SYNTHESIS OF FUSED POLYCYCLES BY 1,4-PALLADIUM MIGRATION CHEMISTRY

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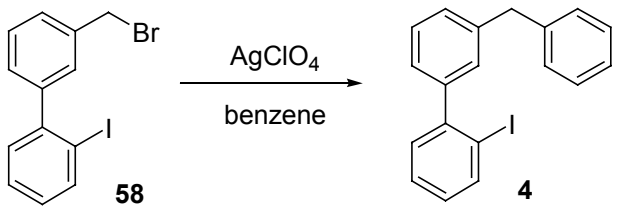
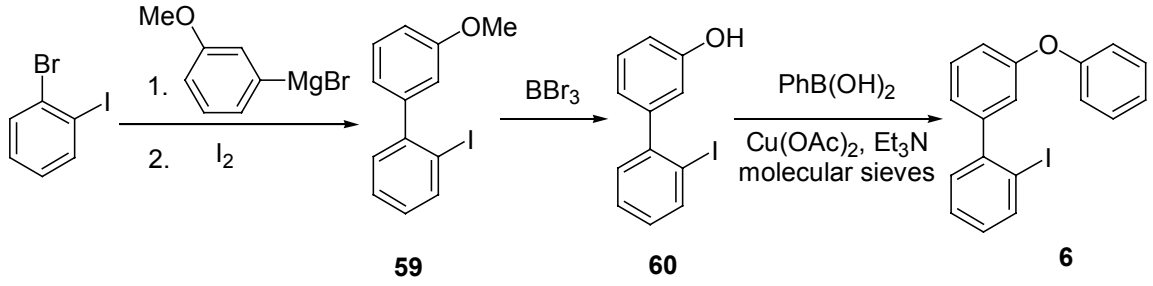
General procedures. All ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75.5 MHz or 400 and 100 MHz respectively. Thin-layer chromatography was performed using commercially prepared 60-mesh silica gel plates (Whatman K6F), and visualization was effected with short wavelength UV light (254 nm) and/or a basic $KMnO_4$ solution [3 g of $KMnO_4$ + 20 g of K_2CO_3 + 5 mL of NaOH (5 %) + 300 mL of H_2O]. All melting points are uncorrected. High resolution mass spectra were recorded on a Kratos MS50TC double focusing magnetic sector mass spectrometer using EI at 70 eV. Compounds **19**,[1] **20**,[1] **36**,[1] and **49**[1] were prepared according to literature procedures.



58 **4**

3'-Benzyl-2-iodobiphenyl (4). This biphenyl was prepared from 3'-bromomethyl-2-iodobiphenyl (**58**)[1] by following a procedure from the literature.[2] To a suspension of $AgClO_4$ (0.28 g, 1.4 mmol) in benzene (4.0 mL) was added compound **58** (0.261 g, 0.7 mmol) in benzene (4.0 mL) and the resulting mixture was stirred overnight at room temperature in the dark. The reaction mixture was diluted with diethyl ether (50 mL), filtered and washed with brine (25 mL). The organic layer was dried (Na_2SO_4), filtered and the solvent evaporated under reduced pressure. The residue was purified by silica gel column chromatography using 50:1 hexane/EtOAc to afford 0.187 g (72 %) of the indicated compound **4** as a colorless oil: ^{1}H NMR ($CDCl_3$) δ 4.03 (s, 3H), 6.97-7.01 (m, 1H), 7.15-7.34 (m, 11H), 7.92 (dd, J = 1.0, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 42.0, 98.8, 126.2, 127.1, 128.2, 128.2, 128.3, 128.6, 128.8,

129.1, 130.1, 130.2, 139.6, 140.8, 141.0, 144.3, 146.6; IR (CH_2Cl_2) 3056, 3025, 2917, 1601, 1583, 1494, 1461 cm^{-1}; HRMS *m/z* 370.0224 (calcd for $C_{19}H_{15}I$, 370.0218).

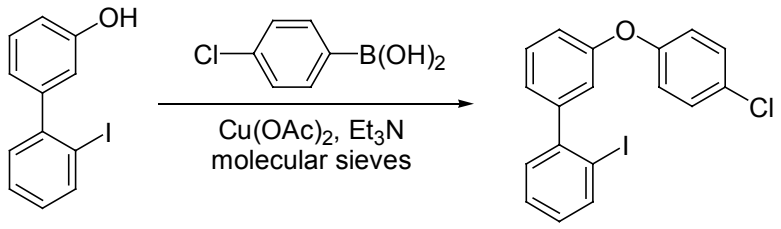


59 **60** **6**

2-Iodo-3'-methoxybiphenyl (59). Compound **59** was prepared by a procedure reported by Hart *et al*.[3] A solution of 2-bromoiodobenzene (1.415 g, 5.0 mmol) in THF (10 mL) was added slowly (90 min) to a solution of 3-methoxyphenylmagnesium bromide [prepared from 3-bromoanisole (1.87 g, 10 mmol) and Mg (0.246 g, 10 mmol) in THF (30 mL)], and the mixture was stirred under Ar for an additional 14 h at room temperature. The reaction was quenched by adding I_2 (3.8 g, 15 mmol), and the mixture was stirred for an additional 30 min at room temperature. The excess I_2 was destroyed by adding 10 % aq $NaHSO_3$ (35 mL) and the organic layer was separated and washed with brine (20 mL). Finally, the organic layer was dried ($MgSO_4$), filtered, and the solvent removed under reduced pressure. The residue was chromatographed using 30:1 hexane/EtOAc to afford 0.620 g (40 %) of the desired compound **59** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 3.84 (s, 3H), 6.88-6.95 (m, 3H), 7.01-7.05 (m, 1H), 7.29-7.38 (m, 3H), 7.95 (dd, *J* = 1.2, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 55.4, 98.5, 113.4, 115.0, 121.8, 128.1, 128.9, 129.1, 130.1, 139.6, 145.5, 146.5, 159.1; HRMS *m/z* 309.9859 (calcd for $C_{13}H_{11}IO$, 309.9855).

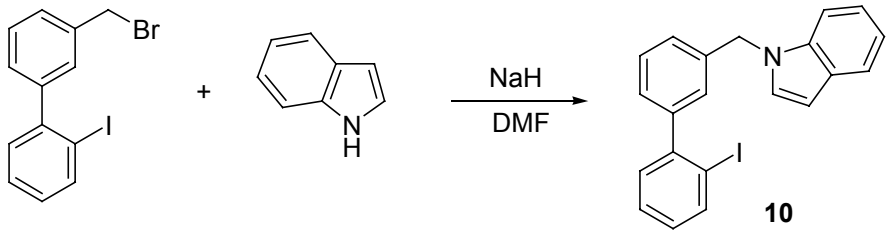
2-Iodo-3'-phenoxybiphenyl (6). This biphenyl was prepared in two steps from 2-iodo-3-methoxybiphenyl (**59**). To a solution of compound **59** (0.97 g, 3.14 mmol) in CH_2Cl_2 (20

mL) at -78 ^{o}C was added 1.0 M BBr_3 in CH_2Cl_2 (4.1 mL, 4.1 mmol). The resulting solution was allowed to warm to room temperature and stirred for 2 h. The mixture was worked up with ice (15 g) and extracted with diethyl ether (75 mL). The organic layer was dried (Na_2SO_4), filtered and the solvent evaporated under reduced pressure. The residue was purified by silica gel column chromatography using 3:1 hexane/EtOAc to afford 0.91 g (98 %) of 3-(2-iodophenyl)phenol (**60**) as a clear oil: ^{1}H NMR ($CDCl_3$) δ 5.04 (br s, 1H), 6.80-6.81 (m, 1H), 6.85-6.90 (m, 2H), 7.00-7.05 (m, 1H), 7.25-7.31 (m, 2H), 7.37 (dt, *J* = 0.8, 7.6 Hz, 1H), 7.94 (dd, *J* = 0.8, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 98.4, 114.7, 116.4, 122.0, 128.1, 128.9, 129.3, 130.0, 139.5, 145.8, 146.2, 155.0. 3-(2-Iodophenyl)phenol (**60**) was phenylated by a literature procedure.[4] A suspension of 3-(2-iodophenyl)phenol (0.222 g, 0.75 mmol), phenylboronic acid (0.183 g, 1.5 mmol), $Cu(OAc)_2$ (0.163 g, 0.90 mmol), Et_3N (0.38 g, 3.75 mmol), and 5 Angstrom molecular sieves (0.2 g) in CH_2Cl_2 (6.0 mL) was stirred under O_2 (1 atm) for 2 d at room temperature. The reaction mixture was diluted with diethyl ether (50 mL), filtered, and the solvent evaporated under reduced pressure. The residue was purified by silica gel column chromatography using 15:1 hexane/EtOAc to afford 0.129 g (46 %) of the indicated compound **6** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 7.00-7.12 (m, 7H), 7.25-7.40 (m, 5H), 7.92 (dd, *J* = 1.2, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 98.4, 118.2, 119.1, 119.8, 123.4, 124.2, 128.2, 129.0, 129.4, 129.8, 130.0, 139.6, 145.9, 146.0, 156.8, 157.1; IR (CH_2Cl_2) 3058, 1578, 1488, 1460, 1222, cm^{-1}; HRMS *m/z* 372.0020 (calcd for $C_{18}H_{13}IO$, 372.0011).



60 **8**

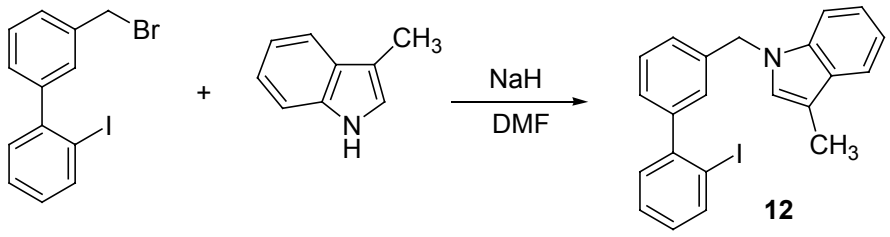
2-Iodo-3'-(*p*-chlorophenoxy)biphenyl (8). This biphenyl was prepared by a procedure similar to that used for compound **6**. A suspension of 3-(2-iodophenyl)phenol (**60**) (0.222 g, 0.75 mmol), *p*-chlorophenylboronic acid (0.235 g, 1.5 mmol), $Cu(OAc)_2$ (0.163 g, 0.90 mmol), Et_3N (0.38 g, 3.75 mmol), and 5 Angstrom molecular sieves (0.2 g) in CH_2Cl_2 (6.0 mL) was stirred under O_2 (1 atm) for 2 d at room temperature. The reaction mixture was diluted with diethyl ether (50 mL), filtered, and the solvent evaporated under reduced pressure. The residue was purified by chromatography on a silica gel column using 30:1 hexanes/ethyl acetate to afford 79.5 mg (26 %) of the indicated compound **8** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 6.96-7.09 (m, 6H), 7.27-7.41 (m, 5H), 7.93 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 98.4, 118.2, 119.9, 120.3, 124.6, 128.2, 128.4, 129.1, 129.6, 129.8, 130.0, 139.6, 145.8, 146.0, 155.8, 156.4; IR (CH_2Cl_2) 3057, 1576, 1484, 1460, 1228 cm^{-1}; HRMS *m/z* 405.9632 (calcd for $C_{18}H_{12}IClO$, 405.9621).



10

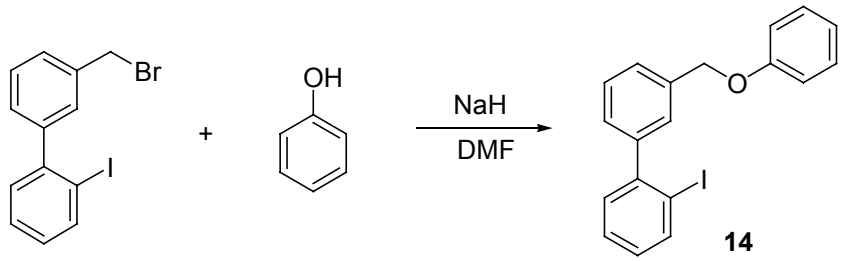
1-[3-(2-Iodophenyl)benzyl]indole (10). To a suspension of NaH (0.031 g, 1.30 mmol) in DMF (2 mL) at 0 ^{0}C was added 1*H*-indole (0.117 g, 1.0 mmol) in DMF (3 mL) and the

mixture was stirred at room temperature for 30 min. At this point 3'-bromomethyl-2-iodobiphenyl (**58**)[1] (0.347 g, 0.93 mmol) in DMF (3 mL) was added and the reaction mixture was stirred at 50 ^{o}C for 3 h. The reaction mixture was diluted with diethyl ether (50 mL) and washed with brine (60 mL). The aqueous layer was reextracted with diethyl ether (15 mL) and the organic layers were combined, dried ($MgSO_4$), and the solvent evaporated under reduced pressure. The residue was purified by column chromatography using 12:1 hexanes/ethyl acetate to afford 0.335 g (88 %) of the desired compound **10** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 5.34 (s, 2H), 6.54 (d, *J* = 2.8 Hz, 1H), 6.98 (td, *J* = 7.6, 1.6 Hz, 1H), 7.09-7.23 (m, 7H), 7.30-7.34 (m, 3H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.90 (dd, *J* = 8.0, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 50.1, 98.6, 101.9, 109.9, 119.6, 121.1, 121.8, 126.2, 128.0, 128.2, 128.4, 128.6, 128.6, 128.9, 129.0, 130.1, 136.4, 137.4, 139.6, 144.6, 146.1; IR (CH_2Cl_2) 3052, 2972, 2922, 2863, 1462, 1437, 1316 cm^{-1}; HRMS *m/z* 409.0334 (calcd for $C_{21}H_{16}IN$, 409.0328).



1-[3-(2-Iodophenyl)benzyl]-3-methylindole (12). To a suspension of NaH (0.031 g, 1.30 mmol) in DMF (2 mL) at 0 ^{0}C was added 3-methyl-1*H*-indole (0.131 g, 1.0 mmol) in DMF (3 mL) and the mixture was stirred at room temperature for 30 min. At this point 3'-bromomethyl-2-iodobiphenyl (**58**)[1] (0.347 g, 0.93 mmol) in DMF (3 mL) was added and the reaction mixture was stirred at 50 ^{o}C for 3 h. The reaction mixture was diluted with diethyl ether (50 mL) and washed with brine (60 mL). The aqueous layer was reextracted with

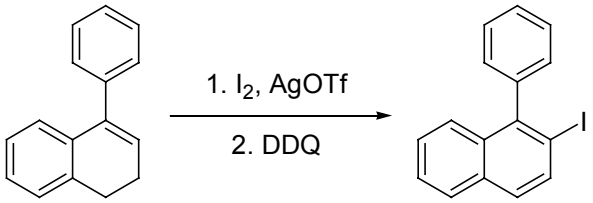
diethyl ether (15 mL) and the organic layers were combined, dried ($MgSO_4$), and the solvent evaporated under reduced pressure. The residue was purified by column chromatography using 12:1 hexanes/ethyl acetate to afford 0.362 g (92 %) of the desired compound **12** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 2.33 (d, J = 0.8 Hz, 3H), 5.29 (s, 2H), 6.92-6.92 (m, 1H), 6.97-6.99 (m, 1H), 7.10-7.24 (m, 6H), 7.27-7.34 (m, 3H), 7.56-7.58 (m, 1H), 7.90-7.92 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 10.1, 50.1, 98.8, 109.9, 111.2, 119.1, 119.3, 121.9, 126.2, 126.4, 128.2, 128.4, 128.7, 128.7, 129.2, 129.3, 130.3, 136.9, 137.9, 139.8, 144.7, 146.4; IR (CH_2Cl_2) 3052, 2914, 1611, 1465, 1330, 1012 cm^{-1}; HRMS *m/z* 423.0491 (calcd for $C_{22}H_{18}IN$, 423.0484).



14

3-(2-Iodophenyl)benzyl phenyl ether (14). To a suspension of NaH (0.031 g, 1.30 mmol) in DMF (2 mL) at 0 ^{0}C was added phenol (0.094 g, 1.0 mmol) in DMF (3 mL) and the mixture was stirred at room temperature for 30 min. At this point, 3'-bromomethyl-2-iodobiphenyl (**58**)[1] (0.347 g, 0.93 mmol) in DMF (3 mL) was added and the reaction mixture was stirred at room temperature for 3 h. The reaction mixture was diluted with diethyl ether (50 mL) and washed with brine (60 mL). The aqueous layer was reextracted with diethyl ether (15 mL) and the organic layers were combined, dried ($MgSO_4$), and the solvent evaporated under reduced pressure. The residue was purified by column chromatography using 12:1 hexanes/ethyl acetate to afford 0.359 g (100 %) of the desired compound **14** as a

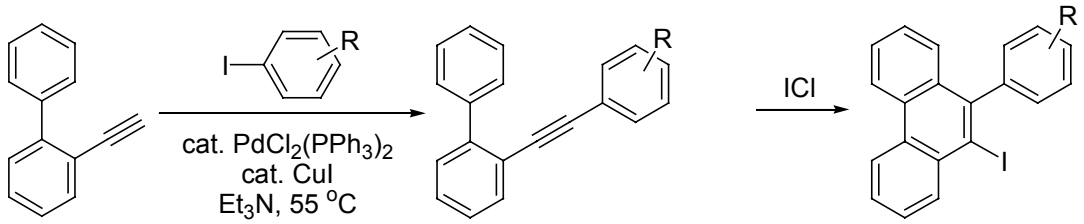
clear oil: ^{1}H NMR ($CDCl_3$) δ 5.13 (s, 2H), 6.96-7.04 (m, 4H), 7.26-7.33 (m, 4H), 7.39-7.46 (m, 4H), 7.94-7.96 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 69.9, 98.6, 115.0, 121.1, 126.8, 128.3, 128.4, 128.5, 129.0, 129.0, 129.6, 130.2, 137.0, 139.6, 144.5, 146.4, 158.8; IR (CH_2Cl_2) 3056, 2919, 1598, 1494, 1238 cm^{-1}; HRMS *m/z* 386.0172 (calcd for $C_{19}H_{15}IO$, 386.0168).



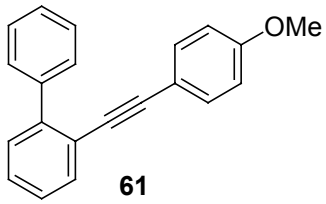
17

2-Iodo-1-phenylnaphthalene (17). To a solution of 3,4-dihydro-1-phenylnaphthalene (1.30 g, 6.3 mmol) and I_2 (2.24 g, 8.8 mmol) in anhydrous CH_3CN (15 mL) was added dropwise AgOTf (1.75 g, 6.8 mmol) in anhydrous CH_3CN (20 mL). The resulting mixture was stirred at room temperature in the dark for 1 h. The reaction was diluted with diethyl ether (70 mL) and washed with satd aq $Na_2S_2O_3$ (25 mL). The organic layer was dried (Na_2SO_4), filtered and the solvent removed under reduced pressure. The residue was dissolved in benzene (25 mL). To this solution was added DDQ (2.86 g, 12.6 mmol) and the reaction was heated at 65 ^{o}C for 2 d. The resulting mixture was filtered and washed with 10 % aq Na_2CO_3 (25 mL). The organic layer was filtered, dried (Na_2SO_4) and the solvent removed under reduced pressure. The residue was purified by silica gel column chromatography using 50:1 hexane/EtOAc to afford 1.47 g (70 %) of the indicated compound **17** as a clear oil: ^{1}H NMR ($CDCl_3$) δ 7.22-7.26 (m, 2H), 7.32-7.34 (m, 1H), 7.38-7.56 (m, 6H), 7.80-7.83 (m, 1H), 7.95 (d, J = 8.7 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 98.7, 126.5, 127.0, 127.4, 128.1, 128.1, 128.7, 129.3, 130.2, 133.1, 133.6, 135.8, 143.5, 144.7; IR

(CH_2Cl_2) 3053, 1577, 1502, 1442, 1382, 1306 cm^{-1}; HRMS *m/z* 329.9910 (calcd for $C_{16}H_{11}I$, 329.9906).

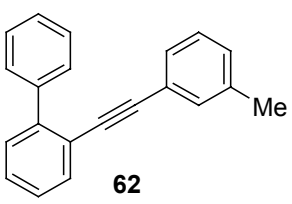


General procedure for preparation of the 2-(arylethynyl)biphenyls. To a solution of the corresponding aryl iodide (1.0 mmol) and the terminal alkyne (1.2 mmol, 1.2 equiv) in Et_3N (4.0 mL) were added $PdCl_2(PPh_3)_2$ (1.4 mg, 2 mol %) and CuI (2.0 mg, 1 mol %). The resulting mixture was then heated under an N_2 atmosphere at 55 °C for 3 h. The mixture was allowed to cool to room temperature, and the ammonium salt was removed by filtration. The solvent was removed under reduced pressure and the residue was purified by column chromatography on silica gel to afford the corresponding product.



61

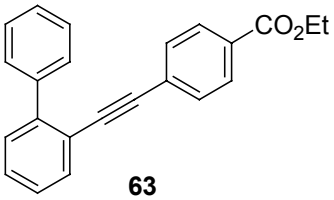
2-[(4-Methoxyphenyl)ethynyl]biphenyl (61). 2-Ethynylbiphenyl[5] and 4-iodoanisole were employed. Purification by flash chromatography (30:1 hexane/EtOAc) afforded 0.21 g (74 %) of the product as a clear liquid: ^{1}H NMR ($CDCl_3$) δ 3.80 (s, 3H), 6.84 (dd, *J* = 2.4, 6.9 Hz, 2H), 7.30 (dd, *J* = 2.1, 6.9 Hz, 2H), 7.34-7.50 (m, 6H), 7.64-7.73 (m, 3H); ^{13}C NMR ($CDCl_3$) δ 55.5, 88.4, 92.5, 114.2, 115.9, 122.2, 127.3, 127.6, 128.1, 128.4, 129.6, 129.7, 132.9, 133.1, 140.9, 143.9, 159.8.



62

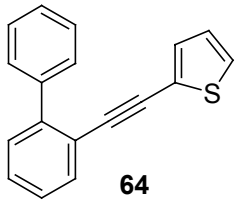
2-[(3-Methylphenyl)ethynyl]biphenyl (62). 2-Ethynylbiphenyl[5] and 3-iodotoluene were employed. Purification by flash

chromatography (40:1 hexane/EtOAc) afforded 0.26 g (95 %) of the product as a clear liquid: ^{1}H NMR ($CDCl_3$) δ 2.34 (s, 3H), 7.12-7.22 (m, 4H), 7.33-7.53 (m, 6H), 7.67-7.74 (m, 3H); ^{13}C NMR ($CDCl_3$) δ 21.5, 89.3, 92.7, 122.0, 123.5, 127.3, 127.7, 128.2, 128.4, 128.7, 128.7, 129.3, 129.7, 129.7, 132.2, 133.1, 138.2, 140.9, 144.1.



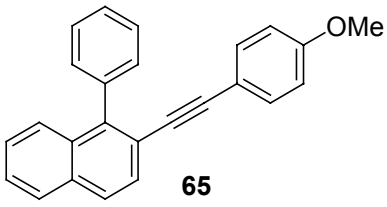
63

Ethyl 4-(biphen-2-ylethynyl)benzoate (63). 2-Ethynylbiphenyl[5] and ethyl 4-iodobenzoate were employed. Purification by flash chromatography (15:1 hexane/EtOAc) afforded 0.27 g (84 %) of the product as a white solid: mp 58-60 ºC; ^{1}H NMR ($CDCl_3$) δ 1.38 (t, J = 6.9 Hz, 3H), 4.36 (q, J = 7.2 Hz, 2H), 7.32-7.48 (m, 8H), 7.64-7.66 (m, 3H), 7.96 (d, J = 8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 14.6, 61.3, 91.7, 92.6, 121.3, 127.4, 127.9, 128.2, 128.3, 129.3, 129.63, 129.64, 129.8, 129.9, 131.4, 133.2, 140.6, 144.5, 166.3.



64

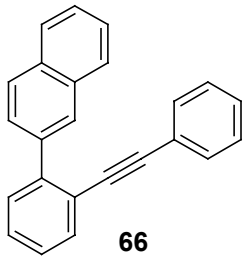
2-(Biphen-2-ylethynyl)thiophene (64). 2-Ethynylbiphenyl[5] and 2-iodothiophene were employed. Purification by flash chromatography (15:1 hexane/EtOAc) afforded 0.22 g (85 %) of the product as a light yellow liquid: ^{1}H NMR ($CDCl_3$) δ 6.98-7.00 (m, 1H), 7.15-7.17 (m, 1H), 7.25-7.27 (m, 1H), 7.37-7.55 (m, 6H), 7.66-7.75 (m, 3H); ^{13}C NMR ($CDCl_3$) δ 85.9, 93.5, 121.6, 123.8, 127.3, 127.4, 127.5, 127.8, 128.3, 129.0, 129.6, 129.8, 131.8, 132.8, 140.7, 144.0.



65

2-[(4-Methoxyphenyl)ethynyl]-1-phenylnaphthalene (65). 2-Iodo-1-phenylnaphthalene and 4-ethynylanisole[6] were employed. Purification by flash chromatography (20:1

hexane/EtOAc) afforded 0.27 g (82 %) of the product as a clear oil: ^{1}H NMR ($CDCl_3$) δ 3.81 (s, 3H), 6.82 (dd, *J* = 6.9, 2.1 Hz, 2H), 7.17 (dd, *J* = 6.9, 2.1 Hz, 2H), 7.43-7.60 (m, 7H), 7.68-7.72 (m, 2H), 7.83-7.94 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 55.4, 88.9, 93.5, 114, 115.7, 120.7, 126.4, 126.6, 126.8, 127.6, 127.6, 128.1, 128.2, 128.4, 130.9, 132.4, 133.0, 133.1, 139.3, 142.8, 159.7.

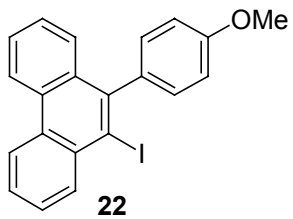


66

2-[2-(Phenylethynyl)phenyl]naphthalene (66). 2-(2-Iodophenyl)naphthalene[15] and phenylacetylene were employed. Purification by flash chromatography (40:1 hexane/EtOAc) afforded 0.29 g (96 %) of the product as a light yellow liquid: ^{1}H NMR ($CDCl_3$) δ 7.24-7.58 (m, 10H), 7.70-7.72 (m, 1H), 7.86-7.97 (m, 4H), 8.17 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 89.7, 92.7, 122.0, 123.6, 126.2, 126.3, 127.4, 127.5, 127.9, 128.0, 128.3, 128.4, 128.5, 128.9, 130.0, 131.6, 132.9, 133.3, 133.5, 138.3, 144.0 (one sp^2 carbon missing due to overlap).

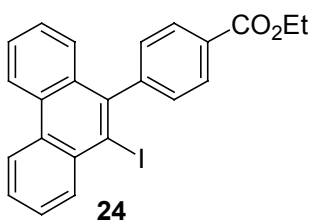
General procedure for synthesis of the phenanthrenes[7]

The following procedure was used to prepare phenanthrenes **22**, **24**, **26**, **28**, **30** and chrysene **32**. To a solution of 2-(arylethynyl)biphenyl (0.30 mmol) in CH_2Cl_2 (3 mL) under N_2 was added ICl (1.2 equiv) in CH_2Cl_2 (0.5 mL) at -78 °C. The reaction mixture was stirred at -78 °C for 1 h unless otherwise indicated. The reaction mixture was then diluted with diethyl ether (50 mL), washed with 25 mL of satd aq $Na_2S_2O_3$, dried ($MgSO_4$), and filtered. The solvent was evaporated under reduced pressure and the product was purified by chromatography on a silica gel column.



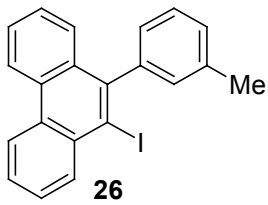
22

9-Iodo-10-(4-methoxyphenyl)phenanthrene (22). Purification by flash chromatography (30:1 hexane/EtOAc) afforded 0.122 g (99 %) of the product as a white solid: mp 170-171 ºC; ^{1}H NMR ($CDCl_3$) δ 3.94 (s, 3H), 7.09 (dd, *J* = 2.1, 6.6 Hz, 2H), 7.21 (dd, *J* = 2.1, 6.6 Hz, 2H), 7.40-7.49 (m, 2H), 7.64-7.72 (m, 3H), 8.45-8.49 (m, 1H), 8.67-8.78 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 55.6, 107.7, 114.0, 122.8, 122.9, 127.2, 127.3, 127.7, 128.3, 129.0, 130.5, 130.8, 131.3, 132.7, 132.9, 135.0, 138.2, 145.3, 159.4; IR (neat) 3066, 3024, 2834, 1610 cm^{-1}; HRMS *m/z* 410.0172 (calcd for $C_{21}H_{15}IO$, 410.0168).



24

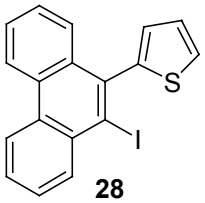
Ethyl 4-(10-iodophenanthren-9-yl)benzoate (24). The reaction mixture was stirred at room temperature for 1 h. Purification by flash chromatography (15:1 hexane/EtOAc) afforded 0.136 g (100 %) of the product as a white solid: mp 152-153 ºC; ^{1}H NMR ($CDCl_3$) δ 1.46 (t, *J* = 7.2 Hz, 3H), 4.47 (q, *J* = 7.2 Hz, 2H), 7.30-7.45 (m, 4H), 7.66-7.75 (m, 3H), 8.26 (dd, *J* = 1.8, 6.6 Hz, 2H), 8.45-8.49 (m, 1H), 8.68-8.78 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 14.6, 61.4, 106.0, 122.9, 123.0, 127.4, 127.5, 128.0, 128.4, 128.5, 130.1, 130.3, 130.4, 130.5, 130.8, 132.1, 132.5, 134.9, 144.6, 150.0, 166.7; IR (CH_2Cl_2) 3069, 2979, 1714 cm^{-1}; HRMS *m/z* 452.0278 (calcd for $C_{23}H_{17}IO_2$, 452.0273).



26

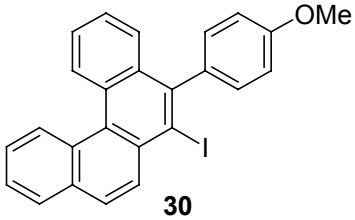
9-Iodo-10-(3-methylphenyl)phenanthrene (26). Purification by flash chromatography (30:1 hexane/EtOAc) afforded 0.117 g (99 %) of the product as a white solid: mp 134-135 ºC; ^{1}H NMR ($CDCl_3$) δ 2.44 (s, 3H), 7.07-7.09 (m, 2H), 7.30-7.32 (m, 1H), 7.41-7.45 (m, 3H), 7.63-7.70 (m, 3H), 8.45-8.48 (m, 1H), 8.67-8.73 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 21.7, 106.5, 122.6, 122.7, 127.1, 127.1, 127.5, 128.1, 128.4, 128.5, 128.8, 130.3, 130.6, 130.6, 132.5, 132.5, 134.7, 138.1,

145.4, 145.5 (one sp^2 carbon missing due to overlap); IR (CH_2Cl_2) 3067, 2971, 2921, 1602, 1563 cm^{-1}; HRMS *m/z* 394.0226 (calcd for $C_{21}H_{15}I$, 394.0219).



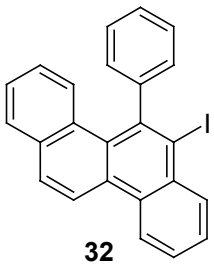
28

9-Iodo-10-(thiophen-2-yl)phenanthrene (28). Purification by flash chromatography (30:1 hexane/EtOAc) afforded 0.111 g (96 %) of the product as a white solid: mp 140-142 ºC; ^{1}H NMR ($CDCl_3$) δ 7.06-7.08 (m, 1H), 7.23-7.26 (m, 1H), 7.45-7.76 (m, 6H), 8.44-8.49 (m, 1H), 8.66-8.75 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 110.5, 122.7, 122.9, 126.5, 127.2, 127.5, 128.2, 128.4, 128.7, 128.8, 130.3, 131.1, 132.6, 133.2, 135.3, 138.4, 146.5; IR (neat) 2925, 1464, 1216 cm^{-1}; HRMS *m/z* 385.9631 (calcd for $C_{18}H_{11}IS$, 385.9626).



30

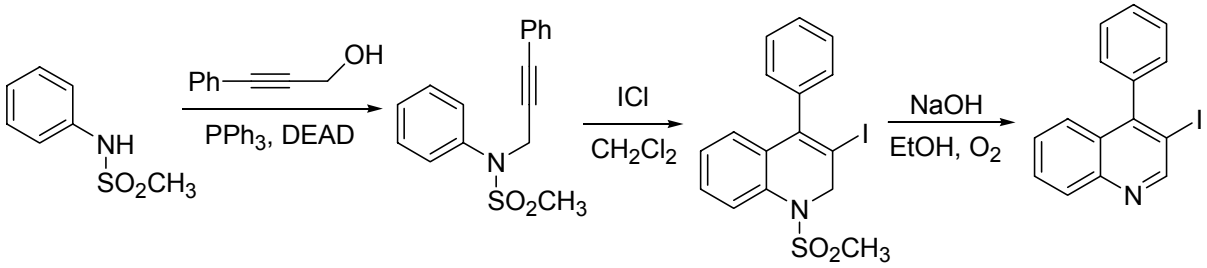
6-Iodo-5-(4-methoxyphenyl)benzo[*c*]phenanthrene (30). Purification by flash chromatography (30:1 hexane/EtOAc) afforded 0.138 g (97 %) of the product as a white solid: mp 186-187 ºC; ^{1}H NMR ($CDCl_3$) δ 3.94 (s, 3H), 7.08-7.12 (m, 2H), 7.23-7.26 (m, 2H), 7.42-7.47 (m, 1H), 7.57-7.69 (m, 4H), 7.94 (d, *J* = 9.0 Hz, 1H), 8.04-8.06 (m, 1H), 8.42 (d, *J* = 9.0 Hz, 1H), 9.01-9.04 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 55.6, 107.3, 114.1, 126.4, 126.6, 126.7, 126.8, 128.4, 128.4, 128.6, 128.6, 128.8, 129.0, 129.7, 130.2, 131.3, 131.5, 132.4, 133.8, 133.8, 138.0, 145.0, 159.4; IR (neat) 2950, 1606, 1506 cm^{-1}; HRMS *m/z* 460.0330 (calcd for $C_{25}H_{17}IO$, 460.0324).



32

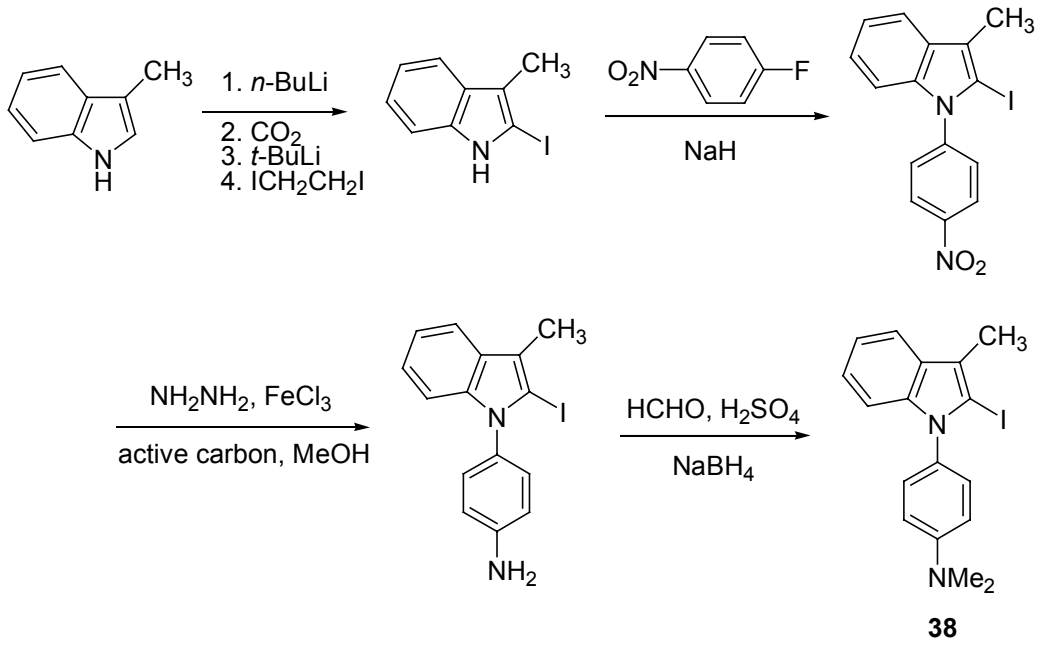
6-Iodo-5-phenylchrysene (32). Purification by flash chromatography (40:1 hexane/EtOAc) afforded 98 mg (76%) of the product as a yellow solid: mp 168-169 ºC; ^{1}H NMR ($CDCl_3$) δ 7.07 (t, *J* = 6.9 Hz, 1H), 7.33-7.57 (m, 7H), 7.71-7.76 (m, 2H), 8.89 (d, *J* = 6.5 Hz, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 8.56-8.60 (m, 1H), 8.78 (d, *J* = 7.0 Hz, 2H); ^{13}C NMR ($CDCl_3$) δ 111.5, 121.3,

123.7, 125.4, 126.1, 127.7, 128.2, 128.4, 128.6, 128.9, 129.0, 129.2, 129.3, 130.4, 130.7, 130.8, 131.1, 133.5, 133.8, 135.3, 144.3, 150.0; IR (neat) 2922 cm^{-1}; HRMS *m/z* 430.0025 (calcd for $C_{24}H_{15}I$, 430.0219).



3-Iodo-4-phenylquinoline (34). To a solution of *N*-phenylmethanesulfonamide[8] (0.513 g, 3.0 mmol), PPh_3 (1.18 g, 4.5 mmol) and 3-phenylpropargyl alcohol (0.594 g, 4.5 mmol) in anhydrous THF (30 mL) at 0 °C was added DEAD (0.784 g, 4.5 mmol). The resulting solution was stirred at 0 °C for 1 h and an additional 3 h at room temperature. The mixture was washed with brine (30 mL) and the organic layer was dried (Na_2SO_4), filtered, and the solvent removed under reduced pressure. The residue was purified by chromatography on a silica gel column using 3:1 hexanes/ethyl acetate to obtain 0.534 g (63 %) of *N*-phenyl-*N*-(3-phenyl-2-propyn-1-yl)methanesulfonamide as a white solid: mp 76-77 °C; ^{1}H NMR ($CDCl_3$) δ 3.08 (s, 3H), 4.67 (s, 2H), 7.34-7.46 (m, 8H), 7.62-7.66 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 39.2, 42.3, 84.4, 86.3, 122.3, 127.7, 128.4, 128.7, 129.1, 129.7, 131.9, 140.5. To a solution of *N*-phenyl-*N*-(3-phenyl-2-propyn-1-yl)methanesulfonamide (71.2 mg, 0.25 mmol) in CH_2Cl_2 (3.0 mL) at -78 °C was added ICl (48.7 mg, 0.3 mmol) in CH_2Cl_2 (0.5 mL) and the resulting solution was stirred at this temperature for 1 h. The reaction mixture was washed with satd aq $Na_2S_2O_3$ (20 mL) and the organic layer dried (Na_2SO_4), filtered and the solvent removed under reduced pressure. The residue was purified by chromatography on a silica gel column

using 5:1 hexanes/ethyl acetate to obtain 82.2 mg (80 %) of 3-iodo-1-methanesulfonyl-4-phenyl-1,2-dihydroquinoline as a white solid: mp 173-175 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 2.89 (s, 3H), 4.82 (s, 2H), 6.80 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.11-7.16 (m, 3H), 7.30-7.33 (m, 1H), 7.44-7.48 (m, 3H), 7.62 (dd, *J* = 8.1, 0.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 38.6, 56.7, 92.0, 126.9, 127.2, 127.2, 128.6, 128.8, 129.0, 129.2, 130.7, 134.5, 140.3, 143.9. A solution of 3-iodo-1-methanesulfonyl-4-phenyl-1,2-dihydroquinoline (0.103 g, 0.25 mmol) and NaOH (0.10 g, 2.5 mmol) in EtOH (10 mL) was stirred at 50 ^{o}C under O_2 (1 atm) for 12 h. The reaction mixture was diluted with diethyl ether (50 mL) and washed with brine (50 mL). The organic layer was dried (Na_2SO_4), filtered, and the solvent removed under reduced pressure. The residue was purified by column chromatography on a silica gel column using 5:1 hexanes/ethyl acetate to afford 76.1 mg (92 %) of the desired compound **34** as a white solid: mp 131-132 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.25-7.28 (m, 2H), 7.42-7.48 (m, 2H), 7.52-7.55 (m, 3H), 7.69-7.74 (m, 1H), 8.12 (d, *J* = 8.8 Hz, 1H), 9.24 (s, 1H); ^{13}C NMR ($CDCl_3$) δ 96.4, 126.8, 127.4, 128.7, 129.0, 129.1, 129.5, 129.8, 140.4, 147.2, 152.4, 156.6 (one sp^2 carbon missing due to overlap); IR (CH_2Cl_2) 3061, 2918, 1566, 1501, 1485 cm^{-1}; HRMS *m/z* 330.9864 (calcd for $C_{15}H_{10}IN$, 330.9858).



38

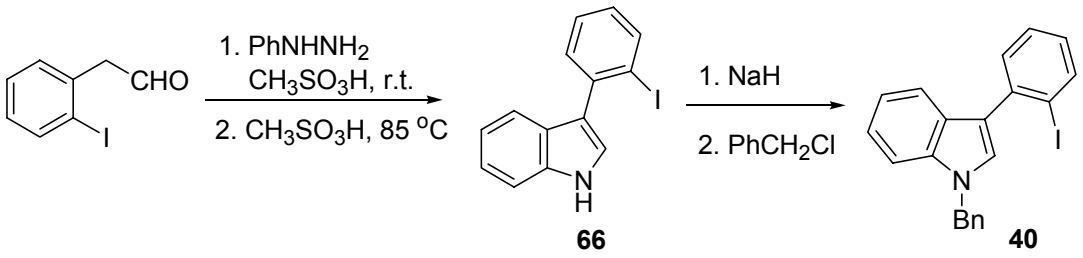
2-Iodo-3-methylindole. To a solution of 3-methylindole (2.64 g, 20.0 mmol) in 55 mL of dry THF was added dropwise 8.4 mL of *n*-BuLi (2.5 M in hexane) at –78 ^{o}C under an Ar atmosphere. The resulting suspension was stirred at –78 ^{o}C for 20 min. Carbon dioxide was bubbled through the reaction mixture for 30 min to form a clear yellow solution. The reaction mixture was allowed to warm to 25 ^{o}C and the solvent was removed under reduced pressure. To the residue was added 50 mL of dry THF and the suspension was cooled to -78 ^{o}C. 12.5 Ml of *t*-BuLi (1.7 M pentane) was added to the suspension and the resulting orange reaction mixture was stirred at -78 ^{o}C for 1 h. A solution of ICH_2CH_2I (5.64 g, 20.0 mmol) in 15 mL of dry THF was added dropwise and the resulting yellow solution was stirred at -78 ^{o}C for 1 h. Then the reaction mixture was allowed to warm to 25 ^{o}C and washed with 50 mL of satd aqueous NH_4Cl. The organic layer was collected, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column (5:1 hexane/EtOAc) to afford 4.98 g of 2-iodo-3-methylindole as a yellow oil in 97 % yield with spectral properties identical to those previously reported.[9]

2-Iodo-3-methyl-1-(4-nitrophenyl)indole. To a suspension of NaH (5.5 mmol) in 20 mL of DMF was added 1.28 g of 2-iodo-3-methylindole (5.0 mmol) at 0 ^{o}C under an Ar atmosphere and lots of bubbles were generated. The resulting yellow suspension was stirred at 0 ^{o}C for 40 min and a solution of 1-fluoro-4-nitrobenzene (0.846 g, 6.0 mmol) in 10 mL of DMF was added dropwise. After 12 h, the reaction was diluted with 30 mL of Et_2O and washed with 30 mL of brine. The organic layer was collected, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by column chromatography (15:1 hexane/EtOAc) to afford 1.07 g of the indicated compound in a 57 % yield as a yellow solid: mp 123-126 ^{o}C; ^{1}H NMR ($CDCl_3$) 2.39 (s, 3H), 7.13-7.20 (m, 3H), 7.54-7.60 (m, 3H), 8.37-8.42 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 12.8, 85.2, 110.3, 118.9, 121.1, 121.5, 123.4, 124.9, 129.2, 129.5, 139.3, 144.7, 147.0.

1-(4-Aminophenyl)-2-iodo-3-methylindole. To a 6 dram vial was added 0.80 g of 2-iodo-3-methyl-1-(4-nitrophenyl)indole (2.1 mmol), 17 mL of CH_3OH, 8.5 mg of $FeCl_3$•$6H_2O$ (0.32 mmol), 4.3 mg of active carbon (3.6 mmol), and 0.21 mL of NH_2NH_2•H_2O (4.2 mmol). The resulting mixture was stirred at 25 ^{o}C for 5 min and was heated to 70 ^{o}C (a sealed tube reaction). After 7 h, the reaction was allowed to cool to 25 ^{o}C and filtered. The colorless filtrate was concentrated under reduced pressure and the residue was purified by column chromatography (2:1 hexane/EtOAc) to afford 0.60 g of the indicated compound in an 82 % yield as a yellow oil: ^{1}H NMR ($CDCl_3$) 2.38 (s, 3H), 3.94 (br s, 2H), 6.78-6.80 (m, 2H), 7.06-7.10 (m, 5H), 7.54-7.56 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 12.7, 88.8, 110.9, 115.4, 118.0, 118.2, 119.7, 122.2, 128.5, 130.2, 140.1, 146.7 (one sp^2 carbon missing due to overlap).

1-(4-Dimethylaminophenyl)-2-iodo-3-methylindole (38). To a mixture of formaldehyde (37% of aqueous solution, 0.40 mL, 4.98 mmol) and H_2SO_4 (3 M, 0.69 mL,

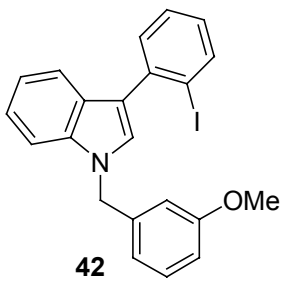
2.1 mmol) was added a slurry of $NaBH_4$ (0.22 g, 5.8 mmol) and 1-(4-aminophenyl)-2-iodo-3-methylindole (0.29 g, 0.83 mmol) in 7 mL of THF at 0 ^oC. Lots of bubbles were generated in this process and the resulting yellow suspension was stirred at 0 ^oC for 10 min. The reaction mixture was diluted with 30 mL of Et_2O, and washed with satd aq $NaHCO_3$ (30 mL) and brine (20 mL). The organic layer was collected, dried over $NaSO_4$, and filtered. Removal of solvent under reduced pressure afforded 0.26 g of the indicated compound in an 83 % yield as a yellow solid: mp 149-150 ^oC; ^1H NMR ($CDCl_3$) 2.38 (s, 3H), 3.04 (s, 6H), 6.79 (d, J = 8.8 Hz, 2H), 7.05-7.10 (m, 3H), 7.16 (d, J = 8.8 Hz, 2H), 7.54-7.56 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 12.7, 40.7, 89.3, 111.0, 112.3, 117.8, 118.2, 119.6, 122.1, 128.1, 128.4, 129.9, 140.2, 150.3; IR (CH_2Cl_2) 3053, 2986, 1524 cm^{-1}; HRMS *m/z* 376.0441 (calcd for $C_{17}H_{17}IN_2$, 376.0437).



3-(2-Iodophenyl)indole (66). To a solution of (2-iodophenyl)acetaldehyde[10] (0.738 g, 3.0 mmol) in 15 mL of absolute ethanol was added 0.356 g of $PhNHNH_2$ (3.3 mmol) and 57.6 mg of CH_3SO_3H (0.6 mmol). The resulting yellow solution was then stirred at room temperature for 1 h. Another 0.519 g of CH_3SO_3H (5.4 mmol) was then added to the reaction mixture and the reaction was stirred at 85 ^oC. After 2 d, the reaction was complete and was allowed to cool to room temperature. The ethanol was removed under reduced pressure and the residue was diluted with Et_2O (30 mL), washed with brine (30 mL), dried over Na_2SO_4,

filtered and concentrated. The residue was purified by flash chromatography (5:1 hexane/EtOAc) to afford 0.41 g of compound **66** (43 % yield) as a yellow oil: ^{1}H NMR ($CDCl_3$) δ 7.01-7.05 (m, 1H), 7.14-7.18 (m, 1H), 7.23-7.27 (m, 1H), 7.38-7.49 (m, 4H), 7.54 (d, J = 8.0 Hz, 1H), 8.01 (dd, J = 1.2, 8.0 Hz, 1H), 8.27 (br s, 1H); ^{13}C NMR ($CDCl_3$) δ 101.0, 111.5, 120.3, 120.4, 122.6, 123.8, 126.8, 128.2, 128.5, 131.6, 135.8, 140.0, 140.1 (one sp^2 carbon missing due to overlap).

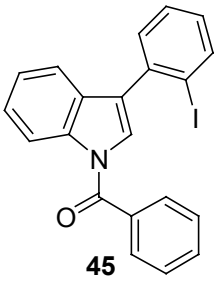
1-Benzyl-3-(2-iodophenyl)indole (40). To a suspension of 30 mg of NaH (0.75 mmol, 60 % in mineral oil) in DMF (2 mL) was added dropwise a solution of compound **66** (0.16 g, 0.5 mmol) in DMF (4 mL) at 0 °C. A lot of bubbles were generated. The resulting brown solution was stirred at 0 °C for 45 min and a solution of $PhCH_2Cl$ (0.127 g, 1.0 mmol) in DMF (1 mL) was added dropwise at 0 °C. The resulting mixture was stirred at 0 °C for 12 h. The reaction mixture was diluted with Et_2O (30 mL), washed with brine (30 mL), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography (20:1 hexane/EtOAc) to afford 0.155 g of the indicated compound **40** (76 % yield) as a colorless oil: ^{1}H NMR ($CDCl_3$) δ 5.38 (s, 2H), 6.98-7.02 (m, 1H), 7.12-7.16 (m, 1H), 7.18-7.33 (m, 8H), 7.37-7.41 (m, 1H), 7.49 (dd, J = 1.6, 7.6 Hz, 1H), 7.54-7.56 (m, 1H), 7.99 (dd, J = 1.2, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 50.4, 101.1, 110.1, 119.2, 120.1, 120.4, 122.3, 127.1, 127.5, 127.9, 128.1, 128.2, 128.4, 129.0, 131.6, 136.3, 137.5, 140.0, 140.1; IR (neat) 3055, 3029, 2921, 1613, 1585 cm^{-1}; HRMS *m/z* 409.0335 (calcd for $C_{21}H_{16}IN$, 409.0328).



42

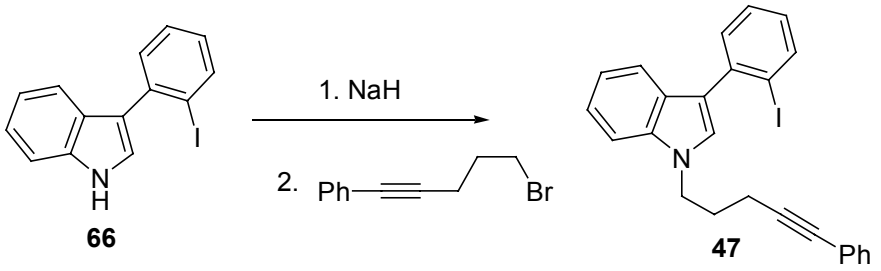
1-(3-Methoxybenzyl)-3-(2-iodophenyl)indole (42). Using the procedure to prepare compound **40**, but employing 0.16 g of 3-

methoxybenzyl chloride (1.0 mmol) afforded 0.193 g of the indicated compound **42** in an 88 % yield as a yellow oil: ^{1}H NMR ($CDCl_3$) δ 3.72 (s, 3H), 5.34 (s, 2H), 6.71 (s, 1H), 6.77-6.81 (m, 2H), 6.98-7.02 (m, 1H), 7.12-7.15 (m, 1H), 7.18-7.24 (m, 2H), 7.31-7.33 (m, 2H), 7.37-7.40 (m, 1H), 7.48-7.50 (m, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 50.3, 55.4, 101.1, 110.1, 112.7, 113.2, 119.2, 119.3, 120.1, 120.4, 122.3, 127.5, 128.1, 128.2, 128.4, 130.0, 131.6, 136.2, 139.1, 140.0, 140.0, 160.2; IR (neat) 3051, 2934, 1586, 1490 cm^{-1}; HRMS *m/z* 439.0439 (calcd for $C_{22}H_{18}ION$, 439.0433).



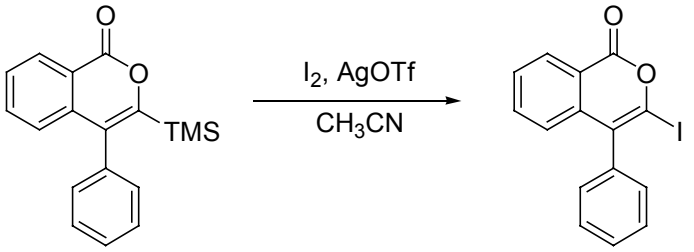
45

1-Benzoyl-3-(2-iodophenyl)indole (45). Using the procedure to prepare compound **40**, but employing of 0.14 g of benzoyl chloride (1.0 mmol) afforded 0.190 g of the indicated compound **45** in a 90 % yield as a pale yellow solid: mp 102-103 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.04-7.08 (m, 1H), 7.32-7.36 (m, 1H), 7.40-7.46 (m, 5H), 7.51-7.55 (m, 2H), 7.58-7.63 (m, 1H), 7.81-7.84 (m, 2H), 7.98 (d, J = 7.6 Hz, 1H), 8.49-8.51 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 100.2, 116.7, 120.5, 124.3, 125.3, 125.5, 126.5, 128.3, 128.8, 129.6, 129.6, 130.1, 131.3, 132.3, 134.6, 136.1, 138.1, 140.1, 168.9; IR (neat) 3051, 1686, 1450, 1364 cm^{-1}; HRMS *m/z* 423.0129 (calcd for $C_{21}H_{14}ION$, 423.0120).



66 **47**

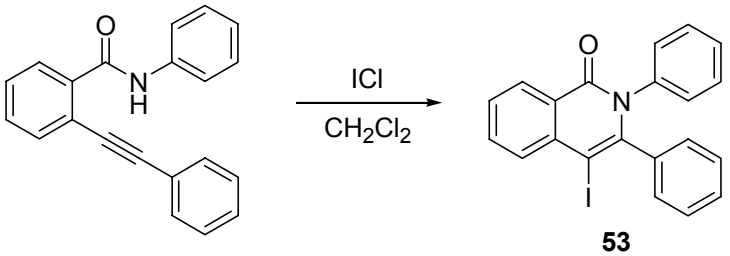
3-(2-Iodophenyl)-1-(5-phenyl-4-pentynyl)indole (47). To a suspension of NaH (45.7 mg, 1.14 mmol, 60 % in mineral oil) in DMF (3 mL) was added dropwise a solution of compound **66** (0.243 g, 0.76 mmol) in DMF (5 mL) at 0 ^{o}C. A lot of bubbles were generated. The resulting brown solution was stirred at 0 ^{o}C for 45 min and a solution of 5-bromo-1-phenyl-1-pentyne (0.34 g, 1.52 mmol) in DMF (2 mL) was added dropwise at 0 ^{o}C. The resulting mixture was stirred at 0 ^{o}C for 12 h, diluted with Et_2O (30 mL), washed with brine (30 mL), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography (20:1 hexane/EtOAc) to afford 0.30 g of the indicated compound **47** (85 % yield) as a yellow oil: ^{1}H NMR ($CDCl_3$) δ 2.13-2.22 (m, 2H), 2.45 (t, *J* = 8.8 Hz, 2H), 4.41 (t, *J* = 8.8 Hz, 2H), 6.98-7.03 (m, 1H), 7.12-7.23 (m, 1H), 7.23-7.33 (m, 4H), 7.37-7.50 (m, 6H), 7.54-7.56 (m, 1H), 8.00 (dd, *J* = 1.6, 10.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 17.0, 29.1, 45.1, 82.3, 88.6, 101.1, 109.8, 118.7, 120.0, 120.4, 122.1, 123.8, 127.5, 128.0, 128.1, 128.2, 128.3, 128.5, 131.5, 131.8, 135.9, 140.1 (one sp^2 carbon missing due to overlap); IR (CH_2Cl_2) 3053, 2985, 1613, 1596, 1548 cm^{-1}; HRMS *m/z* 461.0647 (calcd for $C_{25}H_{20}IN$, 461.0641).



51

3-Iodo-4-phenylisocoumarin (51). A solution of 4-phenyl-3-(trimethylsilyl)isocoumarin[11] (0.435 g, 1.48 mmol), I_2 (1.13 g, 4.45 mmol), and AgOTf (0.76

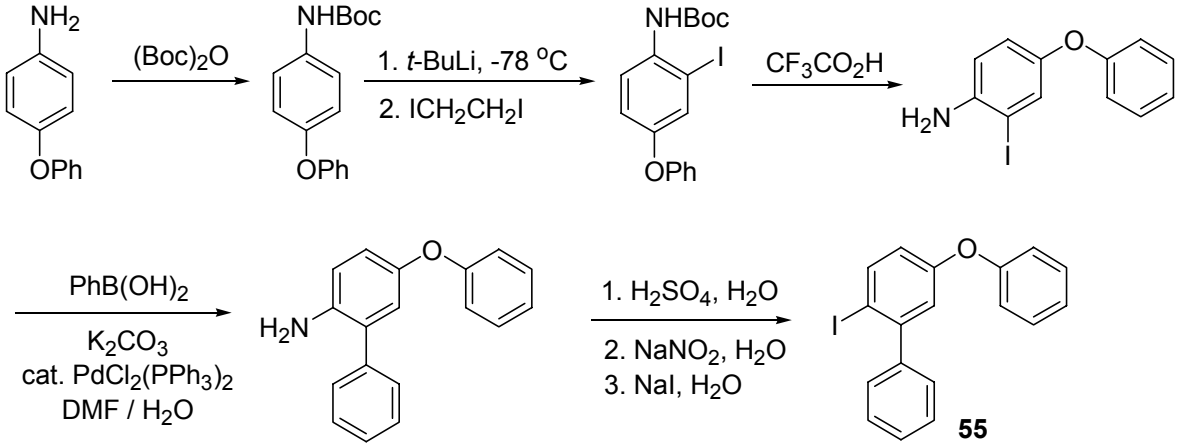
g, 2.96 mmol) in CH_3CN (20 mL) was heated at 55 ^oC for 5 d. The reaction mixture was diluted with diethyl ether (100 mL), and washed with satd aq $Na_2S_2O_3$ (30 mL). The organic layer was dried (Na_2SO_4), filtered, and the solvent removed under reduced pressure to obtain 0.498 g (97 %) of the indicated compound **51** as a yellow solid. Recrystallization from hexanes/ethyl acetate afforded the indicated compound **51** as a yellow solid: mp 170-171 ^oC, ^1H NMR ($CDCl_3$) δ 6.97 (d, J = 8.0 Hz, 1H), 7.26-7.28 (m, 2H), 7.50-7.56 (m, 4H), 7.59-7.63 (m, 1H), 8.31 (dd, J = 8.0, 0.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 107.9, 119.6, 125.6, 127.4, 128.7, 128.9, 129.1, 129.9, 130.5, 135.2, 137.0, 137.3, 161.2; IR (CH_2Cl_2) 1736 cm^{-1}; HRMS *m/z* 347.9652 (calcd for $C_{15}H_9IO_2$, 347.9647).



53

4-Iodo-2,3-diphenyl-2*H*-isoquinolin-1-one (53). To a solution of *N*-phenyl-2-(phenylethynyl)benzamide[12] (74.2 mg, 0.25 mmol) in CH_2Cl_2 (3.0 mL) at room temperature was added ICl (48.7 mg, 0.3 mmol) in CH_2Cl_2 (0.5 mL) and the resulting solution was stirred at this temperature for 1 h. The reaction mixture was washed with satd aq $Na_2S_2O_3$ (20 mL) and the organic layer dried (Na_2SO_4), filtered and the solvent removed under reduced pressure. The residue was purified by chromatography on a silica gel column using 5:1 hexanes/ethyl acetate to obtain 42.3 mg (40 %) of the indicated compound **53** as a yellow solid: mp 129-130 ^oC; ^1H NMR ($CDCl_3$) δ 7.08-7.11 (m, 1H), 7.20-7.30 (m, 3H), 7.33-7.38 (m, 4H), 7.57-7.64 (m, 3H), 7.67-7.72 (m, 1H), 8.03-8.06 (m, 1H), 8.84-8.87 (m, 1H); ^{13}C

NMR ($CDCl_3$) δ 75.2, 124.1, 125.1, 125.1, 125.4, 128.1, 128.7, 128.7, 130.5, 130.9, 132.0, 132.7, 135.7, 140.6, 145.0, 147.8, 152.1; IR (CH_2Cl_2) 2916, 2849, 1642, 1586, 1488, 1445 cm^{-1}; HRMS *m/z* 423.0131 (calcd for $C_{15}H_9IO_2$, 423.0120).



***N*-(4-Phenoxyphenyl)-2,2-dimethylpropanamide.** To a solution of 4-phenoxyaniline (3.33 g, 18.0 mmol) in 70 mL of dried THF was added $(Boc)_2O$ (4.71 g, 21.6 mmol) and the resulting yellow solution was refluxed at 80 °C for 6 h. The solvent was removed under reduced pressure and the reddish residue was recrystallized using hexane and EtOAc to afford 4.84 g of the indicated compound (85 % yield) as white needles: mp 109-111 °C; ^1H NMR ($CDCl_3$) δ 1.52 (s, 9H), 6.43 (br s, 1H), 6.95-6.98 (m, 4H), 7.06 (t, *J* = 3.6 Hz, 1H), 7.29-7.34 (m, 4H); ^{13}C NMR ($CDCl_3$) δ 28.6, 80.7, 118.3, 120.2, 120.5, 123.0, 129.9, 134.2, 152.6, 153.2, 158.1.

***N*-(2-Iodo-4-phenoxyphenyl)-2,2-dimethylpropanamide.** To a solution of *N*-(4-phenoxyphenyl)-2,2-dimethylpropanamide (2.57 g, 9.02 mmol) in 20 mL of dry diethyl ether was added dropwise 10.6 mL of *t*-BuLi (1.7 M in pentane, 18.04 mmol) at -78 °C under Ar. The pale orange solution turned a pale yellow color when half of the *t*-BuLi solution had

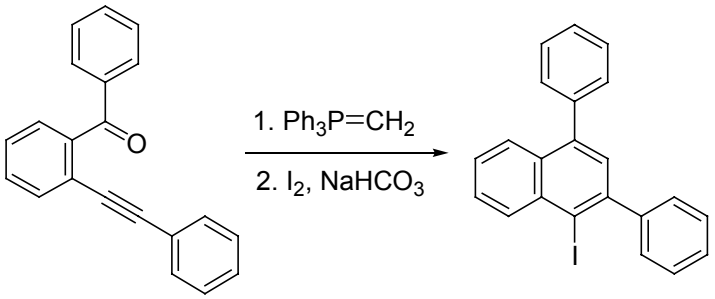
been added and eventually to yellow when all of the *t*-BuLi solution was added. The resulting yellow solution was then stirred at -78 ^{o}C for 30 min. A solution of ICH_2CH_2I (2.81 g, 9.92 mmol, recrystallized from diethyl ether) in 20 mL of dry ether was added dropwise to the reaction mixture and the resulting orange solution was stirred at -78 ^{o}C for another 30 min. The reaction mixture was allowed to warm up to room temperature and quenched by 50 mL of water. The organic layer was separated and dried over Na_2SO_4, filtered, and concentrated. The residue was purified by flash chromatography (15:1 hexane/EtOAc) to afford 2.3 g of the desired compound (62 % yield) as a colorless oil: ^{1}H NMR ($CDCl_3$) δ 1.53 (s, 9H), 6.68 (br s, 1H), 6.96-6.98 (m, 2H), 7.02 (dd, *J* = 2.4, 8.8 Hz, 1H), 7.08-7.12 (m, 1H), 7.30-7.35 (m, 2H), 7.42 (d, *J* = 2.8 Hz, 1H), 7.94 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 28.5, 81.3, 89.5, 118.6, 120.2, 121.6, 123.6, 129.3, 130.0, 134.9, 153.0, 153.0, 157.4.

2-Iodo-4-phenoxyaniline. To a solution of *N*-(2-iodo-4-phenoxyphenyl)-2,2-dimethylpropanamide (0.82 g, 2.0 mmol) in 10 mL of CH_2Cl_2 was added dropwise 2.0 mL of TFA at 0 ^{o}C and the reaction was allowed to warm up to room temperature. The resulting colorless mixture was stirred at room temperature for 16 h, diluted with 20 mL of CH_2Cl_2, washed with brine (30 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by flash chromatography (5:1 hexane/EtOAc) to afford 0.56 g of the indicated compound (91 % yield) as a pale orange solid: mp 54-56 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 4.00 (s, 2H), 6.74 (d, *J* = 8.7 Hz, 1H), 6.88-6.91 (m, 2H), 6.93-6.95 (m, 1H), 7.01-7.07 (m, 1H), 7.26-7.32 (m, 2H), 7.36 (d, *J* = 2.7 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 83.8, 115.2, 117.6, 121.6, 122.8, 129.9, 130.3, 143.5, 148.8, 158.6.

4-Phenoxy-2-phenylaniline. To a 50 mL round-bottom flask was added $PdCl_2(PPh_3)_2$ (0.103 g, 0.147 mmol), $PhB(OH)_2$ (0.358 g, 2.94 mmol), K_2CO_3 (0.406 g, 2.94 mmol), 2-iodo-4-phenoxyaniline (0.457 g, 1.47 mmol), 15 mL of DMF and 3 mL of H_2O. The whole mixture was then stirred at room temperature for 5 min, flushed with Ar and heated to 70 ^oC for 3 h. The reaction was allowed to cool to room temperature, diluted with diethyl ether (30 mL), washed with brine (50 mL), dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography (5:1 hexane/EtOAc) to afford 0.342 g of the indicated compound (88 % yield) as a yellow oil: ^1H NMR ($CDCl_3$) δ 3.71 (br s, 2H), 6.75-6.77 (m, 1H), 6.87-6.90 (m, 2H), 6.97-7.03 (m, 3H), 7.25-7.35 (m, 3H), 7.41-7.60 (m, 4H); ^{13}C NMR ($CDCl_3$) δ 116.9, 117.5, 120.4, 122.2, 122.3, 127.6, 129.0, 129.1, 129.2, 129.7, 139.1, 139.9, 148.9, 159.0.

2-Iodo-5-phenoxybiphenyl (55). To a solution of 4-phenoxy-2-phenylaniline (0.383 g, 1.47 mmol) in DME (4 mL) was added dropwise 3 mL of water containing 0.6 mL of conc H_2SO_4 (95 %). The resulting yellow mixture was cooled to 0 ^oC and a solution of $NaNO_2$ (0.152 g, 2.21 mmol) in water (1 mL) was added over 10 min. The yellow reaction mixture was stirred at 0 ^oC for 20 min and a solution of NaI (1.10 g, 7.35 mmol) in water (3 mL) was added dropwise at 0 ^oC. The reaction mixture turned black when the NaI solution was added. After 10 min, the reaction was diluted with Et_2O (30 mL), and washed by satd $Na_2S_2O_3$ (30 mL), water (30 mL), and brine (30 mL). The organic layer was collected, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography (30:1 hexane/EtOAc) to afford 0.44 g of the indicated compound **55** (81 % yield) as a yellow solid: mp 68-70 ^oC; ^1H NMR ($CDCl_3$) δ 6.73 (dd, J = 3.0, 8.8 Hz, 1H), 6.97 (d, J = 2.8 Hz, 1H), 7.04-7.06 (m, 2H), 7.11-7.15 (m, 1H), 7.31-7.43 (m, 7H), 7.85 (d, J

= 8.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 90.4, 119.4, 119.5, 120.5, 124.1, 128.0, 128.2, 129.4, 130.1, 140.6, 143.9, 148.2, 156.6, 158.0; IR (CH_2Cl_2) 3056, 2981, 1583, 1561, 1490 cm^{-1}; HRMS *m/z* 372.0019 (calcd for $C_{18}H_{13}IO$, 372.0011).

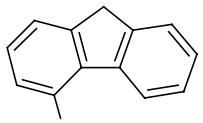


56

1-Iodo-2,4-diphenylnaphthalene (56). To a yellow suspension of $Ph_3P{=}CH_2$ (1.5 mmol) in THF (8 mL) [prepared by the reaction of 0.57 g of methyltriphenylphosphonium bromide (1.6 mmol) in 8 mL of THF and 0.6 mL of *n*-BuLi (2.5 M in hexane, 1.5 mmol) at 0 ^{o}C for 30 min] was added a solution of 2-(phenylethynyl)acetophenone (1.0 mmol) in THF (3 mL). After 1 h, TLC analysis showed that the reaction was not complete and another 1.0 mmol of $Ph_3P{=}CH_2$ in THF (5 mL) was added to the reaction mixture. The reaction reached completion in 10 min. The solvent was removed under reduced pressure and 30 mL of hexane was added to the residue. After being stirred at 25 ^{o}C for 20 min, the mixture was filtered to remove the phosphonium salt. Removal of the solvent under reduced pressure afforded a colorless residue. The colorless residue was added to a stirred mixture of $NaHCO_3$ (0.25 g, 3.0 mmol), I_2 (1.54 g, 6.0 mmol) and CH_3CN (15 mL). The reaction was complete after 20 min at 25 ^{o}C. The reaction mixture was diluted with Et_2O (30 mL) and washed by satd aqueous $Na_2S_2O_3$ (30 mL). The organic layer was collected, dried over $NaSO_4$, filtered, and the solvent was removed under reduced pressure. The residue was purified by chromatograph (50:1 hexane/EtOAc) to afford 0.39 g of the indicated compound

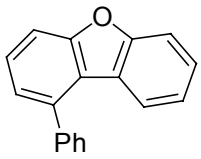
56 in a 97 % yield as a yellow oil: ^{1}H NMR ($CDCl_3$) δ 7.38-7.50 (m, 12H), 7.58-7.63 (m, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 8.43 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 103.6, 126.8, 126.9, 127.8, 128.2, 128.2, 128.6, 128.9, 129.8, 130.2, 131.5, 134.1, 135.3, 139.9, 140.9, 146.0, 146.2 (one sp^2 carbon missing due to overlap); IR (neat) 3058, 3028, 2927, 1599 cm^{-1}; HRMS *m/z* 406.0225 (calcd for $C_{22}H_{15}I$, 406.0218).

Representative procedure for the palladium-catalyzed migration reactions. The appropriate aryl iodide (0.25 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), 1,1-*bis*(diphenylphosphino)methane (dppm) (4.8 mg, 0.0125 mmol) and CsO_2CCMe_3 (CsPiv) (0.117 g, 0.5 mmol) in DMF (4 mL) were stirred under Ar at 100 °C for the specified period of time. The reaction mixture was allowed to cool to room temperature, diluted with diethyl ether (35 mL) and washed with brine (30 mL). The aqueous layer was reextracted with diethyl ether (15 mL). The organic layers were combined, dried ($MgSO_4$), filtered, and the solvent removed under reduced pressure. The residue was purified by flash chromatography on silica gel.



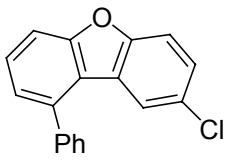
5

1-Phenyl-9*H*-fluorene (5). Compound **4** (92.5 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 °C for 3 d. The reaction mixture was chromatographed using 30:1 hexane/EtOAc to afford 24.2 mg (40 %) of the indicated compound **2** as a colorless oil: ^{1}H NMR ($CDCl_3$) δ 3.95 (s, 2H), 6.94 (d, *J* = 7.6 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 7.19-7.22 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.45-7.55 (m, 7H); ^{13}C NMR ($CDCl_3$) δ 37.0, 122.9, 124.0, 124.8, 126.3, 126.4, 127.5, 128.5, 128.8, 129.2, 137.9, 138.7, 141.3, 141.6, 143.7, 143.9 (one sp^2 carbon missing due to overlap); IR (CH_2Cl_2) 3056, 3025, 1454, 1417, 1478 cm^{-1}; HRMS *m/z* 242.1101 (calcd for $C_{19}H_{14}$, 242.1096).



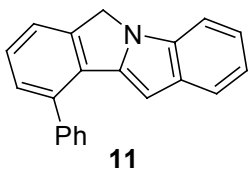
7

1-Phenyldibenzofuran (7). Compound **6** (93.0 mg, 0.25 mmol) or compound **55** (93.0 mg, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d. The reaction mixtures were chromatographed using 30:1 hexane/EtOAc to afford 54.4 mg (89 %) (entry 2, Table 2) or 54.0 mg (88 %) (entry 8, Table 2) of the indicated compound **7**, respectively, as a white solid: mp 62-63 ^{o}C (lit[13] mp 63-64 ^{o}C); ^{1}H NMR ($CDCl_3$) δ 7.10-7.14 (m, 1H), 7.24-7.26 (m, 1H), 7.37-7.42 (m, 1H), 7.46-7.64 (m, 9H); ^{13}C NMR ($CDCl_3$) δ 110.5, 111.6, 121.8, 122.3, 122.5, 123.9, 124.0, 127.1, 127.1, 127.9, 128.6, 129.0, 138.0, 140.0, 156.4, 156.5. The other spectral properties were identical to those previously reported.[13]



9

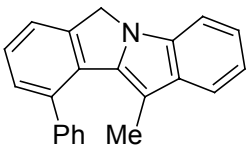
7-Chloro-1-phenyldibenzofuran (9). Compound **8** (0.101 g, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d. The reaction mixture was chromatographed using 50:1 hexanes/ethyl acetate to afford 57.1 mg (82 %) of the indicated compound **9** as a colorless oil: ^{1}H NMR ($CDCl_3$) δ 7.25 (dd, *J* = 6.8, 1.2 Hz, 1H), 7.34 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.45-7.60 (m, 9H); ^{13}C NMR ($CDCl_3$) δ 110.7, 112.5, 121.0, 122.1, 124.3, 125.3, 127.1, 127.7, 127.8, 128.3, 128.8, 128.9, 138.2, 139.4, 154.7, 157.1; IR (CH_2Cl_2) 3061, 3032, 1444, 1400, 1199, 1243 cm^{-1}; HRMS *m/z* 278.0501 (calcd for $C_{18}H_{11}ClO$, 278.0498).



11

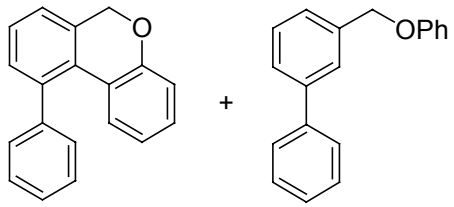
10-Phenyl-6*H*-isoindolo[2,1-*a*]indole (11). Compound **10** (0.102 g, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d. The reaction mixture was chromatographed using 12:1 hexanes/ethyl acetate to afford 49.2 mg (70 %) of the indicated compound **11** as a white solid: mp 139-140 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 5.08 (s, 2H), 6.16 (s, 1H), 7.03-7.07 (m, 1H), 7.14-7.18 (m, 1H), 7.32-7.54 (m, 8H), 7.64-7.66 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 48.2, 94.3,

109.1, 119.7, 121.7, 122.4, 127.3, 128.0, 128.5, 128.8, 129.3, 131.0, 132.4, 133.7, 137.0, 139.9, 142.5, 143.2 (one sp^2 carbon missing due to overlap); IR (CH_2Cl_2) 3053, 2916, 2850, 1471, 1551, 1446 cm^{-1}; HRMS *m/z* 281.1210 (calcd for $C_{21}H_{15}N$, 281.1204).



13

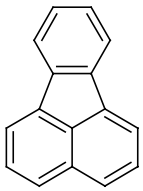
2-Methyl-10-phenyl-6*H*-isoindolo[2,1-*a*]indole (13). Compound **12** (0.106 g, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d. The reaction mixture was chromatographed using 12:1 hexanes/ethyl acetate to afford 52.4 mg (71 %) of the indicated compound **13** as a white solid: mp 143-145 ^oC (decomposes); ^1H NMR ($CDCl_3$) δ 1.41 (s, 3H), 5.06 (s, 2H), 7.03-7.07 (m, 1H), 7.16-7.20 (m, 1H), 7.23-7.31 (m, 3H), 7.40-7.50 (m, 7H); ^{13}C NMR ($CDCl_3$) δ 9.5, 48.1, 104.2, 109.0, 119.1, 120.0, 122.0, 122.4, 126.5, 127.9, 128.7, 129.9, 130.2, 132.6, 133.8, 134.0, 137.0, 140.0, 142.6, 142.8; IR (CH_2Cl_2) 3048, 2976, 2853, 1469, 2976, 2853, 1469, 1411 cm^{-1}; HRMS *m/z* 295.1369 (calcd for $C_{22}H_{17}N$, 295.1361).



15 **16**

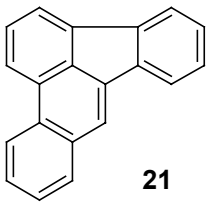
10-Phenyl-6*H*-benzo[*c*]chromene (15) and phenyl 3-phenylbenzyl ether (16). Compound **14** (96.5 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 120 ^oC for 2 d. The reaction mixture was chromatographed using 50:1 hexanes/ethyl acetate to afford 47.8 mg (75 %) of a 60:40 inseparable mixture of compounds **15** and **16** respectively. Major isomer **15**: ^1H NMR ($CDCl_3$) δ 5.02 (s, 2H) as a characteristic peak; HRMS *m/z* 258.1050 (calcd for $C_{19}H_{14}O$, 258.1045). Minor isomer **16**: ^1H NMR ($CDCl_3$) δ 5.11 (s, 2H) as a characteristic peak; HRMS *m/z* 260.1206 (calcd for $C_{19}H_{16}O$, 260.1201). Mixture: ^{13}C NMR ($CDCl_3$) δ 69.9, 70.2, 115.1, 117.6, 121.3, 121.3, 123.6, 124.1, 126.6, 126.7, 127.1, 127.4, 127.4, 127.5, 127.5, 127.7, 128.4, 128.9, 128.9, 128.9, 129.1, 129.1, 129.3, 129.4, 129.4, 129.8, 132.0,

135.5, 137.8, 139.3, 141.2, 141.9, 142.5, 156.6, 159.0; IR (neat) 3058, 3029, 1599, 1495, 1453, 1243 cm^{-1}.



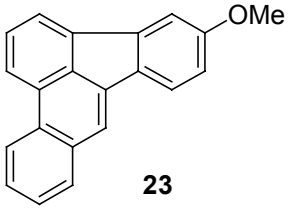
18

Fluoranthene (18). Compound **17** (82.5 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 ^{o}C for 1 d. The reaction mixture was chromatographed using 50:1 hexane/EtOAc to afford 41.0 mg (81 %) of the indicated compound **6** as a white solid: mp 107-108 ^{o}C (lit[14] mp 106-108 ^{o}C). The other spectral properties were identical to those previously reported.[15]



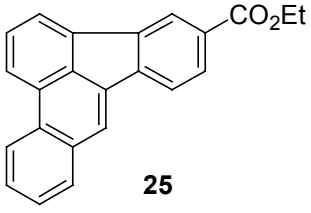
21

Benzo[*e*]acephenanthrylene (21). Compound **20**[1] (95.0 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 ^{o}C for 2 d. The reaction mixture was chromatographed using 50:1 hexane/EtOAc to afford 49.2 mg (78 %) of the indicated compound **8** as a white solid: mp 166-167 ^{o}C (lit[16] mp 165-166 ^{o}C). The other spectral properties were identical to those previously reported.[17]



23

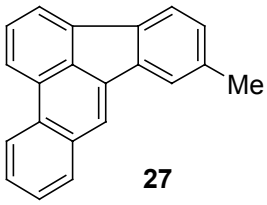
5-Methoxybenzo[*e*]acephenanthrylene (23). Compound **22** (0.103 g, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 ^{o}C for 2 d. The reaction mixture was chromatographed using 30:1 hexanes/ethyl acetate to afford 50.1 mg (71 %) of the indicated compound **23** as a white solid: mp 188-189 ^{o}C (lit[17] mp 189-190 ^{o}C). The other spectral properties were identical to those previously reported.[17]



25

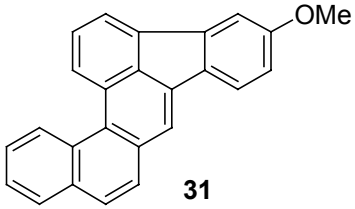
Ethyl benzo[*e*]acephenanthrylene-5-carboxylate (25). Compound **24** (0.113 g, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 ^{o}C for 2 d. The reaction

mixture was chromatographed using 9:1 hexanes/ethyl acetate to afford 40.5 mg (50 %) of the indicated compound **25** as a white solid: mp 153-154 °C; ^{1}H NMR ($CDCl_3$) δ 1.46 (t, *J* = 7.2 Hz, 3H), 4.45 (q, *J* = 7.2 Hz, 2H), 7.63-7.65 (m, 1H), 7.68-7.70 (m, 1H), 7.74-7.78 (m, 1H), 7.98-8.04 (m, 3H), 8.09 (dd, *J* = 7.6, 1.6 Hz, 1H), 8.24 (s, 1H), 8.45 (d, *J* = 8.0 Hz, 1H), 8.54 (d, *J* = 0.8 Hz, 1H), 8.64 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 14.5, 61.2, 120.1, 121.5, 122.1, 122.5, 123.2, 123.3, 127.0, 127.6, 127.7, 128.5, 129.0, 129.9, 130.6, 131.1, 132.4, 133.8, 134.0, 136.2, 140.7, 142.6, 166.9; IR (CH_2Cl_2) 2979, 1710, 1240, 1290 cm^{-1}; HRMS *m/z* 324.1157 (calcd for $C_{23}H_{16}O_2$, 324.1150).



27

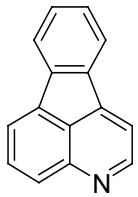
6-Methylbenzo[*e*]acephenanthrylene (27). Compound **26** (98.5 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 °C for 2 d. The reaction mixture was chromatographed using 50:1 hexane/EtOAc to afford 37.2 mg (56 %) of the indicated compound **27** as a white solid: mp 149-151 °C; ^{1}H NMR ($CDCl_3$) δ 2.50 (s, 3H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.59-7.80 (m, 5H), 7.91 (d, *J* = 7.2 Hz, 1H), 8.01-8.02 (m, 1H), 8.17 (s, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.63 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 21.9, 119.2, 121.2, 121.3, 121.3, 122.8, 123.2, 126.8, 127.0, 127.6, 128.3, 129.0, 130.2, 130.8, 132.4, 134.1, 135.3, 137.2, 137.5, 138.2, 138.9; IR (CH_2Cl_2) 2921, 2852, 1460, 1600, 1374 cm^{-1}; HRMS *m/z* 266.1099 (calcd for $C_{21}H_{14}$, 266.1096).



31

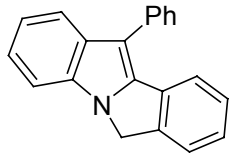
10-Methoxydibenz[*e,l*]acephenanthrylene (31). Compound **30** (0.115 g, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 °C for 2 d. The reaction mixture was chromatographed using 50:1 hexanes/ethyl acetate to afford 54.0 mg (65 %) of the indicated compound **31** as a white solid: mp 178-179 °C; ^{1}H NMR ($CDCl_3$) δ 3.95 (s,

3H), 6.93 (dd, J = 8.1, 2.4 Hz, 1H), 7.46 (d, J = 2.1 Hz, 1H), 7.60-7.66 (m, 1H), 7.70-8.03 (m, 7H), 8.11 (s, 1H), 8.98 (d, J = 8.4 Hz, 1H), 9.19 (d, J = 8.7 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 55.9, 107.4, 113.4, 119.6, 121.0, 122.8, 122.8, 126.0, 126.8, 127.3, 127.5, 127.8, 128.3, 128.4, 128.6, 128.7, 129.0, 131.5, 131.5, 133.8, 133.8, 136.1, 137.4, 142.6, 160.6; IR (CH_2Cl_2) 2921, 2849, 1608, 1461, 1285, 1213 cm^{-1}; HRMS *m/z* 332.1209 (calcd for $C_{25}H_{16}O$, 332.1201).



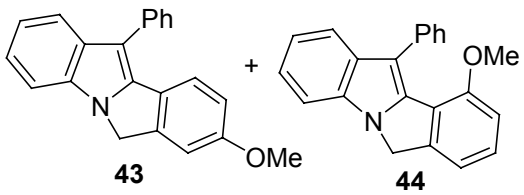
35

Indeno[1,2,3-*de*]quinoline (35). Compound **34** (82.8 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 °C for 2.5 d. The reaction mixture was chromatographed using 3:2 hexanes/ethyl acetate to afford 27.4 mg (54 %) of the indicated compound **35** as a white solid: mp 100-101 °C (lit[18] mp 102-103 °C); ^{1}H NMR ($CDCl_3$) δ 7.35-7.51 (m, 2H), 7.72-7.77 (m, 2H), 7.84-7.91 (m, 3H), 7.99 (d, J = 8.4 Hz, 1H), 9.07 (d, J = 4.2 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 114.4, 121.0, 122.2, 123.7, 128.2, 128.4, 130.4, 131.7, 135.4, 138.2, 138.2, 140.5, 145.1, 145.7, 152.9. The other spectral properties were identical to those previously reported.[19]



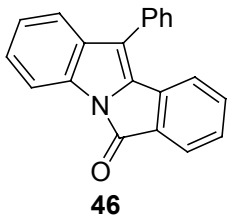
41

11-Phenyl-6*H*-isoindolo[2,1-*a*]indole (41). Compound **40** (103 mg, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d affording a 92 % yield of the indicated compound **41**, which is unstable on silica gel, as determined by ^{1}H NMR spectroscopy. To obtained pure compound **41**, the crude product was recrystallized (hexane/EtOAc) to afford a pale purple solid: mp 148-151 ºC; ^{1}H NMR (DMSO-d_6) δ 5.27 (s, 2H), 7.09-7.13 (m, 1H), 7.21-7.25 (m, 1H), 7.36-7.39 (m, 3H), 7.51-7.58 (m, 3H), 7.63-7.65 (m, 1H), 7.68-7.70 (m, 3H), 7.74-7.76 (m, 1H); ^{13}C NMR (DMSO-d_6) δ 48.2, 108.0, 110.2, 119.5, 120.0, 120.2, 122.0, 124.2, 126.2, 127.6, 128.0, 128.7, 128.9, 130.4, 131.9, 133.5, 134.4, 139.3, 142.7; IR (CH_2Cl_2) 3053, 2985, 1616, 1603, 1497 cm^{-1}; HRMS *m/z* 281.1209 (calcd for $C_{21}H_{15}N$, 281.1205).



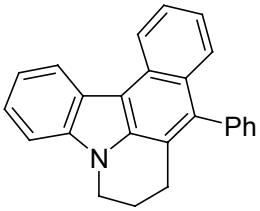
43 **44**

8-Methoxy-11-phenyl-6*H*-isoindolo[2,1-*a*]indole (43) and 10-methoxy-11-phenyl-6*H*-isoindolo[2,1-*a*]indole (44). Compound **42** (0.110 g, 0.25 mmol) was allowed to react under our standard reaction conditions for 12 h. The reaction mixture was chromatographed using 9:1 hexane/EtOAc to afford 61 mg (78 %) of the compound **43** as a yellow solid and 9 mg (12 %) of the compound **44**. Compound **43**: mp 196-198 ^{o}C; ^{1}H NMR (DMSO-d_6) δ 3.83 (s, 3H), 5.23 (s, 2H), 6.97 (d, J = 8.4 Hz, 1H), 7.07-7.10 (m, 1H), 7.17-7.21 (m, 1H), 7.27 (s, 1H), 7.34-7.37 (m, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.53-7.57 (m, 2H), 7.66-7.68 (m, 4H); ^{13}C NMR (DMSO-d_6) δ 48.4, 55.8, 108.1, 109.3, 109.8, 113.7, 120.0, 120.3, 121.9, 122.1, 126.0, 126.2, 128.9, 129.3, 131.6, 134.1, 135.4, 140.3, 144.2, 159.7; IR (CH_2Cl_2) 3051, 1686, 1450 cm^{-1}; HRMS *m/z* 311.1316 (calcd for $C_{22}H_{17}ON$, 311.1310).



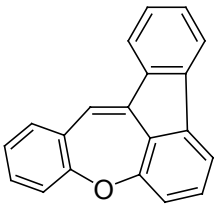
46

11-Phenyl-6*H*-isoindolo[2,1-*a*]indol-6-one (46). Compound **45** (0.106 g, 0.25 mmol) was allowed to react under our standard reaction conditions for 1 d. The reaction mixture was chromatographed using 10:1 hexane/EtOAc to afford 24 mg (33 %) of the indicated compound **46** as a yellow solid: mp 222-223 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 7.17-7.21 (m, 1H), 7.31-7.36 (m, 2H), 7.40-7.44 (m, 1H), 7.45-7.49 (m, 1H), 7.54-7.60 (m, 4H), 7.70-7.72 (m, 2H), 7.79 (d, J = 7.6 Hz, 1H), 7.97 (d, J = 7.6 Hz, 1H); ^{13}C NMR ($CDCl_3$) δ 113.8, 120.8, 121.4, 121.5, 124.3, 125.6, 127.0, 128.6, 129.0, 129.2, 129.3, 132.4, 133.9, 134.0, 134.1, 134.2, 134.4, 134.9, 162.8; IR (CH_2Cl_2) 3053, 2987, 1731, 1264 cm^{-1}; HRMS *m/z* 295.1003 (calcd for $C_{21}H_{13}ON$, 295.0997).



48

9-Phenyl-7,8-dihydro-6*H*-benzo[*c*]pyrido[1,2,3-*lm*]carbazole (48). Compound **47** (116 mg, 0.25 mmol) was allowed to react under our standard reaction conditions for 12 h. The reaction mixture was chromatographed using 20:1 hexane/EtOAc to afford 54 mg (65 %) of the indicated compound **48** as a yellow solid: mp 239-241 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 2.21-2.29 (m, 2H), 2.87 (t, *J* = 6.0 Hz, 2H), 4.31 (t, *J* = 5.7 Hz, 2H), 7.28-7.34 (m, 1H), 7.35-7.55 (m, 8H), 7.61-7.65 (m, 2H), 8.58 (d, *J* = 7.8 Hz, 1H), 8.74-8.77 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 22.8, 24.8, 41.3, 109.1, 112.5, 119.9, 121.1, 122.3, 122.6, 123.2, 123.7, 123.9, 125.9, 127.4, 127.9, 128.5, 129.1, 129.2, 130.8, 135.3, 135.7, 139.1, 139.2; IR (CH_2Cl_2) 3053, 2986, 1421, 1265 cm^{-1}; HRMS *m/z* 333.1523 (calcd for $C_{25}H_{19}N$, 333.1518). Anal. Calcd for $C_{25}H_{19}N$: C, 90.06; H, 5.74; N, 4.20. Found: C, 90.27; H, 5.44; N, 4.17.



50

Benzo[*f*]fluoreno[1,9-*bc*]oxepine (50). Compound **49** (99.1 mg, 0.25 mmol) was allowed to react under our standard reaction conditions at 110 ^{o}C for 2 d. The reaction mixture was chromatographed using 18:1 hexanes/ethyl acetate to afford 53.6 mg (80 %) of the indicated compound **50** as a white solid: mp 106-107 ^{o}C; ^{1}H NMR ($CDCl_3$) δ 6.69 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.83 (s, 1H), 6.93-6.95 (m, 1H), 6.97-6.99 (m, 1H), 7.05-7.07 (m, 1H), 7.16-7.30 (m, 5H), 7.58-7.59 (m, 1H), 7.62-7.64 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 115.4, 117.2, 120.4, 120.6, 122.3, 124.8, 126.0, 127.2, 128.3, 128.7, 129.1, 131.3, 131.4, 132.4, 137.1, 137.6, 139.9, 141.0, 154.8, 155.6; IR (CH_2Cl_2) 3050, 1580, 1238, 1450, 1426 cm^{-1}; HRMS *m/z* 268.0892 (calcd for $C_{20}H_{12}O$, 268.0888).

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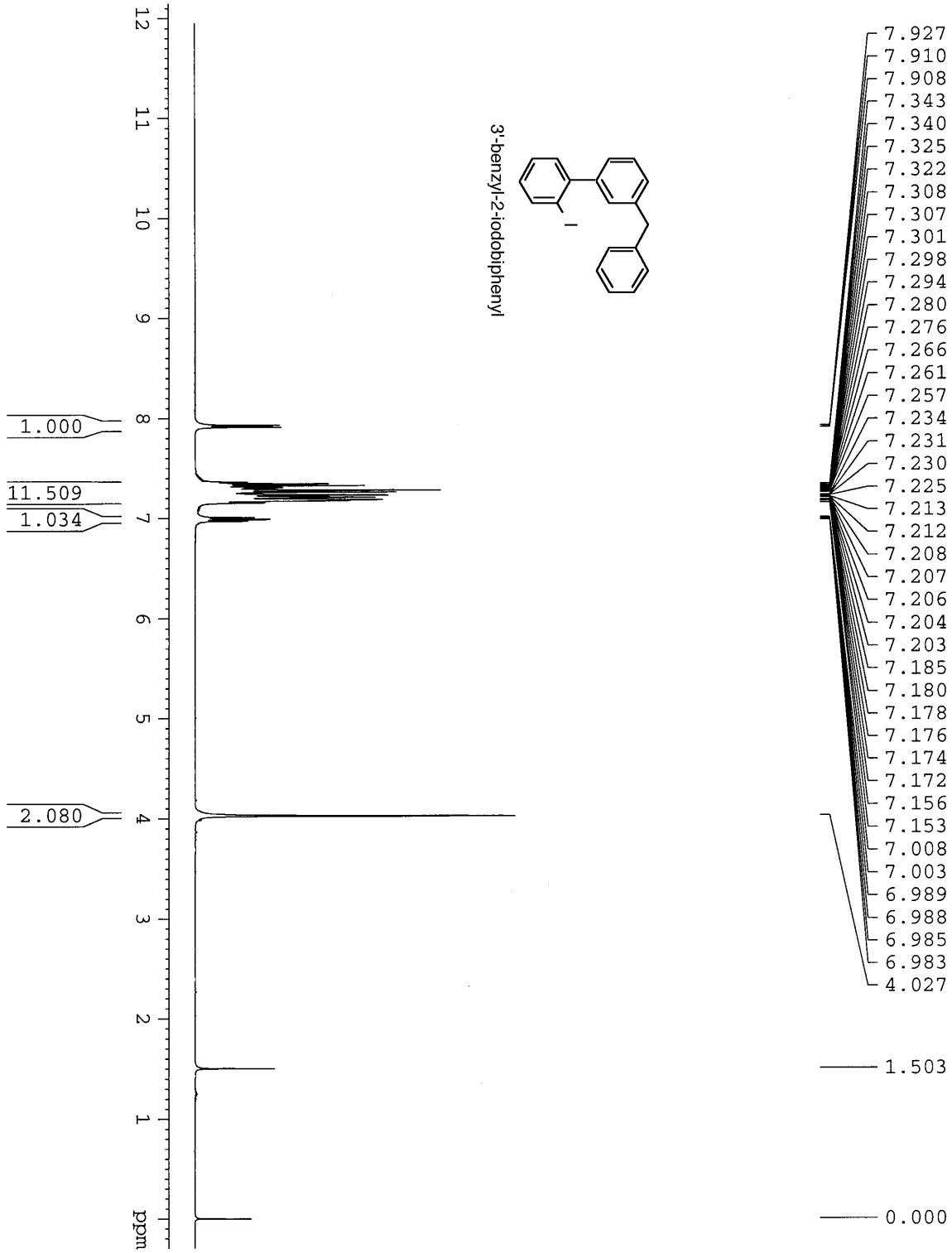
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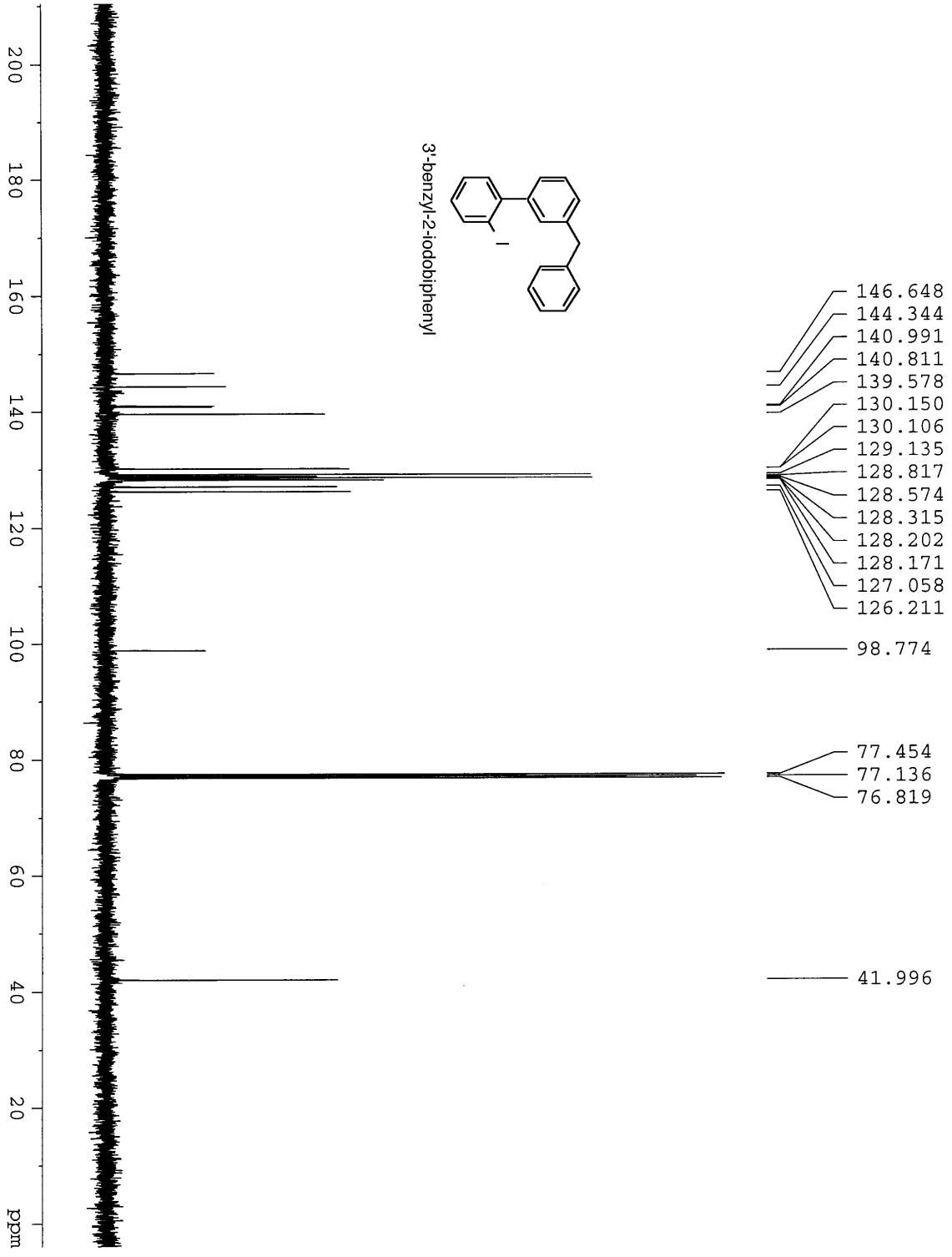
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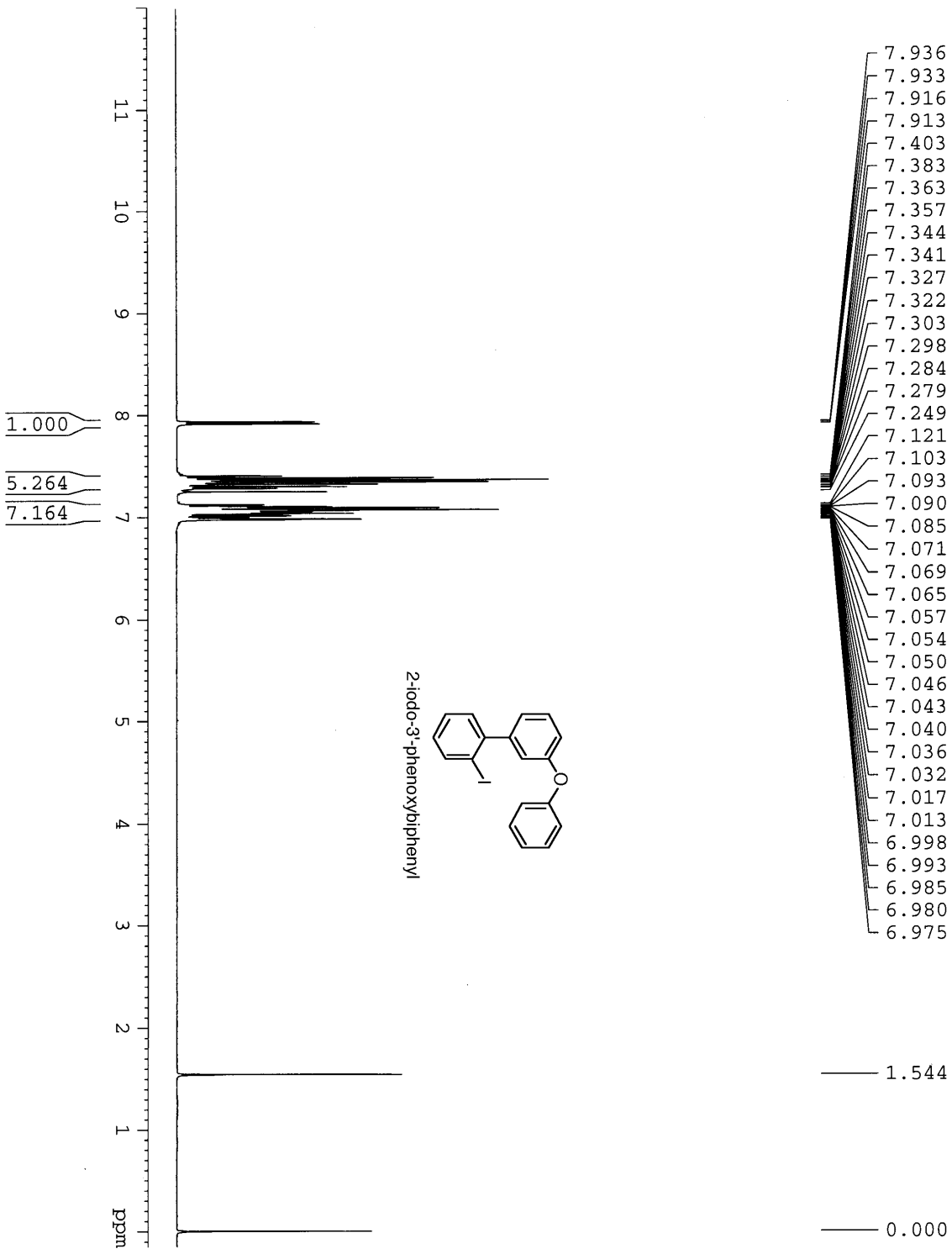
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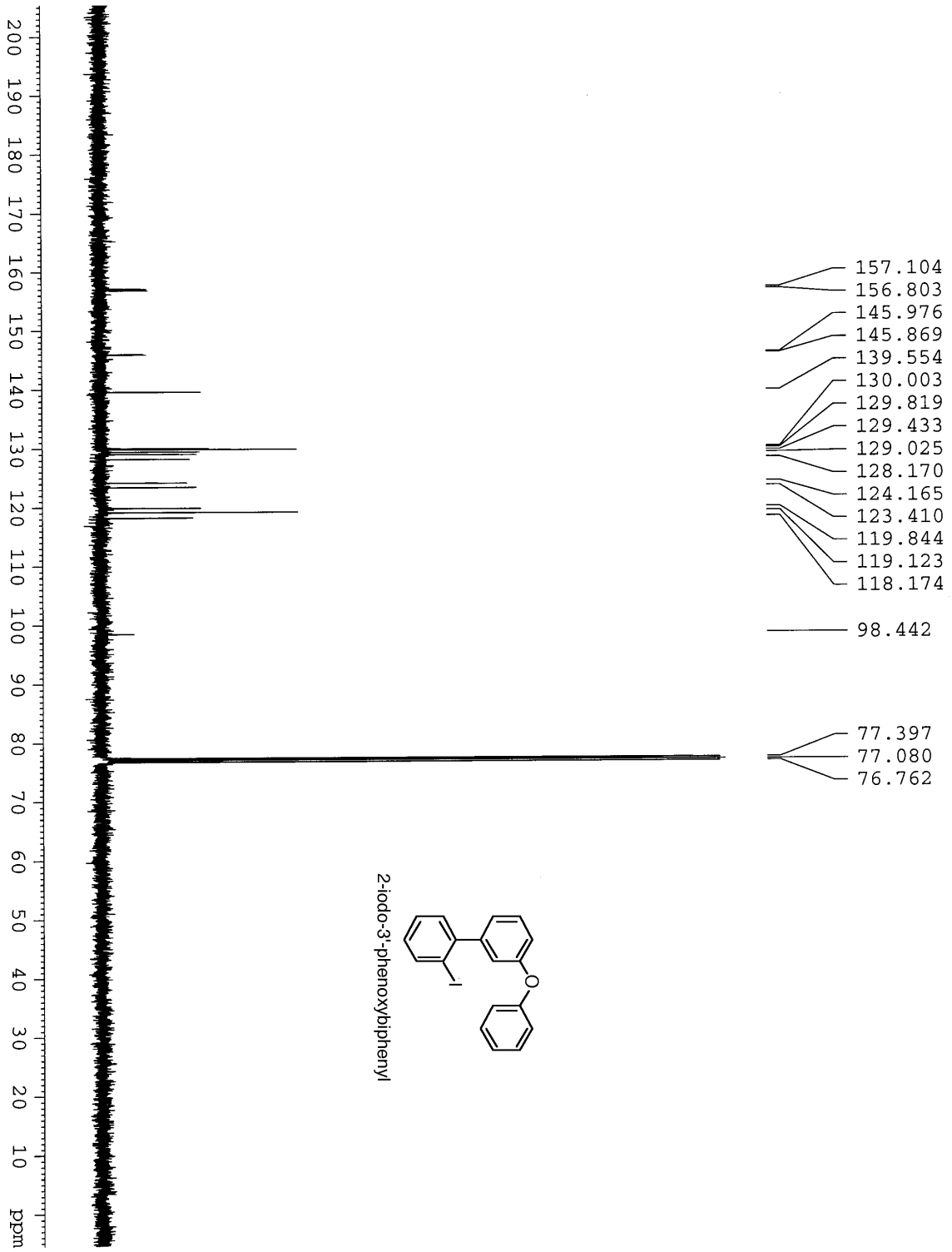
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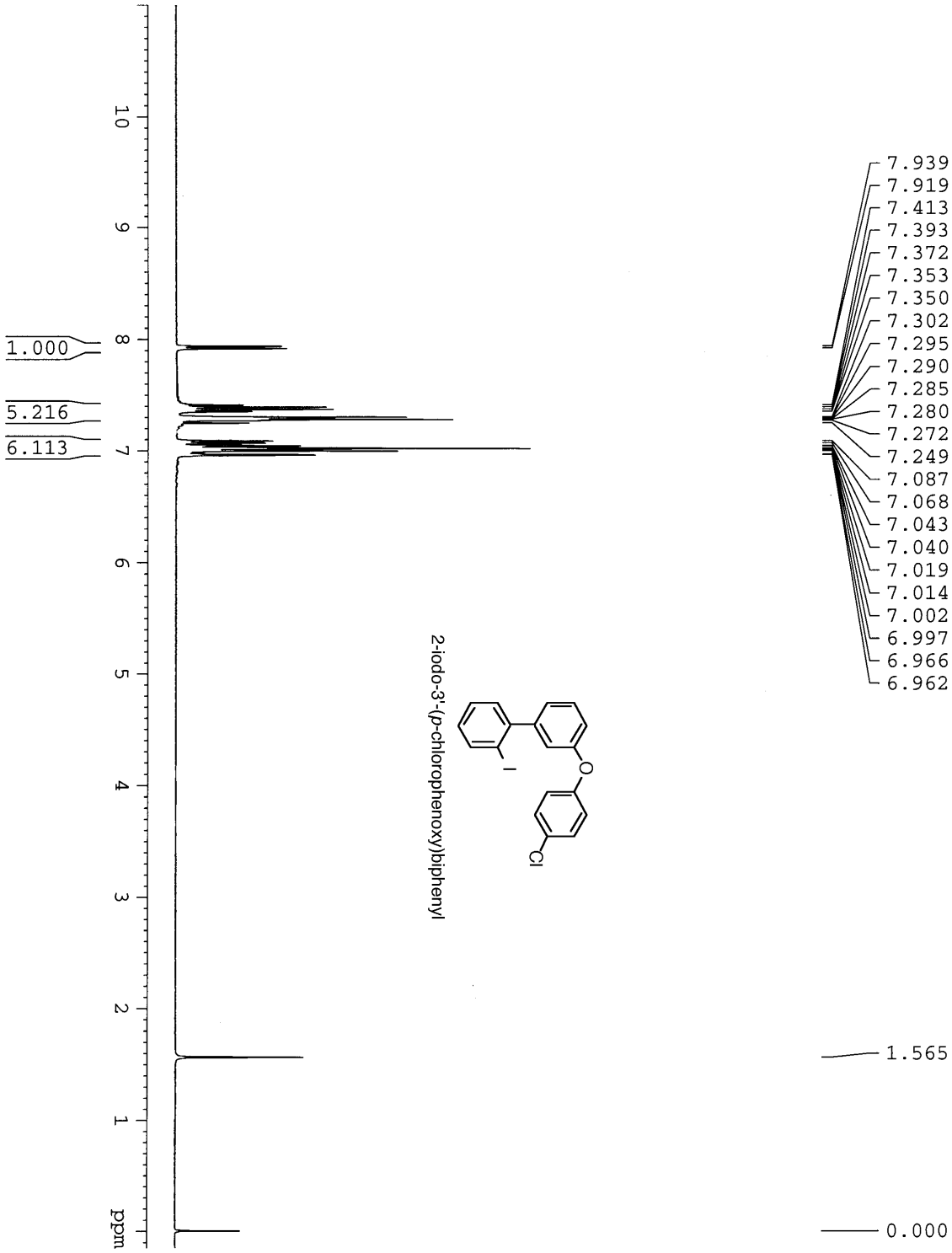
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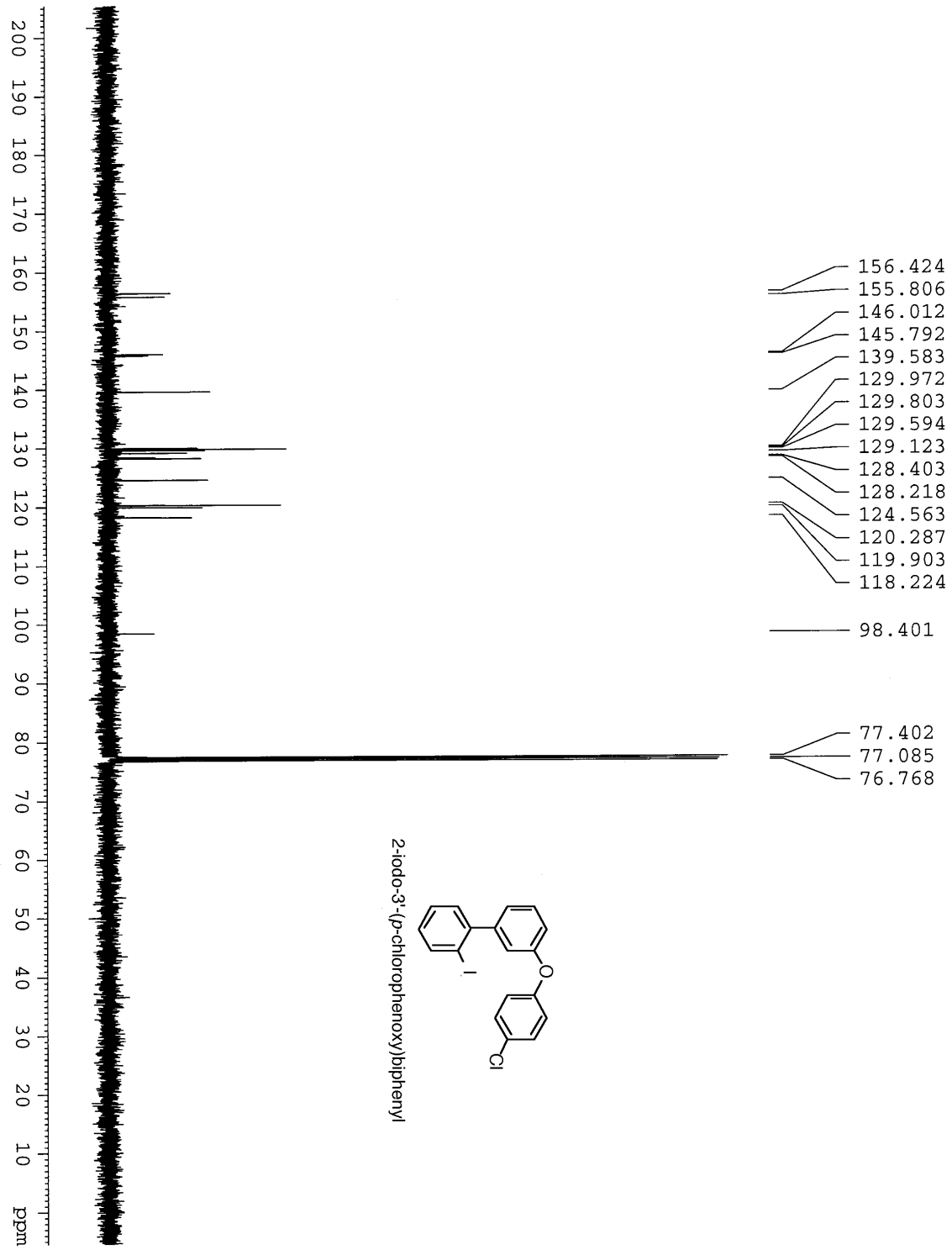
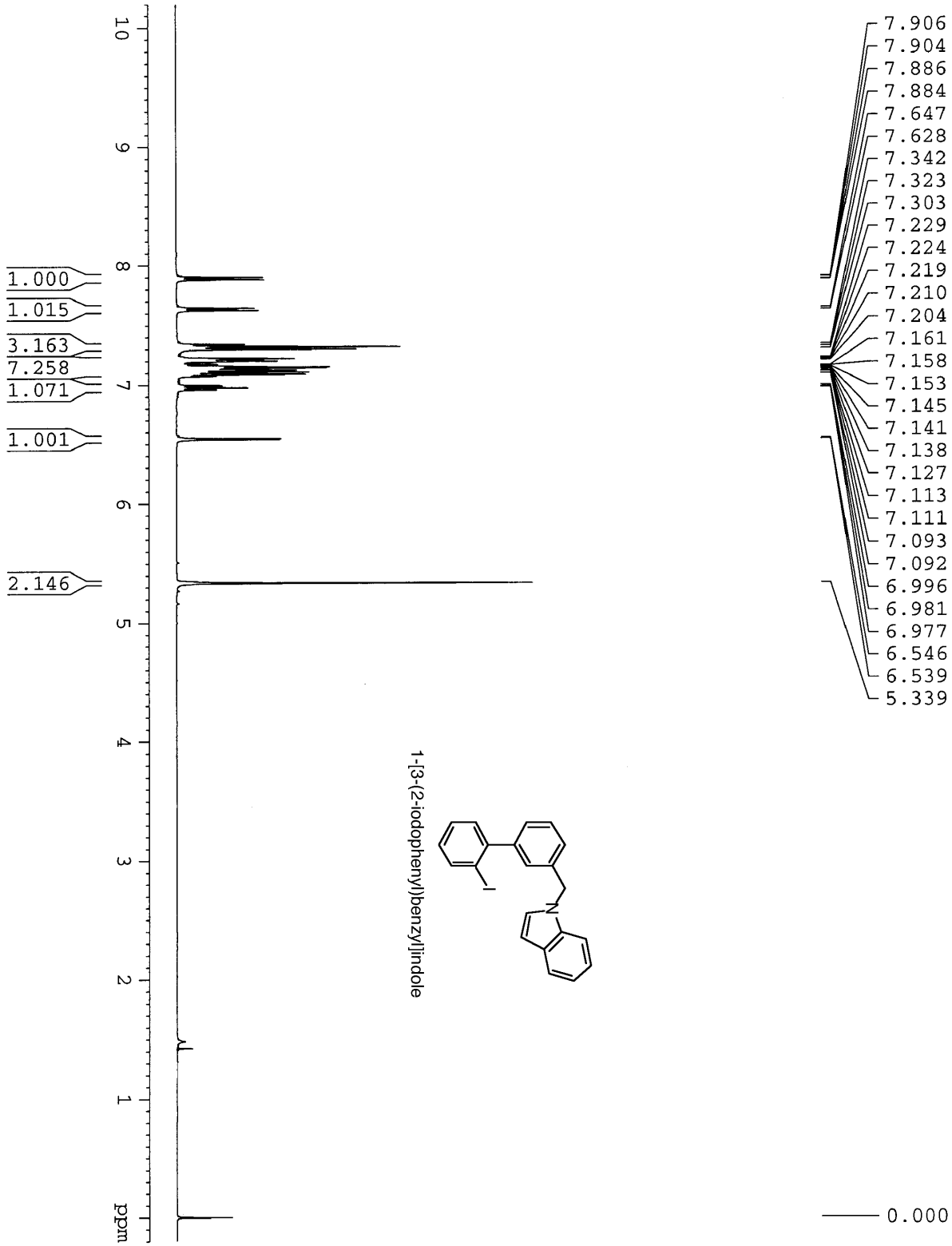
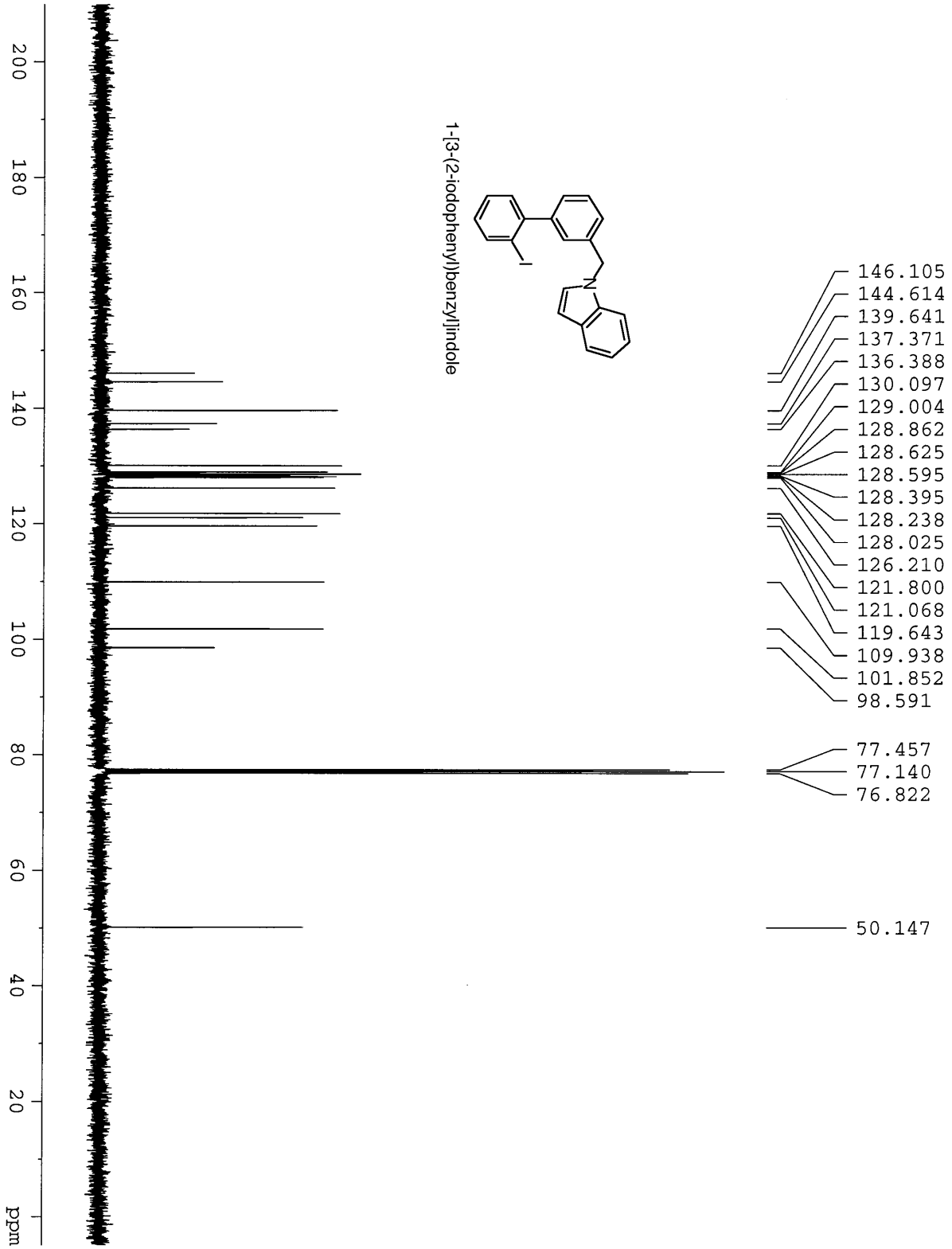
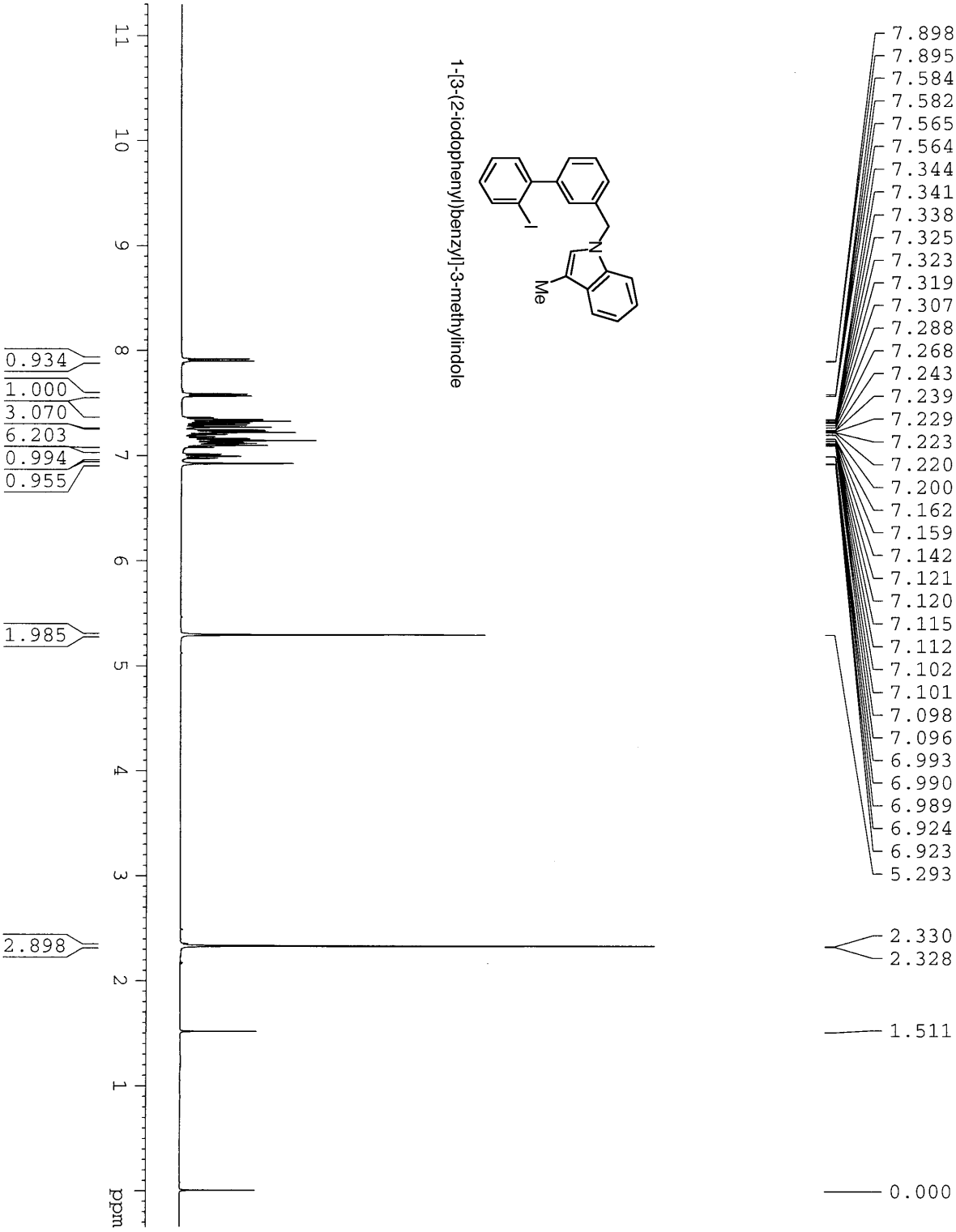
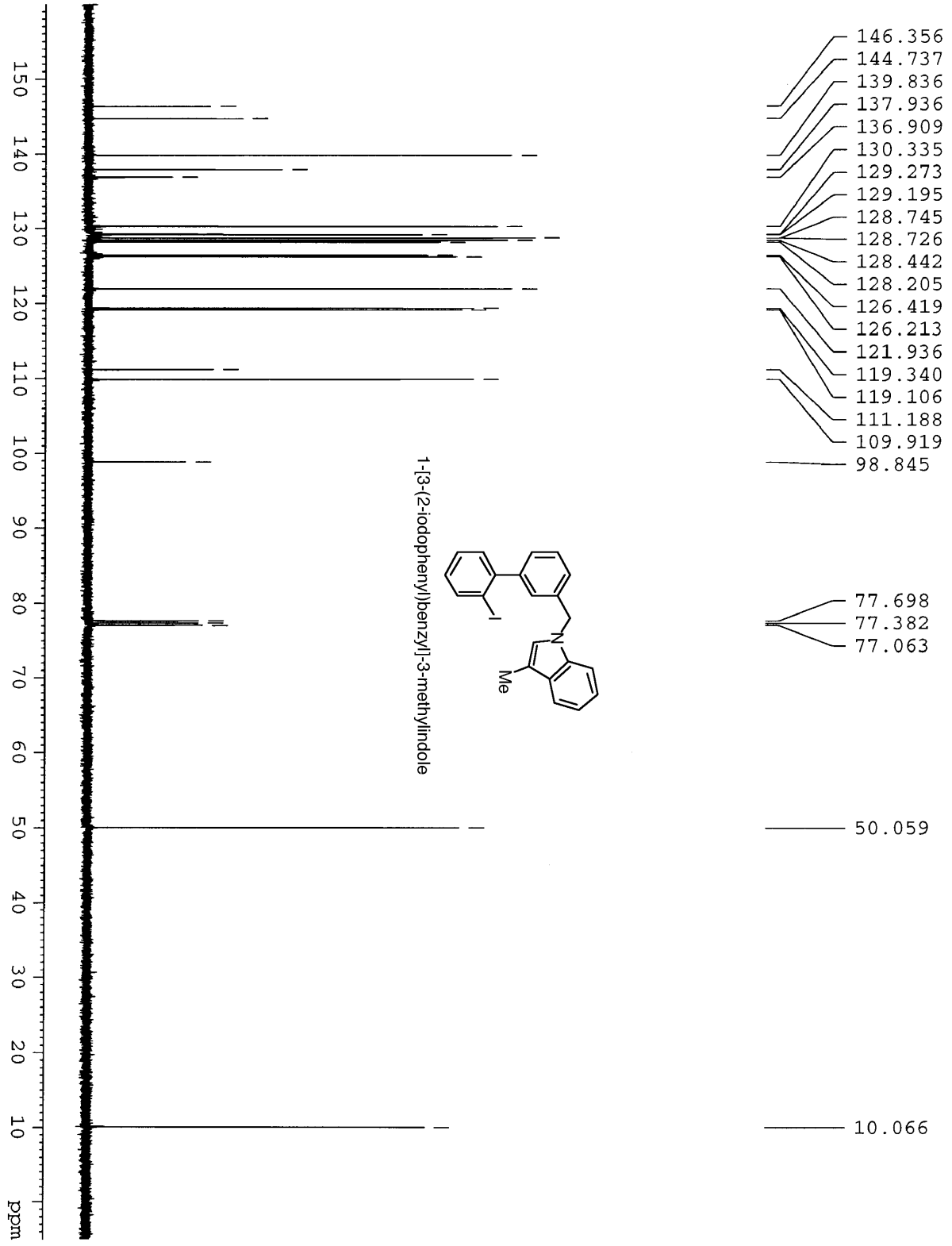
7.353
7.350
7.302
7.295
7.290
7.285
7.280
7.272
7.249
7.087
7.068
7.043
7.040
7.019
7.014
7.002
6.997
6.966
6.962
1.565
0.000
1.000
5.216
6.113
10
9
8
7
6
5
4
3
2
1
ppm
2-iodo-3'-(p-chlorophenoxy)biphenyl
I
O
Cl

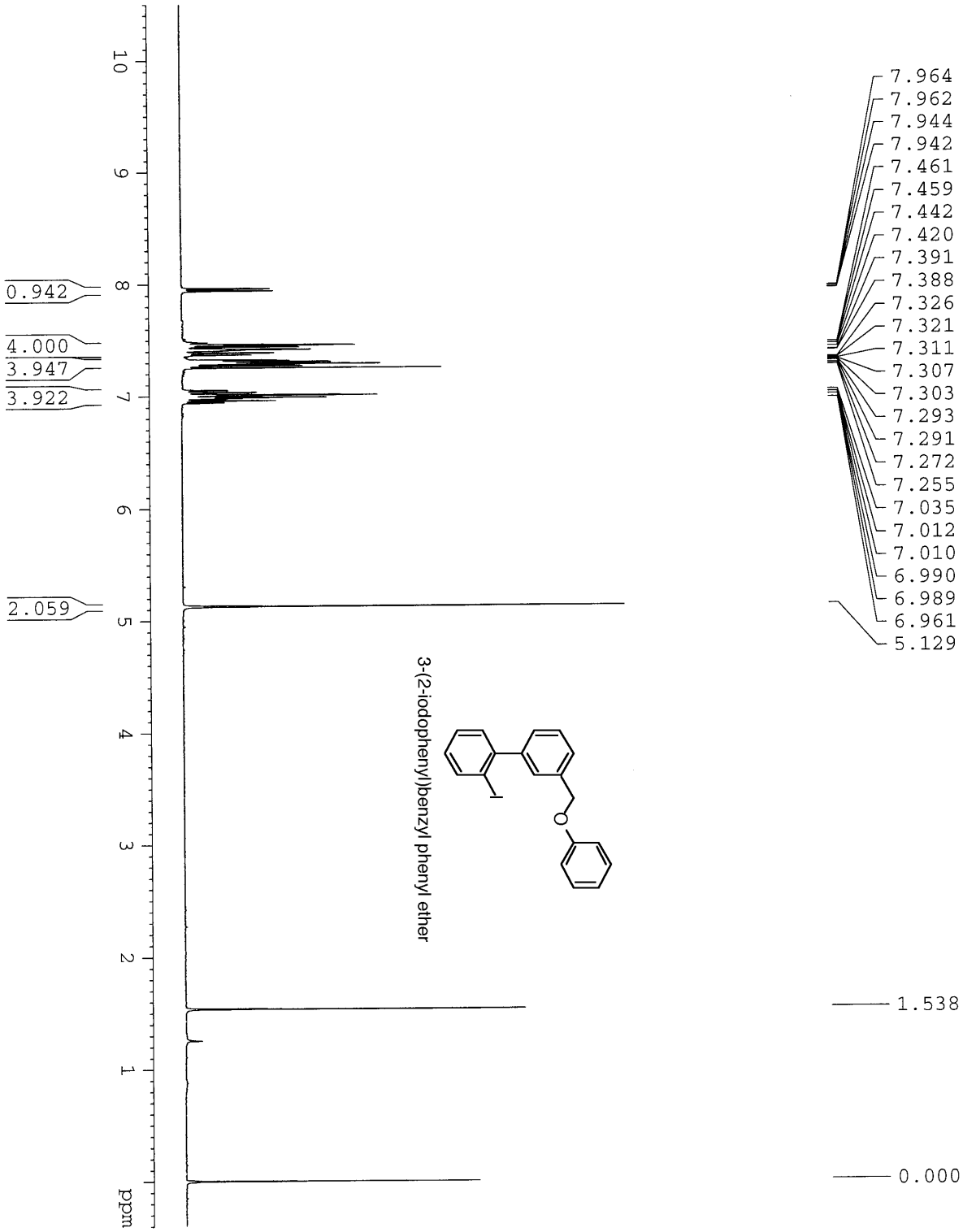

156.424
155.806
146.012
145.792
139.583
129.972
129.803
129.594
129.123
128.403
128.218
124.563
120.287
119.903
118.224
98.401
77.402
77.085
76.768
2-iodo-3'-(p-chlorophenoxy)biphenyl
I
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

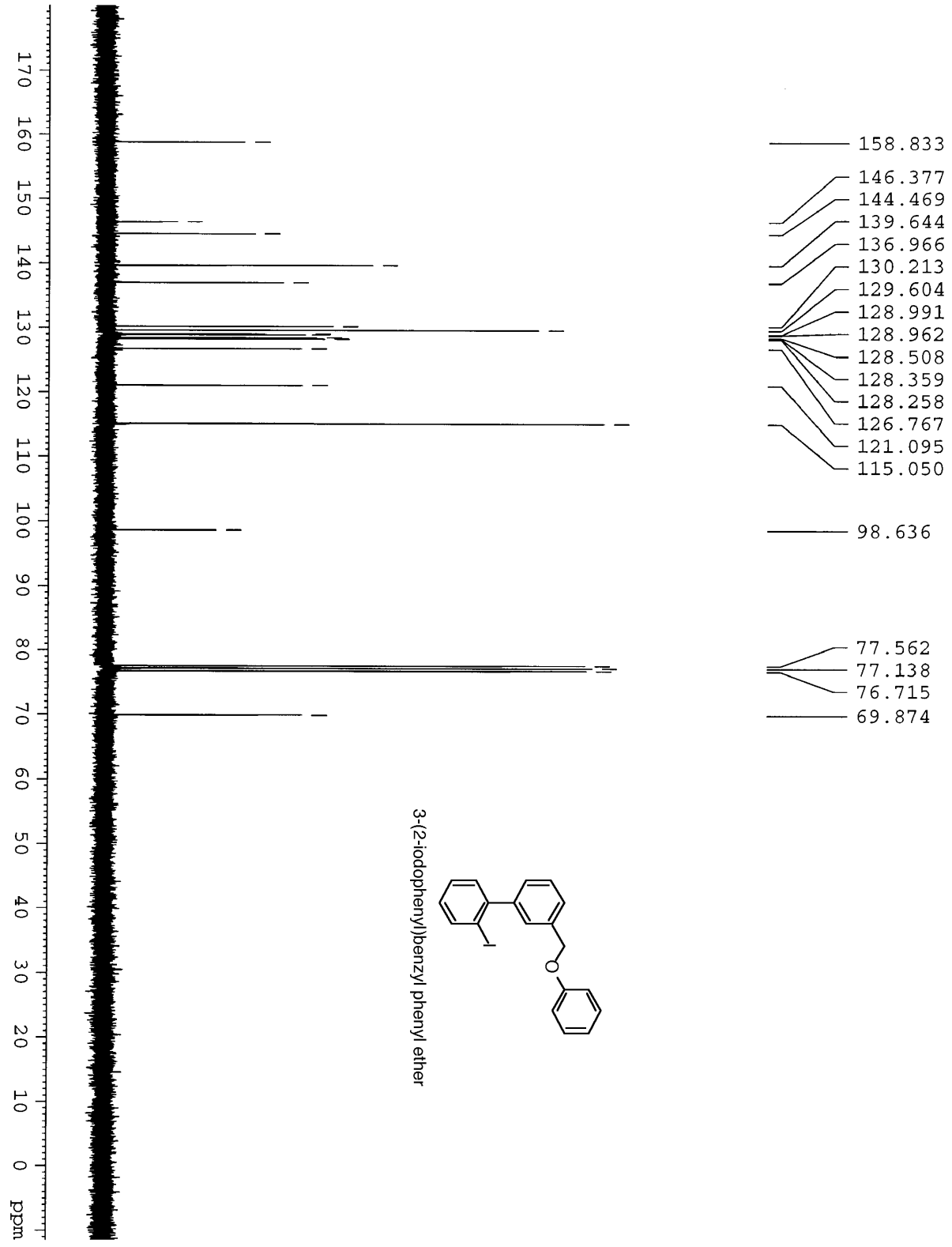

7.906
7.904
7.886
7.884
7.647
7.628
7.342
7.323
7.303
7.229
7.224
7.219
7.210
7.204
7.161
7.158
7.153
7.145
7.141
7.138
7.127
7.113
7.111
7.093
7.092
6.996
6.981
6.977
6.546
6.539
5.339
1.000
1.015
3.163
7.258
1.071
1.001
2.146
10
9
8
7
6
5
4
3
2
1
ppm
0.000
1-[3-(2-iodophenyl)benzyl]indole
I
N

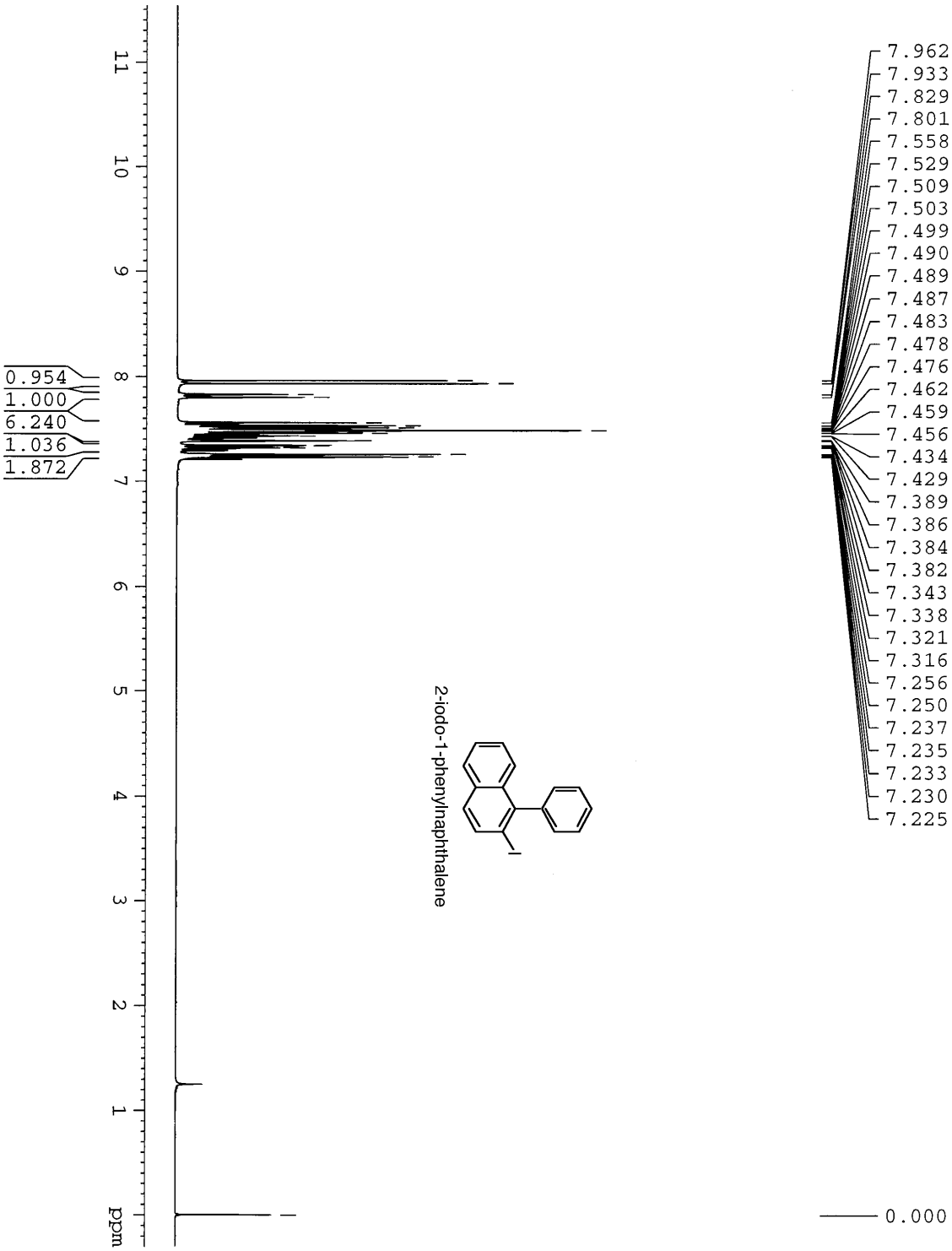

1-[3-(2-iodophenyl)benzyl]indole
I
N
146.105
144.614
139.641
137.371
136.388
130.097
129.004
128.862
128.625
128.595
128.395
128.238
128.025
126.210
121.800
121.068
119.643
109.938
101.852
98.591
77.457
77.140
76.822
50.147
200
180
160
140
120
100
80
60
40
20
ppm

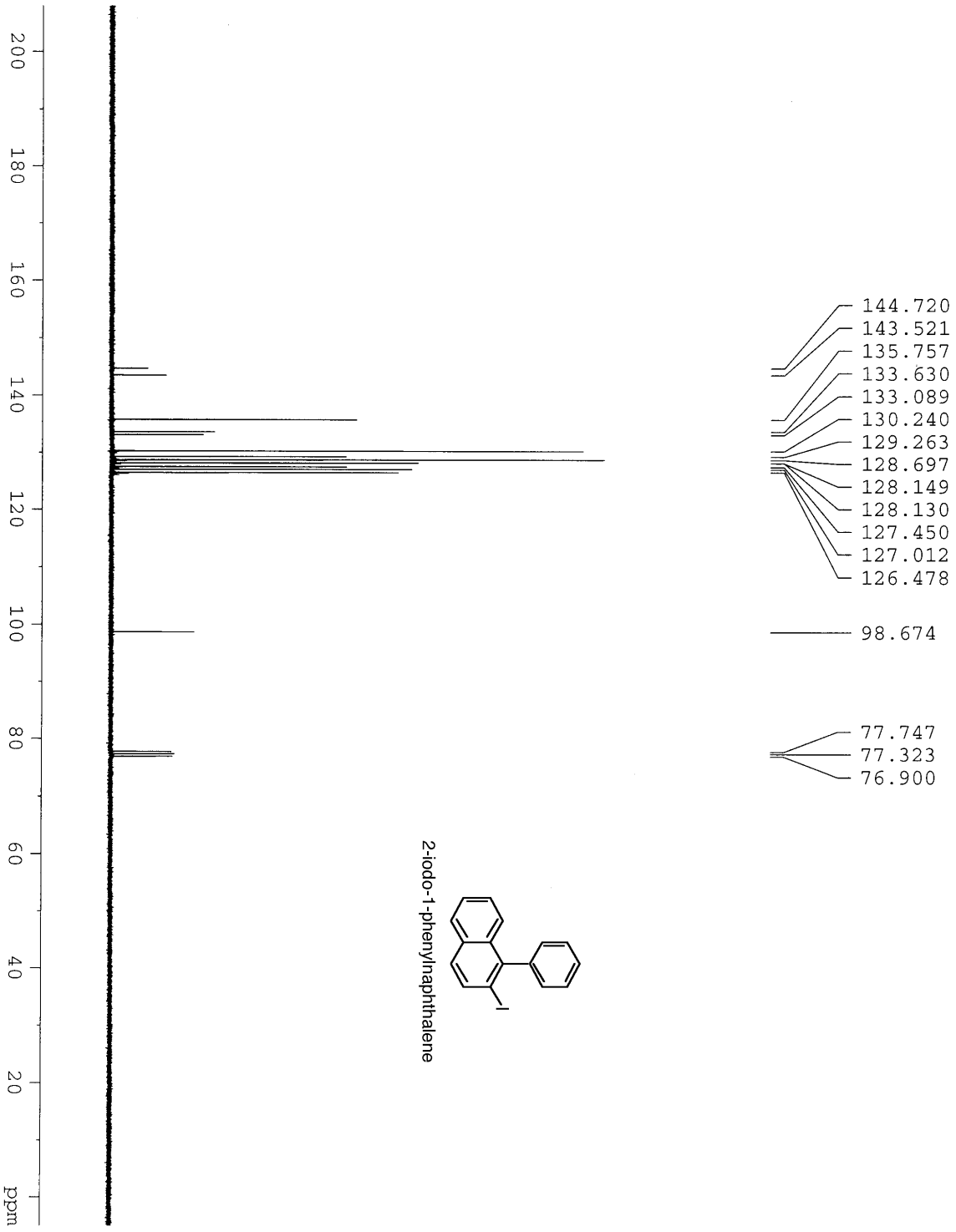

1-[3-(2-iodophenyl)benzyl]-3-methylindole
Me
I
N
7.898
7.895
7.584
7.582
7.565
7.564
7.344
7.341
7.338
7.325
7.323
7.319
7.307
7.288
7.268
7.243
7.239
7.229
7.223
7.220
7.200
7.162
7.159
7.142
7.121
7.120
7.115
7.112
7.102
7.101
7.098
7.096
6.993
6.990
6.989
6.924
6.923
5.293
2.330
2.328
1.511
0.000
0.934
1.000
3.070
6.203
0.994
0.955
1.985
2.898
ppm

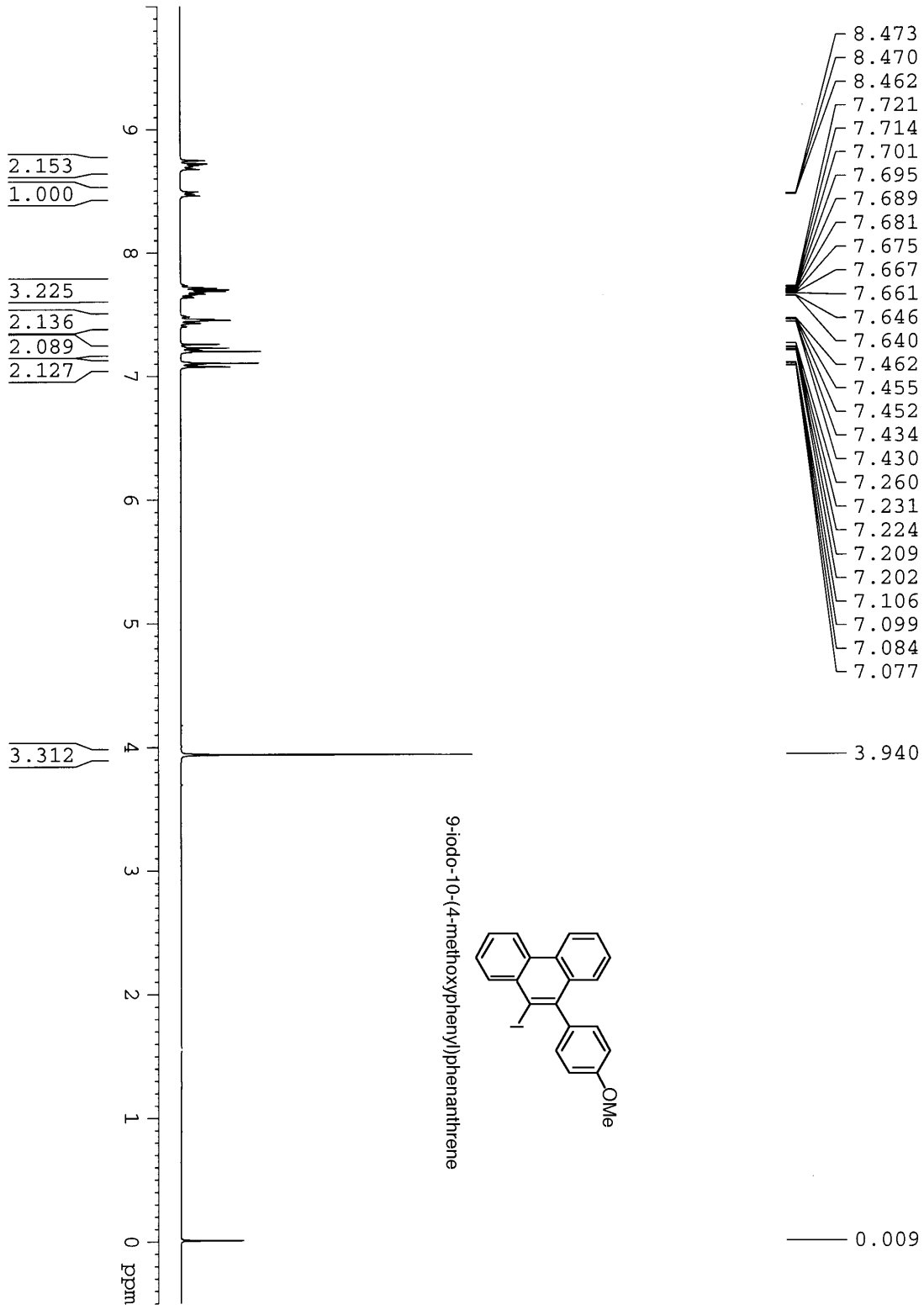

146.356
144.737
139.836
137.936
136.909
130.335
129.273
129.195
128.745
128.726
128.442
128.205
126.419
126.213
121.936
119.340
119.106
111.188
109.919
98.845
77.698
77.382
77.063
50.059
10.066
1-[3-(2-iodophenyl)benzyl]-3-methylindole
I
N
Me
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

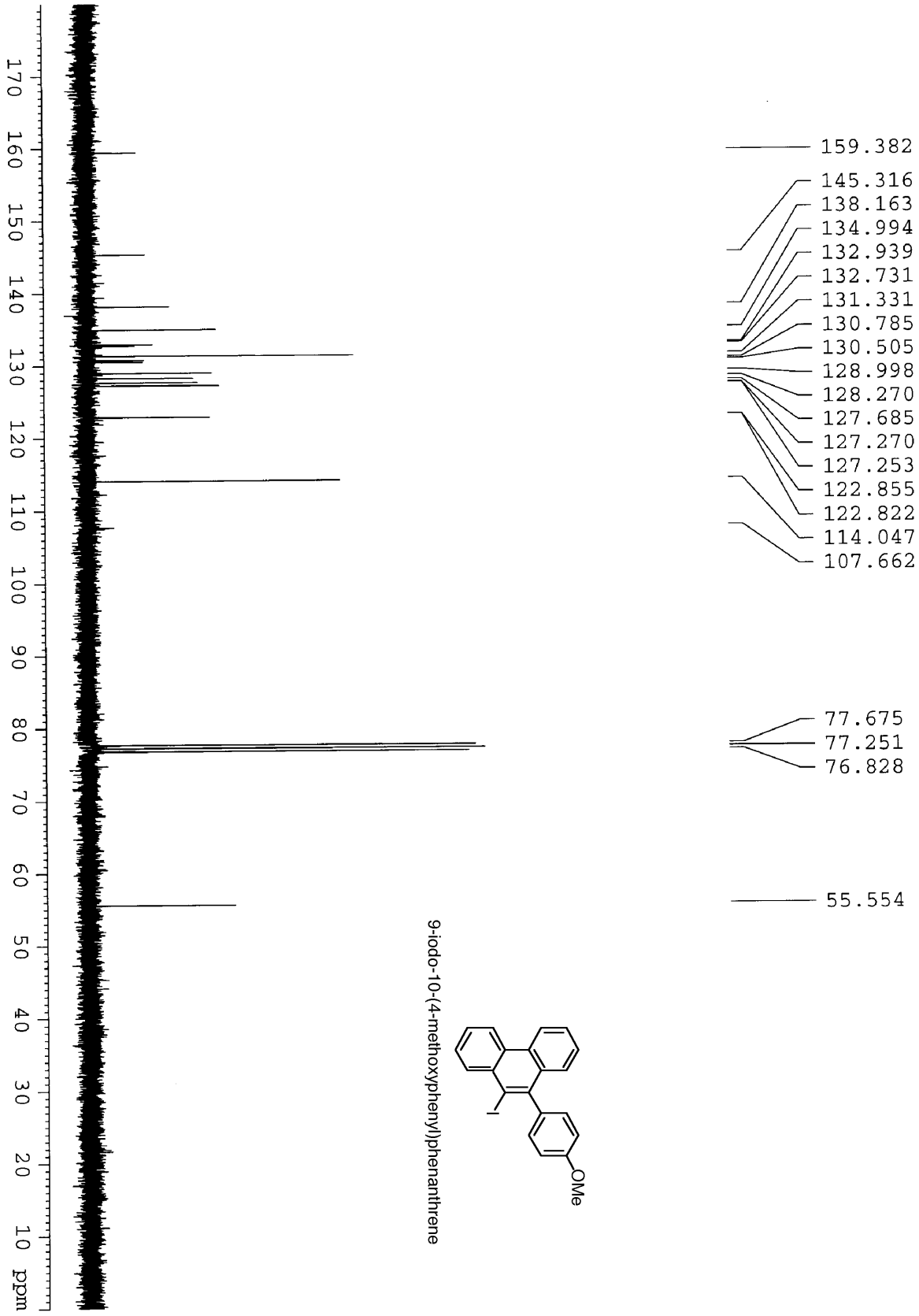

7.964
7.962
7.944
7.942
7.461
7.459
7.442
7.420
7.391
7.388
7.326
7.321
7.311
7.307
7.303
7.293
7.291
7.272
7.255
7.035
7.012
7.010
6.990
6.989
6.961
5.129
1.538
0.000
0.942
4.000
3.947
3.922
2.059
10
9
8
7
6
5
4
3
2
1
ppm
3-(2-iodophenyl)benzyl phenyl ether
I
O

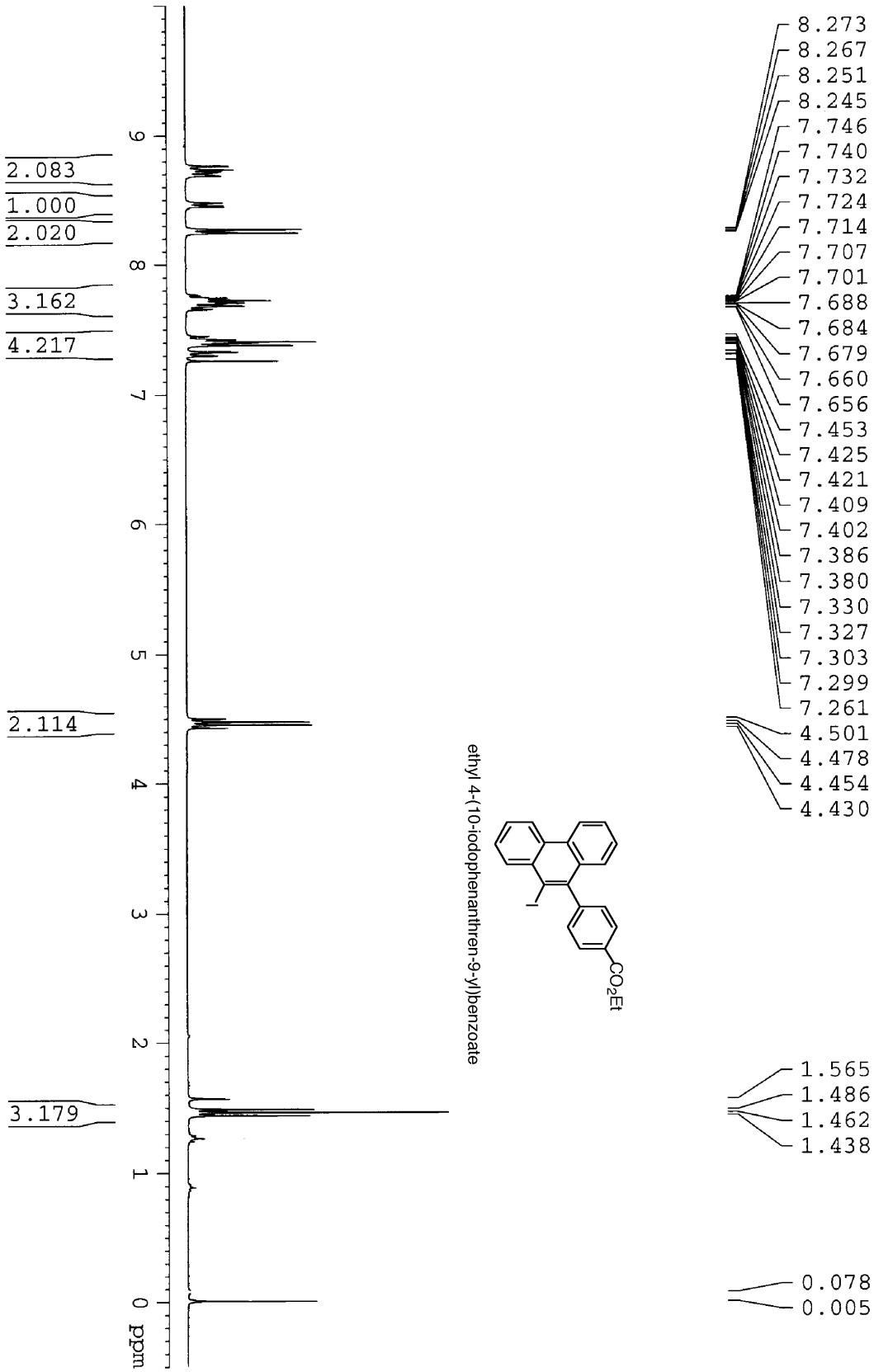

158.833
146.377
144.469
139.644
136.966
130.213
129.604
128.991
128.962
128.508
128.359
128.258
126.767
121.095
115.050
98.636
77.562
77.138
76.715
69.874
3-(2-iodophenyl)benzyl phenyl ether
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

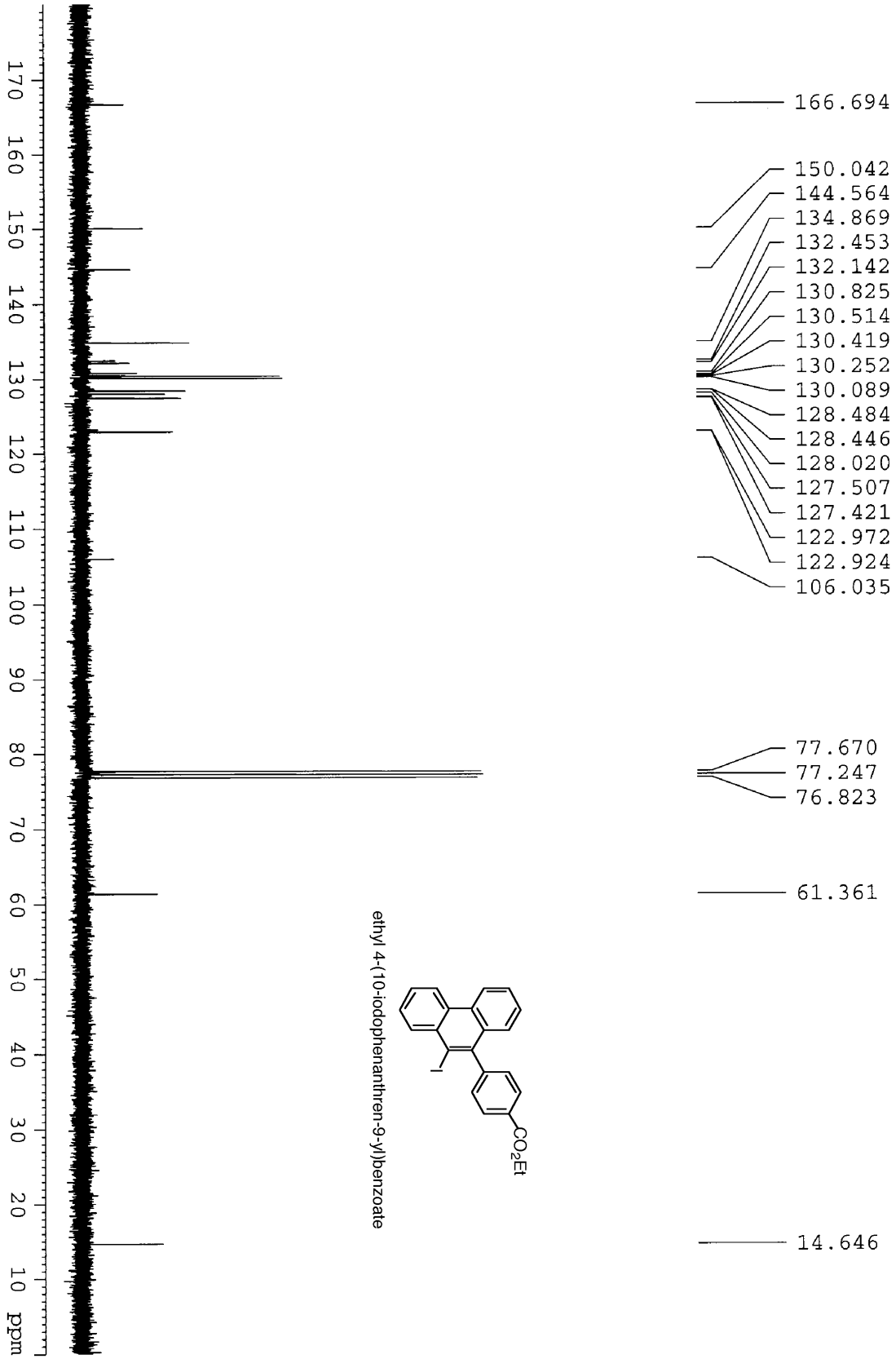

0.954
1.000
6.240
1.036
1.872
11
10
9
8
7
6
5
4
3
2
1
ppm
2-iodo-1-phenylnaphthalene
7.962
7.933
7.829
7.801
7.558
7.529
7.509
7.503
7.499
7.490
7.489
7.487
7.483
7.478
7.476
7.462
7.459
7.456
7.434
7.429
7.389
7.386
7.384
7.382
7.343
7.338
7.321
7.316
7.256
7.250
7.237
7.235
7.233
7.230
7.225
0.000

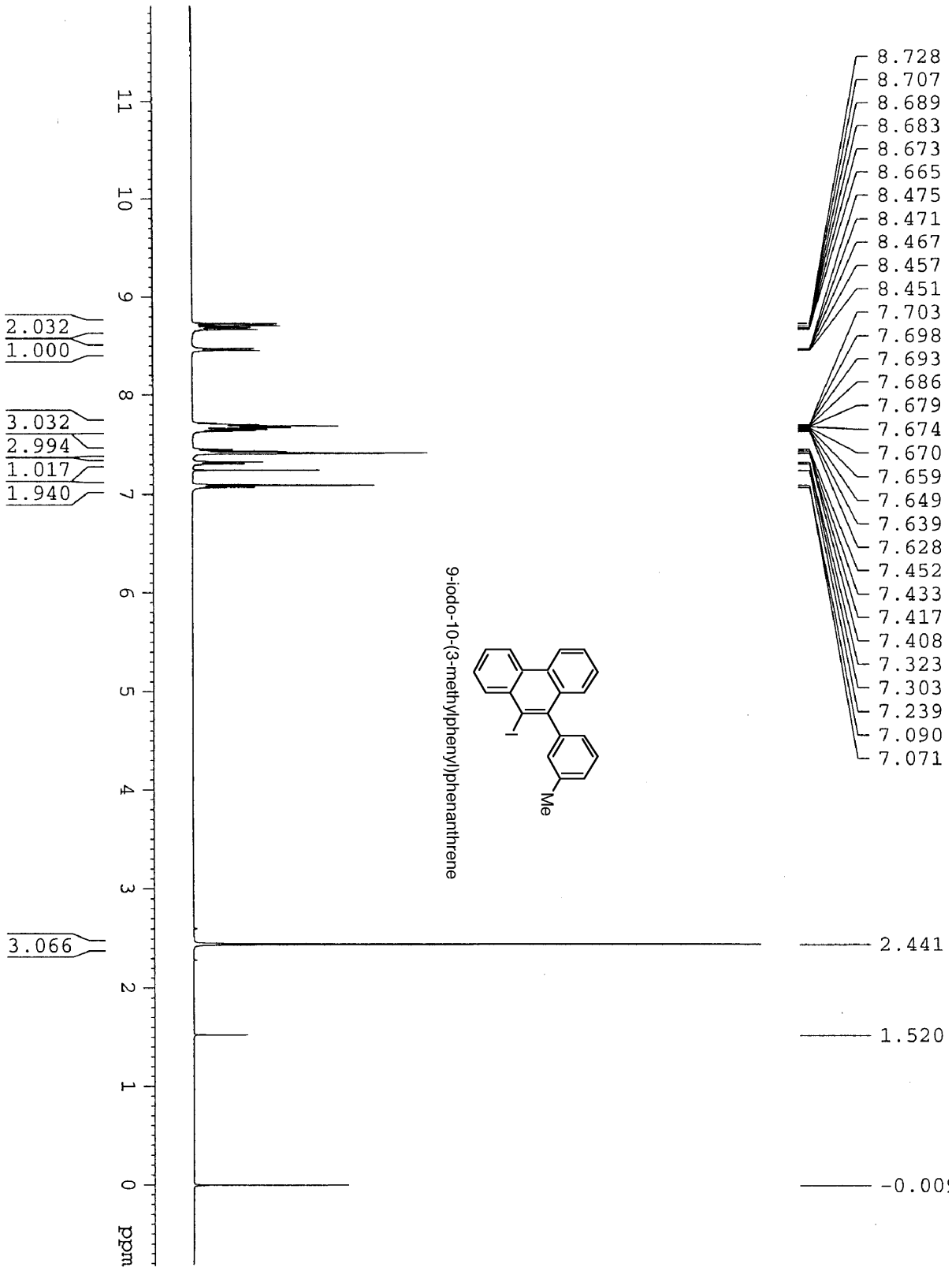

200
180
160
140
120
100
80
60
40
20
ppm
144.720
143.521
135.757
133.630
133.089
130.240
129.263
128.697
128.149
128.130
127.450
127.012
126.478
98.674
77.747
77.323
76.900
2-iodo-1-phenylnaphthalene
I

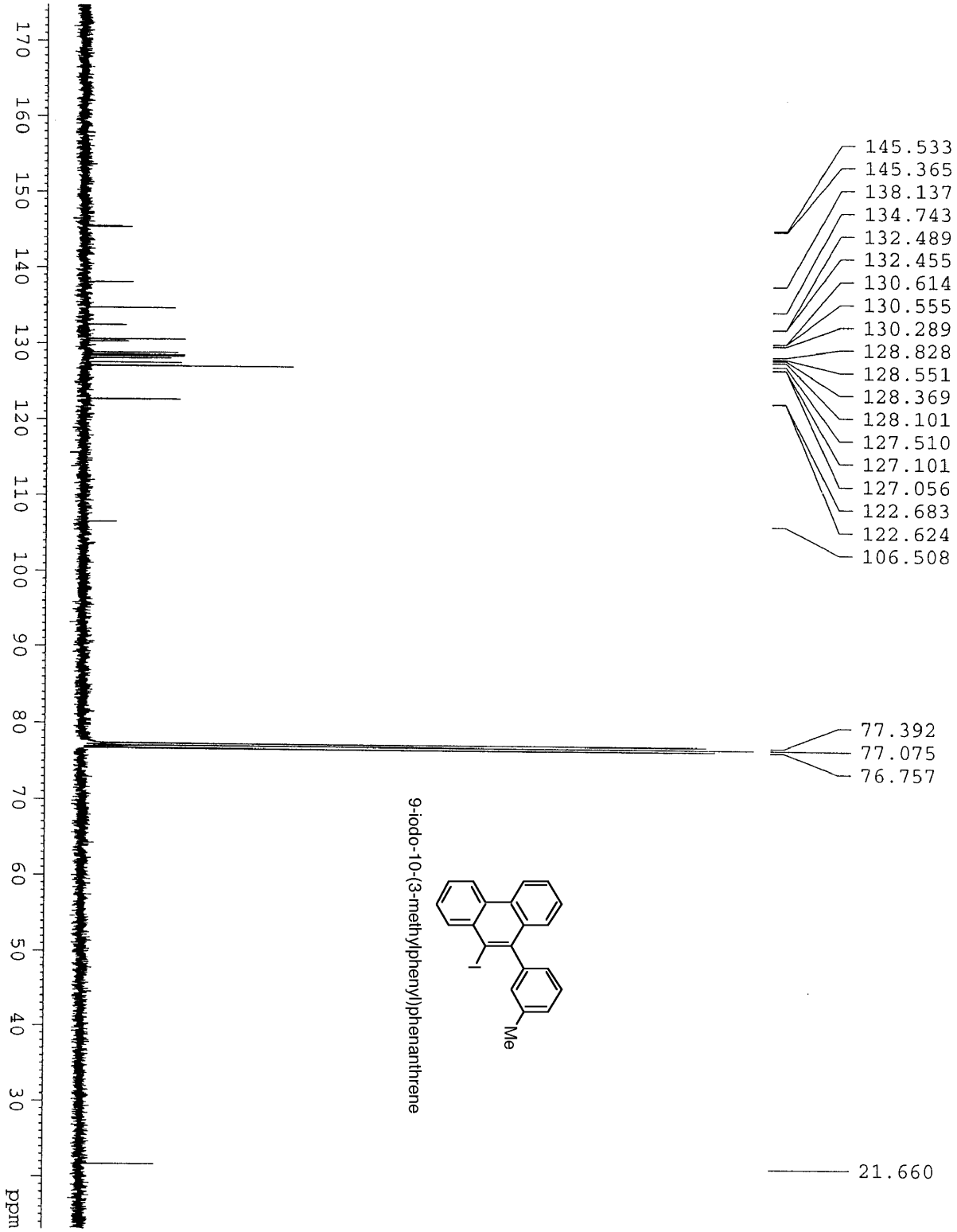

8.473
8.470
8.462
7.721
7.714
7.701
7.695
7.689
7.681
7.675
7.667
7.661
7.646
7.640
7.462
7.455
7.452
7.434
7.430
7.260
7.231
7.224
7.209
7.202
7.106
7.099
7.084
7.077
3.940
0.009
2.153
1.000
3.225
2.136
2.089
2.127
3.312
ppm
9-iodo-10-(4-methoxyphenyl)phenanthrene
OMe

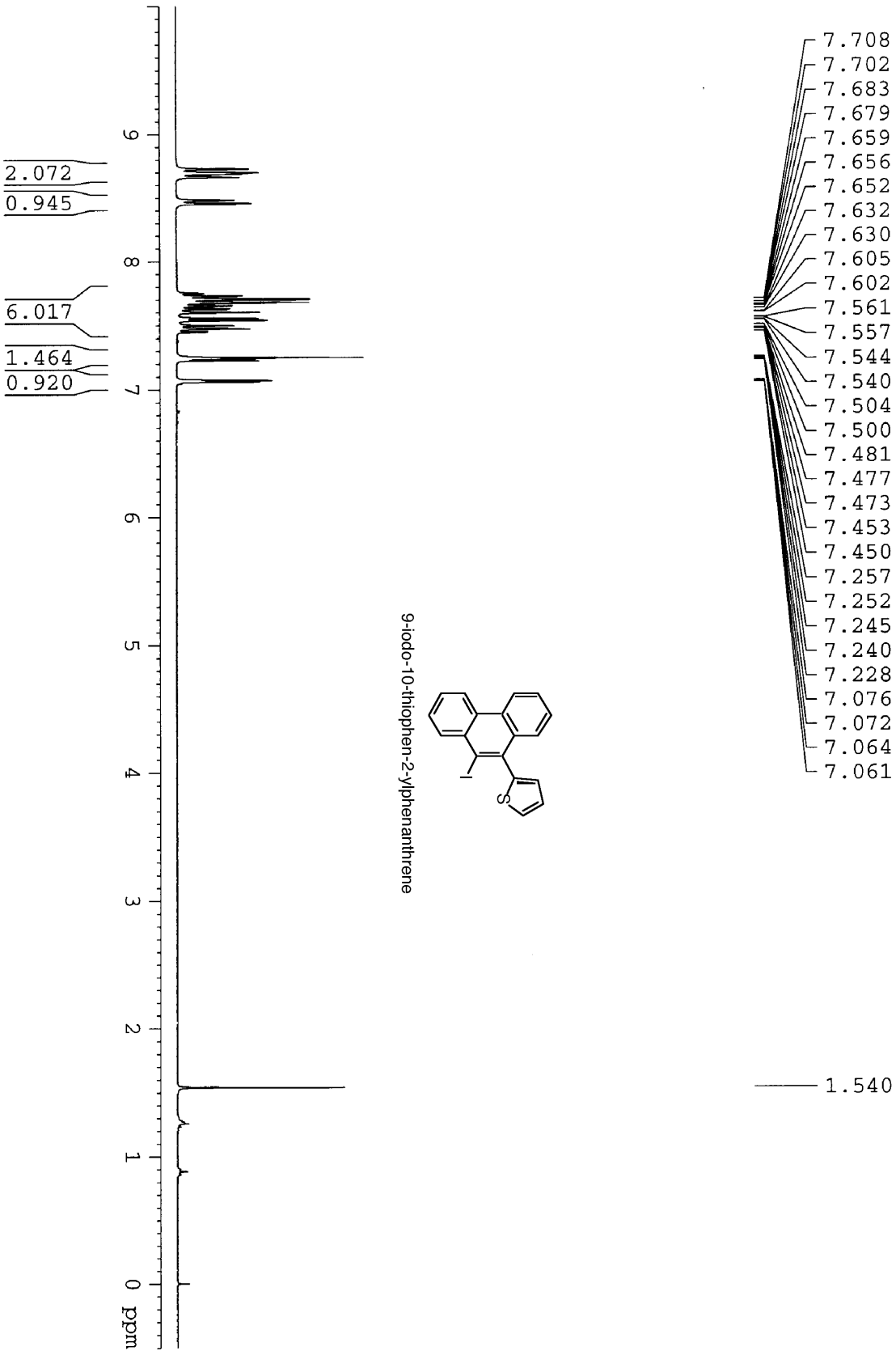

159.382
145.316
138.163
134.994
132.939
132.731
131.331
130.785
130.505
128.998
128.270
127.685
127.270
127.253
122.855
122.822
114.047
107.662
77.675
77.251
76.828
55.554
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
9-iodo-10-(4-methoxyphenyl)phenanthrene
I
OMe

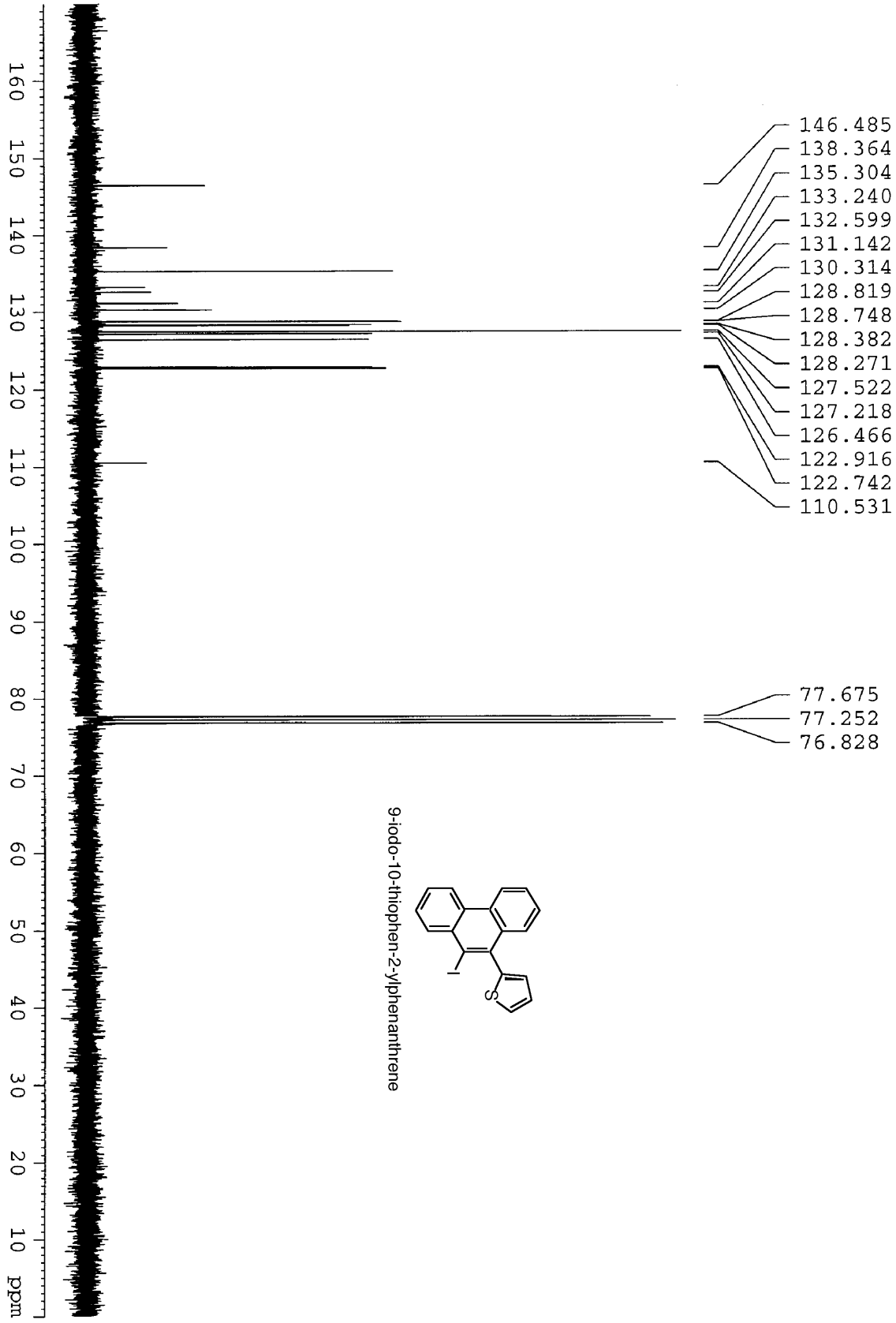

8.273
8.267
8.251
8.245
7.746
7.740
7.732
7.724
7.714
7.707
7.701
7.688
7.684
7.679
7.660
7.656
7.453
7.425
7.421
7.409
7.402
7.386
7.380
7.330
7.327
7.303
7.299
7.261
4.501
4.478
4.454
4.430
1.565
1.486
1.462
1.438
0.078
0.005
2.083
1.000
2.020
3.162
4.217
2.114
3.179
ppm
ethyl 4-(10-iodophenanthren-9-yl)benzoate
CO2Et

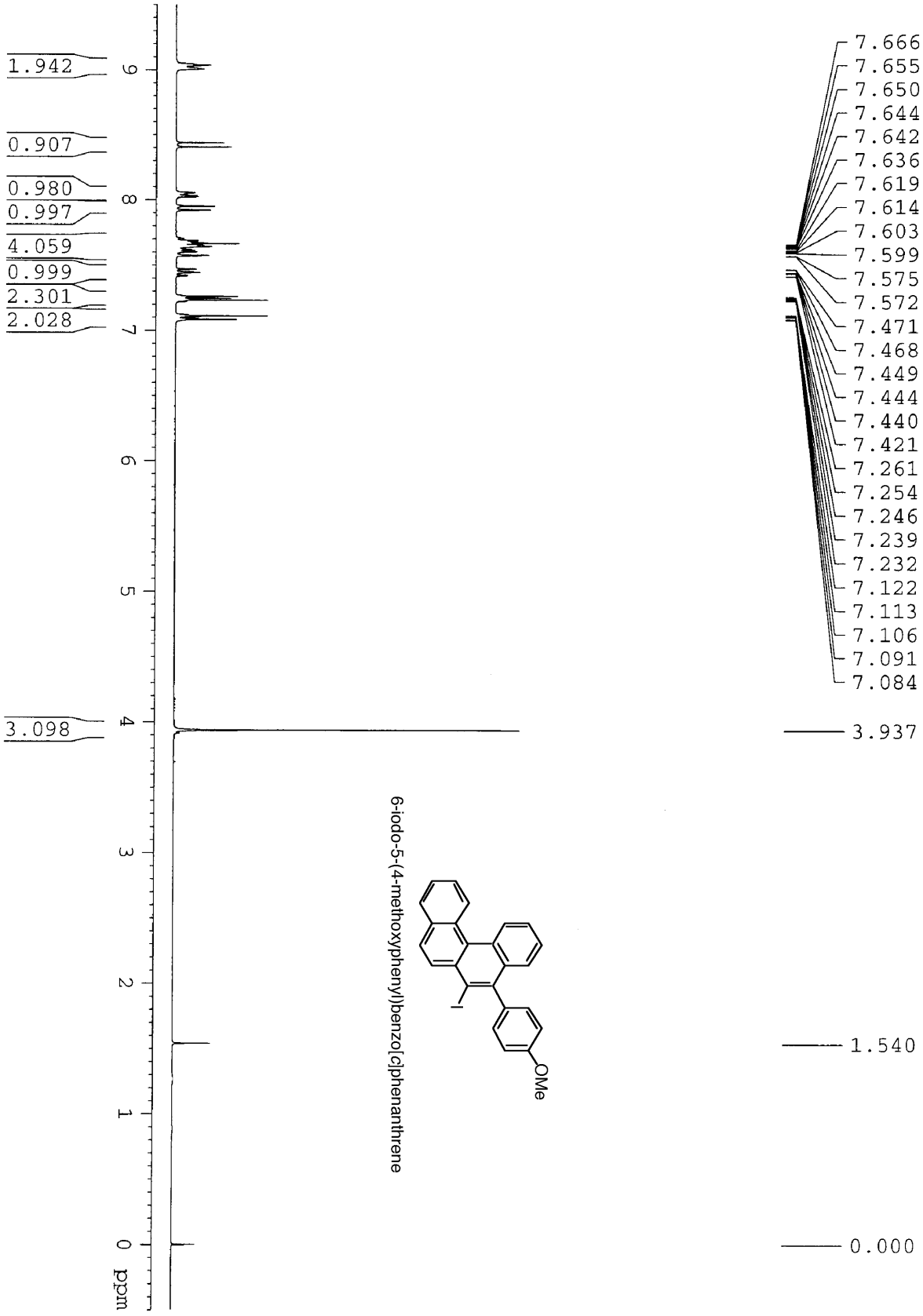

166.694
150.042
144.564
134.869
132.453
132.142
130.825
130.514
130.419
130.252
130.089
128.484
128.446
128.020
127.507
127.421
122.972
122.924
106.035
77.670
77.247
76.823
61.361
14.646
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
ethyl 4-(10-iodophenanthren-9-yl)benzoate
I
CO2Et

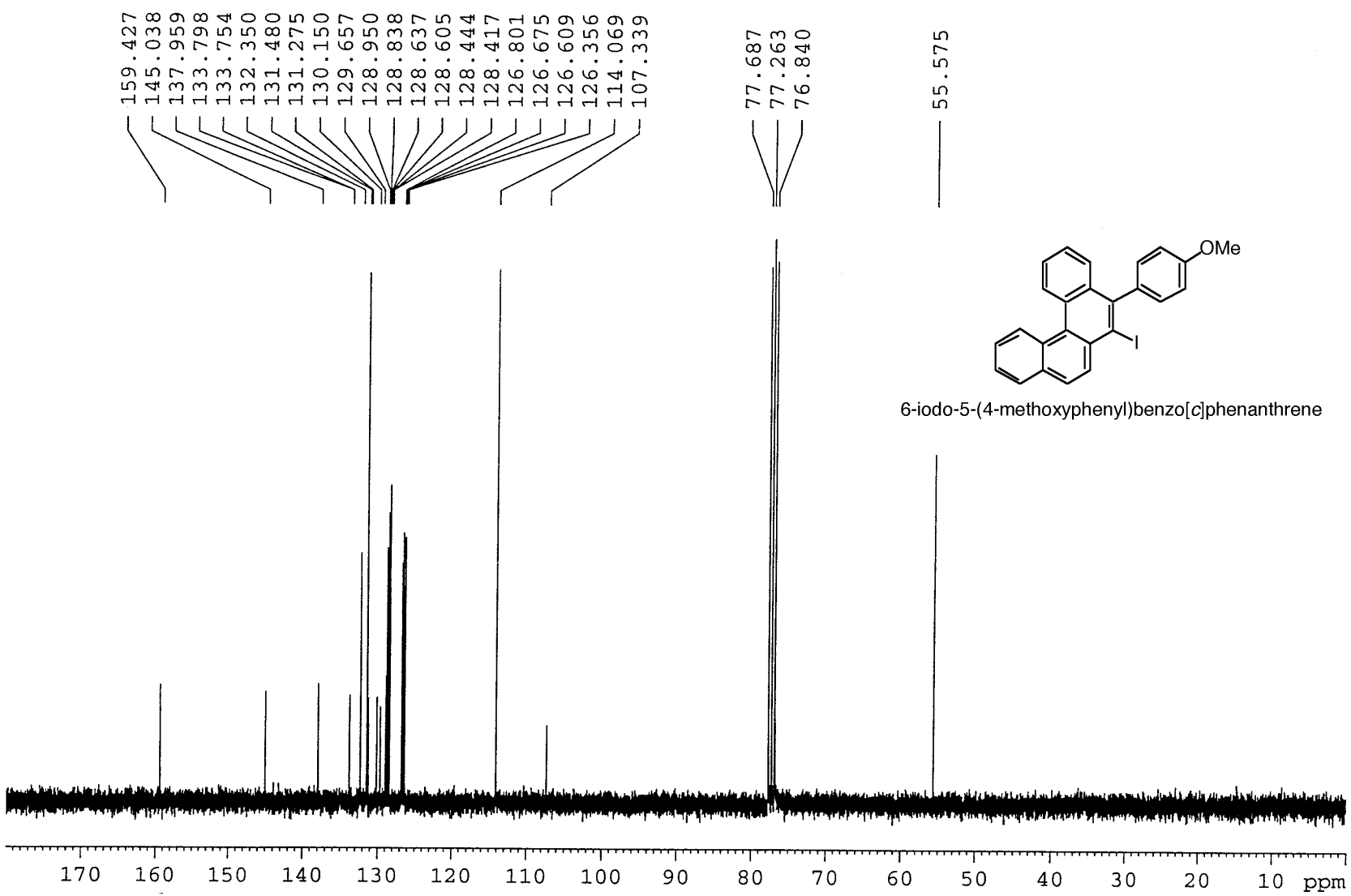

8.728
8.707
8.689
8.683
8.673
8.665
8.475
8.471
8.467
8.457
8.451
7.703
7.698
7.693
7.686
7.679
7.674
7.670
7.659
7.649
7.639
7.628
7.452
7.433
7.417
7.408
7.323
7.303
7.239
7.090
7.071
2.032
1.000
3.032
2.994
1.017
1.940
3.066
2.441
1.520
-0.00
ppm
9-iodo-10-(3-methylphenyl)phenanthrene
Me


145.533
145.365
138.137
134.743
132.489
132.455
130.614
130.555
130.289
128.828
128.551
128.369
128.101
127.510
127.101
127.056
122.683
122.624
106.508
77.392
77.075
76.757
21.660
9-iodo-10-(3-methylphenyl)phenanthrene
I
Me
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

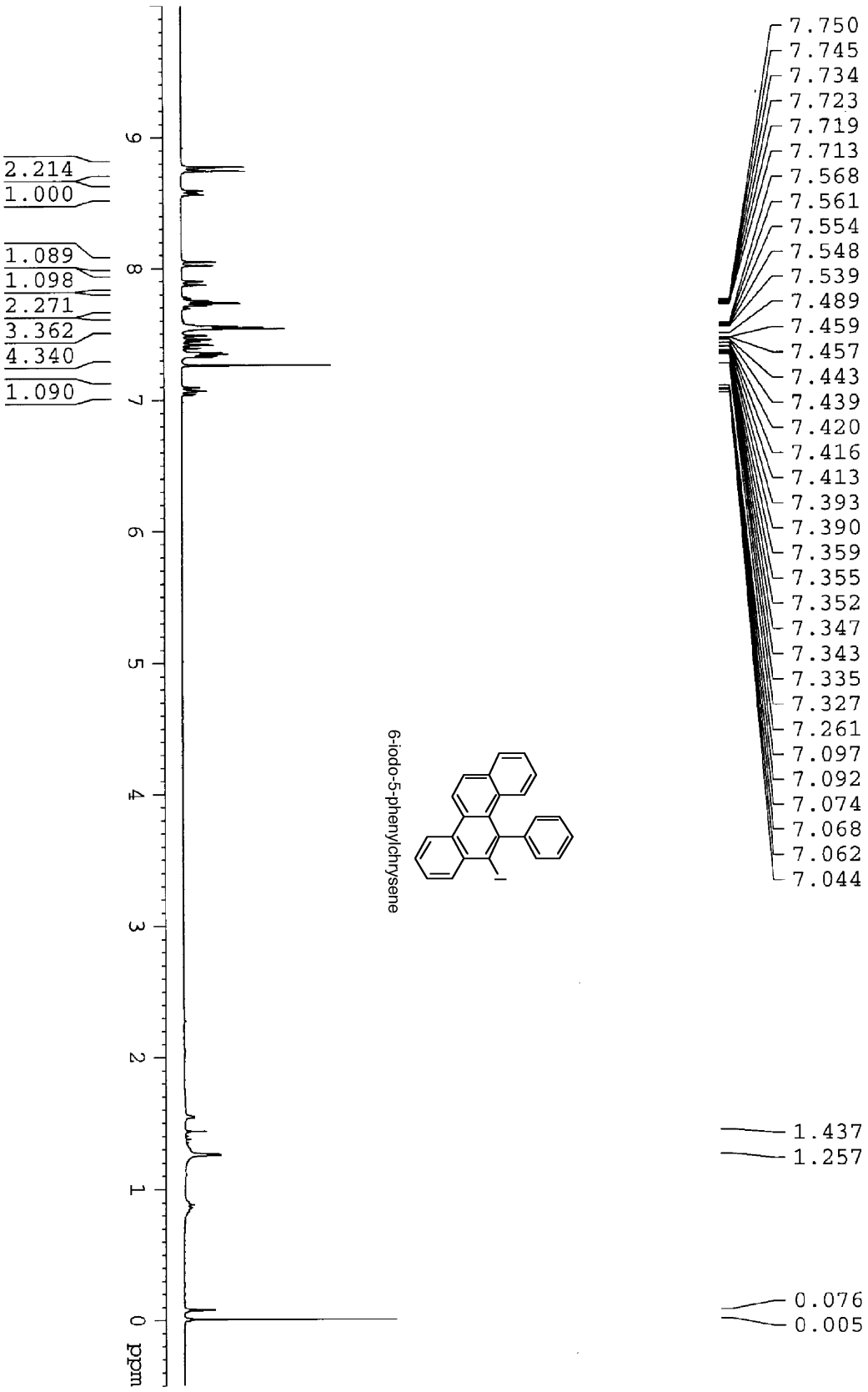

2.072
0.945
6.017
1.464
0.920
9
8
7
6
5
4
3
2
1
0 ppm
9-iodo-10-thiophen-2-ylphenanthrene
I
S
7.708
7.702
7.683
7.679
7.659
7.656
7.652
7.632
7.630
7.605
7.602
7.561
7.557
7.544
7.540
7.504
7.500
7.481
7.477
7.473
7.453
7.450
7.257
7.252
7.245
7.240
7.228
7.076
7.072
7.064
7.061
1.540

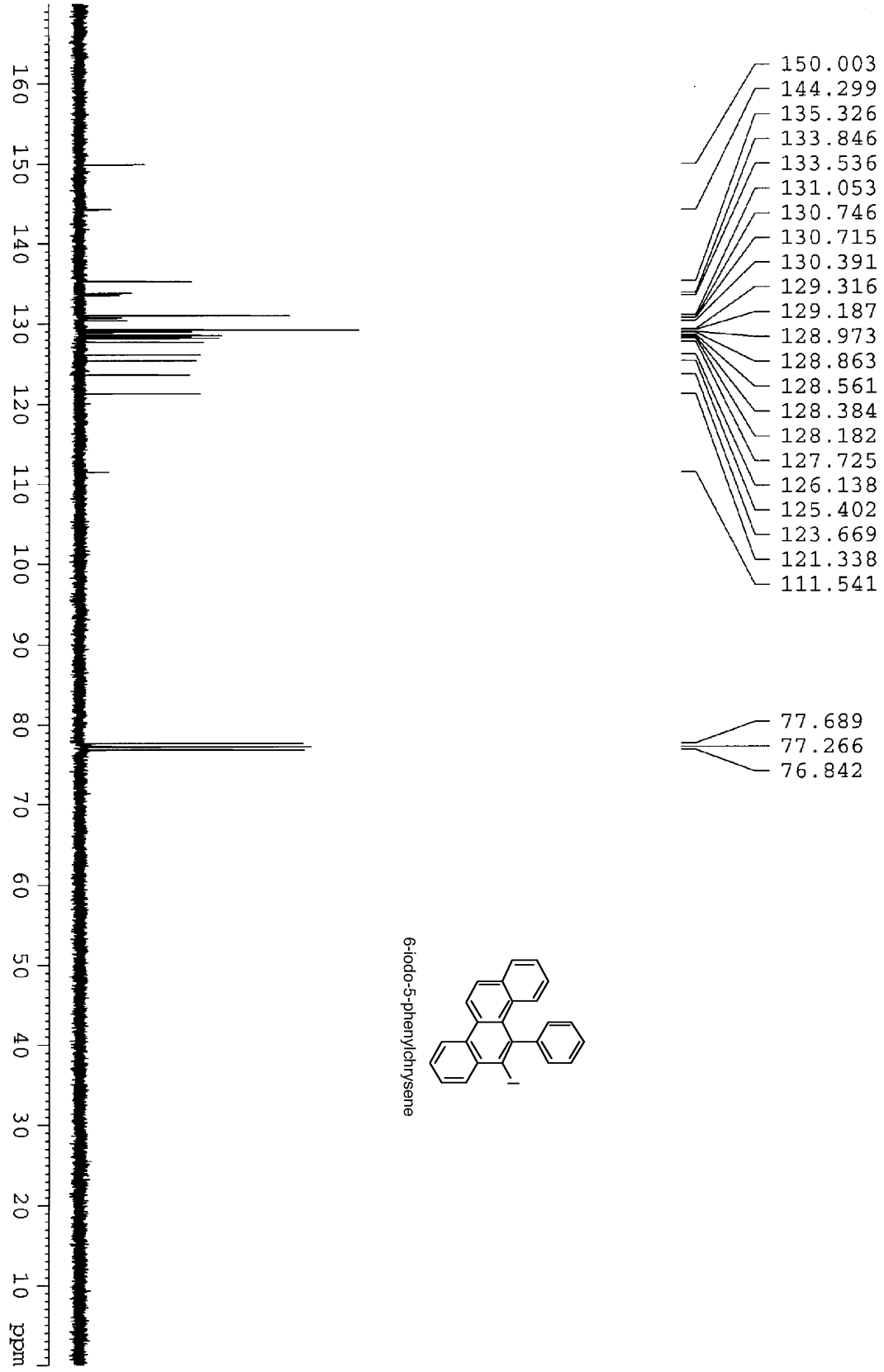

146.485
138.364
135.304
133.240
132.599
131.142
130.314
128.819
128.748
128.382
128.271
127.522
127.218
126.466
122.916
122.742
110.531
77.675
77.252
76.828
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
9-iodo-10-thiophen-2-ylphenanthrene
I
S

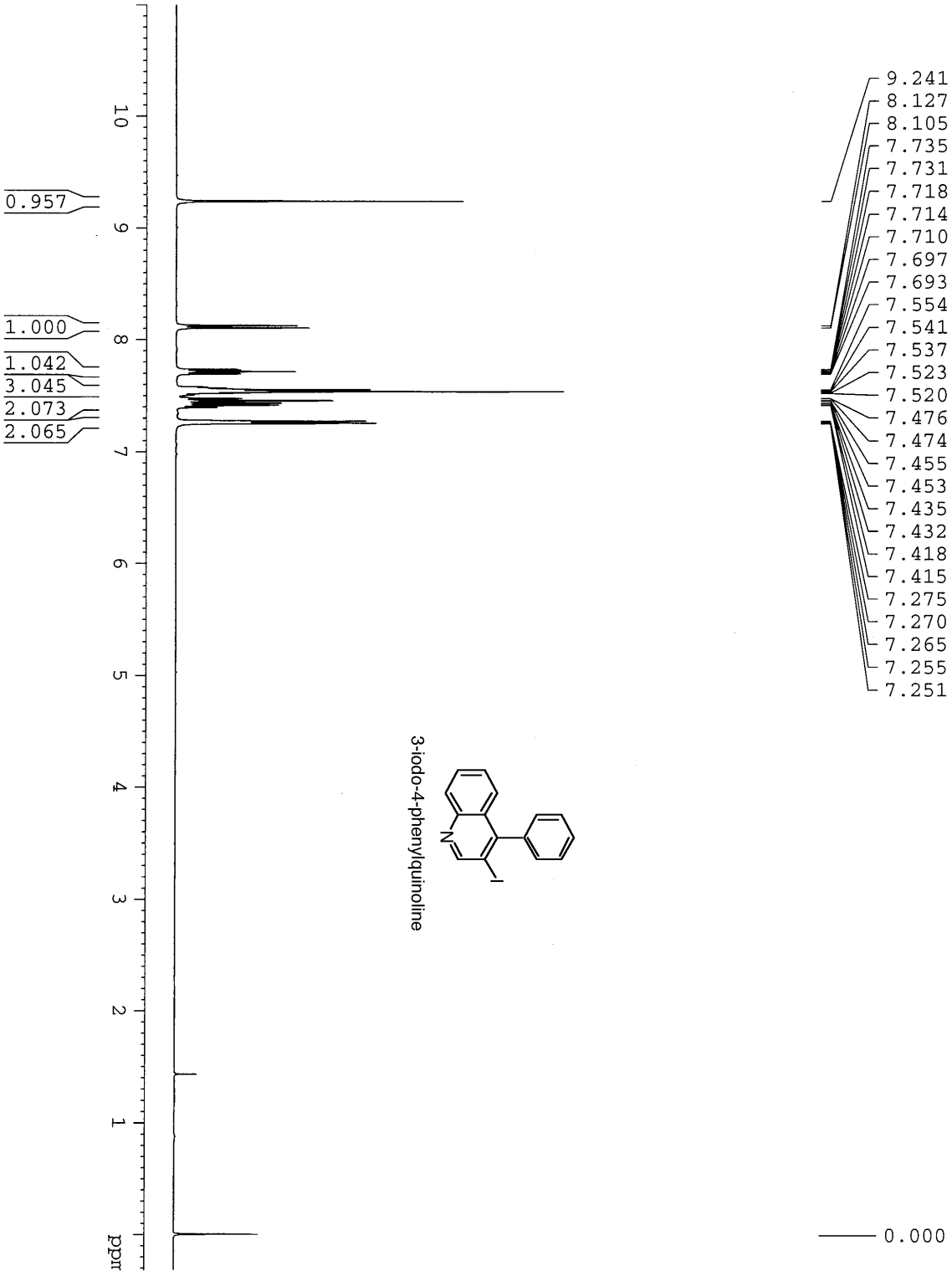

1.942
0.907
0.980
0.997
4.059
0.999
2.301
2.028
3.098
9
8
7
6
5
4
3
2
1
0
ppm
7.666
7.655
7.650
7.644
7.642
7.636
7.619
7.614
7.603
7.599
7.575
7.572
7.471
7.468
7.449
7.444
7.440
7.421
7.261
7.254
7.246
7.239
7.232
7.122
7.113
7.106
7.091
7.084
3.937
1.540
0.000
6-iodo-5-(4-methoxyphenyl)benzo[c]phenanthrene
I
OMe

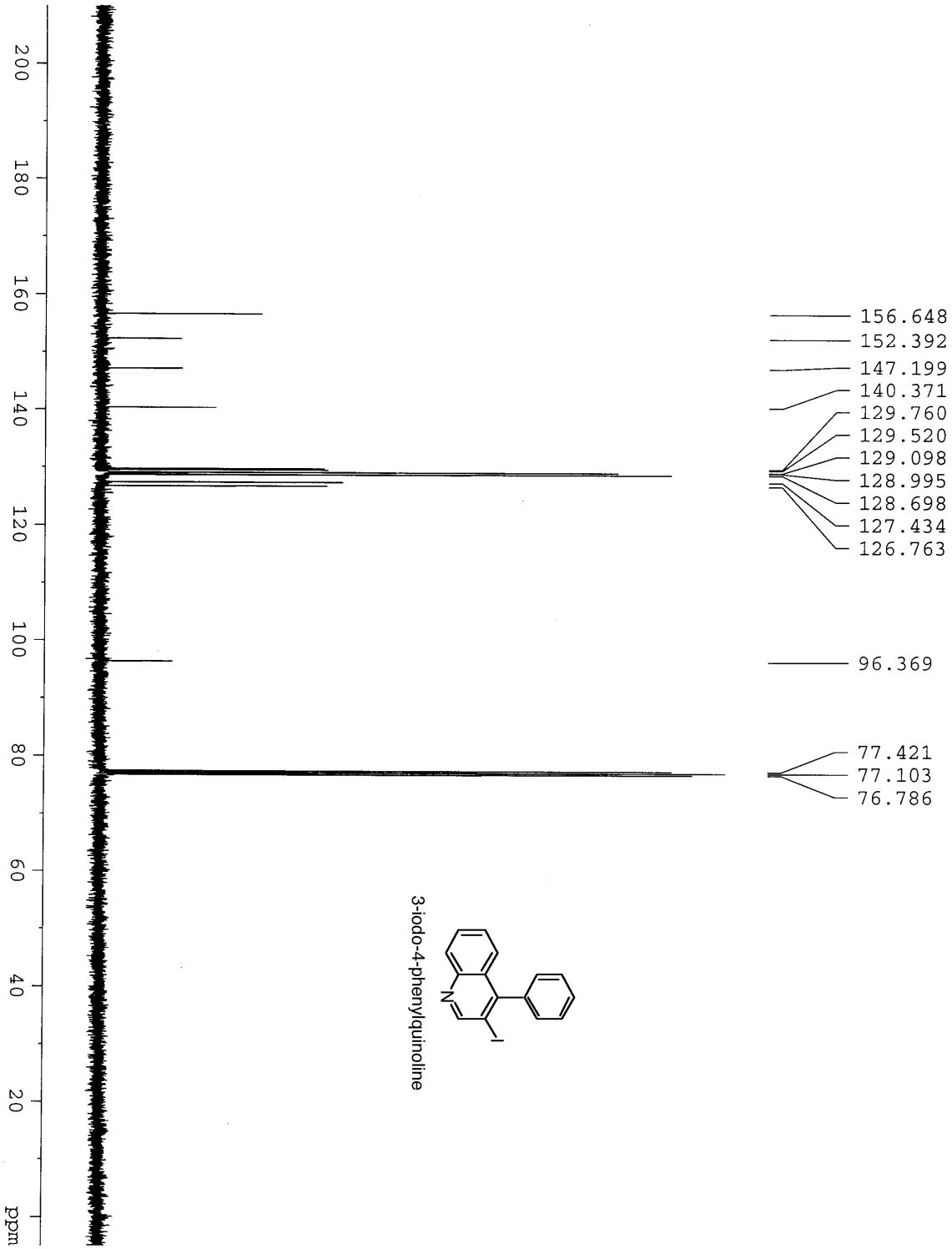


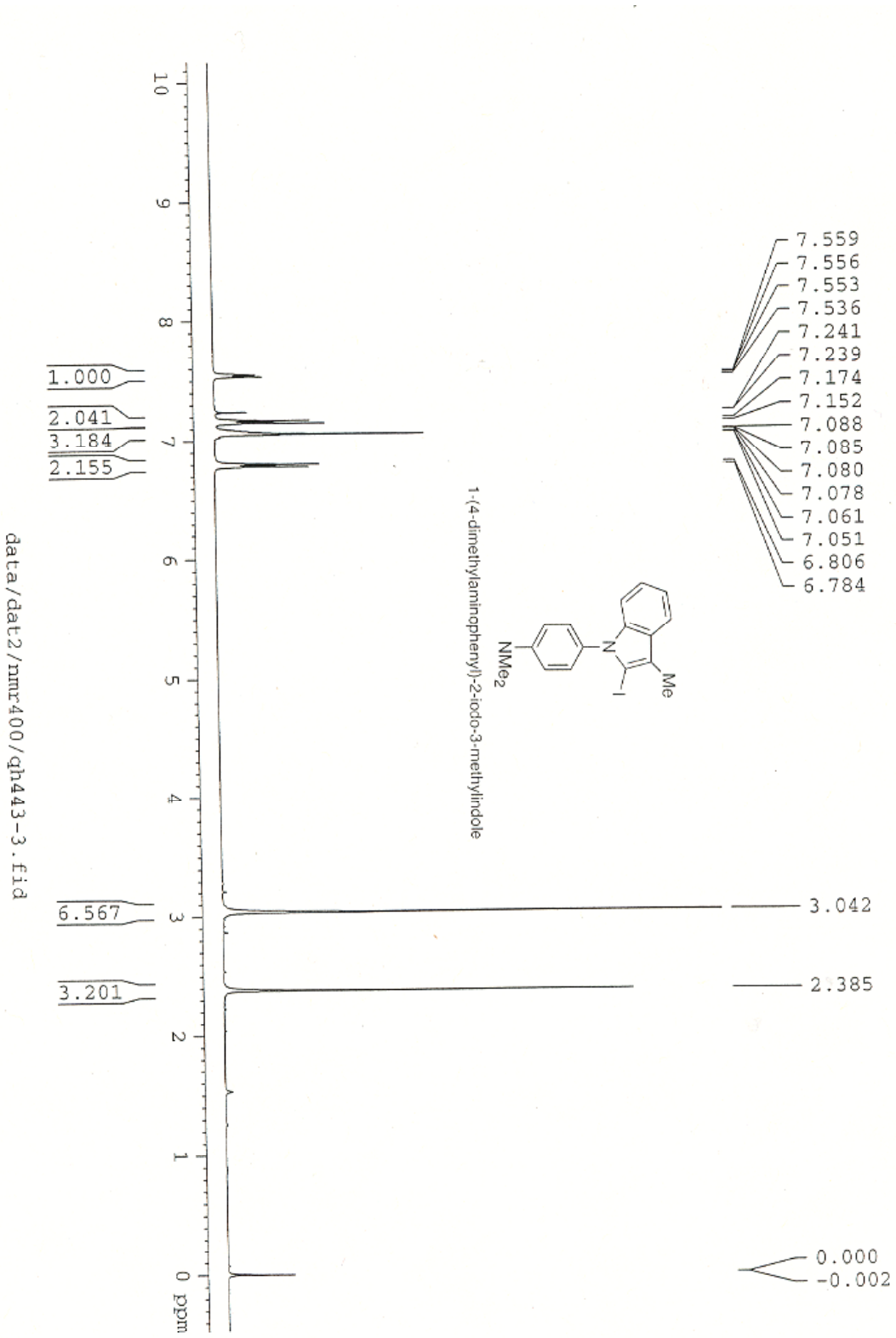
6-iodo-5-(4-methoxyphenyl)benzo[*c*]phenanthrene

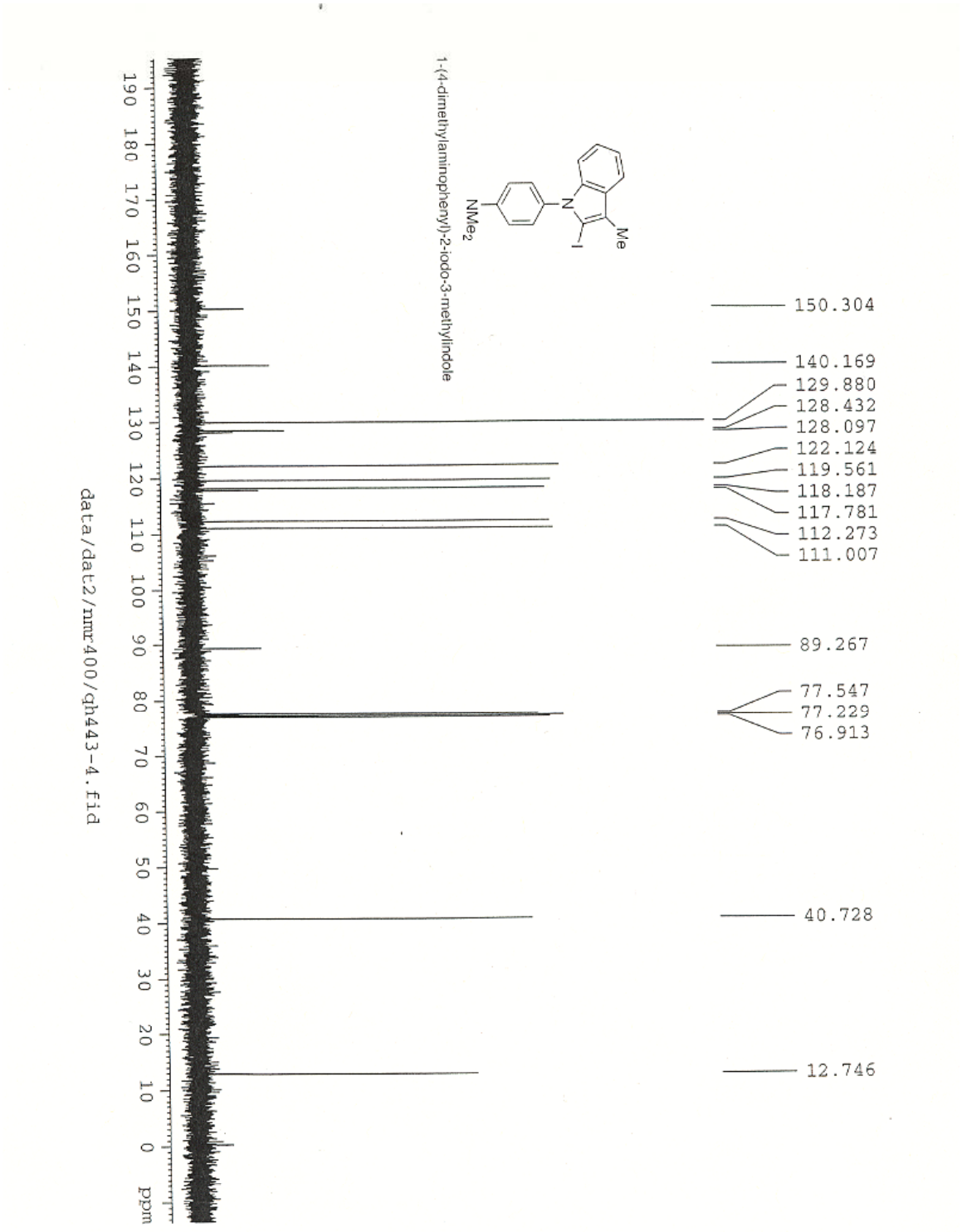

2.214
1.000
1.089
1.098
2.271
3.362
4.340
1.090
9
8
7
6
5
4
3
2
1
0
ppm
7.750
7.745
7.734
7.723
7.719
7.713
7.568
7.561
7.554
7.548
7.539
7.489
7.459
7.457
7.443
7.439
7.420
7.416
7.413
7.393
7.390
7.359
7.355
7.352
7.347
7.343
7.335
7.327
7.261
7.097
7.092
7.074
7.068
7.062
7.044
6-iodo-5-phenylchrysene
I
1.437
1.257
0.076
0.005

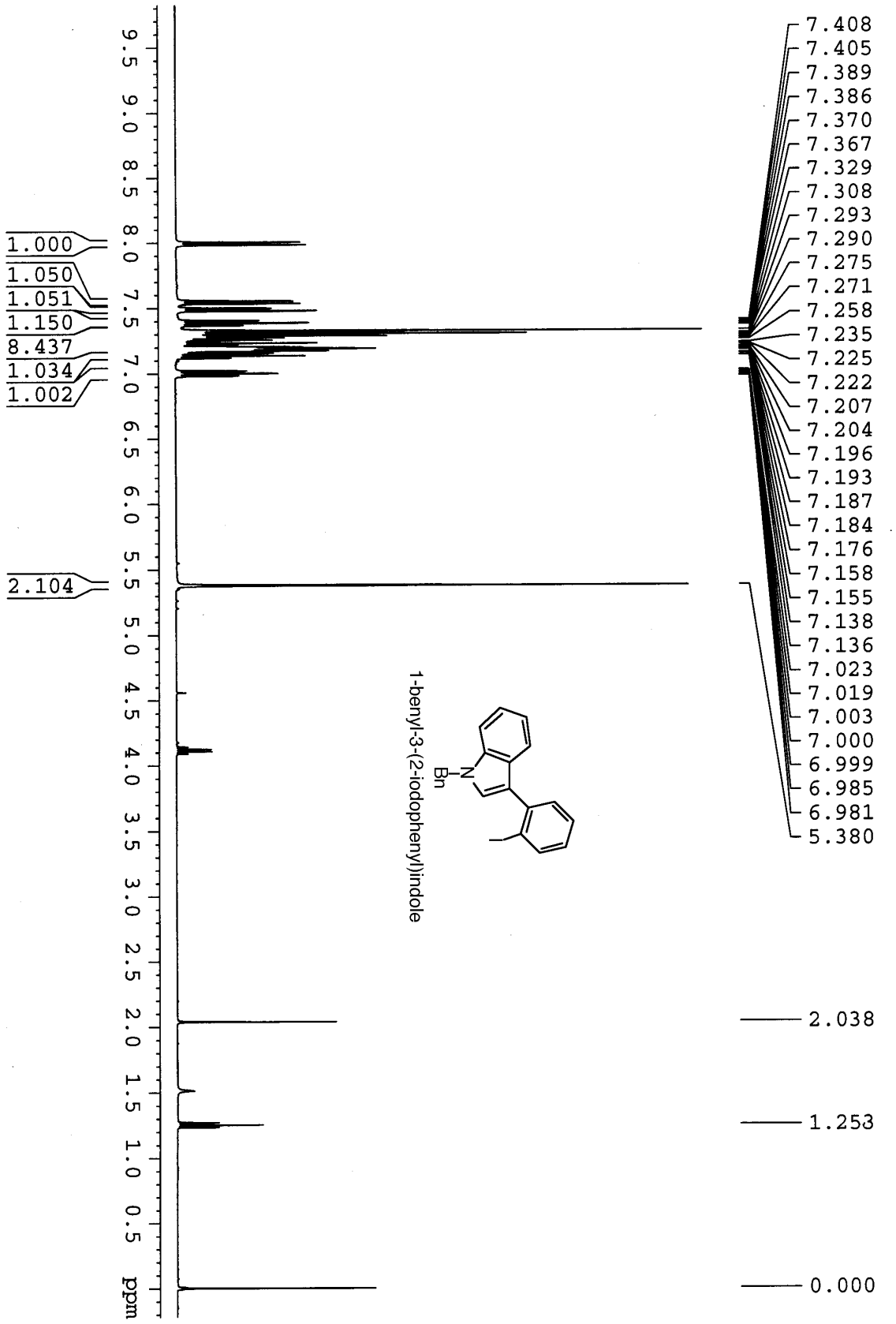

150.003
144.299
135.326
133.846
133.536
131.053
130.746
130.715
130.391
129.316
129.187
128.973
128.863
128.561
128.384
128.182
127.725
126.138
125.402
123.669
121.338
111.541
77.689
77.266
76.842
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
6-iodo-5-phenylchrysene
I

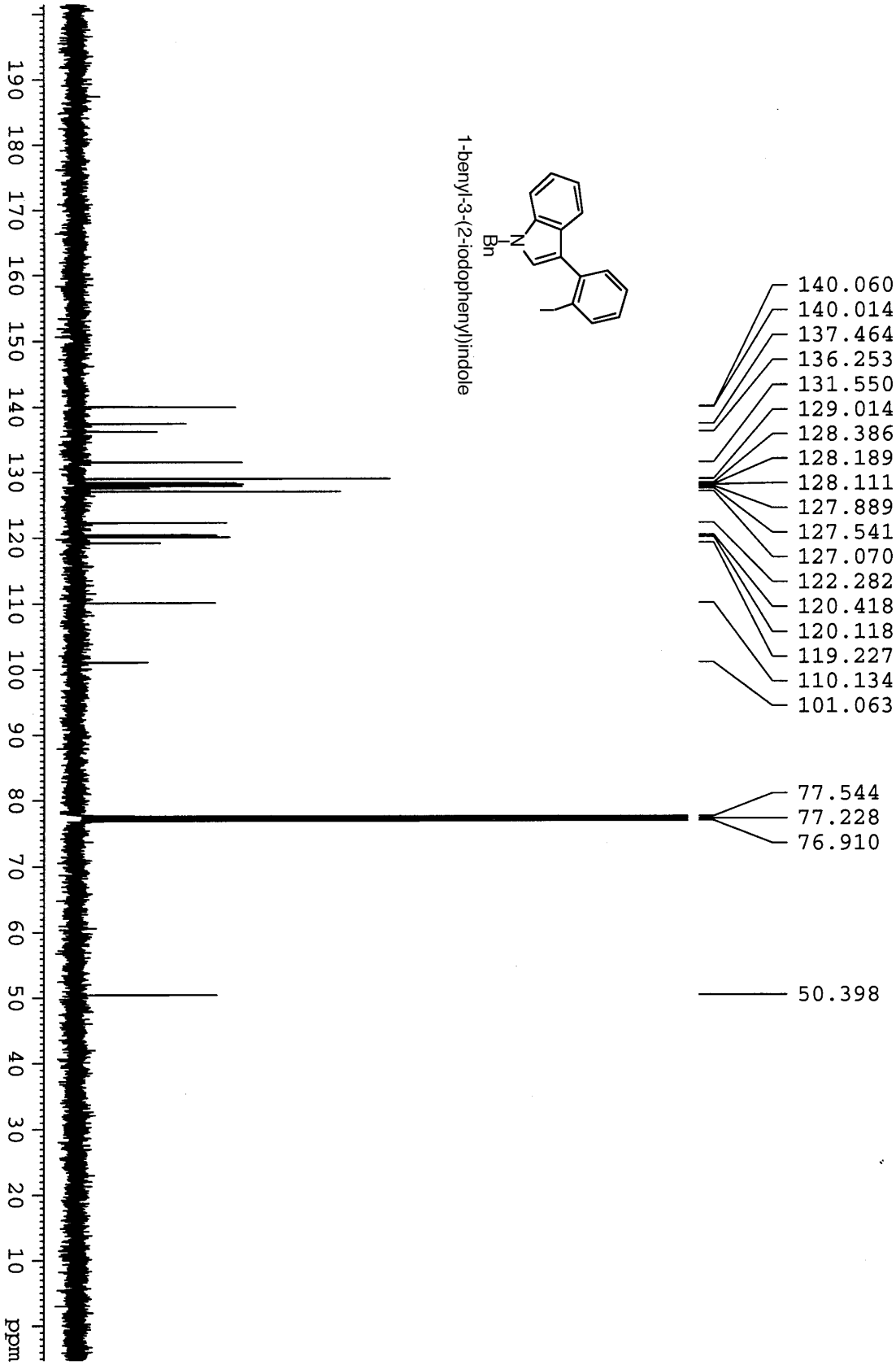

9.241
8.127
8.105
7.735
7.731
7.718
7.714
7.710
7.697
7.693
7.554
7.541
7.537
7.523
7.520
7.476
7.474
7.455
7.453
7.435
7.432
7.418
7.415
7.275
7.270
7.265
7.255
7.251
0.957
1.000
1.042
3.045
2.073
2.065
10
9
8
7
6
5
4
3
2
1
ppm
3-iodo-4-phenylquinoline
N
I
0.000

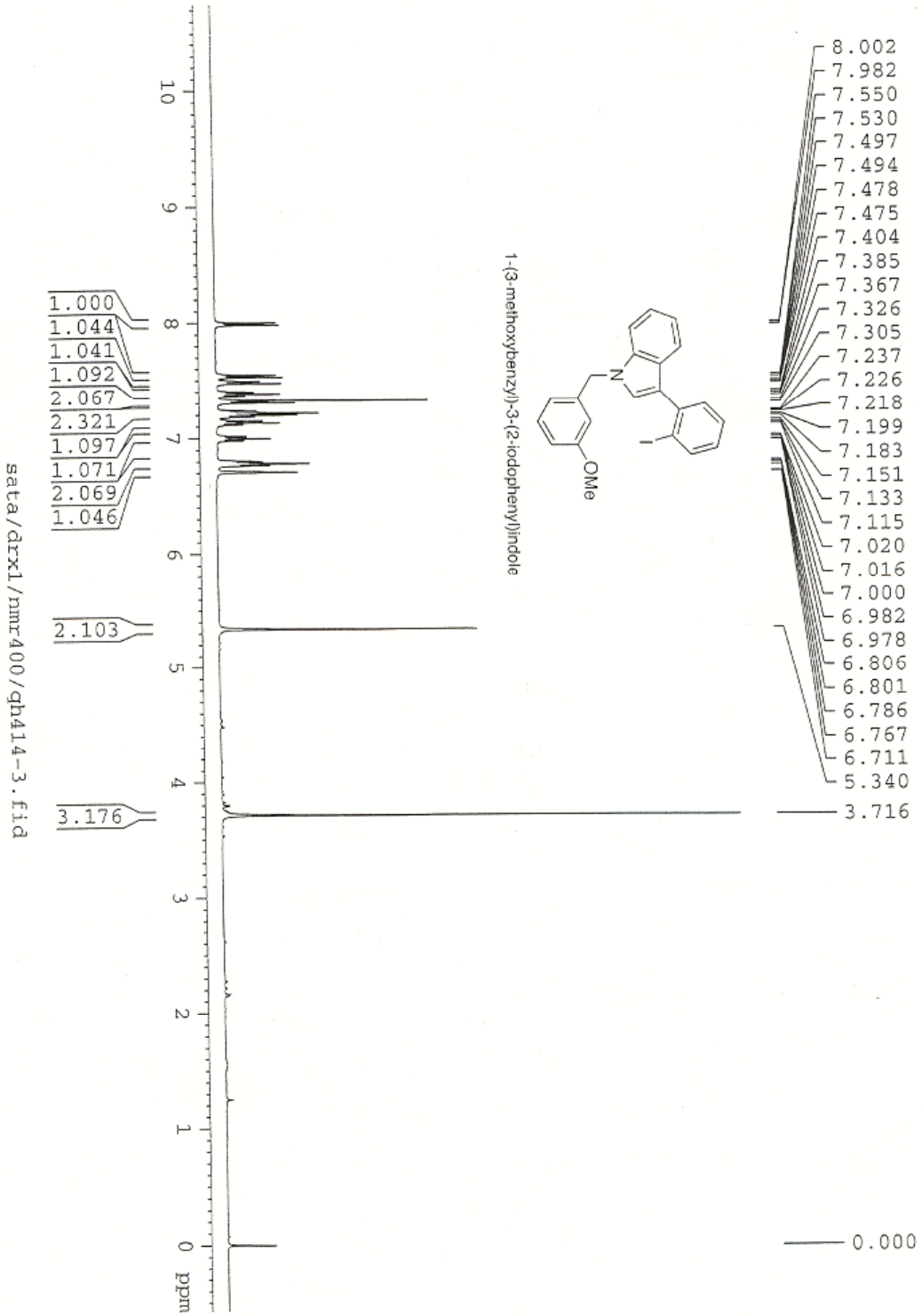

156.648
152.392
147.199
140.371
129.760
129.520
129.098
128.995
128.698
127.434
126.763
96.369
77.421
77.103
76.786
3-iodo-4-phenylquinoline
200
180
160
140
120
100
80
60
40
20
ppm

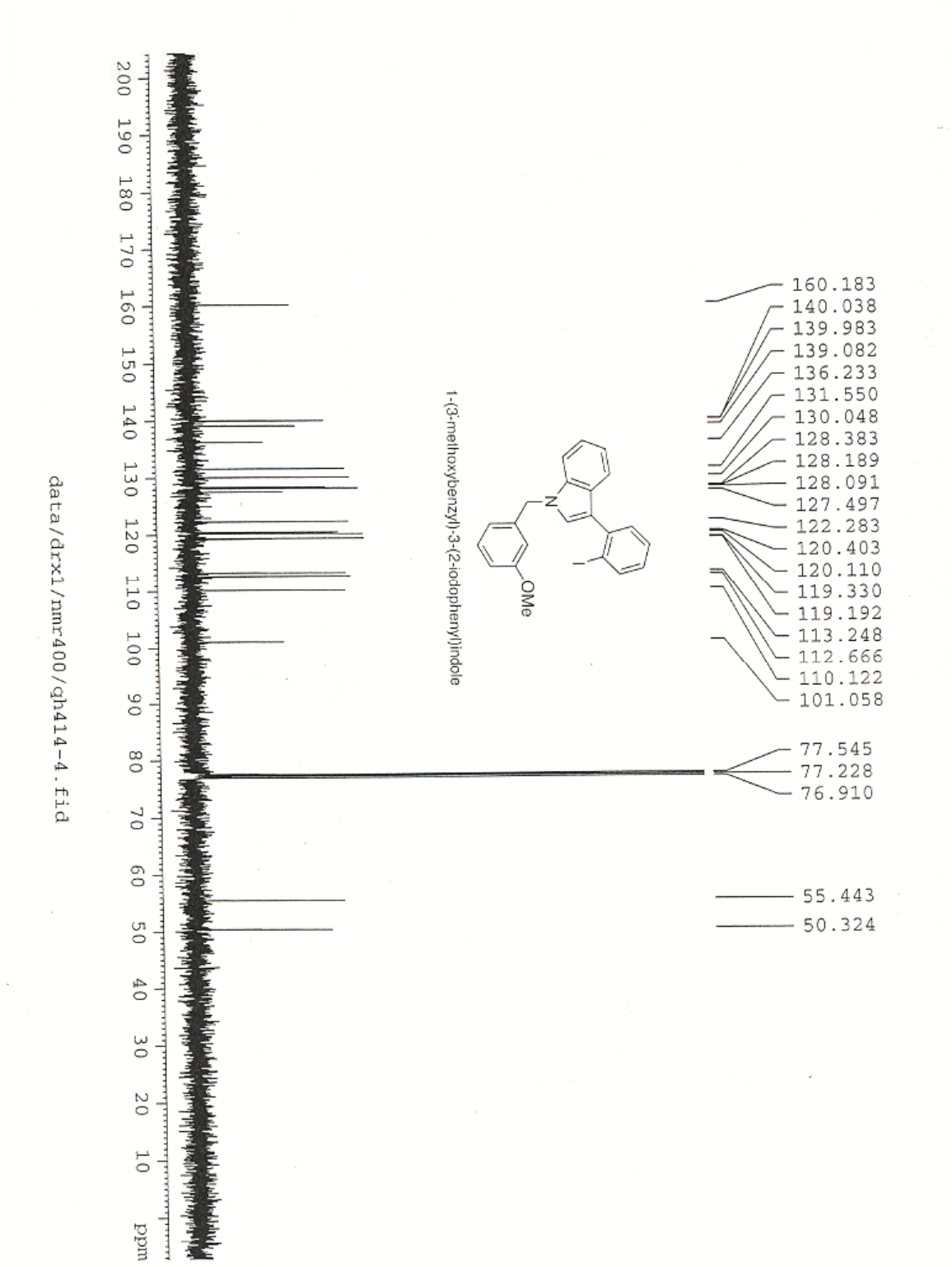

7.559
7.556
7.553
7.536
7.241
7.239
7.174
7.152
7.088
7.085
7.080
7.078
7.061
7.051
6.806
6.784
1.000
2.041
3.184
2.155
6.567
3.201
3.042
2.385
0.000
-0.002
1-(4-dimethylaminophenyl)-2-iodo-3-methylindole
NMe2
N
Me
I
data/dat2/nmr400/qh443-3.fid
ppm

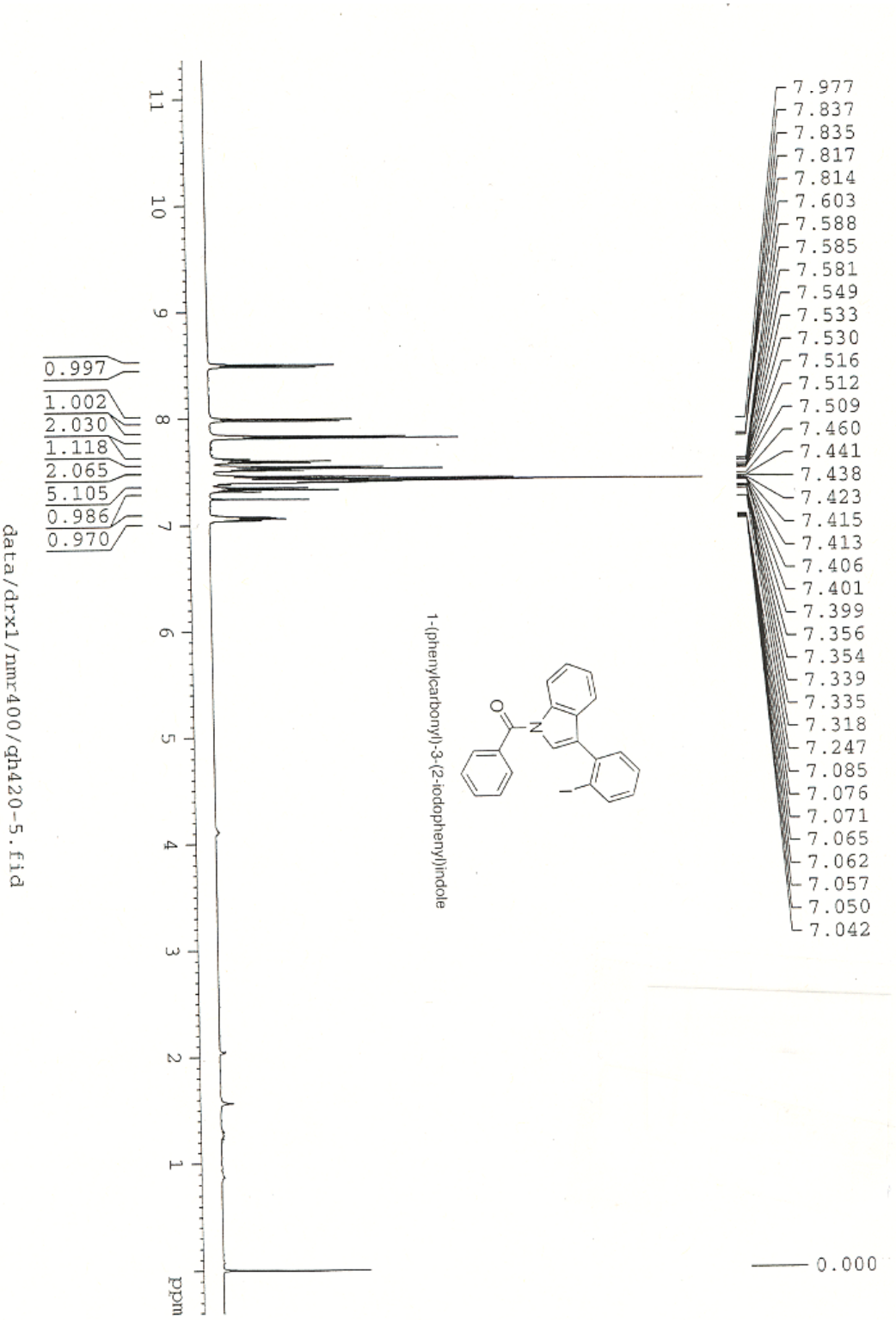

1-(4-dimethylaminophenyl)-2-iodo-3-methylindole
NMe2
N
I
Me
150.304
140.169
129.880
128.432
128.097
122.124
119.561
118.187
117.781
112.273
111.007
89.267
77.547
77.229
76.913
40.728
12.746
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
data/dat2/nmr400/qh443-4.fid

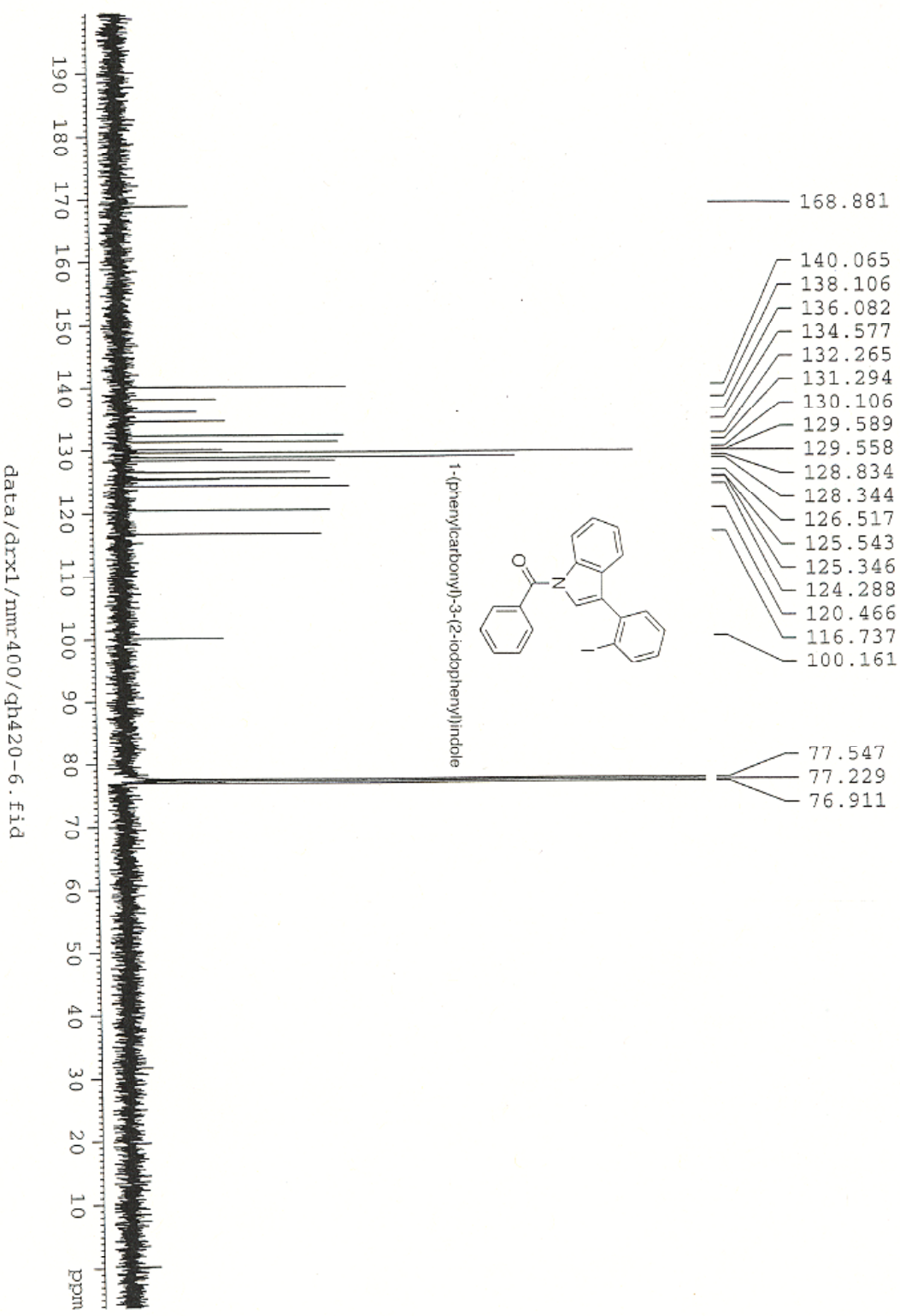

1.000
1.050
1.051
1.150
8.437
1.034
1.002
2.104
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
7.408
7.405
7.389
7.386
7.370
7.367
7.329
7.308
7.293
7.290
7.275
7.271
7.258
7.235
7.225
7.222
7.207
7.204
7.196
7.193
7.187
7.184
7.176
7.158
7.155
7.138
7.136
7.023
7.019
7.003
7.000
6.999
6.985
6.981
5.380
2.038
1.253
0.000
1-benyl-3-(2-iodophenyl)indole
N
Bn

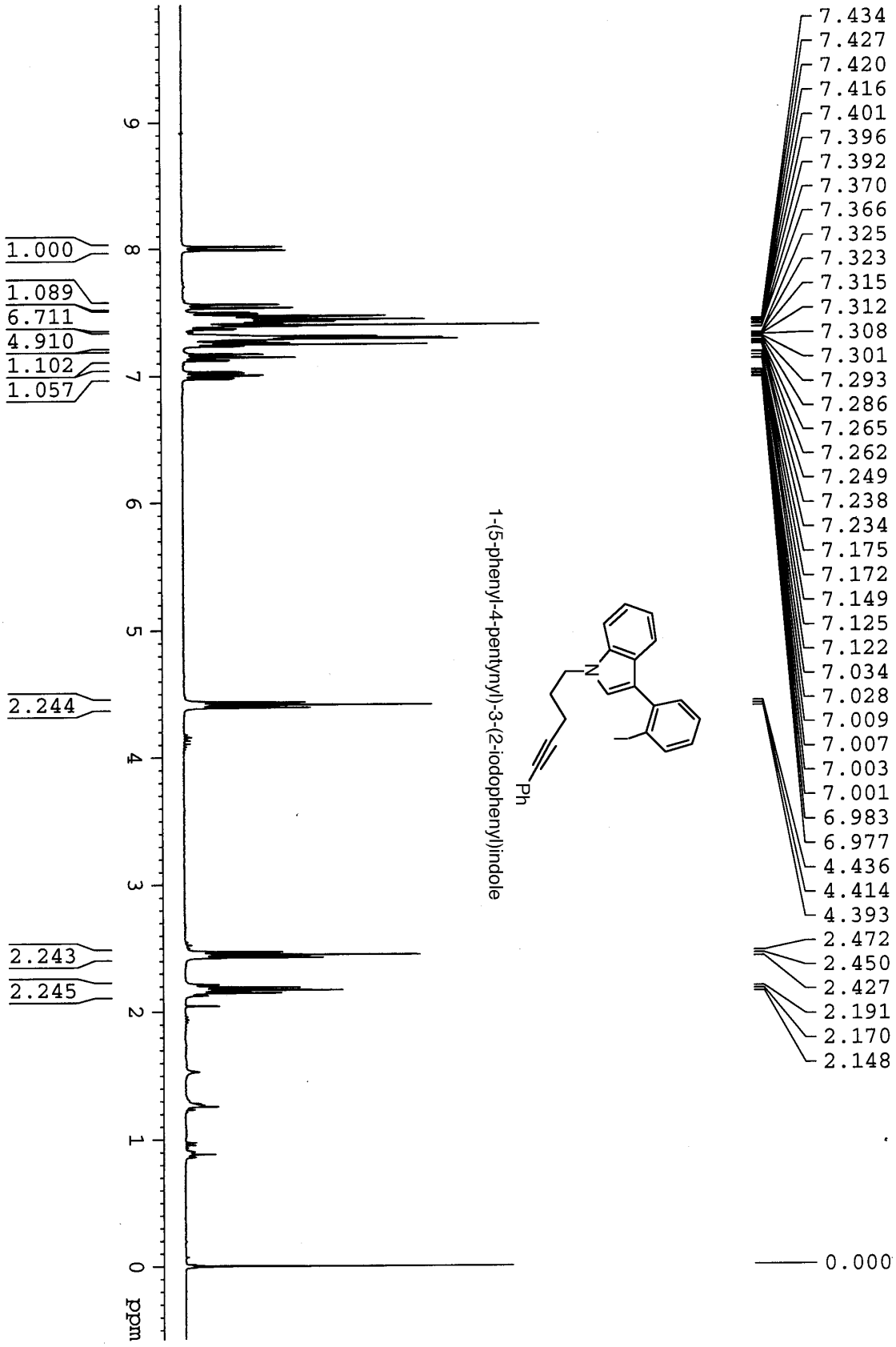

1-benyl-3-(2-iodophenyl)indole
N
Bn
140.060
140.014
137.464
136.253
131.550
129.014
128.386
128.189
128.111
127.889
127.541
127.070
122.282
120.418
120.118
119.227
110.134
101.063
77.544
77.228
76.910
50.398
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

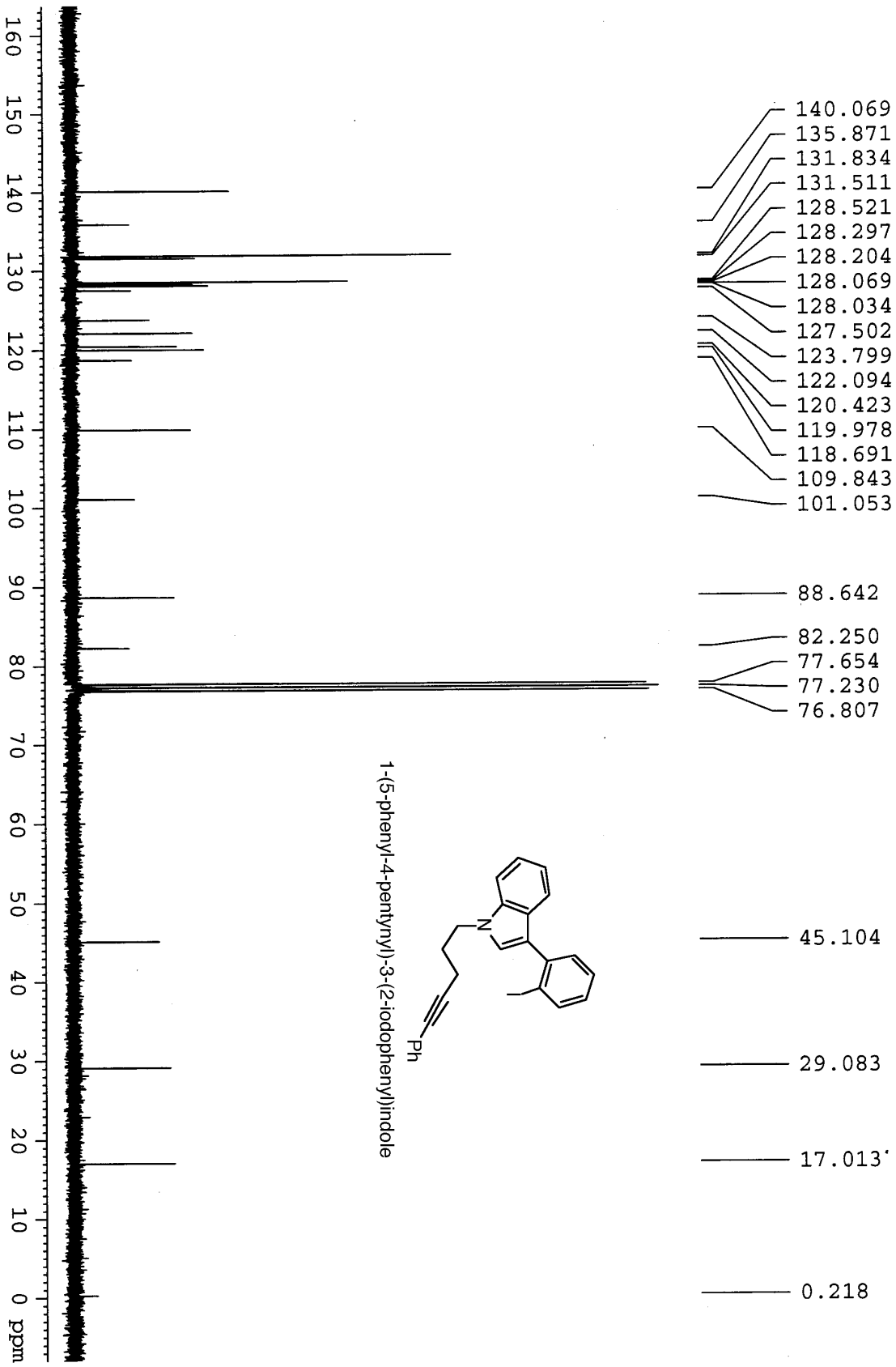

8.002
7.982
7.550
7.530
7.497
7.494
7.478
7.475
7.404
7.385
7.367
7.326
7.305
7.237
7.226
7.218
7.199
7.183
7.151
7.133
7.115
7.020
7.016
7.000
6.982
6.978
6.806
6.801
6.786
6.767
6.711
5.340
3.716
0.000
1-(3-methoxybenzyl)-3-(2-iodophenyl)indole
OMe
I
N
1.000
1.044
1.041
1.092
2.067
2.321
1.097
1.071
2.069
1.046
2.103
3.176
10
9
8
7
6
5
4
3
2
1
0
ppm
sata/drx1/nmr400/qh414-3.fid

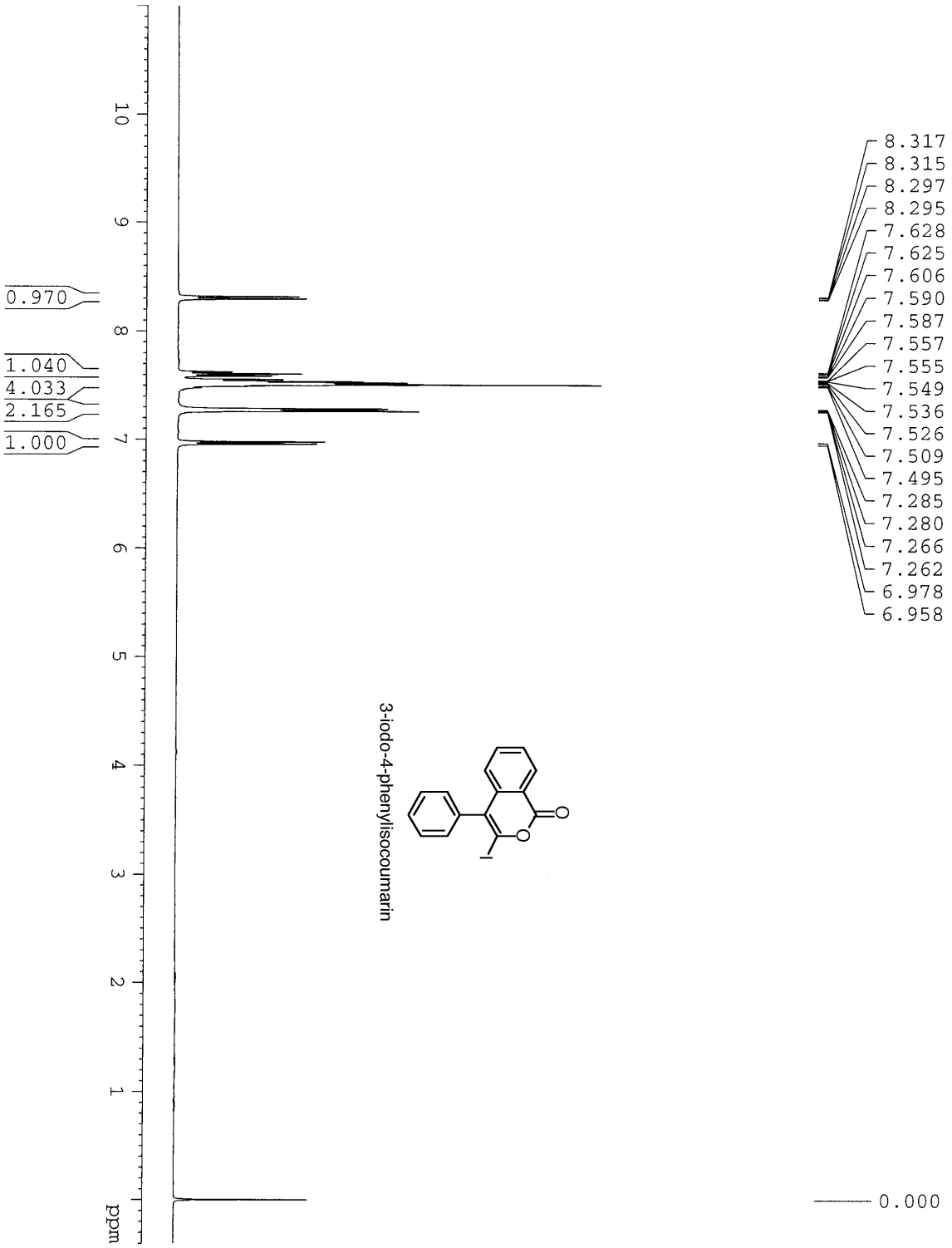

160.183
140.038
139.983
139.082
136.233
131.550
130.048
128.383
128.189
128.091
127.497
122.283
120.403
120.110
119.330
119.192
113.248
112.666
110.122
101.058
77.545
77.228
76.910
55.443
50.324
1-(3-methoxybenzyl)-3-(2-iodophenyl)indole
OMe
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
data/drx1/nmr400/qh414-4.fid

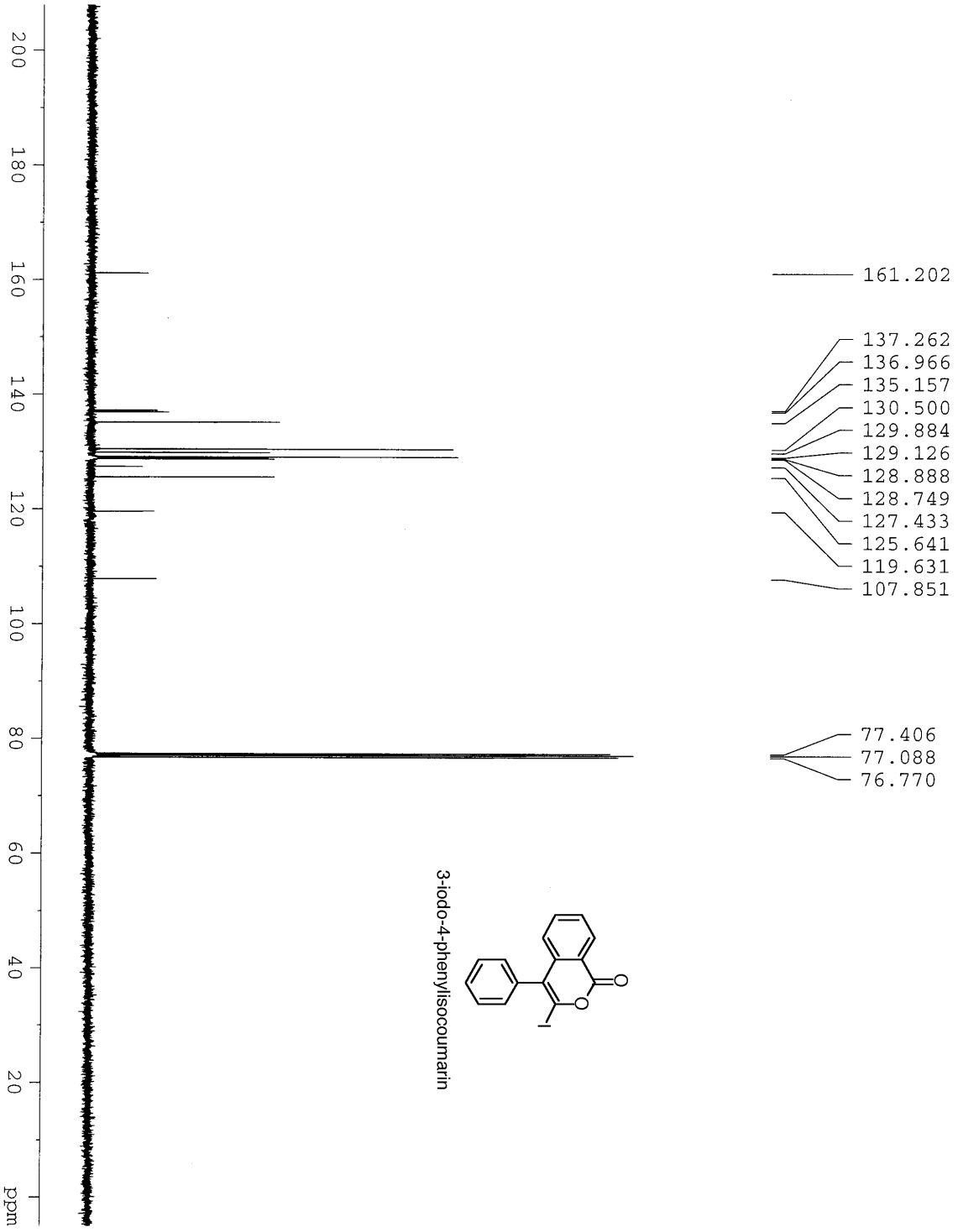

7.977
7.837
7.835
7.817
7.814
7.603
7.588
7.585
7.581
7.549
7.533
7.530
7.516
7.512
7.509
7.460
7.441
7.438
7.423
7.415
7.413
7.406
7.401
7.399
7.356
7.354
7.339
7.335
7.318
7.247
7.085
7.076
7.071
7.065
7.062
7.057
7.050
7.042
0.997
1.002
2.030
1.118
2.065
5.105
0.986
0.970
1-(phenylcarbonyl)-3-(2-iodophenyl)indole
O
N
I
0.000
ppm
data/drx1/nmr400/qh420-5.fid

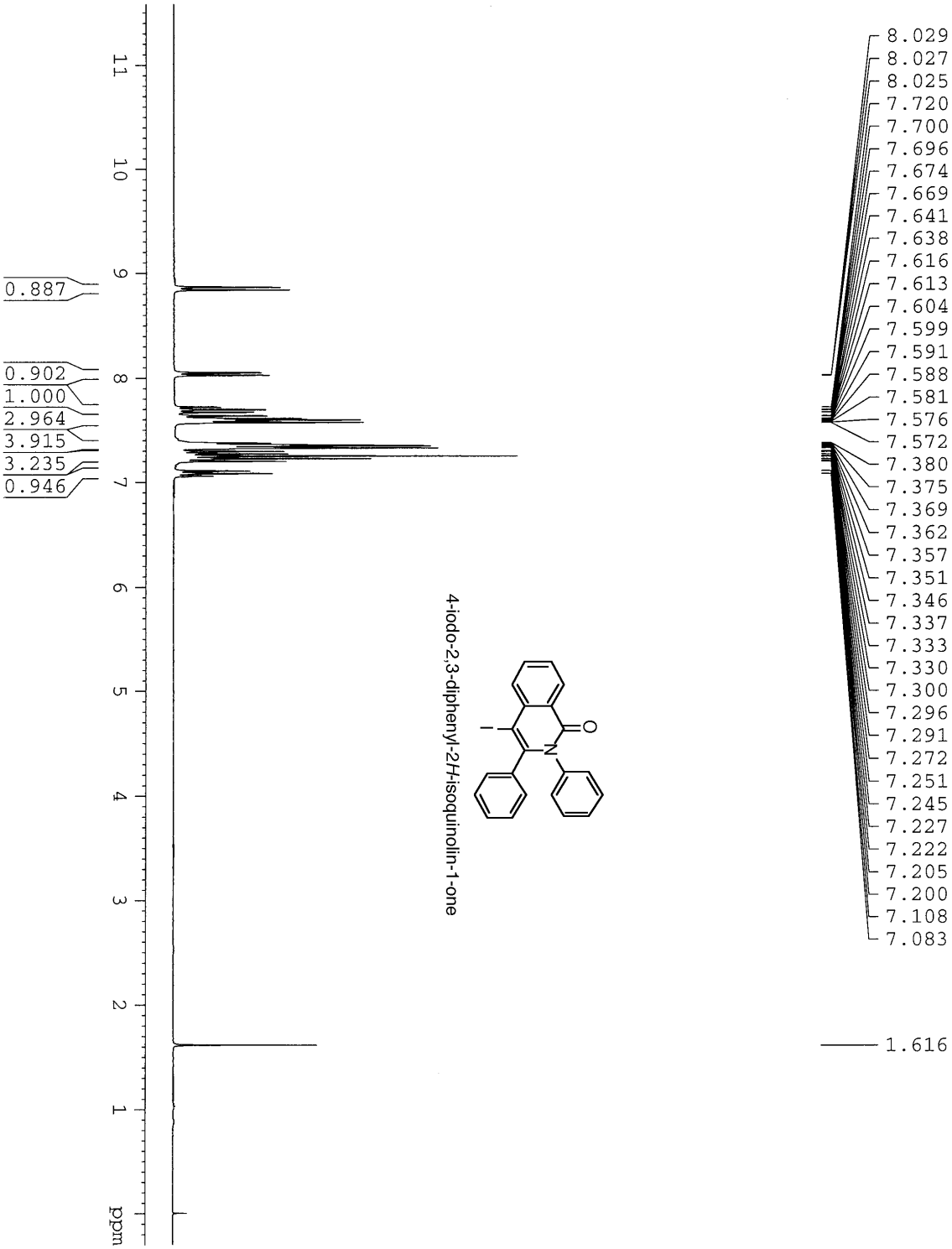

168.881
140.065
138.106
136.082
134.577
132.265
131.294
130.106
129.589
129.558
128.834
128.344
126.517
125.543
125.346
124.288
120.466
116.737
100.161
77.547
77.229
76.911
1-(phenylcarbonyl)-3-(2-iodophenyl)indole
data/drxl/nmr400/qh420-6.fid
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

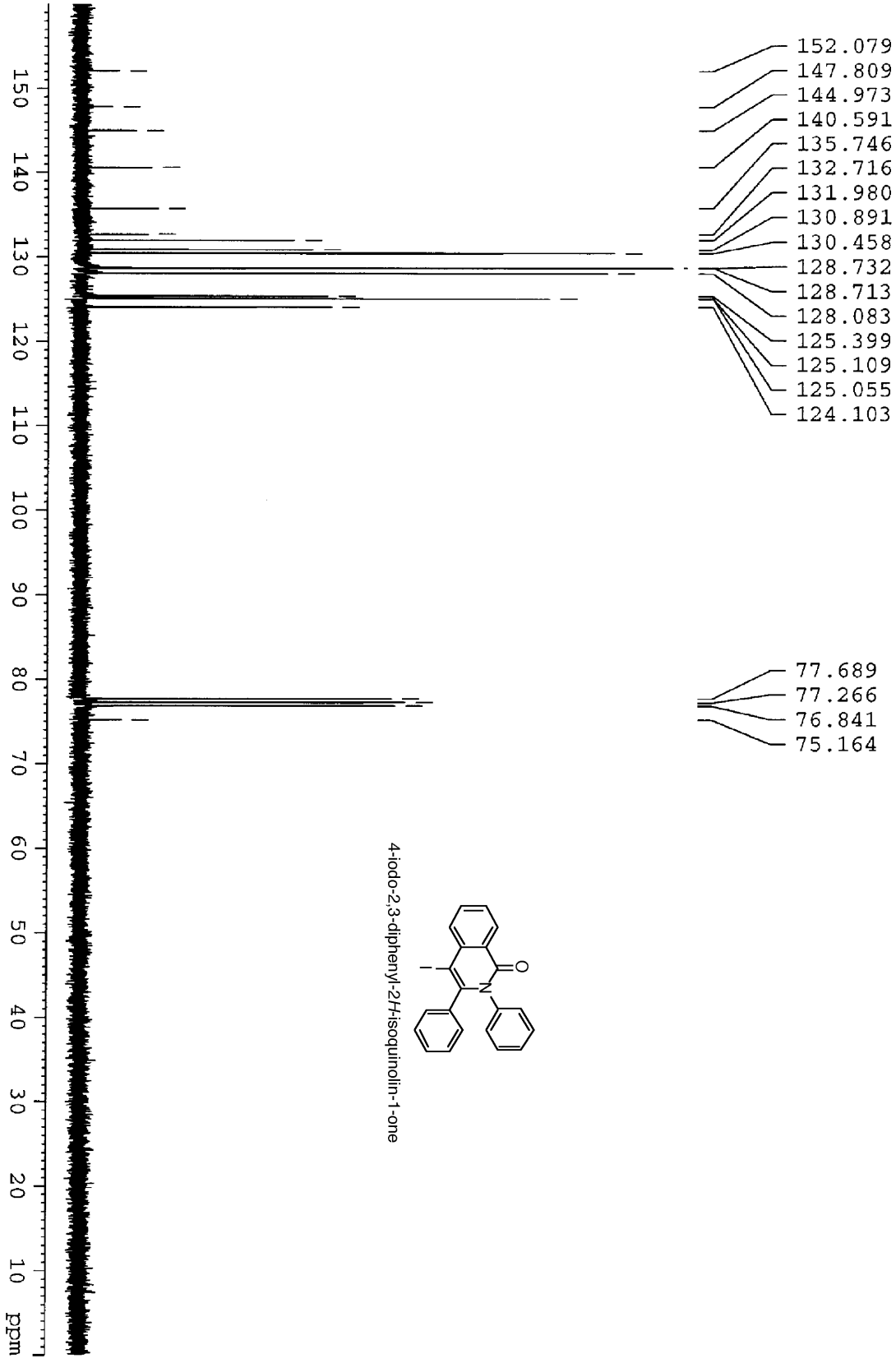

7.434
7.427
7.420
7.416
7.401
7.396
7.392
7.370
7.366
7.325
7.323
7.315
7.312
7.308
7.301
7.293
7.286
7.265
7.262
7.249
7.238
7.234
7.175
7.172
7.149
7.125
7.122
7.034
7.028
7.009
7.007
7.003
7.001
6.983
6.977
4.436
4.414
4.393
2.472
2.450
2.427
2.191
2.170
2.148
0.000
1.000
1.089
6.711
4.910
1.102
1.057
2.244
2.243
2.245
ppm
1-(5-phenyl-4-pentynyl)-3-(2-iodophenyl)indole
N
Ph

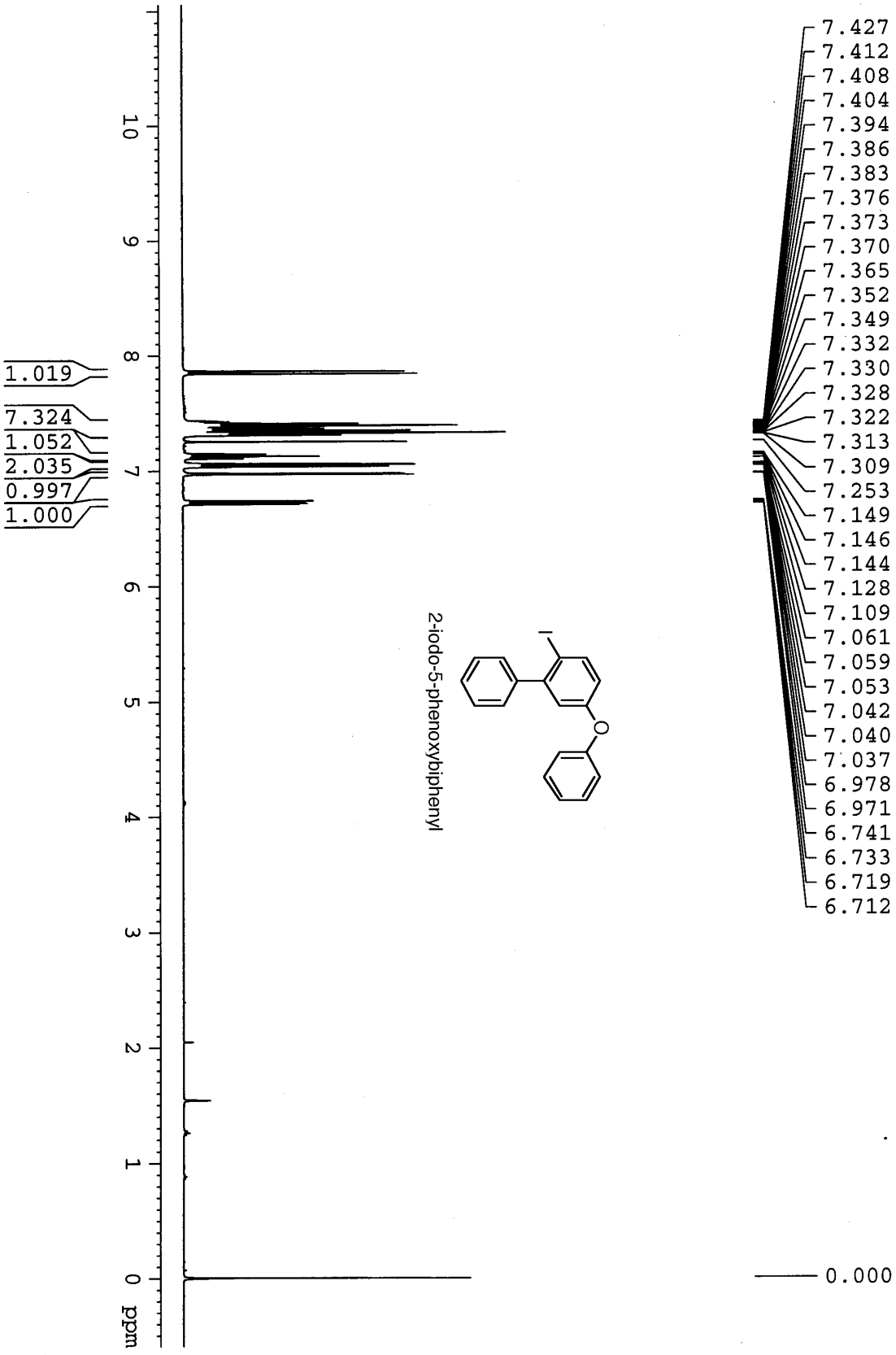

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm
140.069
135.871
131.834
131.511
128.521
128.297
128.204
128.069
128.034
127.502
123.799
122.094
120.423
119.978
118.691
109.843
101.053
88.642
82.250
77.654
77.230
76.807
45.104
29.083
17.013
0.218
1-(5-phenyl-4-pentynyl)-3-(2-iodophenyl)indole
N
Ph

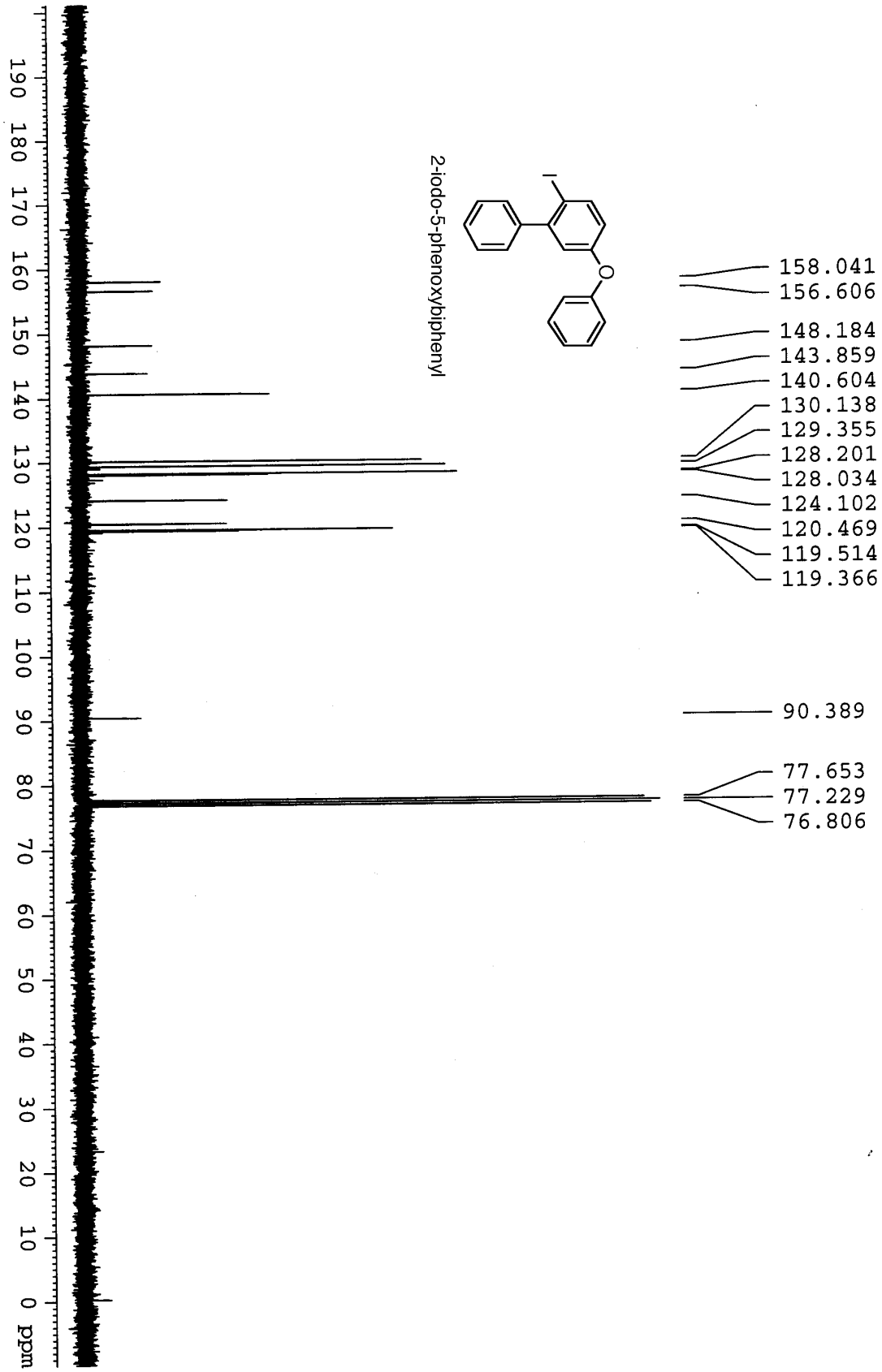

8.317
8.315
8.297
8.295
7.628
7.625
7.606
7.590
7.587
7.557
7.555
7.549
7.536
7.526
7.509
7.495
7.285
7.280
7.266
7.262
6.978
6.958
0.970
1.040
4.033
2.165
1.000
3-iodo-4-phenylisocoumarin
O
O
I
0.000
10
9
8
7
6
5
4
3
2
1
ppm

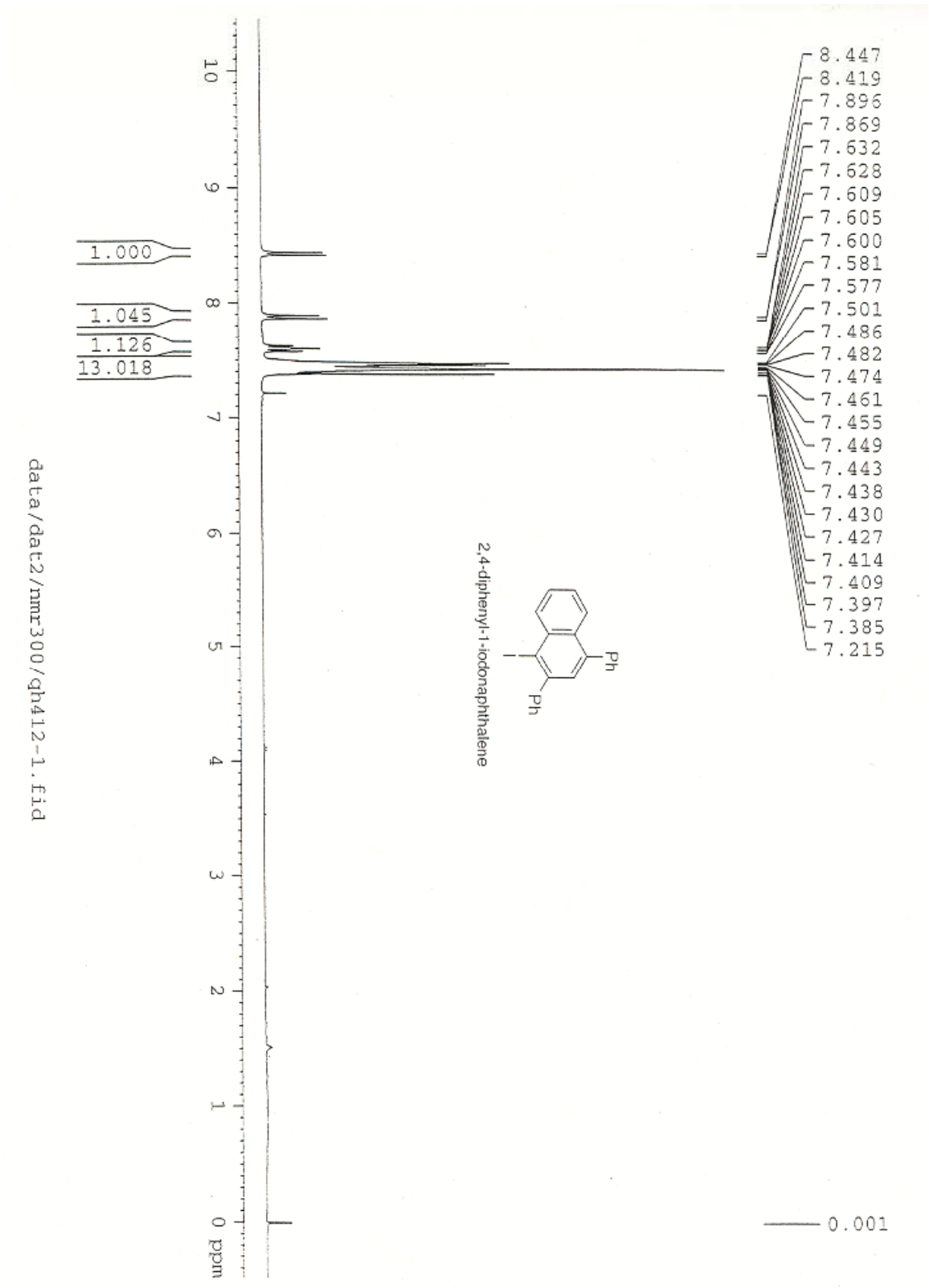

200
180
160
140
120
100
80
60
40
20
ppm
161.202
137.262
136.966
135.157
130.500
129.884
129.126
128.888
128.749
127.433
125.641
119.631
107.851
77.406
77.088
76.770
3-iodo-4-phenylisocoumarin
O
O
I

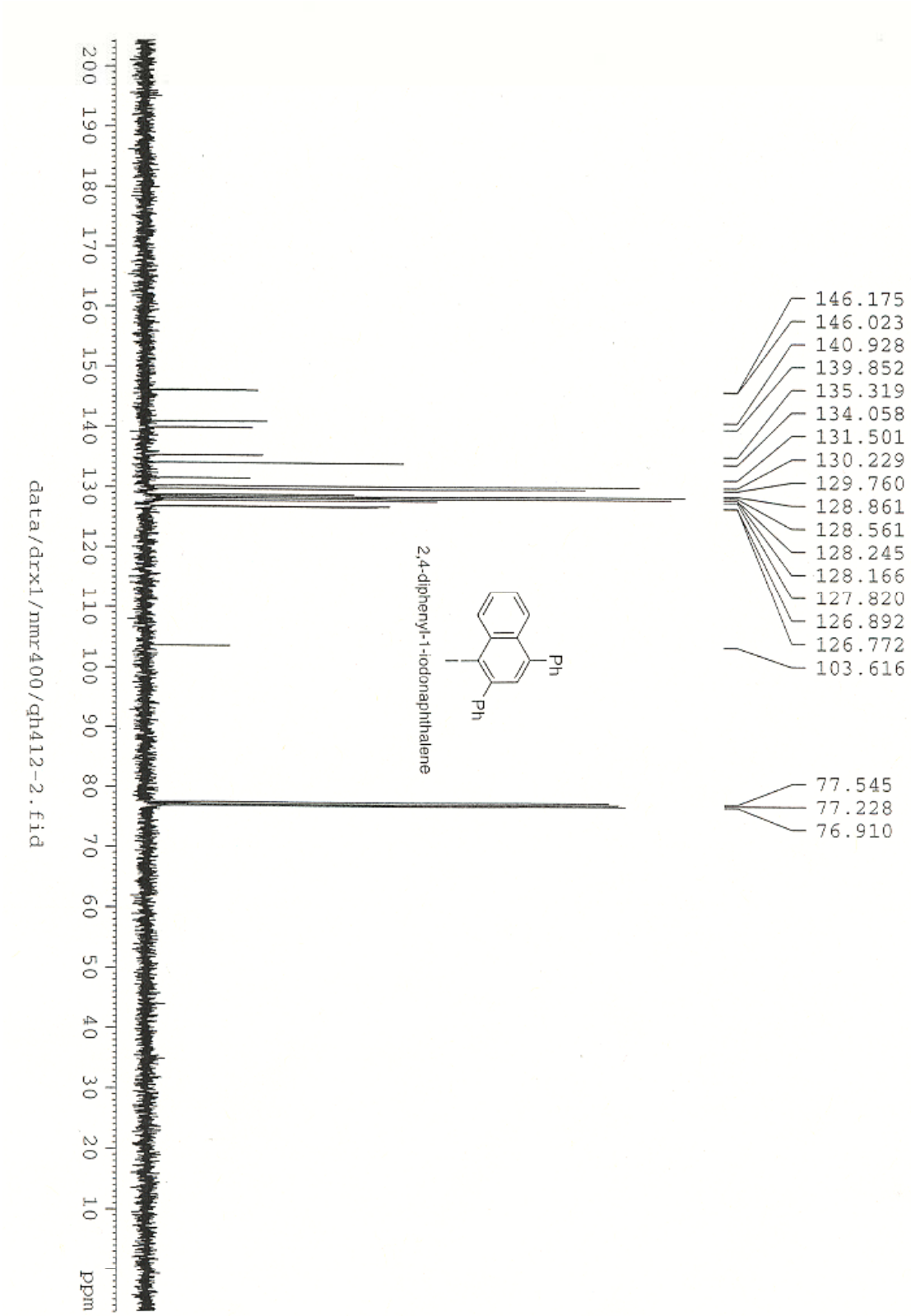

8.029
8.027
8.025
7.720
7.700
7.696
7.674
7.669
7.641
7.638
7.616
7.613
7.604
7.599
7.591
7.588
7.581
7.576
7.572
7.380
7.375
7.369
7.362
7.357
7.351
7.346
7.337
7.333
7.330
7.300
7.296
7.291
7.272
7.251
7.245
7.227
7.222
7.205
7.200
7.108
7.083
1.616
0.887
0.902
1.000
2.964
3.915
3.235
0.946
11
10
9
8
7
6
5
4
3
2
1
ppm
4-iodo-2,3-diphenyl-2H-isoquinolin-1-one
I
O
N

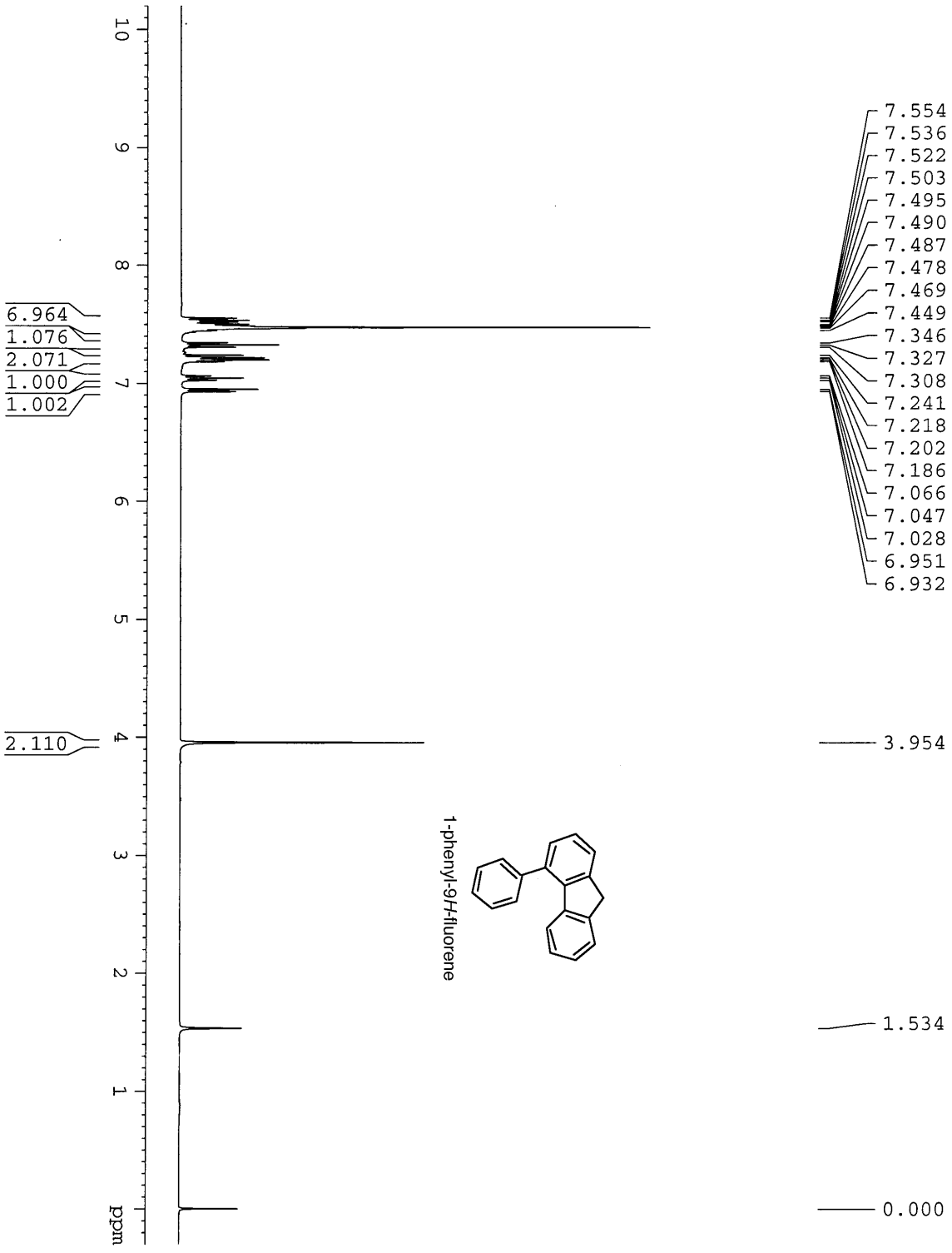

152.079
147.809
144.973
140.591
135.746
132.716
131.980
130.891
130.458
128.732
128.713
128.083
125.399
125.109
125.055
124.103
77.689
77.266
76.841
75.164
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
4-iodo-2,3-diphenyl-2H-isoquinolin-1-one
O
N

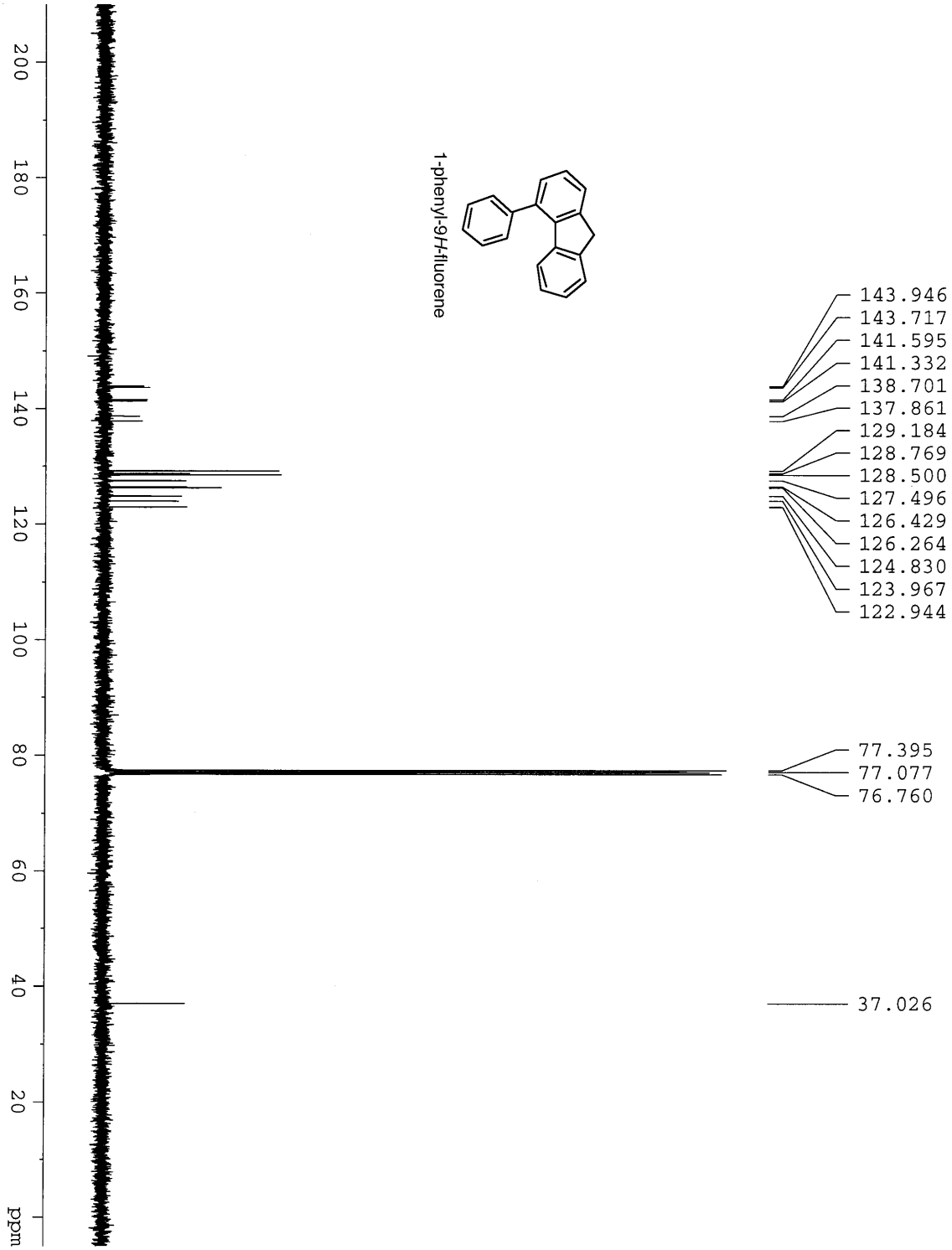

7.427
7.412
7.408
7.404
7.394
7.386
7.383
7.376
7.373
7.370
7.365
7.352
7.349
7.332
7.330
7.328
7.322
7.313
7.309
7.253
7.149
7.146
7.144
7.128
7.109
7.061
7.059
7.053
7.042
7.040
7.037
6.978
6.971
6.741
6.733
6.719
6.712
1.019
7.324
1.052
2.035
0.997
1.000
2-iodo-5-phenoxybiphenyl
I
O
0.000
10
9
8
7
6
5
4
3
2
1
0
ppm

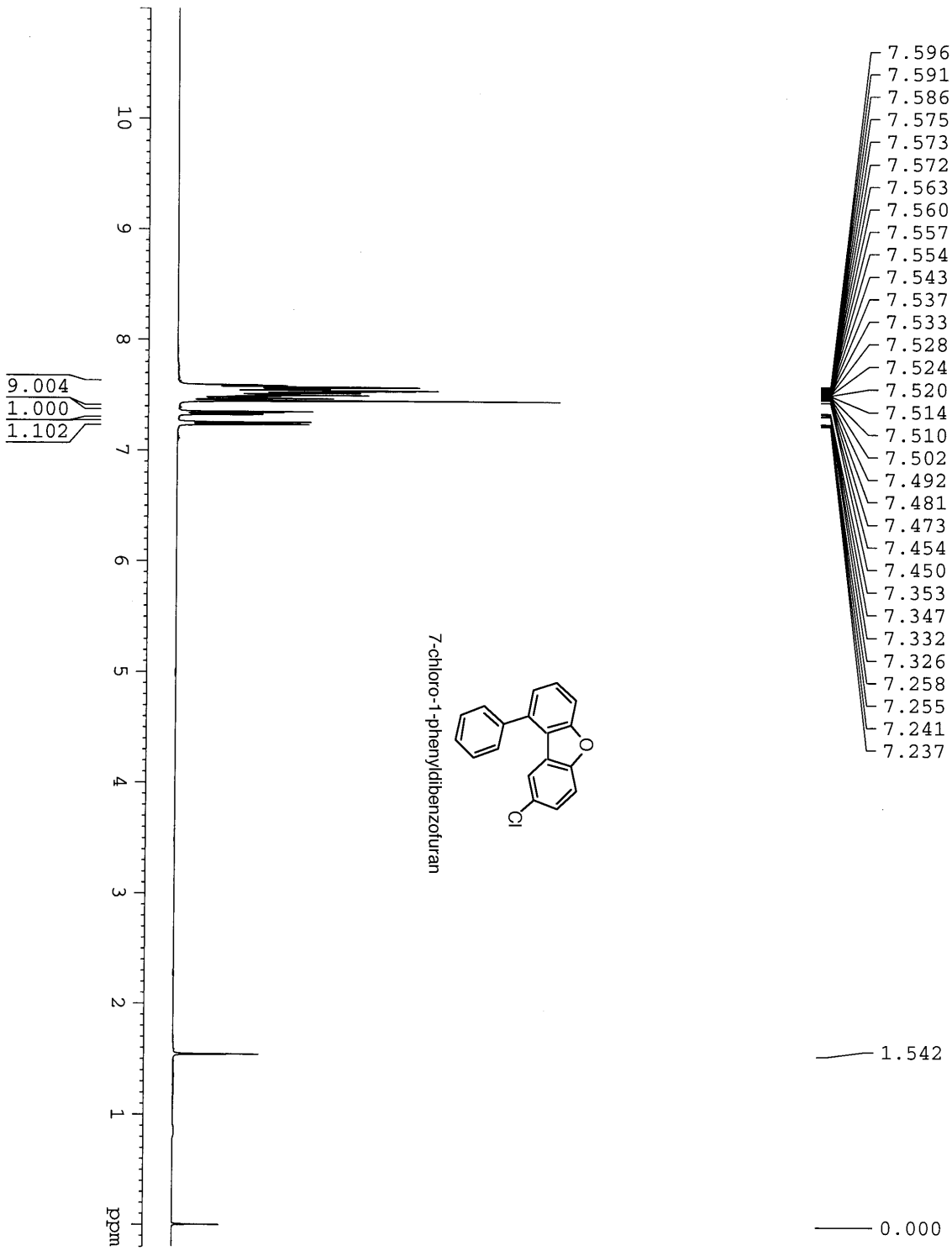

2-iodo-5-phenoxybiphenyl
158.041
156.606
148.184
143.859
140.604
130.138
129.355
128.201
128.034
124.102
120.469
119.514
119.366
90.389
77.653
77.229
76.806
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

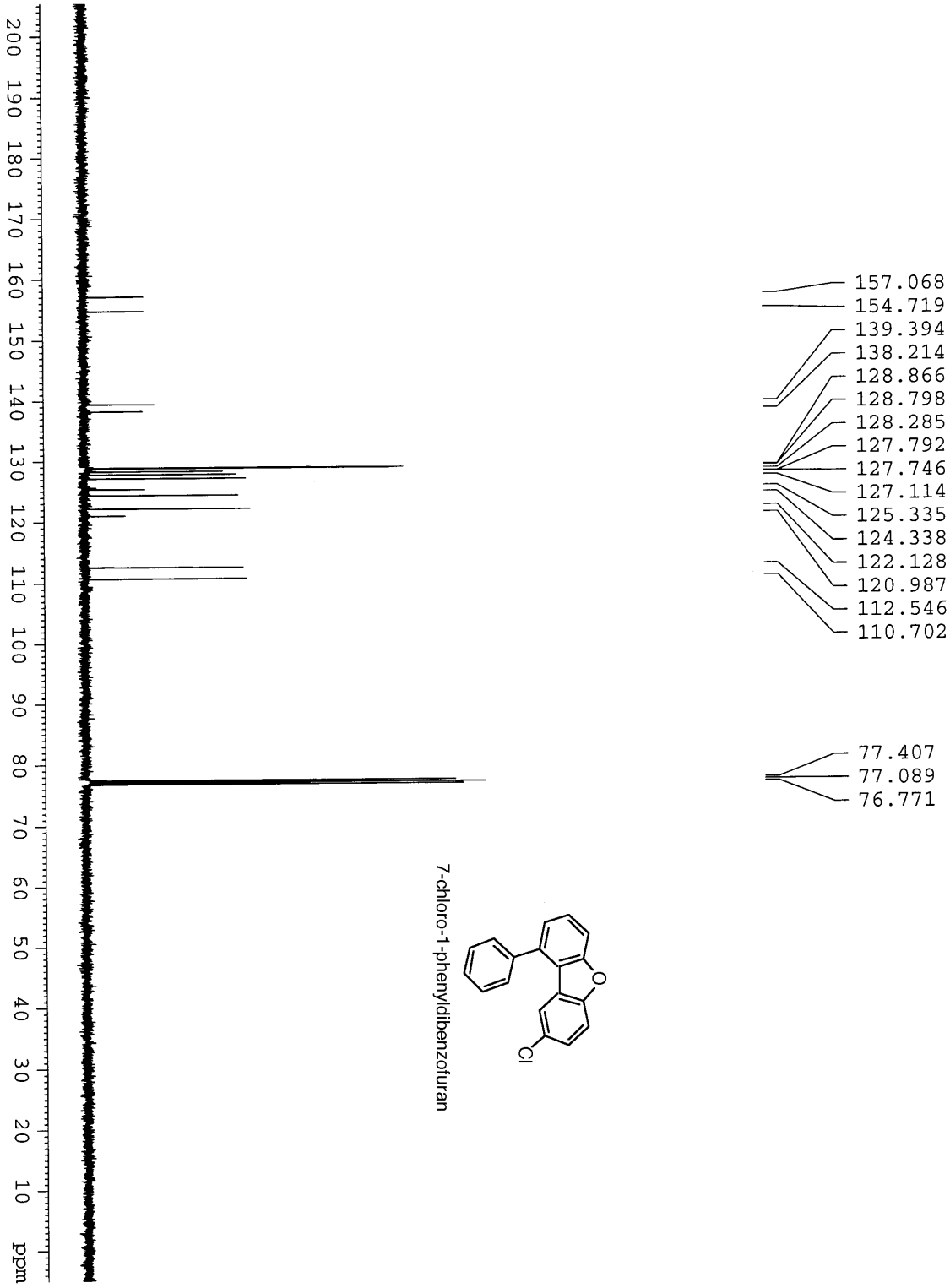

8.447
8.419
7.896
7.869
7.632
7.628
7.609
7.605
7.600
7.581
7.577
7.501
7.486
7.482
7.474
7.461
7.455
7.449
7.443
7.438
7.430
7.427
7.414
7.409
7.397
7.385
7.215
1.000
1.045
1.126
13.018
10
9
8
7
6
5
4
3
2
1
0 ppm
Ph
Ph
2,4-diphenyl-1-iodonaphthalene
0.001
data/dat2/nmr300/qh412-1.fid

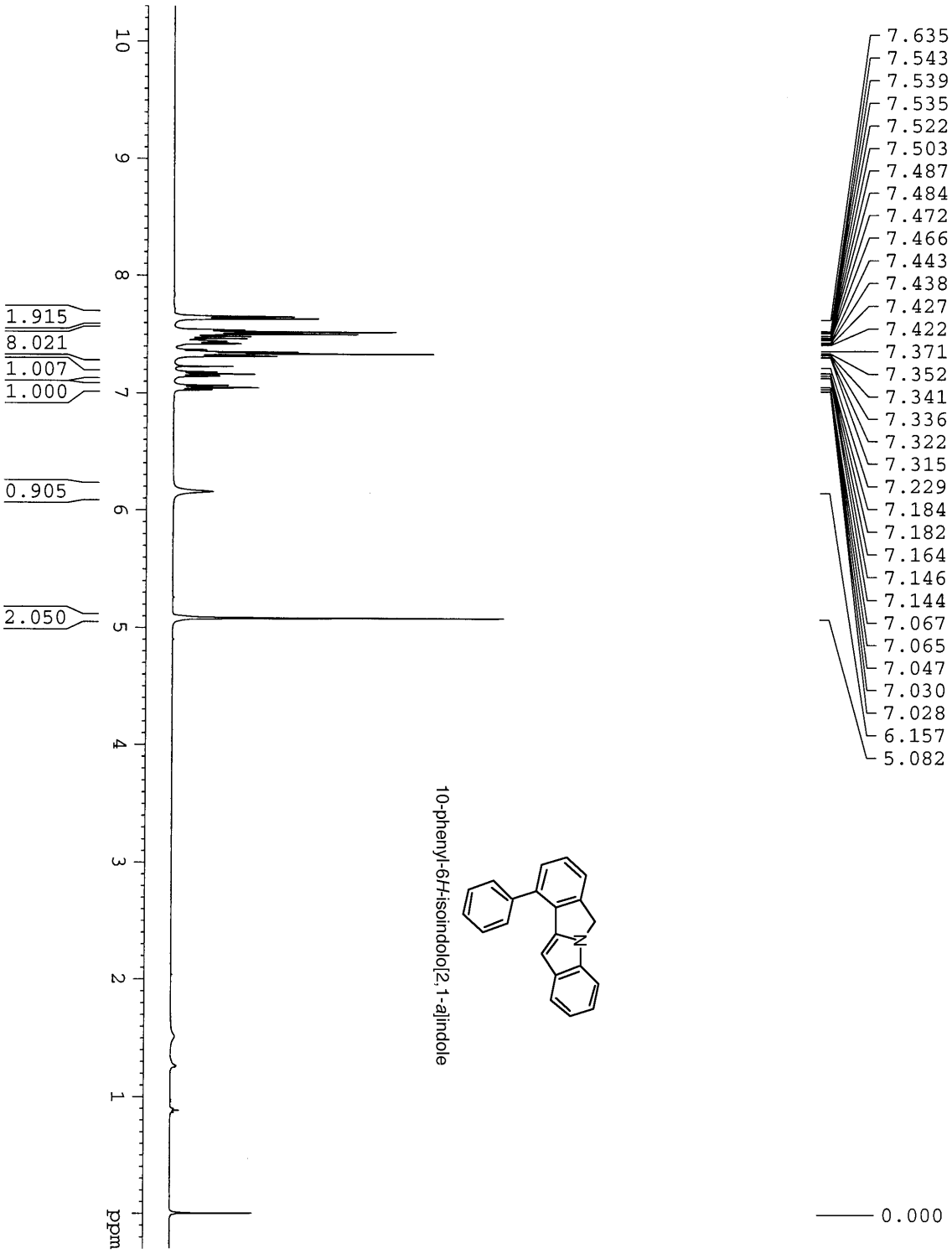

146.175
146.023
140.928
139.852
135.319
134.058
131.501
130.229
129.760
128.861
128.561
128.245
128.166
127.820
126.892
126.772
103.616
77.545
77.228
76.910
2,4-diphenyl-1-iodonaphthalene
Ph
Ph
I
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
data/drx1/nmr400/qh412-2.fid

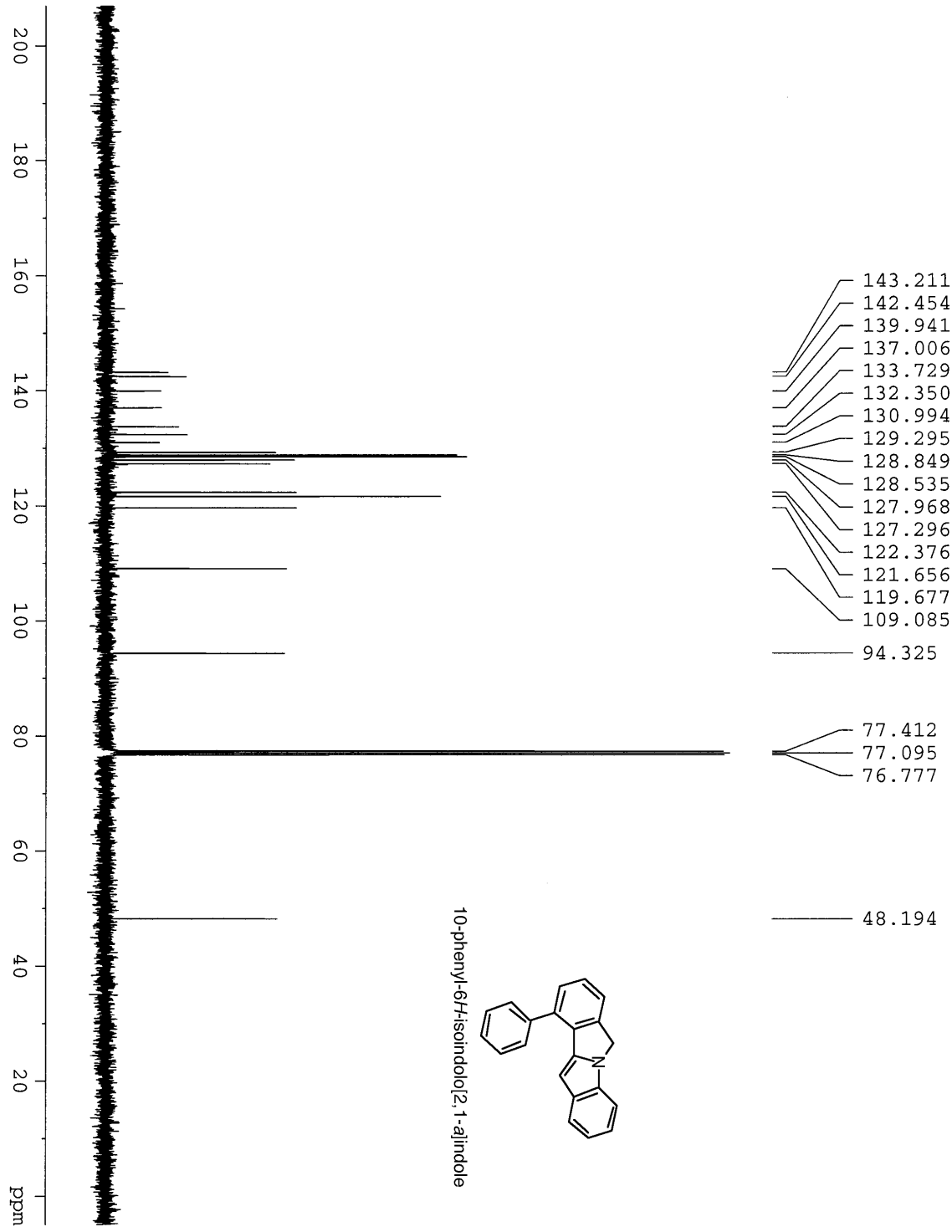

10
9
8
7
6
5
4
3
2
1
ppm
6.964
1.076
2.071
1.000
1.002
2.110
7.554
7.536
7.522
7.503
7.495
7.490
7.487
7.478
7.469
7.449
7.346
7.327
7.308
7.241
7.218
7.202
7.186
7.066
7.047
7.028
6.951
6.932
3.954
1.534
0.000
1-phenyl-9H-fluorene

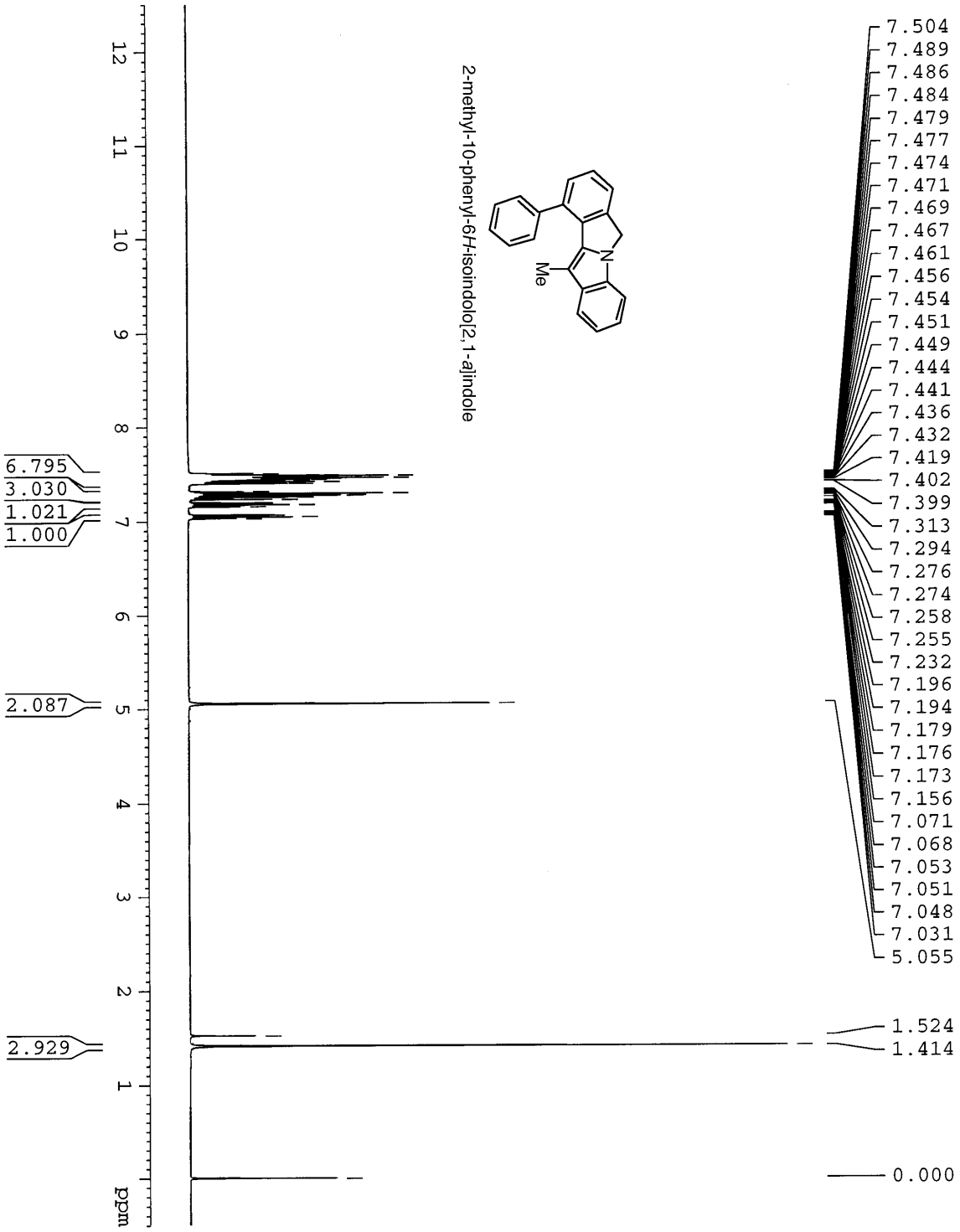

1-phenyl-9H-fluorene
143.946
143.717
141.595
141.332
138.701
137.861
129.184
128.769
128.500
127.496
126.429
126.264
124.830
123.967
122.944
77.395
77.077
76.760
37.026
200
180
160
140
120
100
80
60
40
20
ppm

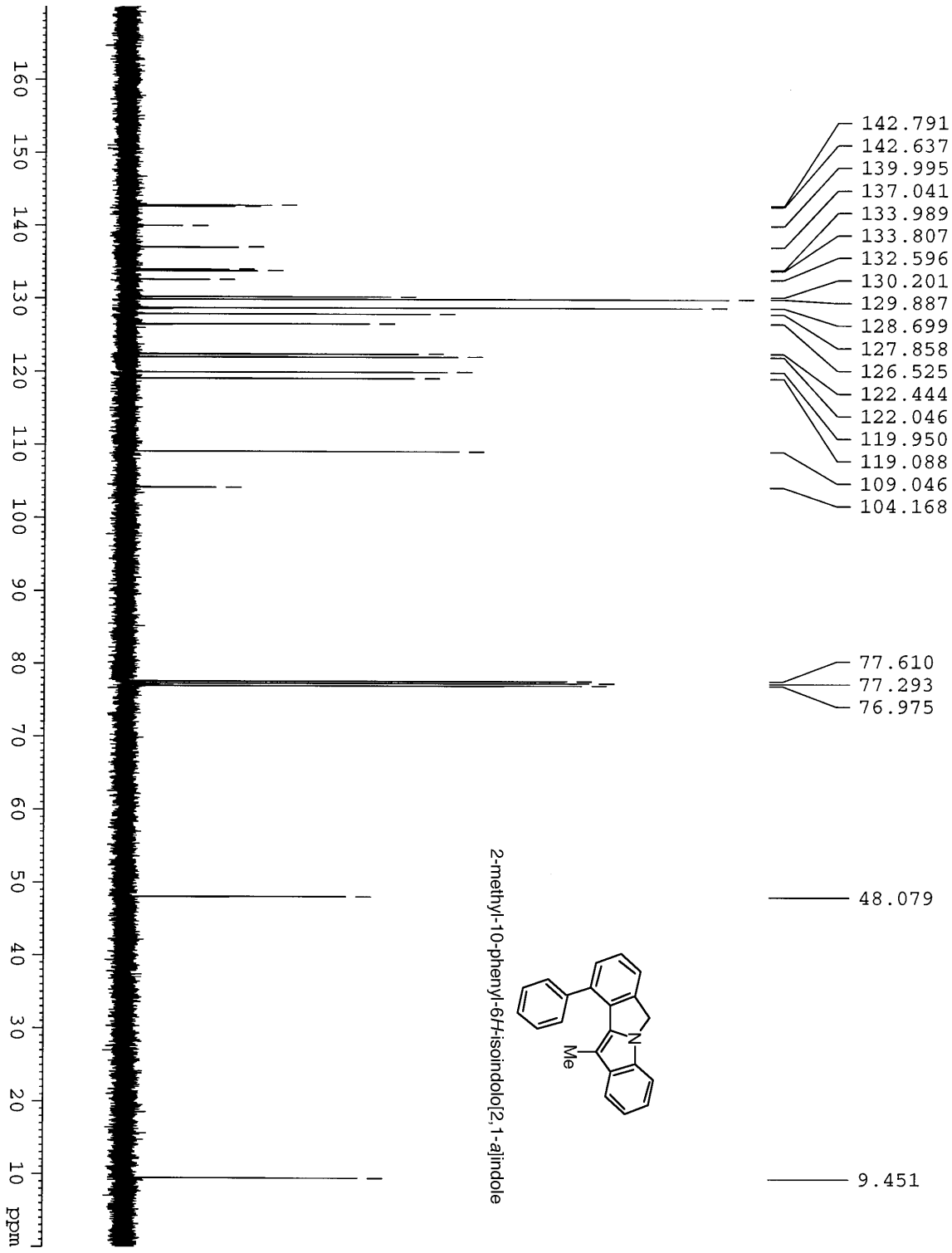

9.004
1.000
1.102
10
9
8
7
6
5
4
3
2
1
ppm
7-chloro-1-phenyldibenzofuran
O
Cl
7.596
7.591
7.586
7.575
7.573
7.572
7.563
7.560
7.557
7.554
7.543
7.537
7.533
7.528
7.524
7.520
7.514
7.510
7.502
7.492
7.481
7.473
7.454
7.450
7.353
7.347
7.332
7.326
7.258
7.255
7.241
7.237
1.542
0.000

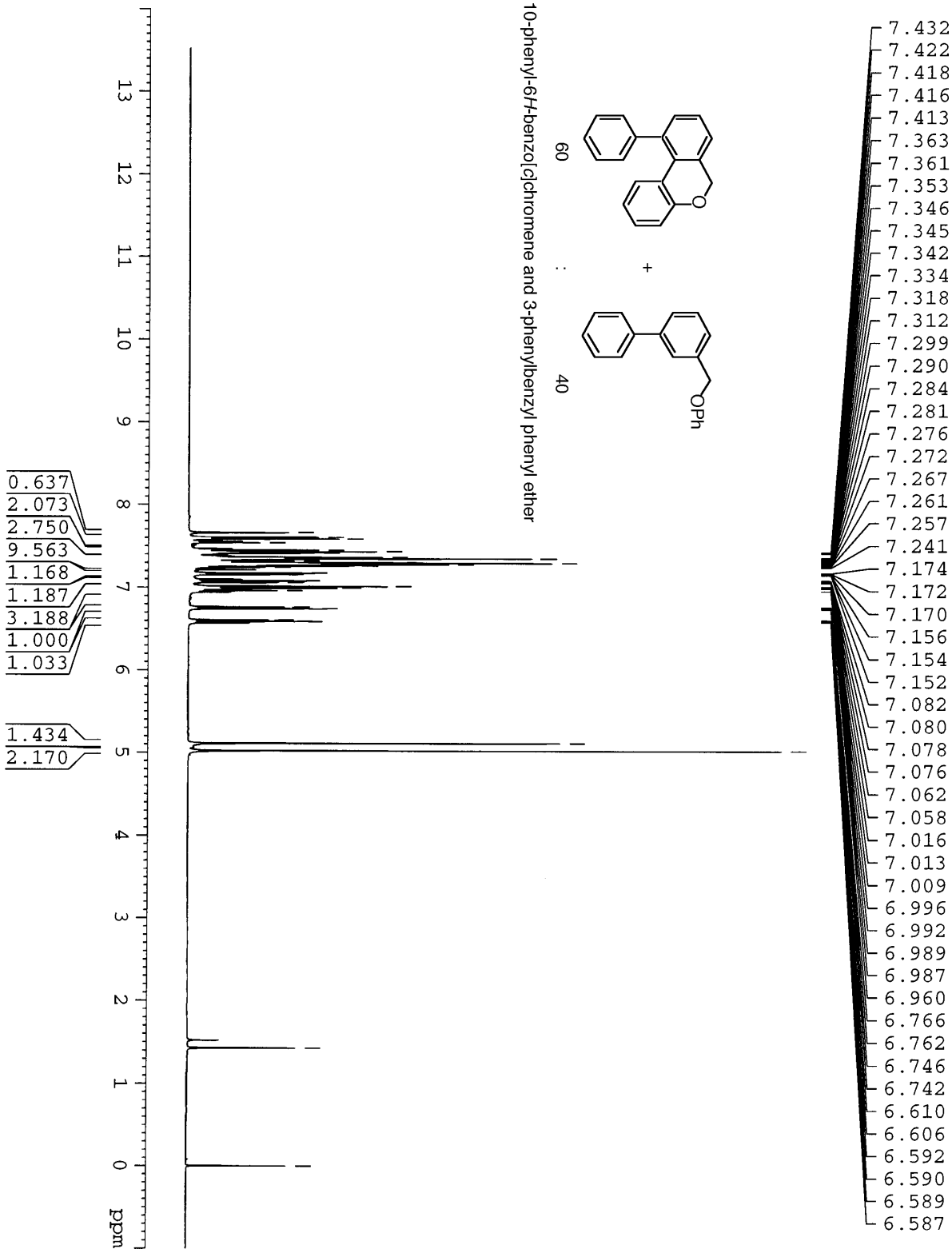

157.068
154.719
139.394
138.214
128.866
128.798
128.285
127.792
127.746
127.114
125.335
124.338
122.128
120.987
112.546
110.702
77.407
77.089
76.771
7-chloro-1-phenyldibenzofuran
O
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

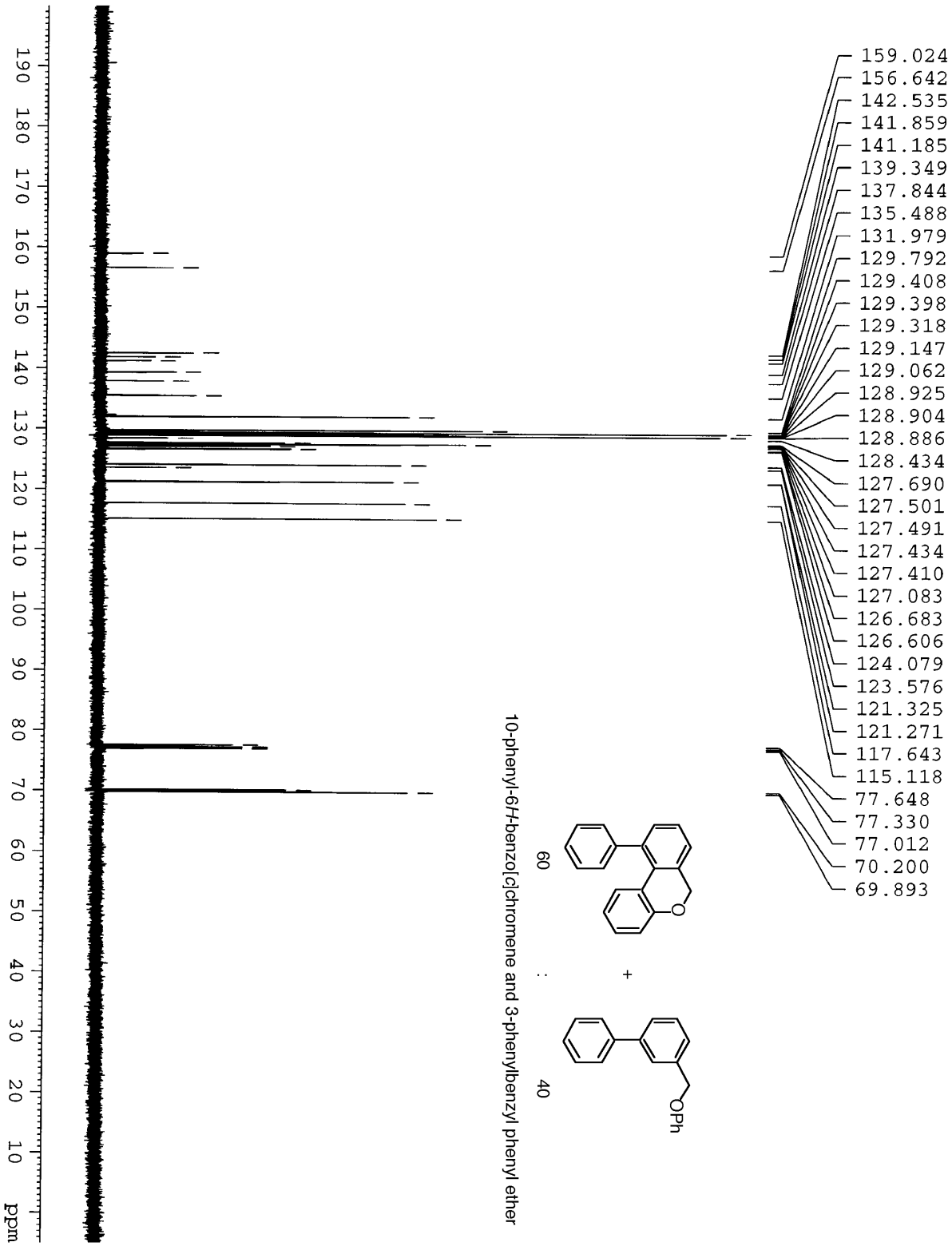

10
9
8
7
6
5
4
3
2
1
ppm
1.915
8.021
1.007
1.000
0.905
2.050
7.635
7.543
7.539
7.535
7.522
7.503
7.487
7.484
7.472
7.466
7.443
7.438
7.427
7.422
7.371
7.352
7.341
7.336
7.322
7.315
7.229
7.184
7.182
7.164
7.146
7.144
7.067
7.065
7.047
7.030
7.028
6.157
5.082
0.000
10-phenyl-6H-isoindolo[2,1-a]indole

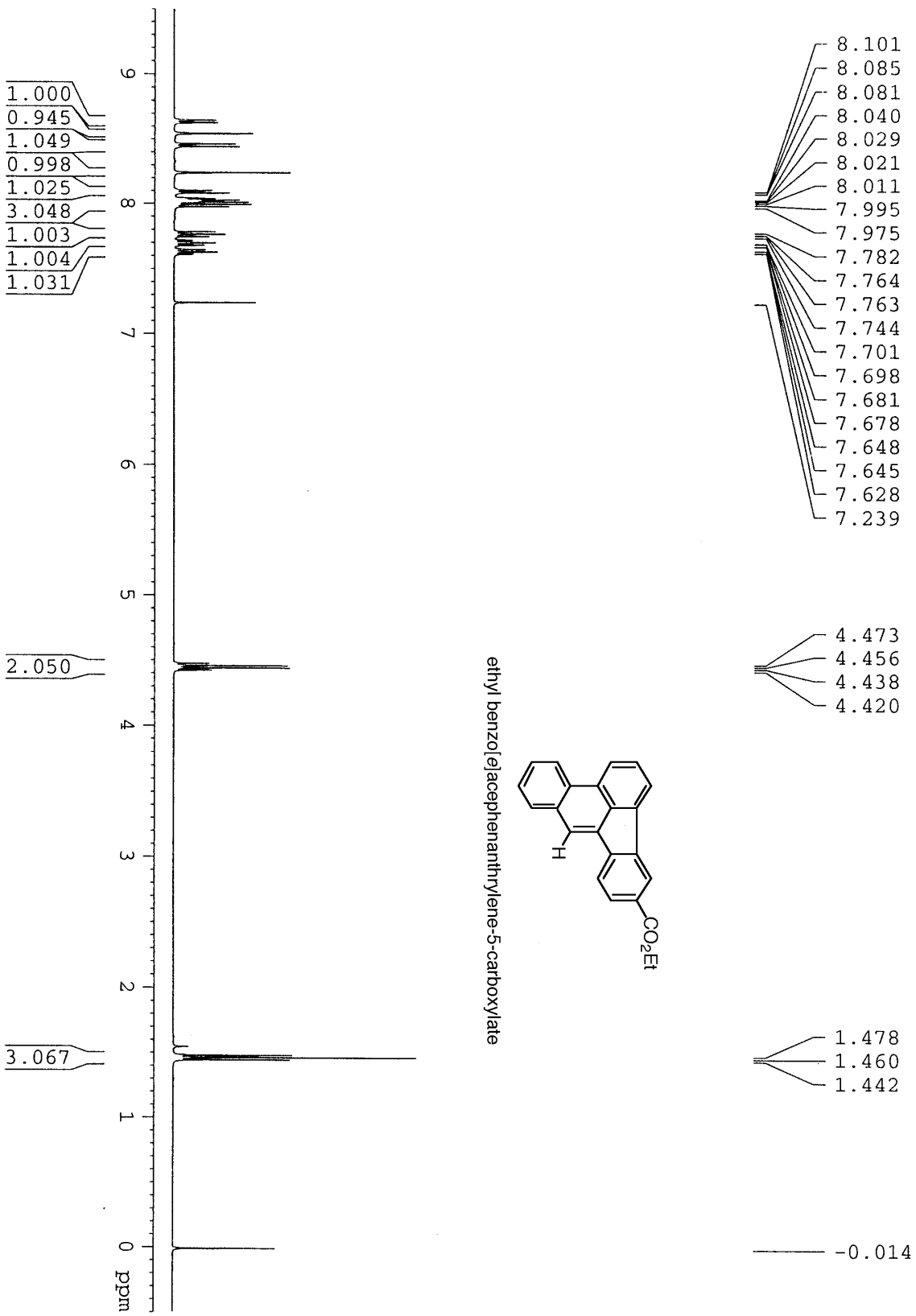

200
180
160
140
120
100
80
60
40
20
ppm
143.211
142.454
139.941
137.006
133.729
132.350
130.994
129.295
128.849
128.535
127.968
127.296
122.376
121.656
119.677
109.085
94.325
77.412
77.095
76.777
48.194
10-phenyl-6H-isoindolo[2,1-a]indole
N

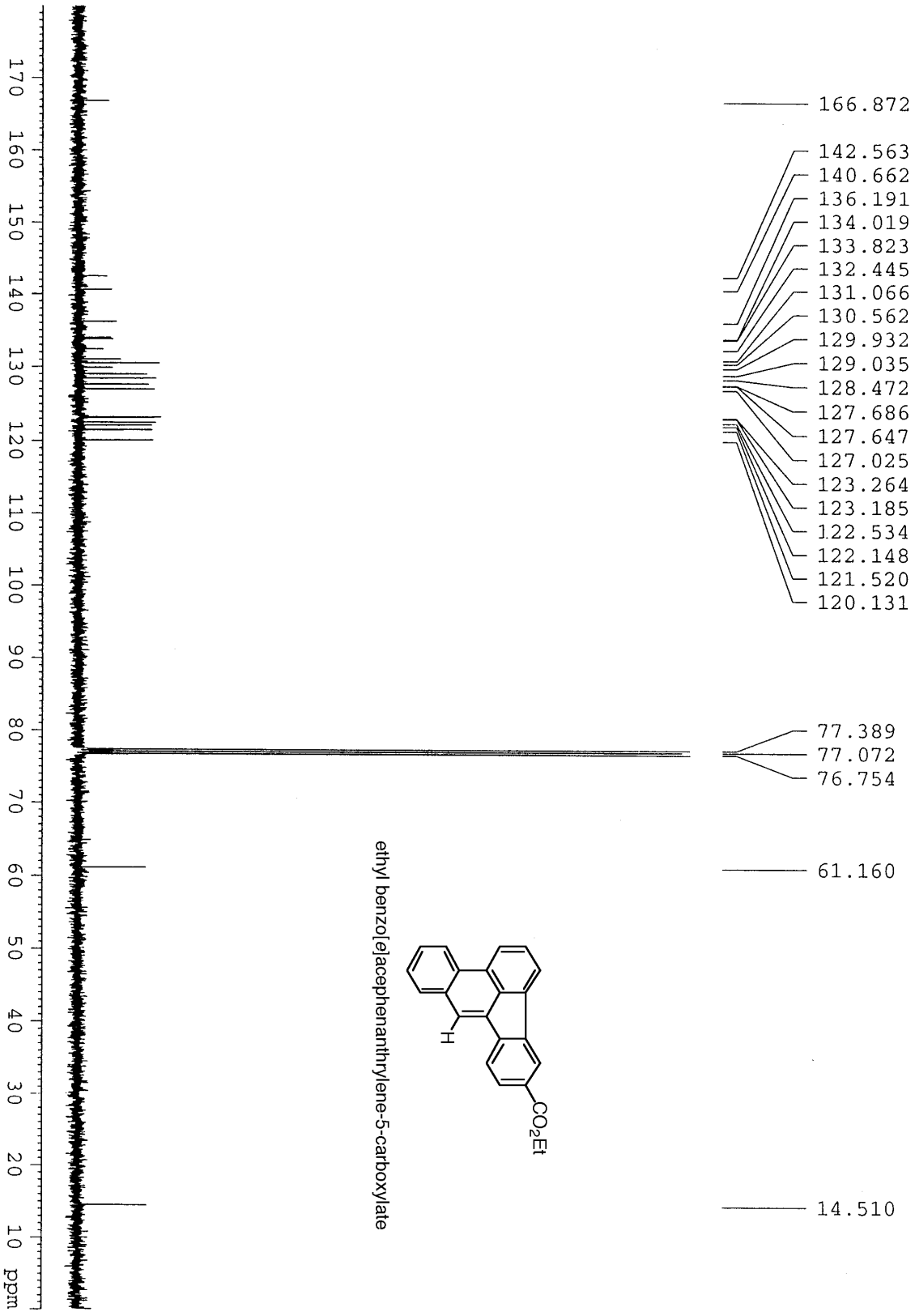

2-methyl-10-phenyl-6H-isoindolo[2,1-a]indole
Me
N
7.504
7.489
7.486
7.484
7.479
7.477
7.474
7.471
7.469
7.467
7.461
7.456
7.454
7.451
7.449
7.444
7.441
7.436
7.432
7.419
7.402
7.399
7.313
7.294
7.276
7.274
7.258
7.255
7.232
7.196
7.194
7.179
7.176
7.173
7.156
7.071
7.068
7.053
7.051
7.048
7.031
5.055
1.524
1.414
0.000
6.795
3.030
1.021
1.000
2.087
2.929
ppm

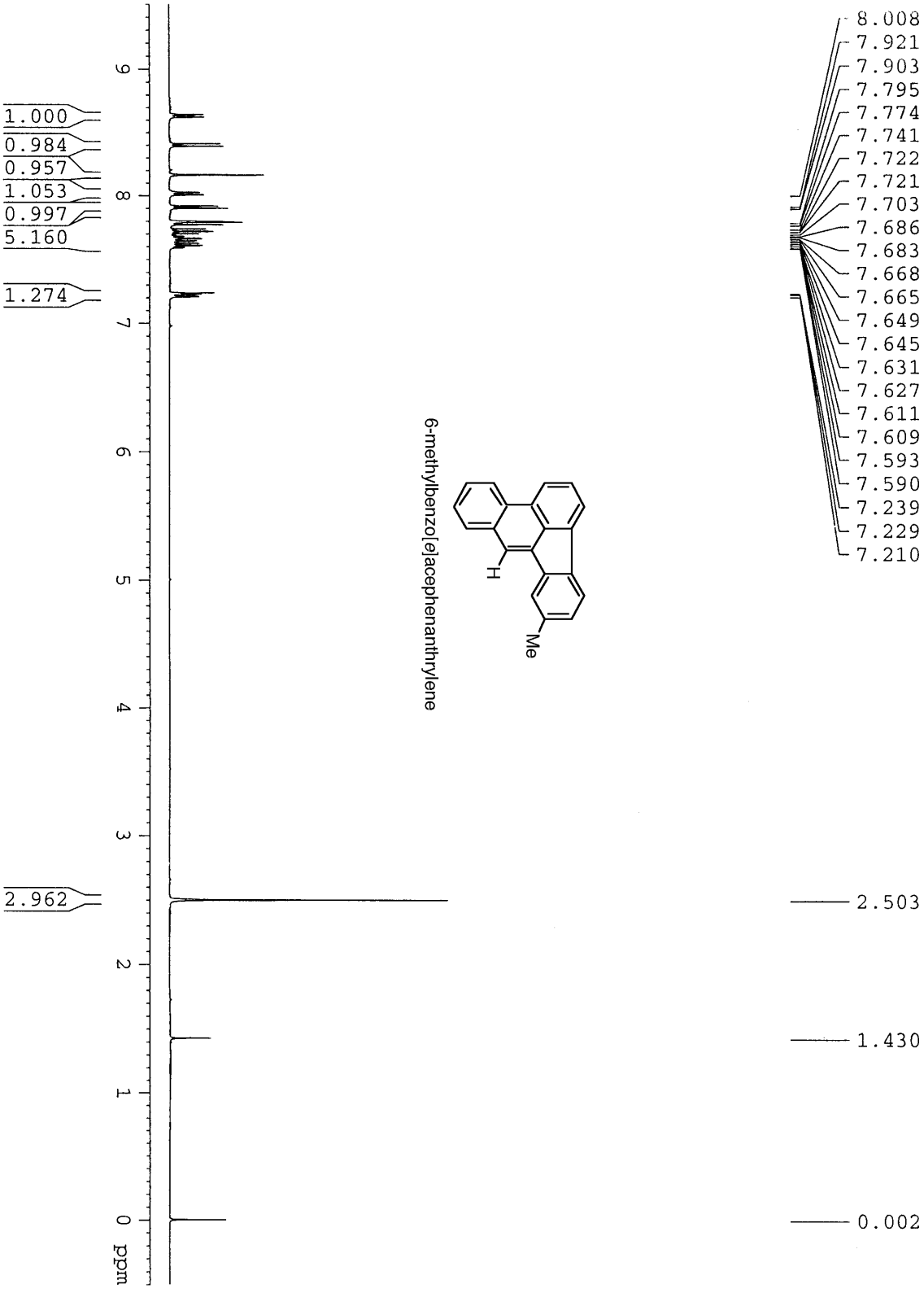

142.791
142.637
139.995
137.041
133.989
133.807
132.596
130.201
129.887
128.699
127.858
126.525
122.444
122.046
119.950
119.088
109.046
104.168
77.610
77.293
76.975
48.079
9.451
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
2-methyl-10-phenyl-6H-isoindolo[2,1-a]indole
Me
N

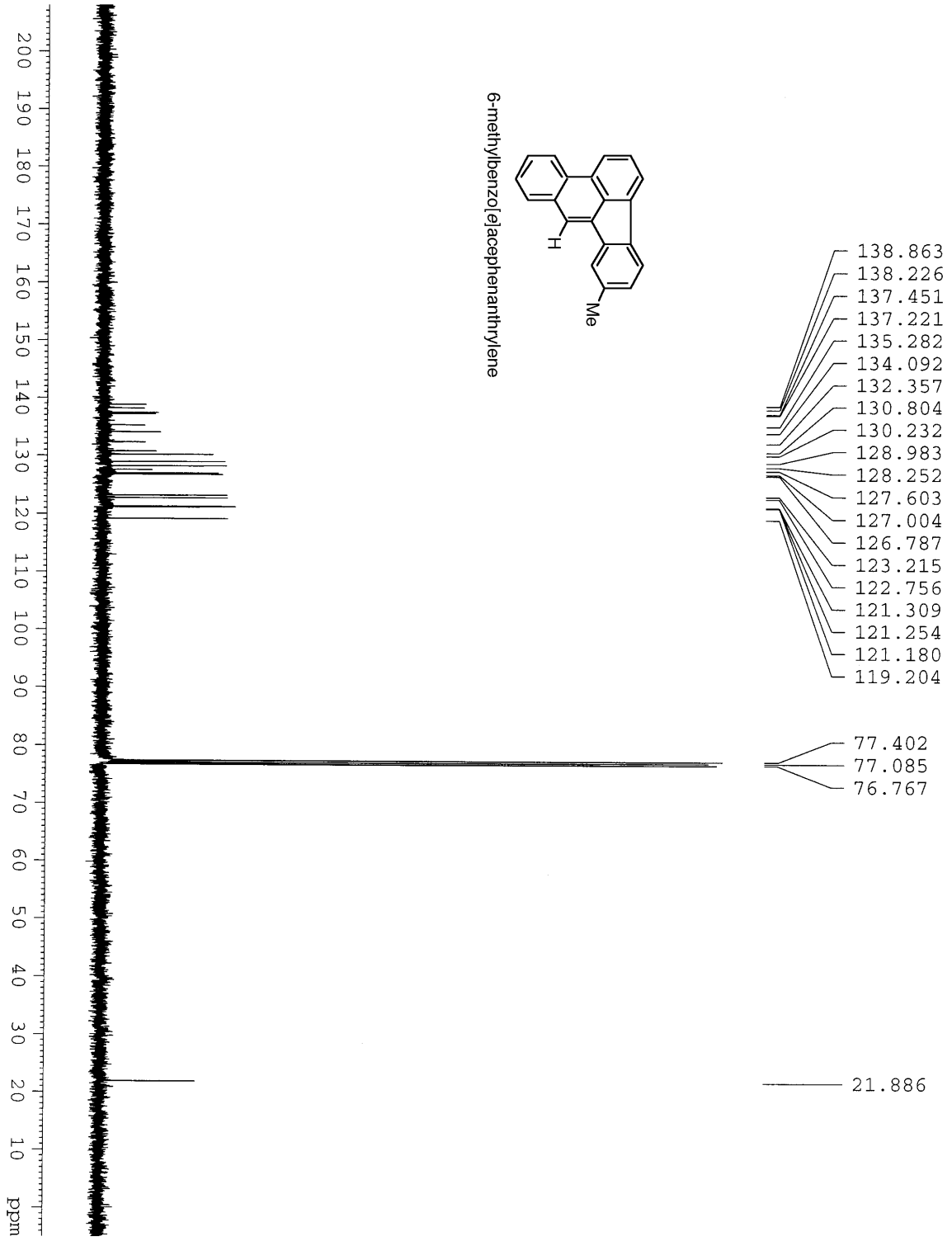

10-phenyl-6*H*-benzo[*c*]chromene and 3-phenylbenzyl phenyl ether
60 : 40
OPh
7.432
7.422
7.418
7.416
7.413
7.363
7.361
7.353
7.346
7.345
7.342
7.334
7.318
7.312
7.299
7.290
7.284
7.281
7.276
7.272
7.267
7.261
7.257
7.241
7.174
7.172
7.170
7.156
7.154
7.152
7.082
7.080
7.078
7.076
7.062
7.058
7.016
7.013
7.009
6.996
6.992
6.989
6.987
6.960
6.766
6.762
6.746
6.742
6.610
6.606
6.592
6.590
6.589
6.587
0.637
2.073
2.750
9.563
1.168
1.187
3.188
1.000
1.033
1.434
2.170
ppm


159.024
156.642
142.535
141.859
141.185
139.349
137.844
135.488
131.979
129.792
129.408
129.398
129.318
129.147
129.062
128.925
128.904
128.886
128.434
127.690
127.501
127.491
127.434
127.410
127.083
126.683
126.606
124.079
123.576
121.325
121.271
117.643
115.118
77.648
77.330
77.012
70.200
69.893
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
10-phenyl-6H-benzo[c]chromene and 3-phenylbenzyl phenyl ether
60 : 40
O
OPh

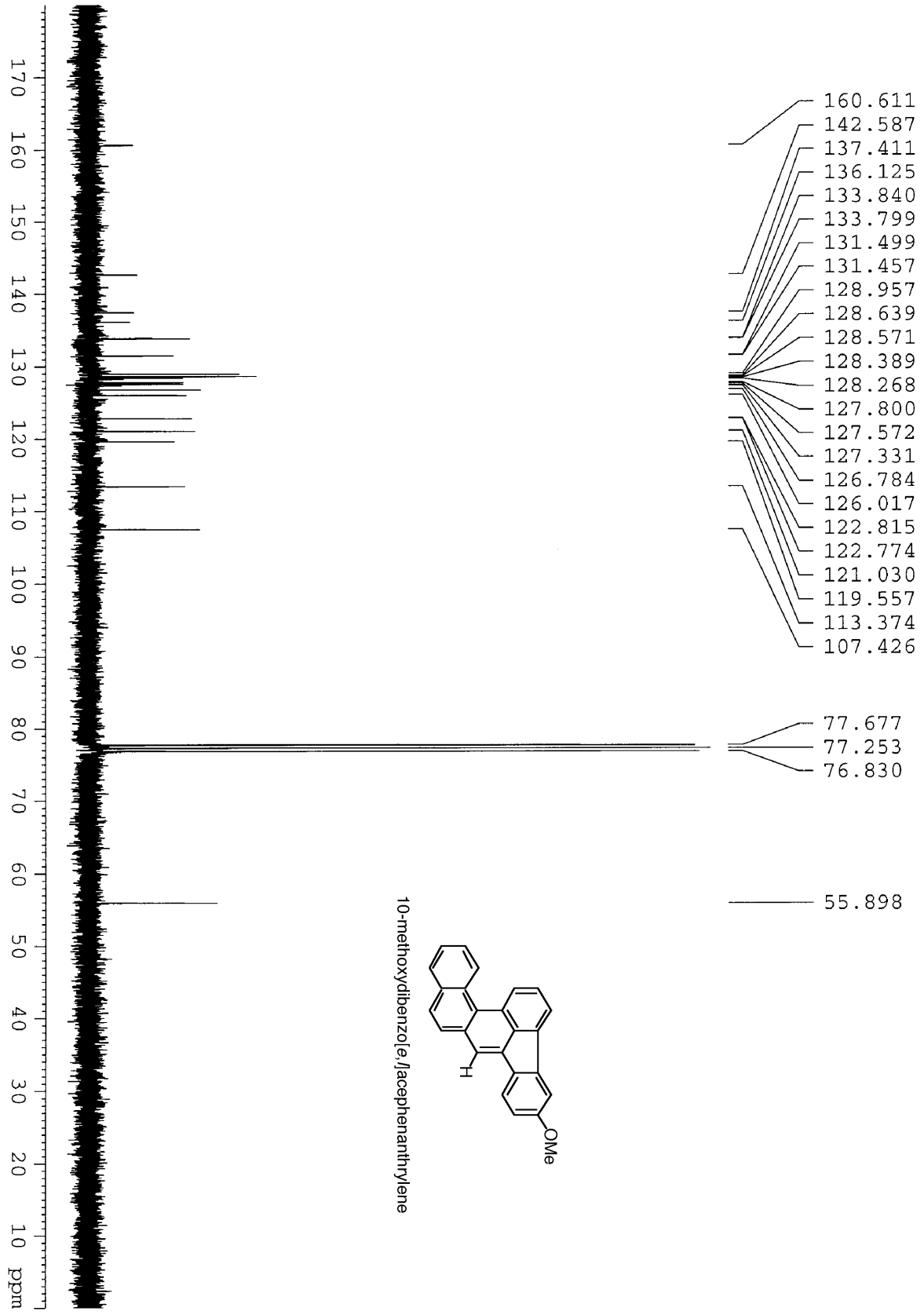

8.101
8.085
8.081
8.040
8.029
8.021
8.011
7.995
7.975
7.782
7.764
7.763
7.744
7.701
7.698
7.681
7.678
7.648
7.645
7.628
7.239
4.473
4.456
4.438
4.420
1.478
1.460
1.442
-0.014
1.000
0.945
1.049
0.998
1.025
3.048
1.003
1.004
1.031
2.050
3.067
9
8
7
6
5
4
3
2
1
0
ppm
ethyl benzo[e]acephenanthrylene-5-carboxylate
H
CO2Et

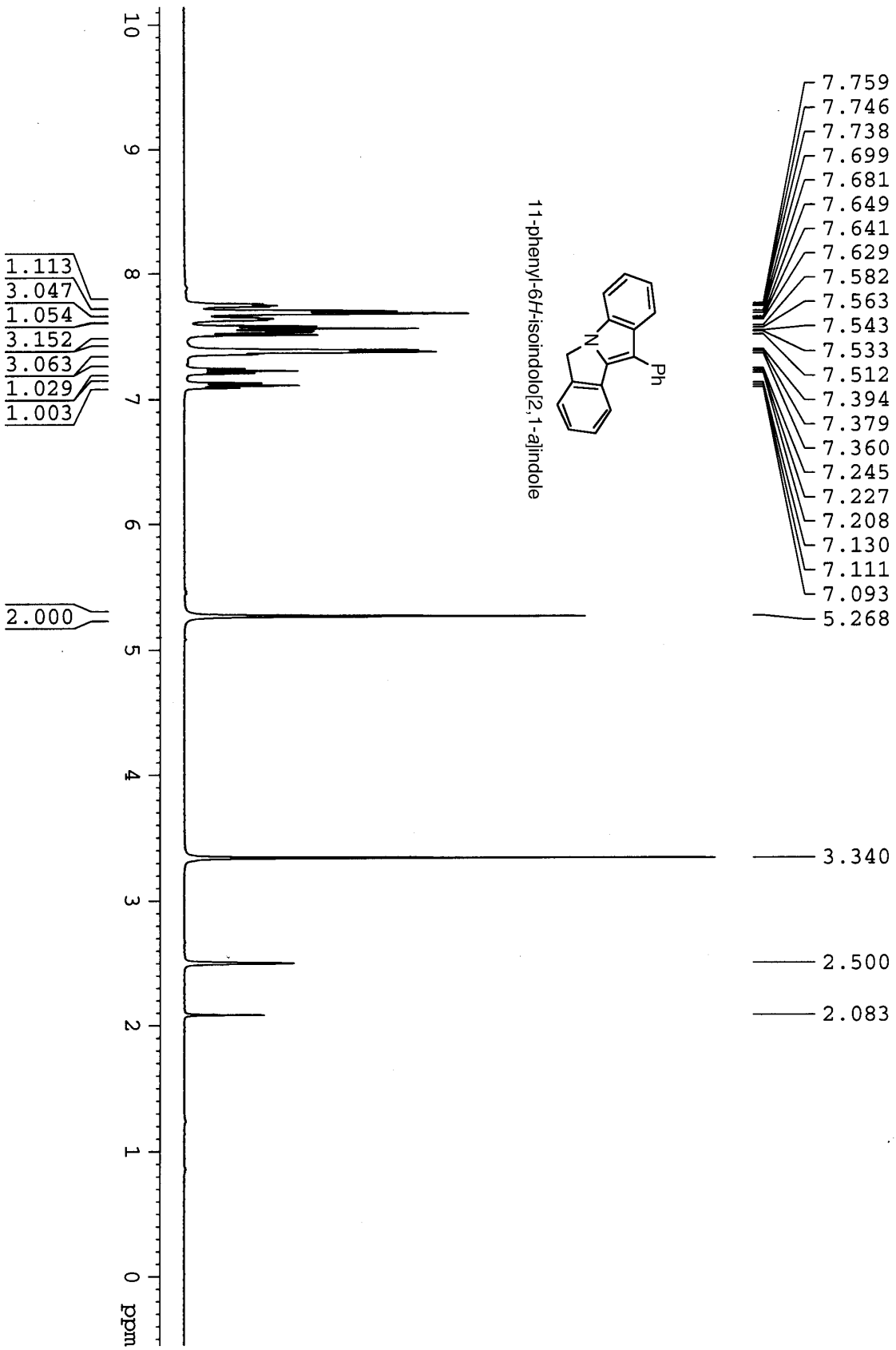

166.872
142.563
140.662
136.191
134.019
133.823
132.445
131.066
130.562
129.932
129.035
128.472
127.686
127.647
127.025
123.264
123.185
122.534
122.148
121.520
120.131
77.389
77.072
76.754
61.160
14.510
ethyl benzo[e]acephenanthrylene-5-carboxylate
H
CO2Et
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

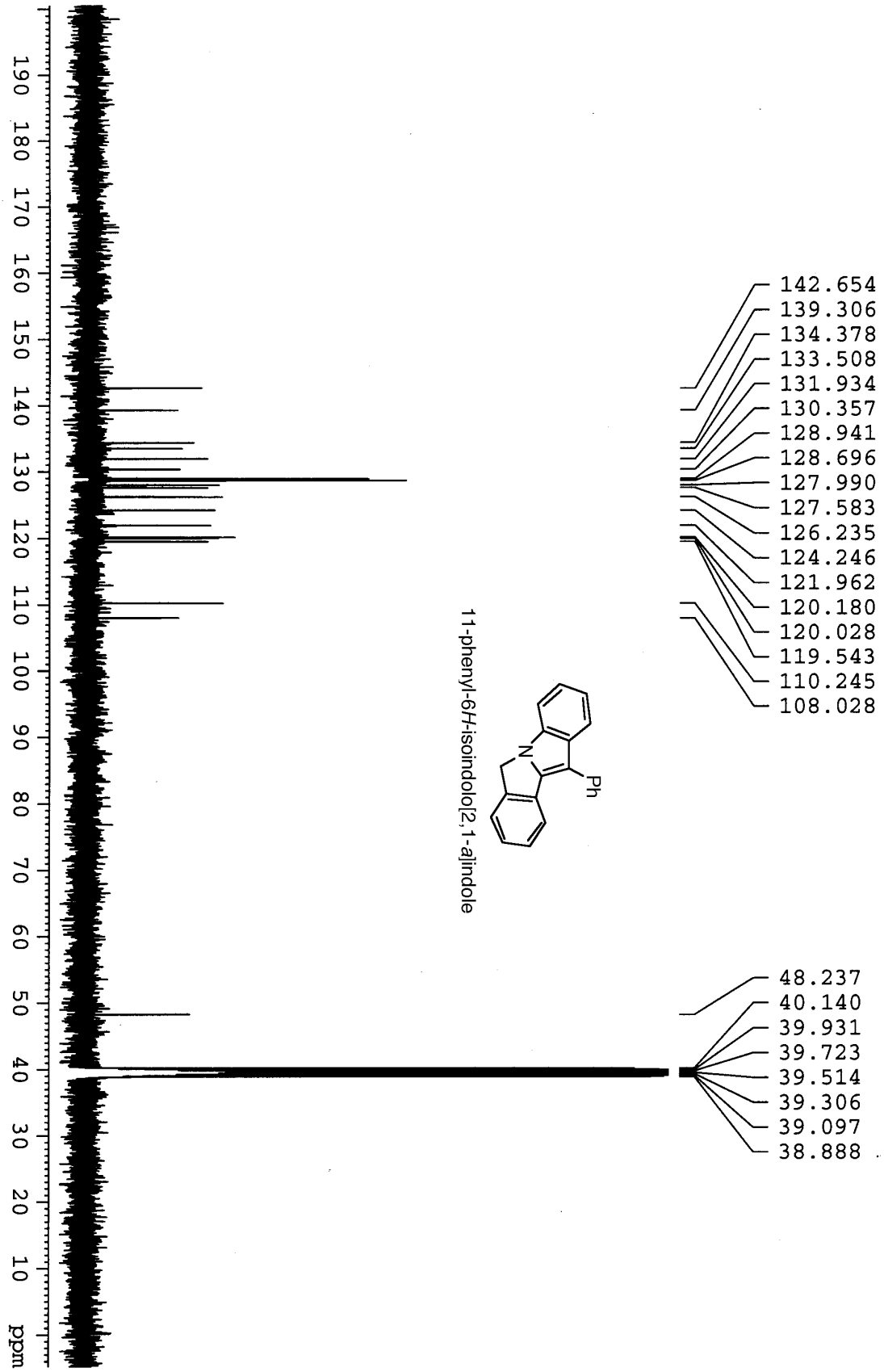

8.008
7.921
7.903
7.795
7.774
7.741
7.722
7.721
7.703
7.686
7.683
7.668
7.665
7.649
7.645
7.631
7.627
7.611
7.609
7.593
7.590
7.239
7.229
7.210
1.000
0.984
0.957
1.053
0.997
5.160
1.274
2.962
2.503
1.430
0.002
6-methylbenzo[e]acephenanthrylene
H
Me
ppm

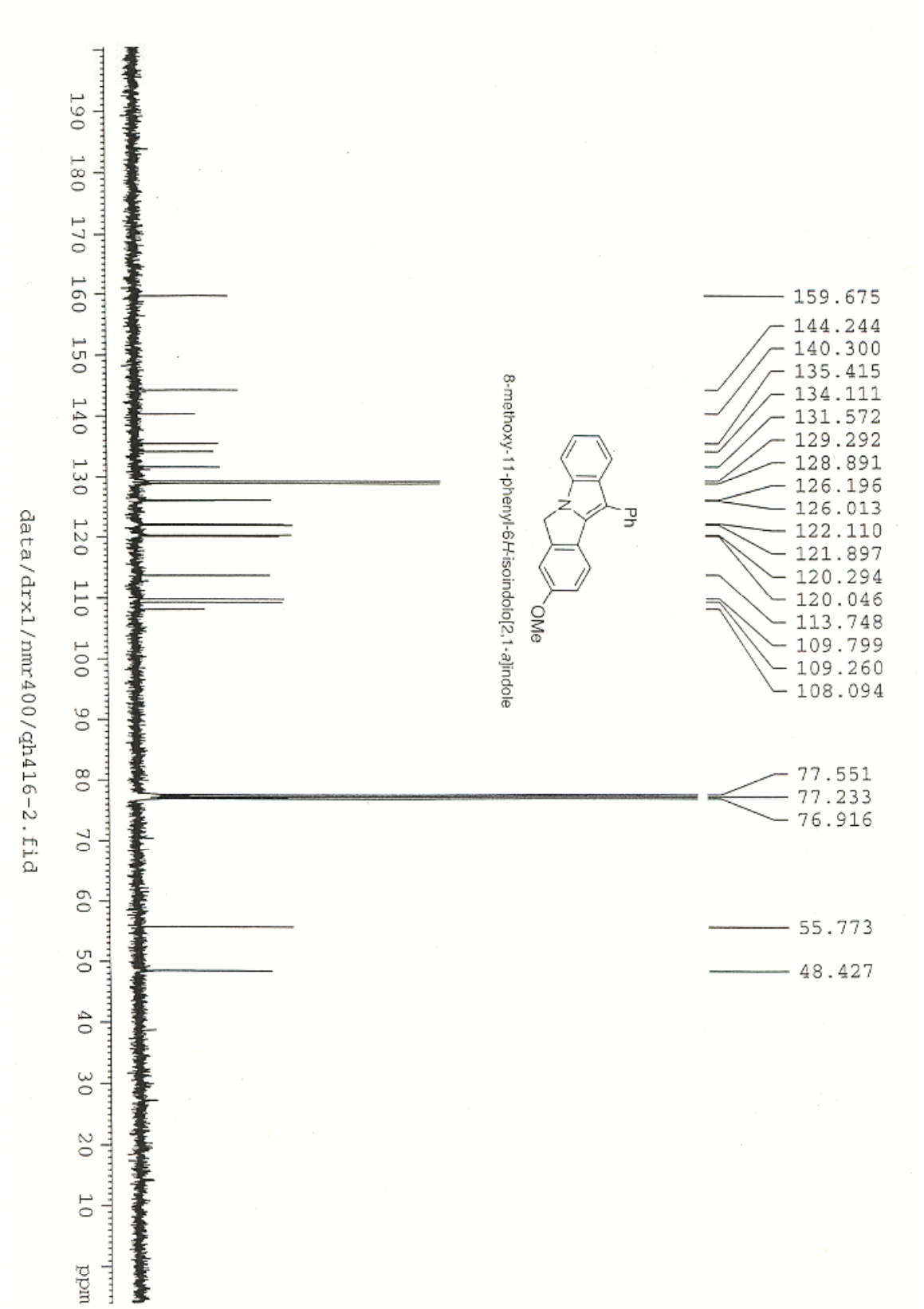

6-methylbenzo[e]acephenanthrylene
H
Me
138.863
138.226
137.451
137.221
135.282
134.092
132.357
130.804
130.232
128.983
128.252
127.603
127.004
126.787
123.215
122.756
121.309
121.254
121.180
119.204
77.402
77.085
76.767
21.886
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

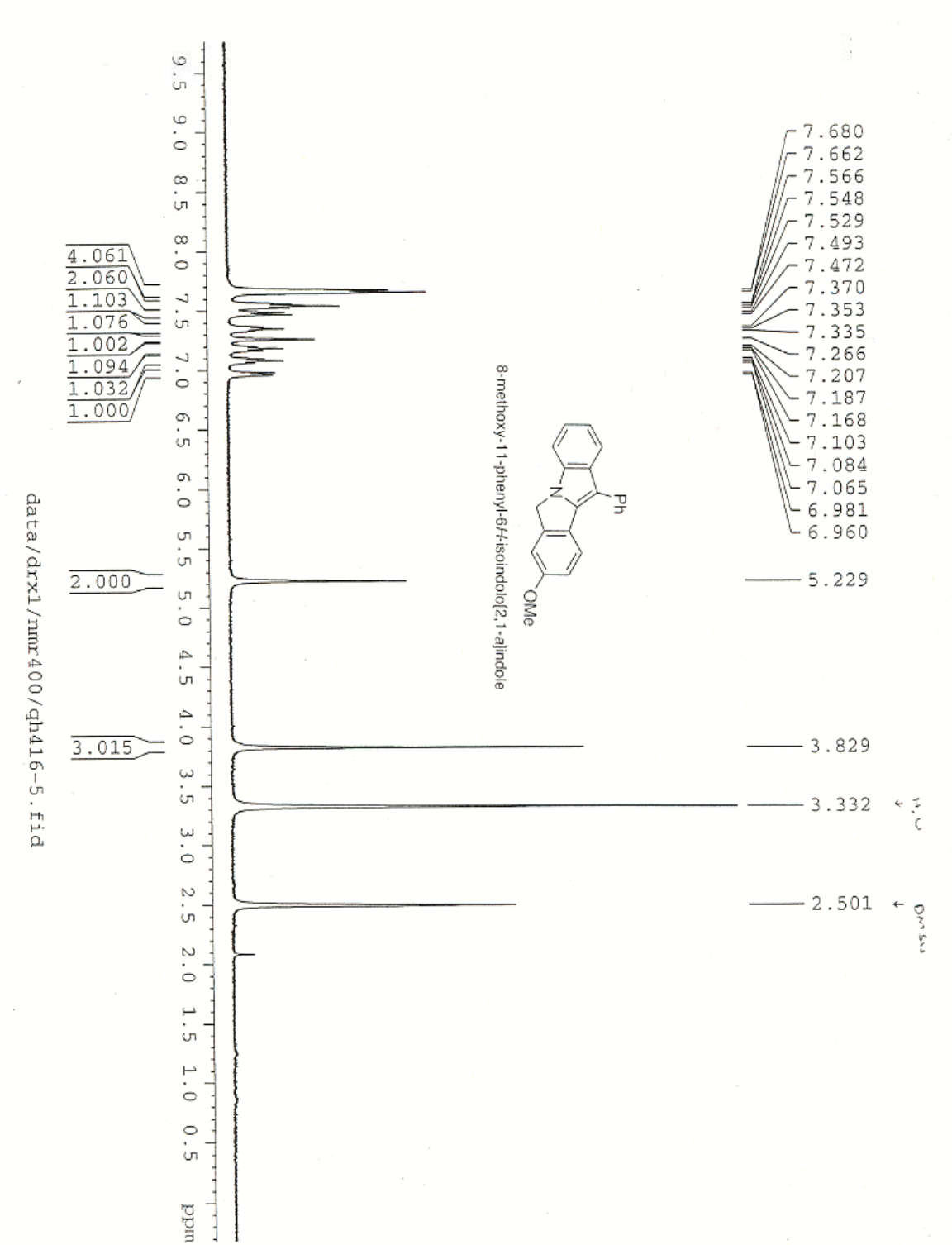
0.951
0.921
1.005
7.176
0.980
0.931
0.942
3.100
9
8
7
6
5
4
3
2
1
0
ppm
7.945
7.902
7.898
7.854
7.826
7.806
7.783
7.778
7.758
7.754
7.735
7.730
7.725
7.707
7.702
7.657
7.653
7.634
7.630
7.627
7.607
7.604
7.459
7.452
7.260
6.944
6.937
6.917
6.909
3.949
1.453
0.027
10-methoxydibenzo[e,fjacephenanthrylene
H
OMe

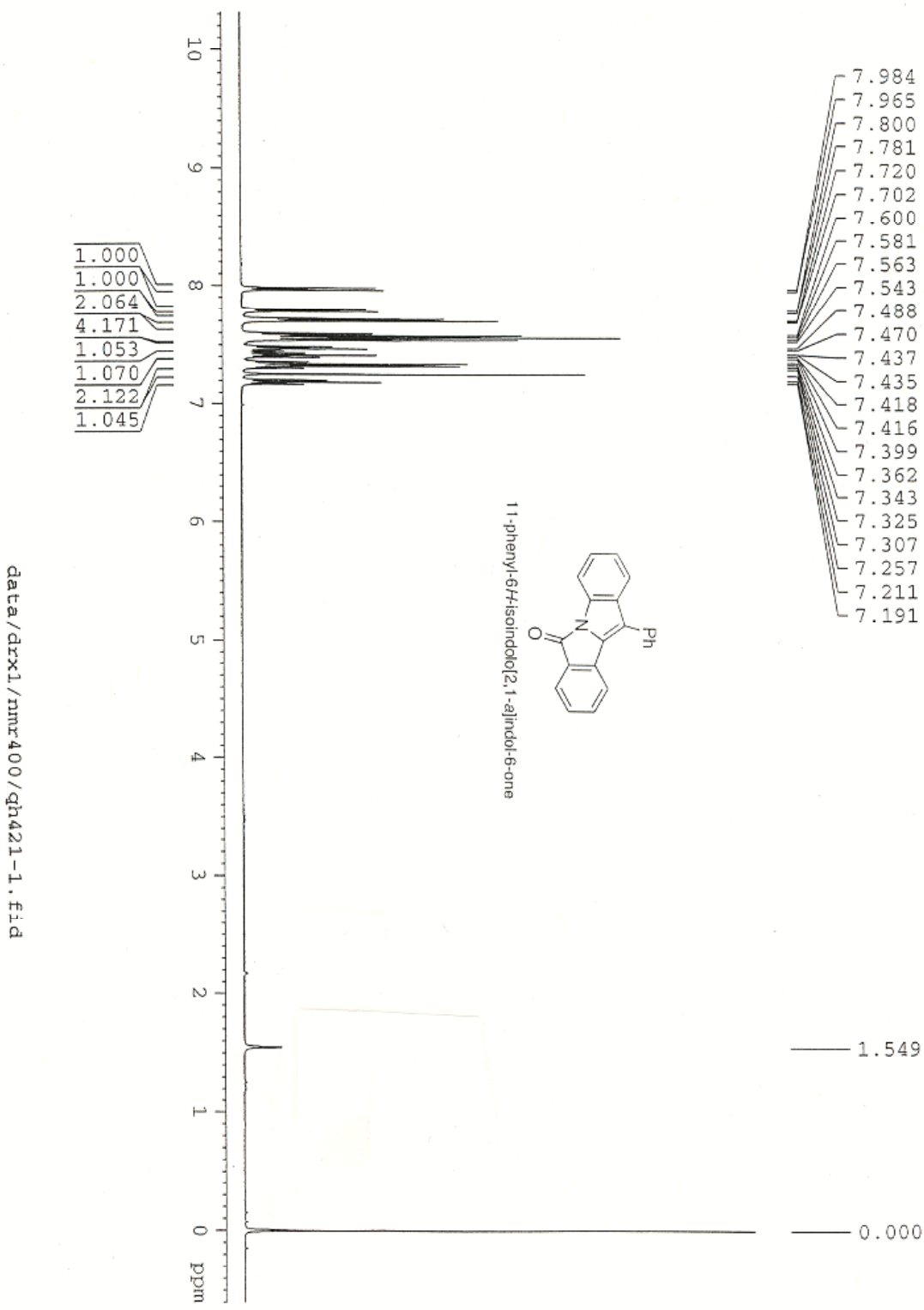

160.611
142.587
137.411
136.125
133.840
133.799
131.499
131.457
128.957
128.639
128.571
128.389
128.268
127.800
127.572
127.331
126.784
126.017
122.815
122.774
121.030
119.557
113.374
107.426
77.677
77.253
76.830
55.898
10-methoxydibenzo[e,/]acephenanthrylene
H
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

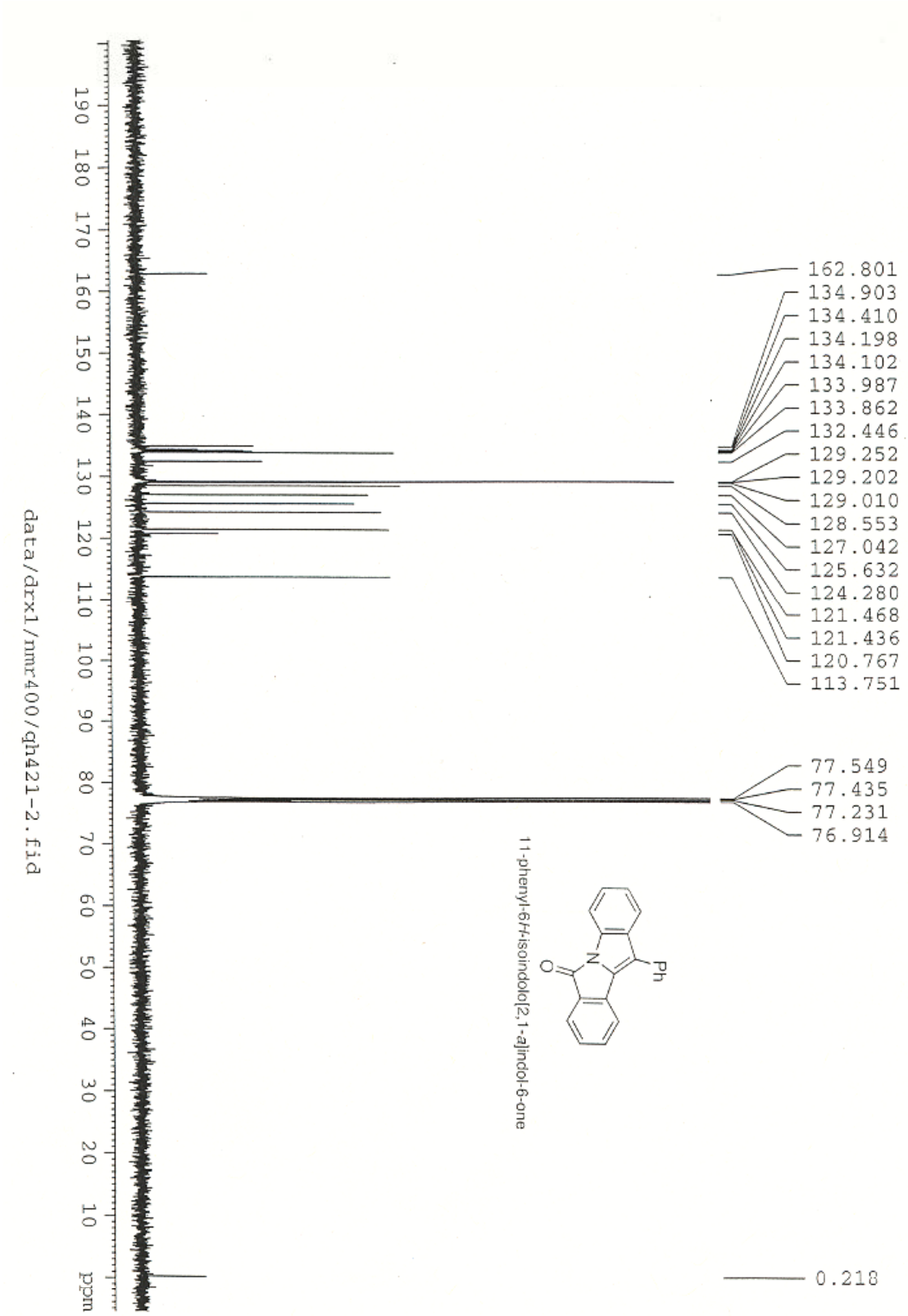

11-phenyl-6H-isoindolo[2,1-a]indole
Ph
N
7.759
7.746
7.738
7.699
7.681
7.649
7.641
7.629
7.582
7.563
7.543
7.533
7.512
7.394
7.379
7.360
7.245
7.227
7.208
7.130
7.111
7.093
5.268
3.340
2.500
2.083
1.113
3.047
1.054
3.152
3.063
1.029
1.003
2.000
10
9
8
7
6
5
4
3
2
1
0
ppm

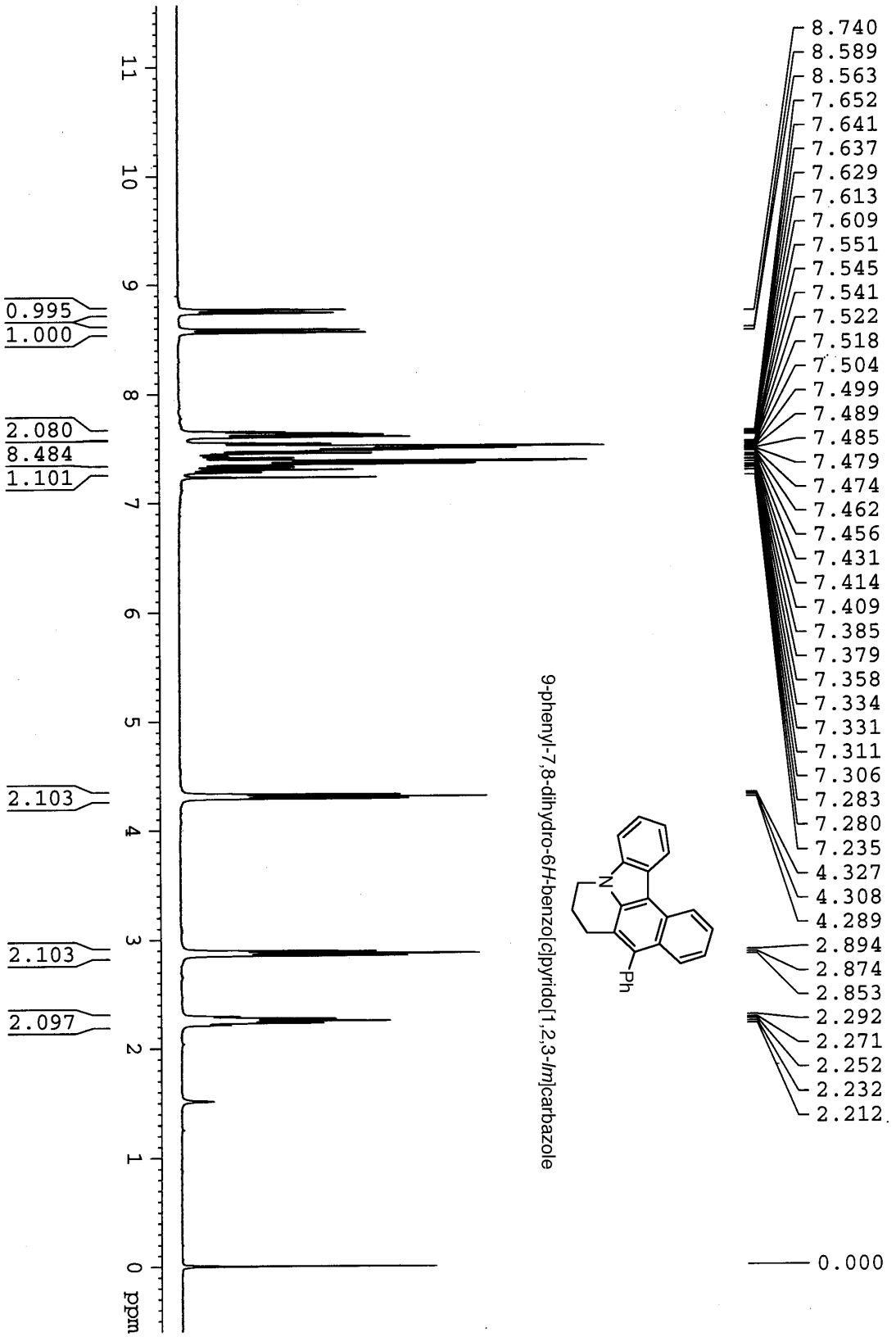

142.654
139.306
134.378
133.508
131.934
130.357
128.941
128.696
127.990
127.583
126.235
124.246
121.962
120.180
120.028
119.543
110.245
108.028
48.237
40.140
39.931
39.723
39.514
39.306
39.097
38.888
11-phenyl-6H-isoindolo[2,1-a]indole
N
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

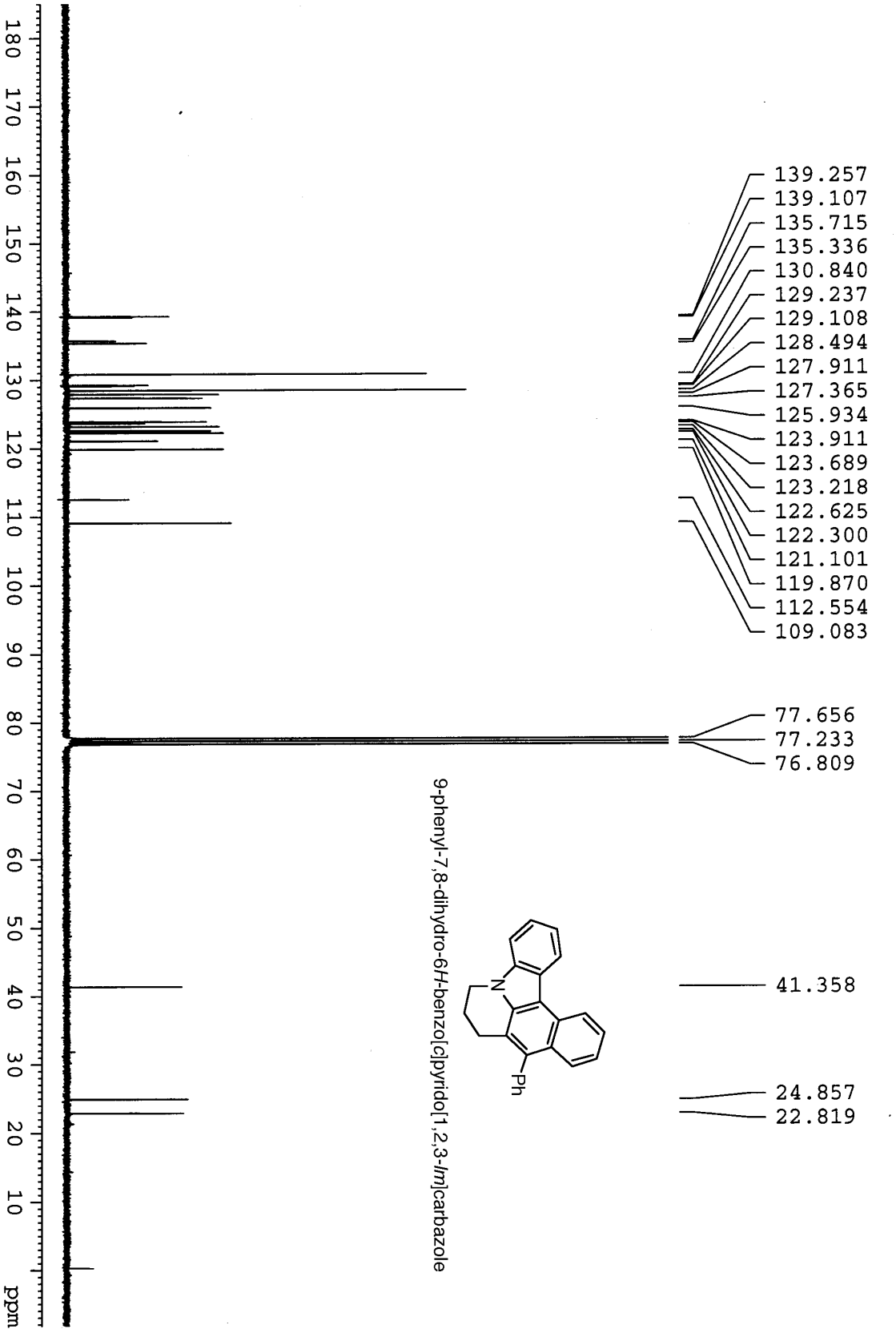

159.675
144.244
140.300
135.415
134.111
131.572
129.292
128.891
126.196
126.013
122.110
121.897
120.294
120.046
113.748
109.799
109.260
108.094
77.551
77.233
76.916
55.773
48.427
8-methoxy-11-phenyl-6H-isoindolo[2,1-a]indole
Ph
OMe
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
data/drx1/nmr400/qh416-2.fid

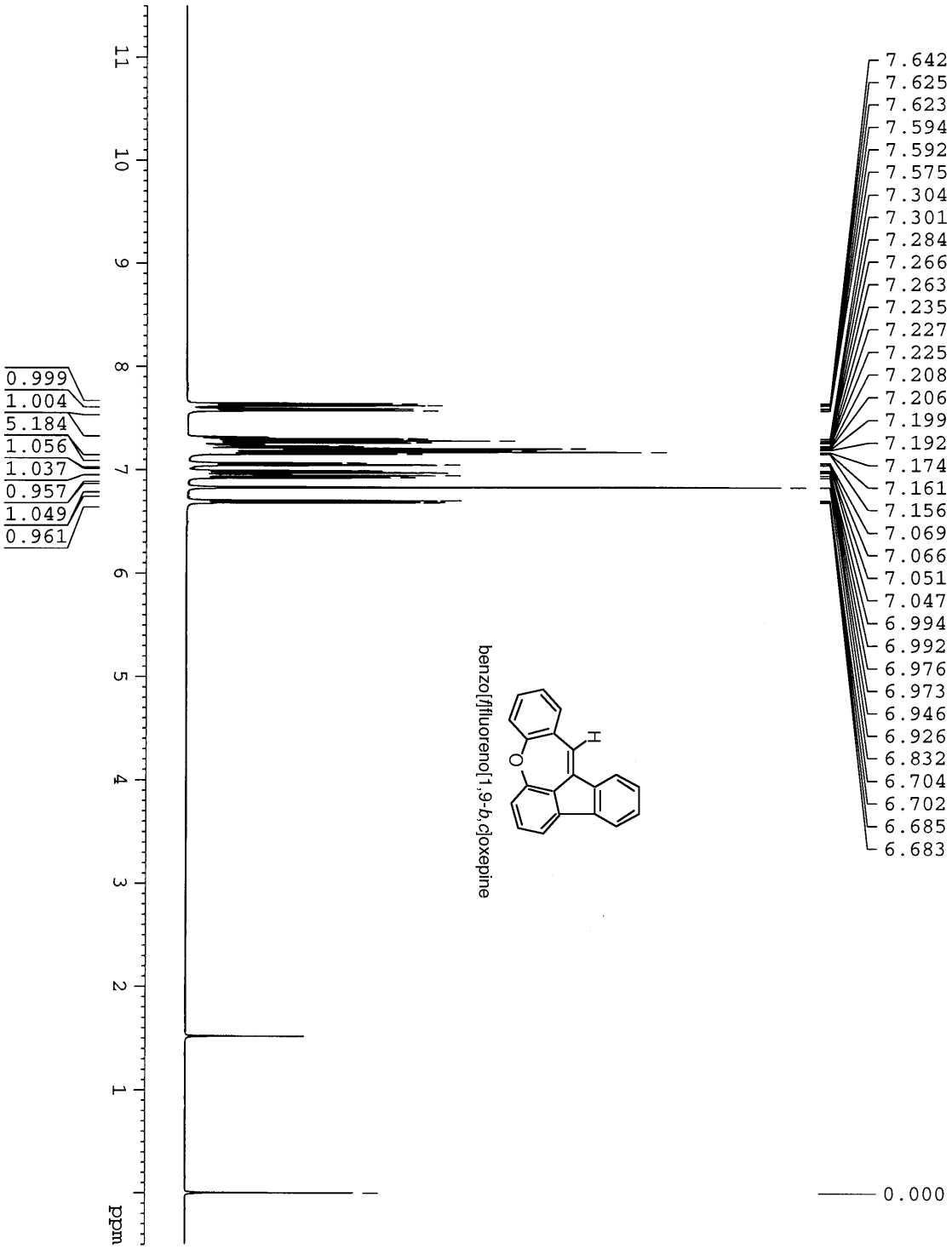

7.680
7.662
7.566
7.548
7.529
7.493
7.472
7.370
7.353
7.335
7.266
7.207
7.187
7.168
7.103
7.084
7.065
6.981
6.960
5.229
3.829
3.332
2.501
4.061
2.060
1.103
1.076
1.002
1.094
1.032
1.000
2.000
3.015
8-methoxy-11-phenyl-6H-isoindolo[2,1-a]indole
OMe
Ph
N
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
data/drx1/nmr400/qh416-5.fid

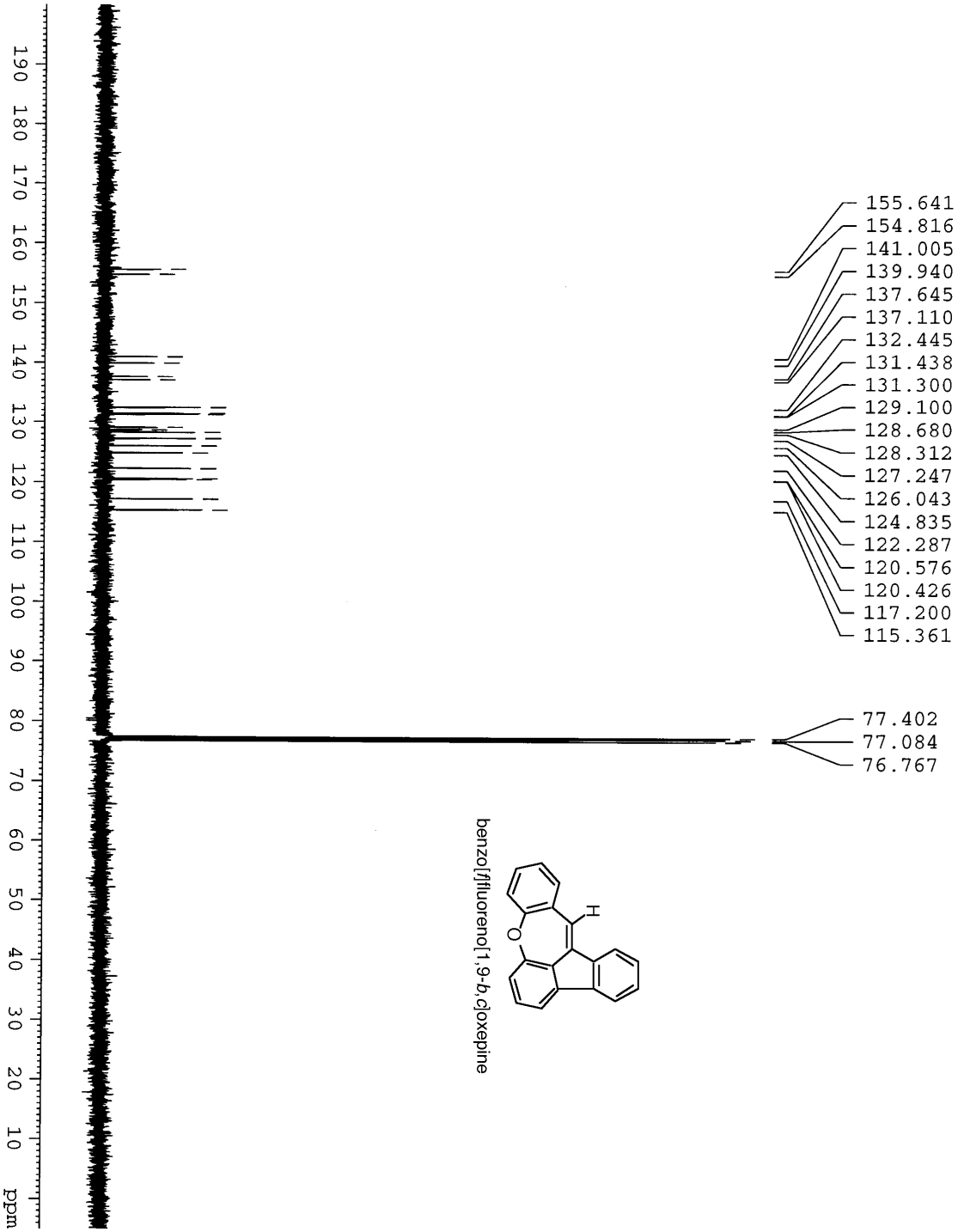

7.984
7.965
7.800
7.781
7.720
7.702
7.600
7.581
7.563
7.543
7.488
7.470
7.437
7.435
7.418
7.416
7.399
7.362
7.343
7.325
7.307
7.257
7.211
7.191
1.000
1.000
2.064
4.171
1.053
1.070
2.122
1.045
11-phenyl-6H-isoindolo[2,1-a]indol-6-one
Ph
N
O
1.549
0.000
ppm
data/drx1/nmr400/qh421-1.fid


162.801
134.903
134.410
134.198
134.102
133.987
133.862
132.446
129.252
129.202
129.010
128.553
127.042
125.632
124.280
121.468
121.436
120.767
113.751
77.549
77.435
77.231
76.914
0.218
11-phenyl-6H-isoindolo[2,1-a]indol-6-one
Ph
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
data/drxl/nmr400/qh421-2.fid


8.740
8.589
8.563
7.652
7.641
7.637
7.629
7.613
7.609
7.551
7.545
7.541
7.522
7.518
7.504
7.499
7.489
7.485
7.479
7.474
7.462
7.456
7.431
7.414
7.409
7.385
7.379
7.358
7.334
7.331
7.311
7.306
7.283
7.280
7.235
4.327
4.308
4.289
2.894
2.874
2.853
2.292
2.271
2.252
2.232
2.212
0.000
0.995
1.000
2.080
8.484
1.101
2.103
2.103
2.097
11
10
9
8
7
6
5
4
3
2
1
0
ppm
9-phenyl-7,8-dihydro-6H-benzo[c]pyrido[1,2,3-lm]carbazole
N
Ph


139.257
139.107
135.715
135.336
130.840
129.237
129.108
128.494
127.911
127.365
125.934
123.911
123.689
123.218
122.625
122.300
121.101
119.870
112.554
109.083
77.656
77.233
76.809
41.358
24.857
22.819
9-phenyl-7,8-dihydro-6H-benzo[c]pyrido[1,2,3-lm]carbazole
N
Ph
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.642
7.625
7.623
7.594
7.592
7.575
7.304
7.301
7.284
7.266
7.263
7.235
7.227
7.225
7.208
7.206
7.199
7.192
7.174
7.161
7.156
7.069
7.066
7.051
7.047
6.994
6.992
6.976
6.973
6.946
6.926
6.832
6.704
6.702
6.685
6.683
0.000
0.999
1.004
5.184
1.056
1.037
0.957
1.049
0.961
11
10
9
8
7
6
5
4
3
2
1
ppm
benzo[f]fluoreno[1,9-b,c]oxepine
O
H


155.641
154.816
141.005
139.940
137.645
137.110
132.445
131.438
131.300
129.100
128.680
128.312
127.247
126.043
124.835
122.287
120.576
120.426
117.200
115.361
77.402
77.084
76.767
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
benzo[f]fluoreno[1,9-b,c]oxepine
O
H