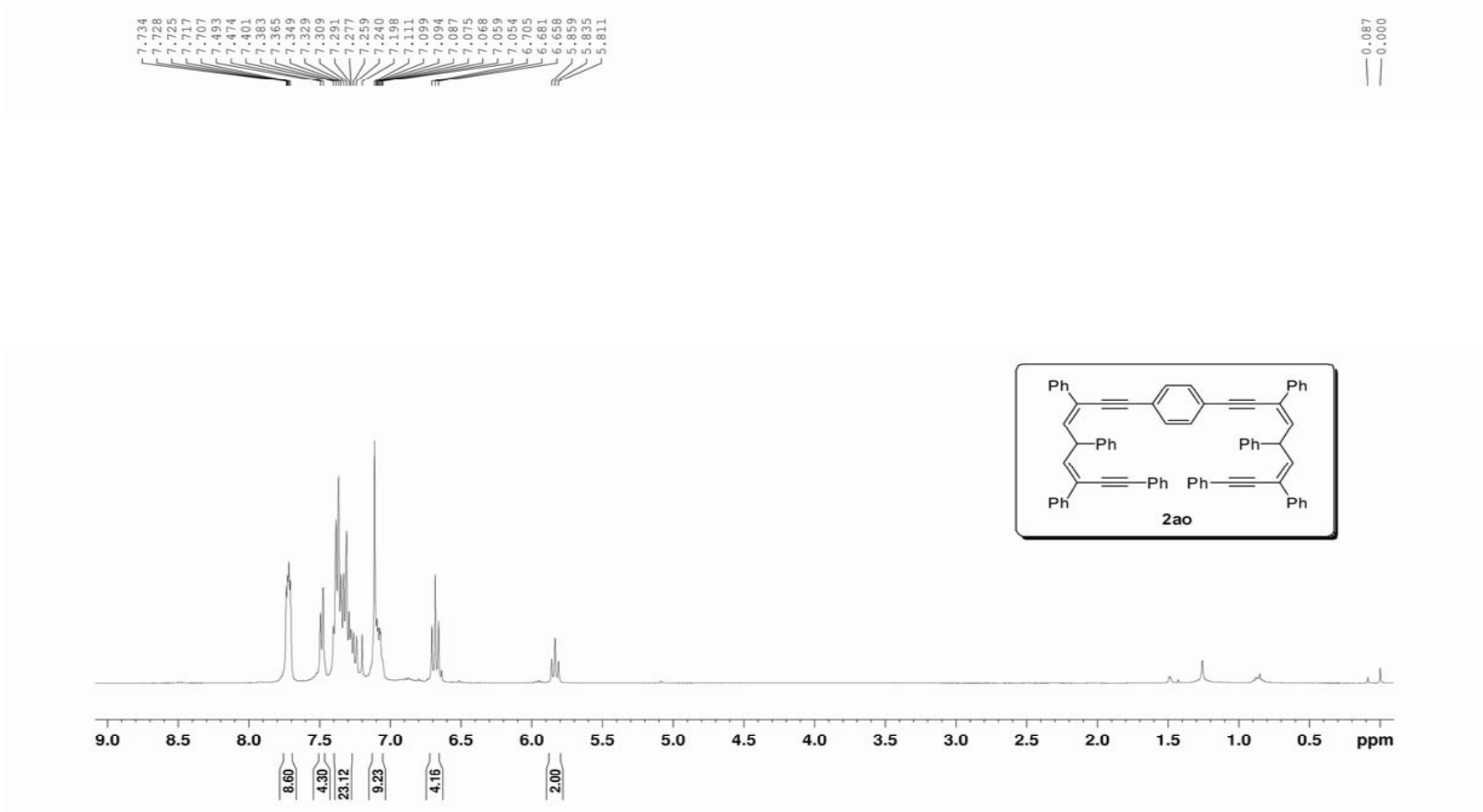
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Ph
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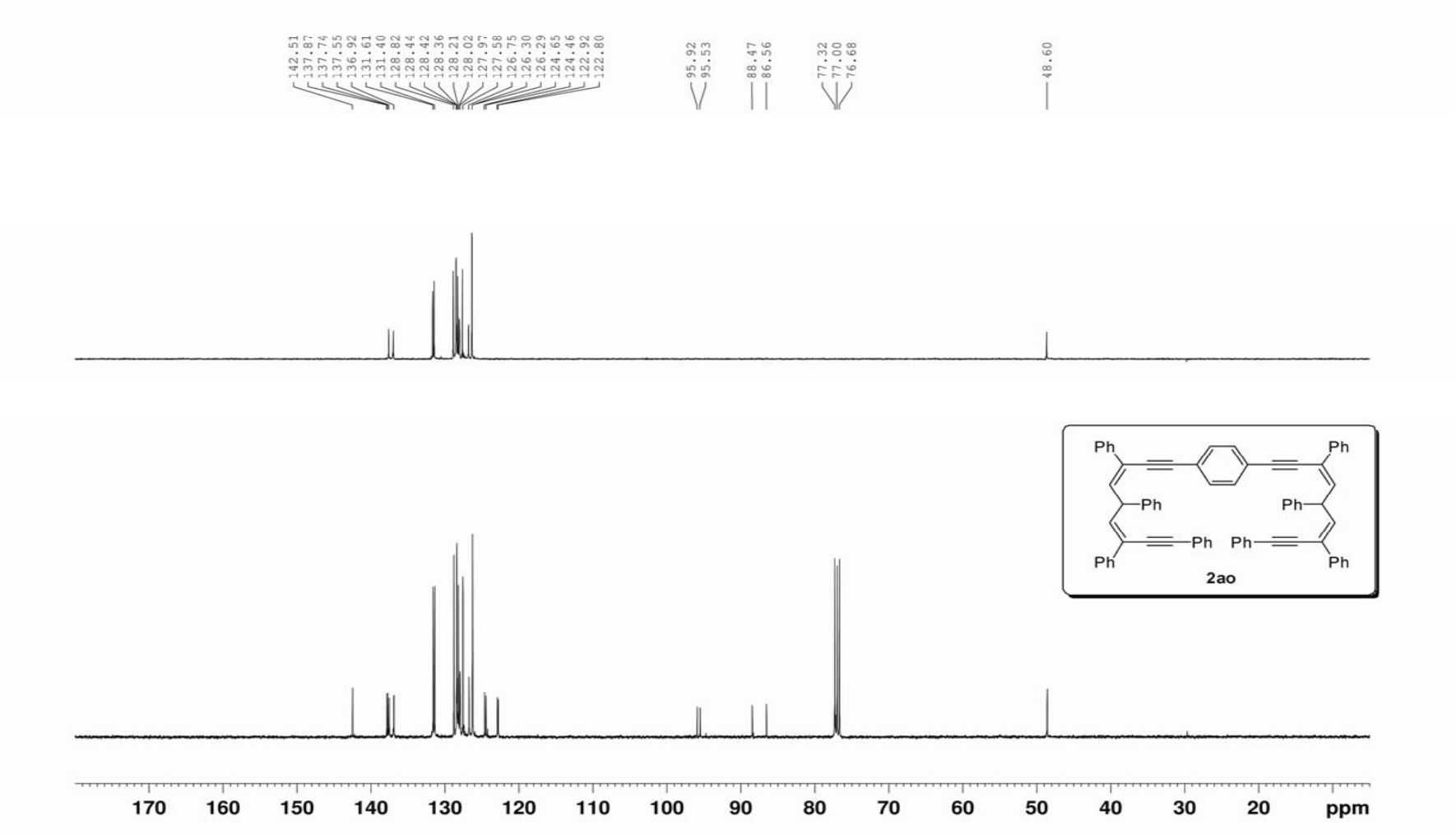
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126.30
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124.46
122.92
122.80
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95.53
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Ph
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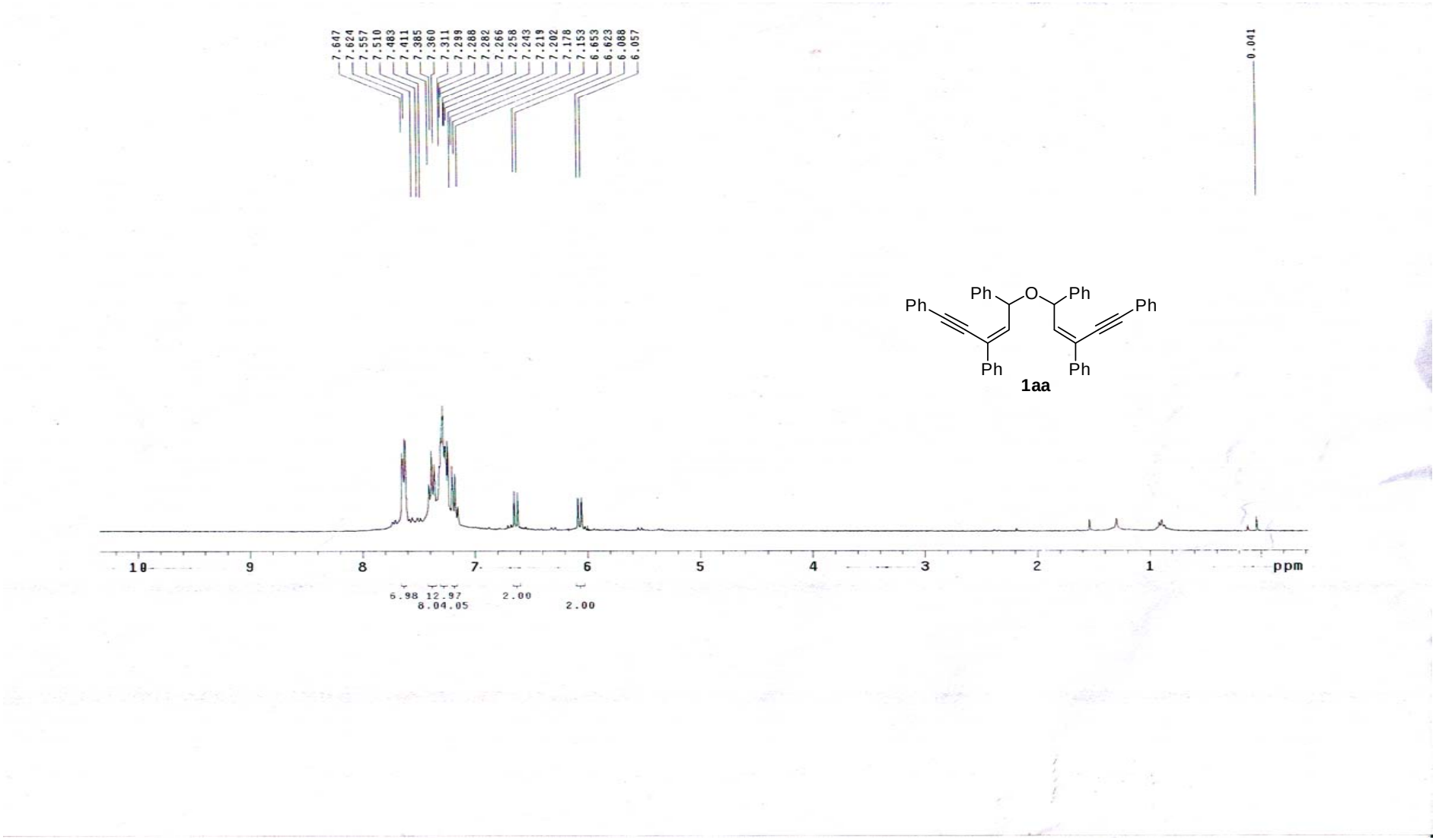
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7.243
7.219
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7.178
7.153
6.653
6.623
6.088
6.057
0.041
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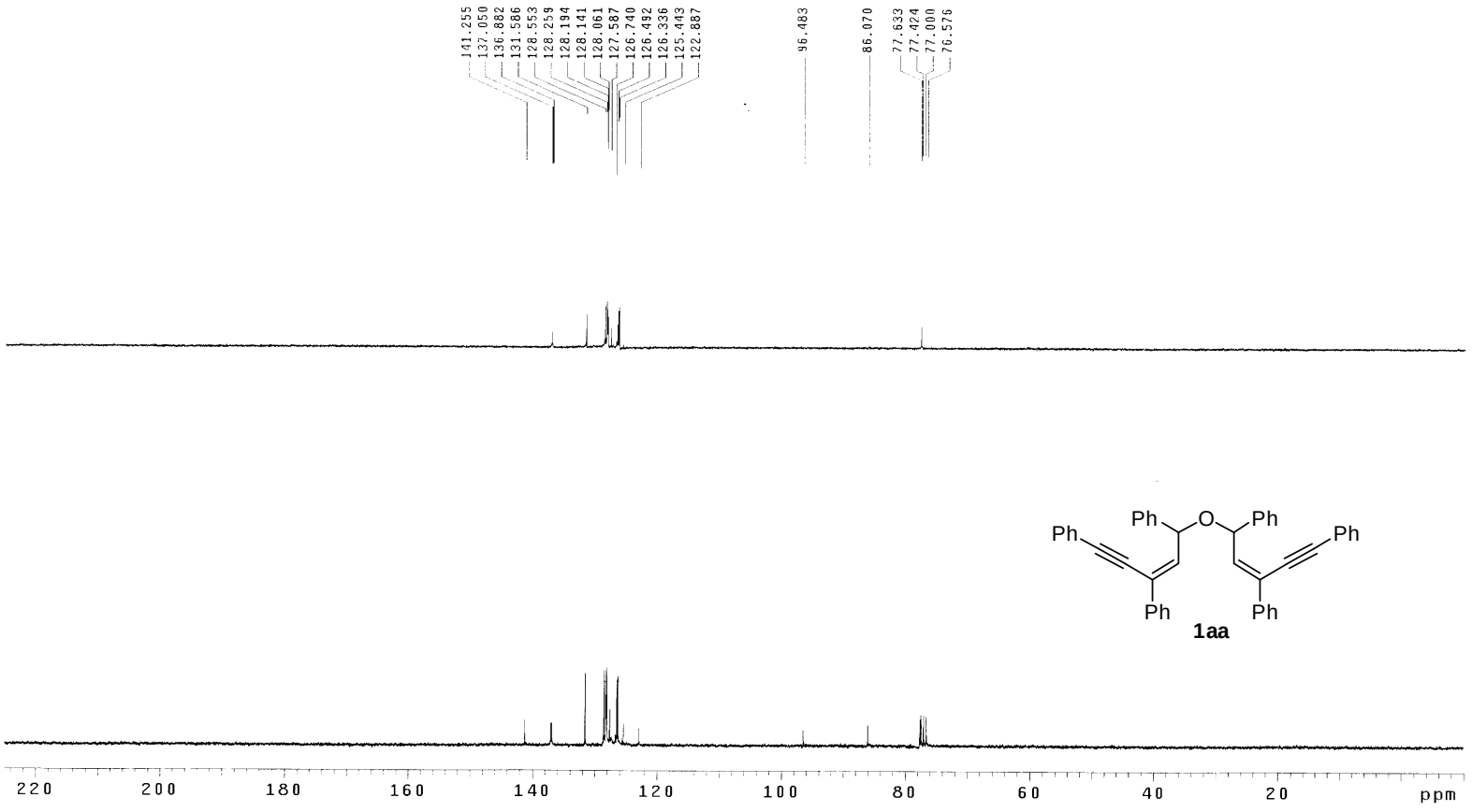
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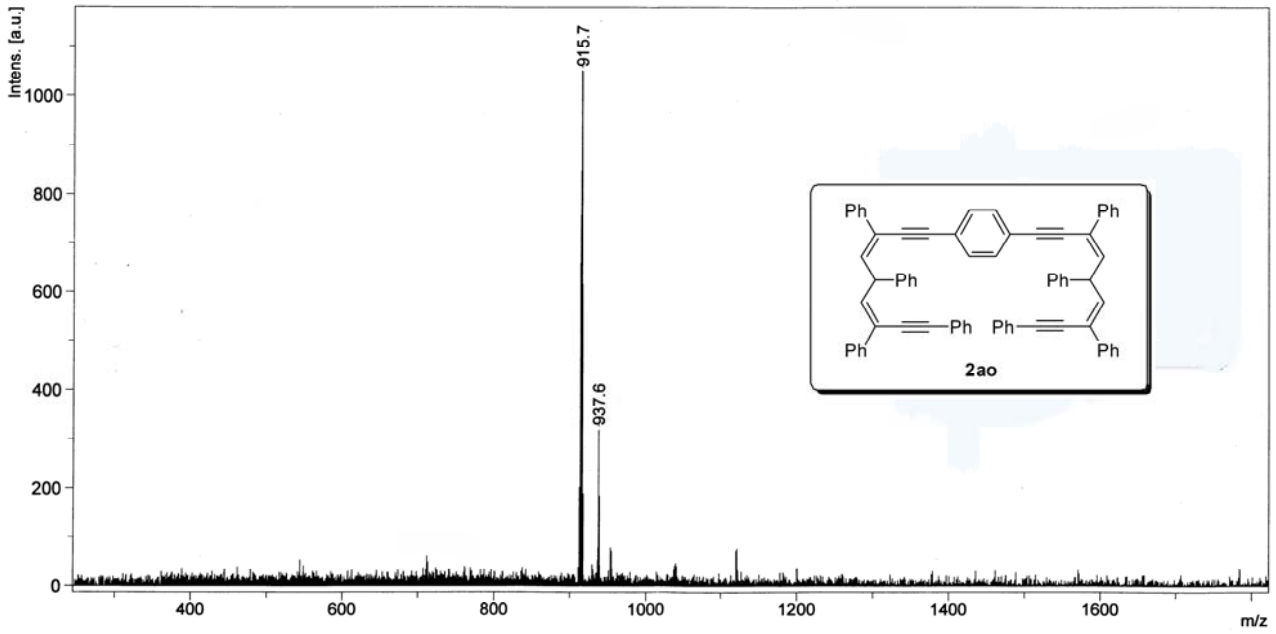
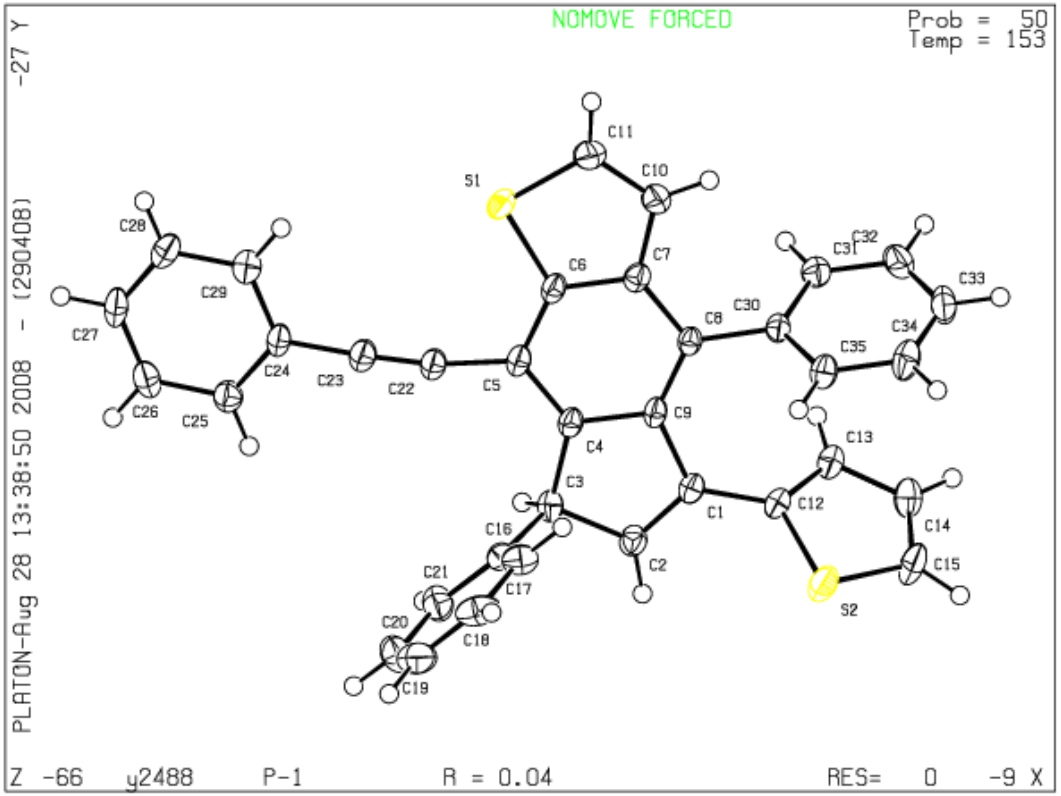
MALDI-TOF,CCA,2008,5,15

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S1
C10
C28
C29
C6
C7
C31
C32
C33
C27
C30
C8
C34
C24
C23
C22
C5
C35
C26
C25
C9
C13
C4
C3
C1
C12
C14
C16
C2
C15
C21
C17
S2
C20
C18
C19

Table 1. Crystal data and structure refinement for **3m**.

Identification code	y2488
Empirical formula	C35 H22 S2
Formula weight	506.65
Temperature	153(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.4462(3) A alpha = 72.464(1) deg. b = 11.3402(3) A beta = 70.535(1) deg. c = 12.9205(4) A gamma = 66.002(1) deg.
Volume	1293.72(6) A^3
Z, Calculated density	2, 1.301 Mg/m^3
Absorption coefficient	0.229 mm^-1
F(000)	528

Crystal size	0.39 x 0.28 x 0.16 mm
Theta range for data collection	3.09 to 27.48 deg.
Limiting indices	-13<=h<=12, -14<=k<=14, -16<=l<=16
Reflections collected / unique	12796 / 5890 [R(int) = 0.0196]
Completeness to theta = 27.48	99.2 %
Absorption correction	Empirical
Max. and min. transmission	0.9643 and 0.9161
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5890 / 0 / 335
Goodness-of-fit on F^2	0.996
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.1018
R indices (all data)	R1 = 0.0524, wR2 = 0.1275
Extinction coefficient	0.0061(17)

Largest diff. peak and hole 0.360 and -0.410 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for y2488.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	5415(1)	4017(1)	8828(1)	31(1)
S(2)	6536(1)	-3251(1)	7643(1)	35(1)
C(1)	6296(2)	-634(2)	7116(1)	22(1)
C(2)	5446(2)	-83(2)	6399(1)	25(1)
C(3)	4692(2)	1378(2)	6351(1)	23(1)
C(4)	5246(2)	1598(2)	7196(1)	21(1)
C(5)	4989(2)	2771(2)	7472(1)	22(1)
C(6)	5643(2)	2699(2)	8291(1)	22(1)
C(7)	6540(2)	1508(2)	8799(1)	22(1)
C(8)	6829(2)	315(2)	8482(1)	20(1)
C(9)	6181(2)	386(2)	7675(1)	21(1)
C(10)	7019(2)	1715(2)	9635(2)	28(1)
C(11)	6495(2)	2993(2)	9728(2)	34(1)

C(12)	7254(2)	-2018(2)	7261(1)	23(1)
C(13)	8749(2)	-2525(2)	7089(1)	26(1)
C(14)	9267(2)	-3925(2)	7279(2)	34(1)
C(15)	8198(2)	-4446(2)	7576(2)	38(1)
C(16)	3059(2)	1778(2)	6588(1)	23(1)
C(17)	2268(2)	1416(2)	7660(2)	31(1)
C(18)	789(2)	1693(2)	7857(2)	39(1)
C(19)	95(2)	2321(2)	6999(2)	42(1)
C(20)	873(2)	2698(2)	5944(2)	43(1)
C(21)	2349(2)	2427(2)	5739(2)	33(1)
C(22)	4166(2)	4039(2)	6952(2)	24(1)
C(23)	3603(2)	5164(2)	6558(2)	26(1)
C(24)	2958(2)	6534(2)	6126(2)	24(1)
C(25)	2398(2)	6949(2)	5183(2)	27(1)
C(26)	1792(2)	8285(2)	4781(2)	31(1)
C(27)	1741(2)	9203(2)	5306(2)	31(1)
C(28)	2297(2)	8804(2)	6239(2)	31(1)
C(29)	2914(2)	7473(2)	6645(2)	29(1)
C(30)	7793(2)	-933(2)	9022(1)	21(1)
C(31)	9247(2)	-1117(2)	8855(2)	28(1)
C(32)	10156(2)	-2296(2)	9334(2)	36(1)
C(33)	9625(2)	-3282(2)	10000(2)	35(1)
C(34)	8178(2)	-3102(2)	10179(2)	33(1)
C(35)	7267(2)	-1933(2)	9693(1)	26(1)

Table 3. Bond lengths [A] and angles [deg] for y2488.

S(1)-C(11)	1.723(2)
S(1)-C(6)	1.7312(16)
S(1)-S(2)#1	3.4948(6)
S(2)-C(15)	1.708(2)
S(2)-C(12)	1.7182(17)
C(1)-C(2)	1.336(2)
C(1)-C(12)	1.473(2)
C(1)-C(9)	1.485(2)
C(2)-C(3)	1.509(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.513(2)
C(3)-C(16)	1.522(2)
C(3)-H(3)	1.0000
C(4)-C(5)	1.379(2)
C(4)-C(9)	1.423(2)
C(5)-C(6)	1.406(2)
C(5)-C(22)	1.433(2)
C(6)-C(7)	1.406(2)
C(7)-C(8)	1.418(2)
C(7)-C(10)	1.442(2)
C(8)-C(9)	1.388(2)
C(8)-C(30)	1.490(2)
C(10)-C(11)	1.353(3)

C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(13)	1.390(2)
C(13)-C(14)	1.424(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.363(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.381(2)
C(16)-C(17)	1.393(3)
C(17)-C(18)	1.394(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.379(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.376(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.390(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.196(2)
C(23)-C(24)	1.434(2)
C(24)-C(25)	1.397(2)
C(24)-C(29)	1.398(2)
C(25)-C(26)	1.389(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.379(3)

C(26)-H(26)	0.9500
C(27)-C(28)	1.385(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.388(2)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(35)	1.392(2)
C(30)-C(31)	1.396(2)
C(31)-C(32)	1.390(3)
C(31)-H(31)	0.9500
C(32)-C(33)	1.381(3)
C(32)-H(32)	0.9500
C(33)-C(34)	1.387(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.389(2)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500

C(11)-S(1)-C(6)	90.97(8)
C(11)-S(1)-S(2)#1	106.29(7)
C(6)-S(1)-S(2)#1	132.06(6)
C(15)-S(2)-C(12)	92.30(9)
C(2)-C(1)-C(12)	124.46(15)
C(2)-C(1)-C(9)	109.14(14)
C(12)-C(1)-C(9)	126.29(15)
C(1)-C(2)-C(3)	112.78(15)

C(1)-C(2)-H(2)	123.6
C(3)-C(2)-H(2)	123.6
C(2)-C(3)-C(4)	101.17(13)
C(2)-C(3)-C(16)	112.52(14)
C(4)-C(3)-C(16)	115.62(13)
C(2)-C(3)-H(3)	109.1
C(4)-C(3)-H(3)	109.1
C(16)-C(3)-H(3)	109.1
C(5)-C(4)-C(9)	121.64(16)
C(5)-C(4)-C(3)	128.11(15)
C(9)-C(4)-C(3)	110.19(14)
C(4)-C(5)-C(6)	116.51(15)
C(4)-C(5)-C(22)	124.69(16)
C(6)-C(5)-C(22)	118.74(15)
C(5)-C(6)-C(7)	122.87(15)
C(5)-C(6)-S(1)	125.24(12)
C(7)-C(6)-S(1)	111.86(13)
C(6)-C(7)-C(8)	119.94(15)
C(6)-C(7)-C(10)	111.10(15)
C(8)-C(7)-C(10)	128.94(15)
C(9)-C(8)-C(7)	117.22(14)
C(9)-C(8)-C(30)	123.70(14)
C(7)-C(8)-C(30)	119.07(14)
C(8)-C(9)-C(4)	121.75(14)
C(8)-C(9)-C(1)	131.56(14)
C(4)-C(9)-C(1)	106.66(14)

C(11)-C(10)-C(7)	112.32(16)
C(11)-C(10)-H(10)	123.8
C(7)-C(10)-H(10)	123.8
C(10)-C(11)-S(1)	113.75(15)
C(10)-C(11)-H(11)	123.1
S(1)-C(11)-H(11)	123.1
C(13)-C(12)-C(1)	129.01(15)
C(13)-C(12)-S(2)	111.35(12)
C(1)-C(12)-S(2)	119.59(12)
C(12)-C(13)-C(14)	111.34(16)
C(12)-C(13)-H(13)	124.3
C(14)-C(13)-H(13)	124.3
C(15)-C(14)-C(13)	113.35(17)
C(15)-C(14)-H(14)	123.3
C(13)-C(14)-H(14)	123.3
C(14)-C(15)-S(2)	111.66(14)
C(14)-C(15)-H(15)	124.2
S(2)-C(15)-H(15)	124.2
C(21)-C(16)-C(17)	118.88(17)
C(21)-C(16)-C(3)	121.01(16)
C(17)-C(16)-C(3)	119.99(15)
C(16)-C(17)-C(18)	119.95(18)
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(19)-C(18)-C(17)	120.68(19)
C(19)-C(18)-H(18)	119.7

C(17)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	119.29(19)
C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(19)-C(20)-C(21)	120.5(2)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(16)-C(21)-C(20)	120.69(19)
C(16)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(23)-C(22)-C(5)	170.49(19)
C(22)-C(23)-C(24)	176.7(2)
C(25)-C(24)-C(29)	119.38(15)
C(25)-C(24)-C(23)	121.28(16)
C(29)-C(24)-C(23)	119.33(16)
C(26)-C(25)-C(24)	119.76(17)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(27)-C(26)-C(25)	120.42(17)
C(27)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(28)	120.39(16)
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-H(27)	119.8
C(27)-C(28)-C(29)	119.80(17)
C(27)-C(28)-H(28)	120.1

C(29)-C(28)-H(28)	120.1
C(28)-C(29)-C(24)	120.24(17)
C(28)-C(29)-H(29)	119.9
C(24)-C(29)-H(29)	119.9
C(35)-C(30)-C(31)	119.01(15)
C(35)-C(30)-C(8)	120.85(15)
C(31)-C(30)-C(8)	120.14(15)
C(32)-C(31)-C(30)	120.14(17)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(33)-C(32)-C(31)	120.48(18)
C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8
C(32)-C(33)-C(34)	119.71(17)
C(32)-C(33)-H(33)	120.1
C(34)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	120.16(18)
C(33)-C(34)-H(34)	119.9
C(35)-C(34)-H(34)	119.9
C(34)-C(35)-C(30)	120.49(17)
C(34)-C(35)-H(35)	119.8
C(30)-C(35)-H(35)	119.8

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for y2488.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	30(1)	18(1)	46(1)	-9(1)	-13(1)	-6(1)
S(2)	31(1)	20(1)	50(1)	-6(1)	-7(1)	-8(1)
C(1)	24(1)	17(1)	22(1)	-2(1)	-4(1)	-7(1)
C(2)	27(1)	21(1)	24(1)	-6(1)	-6(1)	-5(1)
C(3)	24(1)	20(1)	21(1)	-2(1)	-5(1)	-5(1)
C(4)	21(1)	17(1)	23(1)	-1(1)	-4(1)	-7(1)
C(5)	20(1)	16(1)	26(1)	-2(1)	-3(1)	-5(1)
C(6)	19(1)	15(1)	29(1)	-2(1)	-3(1)	-6(1)
C(7)	18(1)	19(1)	26(1)	-3(1)	-2(1)	-7(1)
C(8)	18(1)	16(1)	21(1)	-1(1)	-3(1)	-6(1)
C(9)	19(1)	15(1)	24(1)	0(1)	-3(1)	-5(1)
C(10)	25(1)	27(1)	32(1)	-7(1)	-10(1)	-6(1)
C(11)	32(1)	30(1)	46(1)	-14(1)	-15(1)	-7(1)
C(12)	27(1)	16(1)	24(1)	-3(1)	-5(1)	-7(1)
C(13)	29(1)	19(1)	24(1)	-4(1)	-4(1)	-5(1)
C(14)	28(1)	26(1)	37(1)	-6(1)	-7(1)	0(1)
C(15)	38(1)	16(1)	50(1)	-6(1)	-6(1)	-4(1)

C(16)	25(1)	19(1)	26(1)	-8(1)	-8(1)	-4(1)
C(17)	33(1)	36(1)	28(1)	-9(1)	-5(1)	-16(1)
C(18)	35(1)	48(1)	42(1)	-24(1)	3(1)	-22(1)
C(19)	25(1)	44(1)	63(1)	-31(1)	-9(1)	-6(1)
C(20)	36(1)	39(1)	53(1)	-15(1)	-22(1)	1(1)
C(21)	34(1)	31(1)	30(1)	-7(1)	-11(1)	-4(1)
C(22)	23(1)	19(1)	28(1)	-2(1)	-6(1)	-6(1)
C(23)	26(1)	20(1)	31(1)	-2(1)	-6(1)	-7(1)
C(24)	21(1)	16(1)	30(1)	0(1)	-5(1)	-4(1)
C(25)	25(1)	24(1)	31(1)	-2(1)	-7(1)	-8(1)
C(26)	24(1)	29(1)	32(1)	4(1)	-10(1)	-7(1)
C(27)	21(1)	18(1)	41(1)	4(1)	-5(1)	-3(1)
C(28)	31(1)	19(1)	39(1)	-7(1)	-5(1)	-7(1)
C(29)	30(1)	24(1)	30(1)	-4(1)	-8(1)	-7(1)
C(30)	22(1)	17(1)	21(1)	-4(1)	-6(1)	-4(1)
C(31)	26(1)	25(1)	35(1)	-5(1)	-9(1)	-8(1)
C(32)	26(1)	34(1)	47(1)	-12(1)	-17(1)	-1(1)
C(33)	42(1)	23(1)	33(1)	-6(1)	-19(1)	4(1)
C(34)	43(1)	21(1)	27(1)	1(1)	-6(1)	-6(1)
C(35)	26(1)	21(1)	25(1)	-1(1)	-3(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for y2488.

	x	y	z	U(eq)
H(2)	5329	-559	5965	30
H(3)	5057	1857	5592	28
H(10)	7632	1031	10071	33
H(11)	6703	3298	10241	40
H(13)	9347	-2005	6873	31
H(14)	10260	-4444	7206	41
H(15)	8358	-5362	7727	46
H(17)	2737	980	8256	37
H(18)	253	1448	8590	46
H(19)	-910	2491	7134	50
H(20)	399	3146	5352	51
H(21)	2874	2692	5007	39
H(25)	2431	6321	4819	33
H(26)	1411	8568	4140	37
H(27)	1321	10114	5026	37
H(28)	2257	9440	6599	37
H(29)	3309	7198	7278	35

H(31)	9616	-436	8412	34
H(32)	11150	-2423	9202	43
H(33)	10248	-4081	10334	42
H(34)	7810	-3780	10635	40
H(35)	6277	-1816	9818	31

Table 6. Torsion angles [deg] for y2488.

C(12)-C(1)-C(2)-C(3)	-174.50(15)
C(9)-C(1)-C(2)-C(3)	2.0(2)
C(1)-C(2)-C(3)-C(4)	-0.59(19)
C(1)-C(2)-C(3)-C(16)	-124.57(16)
C(2)-C(3)-C(4)-C(5)	176.15(16)
C(16)-C(3)-C(4)-C(5)	-62.0(2)
C(2)-C(3)-C(4)-C(9)	-1.09(17)
C(16)-C(3)-C(4)-C(9)	120.76(15)
C(9)-C(4)-C(5)-C(6)	-2.9(2)
C(3)-C(4)-C(5)-C(6)	-179.88(15)
C(9)-C(4)-C(5)-C(22)	174.20(15)
C(3)-C(4)-C(5)-C(22)	-2.8(3)
C(4)-C(5)-C(6)-C(7)	1.2(2)
C(22)-C(5)-C(6)-C(7)	-176.08(15)
C(4)-C(5)-C(6)-S(1)	-176.70(12)
C(22)-C(5)-C(6)-S(1)	6.0(2)

C(11)-S(1)-C(6)-C(5)	177.75(16)
S(2)#1-S(1)-C(6)-C(5)	-69.11(16)
C(11)-S(1)-C(6)-C(7)	-0.37(13)
S(2)#1-S(1)-C(6)-C(7)	112.78(12)
C(5)-C(6)-C(7)-C(8)	0.6(2)
S(1)-C(6)-C(7)-C(8)	178.76(12)
C(5)-C(6)-C(7)-C(10)	-177.85(15)
S(1)-C(6)-C(7)-C(10)	0.32(18)
C(6)-C(7)-C(8)-C(9)	-0.7(2)
C(10)-C(7)-C(8)-C(9)	177.43(16)
C(6)-C(7)-C(8)-C(30)	179.45(14)
C(10)-C(7)-C(8)-C(30)	-2.4(3)
C(7)-C(8)-C(9)-C(4)	-1.0(2)
C(30)-C(8)-C(9)-C(4)	178.86(15)
C(7)-C(8)-C(9)-C(1)	176.67(16)
C(30)-C(8)-C(9)-C(1)	-3.5(3)
C(5)-C(4)-C(9)-C(8)	2.9(2)
C(3)-C(4)-C(9)-C(8)	-179.63(14)
C(5)-C(4)-C(9)-C(1)	-175.24(14)
C(3)-C(4)-C(9)-C(1)	2.21(18)
C(2)-C(1)-C(9)-C(8)	179.50(17)
C(12)-C(1)-C(9)-C(8)	-4.1(3)
C(2)-C(1)-C(9)-C(4)	-2.58(18)
C(12)-C(1)-C(9)-C(4)	173.80(15)
C(6)-C(7)-C(10)-C(11)	-0.1(2)
C(8)-C(7)-C(10)-C(11)	-178.34(17)

C(7)-C(10)-C(11)-S(1)	-0.2(2)
C(6)-S(1)-C(11)-C(10)	0.34(16)
S(2)#1-S(1)-C(11)-C(10)	-134.33(14)
C(2)-C(1)-C(12)-C(13)	118.6(2)
C(9)-C(1)-C(12)-C(13)	-57.2(3)
C(2)-C(1)-C(12)-S(2)	-58.5(2)
C(9)-C(1)-C(12)-S(2)	125.62(16)
C(15)-S(2)-C(12)-C(13)	-0.15(15)
C(15)-S(2)-C(12)-C(1)	177.49(15)
C(1)-C(12)-C(13)-C(14)	-177.46(17)
S(2)-C(12)-C(13)-C(14)	-0.10(19)
C(12)-C(13)-C(14)-C(15)	0.4(2)
C(13)-C(14)-C(15)-S(2)	-0.5(2)
C(12)-S(2)-C(15)-C(14)	0.37(18)
C(2)-C(3)-C(16)-C(21)	-106.42(18)
C(4)-C(3)-C(16)-C(21)	138.02(17)
C(2)-C(3)-C(16)-C(17)	69.5(2)
C(4)-C(3)-C(16)-C(17)	-46.1(2)
C(21)-C(16)-C(17)-C(18)	0.9(3)
C(3)-C(16)-C(17)-C(18)	-175.05(16)
C(16)-C(17)-C(18)-C(19)	0.3(3)
C(17)-C(18)-C(19)-C(20)	-1.4(3)
C(18)-C(19)-C(20)-C(21)	1.3(3)
C(17)-C(16)-C(21)-C(20)	-1.0(3)
C(3)-C(16)-C(21)-C(20)	174.92(17)
C(19)-C(20)-C(21)-C(16)	-0.1(3)

C(4)-C(5)-C(22)-C(23)	-151.9(11)
C(6)-C(5)-C(22)-C(23)	25.1(12)
C(5)-C(22)-C(23)-C(24)	-22(4)
C(22)-C(23)-C(24)-C(25)	169(3)
C(22)-C(23)-C(24)-C(29)	-10(4)
C(29)-C(24)-C(25)-C(26)	-0.7(3)
C(23)-C(24)-C(25)-C(26)	-179.41(16)
C(24)-C(25)-C(26)-C(27)	0.0(3)
C(25)-C(26)-C(27)-C(28)	0.3(3)
C(26)-C(27)-C(28)-C(29)	0.2(3)
C(27)-C(28)-C(29)-C(24)	-0.9(3)
C(25)-C(24)-C(29)-C(28)	1.1(3)
C(23)-C(24)-C(29)-C(28)	179.87(17)
C(9)-C(8)-C(30)-C(35)	-64.4(2)
C(7)-C(8)-C(30)-C(35)	115.41(17)
C(9)-C(8)-C(30)-C(31)	115.08(18)
C(7)-C(8)-C(30)-C(31)	-65.1(2)
C(35)-C(30)-C(31)-C(32)	1.3(3)
C(8)-C(30)-C(31)-C(32)	-178.22(16)
C(30)-C(31)-C(32)-C(33)	-1.5(3)
C(31)-C(32)-C(33)-C(34)	0.9(3)
C(32)-C(33)-C(34)-C(35)	-0.2(3)
C(33)-C(34)-C(35)-C(30)	0.0(3)
C(31)-C(30)-C(35)-C(34)	-0.6(3)
C(8)-C(30)-C(35)-C(34)	178.94(16)

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z

Table 7. Hydrogen bonds for y2488 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)