BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Facile approach to N,O,S-heteropentacycles via condensation of sterically crowded 3*H*-phenoxazin-3-one with *ortho*-substituted anilines

Eugeny Ivakhnenko, Vasily Malay, Pavel Knyazev, Nikita Merezhko, Nadezhda Makarova, Oleg Demidov, Gennady Borodkin, Andrey Starikov and Vladimir Minkin

Beilstein J. Org. Chem. **2024,** *20,* 336–345. doi:10.3762/bjoc.20.34

Synthetic details, compound characterization and additional analytic data, including copies of spectra and Cartesian coordinates

Table of Contents

1. Synthesis

General procedure for the synthesis of compounds **4a**–**h**

309 mg (1 mmol) of 6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**1**) powder was mixed with 3 mmol of the corresponding amine powder, placed in a round-bottom flask, and heated in a glycerin bath for 30 minutes at a temperature of 250°C, stirring the melt with a spatula every 10 minutes. For compounds **4a**–**h**, the reaction mixture was separated by column chromatography (Al_2O_3, eluent toluene), and the resulting fraction was recrystallized from diethyl ether.

6,8-Di-*tert*-butyl-2-(phenylamino)-3*H*-phenoxazin-3-one (**4a**)

Dark orange solid with m.p. 145-147 °C. Yield 80% (320 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3269 (N-H), 2950 (t-Bu), 2903 (t-Bu), 2863 (t-Bu), 1566 (C=O), 1519 (C=N), 1266 (C-N), 1239 (C-N), 1182 (C-O), 1159 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.63 (d, *J* = 2.1 Hz, 1H), 7.49 (d, *J* = 2.1 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 7.12 (t, *J* = 7.8 Hz, 1H), 7.00 (s, 1H), 6.52 (s, 1H), 1.51 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 180.08, 149.34, 147.85, 147.53, 141.98, 139.45, 138.94, 136.75, 134.20, 129.57, 125.33, 124.39, 123.81, 121.39, 103.20, 99.48, 35.17, 34.87, 31.40, 30.08. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{29}N_2O_2$ 401.2224; Found 401.2229.

6,8-Di-*tert*-butyl-2-((2-iodophenyl)amino)-3*H*-phenoxazin-3-one (**4b**)

Orange needles with m.p. 170-173 °C. Yield 82% (431 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3243 (N-H), 2961 (t-Bu), 2902 (t-Bu), 2868 (t-Bu), 1580 (C=O), 1529 (C=N), 1264 (C-N), 1208 (C-N), 1162 (C-O), 1150 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.9, 1H), 7.78 (s, 1H), 7.62 (d, *J* = 2.3 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 2.3 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 6.89 (t, *J* = 7.9 Hz, 1H), 6.85 (s, 1H), 6.55 (s, 1H), 1.51 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 179.74, 149.28, 147.88, 147.45, 141.81, 140.03, 139.86, 136.78, 134.08, 129.21, 126.17, 125.60, 123.83, 122.13, 103.33, 100.05, 93.67, 35.15, 34.84, 31.36, 30.03. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{28}IN_2O_2$ 527.1132; Found 527.1135.

6,8-Di-*tert*-butyl-2-((3-methoxyphenyl)amino)-3*H*-phenoxazin-3-one (**4c**)

Brown needles with m.p. 163-165 °C. Yield 87% (374 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3316 (N-H), 2952 (t-Bu), 2904 (t-Bu), 2868 (t-Bu), 1580 (C=O), 1523 (C=N), 1256 (C-

N), 1238 (C-N), 1174 (C-O), 1143 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.64 (d, *J* = 2.3 Hz, 1H), 7.49 (d, *J* = 2.3 Hz, 1H), 7.28 (t, *J* = 8.1 Hz, 1H), 7.03 (s, 1H), 6.94 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.85 (t, *J* = 2.2 Hz, 1H), 6.68 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.51 (s, 1H), 3.81 (s, 3H), 1.51 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 180.03, 160.69, 149.29, 147.83, 147.48, 141.80, 140.10, 139.41, 136.71, 134.18, 130.27, 125.34, 123.78, 113.63, 109.73, 107.41, 103.14, 99.94, 55.36, 35.13, 34.83, 31.36, 30.03. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{27}H_{31}N_2O_3$ 431.2329; Found 431.2339.

6,8-Di-*tert*-butyl-2-((3-chlorophenyl)amino)-3*H*-phenoxazin-3-one (**4d**)

Brown needles with m.p. 171-174 °C. Yield 79% (344 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3274 (N-H), 2952 (t-Bu), 2905 (t-Bu), 2866 (t-Bu), 1574 (C=O), 1519 (C=N), 1264 (C-N), 1239 (C-N), 1207 (C-O), 1157 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.65 (d, *J* = 2.3 Hz, 1H), 7.51 (d, *J* = 2.3 Hz, 1H), 7.34 (t, *J* = 2.0 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.20 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.09 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.01 (s, 1H), 6.52 (s, 1H), 1.51 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 179.69, 149.26, 147.97, 147.29, 141.27, 140.25, 139.46, 136.76, 135.25, 134.09, 130.49, 125.71, 124.21, 123.86, 120.86, 119.19, 103.15, 100.35, 35.12, 34.83, 31.32, 30.00. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{28}ClN_2O_2$ 435.1834; Found 435.1837.

6,8-Di-*tert*-butyl-2-((4-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4e**)

Dark orange powder with m.p. 180-183 °C. Yield 88% (391 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3250 (N-H), 2953 (t-Bu), 2904 (t-Bu), 2866 (t-Bu), 1637 (C=O), 1582 (C=N), 1574 (N=O), 1269 (C-N), 1240 (C-N), 1155 (C-O), 1111 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.6 Hz, 2H), 8.15 (s, 1H), 7.67 (s, 1H), 7.56 (s, 1H), 7.41 (d, *J* = 8.6 Hz, 2H), 7.22 (s, 1H), 6.55 (s, 1H), 1.51 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 179.39, 149.32, 148.37, 146.97, 145.27, 142.72, 139.75, 139.71, 136.98, 134.15, 126.73, 125.73, 124.24, 118.89, 103.50, 103.33, 35.22, 34.92, 31.35, 30.05. HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{26}H_{26}N_2O_2$ 444.1929; found 444.1933.

6,8-Di-*tert*-butyl-2-((2-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4f**)

Orange needles with m.p. 178-180 °C. Yield 93% (414 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3221 (N-H), 2997 (t-Bu), 2961 (t-Bu), 2869 (t-Bu), 1589 (C=O), 1572 (N=O), 1509 (C=N), 1262 (C-N), 1241 (C-N), 1153 (C-O), 1111 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.23 (d, *J* = 8.4, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 2.3 Hz, 1H), 7.62 (t, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 2.3 Hz, 1H), 7.13 (t, *J* = 8.4 Hz, 1H), 6.56 (s, 1H), 1.51 (s, 9H), 1.36 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 179.46, 149.08, 148.10, 147.26, 140.27, 139.73, 138.71, 136.94, 136.08, 135.04, 134.00, 126.91, 126.51, 124.15, 122.29, 120.56, 104.37, 103.76, 35.18, 34.86, 31.33, 30.01. HRMS (ESI) m/z: $[M-Na]^+$ calcd for $C_{26}H_{27}N_3NaO_4$ 468.1894; found 468.1887.

2-((4-Aminophenyl)amino)-6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**4g**)

Dark green powder with m.p. 156-158 °C. Yield 68% (282 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3410 (N-H), 3262 (N-H), 3208 (N-H), 2953 (t-Bu), 2902 (t-Bu), 2867 (t-Bu), 1637 (C=O), 1573 (C=N), 1265 (C-N), 1240 (C-N), 1182 (C-O), 1155 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 2.3 Hz, 1H), 7.49 (s, 1H), 7.45 (d, *J* = 2.3 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 2H), 6.74 (s, 1H), 6.69 (d, *J* = 8.6 Hz, 2H), 6.48 (s, 1H), 3.69 (s, 2H), 1.50 (s, 9H), 1.35 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 180.22, 149.42, 147.63, 147.44, 143.86, 143.14, 139.24, 136.60, 134.18, 129.63, 124.71, 123.87, 123.50, 115.82, 103.04, 97.89, 35.08, 34.78, 31.34, 30.01. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{30}N_3O_2$ 416.2342; Found 416.2333.

Methyl 4-((6,8-di-*tert*-butyl-3-oxo-3H-phenoxazin-2-yl)amino)benzoate (**4h**)

Red brown powder with m.p. 174-177 °C. Yield 81% (371 mg). Rf ~ 0.70. IR (neat, cm^{-1}): 3264 (N-H), 2950 (t-Bu), 2902 (t-Bu), 2869 (t-Bu), 1713 (C=O), 1580 (C=O), 1531 (C=N), 1280 (C-N), 1265 (C-N), 1182 (C-O), 1156 (C-O), 1111 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.7 Hz, 2H), 7.95 (s, 1H), 7.66 (d, *J* = 2.3 Hz, 1H), 7.52 (d, *J* = 2.3 Hz, 1H), 7.36 (d, *J* = 8.7 Hz, 2H), 7.16 (s, 1H), 6.53 (s, 1H), 3.90 (s, 3H), 1.51 (s, 9H), 1.37 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 179.68, 166.39, 149.26, 148.06, 147.26, 143.35, 140.44, 139.55, 136.82, 134.14, 131.31, 126.00, 125.01, 124.02, 119.22, 103.23, 101.81, 51.98, 35.15, 34.86, 31.34, 30.02. HRMS (ESI) m/z: $[M-H]^-$ Calcd. for $C_{28}H_{29}N_2O_4$ 457.2133; Found 457.2131.

General procedure for the synthesis of compounds **5a**–**c**

309 mg (1 mmol) of 6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**1**) powder was mixed with 3 mmol of the corresponding *o*-phenylenediamine powder, placed in a round-bottom flask, and heated in a glycerin bath for 30 minutes at a temperature of 250 °C, stirring the melt with a spatula every 10 minutes. The reaction mixture was separated by column chromatography (Al_2O_3, eluent dichloromethane and isopropanol, *l* = 40 cm, *d* = 15 mm). The resulting fraction was recrystallized from isopropanol.

2,4-Di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**)

Red powder with m.p. > 260 °C. Yield 93% (369 mg). Rf ~ 0.45. IR (neat, cm^{-1}): 3264 (N-H), 3087 (t-Bu), 2949 (t-Bu), 2902 (t-Bu), 2865 (t-Bu), 1618 (C=N), 1593 (C=N), 1235 (C-N), 1211 (C-N), 1179 (C-N), 1139 (C-O), 1113 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (s 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 2H) 7.26 (s, 1H), 6.85 (s, 1H), 6.74 (d, *J* = 2.4 Hz, 1H), 6.42 (d, *J* = 2.4 Hz, 1H), 1.46 (s, 9H), 1.13 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.97, 146.46, 144.11, 143.58, 142.19, 141.67, 138.09, 136.94, 136.53, 129.10, 128.98, 128.02, 127.80, 127.28, 117.04, 109.69, 109.64, 102.35, 34.93, 34.38, 31.20, 29.98. ^{15}N NMR (60 MHz, $CDCl_3$) δ 314.85, 296.56, 92.79. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{28}N_3O$ 398.2227; Found 398.2218.

2,4-Di-*tert*-butyl-9,10-dimethyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5b**)

Red powder with m.p. > 260 °C. Yield 69% (293 mg). Rf ~ 0.48. IR (neat, cm^{-1}): 3245 (N-H), 2952 (t-Bu), 2867 (t-Bu), 1615 (C=N), 1592 (C=N), 1238 (C-N), 1212 (C-N), 1168 (C-N), 1110 (C-O), 1032 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.65 (s, 1H), 7.25 (s, 1H), 6.79 (s, 1H), 6.74 (d, *J* = 1.9 Hz, 1H), 6.42 (d, *J* = 1.9 Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H), 1.46 (s, 9H), 1.15 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.36, 146.23, 143.42, 142.80, 141.43, 140.93, 140.04, 138.90, 138.12, 136.90, 135.83, 127.63, 127.61, 126.71, 116.87, 109.79, 109.48, 102.86, 34.91, 34.36, 31.20, 29.95, 20.35, 20.26. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{28}H_{32}N_3O$ 426.2540; Found 426.2534.

Ethyl 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine-10-carboxylate (**5c**)

Violet powder with m.p. > 260 °C. Yield 63% (295 mg). Rf ~ 0.54. IR (neat, cm^{-1}): 3330 (N-H), 2952 (t-Bu), 2902 (t-Bu), 2866 (t-Bu), 1701 (C=O), 1646 (C=N), 1592 (C=N), 1261 (C-N), 1233 (C-N), 1196 (C-N), 1174 (C-O), 1088 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) (600 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.11 (d, *J* = 8.8 Hz, 1H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.65 – 7.45 (m, 2H), 6.84 (s, 1H), 6.80 (s, 1H), 6.46 (s, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.44 (s, 9H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.18 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.08, 150.01, 146.82, 145.07, 144.82, 143.39, 141.54, 138.03, 137.21, 136.64, 131.11, 130.57, 129.04, 127.32, 126.97, 117.49, 109.79, 109.55, 102.72, 61.35, 34.96,

34.49, 31.25, 29.96, 14.25. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{29}H_{31}N_3O_3$ 470.2438; Found 470.2444.

General procedure for the synthesis of compounds **6a**,**b**

100 mg (0.25 mmol) of 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-b]phenoxazine (**5a**) in 15 ml of acetone was added to 40 mg (1 mmol) of sodium hydroxide. After the solution took on an intense blue color, 0.1 ml (1.6 mmol) methyl iodide was added for **6a** or 254 mg (1 mmol) 1-iodonanane for **6b**. This was stirred at room temperature for 4 hours. The reaction mixture was filtered, and the mother liquor was recrystallized from acetone.

2,4-Di-*tert*-butyl-14-methyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6a**)

Red powder with m.p. 232-235 °C. Yield 97% (398 mg). Rf ~ 0.80. IR (neat, cm^{-1}): 2950 (t-Bu), 2924 (t-Bu), 2860 (t-Bu), 1579 (C=N), 1563 (C=N), 1342 (C-N), 1301 (C-N), 1236 (C-N), 1222 (C-N), 1128 (C-O), 1070 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 8.1 Hz, 1H), 7.34 (s, 1H), 6.94 (s, 1H), 6.93 (d, *J* = 2.1, 1H), 6.71 (d, *J* = 2.1, 1H), 3.37 (s, 3H), 1.46 (s, 9H), 1.31 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.45, 146.30, 144.48, 143.17, 142.70, 141.90, 140.04, 139.19, 136.92, 130.84, 129.07, 128.90, 128.49, 128.31, 117.35, 109.17, 108.55, 103.54, 34.97, 34.83, 32.45, 31.45, 30.03. ^{15}N NMR (60 MHz, $CDCl_3$) δ 311.64, 305.64, 83.69. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{27}H_{30}N_3O$ 412.2383; Found 412.2389.

2,4-Di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**)

Red powder with m.p. 154-157 °C. Yield 91% (476 mg). Rf ~ 0.73. IR (neat, cm^{-1}): 2948 (t-Bu), 2927 (t-Bu), 2863 (t-Bu), 1582 (C=N), 1568 (C=N), 1346 (C-N), 1299 (C-N), 1231 (C-N), 1220 (C-N), 1128 (C-O), 1083 (C-O). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 8.1 Hz, 1H), 7.59 (t, *J* = 8.1 Hz, 1H), 7.29 (s, 1H), 6.91 (s, 1H), 6.90 (d, *J* = 2.1, 1H), 6.70 (d, *J* = 2.1, 1H), 3.79 (t, *J* = 8.3, 2H), 1.85 (qvin, *J* = 7.6, 2H), 1.53 (m, 2H), 1.50 (m, 2H), 1.45 (s, 9H), 1.42 (m 2H), 1.35 (m, 2H), 1.32 (m, 2H), 1.31 (s, 9H), 1.28 (m, 2H), 0.89 (t, *J* = 7.0, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.87, 146.04, 144.76, 143.29, 142.74, 141.90, 139.44, 137.50, 136.82, 129.19, 129.02, 128.89, 128.34, 128.17, 117.25, 108.99, 108.41, 102.76, 45.61, 34.99, 34.77, 31.83, 31.41, 29.99, 29.54, 29.39, 29.21, 26.97, 24.74, 22.65, 14.07. ^{15}N NMR (60 MHz, $CDCl_3$) δ 310.36, 303.85, 96.38. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{35}H_{46}N_3O$ 524.3635; Found 524.3640.

General procedure for the synthesis of compounds **10a**,**b**

309 mg (1 mmol) of 6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**1**) powder was mixed with 3 mmol of the corresponding *o*-aminophenol powder, placed in a round-bottom flask, and heated in a glycerin bath for 30 minutes at a temperature of 250 °C, stirring the melt with a spatula every 10 minutes. The structure of the obtained products **10a**,**b** corresponded to those previously described [20].

2,4-Di-*tert*-butylbenzo[5,6][1,4]oxazino[2,3-*b*]phenoxazine (**10a**)

The reaction mixture was separated by column chromatography on Al_2O_3, eluent toluene, Rf ~ 0.70. Red powder. Yield 55% (219 mg). M.p. 228–229 °C.

2,4-Di-*tert*-butyl-9-nitrobenzo[5,6][1,4]oxazino[2,3-*b*]phenoxazine (**10b**)

The reaction mixture was separated by column chromatography on Al_2O_3, eluent toluene, Rf ~ 0.75. Red powder. Yield 65% (288 mg). M.p. > 260 °C.

Synthesis of 2,4-di-*tert*-butylbenzo[5,6][1,4]oxazino[2,3-*b*]phenothiazine (**10c**)

309 mg (1 mmol) of 6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**1**) powder was mixed with 375 mg (3 mmol) of 2-aminobenzenethiol powder, placed in a round-bottom flask, and heated in a glycerin bath for 30 minutes at a temperature of 220 °C, stirring the melt with a spatula every 10 minutes. The reaction mixture was separated by column chromatography (Al_2O_3, eluent dichloromethane, *l* = 40 cm, *d* = 15 mm). Violet powder with m.p. 211-215 °C. Yield 36% (149 mg). Rf ~ 0.80. IR (neat, cm^{-1}): 2943 (t-Bu), 2867 (t-Bu), 1569 (C=N), 1516 (C=N), 1333 (C-N), 1310 (C-N), 1267 (C-N), 1241 (C-N), 1141 (C-O), 1122 (C-O), 569 (C-S). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 2.3 Hz, 1H), 7.24 (d, *J* = 2.3 Hz, 1H), 7.23 – 7.19 (m, 1H), 7.13 – 7.07 (m, 2H), 6.76 (s, 1H), 6.57 (s, 1H), 1.43 (s, 9H), 1.30 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.00, 149.15, 148.33, 147.26, 141.26, 141.17, 136.09, 135.39, 132.07, 131.27, 127.73, 127.70, 124.78, 124.71, 123.75, 121.77, 118.80, 108.44, 34.90, 34.62, 31.30, 29.89. HRMS (ESI) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{27}N_2OS$ 415.1839; Found 415.1845.

Table S1: Compounds and reaction conditions (yield, temperature, solvent, time).

compound	yield %, *T*, 30 min	yield %, 144 °C, *o*-xylene, 120 min	yield %, 144 °C, *o*-xylene, *p*-TSA, 120 min	yield %, 110 °C, toluene, 120 min	yield %, 110 °C, toluene, p-TSA, 120 min	yield %, 82 °C, isopropanol, 120 min	yield %, 82 °C, isopropanol, CF_3CO_2H, 120 min
5a	93, 250 °C	—	—	—	—	—	—
5b	69, 250 °C	—	—	—	—	—	—
5c	63, 250 °C	—	—	—	—	—	—
10a	55, 250 °C	—	11	—	7	3	5
10b	65, 250 °C	—	10	—	9	2	7
10c	36, 220 °C	—	8	—	6	—	—

2. XRD study. Molecular geometries. Crystallographic parameters.

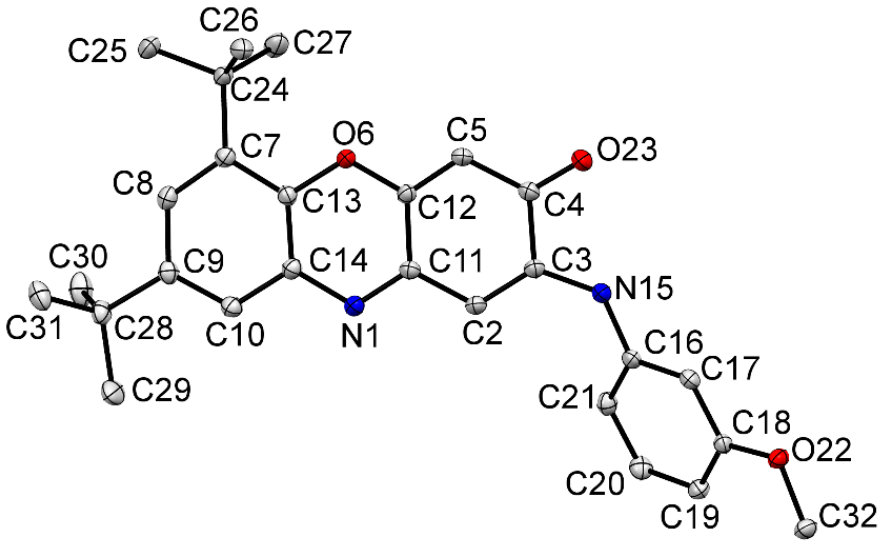


Figure S1: Molecular structure of 6,8-di-*tert*-butyl-2-((3-methoxyphenyl)amino)-3*H*-phenoxazin-3-one (**4c**).

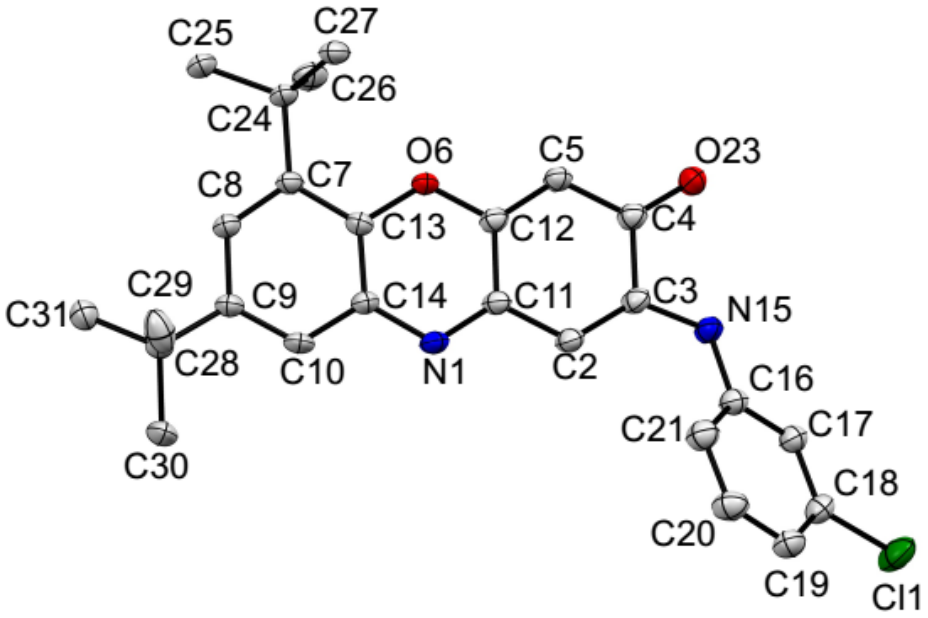


Figure S2: Molecular structure of 6,8-di-*tert*-butyl-2-((3-chlorophenyl)amino)-3*H*-phenoxazin-3-one (**4d**).

Table S2: Crystal data and structure refinement for **4c**,**d**,**f**.

parameter	**4c**	**4d**	**4f**
CCDC Number	2292841	2292840	2292847
Empirical formula	$C_{27}H_{30}N_2O_3$	$C_{26}H_{27}ClN_2O_2$	$C_{26}H_{27}N_3O_4$
Formula weight	430.53	434.94	445.50
Temperature/K	100.01(10)	100.01(13)	100.00(10)
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$	$P2_1/n$	$P2_12_12_1$
a/Å	16.93490(10)	18.2211(3)	7.06800(10)
b/Å	15.04900(10)	18.0052(3)	16.9207(2)
c/Å	19.7911(2)	21.6236(4)	18.5820(2)
α/°	90	90	90
β/°	114.6770(10)	105.415(2)	90
γ/°	90	90	90
Volume/Å^3	4583.20(7)	6838.9(2)	2222.32(5)
Z	8	12	4
ρ_{calc}g/cm^3	1.248	1.267	1.332
μ/mm^{-1}	0.647	1.676	0.736
F(000)	1840.0	2760.0	944.0
Crystal size/mm^3	0.262 × 0.179 × 0.092	0.298 × 0.096 × 0.069	0.344 × 0.124 × 0.112
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.66 to 152.642	7.03 to 152.84	7.066 to 152.536
Index ranges	-21 ≤ h ≤ 21, -15 ≤ k ≤ 18, -24 ≤ l ≤ 24	-22 ≤ h ≤ 14, -22 ≤ k ≤ 22, -23 ≤ l ≤ 27	-8 ≤ h ≤ 8, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23
Reflections collected	50573	60385	13501
Independent reflections	9568 [R_{int} = 0.0290, R_{sigma} = 0.0198]	14134 [R_{int} = 0.0376, R_{sigma} = 0.0291]	4476 [R_{int} = 0.0183, R_{sigma} = 0.0203]
Data/restraints/parameters	9568/0/599	14134/99/887	4476/0/353
Goodness-of-fit on F^2	1.036	1.069	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0358, wR_2 = 0.0908	R_1 = 0.0676, wR_2 = 0.1835	R_1 = 0.0286, wR_2 = 0.0774
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.0949	R_1 = 0.0805, wR_2 = 0.1947	R_1 = 0.0298, wR_2 = 0.0786
Largest diff. peak/hole / e Å^{-3}	0.23/-0.27	1.09/-0.70	0.26/-0.19
	-	-	0.65(6)

Table S3: X-ray-determined bond lengths and valence angles of **4c**. Bond lengths, Å.

O6-C12	1.3526(12)	C21-C20	1.3874(15)
O6-C13	1.3779(12)	C9-C28	1.5374(14)
O22-C18	1.3676(12)	C24-C26	1.5393(15)
O22-C32	1.4291(12)	C24-C25	1.5356(14)
O23-C4	1.2370(13)	C24-C27	1.5420(14)
N15-C3	1.3584(13)	C20-C19	1.3946(14)
N15-C16	1.4027(13)	C28-C30	1.5332(15)
N1-C11	1.3117(13)	C28-C31	1.5361(15)
N1-C14	1.3852(13)	C28-C29	1.5312(16)
C18-C17	1.3895(14)	C10-C14	1.4032(14)
C18-C19	1.3935(14)	C10-C9	1.3803(14)
C3-C2	1.3651(14)	C5-C4	1.4361(14)
C3-C4	1.5048(13)	C14-C13	1.3982(14)
C2-C11	1.4295(14)	C7-C8	1.3953(14)
C11-C12	1.4619(13)	C7-C13	1.4058(14)
C16-C17	1.3929(14)	C7-C24	1.5414(13)
C16-C21	1.3996(14)	C8-C9	1.4133(14)
C12-C5	1.3494(14)		

Valence angles of **4c**, deg.

C12-O6-C13	119.82(8)	C10-C9-C8	118.01(9)
C18-O22-C32	116.75(8)	C10-C9-C28	121.86(9)
C3-N15-C16	130.41(9)	C8-C9-C28	120.11(9)
C11-N1-C14	117.53(9)	C7-C24-C27	109.08(9)
O22-C18-C17	115.22(9)	C26-C24-C7	111.53(8)
O22-C18-C19	124.35(9)	C26-C24-C27	109.95(9)
C17-C18-C19	120.41(9)	C25-C24-C7	111.17(9)
N15-C3-C2	128.42(9)	C25-C24-C26	107.54(9)
N15-C3-C4	111.18(9)	C25-C24-C27	107.48(9)
C2-C3-C4	120.39(9)	C21-C20-C19	121.85(9)
C3-C2-C11	120.77(9)	C18-C19-C20	118.53(9)
N1-C11-C2	119.97(9)	C30-C28-C9	109.11(9)
N1-C11-C12	121.94(9)	C30-C28-C31	109.24(9)
C2-C11-C12	118.08(9)	C31-C28-C9	110.00(8)
C17-C16-N15	116.78(9)	C29-C28-C9	111.73(9)
C17-C16-C21	119.78(9)	C29-C28-C30	108.91(10)
C21-C16-N15	123.41(9)	C29-C28-C31	107.81(10)
O6-C12-C11	118.93(9)	C8-C7-C24	123.13(9)
C5-C12-O6	118.44(9)	C13-C7-C24	121.77(9)
C5-C12-C11	122.62(9)	C7-C8-C9	124.16(9)
C9-C10-C14	120.63(10)	O23-C4-C3	119.02(9)
C12-C5-C4	120.15(9)	O23-C4-C5	123.27(9)
N1-C14-C10	118.16(9)	C5-C4-C3	117.70(9)
N1-C14-C13	122.72(9)	O6-C13-C14	118.85(9)
C13-C14-C10	119.12(9)	O6-C13-C7	118.24(9)
C18-C17-C16	120.47(9)	C14-C13-C7	122.92(9)
C8-C7-C13	115.09(9)	C20-C21-C16	118.94(9)

Table S4: X-ray-determined bond lengths and valence angles of **4d**. Bond lengths, Å.

Cl1-C18	1.734(3)	C17-C16	1.389(3)
O6-C12	1.353(3)	C17-C18	1.386(4)
O6-C13	1.378(3)	C28-C31	1.535(4)
O23-C4	1.233(3)	C28-C29	1.519(4)
N1-C11	1.311(3)	C28-C30	1.536(4)
N1-C14	1.387(3)	C28-C34	1.501(19)
N15-C3	1.365(3)	C28-C33	1.559(18)
N15-C16	1.400(3)	C28-C32	1.546(19)
C12-C11	1.465(3)	C18-C19	1.379(4)
C12-C5	1.345(3)	C19-C20	1.385(4)
C13-C14	1.395(3)	C21-C20	1.387(4)
C13-C7	1.403(3)	C5-C4	1.442(3)
C11-C2	1.423(3)	C4-C3	1.496(3)
C9-C8	1.407(3)	C7-C24	1.537(3)
C9-C10	1.381(3)	C2-C3	1.362(3)
C9-C28	1.531(3)	C24-C27	1.540(3)
C14-C10	1.403(3)	C24-C25	1.526(3)
C7-C8	1.391(3)	C24-C26	1.542(3)

Valence angles of **4d**, deg.

C12-O6-C13	119.85(18)	N15-C16-C21	122.0(2)
C11-N1-C14	117.3(2)	C17-C16-N15	118.5(2)
C3-N15-C16	127.3(2)	C17-C16-C21	119.4(2)
O6-C12-C11	118.9(2)	C9-C28-C31	111.4(2)
C5-C12-O6	118.9(2)	C9-C28-C30	111.1(2)
C5-C12-C11	122.2(2)	C9-C28-C33	113.5(12)
O6-C13-C14	118.8(2)	C9-C28-C32	109.6(19)
O6-C13-C7	118.7(2)	C31-C28-C30	107.6(2)
C14-C13-C7	122.5(2)	C29-C28-C9	107.9(2)
N1-C11-C12	122.0(2)	C29-C28-C31	108.4(3)
N1-C11-C2	119.6(2)	C29-C28-C30	110.5(3)
C2-C11-C12	118.4(2)	C34-C28-C9	105.1(18)
C8-C9-C28	120.5(2)	C34-C28-C33	112(2)
C10-C9-C8	117.8(2)	C34-C28-C32	117(3)
C10-C9-C28	121.5(2)	C32-C28-C33	99(2)
N1-C14-C13	123.0(2)	C17-C18-Cl1	119.5(2)
N1-C14-C10	117.8(2)	C19-C18-Cl1	117.7(2)
C13-C14-C10	119.1(2)	C19-C18-C17	122.8(2)
C13-C7-C24	122.6(2)	C18-C19-C20	117.7(2)
C8-C7-C13	115.6(2)	C20-C21-C16	119.8(2)
C8-C7-C24	121.7(2)	C19-C20-C21	121.4(2)
C7-C8-C9	124.2(2)	C2-C3-N15	126.9(2)
C3-C2-C11	121.1(2)	C2-C3-C4	119.9(2)
C12-C5-C4	119.9(2)	C9-C10-C14	120.7(2)

O23-C4-C5	122.2(2)	C18-C17-C16	118.9(2)
O23-C4-C3	119.5(2)	C25-C24-C7	112.14(19)
C5-C4-C3	118.4(2)	C25-C24-C27	107.4(2)
C7-C24-C27	108.97(19)	C25-C24-C26	107.7(2)
C7-C24-C26	110.2(2)	N15-C3-C4	113.2(2)
C27-C24-C26	110.4(2)		

Table S5: X-ray-determined bond lengths and valence angles of **4f**. Bond lengths, Å.

O6-C12	1.3539(17)	C13-C7	1.405(2)
O6-C13	1.3813(17)	C13-C14	1.3997(19)
O23-C4	1.2314(19)	C11-C2	1.4374(19)
O31-N22	1.236(2)	C8-C7	1.392(2)
O32-N22	1.2247(19)	C7-C24	1.5444(18)
N15-C3	1.3765(19)	C3-C2	1.359(2)
N15-C16	1.383(2)	C24-C23	1.538(2)
N1-C11	1.3061(19)	C24-C26	1.534(2)
N1-C14	1.3836(18)	C24-C25	1.536(2)
N22-C17	1.458(2)	C16-C21	1.406(2)
C10-C9	1.377(2)	C16-C17	1.420(2)
C10-C14	1.398(2)	C21-C20	1.386(2)
C9-C8	1.413(2)	C17-C18	1.393(2)
C9-C27	1.5304(19)	C30-C27	1.534(2)
C12-C5	1.350(2)	C27-C28	1.537(2)
C12-C11	1.4578(19)	C27-C29	1.536(2)
C4-C5	1.444(2)	C18-C19	1.375(3)
C4-C3	1.508(2)	C20-C19	1.386(3)

Valence angles of **4f**, deg.

C12-O6-C13	119.84(11)	N1-C14-C13	122.55(13)
C3-N15-C16	131.12(14)	C10-C14-C13	119.70(13)
C11-N1-C14	117.55(12)	N15-C3-C4	110.51(13)
O31-N22-C17	119.13(13)	C2-C3-N15	130.07(14)
O32-N22-O31	122.25(15)	C2-C3-C4	119.41(13)
O32-N22-C17	118.61(15)	C23-C24-C7	111.32(12)
C9-C10-C14	120.63(13)	C26-C24-C7	109.04(13)
C10-C9-C8	117.66(13)	C26-C24-C23	107.78(13)
C10-C9-C27	122.71(13)	C26-C24-C25	109.95(13)
C8-C9-C27	119.63(13)	C25-C24-C7	111.14(13)
O6-C12-C11	118.59(13)	C25-C24-C23	107.55(13)
C5-C12-O6	119.59(13)	N15-C16-C21	122.45(14)
C5-C12-C11	121.81(13)	N15-C16-C17	121.93(15)
O23-C4-C5	122.33(14)	C21-C16-C17	115.62(14)
O23-C4-C3	119.34(13)	C3-C2-C11	121.33(14)
C5-C4-C3	118.32(13)	C20-C21-C16	121.71(16)

O6-C13-C7	118.88(12)	C16-C17-N22	122.19(14)
O6-C13-C14	118.84(13)	C18-C17-N22	115.78(14)
C14-C13-C7	122.28(13)	C18-C17-C16	122.02(16)
C12-C5-C4	120.37(14)	C9-C27-C30	109.12(13)
N1-C11-C12	122.56(13)	C9-C27-C28	111.62(12)
N1-C11-C2	118.74(13)	C9-C27-C29	109.58(13)
C2-C11-C12	118.70(13)	C30-C27-C28	108.36(14)
C7-C8-C9	124.54(13)	C30-C27-C29	109.79(13)
C13-C7-C24	122.65(13)	C29-C27-C28	108.35(14)
C8-C7-C13	115.17(13)	C19-C18-C17	120.32(16)
C8-C7-C24	122.17(13)	C21-C20-C19	121.10(17)
N1-C14-C10	117.75(13)	C18-C19-C20	119.06(16)

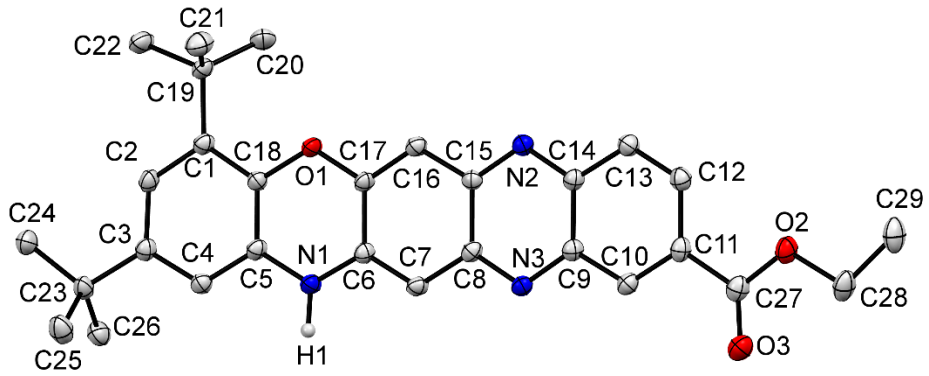


Figure S3: Molecular structure of ethyl 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine-10-carboxylate (**5c**).

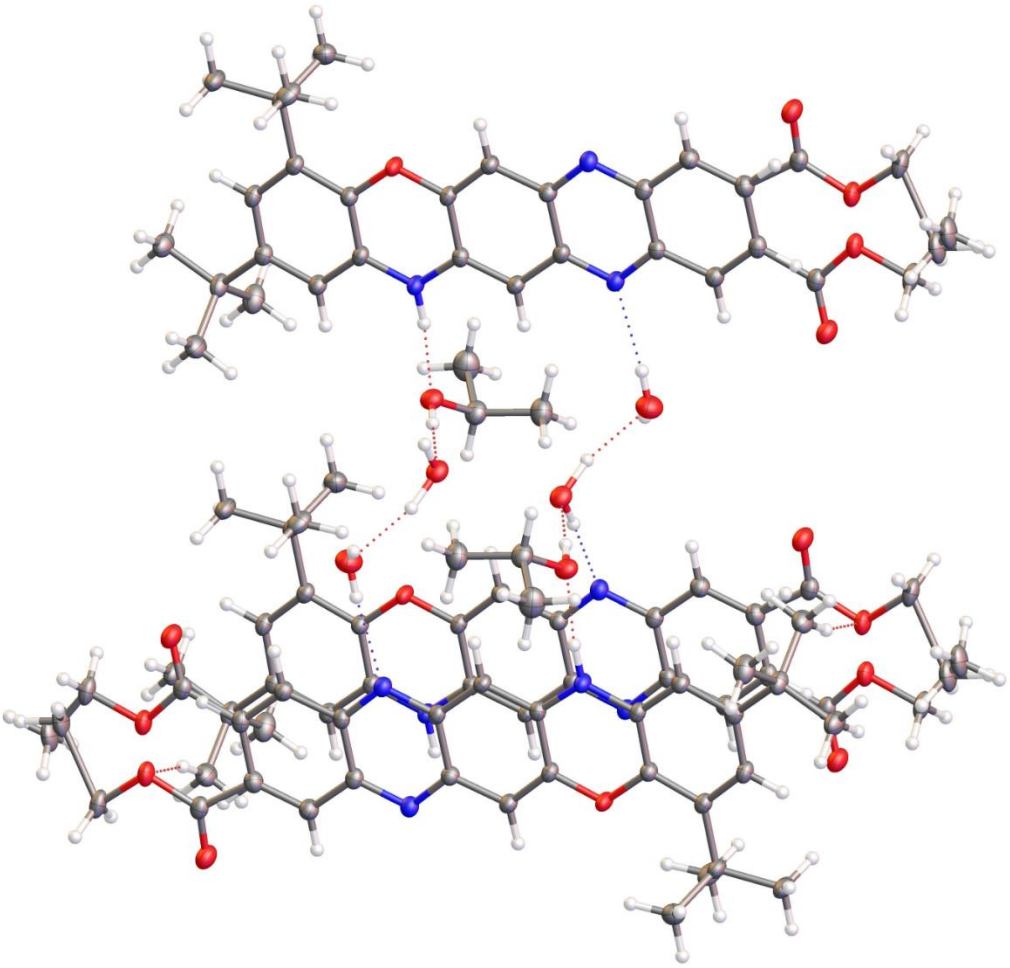


Figure S4: Molecular structure of the solvate of **5c**.

Table S6: Crystal data and structure refinement for **5c**.

parameter	**5c**
CCDC Number	2308520
Empirical formula	$C_{32}H_{43}N_3O_6$
Formula weight	565.69
Temperature/K	100.15
Crystal system	triclinic
Space group	P-1
a/Å	8.8807(3)
b/Å	9.8727(3)
c/Å	17.3935(8)
α/°	99.624(3)
β/°	91.935(3)
γ/°	97.449(3)
Volume/Å^3	1488.46(9)
Z	2
ρ_{calc}g/cm^3	1.262
μ/mm^{-1}	0.705
F(000)	608.0
Crystal size/mm^3	0.24 × 0.09 × 0.04
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/°	9.172 to 152.93
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -21 ≤ l ≤ 21
Reflections collected	11566
Independent reflections	11566 [R_{int} = ?, R_{sigma} = 0.0372]
Data/restraints/parameters	11566/2/414
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0529, wR_2 = 0.1599
Final R indexes [all data]	R_1 = 0.0693, wR_2 = 0.1735
Largest diff. peak/hole / e $Å^{-3}$	0.56/-0.25

Table S7: X-ray-determined bond lengths and valence angles of **5c**. Bond lengths, Å.

O4-C30	1.442(3)	C19-C22	1.540(3)
O1-C18	1.396(2)	C19-C21	1.533(3)
O1-C17	1.369(2)	C17-C16	1.358(3)
O2-C27	1.348(3)	C1-C2	1.407(3)
O2-C28	1.452(3)	C4-C3	1.393(3)
O3-C27	1.203(3)	C13-C14	1.419(3)
N2-C15	1.336(3)	C13-C12	1.369(3)
N2-C14	1.362(3)	C9-C14	1.426(3)
N3-C9	1.355(3)	C9-C10	1.421(3)
N3-C8	1.337(3)	C30-C32	1.511(3)
N1-C5	1.391(3)	C30-C31	1.516(3)
N1-C6	1.365(3)	C7-C8	1.417(3)
C5-C18	1.394(3)	C12-C11	1.428(3)
C5-C4	1.391(3)	C2-C3	1.392(3)
C18-C1	1.399(3)	C10-C11	1.371(3)
C15-C16	1.432(3)	C3-C23	1.534(3)
C15-C8	1.453(3)	C11-C27	1.490(3)
C6-C17	1.441(3)	C23-C26	1.540(3)
C6-C7	1.373(3)	C23-C25	1.532(3)
C19-C1	1.530(3)	C23-C24	1.527(3)
C19-C20	1.532(3)	C29-C28	1.513(4)

Valence angles of **5c**, deg.

C17-O1-C18	120.09(16)	N3-C9-C10	118.81(19)
C27-O2-C28	114.47(19)	C10-C9-C14	118.94(19)
C15-N2-C14	116.85(18)	N2-C14-C13	119.52(19)
C8-N3-C9	116.60(18)	N2-C14-C9	121.13(18)
C6-N1-C5	122.15(18)	C13-C14-C9	119.35(18)
N1-C5-C18	119.54(18)	O4-C30-C32	106.9(2)
C4-C5-N1	120.06(18)	O4-C30-C31	111.52(19)
C4-C5-C18	120.36(18)	C32-C30-C31	112.3(2)
O1-C18-C1	118.51(18)	C6-C7-C8	120.86(18)
C5-C18-O1	119.85(17)	C13-C12-C11	120.36(19)
C5-C18-C1	121.63(18)	C3-C2-C1	124.22(18)
N2-C15-C16	119.55(18)	C11-C10-C9	120.7(2)
N2-C15-C8	121.71(18)	C4-C3-C23	119.68(19)
C16 C15 C8	118.75(18)	C2-C3-C4	117.61(19)
N1-C6-C17	117.66(18)	C2-C3-C23	122.68(18)

N1-C6-C7	122.79(19)	C12-C11-C27	122.30(19)
C7-C6-C17	119.54(19)	C10-C11-C12	120.16(19)
C1-C19-C20	111.73(17)	C10-C11-C27	117.5(2)
C1-C19-C22	110.66(17)	C17-C16-C15	119.95(18)
C1-C19-C21	109.39(17)	N3-C8-C15	121.45(18)
C20-C19-C22	106.85(18)	N3-C8-C7	119.40(18)
C20-C19-C21	110.27(19)	C7-C8-C15	119.15(17)
C21-C19-C22	107.85(18)	C3-C23-C26	109.57(17)
O1-C17-C6	120.69(18)	C25-C23-C3	109.10(17)
C16-C17-O1	117.59(18)	C25-C23-C26	109.11(19)
C16-C17-C6	121.72(18)	C24-C23-C3	112.71(18)
C18-C1-C19	122.96(18)	C24-C23-C26	108.11(18)
C18-C1-C2	115.73(18)	C24-C23-C25	108.17(19)
C2-C1-C19	121.25(17)	O2-C27-C11	112.50(19)
C5-C4-C3	120.37(19)	O3-C27-O2	123.5(2)
C12-C13-C14	120.5(2)	O3-C27-C11	124.0(2)
N3-C9-C14	122.24(18)	O2-C28-C29	107.5(2)

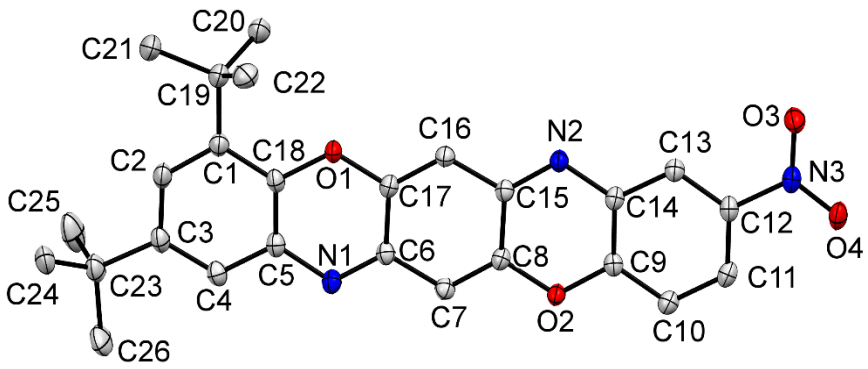


Figure S5: Molecular structure of 2,4-di-*tert*-butyl-9-nitrobenzo[5,6][1,4]oxazino[2,3-*b*]phenoxazine **10b**.

Table S8: Crystal data and structure refinement for **10b**.

parameter	**10b**
CCDC Number	2292848
Empirical formula	$C_{26}H_{25}N_3O_4$
Formula weight	443.49
Temperature/K	100.00(13)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.1069(4)
b/Å	6.68620(10)
c/Å	18.7628(3)
α/°	90
β/°	96.324(2)
γ/°	90
Volume/Å^3	2257.72(7)
Z	4
ρ_{calc}g/cm^3	1.305
μ/mm^{-1}	0.724

F(000)	936.0
Crystal size/mm^3	0.339 × 0.182 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.486 to 152.62
Index ranges	-22 ≤ h ≤ 22, -8 ≤ k ≤ 8, -19 ≤ l ≤ 23
Reflections collected	23366
Independent reflections	4719 [R_{int} = 0.0332, R_{sigma} = 0.0229]
Data/restraints/parameters	4719/0/304
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0464, wR_2 = 0.1296
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.1375
Largest diff. peak/hole / e Å^{-3}	0.29/-0.28

Table S9: X-ray-determined bond lengths and valence angles of **10b**. Bond lengths, Å.

O1-C18	1.3832(15)	C18-C1	1.4014(18)
O1-C17	1.3648(16)	C9-C14	1.4033(19)
O2-C8	1.3681(15)	C17-C16	1.3526(18)
O2-C9	1.3695(15)	C14-C13	1.3977(17)
O3-N3	1.2293(16)	C13-C12	1.3851(18)
O4-N3	1.2306(16)	C5-C4	1.4022(18)
N2-C15	1.3119(17)	C12-C11	1.389(2)
N2-C14	1.3926(16)	C1-C2	1.3982(19)
N1-C6	1.3107(17)	C1-C19	1.534(2)
N1-C5	1.3909(17)	C2-C3	1.405(2)
N3-C12	1.4650(16)	C4-C3	1.381(2)
C8-C15	1.4595(18)	C3-C23	1.5367(18)
C8-C7	1.3491(18)	C19-C22	1.539(2)
C6-C17	1.4549(19)	C19-C20	1.538(2)
C6-C7	1.4349(18)	C19-C21	1.5370(19)
C15-C16	1.4331(18)	C23-C24	1.536(2)
C10-C9	1.3881(18)	C23-C26	1.526(2)
C10-C11	1.3848(18)	C23-C25	1.534(2)
C18-C5	1.400(2)		

Valence angles of **10b**, deg.

C17-O1-C18	119.12(11)	C8-C7-C6	119.98(12)
C8-O2-C9	118.37(10)	N1-C5-C18	122.58(12)
C15-N2-C14	116.19(11)	N1-C5-C4	118.23(12)
C6-N1-C5	116.96(12)	C18-C5-C4	119.19(12)
O3-N3-O4	123.65(11)	C13-C12-N3	118.70(12)
O3-N3-C12	118.56(11)	C13-C12-C11	123.03(12)
O4-N3-C12	117.79(12)	C11-C12-N3	118.26(11)
O2-C8-C15	118.82(11)	C17-C16-C15	120.18(12)
C7-C8-O2	118.02(12)	C10-C11-C12	118.57(12)
C7-C8-C15	123.16(12)	C18-C1-C19	122.29(12)
N1-C6-C17	123.07(12)	C2-C1-C18	115.45(13)
N1-C6-C7	119.98(12)	C2-C1-C19	122.26(12)
C7-C6-C17	116.95(11)	C1-C2-C3	124.09(13)
N2-C15-C8	123.57(12)	C3-C4-C5	120.69(13)

N2-C15-C16	119.75(12)	C2-C3-C23	119.49(13)
C16-C15-C8	116.67(11)	C4-C3-C2	118.01(12)
C11-C10-C9	118.99(12)	C4-C3-C23	122.49(14)
O1-C18-C5	119.42(11)	C1-C19-C22	110.17(12)
O1-C18-C1	118.05(12)	C1-C19-C20	110.08(12)
C5-C18-C1	122.52(12)	C1-C19-C21	111.42(12)
O2-C9-C10	116.70(12)	C20-C19-C22	110.34(12)
O2-C9-C14	120.59(11)	C21-C19-C22	107.30(13)
C10-C9-C14	122.70(12)	C21-C19-C20	107.46(12)
O1-C17-C6	118.76(11)	C24-C23-C3	110.25(13)
C16-C17-O1	118.28(12)	C26-C23-C3	111.54(12)
C16-C17-C6	122.96(12)	C26-C23-C24	107.80(13)
N2-C14-C9	122.40(11)	C26-C23-C25	109.64(15)
N2-C14-C13	119.77(12)	C25-C23-C3	108.43(12)
C13-C14-C9	117.82(12)	C25-C23-C24	109.16(14)
C12-C13-C14	118.86(12)		

3. DFT study

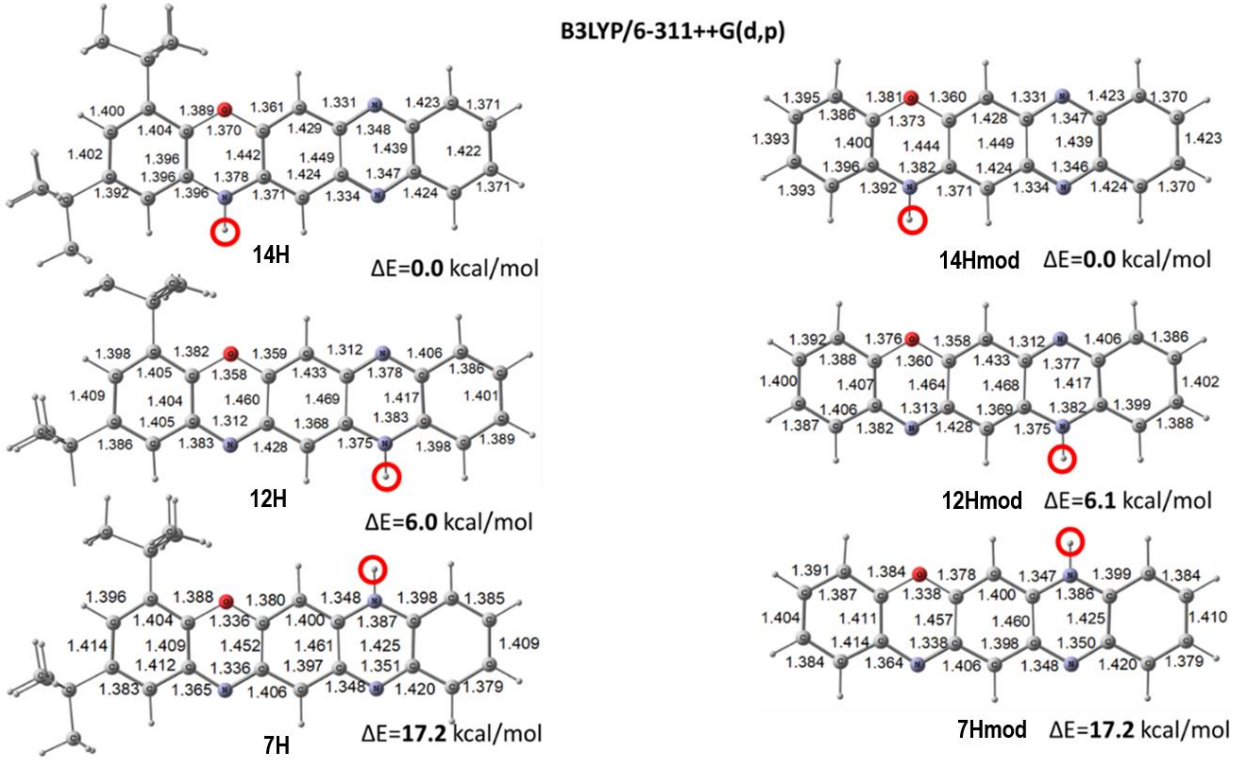


Figure S6: Geometry and relative stability of the tautomeric forms of quinoxaline[2,3-*b*]phenoxazine and corresponding 6,8-di-*tert*-butyl derivatives calculated using the DFT B3LYP/6-311++G(d,p) method.

4. UV–vis and luminescence spectra

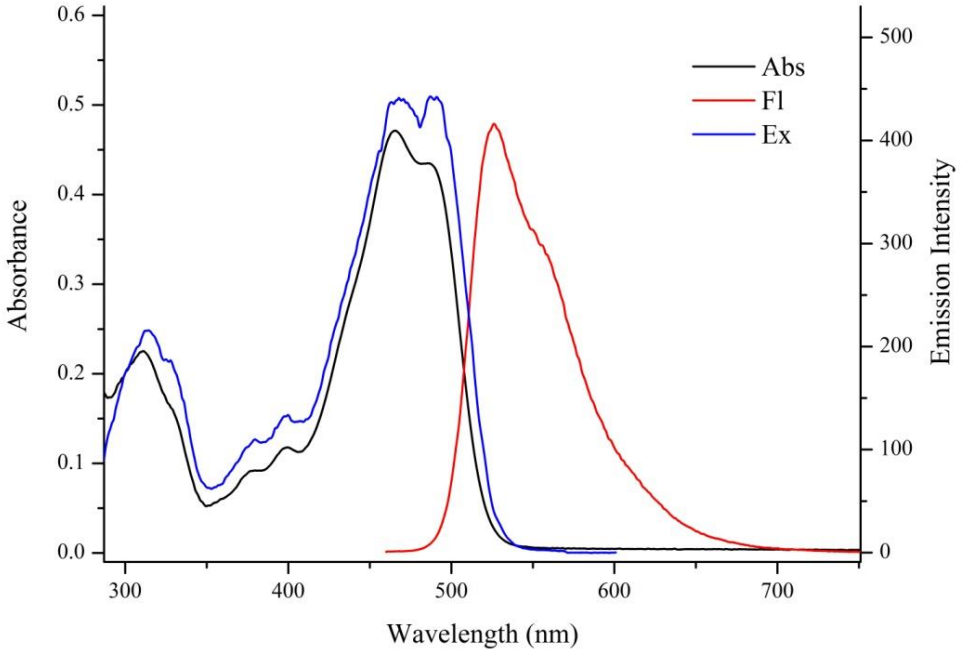


Figure S7: UV–vis, fluorescence emission (λ_{ex} = 365 nm), and fluorescence excitation (λ_{obs} = 610 nm) spectra of compound **5a** (toluene, $c = 2 \cdot 10^{-5}$ M, l = 1 cm, T = 293 K).

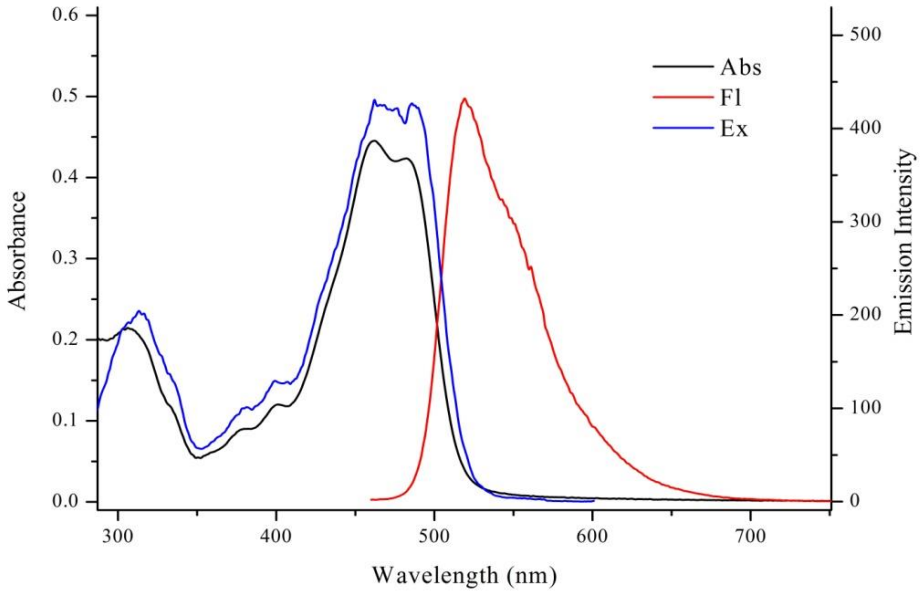


Figure S8: UV–vis, fluorescence emission (λ_{ex} = 365 nm) and fluorescence excitation (λ_{obs} = 610 nm) spectra of compound **5b** (toluene, $c = 2 \cdot 10^{-5}$ M, l = 1 cm, T = 293 K).

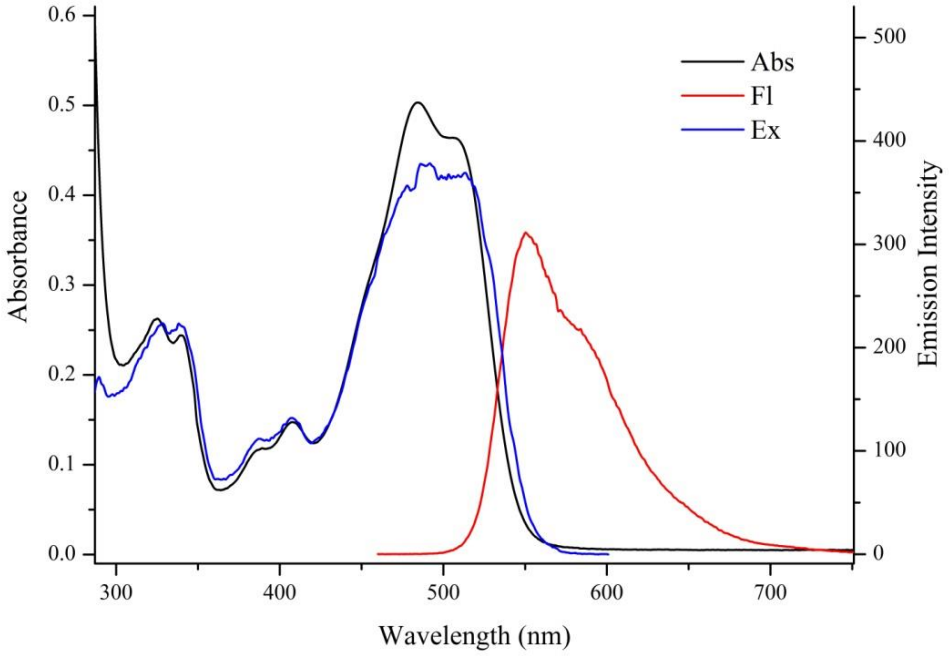


Figure S9: UV–vis, fluorescence emission (λ_{ex} = 365 nm) and fluorescence excitation (λ_{obs} = 630 nm) spectra of compound **5c** (toluene, $c = 2 \cdot 10^{-5}$ M, l = 1 cm, T = 293 K).

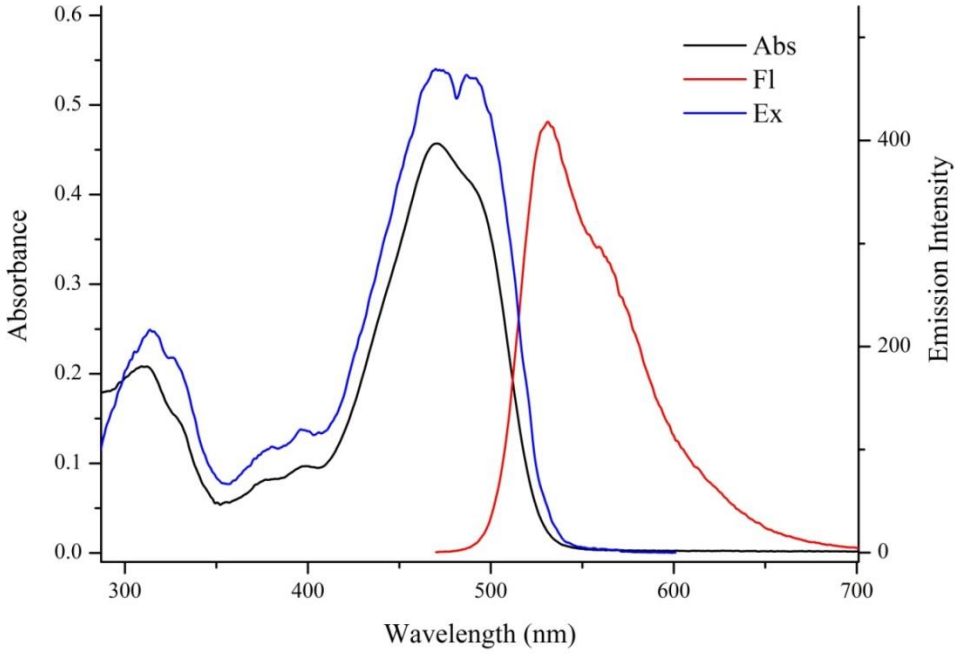


Figure S10: UV–vis, fluorescence emission (λ_{ex} = 365 nm) and fluorescence excitation (λ_{obs} = 610 nm) spectra of compound **6a** (toluene, $c = 2 \cdot 10^{-5}$ M, l = 1 cm, T = 293 K).

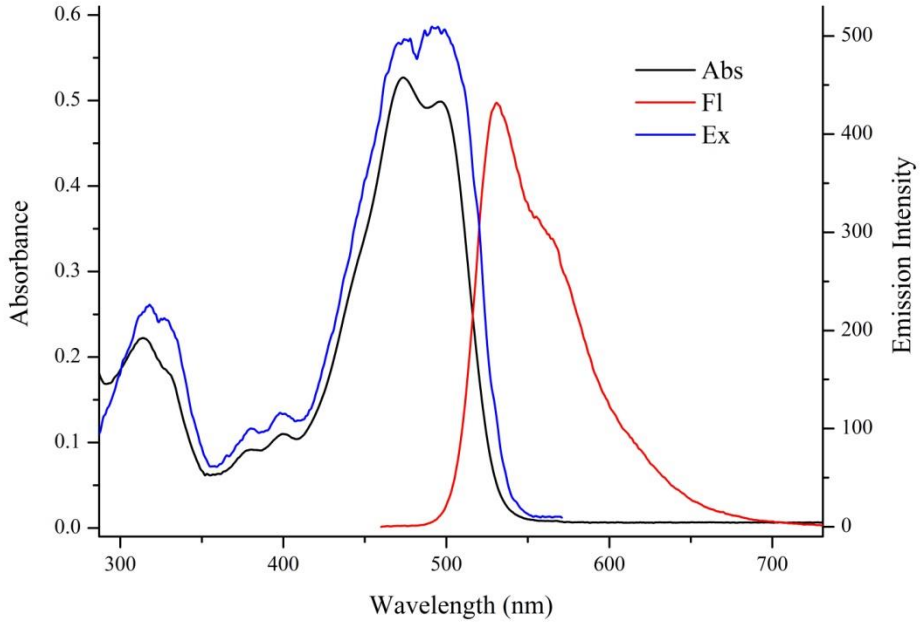


Figure S11: UV–vis, fluorescence emission (λ_{ex} = 365 nm) and fluorescence excitation (λ_{obs} = 610 nm) spectra of compound **6b** (toluene, $c = 2 \cdot 10^{-5}$ M, l = 1 cm, T = 293).

5. Cyclic voltammetry

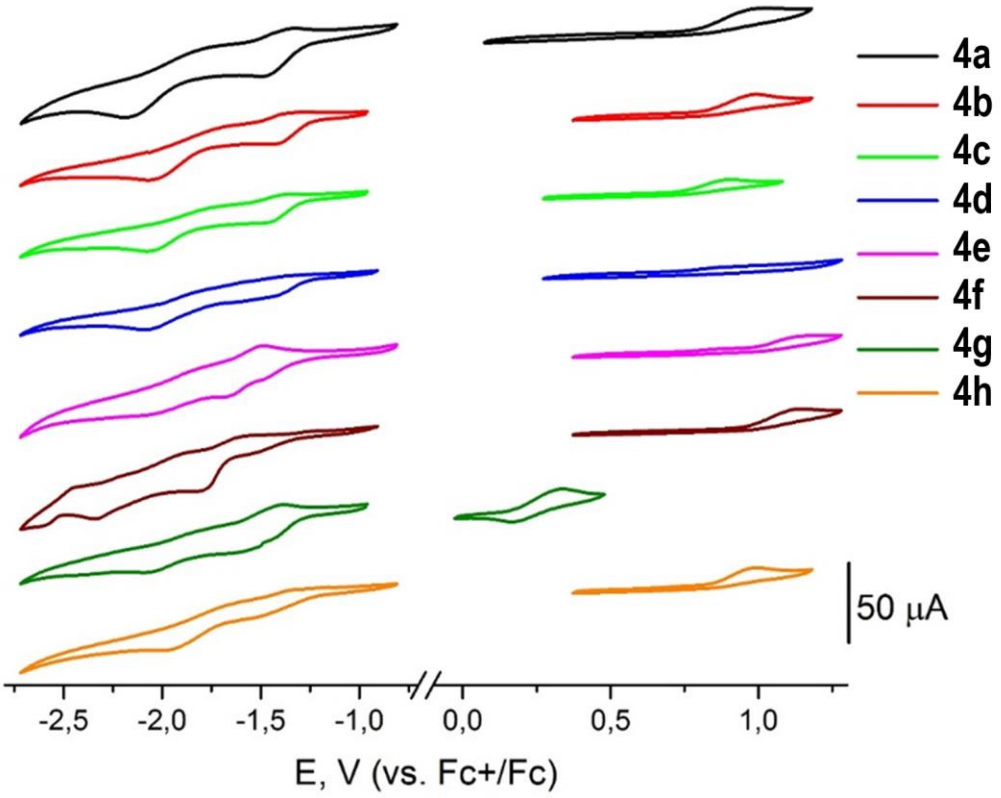


Figure S12: Cyclic voltammetry curves of **4a**–**h** (CH_2Cl_2, 50 mV/sec, *c* = 5 mM).

6. NMR spectra

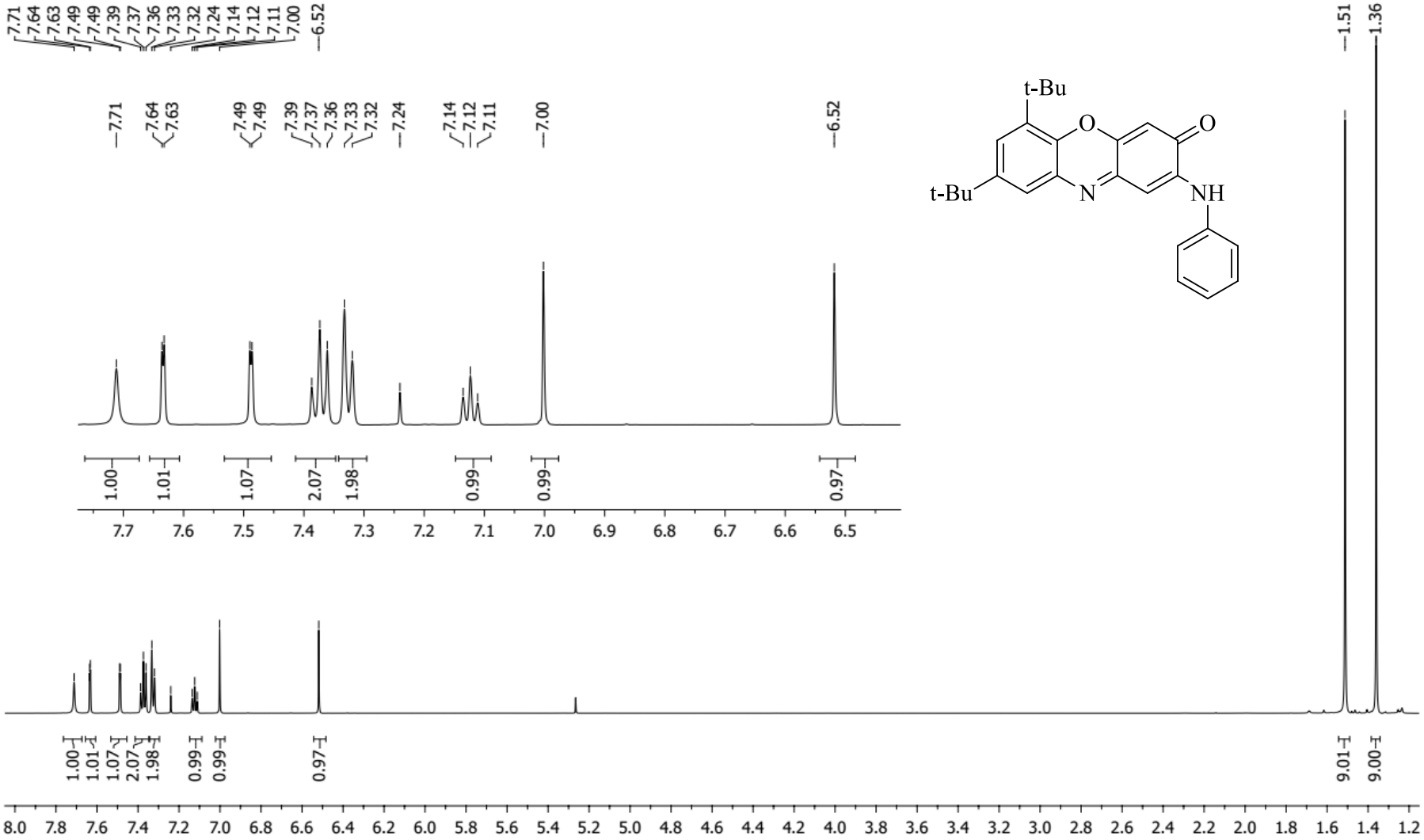


Figure S13: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-(phenylamino)-3*H*-phenoxazin-3-one (**4a**).

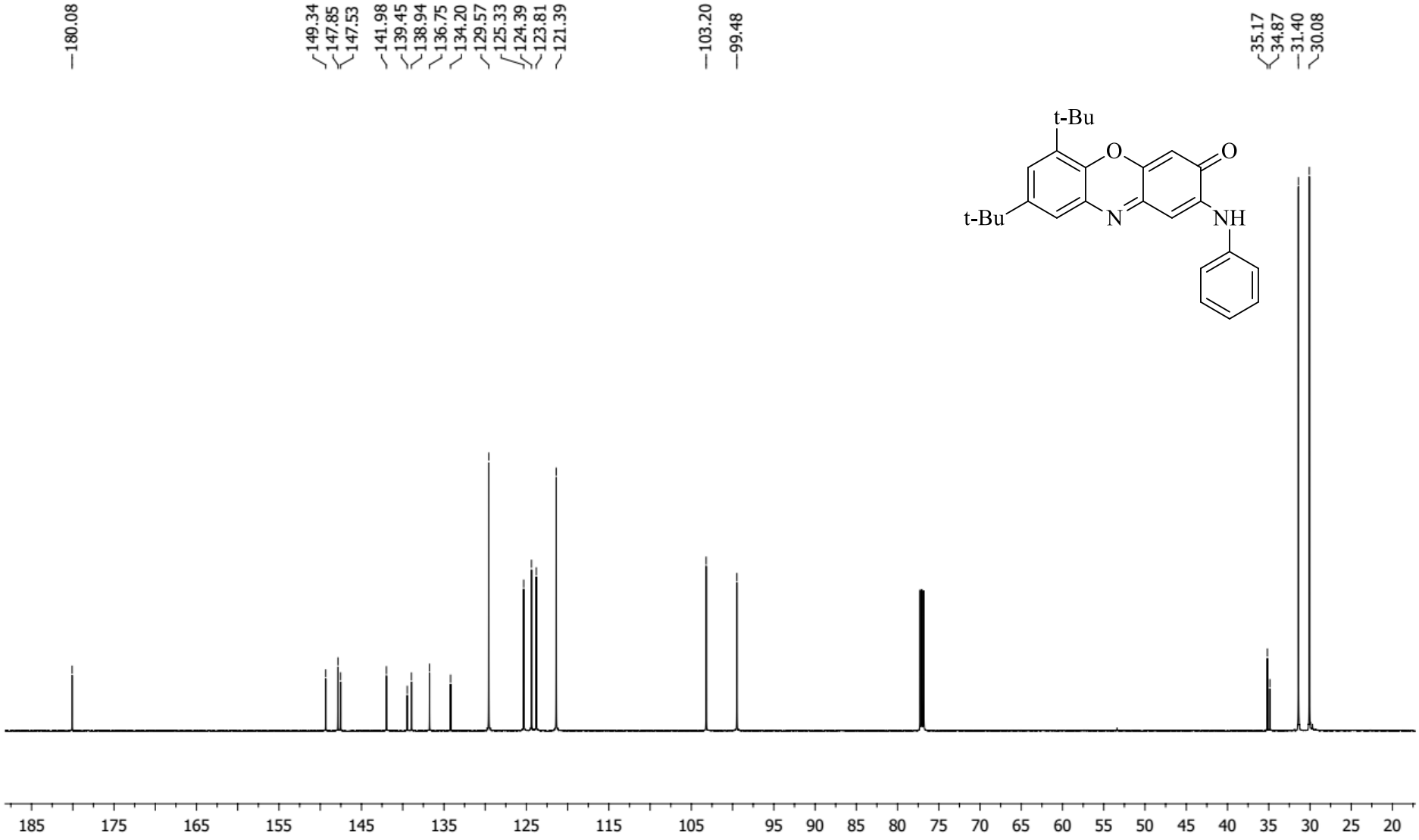


Figure S14: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-(phenylamino)-3*H*-phenoxazin-3-one (**4a**).

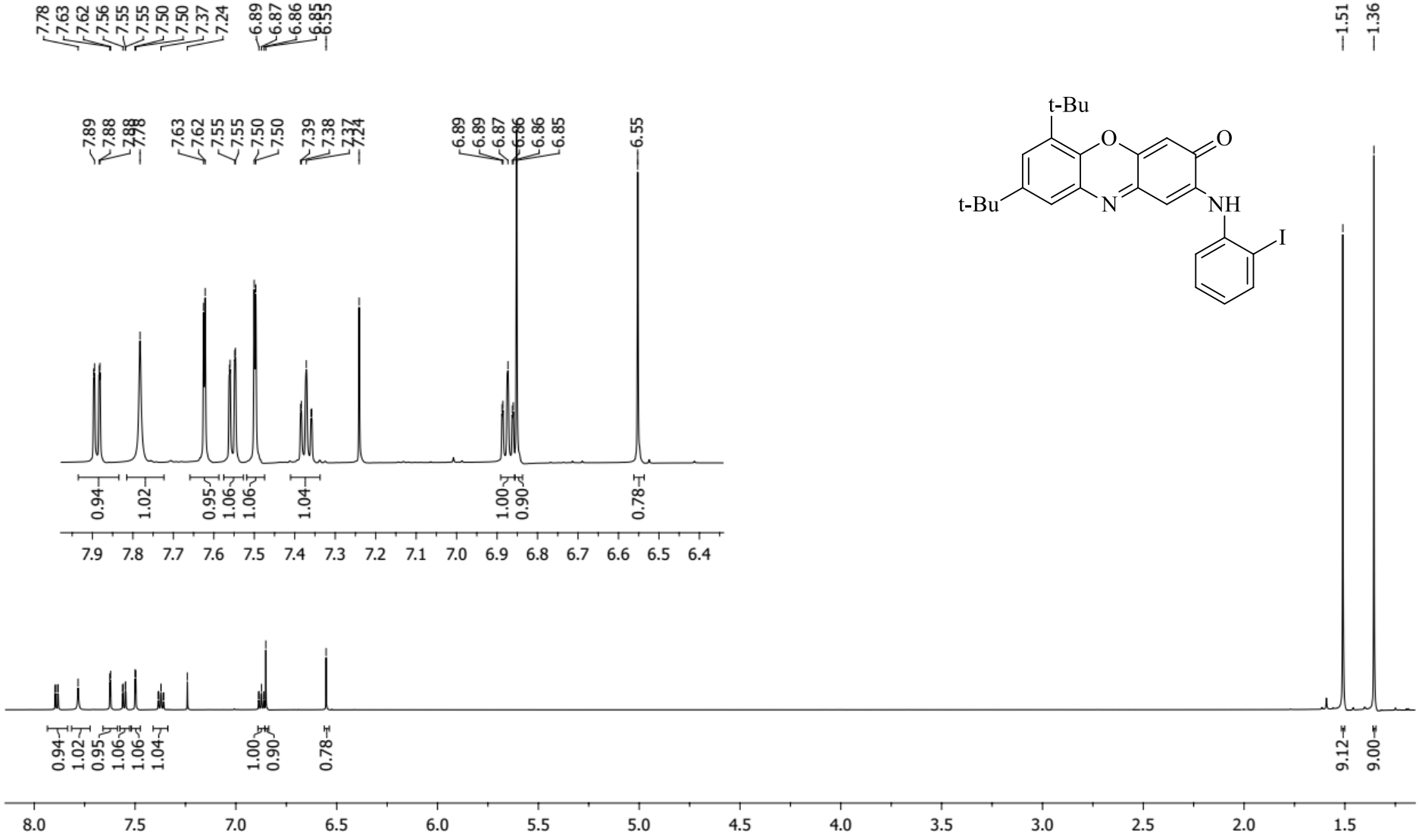


Figure S15: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-((2-iodophenyl)amino)-3*H*-phenoxazin-3-one (**4b**).

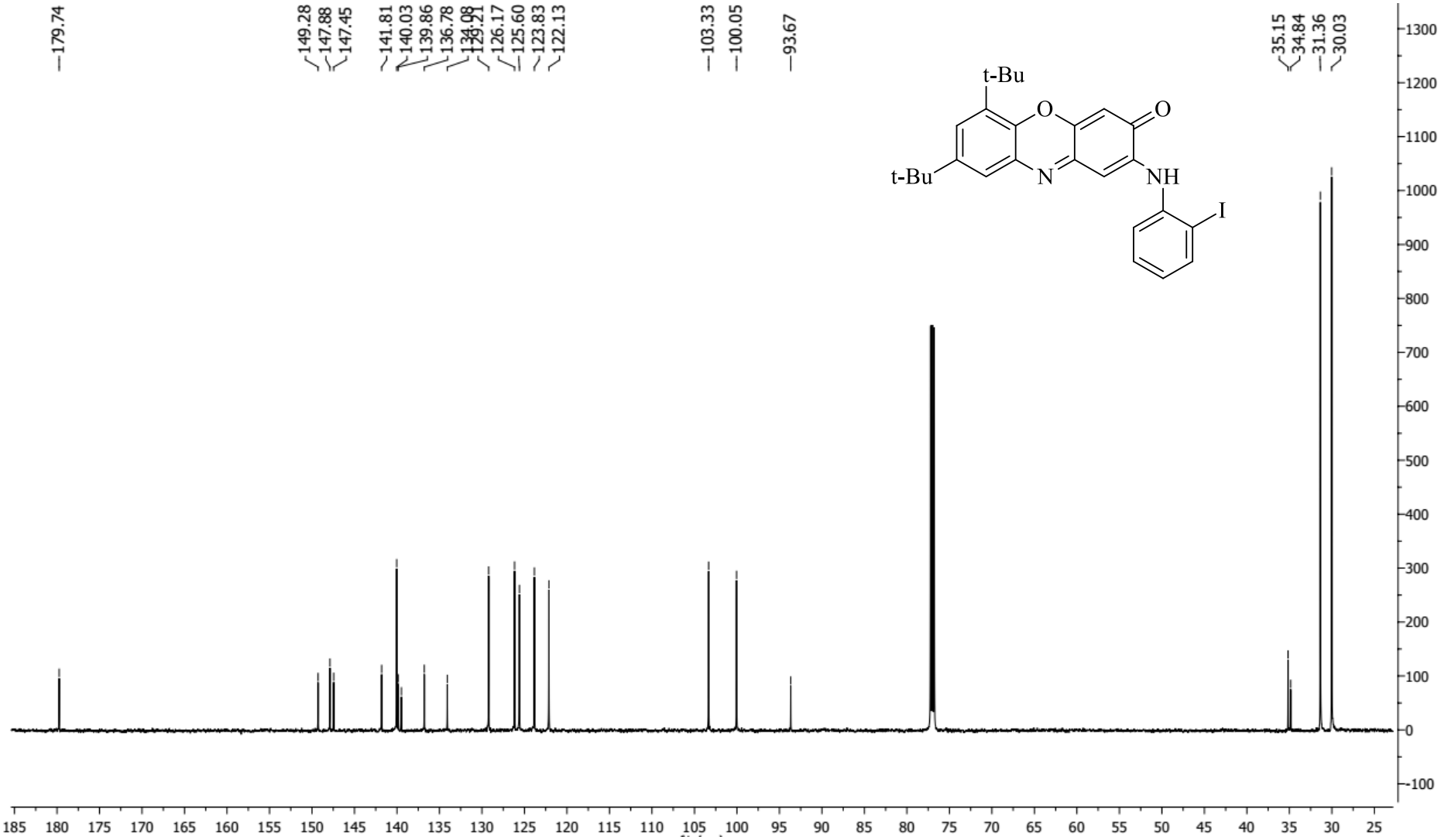


Figure S16: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-((2-iodophenyl)amino)-3*H*-phenoxazin-3-one (**4b**).

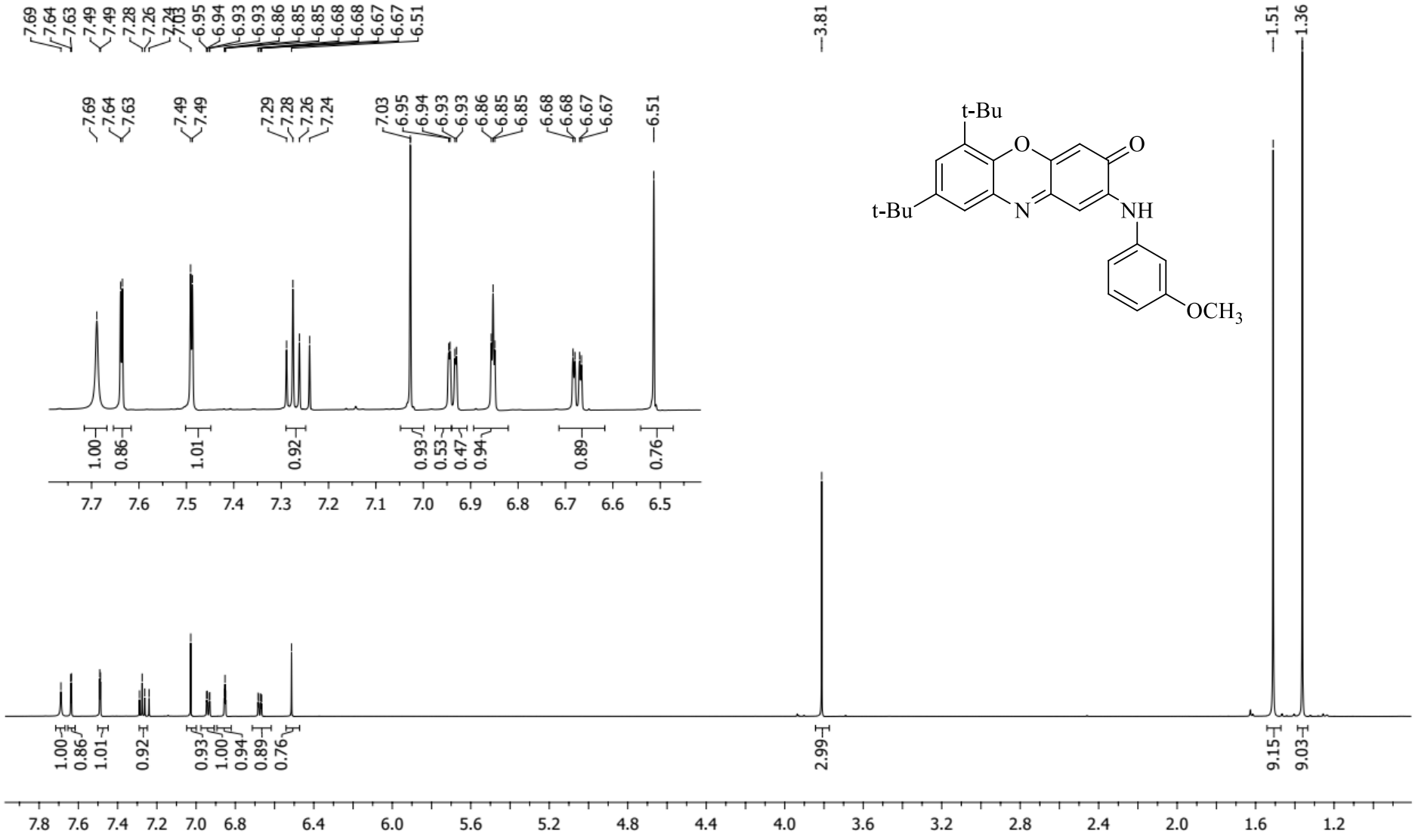


Figure S17: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-((3-methoxyphenyl)amino)-3*H*-phenoxazin-3-one (**4c**).

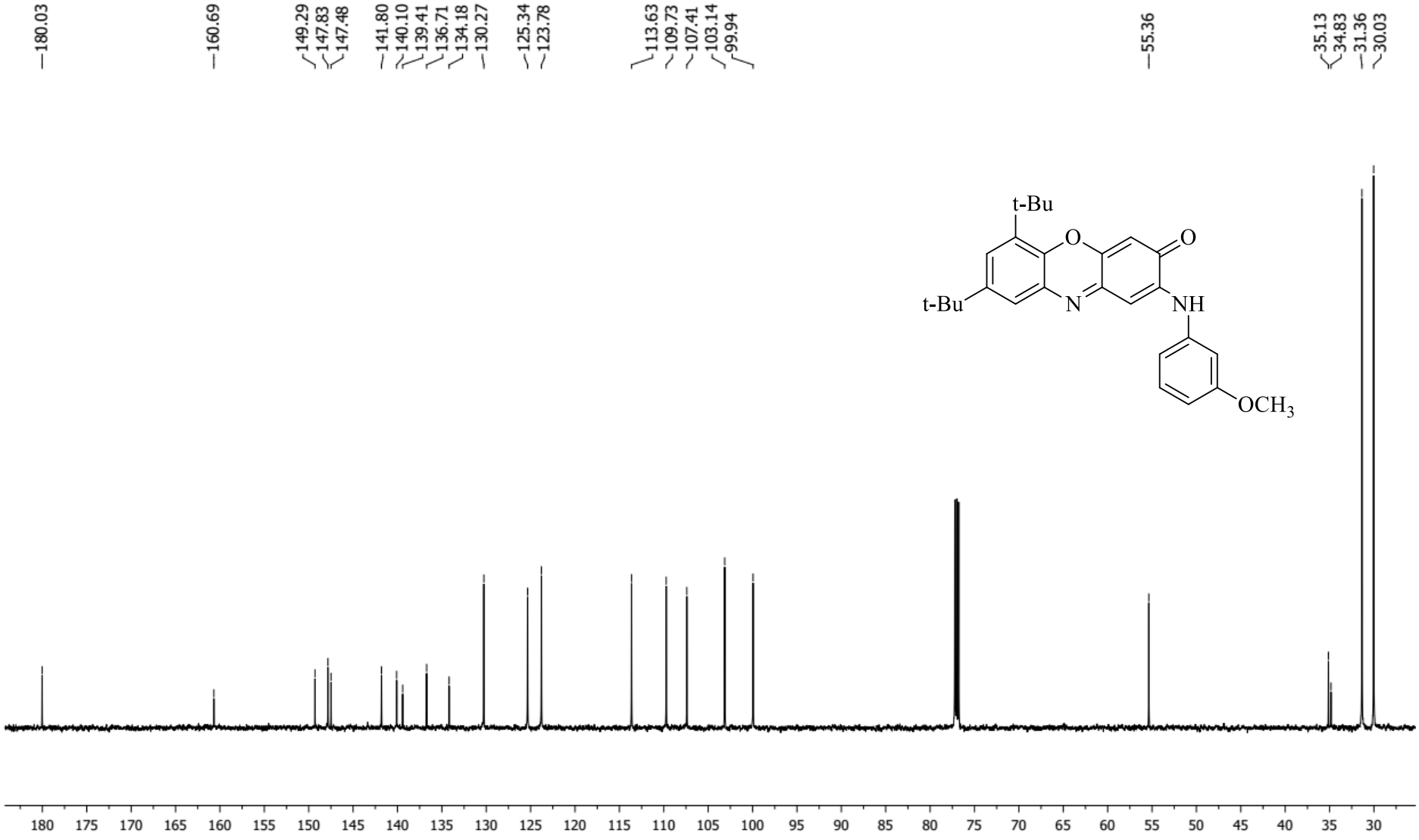


Figure S18: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-((3-methoxyphenyl)amino)-3*H*-phenoxazin-3-one (**4c**).

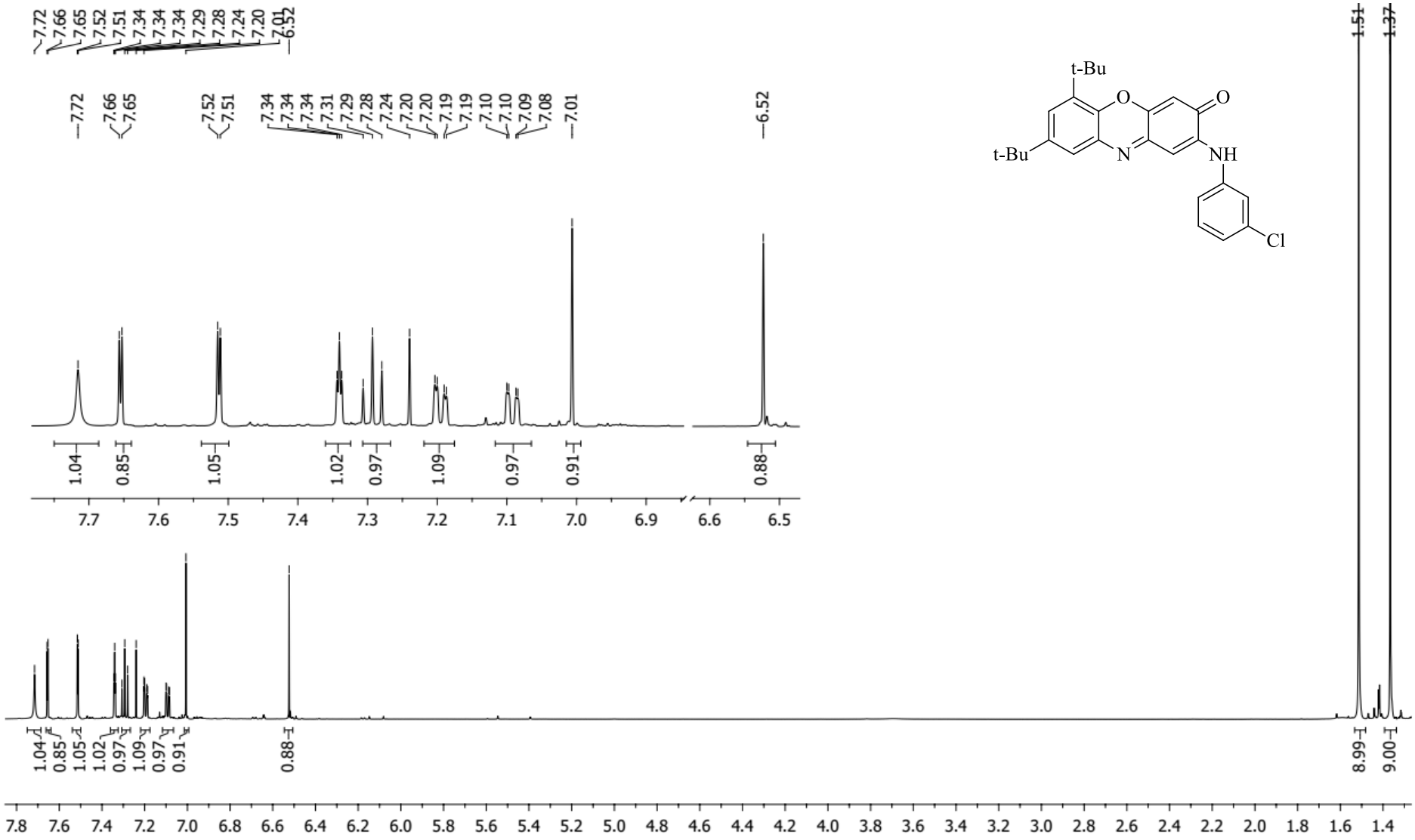


Figure S19: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-((3-chlorophenyl)amino)-3*H*-phenoxazin-3-one (**4d**).

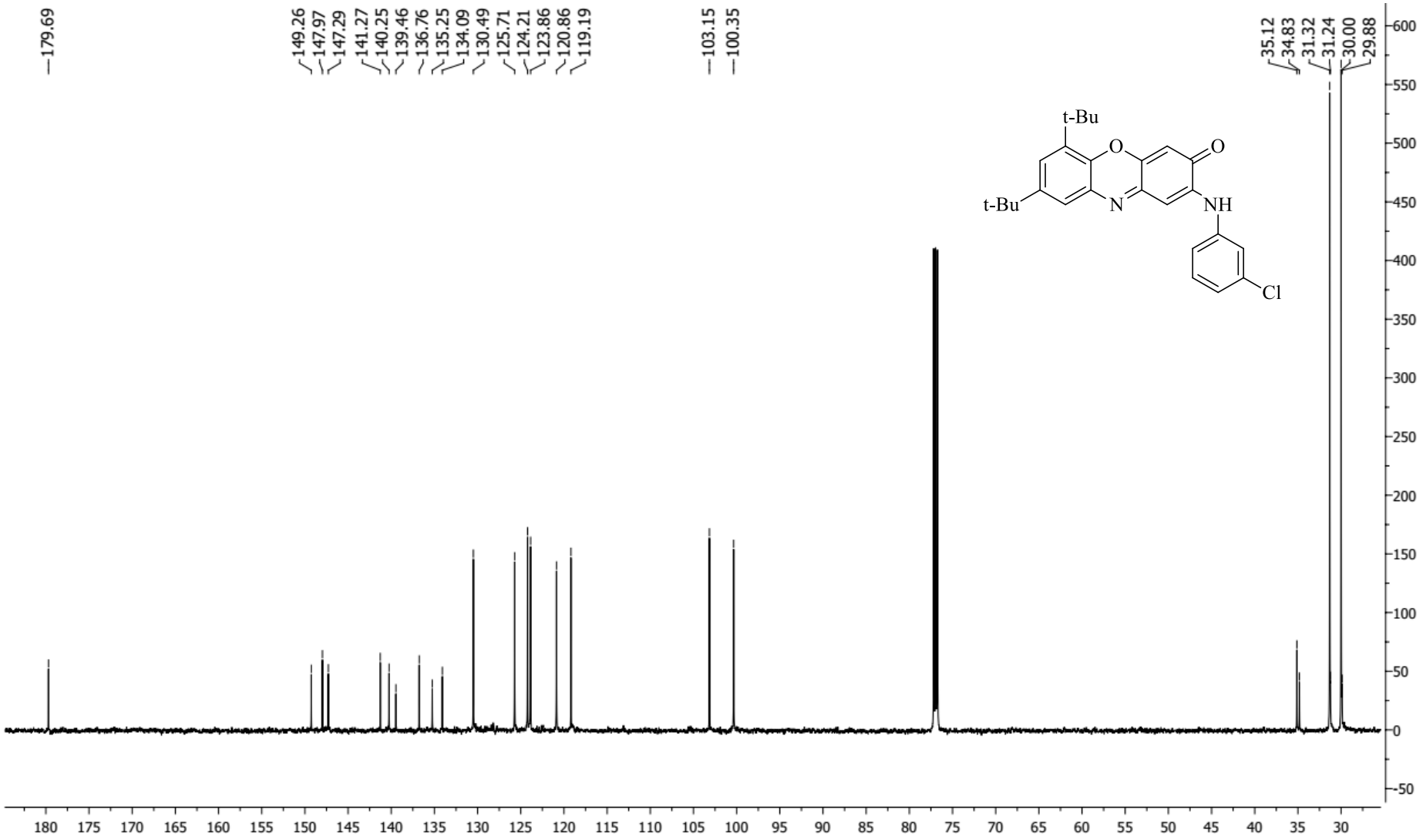


Figure S20: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-((3-chlorophenyl)amino)-3*H*-phenoxazin-3-one (**4d**).

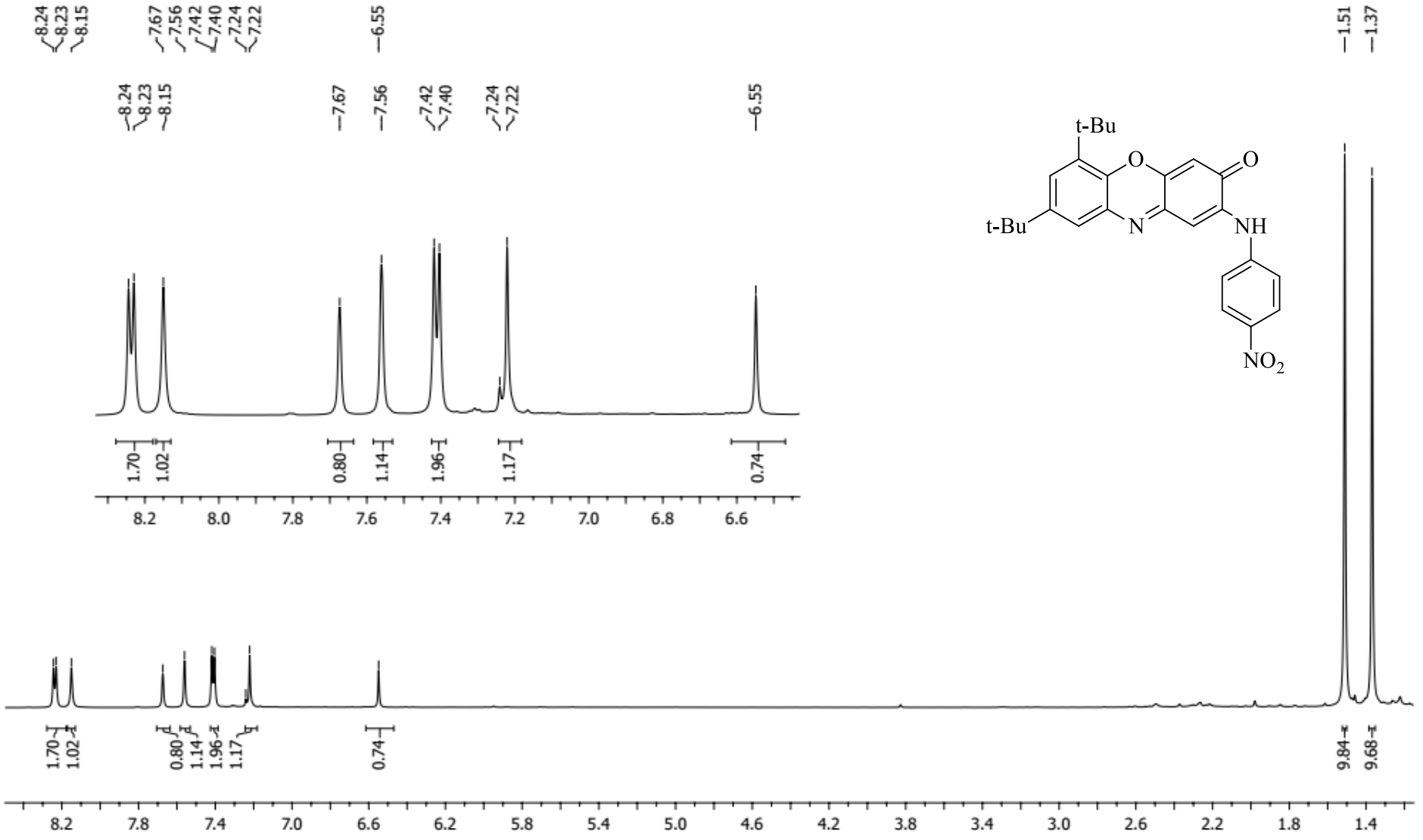


Figure S21: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-((4-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4e**).

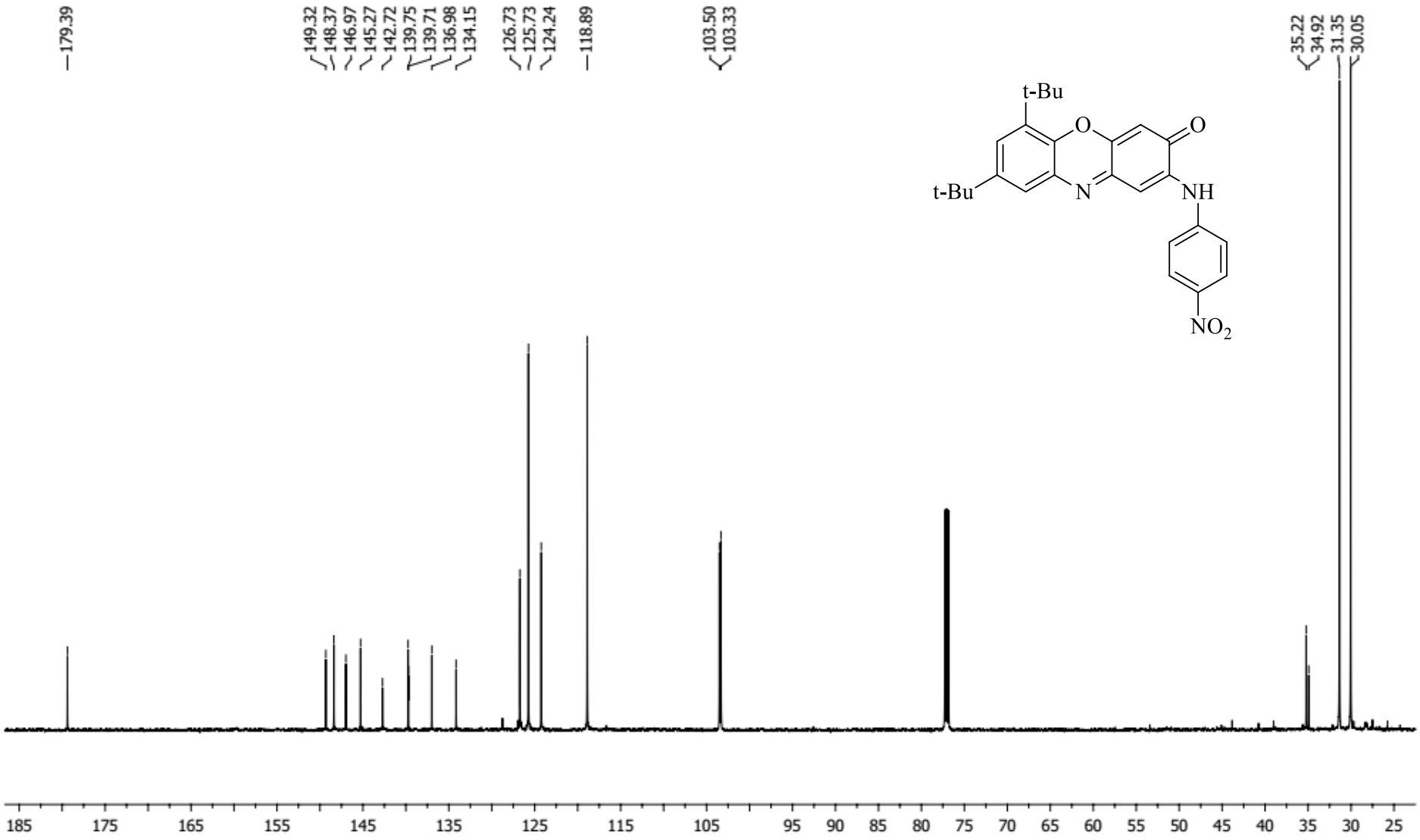


Figure S22: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-((4-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4e**).

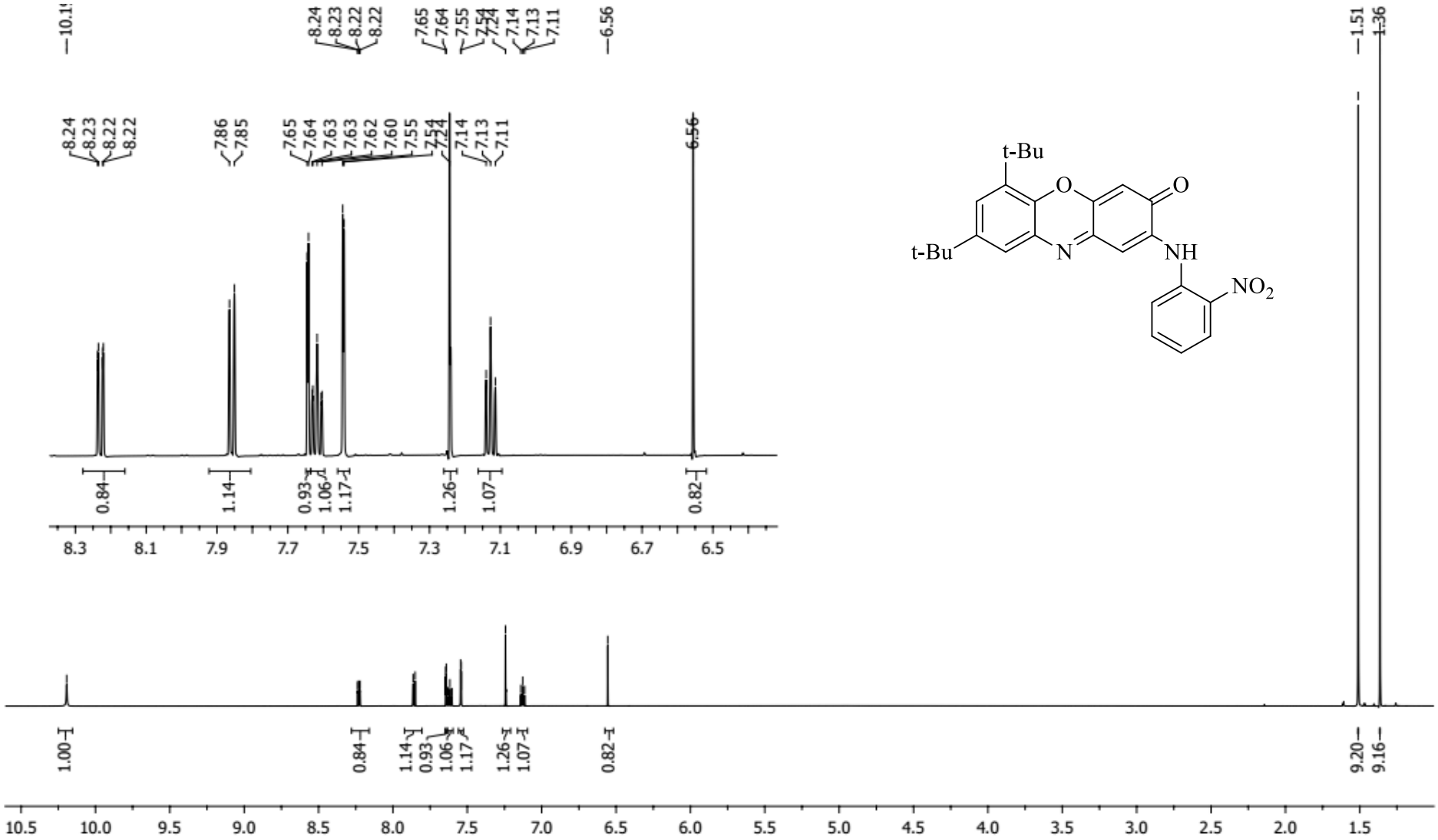


Figure S23: ^{1}H NMR spectrum of 6,8-di-*tert*-butyl-2-((2-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4f**).

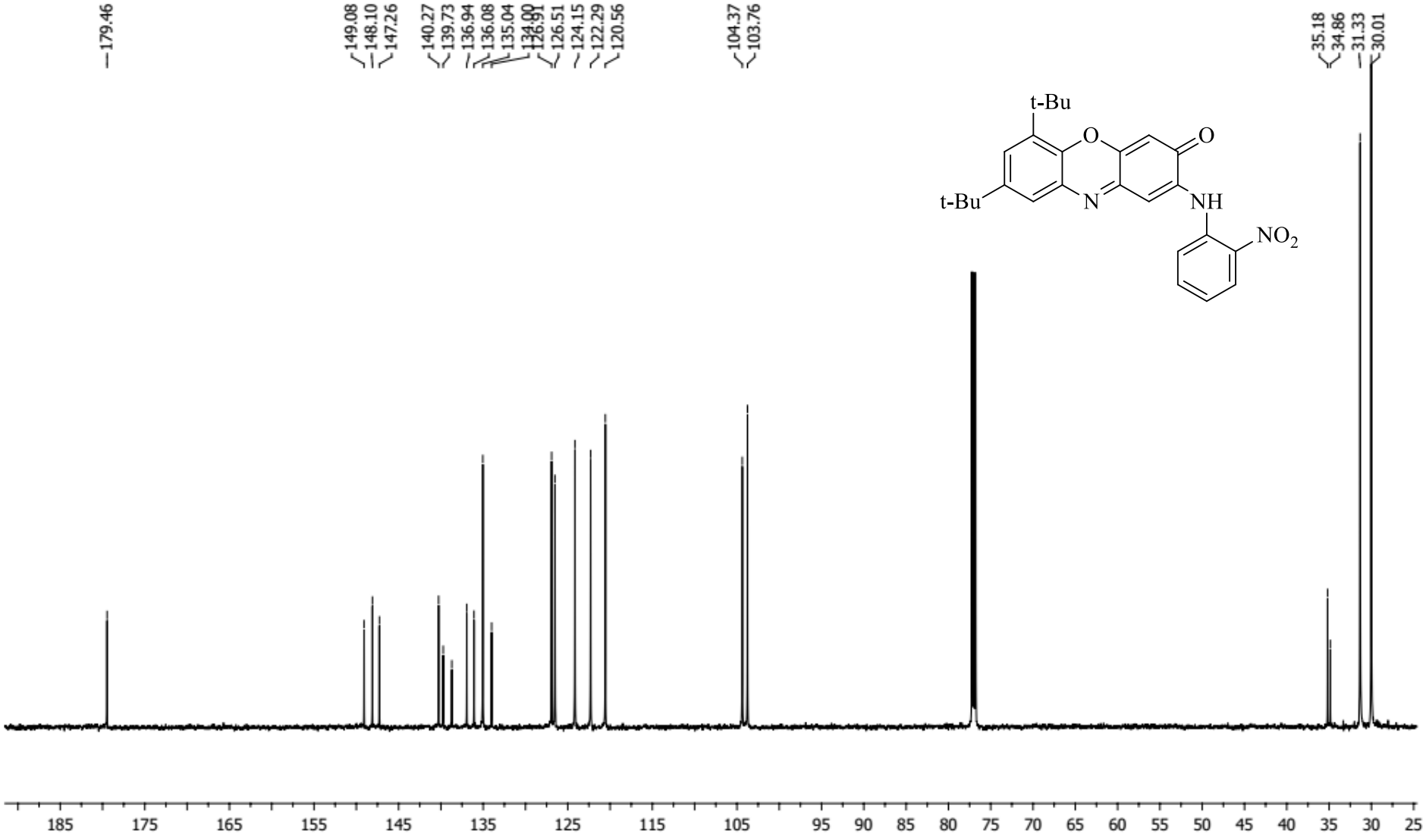


Figure S24: ^{13}C NMR spectrum of 6,8-di-*tert*-butyl-2-((2-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4f**).

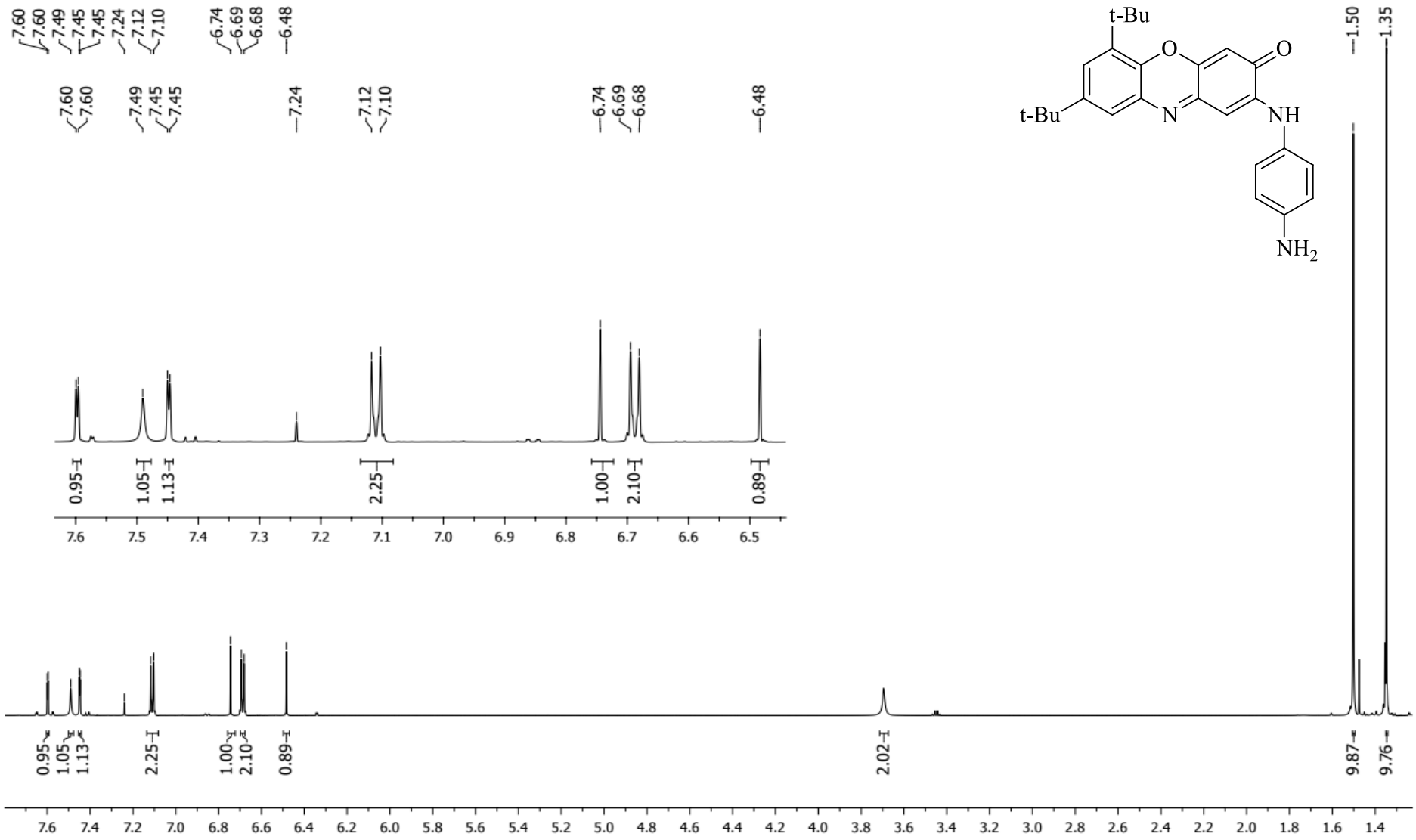


Figure S25: ^{1}H NMR spectrum of 2-((4-aminophenyl)amino)-6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**4g**).

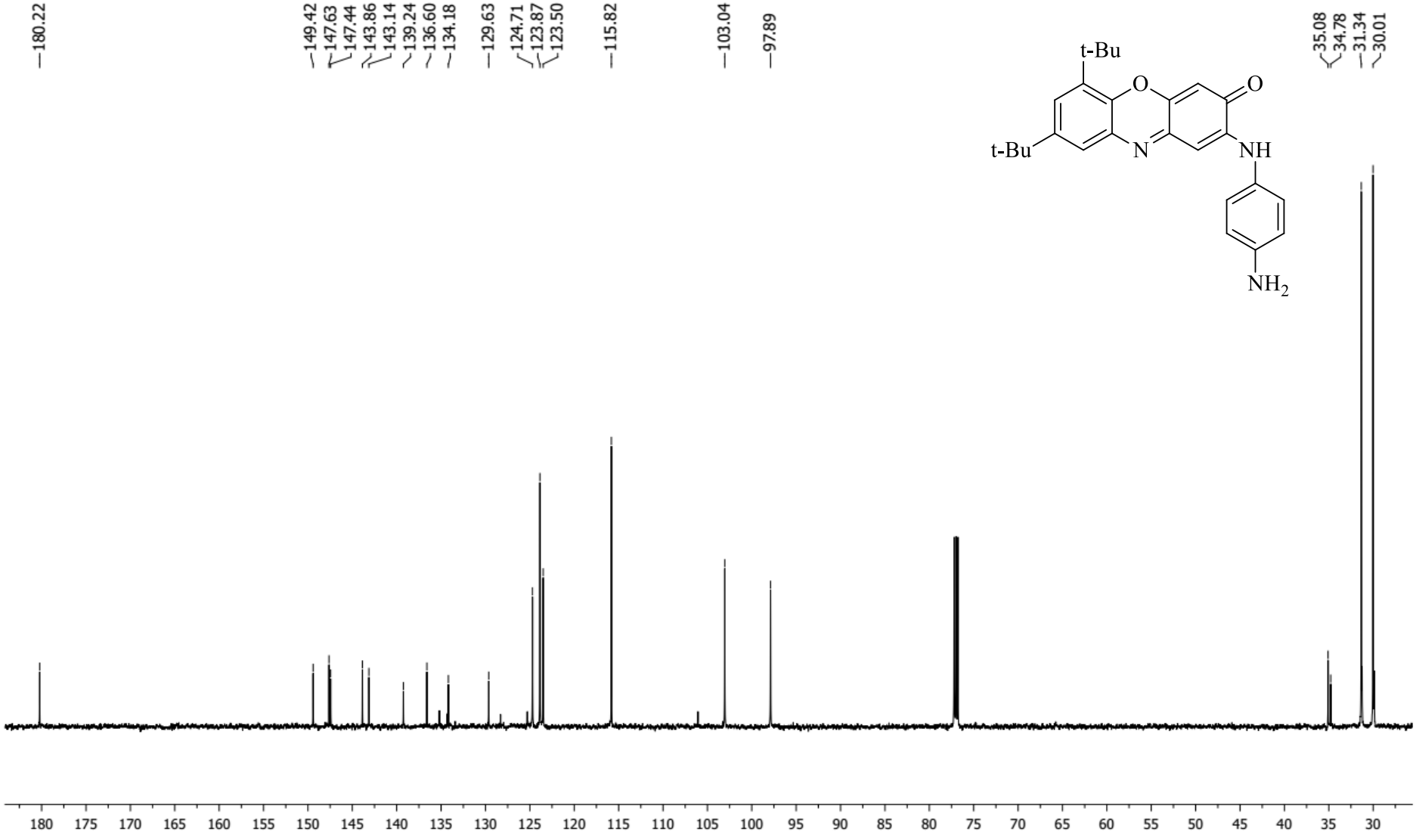


Figure S26: ^{13}C NMR spectrum of 2-((4-aminophenyl)amino)-6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**4g**).

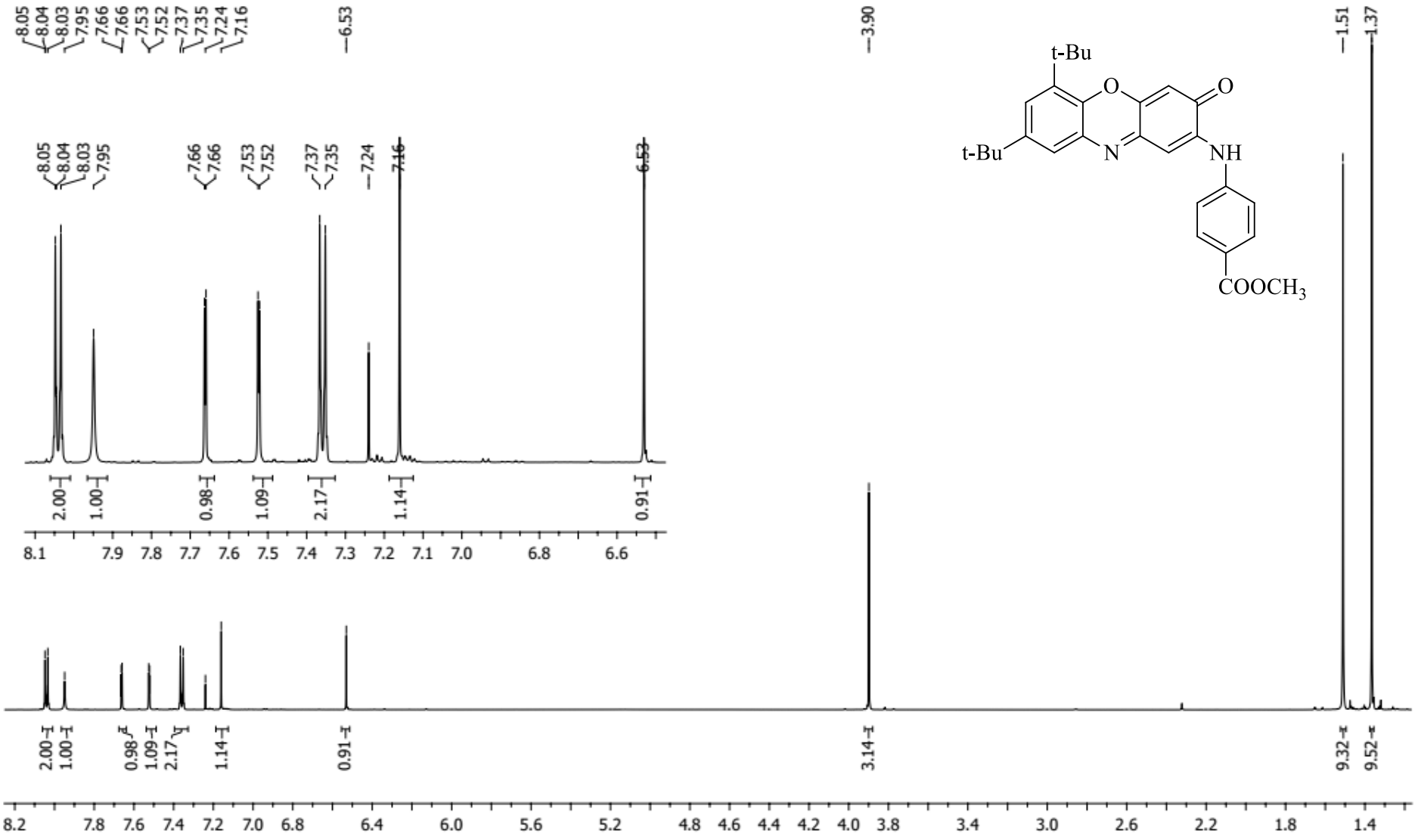


Figure S27: ^{1}H NMR spectrum of methyl 4-((6,8-di-*tert*-butyl-3-oxo-3*H*-phenoxazin-2-yl)amino)benzoate (**4h**).

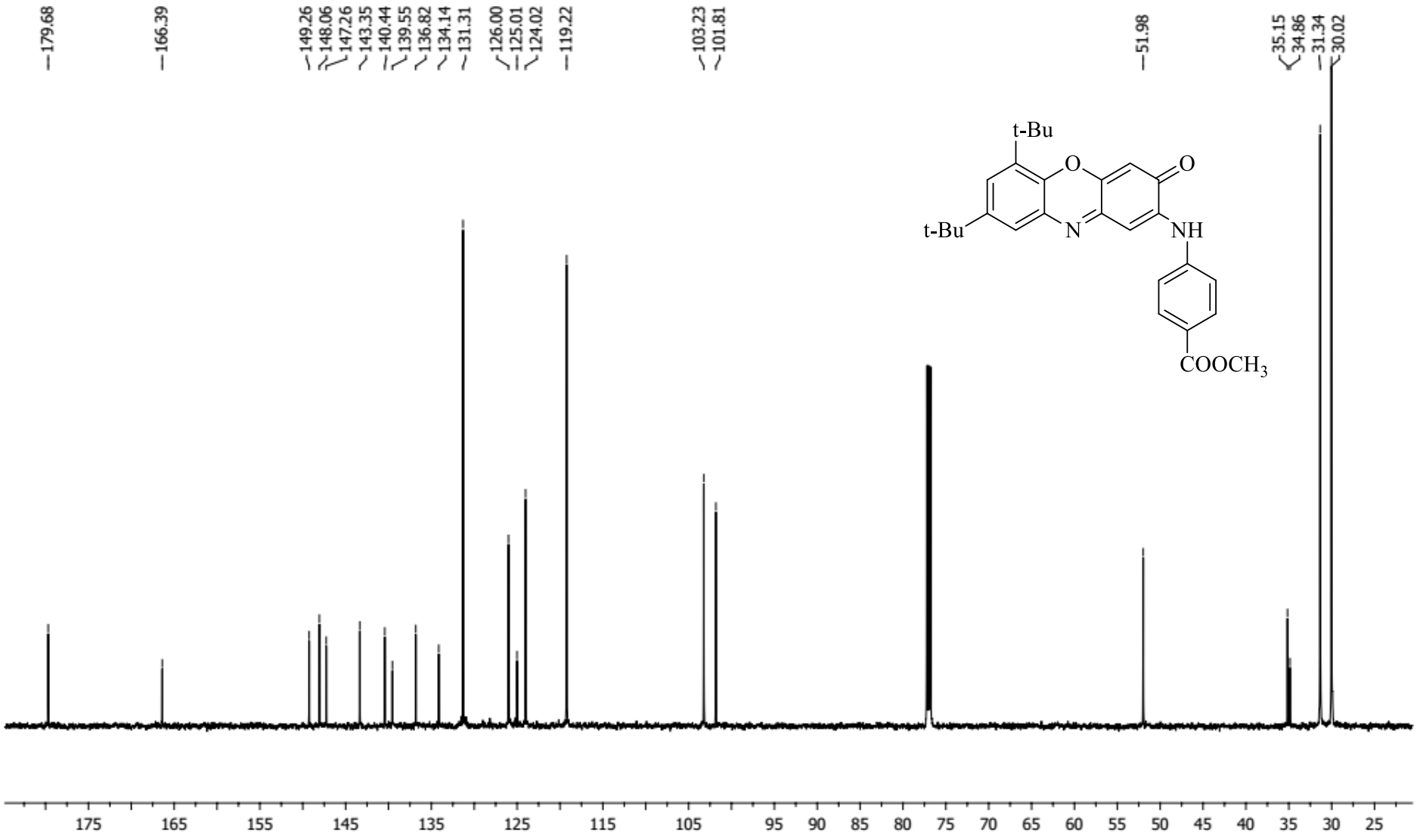


Figure S28: ^{13}C NMR spectrum of methyl 4-((6,8-di-*tert*-butyl-3-oxo-3*H*-phenoxazin-2-yl)amino)benzoate (**4h**).

2,4-Di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**)

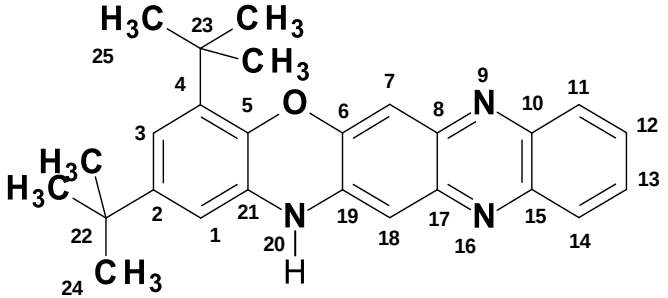


Table S9: Chemical shifts ^{1}H, ^{13}C, and ^{15}N of compound **5a** in $CDCl_3$ at 30°C δ (ppm) and spin–spin coupling constants *J* (Hz).

Compound	**7.** Nucleus	1	2	3	4	5	6	7	8	9(^{15}N)	10	11	12	13	14
5a	^{1}H	6.42		6.74				7.26				7.96	7.48	7.48	7.87
	J_{1H-1H}	2.4		2.4								7.8	7.8	7.8	7.8
	8. $^{13}C/^{15}N$	109.64	136.94	117.04	146.46	138.09	144.11	109.69	143.58	314.95	141.67	128.98	128.02	129.10	127.28

Compound	**9.** Nucleus	15	16(^{15}N)	17	18	19	20(^{15}N)	21	22	23	24	25
5a	^{1}H				6.85						1.46	1.13
	J_{1H-1H}											
	10. $^{13}C/^{15}N$	142.19	296.56	148.97	102.35	136.53	92.79	127.80	34.93	34.38	29.98	31.20

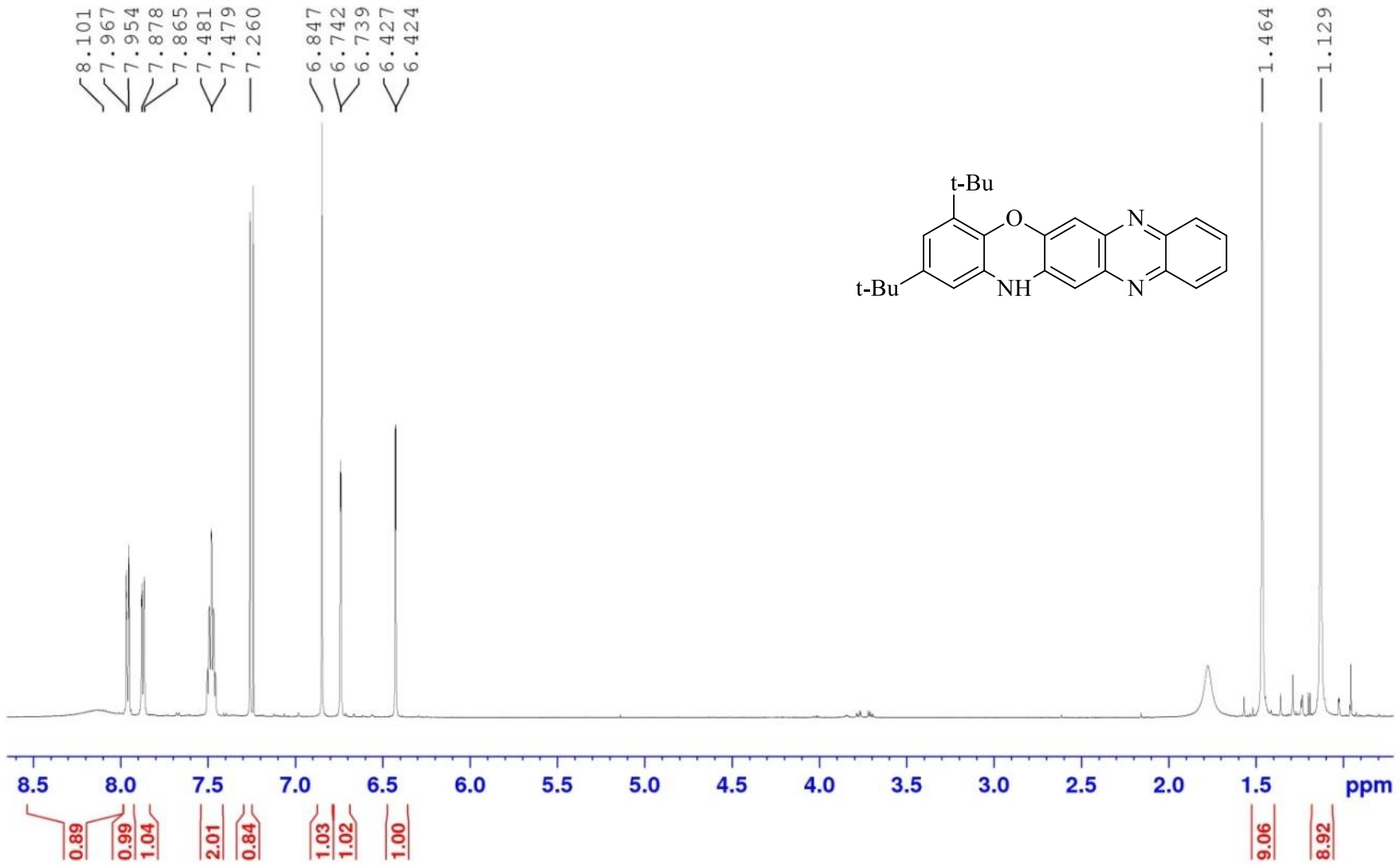


Figure S29: ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**).

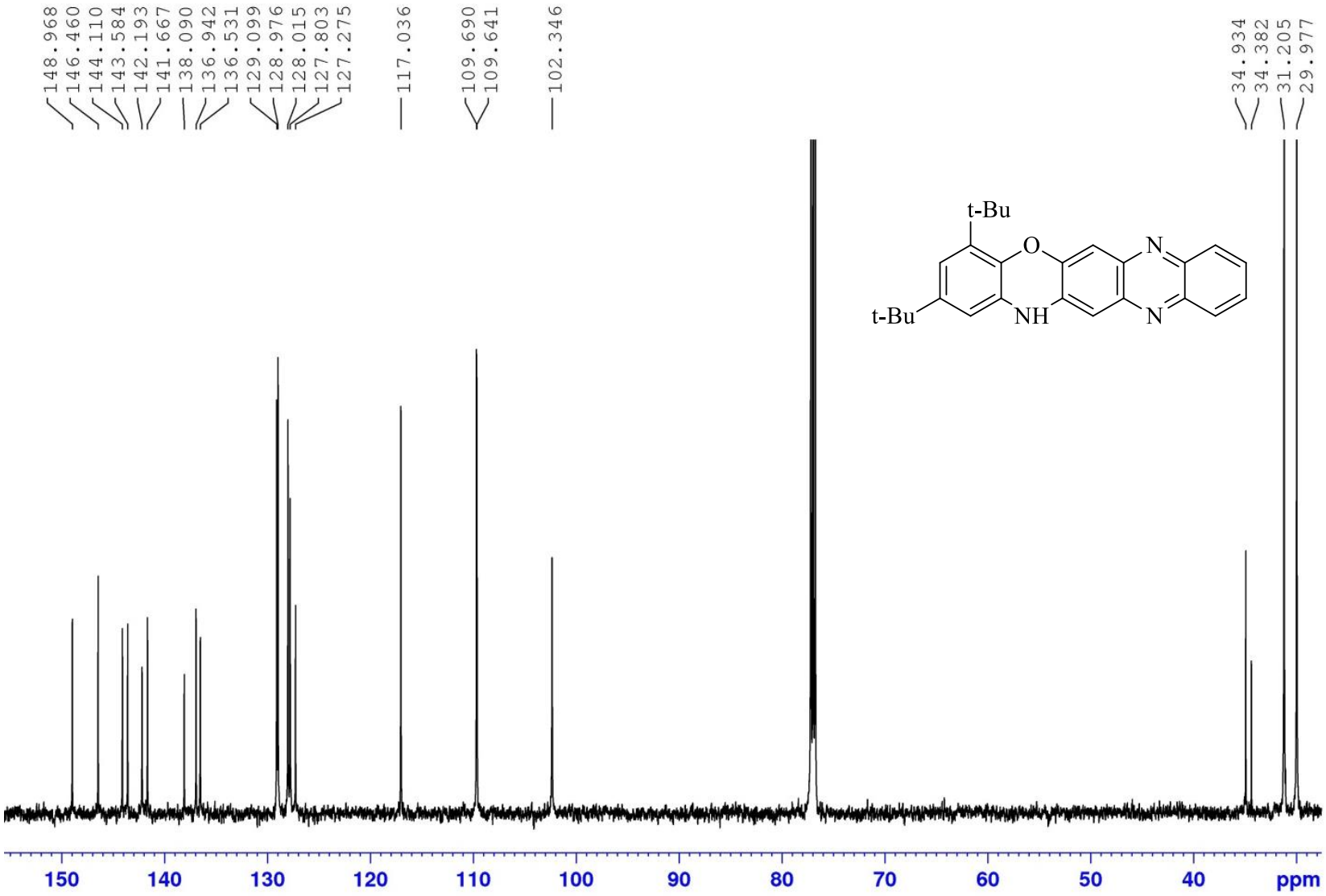


Figure S30: ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**).

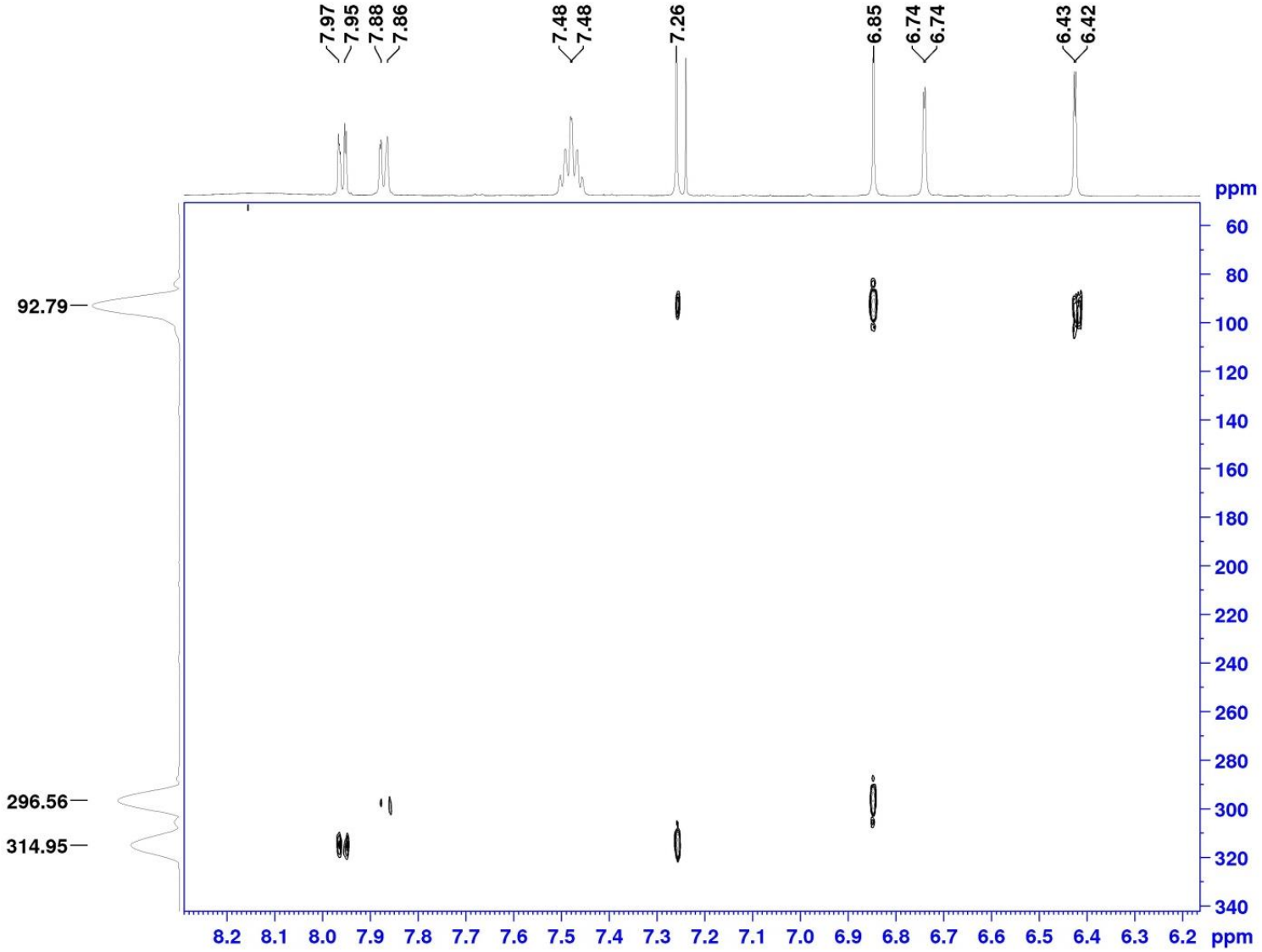


Figure S31: HMBC $^{1}H,^{15}N$ NMR spectrum of 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**).

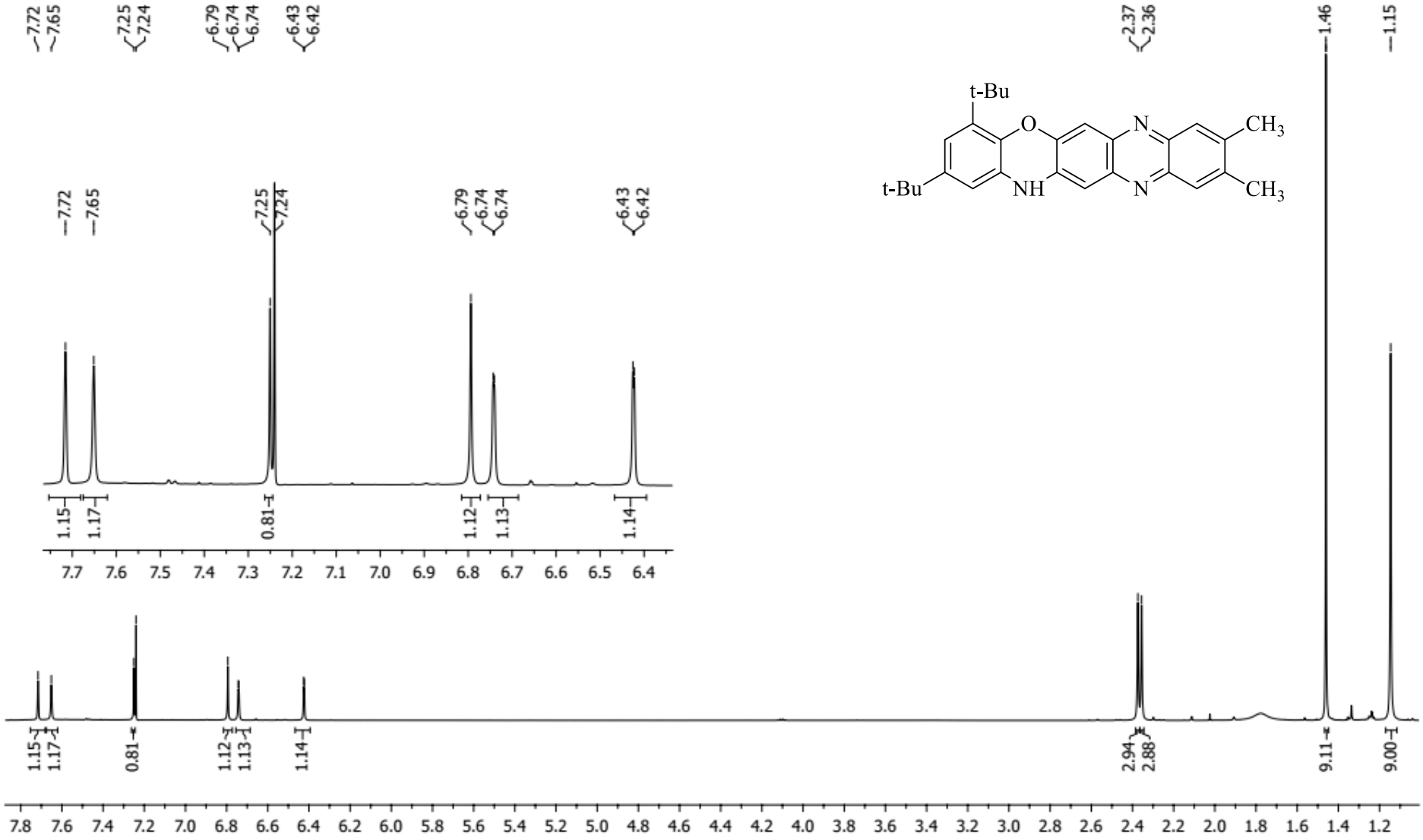


Figure S32: ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-9,10-dimethyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5b**).

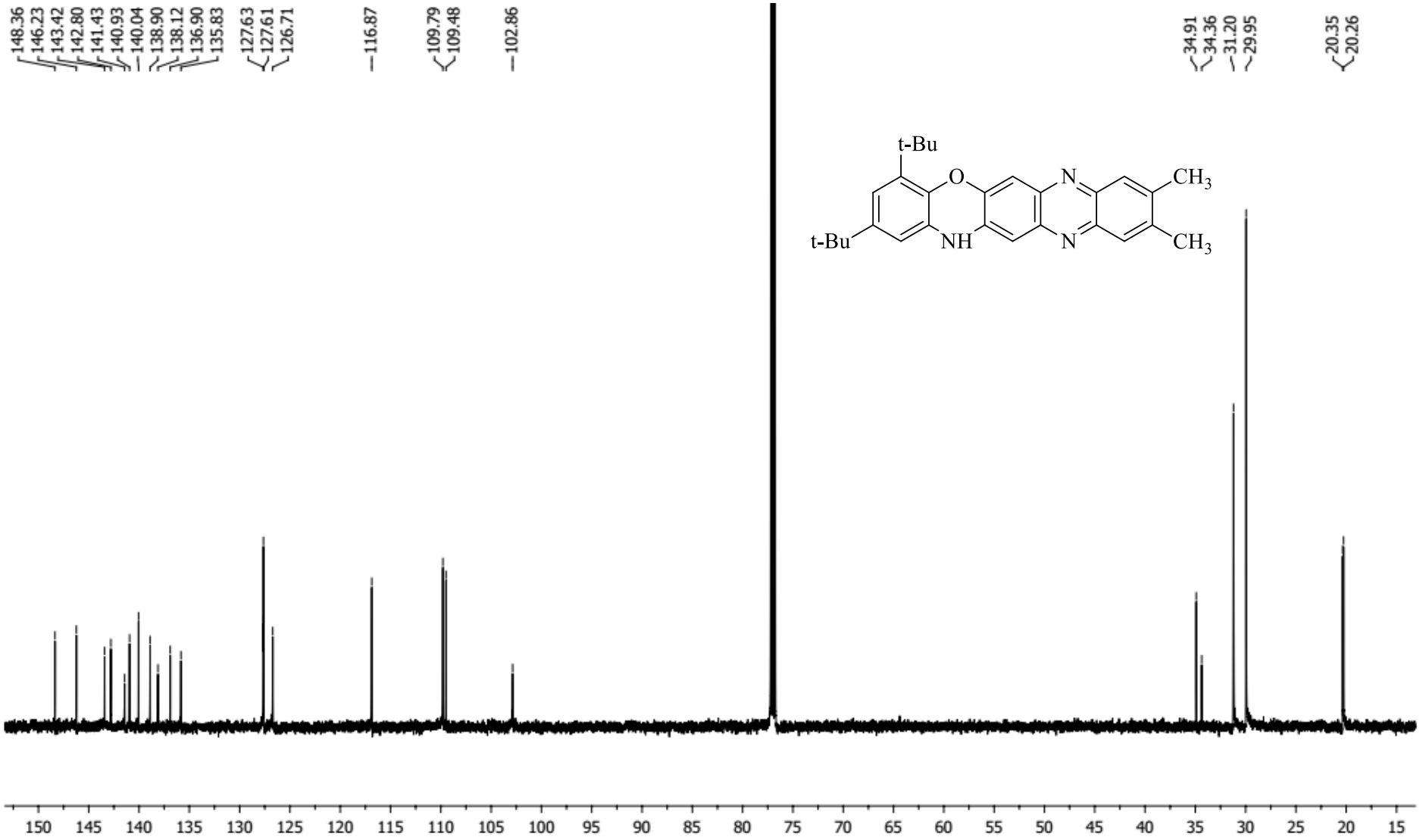


Figure S33: ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-9,10-dimethyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5b**).

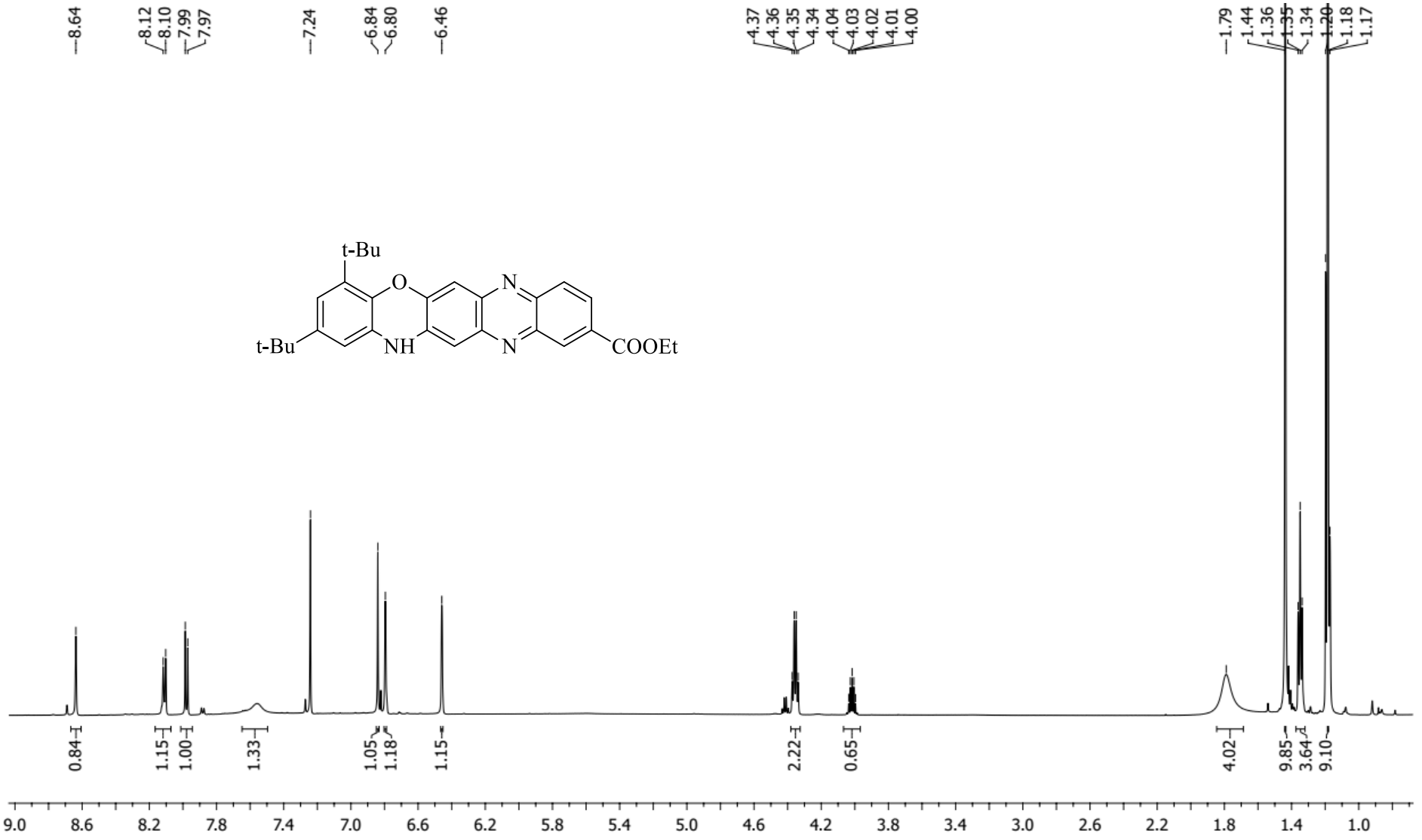


Figure S34: ^{1}H NMR spectrum of ethyl 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine-10-carboxylate (**5c**).

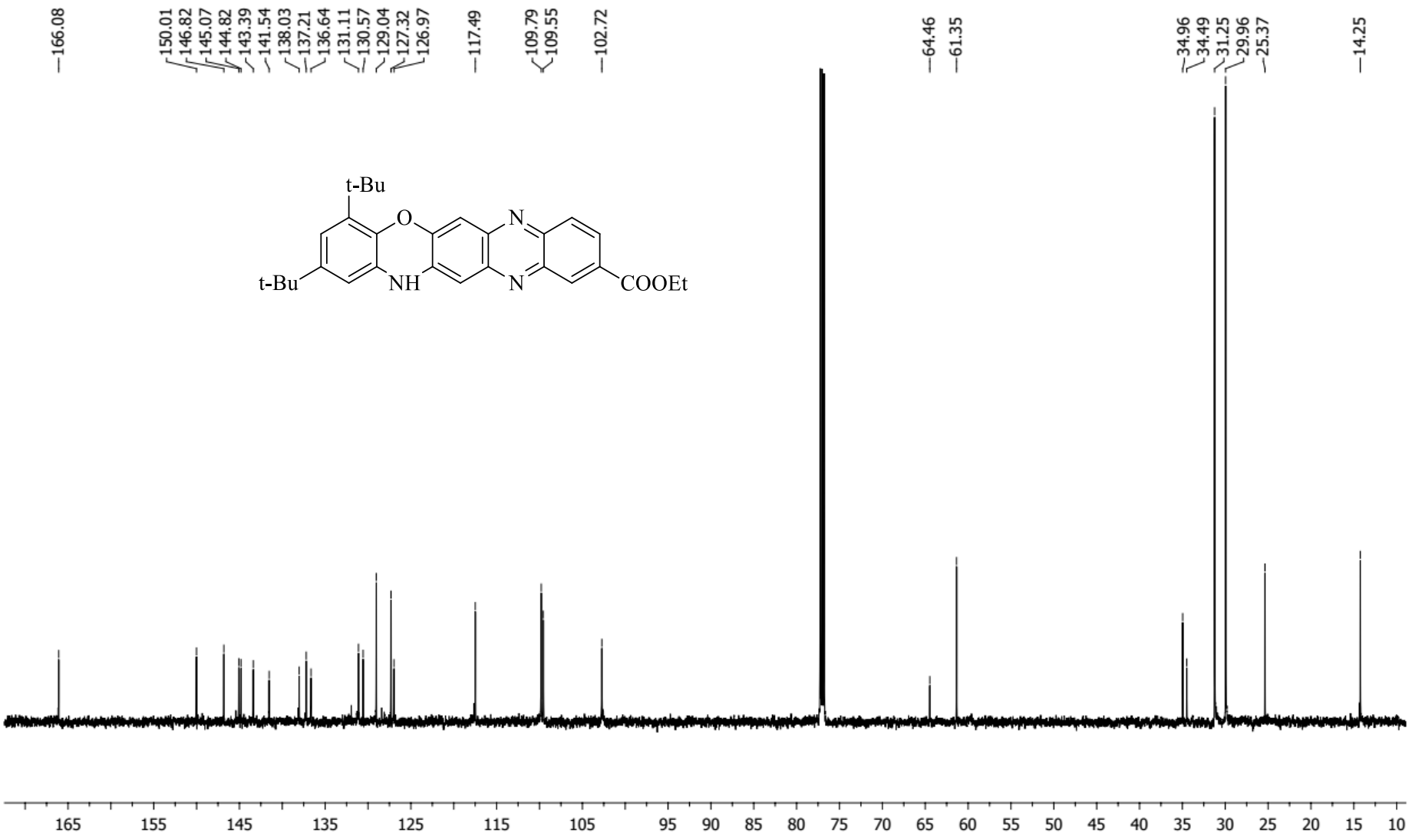


Figure S35: ^{13}C NMR spectrum of ethyl 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine-10-carboxylate (**5c**).

2,4-Di-*tert*-butyl-14-methyl-14H-quinoxalino[2,3-*b*]phenoxazine (**6a**)

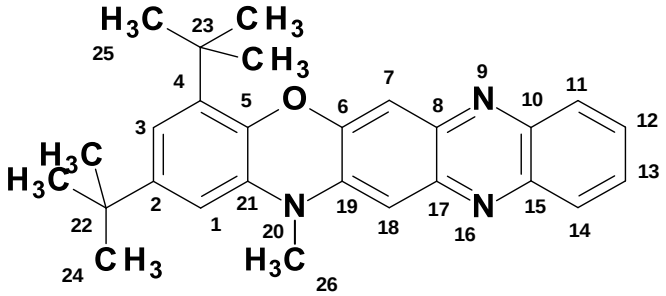


Table S10: Chemical shifts ^{1}H, ^{13}C, and ^{15}N of compound **6a** in $CDCl_3$ at 30°C δ (ppm) and spin–spin coupling constants *J* (Hz).

Compound	**11.** Nucleus	1	2	3	4	5	6	7	8	9(^{15}N)	10	11	12	13	14
6a	^{1}H	6.71		6.93				7.34				8.01	7.60	7.63	7.98
	J_{1H-1H}	2.1		2.1								8.1	8.1	8.1	8.1
	12. $^{13}C/^{15}N$	108.55	136.92	117.35	146.30	140.04	144.48	109.17	143.17	311.64	141.90	128.90	128.31	129.07	128.49

Compound	**13.** Nucleus	15	16(^{15}N)	17	18	19	20(^{15}N)	21	22	23	24	25	26
6a	^{1}H				6.94						1.46	1.31	3.37
	J_{1H-1H}												
	14. $^{13}C/^{15}N$	142.70	305.64	150.45	103.54	139.19	83.69	130.84	34.83	34.97	30.03	31.45	32.45

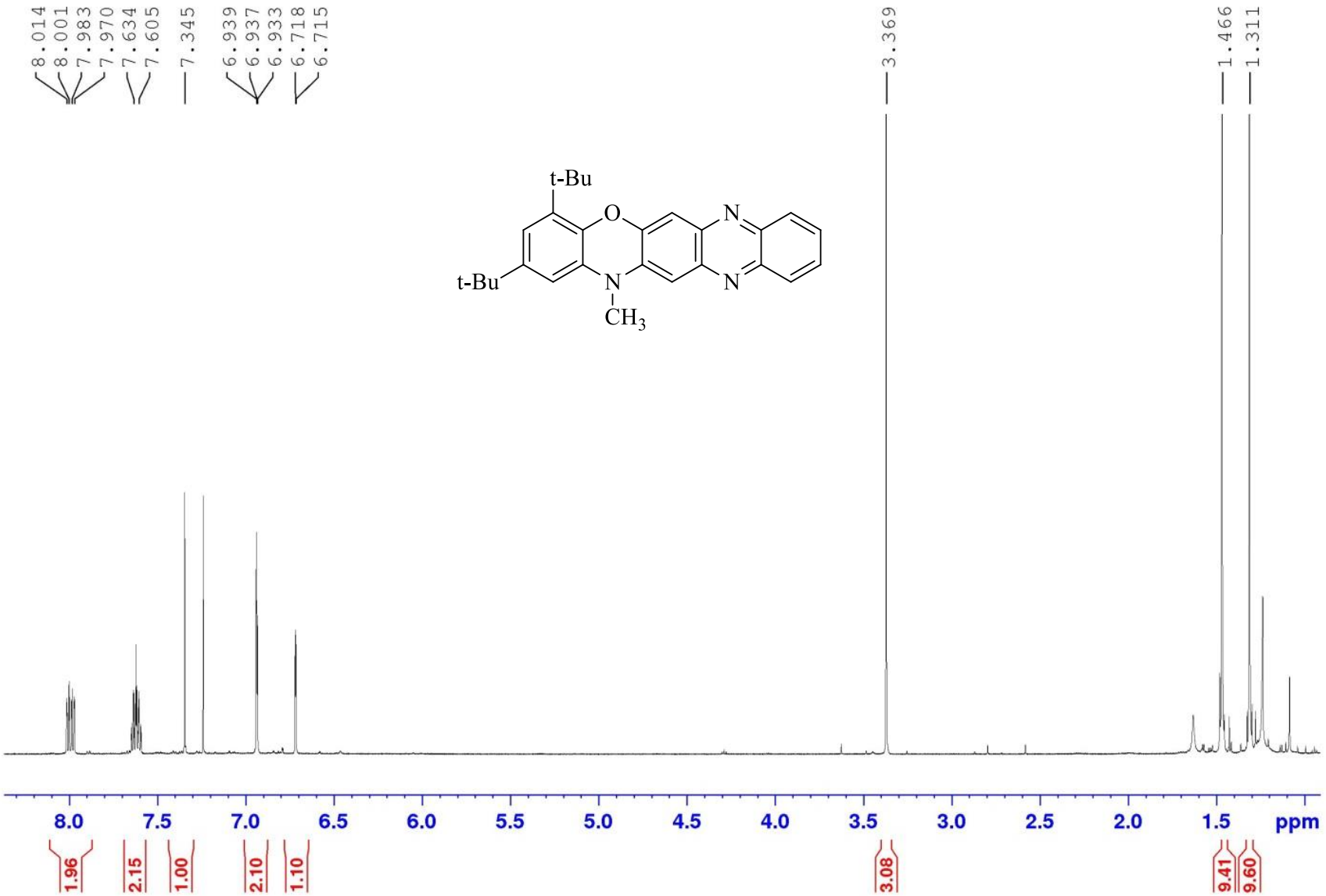


Figure S36: ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-14-methyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6a**).

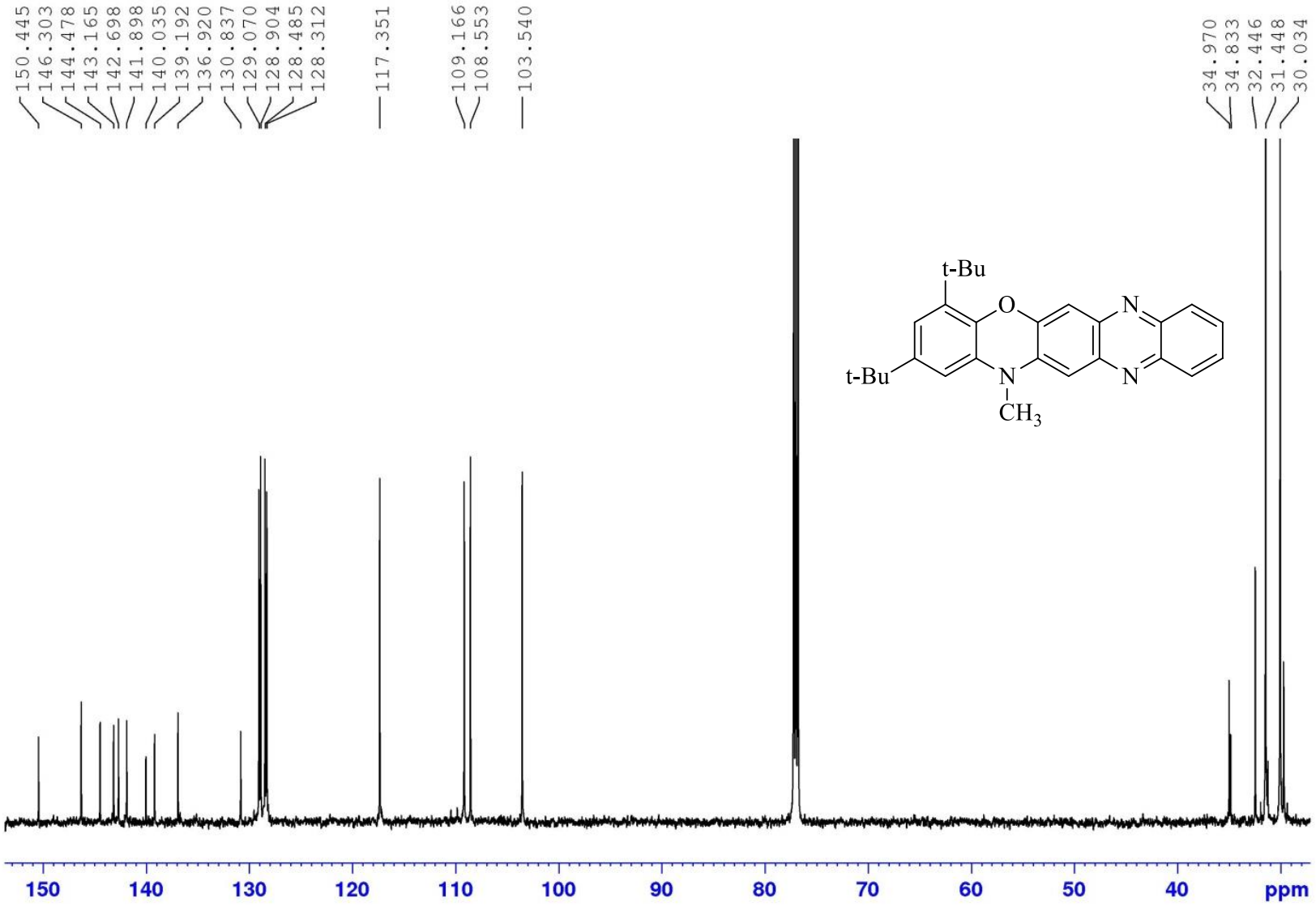


Figure S37: ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-14-methyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6a**).

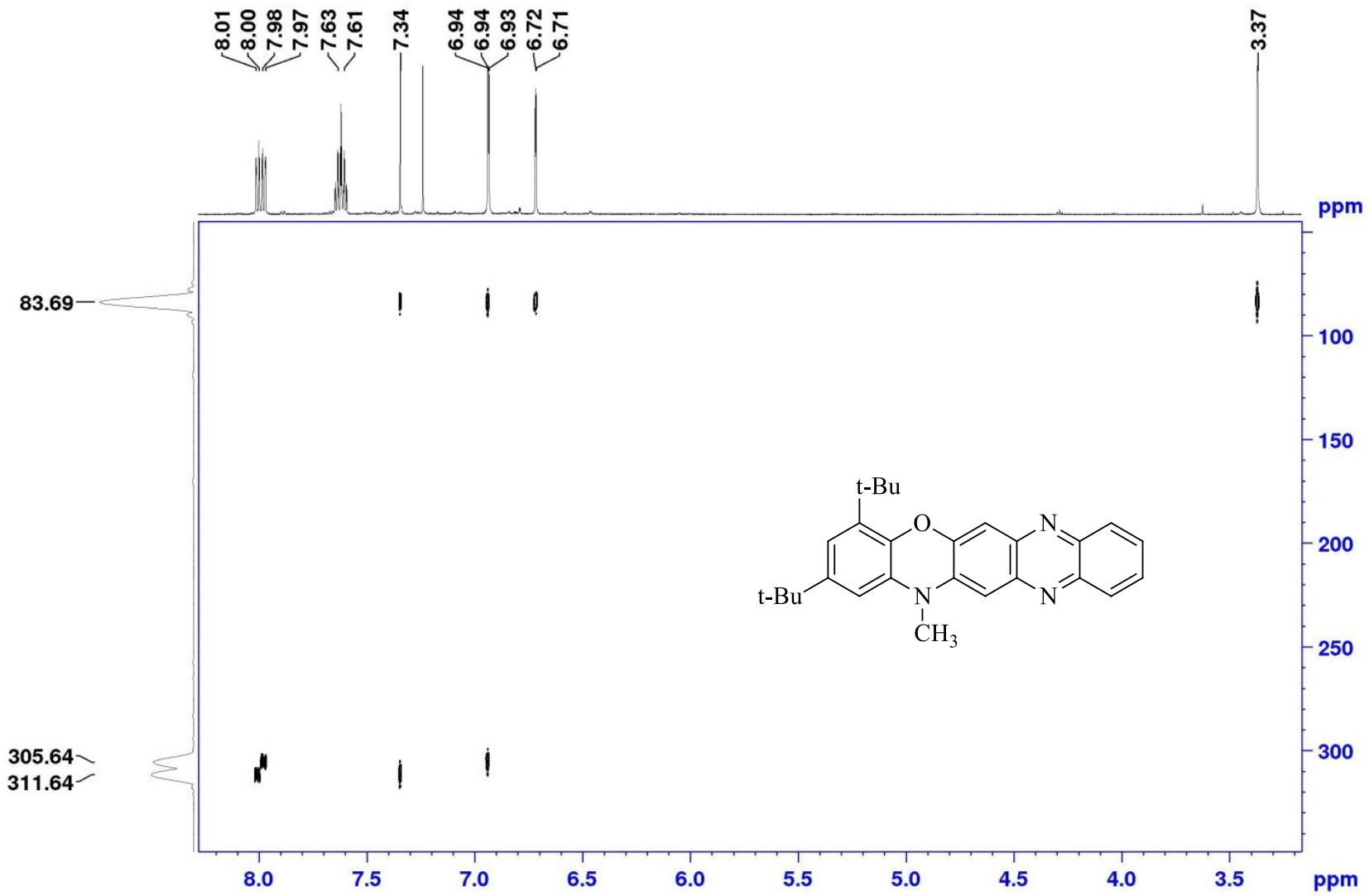


Figure S38: HMBC $^{1}H,^{15}N$ NMR spectrum of 2,4-di-*tert*-butyl-14-methyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6a**). 2,4-Di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**)

2,4-Di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**)

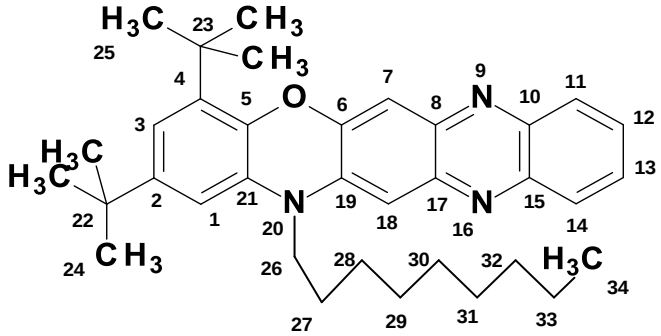


Table S11: Chemical shifts ^{1}H, ^{13}C, and ^{15}N of compound **6b** in $CDCl_3$ at 30°C δ (ppm) and spin–spin coupling constants *J* (Hz).

Compound	**15.** Nucleus	1	2	3	4	5	6	7	8	9(^{15}N)	10	11	12	13	14
6b	^{1}H	6.70		6.90				7.29				7.98	7.59	7.63	7.97
	J_{1H-1H}	2.1		2.1								8.1	8.1	8.1	8.1
	16. ^{13}C/^{15}N	108.41	136.82	117.25	146.04	139.44	144.76	108.99	143.16	310.36	141.91	128.89	128.17	129.08	129.02

Compound	**17.** Nucleus	15	16(^{15}N)	17	18	19	20(^{15}N)	21	22	23	24	25
6b	^{1}H				6.91						1.45	1.31
	J_{1H-1H}											
	18. ^{13}C/^{15}N	142.74	303.85	149.87	102.76	137.50	96.38	129.19	34.77	34.99	29.99	31.41

Compound	**19.** Nucleus	26	27	28	29	30	31	32	33	34
6b	^{1}H	3.79	1.85	1.53	1.50	1.42	1.35	1.32	1.28	0.89
	J_{1H-1H}	t,8.3	qvin,7.6							t,7.0
	20. ^{13}C/^{15}N	45.61	24.74	26.97	31.83	29.54	29.39	29.21	22.65	14.07

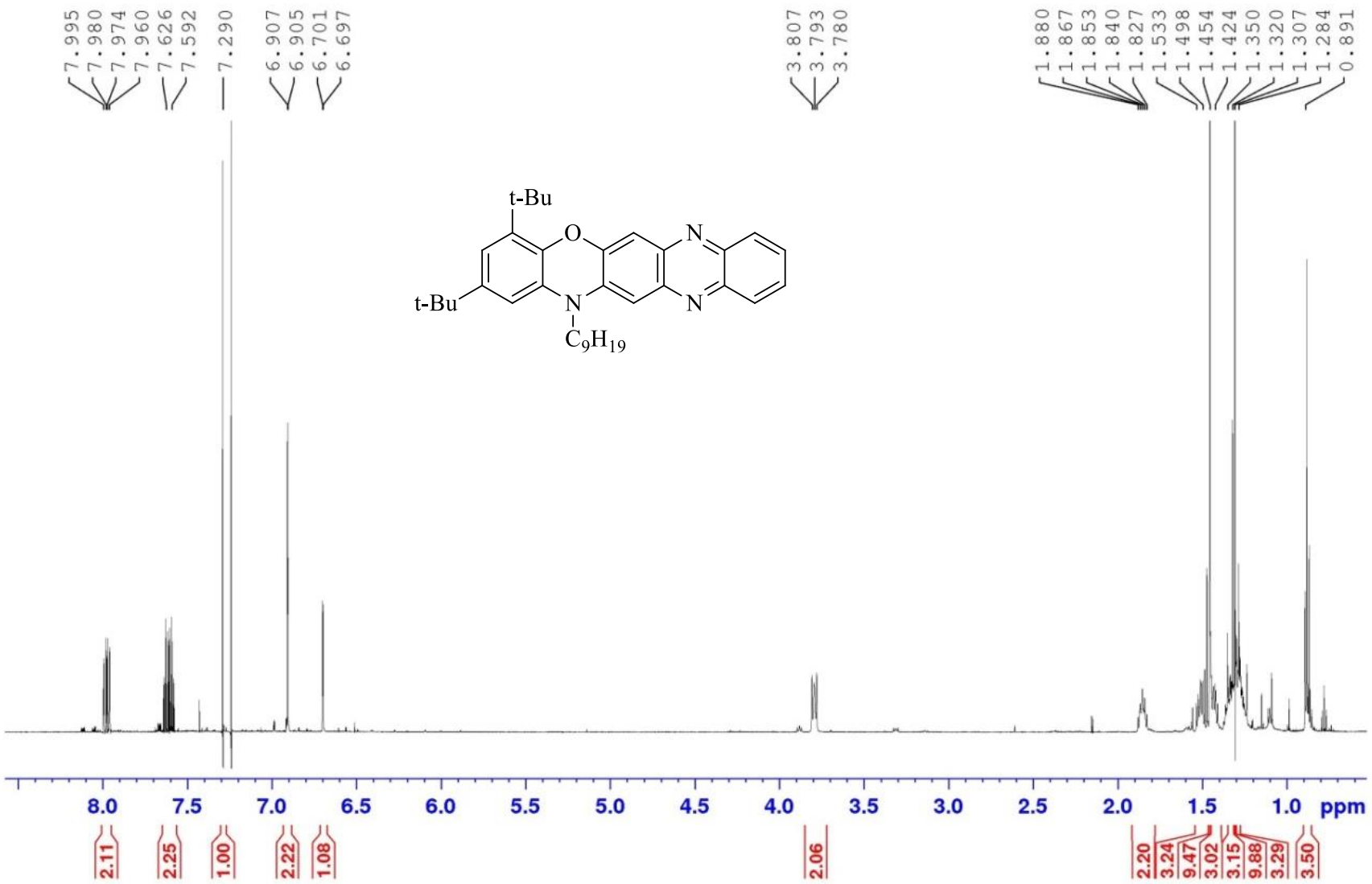


Figure S39: ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**).

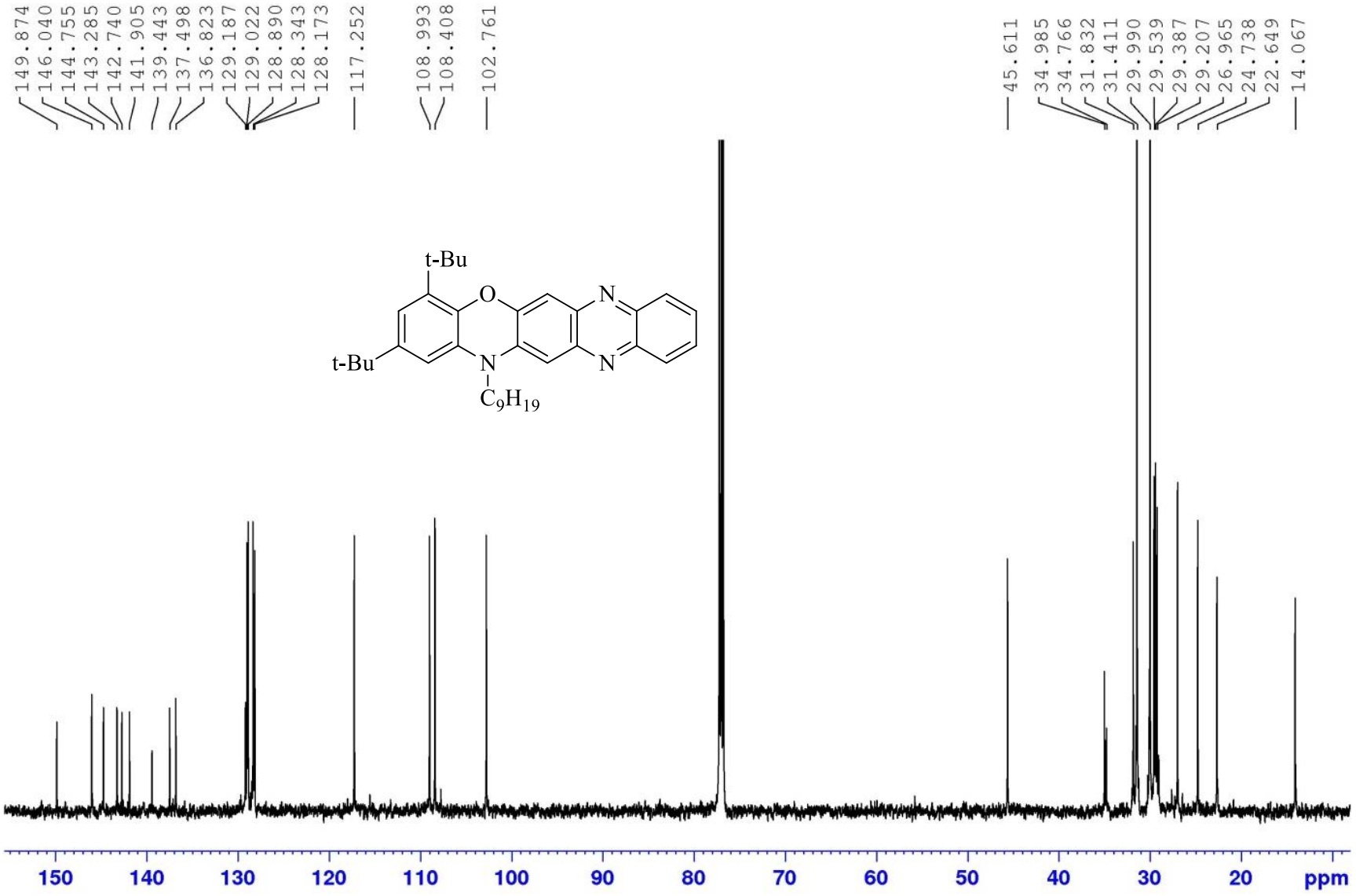


Figure S40: ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**).

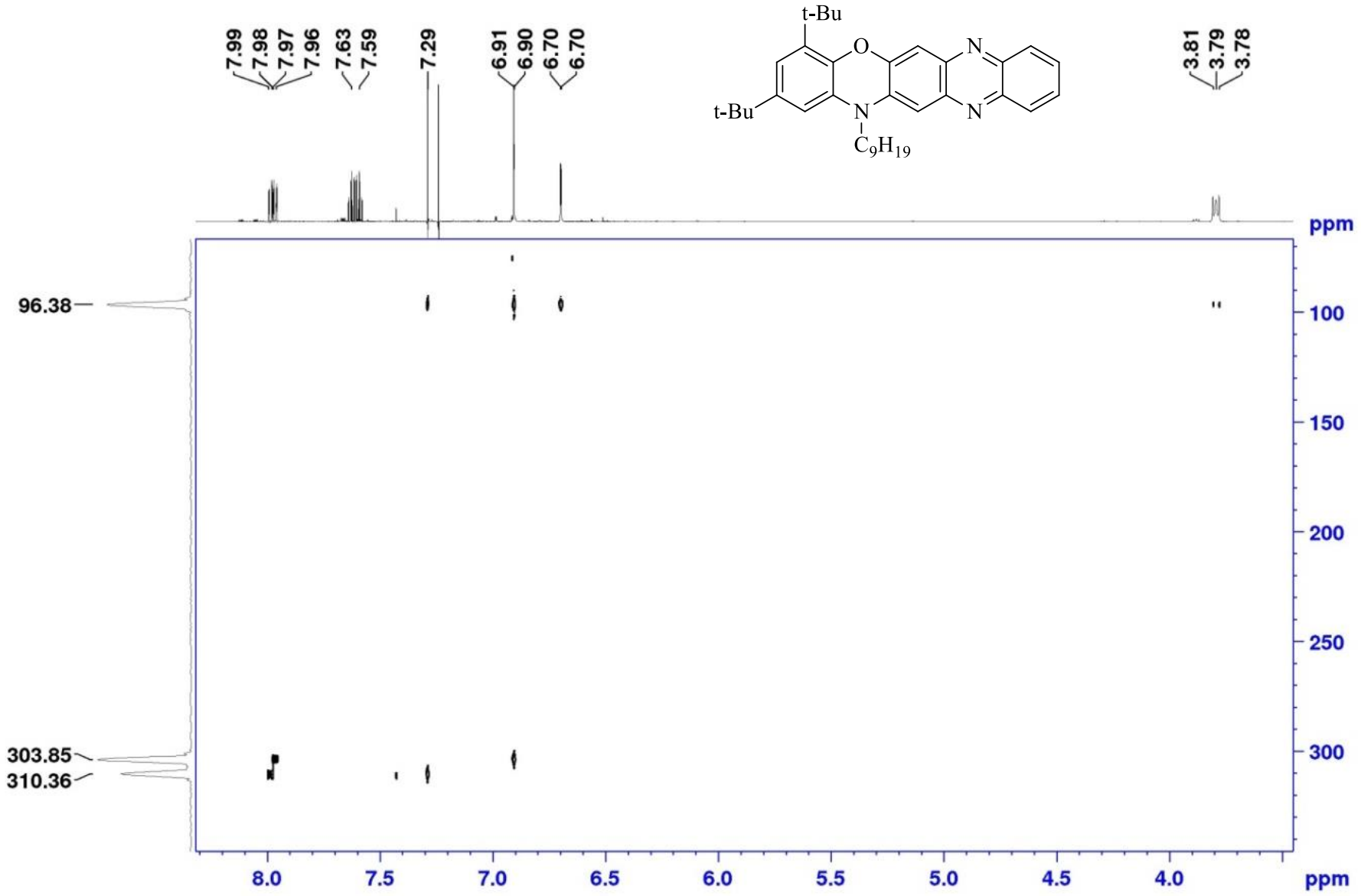


Figure S41: HMBC $^{1}H,^{15}N$ NMR spectrum of 2,4-di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**).

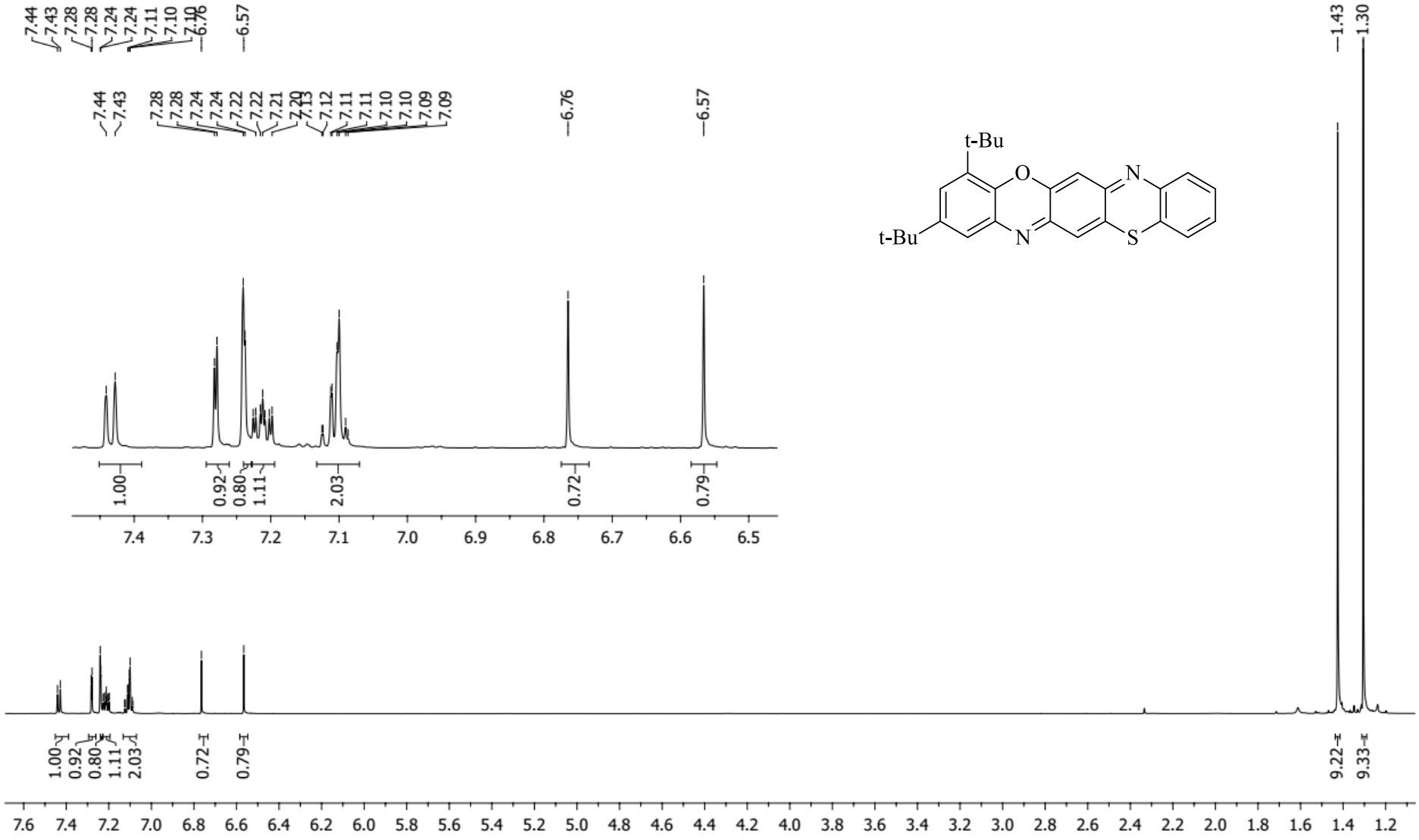


Figure S42: ^{1}H NMR spectrum of 2,4-di-*tert*-butylbenzo[5,6][1,4]oxazino[2,3-*b*]phenothiazine (**10c**).

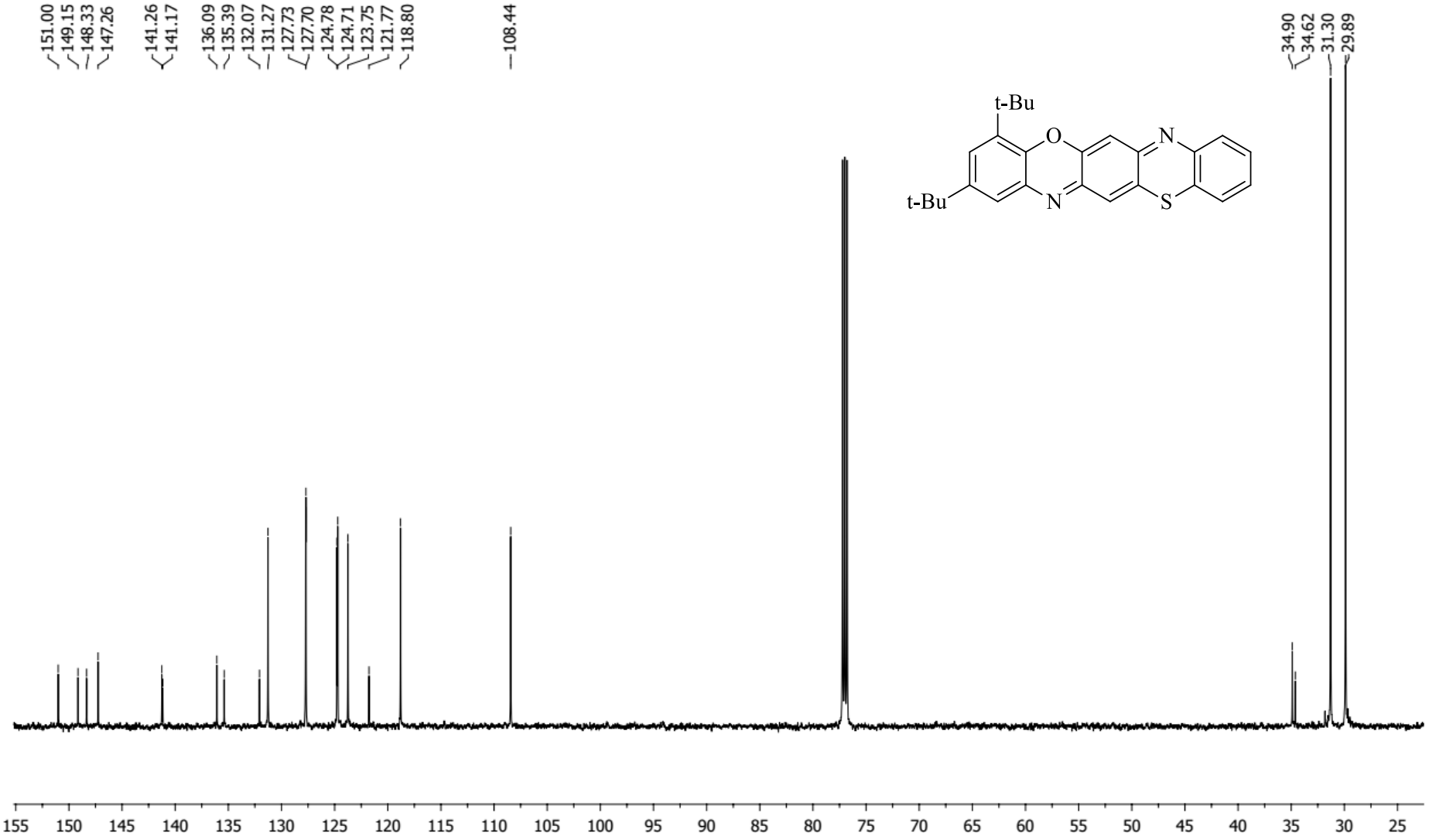


Figure S43: ^{13}C NMR spectrum of 2,4-di-*tert*-butylbenzo[5,6][1,4]oxazino[2,3-*b*]phenothiazine (**10c**).

7. HRMS spectra

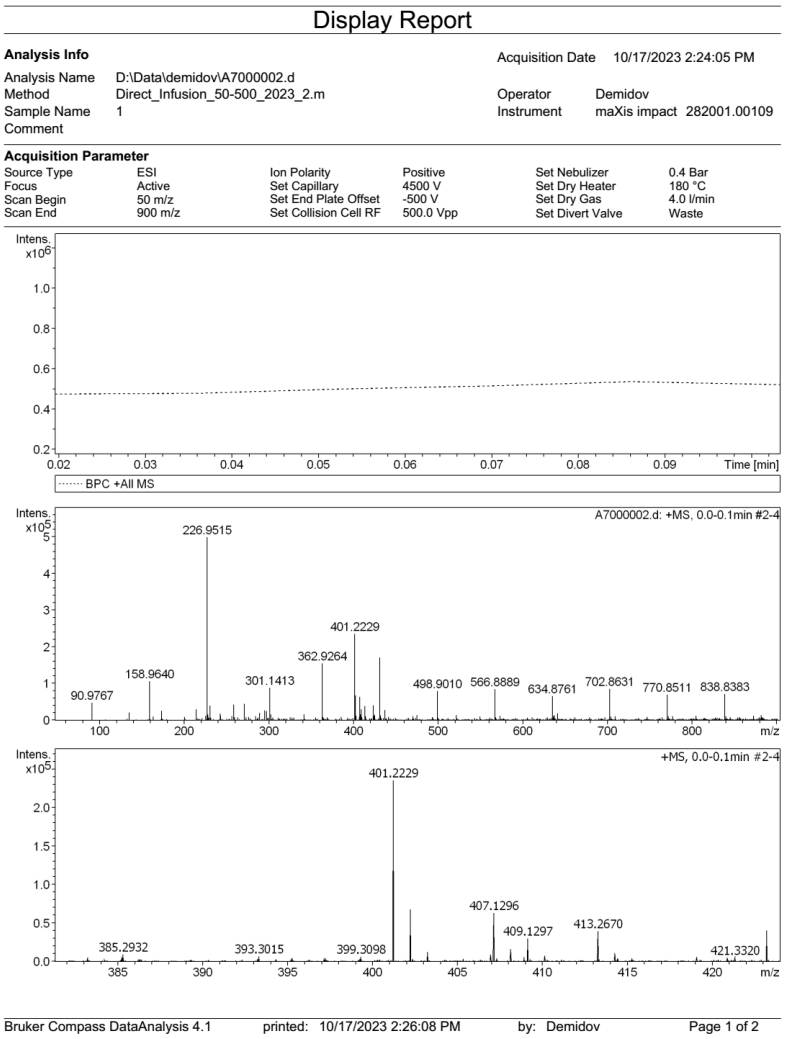
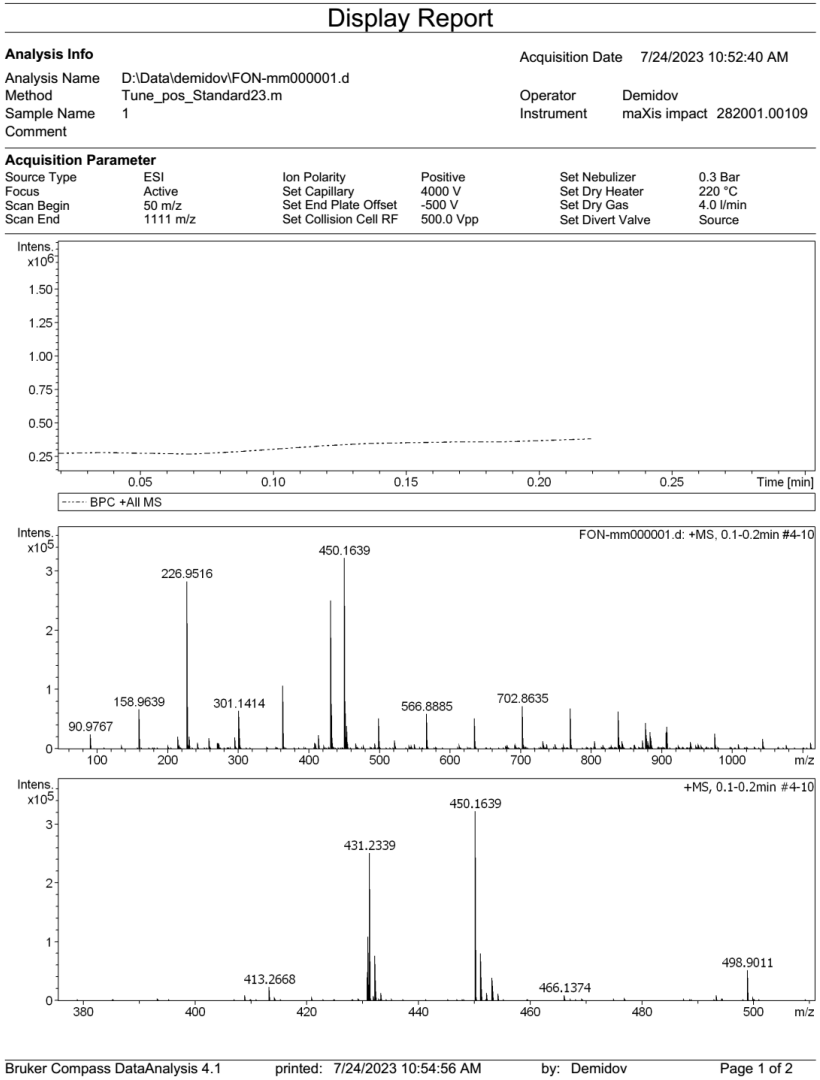


Figure S44: HRMS spectrum of 6,8-di-*tert*-butyl-2-(phenylamino)-3*H*-phenoxazin-3-one (**4a**).



Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
431.2339	1	C27H31N2O3	431.2329	-2.2	0.6	1	100.00	13.5	even	ok
	1	C30H32NaO	431.2345	1.5	12.3	1	100.00	14.5	even	ok
	1	C27H36KO2	431.2347	1.9	31.6	1	100.00	9.5	even	ok
	1	C27H31N2O3	431.2329	-2.2	0.6	1	100.00	13.5	even	ok

+MS, 0.1-0.2min #4-10

Figure S45: HRMS spectrum of 6,8-di-*tert*-butyl-2-((3-methoxyphenyl)amino)-3*H*-phenoxazin-3-one (**4c**).

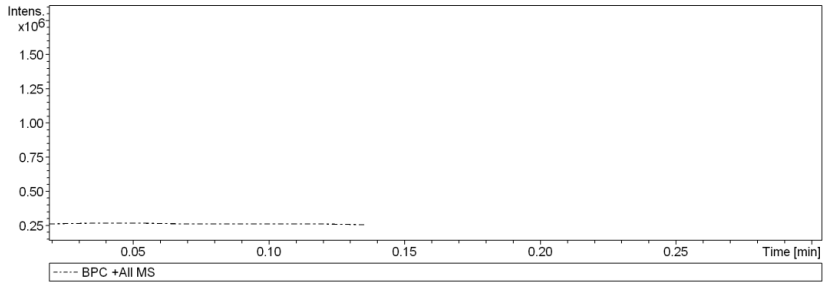
Display Report

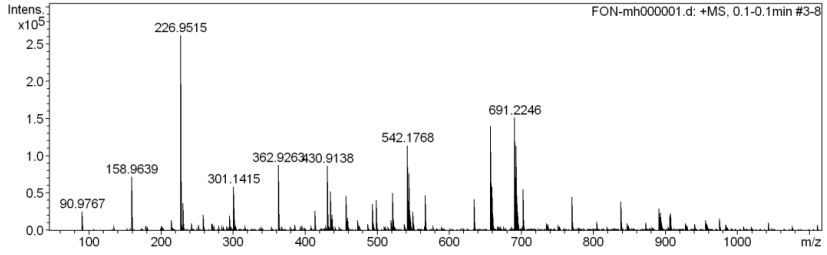
Analysis Info

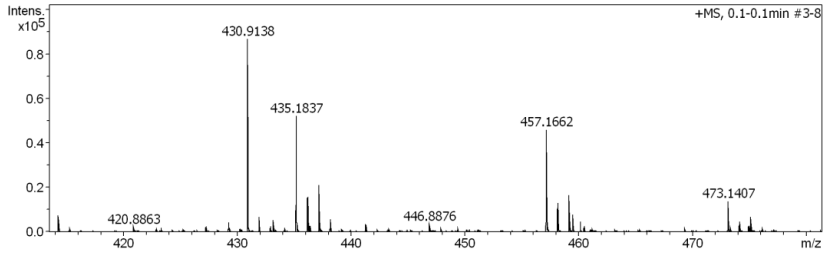
Analysis Name	D:\Data\demidov\FON-mh000001.d	Acquisition Date	7/24/2023 10:48:10 AM
Method	Tune_pos_Standard23.m	Operator	Demidov
Sample Name	1	Instrument	maXis impact 282001.00109
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source







Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e¯ Conf	N-Rule
435.1837	1	C26H28ClN2O2	435.1834	-0.7	18.1	1	100.00	13.5	even	ok
	1	C29H29ClNa	435.1850	3.0	18.9	1	100.00	14.5	even	ok
	1	C26H33ClKO	435.1852	3.3	15.7	1	100.00	9.5	even	ok
	1	C26H28ClN2O2	435.1834	-0.7	18.1	1	100.00	13.5	even	ok

+MS, 0.1-0.1min #3-8

Figure S46: HRMS spectrum of 6,8-di-*tert*-butyl-2-((3-chlorophenyl)amino)-3*H*-phenoxazin-3-one (**4d**).

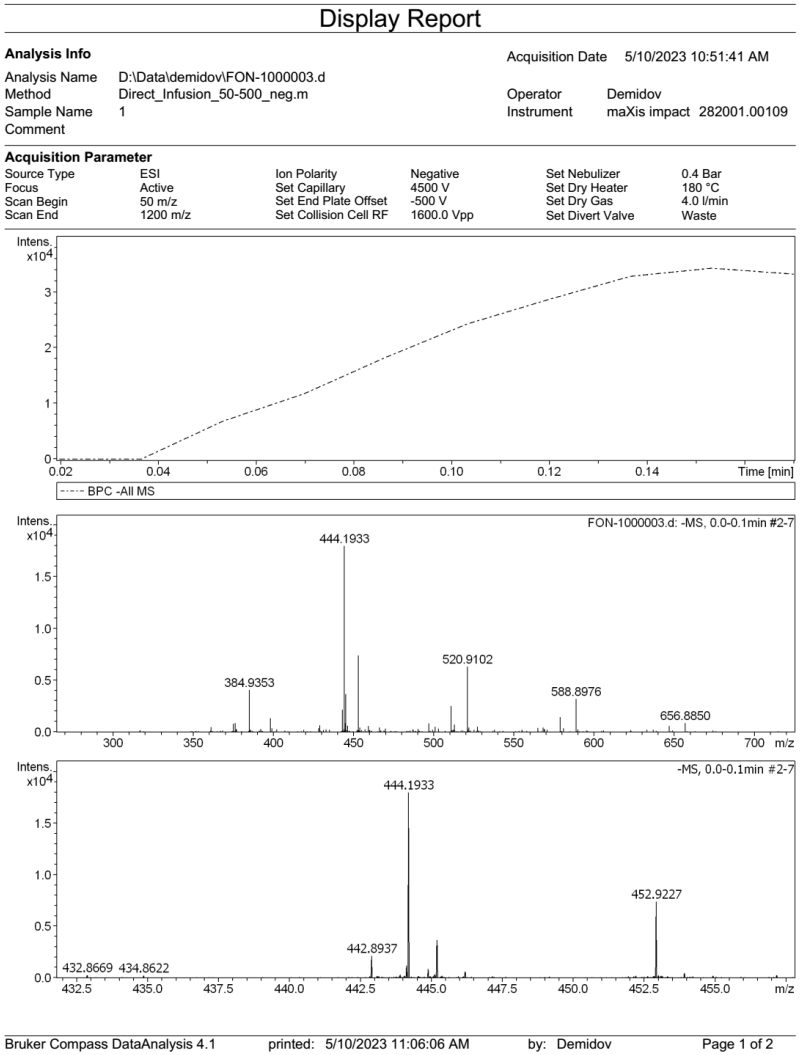


Figure S47: HRMS spectrum of 6,8-di-*tert*-butyl-2-((4-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4e**).

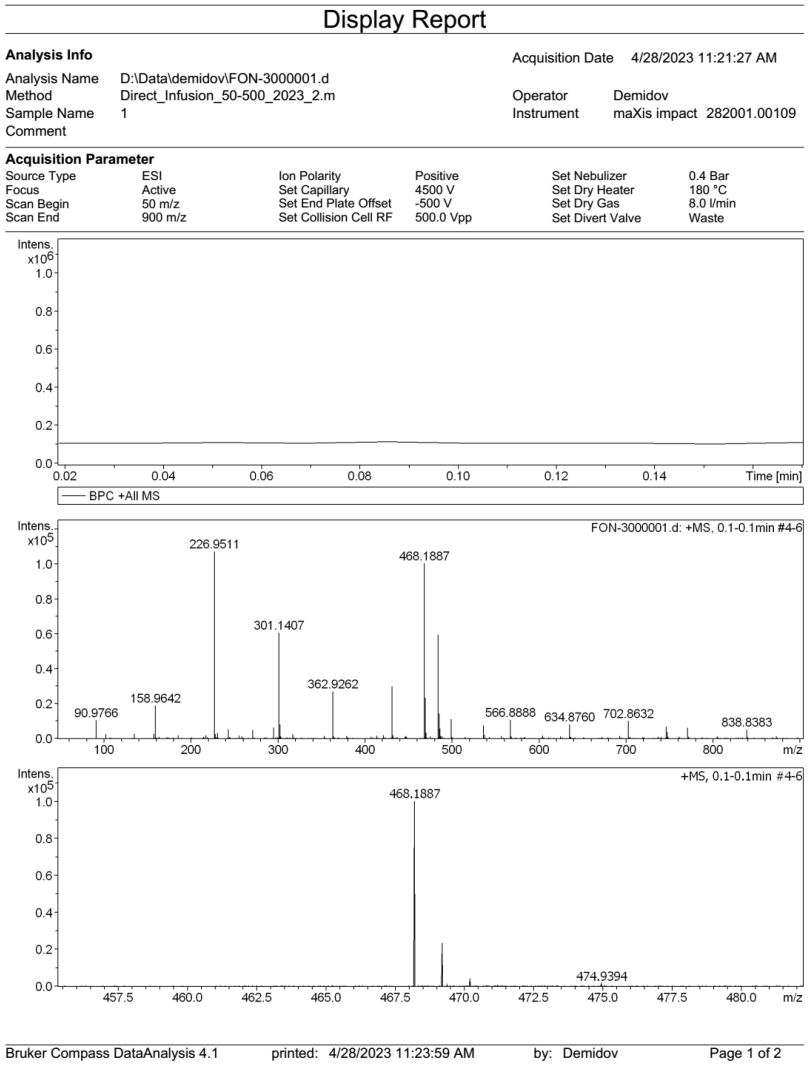


Figure S48: HRMS spectrum of 6,8-di-*tert*-butyl-2-((2-nitrophenyl)amino)-3*H*-phenoxazin-3-one (**4f**).

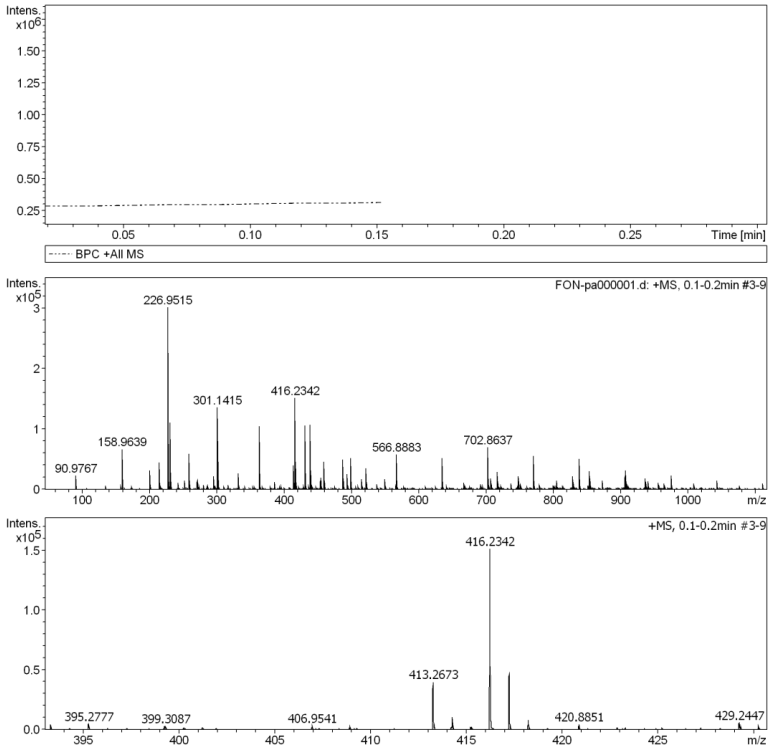
Display Report

Analysis Info

Analysis Name	D:\Data\demidov\FON-pa000001.d	Acquisition Date	7/24/2023 10:56:23 AM
Method	Tune_pos_Standard23.m	Operator	Demidov
Sample Name	1	Instrument	maXis impact 282001.00109
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1111 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Source



Bruker Compass DataAnalysis 4.1 printed: 7/24/2023 10:58:32 AM by: Demidov Page 1 of 2

Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
416.2342	1	C26H30N3O2	416.2333	-2.2	6.1	1	100.00	13.5	even	ok

+MS, 0.1-0.2min #3-9

Bruker Compass DataAnalysis 4.1 printed: 7/24/2023 10:58:32 AM by: Demidov Page 2 of 2

Figure S49: HRMS spectrum of 2-((4-aminophenyl)amino)-6,8-di-*tert*-butyl-3*H*-phenoxazin-3-one (**4g**).

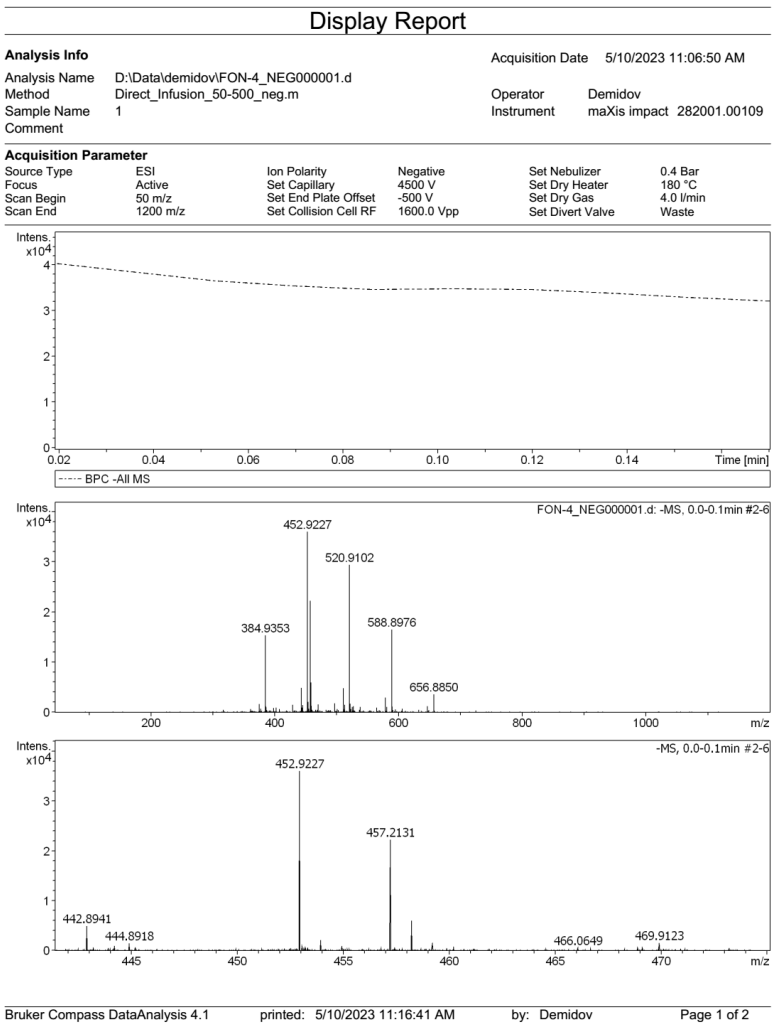


Figure S50: HRMS spectrum of methyl 4-((6,8-di-*tert*-butyl-3-oxo-3*H*-phenoxazin-2-yl)amino)benzoate (**4h**).

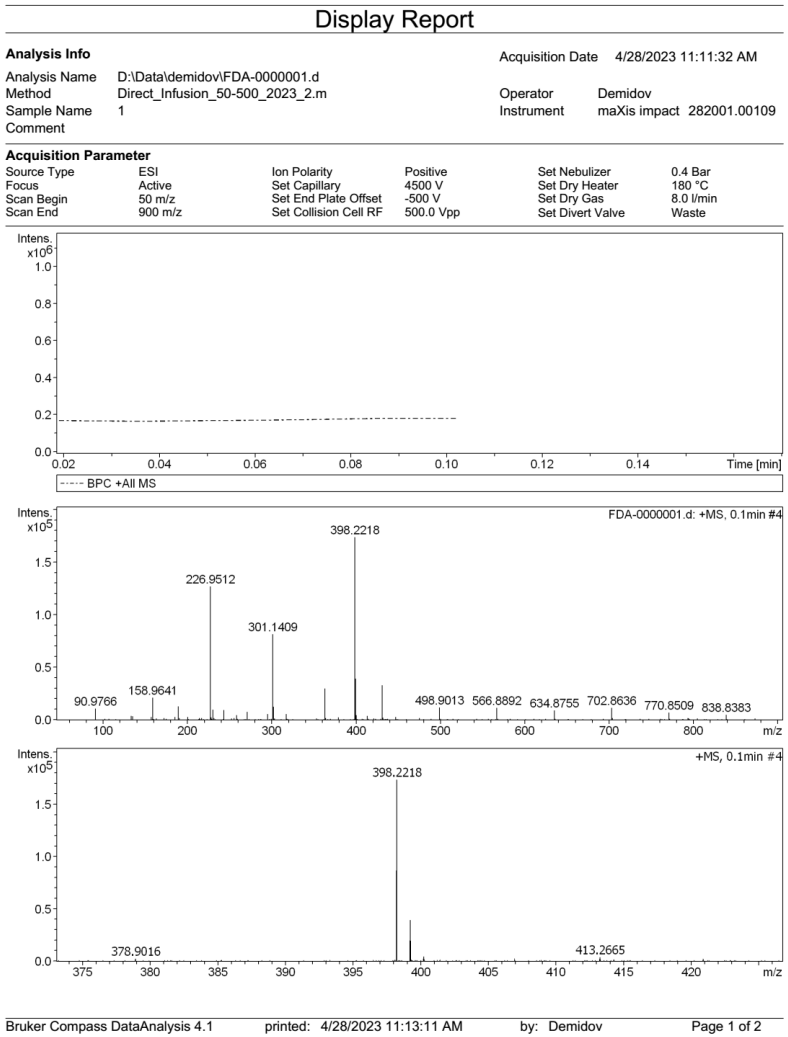


Figure S51: HRMS spectrum of 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5a**).

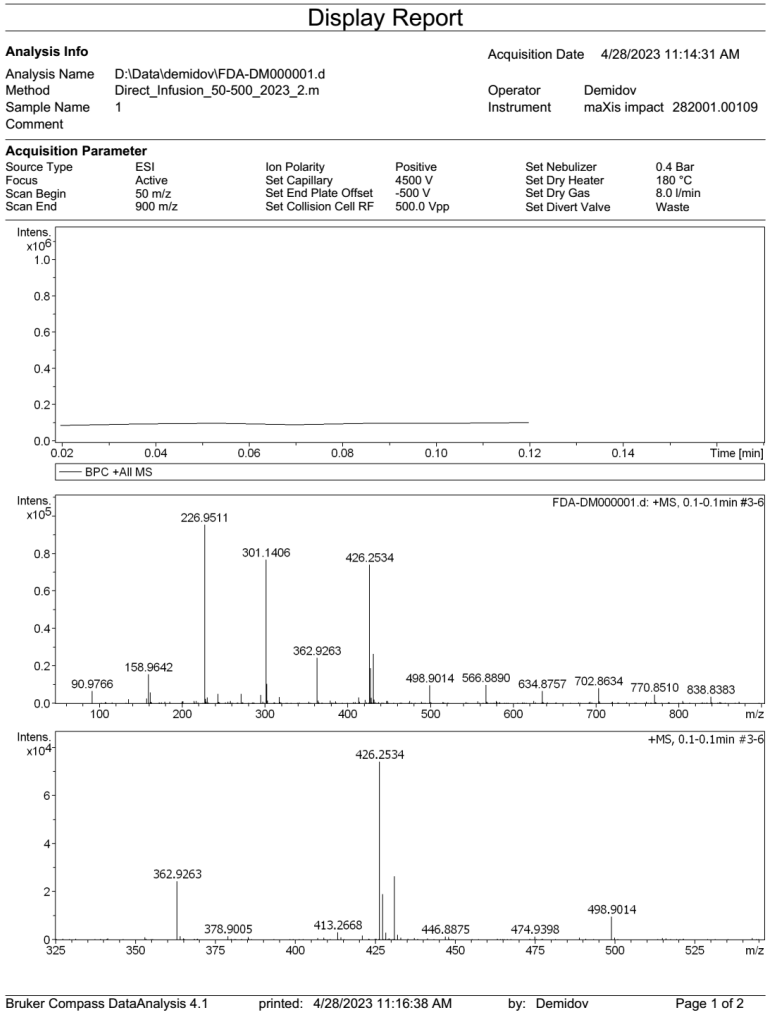


Figure S52: HRMS spectrum of 2,4-di-*tert*-butyl-9,10-dimethyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**5b**).

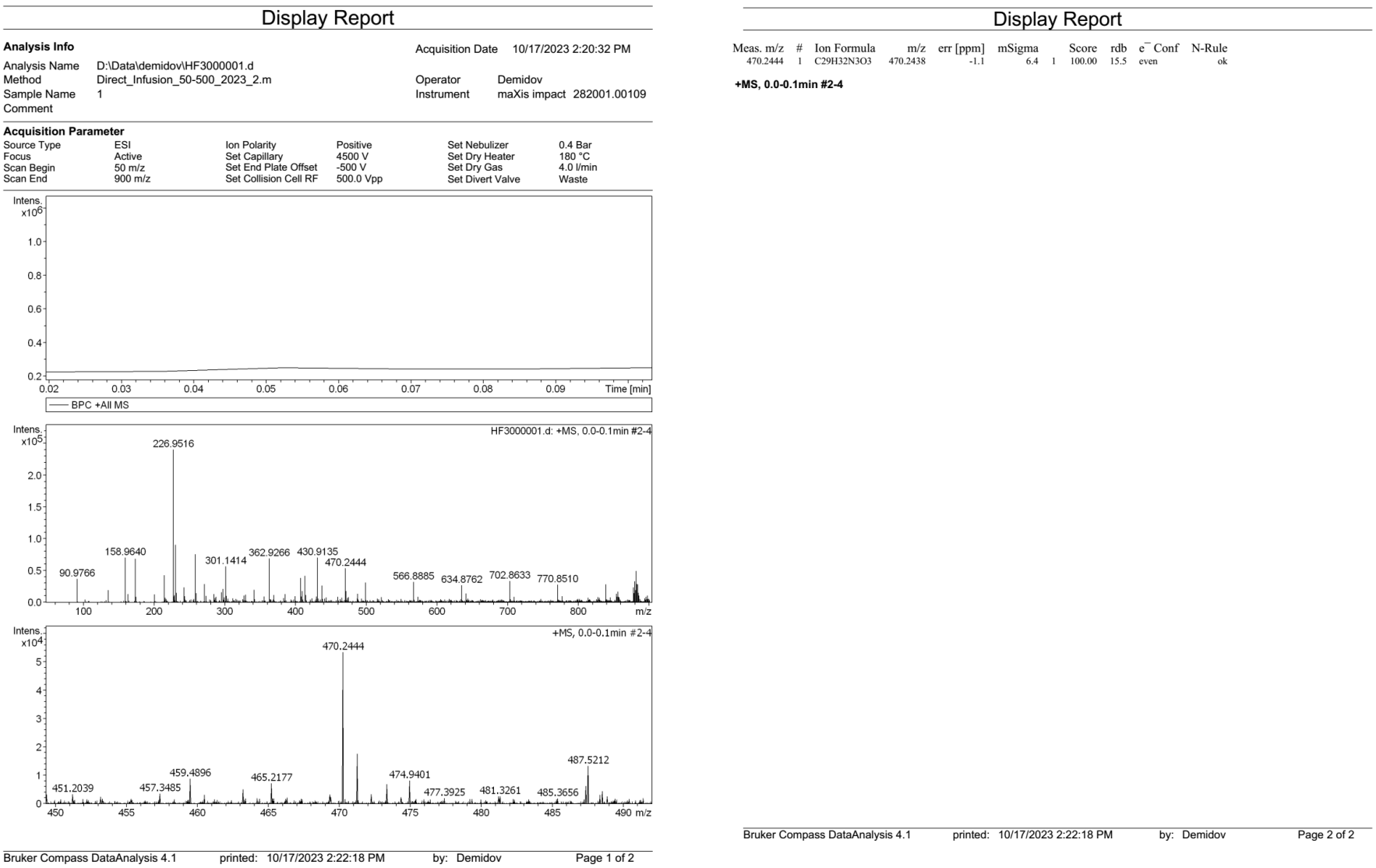


Figure S53: HRMS spectrum of ethyl 2,4-di-*tert*-butyl-14*H*-quinoxalino[2,3-*b*]phenoxazine-10-carboxylate (**5c**).

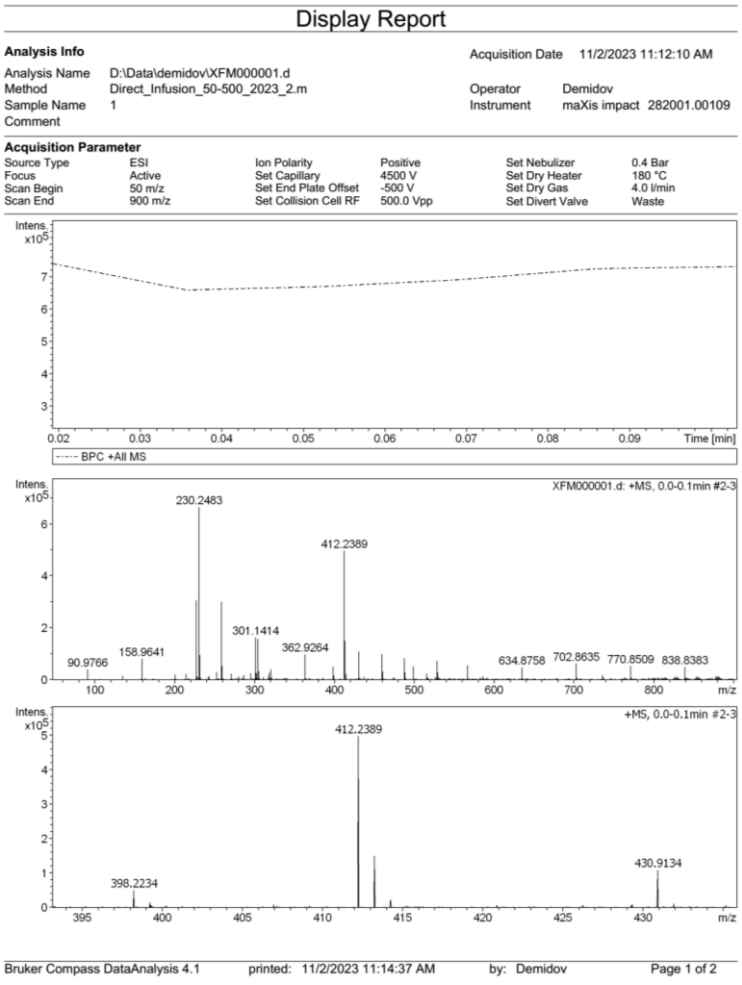


Figure S54: HRMS spectrum of 2,4-di-*tert*-butyl-14-methyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6a**).

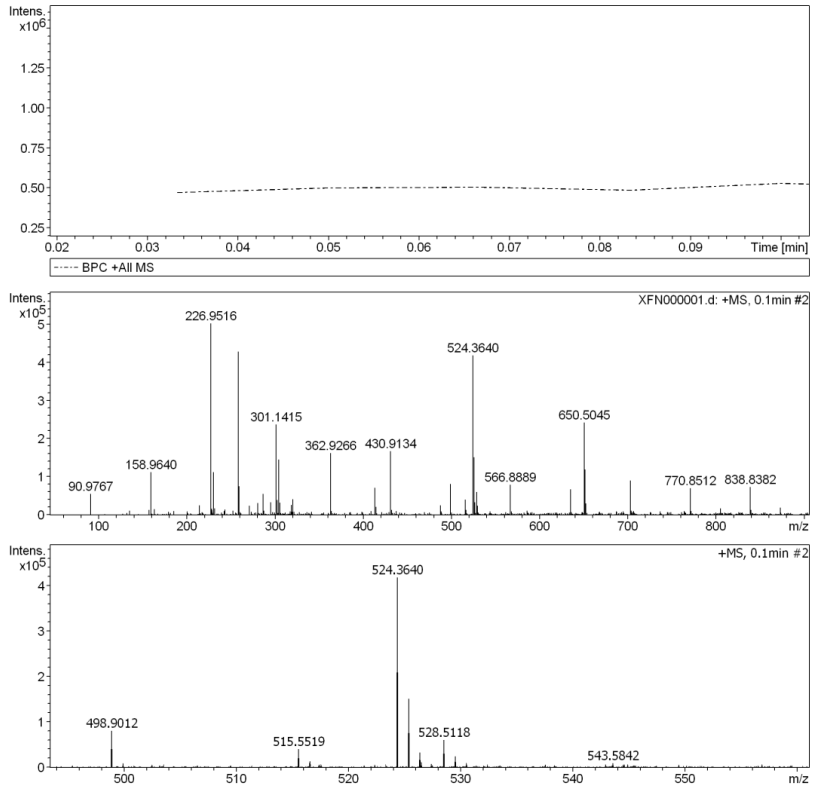
Display Report

Analysis Info

Analysis Name	D:\Data\demidov\XFN000001.d	Acquisition Date	11/2/2023 11:22:25 AM
Method	Direct_Infusion_50-500_2023_2.m	Operator	Demidov
Sample Name	1	Instrument	maXis impact 282001.00109
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	900 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
524.3640	1	C35H46N3O	524.3635	-0.9	16.7	1	100.00	14.5	even	ok
	1	C35H46N3O	524.3635	-0.9	16.7	1	100.00	14.5	even	ok

+MS, 0.1min #2

Figure S55: HRMS spectrum of 2,4-di-*tert*-butyl-14-nonyl-14*H*-quinoxalino[2,3-*b*]phenoxazine (**6b**).

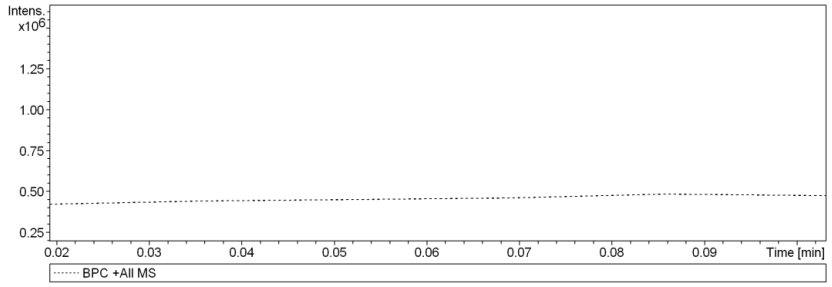
Display Report

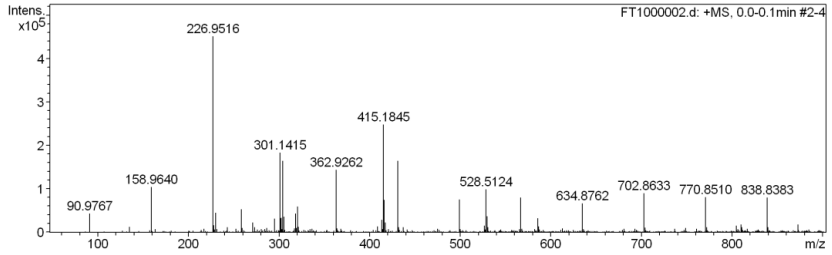
Analysis Info

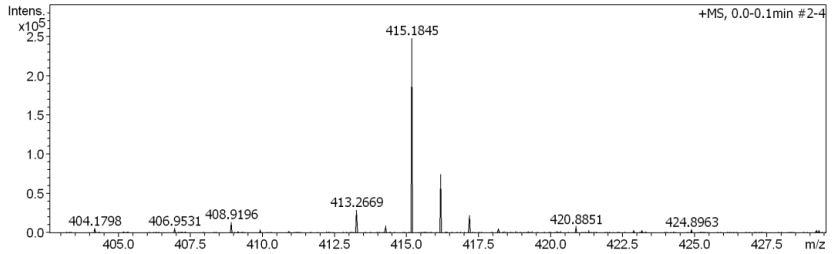
Analysis Name	D:\Data\demidov\FT1000002.d	Acquisition Date	11/2/2023 11:18:59 AM
Method	Direct_Infusion_50-500_2023_2.m	Operator	Demidov
Sample Name	1	Instrument	maXis impact 282001.00109
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	900 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste







Display Report

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e⁻ Conf	N-Rule
415.1845	1	C26H27N2OS	415.1839	-1.5	1.0	1	100.00	14.5	even	ok
	1	C26H27N2OS	415.1839	-1.5	1.0	1	100.00	14.5	even	ok

+MS, 0.0-0.1min #2-4

Figure S56: HRMS spectrum of 2,4-di-*tert*-butylbenzo[5,6][1,4]oxazino[2,3-*b*]phenothiazine (**10c**).

8. Cartesian coordinates of compounds **1**, **7b** (7*H*-tautomer), **7** (12*H*-tautomer), and **7a** (14*H*-tautomer) calculated by the DFT B3LYP/6-311++G(d,p) method.

1

8	-6.085914609	0.070266272	0.000220138
6	-3.432254221	-2.333867993	-0.000050801
1	-3.233269287	-3.399345746	-0.000087314
6	-4.679886954	-1.828604793	0.000047626
6	-4.937481442	-0.368508982	0.000064560
8	-1.435138224	0.806511637	-0.000202675
7	-1.075598268	-1.969048435	-0.000128590
6	-0.164132791	0.290885030	-0.000076202
6	-3.766159244	0.504184208	0.000038630
1	-3.927754100	1.574715074	0.000076731
6	-2.519756848	-0.021159152	-0.000068793
6	-2.273220576	-1.462171773	-0.000099485
6	0.003988409	-1.104431549	-0.000083610
6	0.931818163	1.172884859	0.000014288
6	2.412566175	-0.826291753	0.000030692
6	3.853123174	-1.366529336	0.000049213
6	1.299496866	-1.648703049	-0.000032280
1	1.369106429	-2.727568987	-0.000044451
6	2.189739690	0.567156829	0.000060855
1	3.055412814	1.212815516	0.000114302
6	0.761523633	2.706890857	0.000003704
6	4.593360123	-0.865925012	1.262442288
1	4.091590552	-1.208398474	2.171580972
1	5.618226698	-1.248946151	1.275589167
1	4.647482256	0.224697127	1.300075786
6	2.122183335	3.431759440	-0.000016934
1	2.715907508	3.196796274	-0.887759395
1	1.949107978	4.510770901	-0.000261943
1	2.715728646	3.197151882	0.887937198
6	-0.001477992	3.157169365	-1.269517387
1	-1.005085929	2.736895736	-1.317002050

1	-0.091806961	4.247408380	-1.278447783
1	0.539236379	2.858361494	-2.172101683
6	4.593473896	-0.865722337	-1.262193045
1	4.647592854	0.224905623	-1.299656678
1	5.618345762	-1.248732363	-1.275299707
1	4.091795872	-1.208060329	-2.171433332
6	-0.001469525	3.157253505	1.269497808
1	0.539223679	2.858484263	2.172108033
1	-0.091728643	4.247494636	1.278339831
1	-1.005092808	2.737021680	1.317009458
6	3.891731417	-2.905676819	-0.000075143
1	3.408376156	-3.325498002	-0.886372950
1	4.931019659	-3.244498958	-0.000051330
1	3.408290429	-3.325646172	0.886106245
1	-5.557087675	-2.465251591	0.000115890

7b

8	-0.464808000	1.056262000	-0.000042000
7	-0.494079000	-1.740064000	-0.000063000
6	-1.682062000	0.389788000	-0.000032000
6	1.856869000	1.103520000	0.000006000
1	1.819862000	2.187196000	0.000038000
6	0.685142000	0.375352000	-0.000032000
6	0.665656000	-1.077008000	-0.000057000
6	-1.653118000	-1.018856000	-0.000043000
6	-2.867507000	1.142053000	-0.000011000
6	-4.089862000	-1.013205000	0.000007000
6	-5.454457000	-1.727334000	0.000033000
6	-2.890149000	-1.700621000	-0.000028000
1	-2.836307000	-2.780223000	-0.000040000
6	-4.049297000	0.399724000	0.000009000
1	-4.986930000	0.934919000	0.000015000
6	-2.871831000	2.686160000	-0.000001000
6	-6.250559000	-1.320432000	1.262091000
1	-5.711893000	-1.603912000	2.170506000

1	-7.223583000	-1.821396000	1.273535000
1	-6.430682000	-0.243614000	1.301924000
6	-4.304415000	3.255975000	0.000027000
1	-4.867370000	2.954078000	-0.887047000
1	-4.252139000	4.347843000	0.000072000
1	-4.867365000	2.954007000	0.887080000
6	-2.166206000	3.222127000	-1.269581000
1	-1.122231000	2.914957000	-1.320605000
1	-2.198562000	4.316203000	-1.279286000
1	-2.670950000	2.863535000	-2.171030000
6	-6.250649000	-1.320366000	-1.261944000
1	-6.430772000	-0.243546000	-1.301706000
1	-7.223674000	-1.821330000	-1.273346000
1	-5.712045000	-1.603798000	-2.170410000
6	-2.166161000	3.222102000	1.269561000
1	-2.670902000	2.863527000	2.171019000
1	-2.198478000	4.316179000	1.279266000
1	-1.122197000	2.914892000	1.320566000
6	-5.307660000	-3.259363000	-0.000012000
1	-4.775455000	-3.616360000	-0.885616000
1	-6.298031000	-3.722940000	-0.000014000
1	-4.775434000	-3.616414000	0.885558000
7	4.308906000	-1.692847000	-0.000009000
7	4.251536000	1.076021000	0.000008000
6	5.457221000	-0.981621000	0.000011000
6	1.910316000	-1.731357000	-0.000087000
1	1.925721000	-2.812873000	-0.000093000
6	3.127014000	-1.043951000	-0.000034000
6	3.076483000	0.415714000	-0.000012000
6	5.485314000	0.442824000	0.000020000
6	6.712957000	-1.643567000	0.000028000
6	7.887638000	0.479425000	0.000044000
6	6.683289000	1.163453000	0.000028000
1	6.661802000	2.249414000	0.000020000
6	7.893029000	-0.929566000	0.000045000
1	8.839523000	-1.458122000	0.000058000

1	8.821244000	1.028385000	0.000062000
1	6.703729000	-2.726633000	0.000021000
1	4.235079000	2.088361000	0.000011000

7

8	-0.480028000	1.099783000	0.000049000
7	-0.471477000	-1.707225000	0.000052000
6	-1.680494000	0.415672000	0.000031000
6	1.859125000	1.123684000	-0.000101000
1	1.859997000	2.205769000	-0.000088000
6	0.695781000	0.421193000	-0.000038000
6	0.656634000	-1.038006000	-0.000008000
6	-1.652983000	-0.988157000	0.000052000
6	-2.878798000	1.148812000	0.000005000
6	-4.083933000	-1.018054000	0.000031000
6	-5.439483000	-1.749080000	0.000042000
6	-2.870817000	-1.688865000	0.000050000
1	-2.801720000	-2.767817000	0.000064000
6	-4.052857000	0.390463000	0.000005000
1	-4.995234000	0.918125000	-0.000018000
6	-2.903525000	2.692626000	-0.000020000
6	-6.241269000	-1.352985000	1.261792000
1	-5.699541000	-1.629777000	2.170466000
1	-7.208408000	-1.865320000	1.272922000
1	-6.434052000	-0.278359000	1.301564000
6	-4.343375000	3.243680000	-0.000083000
1	-4.902877000	2.935357000	-0.887420000
1	-4.304721000	4.336035000	-0.000089000
1	-4.902951000	2.935373000	0.887212000
6	-2.203537000	3.236543000	-1.269414000
1	-1.156774000	2.940071000	-1.319157000
1	-2.247140000	4.330145000	-1.277332000
1	-2.705463000	2.874288000	-2.171229000
6	-6.241252000	-1.353056000	-1.261742000
1	-6.434041000	-0.278434000	-1.301573000
1	-7.208386000	-1.865399000	-1.272856000

1	-5.699507000	-1.629895000	-2.170392000
6	-2.203628000	3.236581000	1.269407000
1	-2.705658000	2.874395000	2.171194000
1	-2.247185000	4.330184000	1.277263000
1	-1.156885000	2.940062000	1.319266000
6	-5.271781000	-3.279063000	0.000084000
1	-4.734946000	-3.628971000	-0.885720000
1	-6.255638000	-3.756257000	0.000095000
1	-4.734949000	-3.628922000	0.885908000
7	4.324949000	-1.633719000	-0.000342000
7	4.235963000	1.142199000	-0.000068000
6	5.519358000	-0.936616000	-0.000087000
6	1.914543000	-1.714944000	-0.000061000
1	1.893764000	-2.799008000	-0.000066000
6	3.093754000	-1.020970000	-0.000140000
6	3.122536000	0.447319000	-0.000115000
6	5.442839000	0.478131000	-0.000008000
6	6.758119000	-1.585458000	-0.000002000
6	7.869726000	0.566430000	0.000242000
6	6.642740000	1.210953000	0.000157000
1	6.569370000	2.291848000	0.000215000
6	7.925941000	-0.833899000	0.000170000
1	8.884913000	-1.338732000	0.000244000
1	8.786173000	1.144297000	0.000371000
1	6.799630000	-2.670238000	-0.000070000
1	4.356242000	-2.643466000	-0.000150000

7a

8	-0.440561000	1.072076000	-0.004362000
7	-0.461801000	-1.687132000	-0.004956000
6	-1.656000000	0.399397000	-0.002257000
6	1.904136000	1.106772000	-0.001386000
1	1.882199000	2.188842000	-0.001062000
6	0.747729000	0.389810000	-0.002803000
6	0.761669000	-1.052090000	-0.003308000

6	-1.674506000	-0.996200000	-0.002727000
6	-2.845133000	1.145638000	-0.000275000
6	-4.096040000	-0.986191000	0.000630000
6	-5.461072000	-1.699746000	0.002126000
6	-2.890188000	-1.681512000	-0.001208000
1	-2.864744000	-2.764150000	-0.001597000
6	-4.039499000	0.414833000	0.001053000
1	-4.969700000	0.962518000	0.002504000
6	-2.841198000	2.689891000	0.000224000
6	-6.255427000	-1.292063000	1.264906000
1	-5.717141000	-1.575965000	2.173452000
1	-7.229836000	-1.790202000	1.277018000
1	-6.431532000	-0.214879000	1.303791000
6	-4.270253000	3.268928000	0.002543000
1	-4.837353000	2.972995000	-0.884136000
1	-4.208590000	4.360112000	0.002574000
1	-4.834542000	2.972773000	0.890939000
6	-2.133969000	3.220462000	-1.270831000
1	-1.094041000	2.902241000	-1.324242000
1	-2.155650000	4.314624000	-1.276757000
1	-2.646911000	2.870307000	-2.171276000
6	-6.258235000	-1.291799000	-1.258800000
1	-6.434218000	-0.214577000	-1.297158000
1	-7.232760000	-1.789768000	-1.268777000
1	-5.722054000	-1.575690000	-2.168596000
6	-2.130178000	3.219646000	1.269498000
1	-2.640106000	2.868521000	2.171272000
1	-2.152247000	4.313794000	1.276433000
1	-1.089952000	2.901816000	1.319321000
6	-5.318372000	-3.232533000	0.001808000
1	-4.790837000	-3.592386000	-0.886074000
1	-6.309581000	-3.693620000	0.002932000
1	-4.788726000	-3.592558000	0.888363000
7	4.345272000	-1.681206000	-0.000547000
7	4.288708000	1.157984000	0.000590000
6	5.481134000	-0.957918000	0.000619000

6	1.959906000	-1.719047000	-0.002397000
1	1.997436000	-2.802539000	-0.002753000
6	3.193557000	-1.008480000	-0.001159000
6	3.168105000	0.440634000	-0.000595000
6	5.454016000	0.480916000	0.001219000
6	6.739956000	-1.623091000	0.001267000
6	7.876543000	0.522268000	0.003088000
6	6.683663000	1.197193000	0.002484000
1	6.637039000	2.279869000	0.002933000
6	7.904099000	-0.899839000	0.002460000
1	8.859827000	-1.411934000	0.002938000
1	8.811108000	1.071811000	0.004054000
1	6.738309000	-2.706754000	0.000776000
1	-0.482823000	-2.694588000	-0.004656000

7Hmod

8	-2.358639000	1.339421000	0.000001000
7	-2.401241000	-1.475812000	-0.000024000
6	-3.565892000	0.662517000	-0.000009000
6	-0.038806000	1.368303000	0.000013000
1	-0.073626000	2.452041000	0.000023000
6	-1.213275000	0.647349000	0.000001000
6	-1.241614000	-0.809341000	-0.000013000
6	-3.554476000	-0.748197000	-0.000022000
6	-4.729935000	1.415865000	-0.000007000
6	-5.986388000	-0.650136000	-0.000030000
6	-4.815316000	-1.387905000	-0.000032000
1	-4.825793000	-2.471203000	-0.000042000
6	-5.953030000	0.753029000	-0.000017000
1	-6.874449000	1.322334000	-0.000016000
7	2.399058000	-1.438970000	-0.000004000
7	2.355809000	1.329311000	0.000023000
6	3.550575000	-0.734017000	0.000008000
6	0.000829000	-1.466502000	-0.000015000
1	0.011999000	-2.548043000	-0.000025000
6	1.220662000	-0.784478000	-0.000003000

6	1.177952000	0.675157000	0.000011000
6	3.585523000	0.690542000	0.000022000
6	4.802790000	-1.403235000	0.000007000
6	5.987451000	0.714191000	0.000032000
6	4.787755000	1.405055000	0.000033000
1	4.772342000	2.491023000	0.000044000
6	5.985924000	-0.695439000	0.000019000
1	6.929877000	-1.228375000	0.000018000
1	6.924127000	1.257889000	0.000041000
1	4.787545000	-2.486198000	-0.000003000
1	2.344128000	2.341902000	0.000032000
1	-4.665082000	2.497575000	0.000003000
1	-6.941710000	-1.162565000	-0.000038000

12Hmod

8	2.379513000	-1.377400000	0.000023000
7	2.381743000	1.448286000	-0.000025000
6	3.567942000	-0.683568000	-0.000003000
6	0.041403000	-1.383348000	-0.000002000
1	0.038279000	-2.465430000	0.000019000
6	1.207473000	-0.688019000	-0.000002000
6	1.254004000	0.775286000	-0.000021000
6	3.557826000	0.722994000	-0.000022000
6	4.746974000	-1.415524000	-0.000001000
6	5.985065000	0.664329000	-0.000039000
6	4.798737000	1.383758000	-0.000040000
1	4.790600000	2.467238000	-0.000055000
6	5.961879000	-0.735167000	-0.000020000
1	6.889049000	-1.295821000	-0.000020000
7	-2.412023000	1.384341000	-0.000096000
7	-2.335351000	-1.391202000	0.000022000
6	-3.609127000	0.692828000	-0.000011000
6	-0.001569000	1.455207000	-0.000037000
1	0.023689000	2.539108000	-0.000056000
6	-1.184128000	0.766423000	-0.000042000

6	-1.219227000	-0.701453000	-0.000013000
6	-3.538933000	-0.722353000	0.000034000
6	-4.845252000	1.347168000	0.000004000
6	-5.965566000	-0.800747000	0.000112000
6	-4.741916000	-1.450607000	0.000095000
1	-4.672940000	-2.531754000	0.000129000
6	-6.015572000	0.600254000	0.000068000
1	-6.972491000	1.108922000	0.000083000
1	-6.884659000	-1.374320000	0.000161000
1	-4.882394000	2.432052000	-0.000034000
1	-2.438881000	2.394356000	-0.000039000
1	6.933893000	1.188037000	-0.000053000
1	4.699090000	-2.497922000	0.000014000

14Hmod

8	2.328274000	-1.365100000	-0.003095000
7	2.367159000	1.412658000	-0.002794000
6	3.530563000	-0.685045000	-0.000739000
6	-0.016361000	-1.378116000	-0.001247000
1	0.001548000	-2.460263000	-0.001280000
6	1.144448000	-0.669772000	-0.001940000
6	1.141006000	0.774155000	-0.001883000
6	3.571883000	0.714421000	-0.000625000
6	4.697655000	-1.432843000	0.001096000
6	5.988338000	0.604897000	0.003144000
6	4.813470000	1.353211000	0.001384000
1	4.852122000	2.437636000	0.001491000
6	5.934213000	-0.787411000	0.003012000
1	6.845686000	-1.372158000	0.004410000
7	-2.438455000	1.425623000	-0.000100000
7	-2.401483000	-1.413877000	-0.000124000
6	-3.578950000	0.710439000	0.000410000
6	-0.053165000	1.447137000	-0.001182000
1	-0.084491000	2.530833000	-0.001129000
6	-1.291688000	0.744506000	-0.000624000

6	-1.275797000	-0.704010000	-0.000638000
6	-3.561495000	-0.728953000	0.000402000
6	-4.833220000	1.384482000	0.000973000
6	-5.983976000	-0.753548000	0.001484000
6	-4.796244000	-1.436921000	0.000957000
1	-4.757102000	-2.519852000	0.000942000
6	-6.001871000	0.669045000	0.001492000
1	-6.954176000	1.187422000	0.001916000
1	-6.922395000	-1.296439000	0.001904000
1	-4.824191000	2.468073000	0.000969000
1	2.387475000	2.420170000	-0.001813000
1	4.621206000	-2.513383000	0.000946000
1	6.944730000	1.113876000	0.004659000