Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Synthesis of 3-Phosphinoylbenzofurans via Electrophilic Phosphination Cyclization

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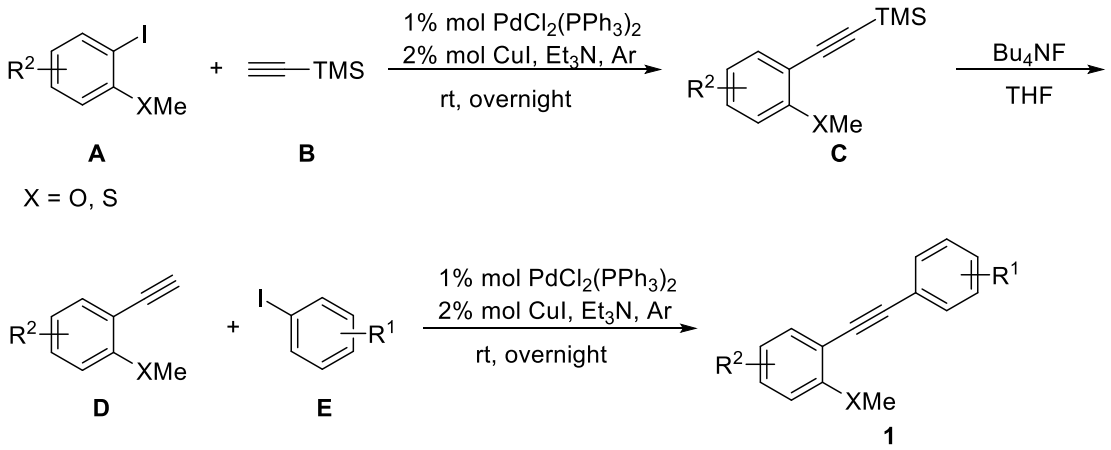
General Remarks

Column chromatography was carried out on silica gel (200-300 mesh). ^{1}H NMR spectra were recorded on 400 MHz, ^{13}C NMR spectra were recorded on 100 MHz and ^{31}P spectra were recorded on 162 MHz in $CDCl_3$. All products were further characterized by high resolution mass spectra (HRMS). Copies of their ^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra are provided in the Supporting Information. THF was distilled over Na/benzophenone. The CH_2Cl_2, DCE, CH_3CN, and toluene were distilled over CaH_2, and other solvents were used without further purification.

General Procedure for Synthesis of substrates 1 (1a-1o, 1q-1t and 1aa-1ac)



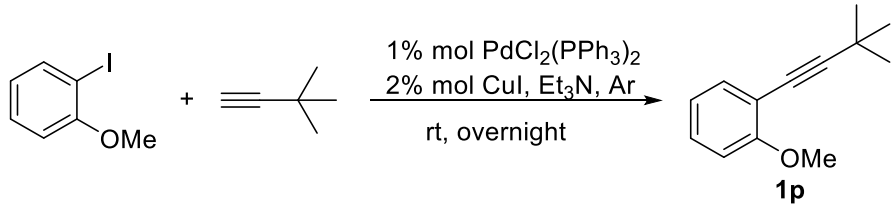
To a soluton of 1-iodo-2-methoxybenzene or (2-iodophenyl)(methyl)sulfane derivatives **A** (10 mmol) in Et_3N (20 mL) was added $PdCl_2(PPh_3)_2$ (1 mol %) and CuI (2 mol %) and the reaction vial was flushed with Ar and the reaction mixture was stirred for 5 minutes. Then, a solution of ethynyltrimethylsilane **B** (1.5 equiv) in Et_3N (5 mL) were then added dropwise through a syringe for 5 minutes. The resulting solution was stirred at room temperature overnight. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched by addition of saturated NH_4Cl (10 mL) and extracted with ethyl acetate (3 x 40 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and organic phase was concentrated under reduced pressure and purified by silica gel flash column chromatography (petroleum ether/EtOAc = 20/1) to give **C**.

To a solution of **C** in THF was added tetrabutylammonium fluoride (2.0 equiv) and the resulting solution was stirred at room temperature for 30 min, When the reaction was considered complete as determined by TLC analysis, the mixture was quenched by water, and extracted with ethyl acetate (3 x 40 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography (petroleum ether/EtOAc = 20/1) to give **D**.

To a soluton of **D** (3 mmol) in Et_3N (20 mL) was added $PdCl_2(PPh_3)_2$ (1 mol %) and CuI (2 mol %) and the reaction vial was flushed with Ar and the reaction mixture

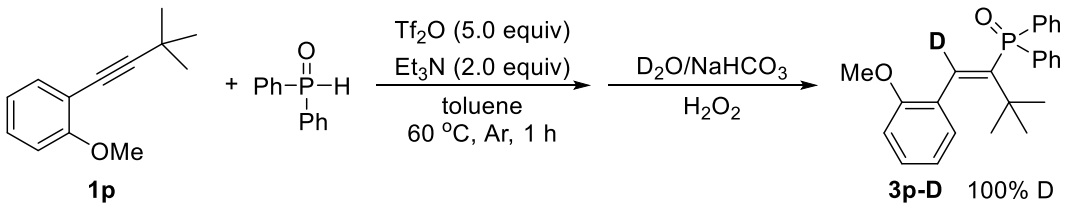
was stirred for 5 minutes. Then, a solution of aryl iodide **E** (1.5 equiv) in Et_3N (5 mL) were then added dropwise. When the reaction was considered complete as determined by TLC analysis, the mixture was quenched by saturated aqueous ammonium chloride (10 mL) and extracted with ethyl acetate (3 x 15 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by silica gel flash column chromatography (petroleum ether/EtOAc = 20/1) to give the substrates **1** (**1a-1o**, **1q-1t and 1aa-1ac**).

Synthesis of 1p



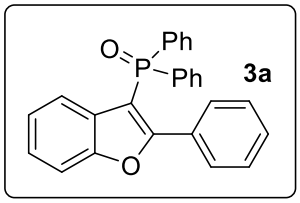
The substrate **1p** was synthesized from 1-iodo-2-methoxybenzene and 3,3-dimethylbut-1-yne according to general procedure as mentioned above.

Deuterium experiment



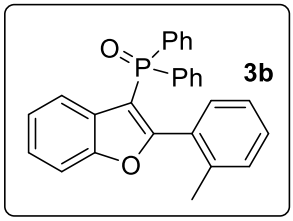
In a schlenk tube, substrates **1p** (0.2 mmol) and diphenylphosphine oxide (0.4 mmol) were placed with a magnetic stir bar under argon atmosphere. Then, toluene (1 mL) and Et_3N (0.4 mmol) were added by a syringe. The resulting mixture was stirred 2 min, Tf_2O (5.0 equiv) was added by a syringe. The reaction mixture was stirred at 60 ℃ for 1 h. After cooling, the reaction mixture was quenched by D_2O and $NaHCO_3$ and oxidized with H_2O_2 (30% aq, 0.5 mL). The resulting mixture was added saturated $Na_2S_2O_3$ and extracted with ethyl acetate (3 x 10 mL). The combined organic layer was washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by silica gel flash column chromatography (petroleum ether/EtOAc = 2/1) to give the product phosphine oxide **3p-D**.

The ^1H and ^2D NMR analyses showed 100% deuterium incorporation of product.

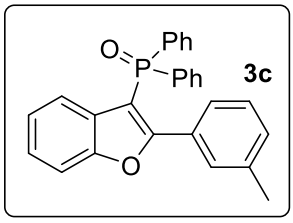


Diphenyl(2-phenylbenzofuran-3-yl)phosphine oxide **3a** White solid (73.3 mg, 93%), mp: 135-137 ℃ ^1H NMR (400 MHz, $CDCl_3$) δ ppm 7.78-7.72 (m, 6H), 7.54 (d, J = 8.4 Hz, 1H), 7.44-7.40 (m, 2H), 7.35-7.31 (m, 4H), 7.27-7.15 (m, 4H), 6.99 (t, J = 7.6

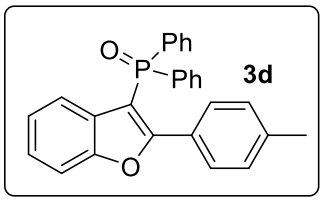
Hz, 1H), 6.55 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.2 (d, *J* = 17 Hz), 154.2 (d, *J* = 11 Hz), 132.7 (d, *J* = 108 Hz), 131.7 (d, *J* = 3 Hz), 131.5 (d, *J* = 10 Hz), 129.7, 129.3, 129.3 (d, *J* = 3 Hz), 129.2, 128.4 (d, *J* = 12 Hz), 127.7, 124.8, 123.3, 121.7, 111.1, 106.6 (d, *J* = 116 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.52. HRMS *m/z* Calcd for $C_{26}H_{19}O_2P$: $[M+H]^+$ = 395.1195. Found: 395.1190.



Diphenyl(2-(*o*-tolyl)benzofuran-3-yl)phosphine oxide **3b** White solid (74.3 mg, 91%), mp: 155-157 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.67-7.62 (m, 4H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.38 (td, *J* = 7.2, 1.2 Hz, 2H), 7.33-7.24 (m, 6H), 7.16-7.08 (m, 3H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.88 (t, *J* = 7.2 Hz, 1H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.8 (d, *J* = 18 Hz), 154.3 (d, *J* = 11 Hz), 137.5, 132.4 (d, *J* = 108 Hz), 131.6 (d, *J* = 3 Hz), 131.4, 131.3, 129.8, 129.6, 129.0, 128.8 (d, *J* = 8 Hz), 128.2, 128.1, 125.0, 123.5, 122.3, 111.1, 108.7 (d, *J* = 118 Hz), 20.0. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.73. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_2P$: $[M+Na]^+$ = 431.1171. Found: 431.1172.

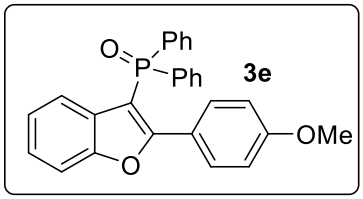


Diphenyl(2-(*m*-tolyl)benzofuran-3-yl)phosphine oxide **3c** White solid (79.2 mg, 97%), mp: 96-98 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.77-7.72 (m, 4H), 7.55 (s, 1H), 7.52 (d, *J* = 5.6 Hz, 2H), 7.43-7.39 (m, 2H), 7.35-7.30 (m, 4H), 7.27-7.23 (m, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 7.02-6.97 (m, 2H), 6.60 (d, *J* = 8.0 Hz, 1H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.4 (d, *J* = 18 Hz), 154.2 (d, *J* = 11 Hz), 137.3, 132.9 (d, *J* = 109 Hz), 131.7 (d, *J* = 3 Hz), 131.5 (d, *J* = 10 Hz), 130.5, 130.2, 129.3 (d, *J* = 9 Hz), 129.1, 128.4 (d, *J* = 12 Hz), 127.7, 126.3, 124.8, 123.3, 121.8, 111.1, 106.6 (d, *J* = 116 Hz), 21.1. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.23. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_2P$: $[M+Na]^+$ = 431.1171. Found: 431.1174.

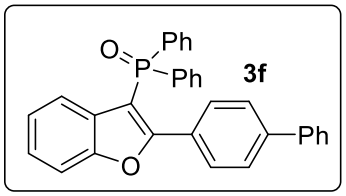


Diphenyl(2-(*p*-tolyl)benzofuran-3-yl)phosphine oxide **3d** White solid (71.0 mg, 87%), mp: 144-146 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.76-7.71 (m, 4H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.43 (td, *J* = 7.6, 1.2 Hz, 2H), 7.34 (td, *J* = 7.6, 2.8 Hz, 4H), 7.25-7.22 (m, 1H), 7.00-6.95 (m, 3H), 6.50 (d, *J* = 8.0 Hz, 1H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.6 (d, *J* = 18 Hz), 154.1 (d, *J* = 12 Hz),

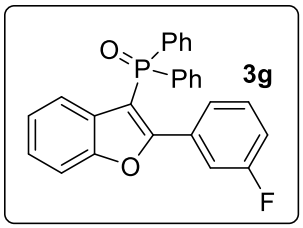
140.0, 133.0 (d, J = 109 Hz), 131.7, 131.6 (d, J = 11 Hz), 129.4 (d, J = 10 Hz), 129.3, 128.5 (d, J = 4 Hz), 128.3, 126.5, 124.6, 123.2, 121.7, 111.1, 106.0 (d, J = 117 Hz), 21.3. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.79. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_2P$: $[M+Na]^+$ = 431.1171. Found: 431.1170.



(2-(4-Methoxyphenyl)benzofuran-3-yl)diphenylphosphine oxide **3e** Pale yellow solid (70.4 mg, 83%), mp: 59-61 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.79-7.72 (m, 6H), 7.52 (d, J = 8.0 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.37-7.33 (m, 4H), 7.23 (t, J = 7.6 Hz, 1H), 6.95 (t, J = 7.6 Hz, 1H), 6.72 (d, J = 8.8 Hz, 2H), 6.44 (d, J = 8.0 Hz, 1H), 3.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.5 (d, J = 17 Hz), 160.7, 154.0 (d, J = 11 Hz), 133.0 (d, J = 108 Hz), 131.7 (d, J = 2 Hz), 131.6 (d, J = 10 Hz), 131.0, 129.5 (d, J = 10 Hz), 128.4 (d, J = 12 Hz), 124.5, 123.2, 121.8, 121.5, 113.3, 111.0, 105.1 (d, J = 116 Hz), 55.2. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.90. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_3P$: $[M+Na]^+$ = 447.1121. Found: 447.1122.

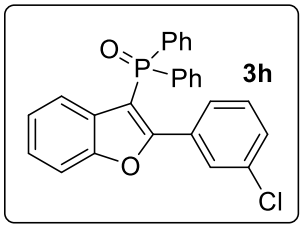


(2-([1,1'-Biphenyl]-4-yl)benzofuran-3-yl)diphenylphosphine oxide **3f** White solid (82.7 mg, 88%), mp: 202-204 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.87-7.85 (m, 2H), 7.79-7.74 (m, 4H), 7.56 (d, J = 8.4 Hz, 1H), 7.52-7.50 (m, 2H), 7.45-7.40 (m, 6H), 7.37-7.33 (m, 5H), 7.27 (t, J = 8.0 Hz, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.55 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.0 (d, J = 18 Hz), 154.2 (d, J = 12 Hz), 142.3, 140.1, 132.8 (d, J = 108 Hz), 131.8 (d, J = 3 Hz), 131.6 (d, J = 10 Hz), 129.8, 129.4 (d, J = 10 Hz), 128.7, 128.5 (d, J = 13 Hz), 128.2, 127.7, 127.0, 126.4, 124.9, 123.4, 121.8, 111.2, 106.8 (d, J = 116 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.82. HRMS *m/z* Calcd for $C_{32}H_{23}NaO_2P$: $[M+Na]^+$ = 493.1328. Found: 493.1326.

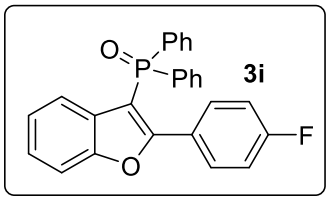


(2-(3-Fluorophenyl)benzofuran-3-yl)diphenylphosphine oxide **3g** Pale yellow solid (61.8 mg, 75%), mp: 126-128 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.78-7.73 (m, 4H), 7.62 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.53-7.50 (m, 1H), 7.49-7.45 (m, 2H), 7.40-7.35 (m, 4H), 7.31-7.27 (m, 1H), 7.18-7.13 (m, 1H), 7.03-6.99 (m, 1H), 6.94 (td, J = 8.4, 2.0 Hz, 1H), 6.52 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.8 (d, $J_{C\text{-}F}$ = 245 Hz), 161.6 (d, J = 2 Hz), 161.4 (d, J = 2 Hz), 154.2 (d, J =

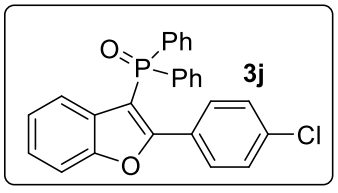
12 Hz), 132.6 (d, *J* = 109 Hz), 132.0 (d, *J* = 3 Hz), 131.6 (d, *J* = 11 Hz), 131.3 (d, *J* = 9 Hz), 129.5, 129.4, 129.1 (d, *J* = 10 Hz), 128.6 (d, *J* = 12 Hz), 125.4 (d, *J* = 3 Hz), 125.3, 123.5, 121.9, 116.8, 116.6, 116.3, 116.1, 111.3, 107.8 (d, *J* = 115 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.48. HRMS *m/z* Calcd for $C_{26}H_{18}FNaO_2P$: $[M+Na]^+$ = 435.0921. Found: 435.0918.



(2-(3-Clhlorophenyl)benzofuran-3-yl)diphenylphosphine oxide **3h** White solid (58.2 mg, 68%), mp: 162-164 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.78-7.73 (m, 5H), 7.72-7.69 (m, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.49-7.45 (m, 2H), 7.40-7.35 (m, 4H), 7.31-7.27 (m, 1H), 7.21-7.19 (m, 1H), 7.11 (t, *J* = 8.0 Hz, 1H), 7.03-6.99 (m, 1H), 6.56 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.3 (d, *J* = 17 Hz), 154.2 (d, *J* = 11 Hz), 133.4 (d, *J* = 70 Hz), 132.0 (d, *J* = 3 Hz), 131.6, 131.5, 130.9, 129.7, 129.2, 129.1, 129.0, 128.5 (d, *J* = 12 Hz), 127.7, 125.3, 123.6, 122.0, 111.3, 108.0 (d, *J* = 115 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.27. HRMS *m/z* Calcd for $C_{26}H_{18}ClNaO_2P$: $[M+Na]^+$ = 451.0625. Found: 451.0627.

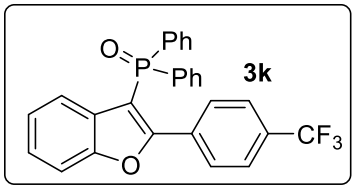


(2-(4-Fluorophenyl)benzofuran-3-yl)diphenylphosphine oxide **3i** White solid (62.6 mg, 76%), mp: 141-143 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.84-7.81 (m, 2H), 7.77-7.72 (m, 4H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.39-7.35 (m, 4H), 7.29-7.25 (m, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.90 (t, *J* = 8.4 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.5 (d, $J_{C\text{-}F}$ = 250 Hz), 162.3 (d, *J* = 17 Hz), 154.2 (d, *J* = 12 Hz), 132.7 (d, *J* = 108 Hz), 131.9 (d, *J* = 2 Hz), 131.6, 131.6, 131.5, 131.5, 129.2 (d, *J* = 10 Hz), 128.5 (d, *J* = 12 Hz), 125.6 (d, *J* = 4 Hz), 125.0, 123.4, 121.7, 115.1, 114.9, 111.2, 106.8 (d, *J* = 116 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.59. HRMS *m/z* Calcd for $C_{26}H_{18}FNaO_2P$: $[M+Na]^+$ = 435.0921. Found: 435.0920.

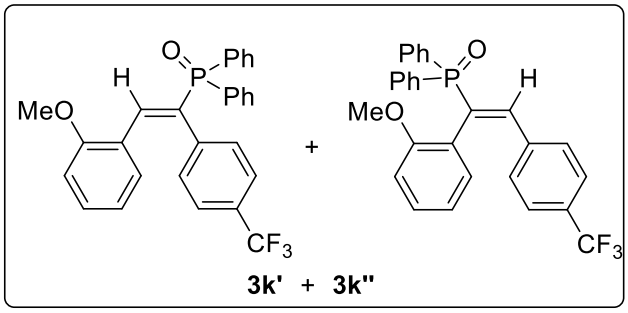


(2-(4-Chlorophenyl)benzofuran-3-yl)diphenylphosphine oxide **3j** White solid (71.9 mg, 84%), mp: 159-161 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.80-7.71 (m, 6H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.40-7.35 (m, 4H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 8.8 Hz, 2H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.46 (d, *J* = 8.0 Hz, 1H).

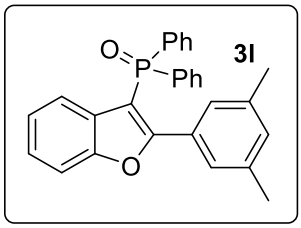
^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.0 (d, J = 16 Hz), 154.2 (d, J = 12 Hz), 136.0, 132.7 (d, J = 109 Hz), 132.0 (d, J = 2 Hz), 131.6 (d, J = 10 Hz), 130.7, 129.2 (d, J = 11 Hz), 128.5 (d, J = 12 Hz), 128.1, 127.8, 125.1, 123.5, 121.85, 111.2, 107.3 (d, J = 115 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.68. HRMS *m/z* Calcd for $C_{26}H_{18}ClNaO_2P$: $[M+Na]^+$ = 451.0625. Found: 451.0626.



Diphenyl(2-(4-(trifluoromethyl)phenyl)benzofuran-3-yl)phosphine oxide **3k** White solid (36.0 mg, 39%), mp: 172-174 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.92 (d, J = 8.4 Hz, 2H), 7.76-7.71 (m, 4H), 7.58 (d, J = 8.4 Hz, 1H), 7.51-7.46 (m, 4H), 7.40-7.36 (m, 4H), 7.34-7.30 (m, 1H), 7.03 (t, J = 7.6 Hz, 1H), 6.55 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.3 (d, J = 18 Hz), 154.4 (d, J = 11 Hz), 132.8, 132.5 (d, J = 109 Hz), 132.1 (d, J = 3 Hz), 131.6 (d, J = 10 Hz), 131.3 (q, $J_{C\text{-}F}$ = 32 Hz), 129.8, 129.1 (d, J = 10 Hz), 128.6 (d, J = 13 Hz), 125.5, 124.7 (q, $J_{C\text{-}F}$ = 4 Hz), 123.7 (q, $J_{C\text{-}F}$ = 271 Hz), 123.7, 122.0, 111.4, 108.7 (d, J = 113 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.61. HRMS *m/z* Calcd for $C_{27}H_{18}F_3NaO_2P$: $[M+Na]^+$ = 485.0889. Found: 485.0888.

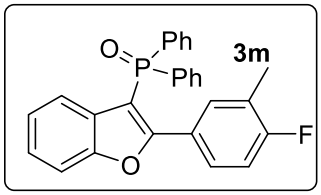


3k' and **3k''** White solid (48.8 mg, 51%), ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.79-7.74 (m, 3H), 7.56-7.39 (m, 13.6H), 7.25-7.18 (m, 4H), 6.95-6.92 (m, 1H), 6.83-6.80 (m, 1.6H), 3.77 (s, 1.5H), 3.17 (s, 3H). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 30.80, 28.79. HRMS *m/z* Calcd for $C_{28}H_{23}F_3O_2P$: $[M+H]^+$ = 479.1382. Found: 479.1378.

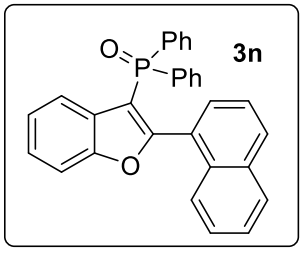


(2-(3,5-Dimethylphenyl)benzofuran-3-yl)diphenylphosphine oxide **3l** White solid (79.3 mg, 94%), mp: 51-53 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.79-7.73 (m, 4H), 7.53 (d, J = 8.4 Hz, 1H), 7.43-7.39 (m, 2H), 7.35-7.30 (m, 6H), 7.27-7.23 (m, 1H), 7.00 (t, J = 8.0 Hz, 1H), 6.82 (s, 1H), 6.64 (d, J = 8.0 Hz, 1H), 2.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.5 (d, J = 17 Hz), 154.2 (d, J = 12 Hz), 137.2, 133.0 (d,

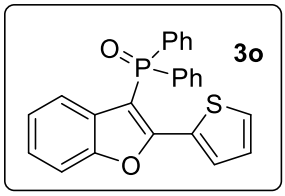
J = 108 Hz), 131.6 (d, *J* = 3 Hz), 131.5, 131.4, 129.3 (d, *J* = 9 Hz), 129.0, 128.3 (d, *J* = 13 Hz), 127.2, 124.7, 123.2, 121.9, 111.0, 106.5 (d, *J* = 117 Hz), 21.0. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.00. HRMS *m/z* Calcd for $C_{28}H_{23}NaO_2P$: $[M+Na]^+$ = 445.1328. Found: 445.1327.



(2-(4-Fluoro-3-methylphenyl)benzofuran-3-yl)diphenylphosphine oxide **3m** Pale yellow solid (74.1 mg, 87%), mp: 116-118 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.78-7.72 (m, 4H), 7.62-7.59 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.47-7.43 (m, 2H), 7.38-7.34 (m, 4H), 7.26 (t, *J* = 8.0 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.86-6.81 (m, 1H), 6.52 (d, *J* = 8.0 Hz, 1H), 2.14 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.1 (d, $J_{C\text{-}F}$ = 248 Hz), 162.5 (d, *J* = 17 Hz), 154.1 (d, *J* = 12 Hz), 133.1, 133.0, 132.8 (d, *J* = 108 Hz), 131.8 (d, *J* = 2 Hz), 131.5 (d, *J* = 10 Hz), 129.2 (d, *J* = 10 Hz), 128.7 (d, *J* = 9 Hz), 128.4 (d, *J* = 13 Hz), 125.2, 125.2, 124.9, 124.5, 124.3, 123.4, 121.8, 114.7, 114.5, 111.1, 106.6 (d, *J* = 115 Hz), 14.3. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.21. HRMS *m/z* Calcd for $C_{27}H_{20}FNaO_2P$: $[M+Na]^+$ = 449.1077. Found: 449.1077.

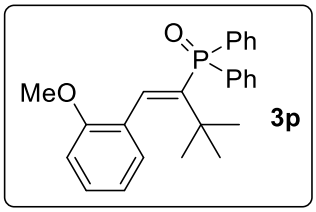


(2-(Naphthalen-1-yl)benzofuran-3-yl)diphenylphosphine oxide **3n** White solid (53.3 mg, 60%), mp: 189-191 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.73-7.65 (m, 3H), 7.59-7.53 (m, 5H), 7.47-7.43 (m, 2H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.38-7.31 (m, 2H), 7.24-7.13 (m, 4H), 7.10-7.06 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.6 (d, *J* = 19 Hz), 154.7 (d, *J* = 12 Hz), 132.9, 132.2 (d, *J* = 109 Hz), 131.8, 131.7 (d, *J* = 12 Hz), 131.4 (d, *J* = 3 Hz), 131.3 (d, *J* = 10 Hz), 130.3 (d, *J* = 11 Hz), 128.8 (d, *J* = 9 Hz), 128.0, 127.9 (d, *J* = 12 Hz), 126.8, 126.7, 126.0, 125.4, 125.3, 124.4, 123.7, 122.4, 111.3, 110.4 (d, *J* = 117 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.35. HRMS *m/z* Calcd for $C_{30}H_{21}NaO_2P$: $[M+Na]^+$ = 467.1171. Found: 467.1171.

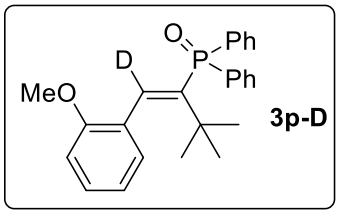


Diphenyl(2-(thiophen-2-yl)benzofuran-3-yl)phosphine oxide **3o** Yellow solid (69.6 mg, 87%), mp: 151-153 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.03 (d, *J* = 7.6 Hz, 1H), 7.78-7.73 (m, 4H), 7.54-7.50 (m, 3H), 7.44-7.40 (m, 4H), 7.34 (d, *J* = 8.8 Hz, 1H), 7.23 (t, *J* = 8.0 Hz, 1H), 6.96-6.89 (m, 2H), 6.25 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR

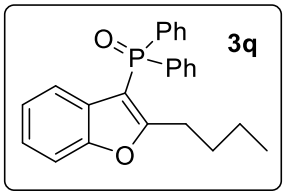
(100 MHz, $CDCl_3$) δ ppm 157.8 (d, J = 17 Hz), 153.7 (d, J = 12 Hz), 132.6 (d, J = 109 Hz), 132.1 (d, J = 3 Hz), 131.9, 131.7 (d, J = 11 Hz), 130.8, 129.3 (d, J = 11 Hz), 129.0, 128.6 (d, J = 12 Hz), 127.9, 124.8, 123.5, 121.2, 111.0, 105.2 (d, J = 116 Hz), 14.3. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 20.02. HRMS *m/z* Calcd for $C_{24}H_{17}NaO_2PS$: $[M+Na]^+$ = 423.0579. Found: 423.0577.



(E)-(1-(2-methoxyphenyl)-3,3-dimethylbut-1-en-2-yl)diphenylphosphine oxide **3p** White solid (74.1 mg, 95%), mp: 112-114 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.84-7.79 (m, 4H), 7.51-7.43 (m, 6H), 7.23 (t, J = 8.0 Hz, 1H), 7.06 (d, J = 7.2 Hz, 1H), 6.89 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.66 (d, J = 27.2 Hz, 1H), 3.85 (s, 3H), 1.18 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.4, 144.7 (d, J = 88 Hz), 141.4 (d, J = 16 Hz), 134.6 (d, J = 100 Hz), 131.8 (d, J = 9 Hz), 131.2 (d, J = 3 Hz), 128.8, 128.5, 128.3 (d, J = 12 Hz), 128.0, 119.9, 110.0, 55.3, 38.5, 31.5. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 39.77. HRMS *m/z* Calcd for $C_{25}H_{27}NaO_2P$: $[M+Na]^+$ = 413.1641. Found: 413.1640.

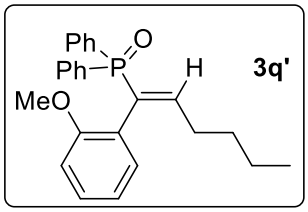


(E)-(1-(2-methoxyphenyl)-3,3-dimethylbut-1-en-2-yl-1-d)diphenylphosphine oxide **3p-D** White solid (64.1 mg, 82%), mp: 118-120 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.84-7.79 (m, 4H), 7.51-7.43 (m, 6H), 7.25-7.21 (m, 1H), 7.08-7.05 (m, 1H), 6.89 (t, J = 7.2 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 3.85 (s, 3H), 1.18 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.4, 144.6 (d, J = 87 Hz), 134.6 (d, J = 100 Hz), 131.8 (d, J = 9 Hz), 131.2 (d, J = 2 Hz), 128.9 (d, J = 2 Hz), 128.5, 128.2 (d, J = 12 Hz), 128.1, 127.9, 119.9, 110.0, 55.3, 38.4 (d, J = 10 Hz), 31.5 (d, J = 4 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 39.64. HRMS *m/z* Calcd for $C_{25}H_{26}DNaO_2P$: $[M+Na]^+$ = 414.1704. Found: 414.1707.

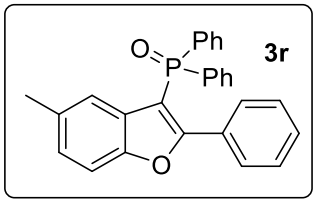


(2-Butylbenzofuran-3-yl)diphenylphosphine oxide **3q** Pale yellow oil (13.5 mg, 18%), mp: 112-114 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.76-7.71 (m, 4H), 7.57-7.55 (m, 2H), 7.49-7.45 (m, 5H), 7.21 (t, J = 7.6 Hz, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.69 (d, J = 8.0 Hz, 1H), 2.94 (t, J = 7.6 Hz, 1H), 1.68-1.60 (m, 2H), 1.68-1.60 (m, 2H), 1.28-1.19

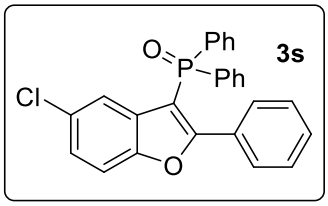
(m, 2H), 0.82 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 168.5 (d, *J* = 19 Hz), 154.1 (d, *J* = 9 Hz), 133.3 (d, *J* = 109 Hz), 132.1 (d, *J* = 3 Hz), 131.7 (d, *J* = 10 Hz), 128.6 (d, *J* = 12 Hz), 124.0, 123.2, 120.9, 110.9, 105.5 (d, *J* = 120 Hz), 30.4, 27.9, 22.3, 13.7. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 21.20. HRMS *m/z* Calcd for $C_{24}H_{23}NaO_2P$: $[M+Na]^+$ = 397.1328. Found: 397.1330.



(E)-(1-(2-methoxyphenyl)hex-1-en-1-yl)diphenylphosphine oxide **3q'** White solid (49.1 mg, 63%), mp: 111-113 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.83-7.78 (m, 4H), 7.55-7.51 (m, 2H), 7.50-7.45 (m, 4H), 7.29 (t, *J* = 6.8 Hz, 2H), 7.08 (d, *J* = 22.8 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 1H), 3.77 (s, 3H), 2.52-2.43 (m, 2H), 1.38-1.34 (m, 2H), 1.19-1.09 (m, 2H), 0.69 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 157.03, 139.4 (d, *J* = 14 Hz), 135.6 (d, *J* = 95 Hz), 132.3 (d, *J* = 101 Hz), 132.1 (d, *J* = 9 Hz), 131.6 (d, *J* = 3 Hz), 129.5, 128.9 (d, *J* = 1 Hz), 128.3 (d, *J* = 12 Hz), 125.0 (d, *J* = 20 Hz), 120.1, 110.5, 55.4, 31.5 (d, *J* = 1 Hz), 28.4 (d, *J* = 10 Hz), 22.7, 13.5. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 34.49. HRMS *m/z* Calcd for $C_{25}H_{27}NaO_2P$: $[M+Na]^+$ = 413.1641. Found: 413.1640.

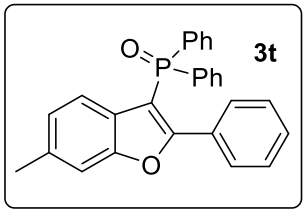


(5-Methyl-2-phenylbenzofuran-3-yl)diphenylphosphine oxide **3r** White solid (76.7 mg, 94%), mp: 130-132 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.76-7.71 (m, 6H), 7.45-7.40 (m, 3H), 7.35-7.31 (m, 4H), 7.22-7.13 (m, 3H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.34 (s, 1H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.1 (d, *J* = 18 Hz), 152.6 (d, *J* = 11 Hz), 132.8 (d, *J* = 109 Hz), 132.7, 131.7 (d, *J* = 3 Hz), 131.6 (d, *J* = 10 Hz), 129.6, 129.4, 129.4 (d, *J* = 10 Hz), 129.3, 128.3 (d, *J* = 13 Hz), 127.7, 126.1, 121.7, 110.5, 106.3 (d, *J* = 116 Hz), 21.3. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 19.14. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_2P$: $[M+Na]^+$ = 431.1171. Found: 431.1173.

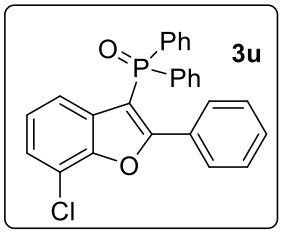


(5-Chloro-2-phenylbenzofuran-3-yl)diphenylphosphine oxide **3s** White solid (81.3 mg, 95%), mp: 188-190 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.75-7.70 (m, 6H), 7.48-7.44 (m, 3H), 7.38-7.34 (m, 4H), 7.25-7.16 (m, 4H), 6.45 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 164.3 (d, *J* = 17 Hz), 152.5 (d, *J* = 12 Hz), 132.3

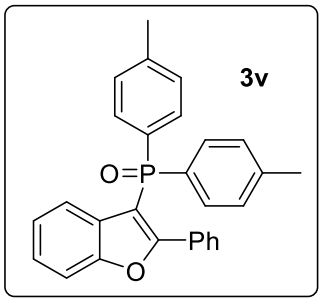
(d, *J* = 109 Hz), 132.0 (d, *J* = 2 Hz), 131.6 (d, *J* = 10 Hz), 131.5 (d, *J* = 10 Hz), 130.7 (d, *J* = 10 Hz), 130.0, 129.3, 128.9 (d, *J* = 15 Hz), 128.5 (d, *J* = 13 Hz), 127.8, 125.1, 121.5, 112.0, 106.7 (d, *J* = 114 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.51. HRMS *m/z* Calcd for $C_{26}H_{18}ClNaO_2P$: $[M+Na]^+$ = 451.0625. Found: 451.0627.



(6-Methyl-2-phenylbenzofuran-3-yl)diphenylphosphine oxide **3t** Yellow solid (60.4 mg, 74%), mp: 60-62 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.77-7.71 (m, 6H), 7.45-7.41 (m, 2H), 7.36-7.31 (m, 5H), 7.24-7.15 (m, 3H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.37 (d, *J* = 8.4 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.7 (d, *J* = 18 Hz), 154.6 (d, *J* = 12 Hz), 135.3, 132.8 (d, *J* = 109 Hz), 131.7 (d, *J* = 3 Hz), 131.6 (d, *J* = 10 Hz), 129.6, 129.4, 129.3, 128.4 (d, *J* = 13 Hz), 127.7, 126.8 (d, *J* = 11 Hz), 124.8, 121.2, 111.3, 106.4 (d, *J* = 116 Hz), 21.5. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.87. HRMS *m/z* Calcd for $C_{27}H_{21}NaO_2P$: $[M+Na]^+$ = 431.1171. Found: 431.1170.

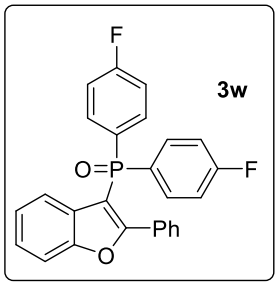


(7-Chloro-2-phenylbenzofuran-3-yl)diphenylphosphine oxide **3u** White solid (83.9 mg, 98%), mp: 70-72 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.77-7.70 (m, 6H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.37-7.32 (m, 4H), 7.28-7.23 (m, 2H), 7.18 (t, *J* = 7.6 Hz, 2H), 6.93 (t, *J* = 8.0 Hz, 1H), 6.48 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.8 (d, *J* = 17 Hz), 150.1 (d, *J* = 11 Hz), 132.3 (d, *J* = 109 Hz), 131.9 (d, *J* = 3 Hz), 131.5 (d, *J* = 10 Hz), 130.9 (d, *J* = 9 Hz), 130.1, 129.5, 128.7, 128.5 (d, *J* = 13 Hz), 127.8, 125.0, 124.2, 120.3, 116.7, 107.5 (d, *J* = 115 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.50. HRMS *m/z* Calcd for $C_{26}H_{18}ClNaO_2P$: $[M+Na]^+$ = 451.0625. Found: 451.0628.

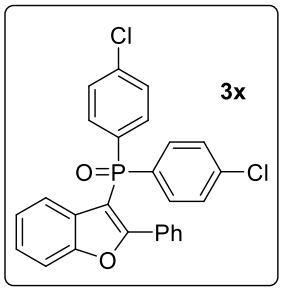


(2-Phenylbenzofuran-3-yl)di-p-tolylphosphine oxide **3v** White solid (72.6 mg, 86%), mp: 157-159 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.77-7.75 (m, 2H), 7.63-7.58 (m, 4H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.27-7.18 (m, 4H), 7.17-7.12 (m, 4H), 7.01 (t, *J* = 8.0

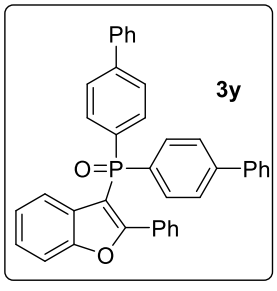
Hz, 1H), 6.64 (d, J = 8.0 Hz, 1H), 2.32 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.0 (d, J = 17 Hz), 154.2 (d, J = 11 Hz), 142.1 (d, J = 13 Hz), 131.6, 131.5, 129.9 (d, J = 111 Hz), 129.5, 129.4, 129.2, 129.1, 127.7, 124.8, 123.3, 122.0, 111.1, 107.2 (d, J = 115 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 19.11. HRMS *m/z* Calcd for $C_{28}H_{23}NaO_2P$: $[M+Na]^+$ = 445.1328. Found: 445.1327.



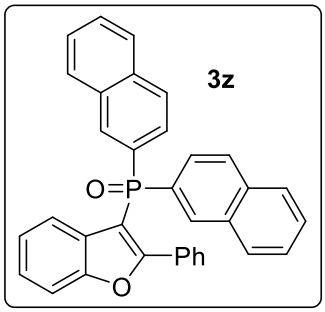
Bis(4-fluorophenyl)(2-phenylbenzofuran-3-yl)phosphine oxide **3w** White solid (73.1 mg, 85%), mp: 64-66 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.75-7.69 (m, 6H), 7.57 (d, J = 8.4 Hz, 1H), 7.32-7.26 (m, 2H), 7.20 (t, J = 7.6 Hz, 2H), 7.07-7.01 (m, 5H), 6.62 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 164.9 (dd, $J_{C\text{-}F}$ = 253 Hz, $J_{C\text{-}P}$ = 4 Hz), 163.4 (d, J = 18 Hz), 154.3 (d, J = 12 Hz), 134.1, 134.0 (d, J = 3 Hz), 133.9, 130.0, 129.4, 129.2 (d, J = 3 Hz), 129.1, 129.0 (d, J = 10 Hz), 128.1 (d, J = 4 Hz), 127.9, 125.1, 123.6, 121.6, 116.0 (d, $J_{C\text{-}F}$ = 21 Hz), 115.8 (d, $J_{C\text{-}F}$ = 21 Hz), 111.3, 106.4 (d, J = 118 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 16.96. HRMS *m/z* Calcd for $C_{26}H_{17}F_2NaO_2P$: $[M+Na]^+$ = 453.0826. Found: 453.0826.



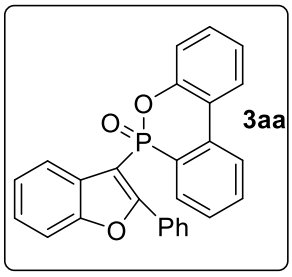
Bis(4-chlorophenyl)(2-phenylbenzofuran-3-yl)phosphine oxide **3x** Pale yellow solid (87.0 mg, 94%), mp: 73-75 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.69-7.61 (m, 6H), 7.57 (d, J = 8.4 Hz, 1H), 7.33-7.27 (m, 6H), 7.20 (t, J = 7.6 Hz, 2H), 7.07 (t, J = 7.6 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.6 (d, J = 18 Hz), 154.3 (d, J = 12 Hz), 138.6 (d, J = 4 Hz), 132.8 (d, J = 11 Hz), 131.1 (d, J = 111 Hz), 130.0, 129.4, 129.0, 128.9 (d, J = 13 Hz), 128.8, 127.9, 125.2, 123.6, 121.6, 111.4, 105.9 (d, J = 119 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 16.93. HRMS *m/z* Calcd for $C_{26}H_{17}Cl_2NaO_2P$: $[M+Na]^+$ = 485.0235. Found: 485.0237.



Di([1,1'-biphenyl]-4-yl)(2-phenylbenzofuran-3-yl)phosphine oxide **3y** White solid (68.8 mg, 63%), mp: 102-104 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.85-7.80 (m, 4H), 7.74-7.72 (m, 2H), 7.58-7.54 (m, 9H), 7.45-7.42 (m, 4H), 7.39-7.35 (m, 2H), 7.31-7.27 (m, 1H), 7.22-7.15 (m, 3H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.2 (d, *J* = 18 Hz), 154.3 (d, *J* = 12 Hz), 144.5 (d, *J* = 3 Hz), 139.8, 132.1 (d, *J* = 11 Hz), 131.4 (d, *J* = 110 Hz), 129.7, 129.5, 129.4, 129.3, 128.7, 128.1, 127.8, 127.2, 127.1, 127.1, 125.0, 123.5, 122.1, 111.2, 107.0 (d, *J* = 117 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.45. HRMS *m/z* Calcd for $C_{38}H_{27}NaO_2P$: $[M+Na]^+$ = 569.1641. Found: 569.1642.

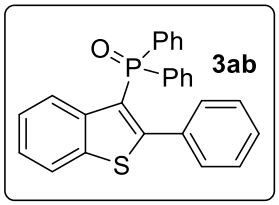


Di(naphthalen-2-yl)(2-phenylbenzofuran-3-yl)phosphine oxide **3z** Pale yellow solid (77.1 mg, 78%), mp: 98-100 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 8.48 (d, *J* = 14.4 Hz, 2H), 7.83 (d, *J* = 7.6 Hz, 2H), 7.77 (d, *J* = 6.8 Hz, 4H), 7.74-7.71 (m, 2H), 7.68-7.63 (m, 2H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.54-7.47 (m, 4H), 7.27-7.23 (m, 1H), 7.03-7.00 (m, 3H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.5 (d, *J* = 17 Hz), 154.3 (d, *J* = 12 Hz), 134.5 (d, *J* = 2 Hz), 133.6 (d, *J* = 9 Hz), 132.4 (d, *J* = 14 Hz), 130.0 (d, *J* = 109 Hz), 129.7, 129.5, 129.3, 129.2 (d, *J* = 2 Hz), 128.8, 128.3 (d, *J* = 12Hz), 128.1, 127.7, 127.6, 126.7, 126.3 (d, *J* = 12 Hz), 124.9, 123.4, 122.0, 111.2, 106.6 (d, *J* = 117 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 18.46. HRMS *m/z* Calcd for $C_{34}H_{23}NaO_2P$: $[M+Na]^+$ = 517.1328. Found: 517.1330.

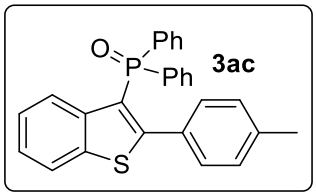


6-(2-Phenylbenzofuran-3-yl)dibenzo[*c*,*e*][1,2]oxaphosphinine 6-oxide **3aa** Pale yellow solid (47.3 mg, 58%), mp: 68-70 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.98-7.93 (m, 2H), 7.85-7.83 (m, 2H), 7.68-7.53 (m, 4H), 7.38-7.28 (m, 6H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 163.5 (d, *J* = 23 Hz), 154.1 (d, *J* = 14 Hz), 148.8 (d, *J* = 8 Hz), 135.3 (d, *J* = 6 Hz), 133.0 (d, *J* = 3 Hz), 130.5, 130.3, 129.9 (d, *J* = 96 Hz), 129.2, 129.1, 128.2 (d, *J* = 15 Hz), 128.0, 126.3, 125.3, 125.0, 124.9, 124.6, 123.9, 123.6 (d, *J* = 10 Hz), 122.0, 121.9, 120.6 (d, *J* = 6 Hz), 111.1, 104.0 (d, *J* = 165 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 17.81. HRMS *m/z* Calcd for $C_{26}H_{17}NaO_3P$: $[M+Na]^+$ = 431.0808. Found:

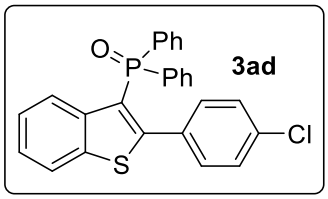
431.0808.



Diphenyl(2-phenylbenzo[*b*]thiophen-3-yl)phosphine oxide **3ab** White solid (45.1 mg, 55%), mp: 190-192 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.91 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.57-7.52 (m, 4H), 7.35-7.30 (m, 3H), 7.24-7.20 (m, 5H), 7.14-7.12 (m, 2H), 7.08-7.05 (m, 1H), 6.96 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 154.8 (d, J = 13 Hz), 141.3 (d, J = 13 Hz), 139.3 (d, J = 13 Hz), 133.3 (d, J = 106 Hz), 132.7, 131.5 (d, J = 10 Hz), 131.4 (d, J = 3 Hz), 129.8, 128.3, 128.2 (d, J = 12 Hz), 127.5, 125.8, 124.8, 124.8, 122.6 (d, J = 104 Hz), 121.4. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 21.72. HRMS *m/z* Calcd for $C_{26}H_{19}NaOPS$: $[M+Na]^+$ = 433.0786. Found: 433.0784.

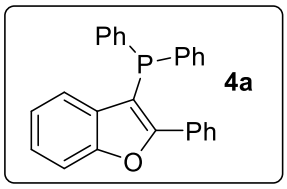


Diphenyl(2-(*p*-tolyl)benzo[*b*]thiophen-3-yl)phosphine oxide **3ac** White solid (40.7 mg, 48%), mp: 198-120 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.91 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.56-7.51 (m, 4H), 7.37-7.30 (m, 3H), 7.24-7.20 (m, 5H), 7.01 (d, J = 8.0 Hz, 2H), 6.74 (d, J = 8.0 Hz, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 155.1 (d, J = 13 Hz), 141.4 (d, J = 13 Hz), 139.3 (d, J = 12 Hz), 138.3, 133.5 (d, J = 106 Hz), 131.6 (d, J = 10 Hz), 131.1 (d, J = 7 Hz), 129.8 (d, J = 2 Hz), 129.7, 128.2, 128.1, 128.1, 125.8, 124.7 (d, J = 9 Hz), 122.6 (d, J = 103 Hz), 121.4, 21.1. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 21.80. HRMS *m/z* Calcd for $C_{27}H_{21}NaOPS$: $[M+Na]^+$ = 447.0943. Found: 447.0946.



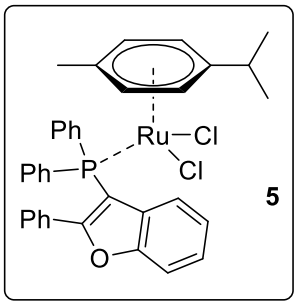
(2-(4-Chlorophenyl)benzo[*b*]thiophen-3-yl)diphenylphosphine oxide **3ad** White solid (45.3 mg, 51%), mp: 229-231 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.88 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.56-7.51 (m, 4H), 7.42-7.38 (m, 2H), 7.34 (t, J = 7.6 Hz, 1H), 7.28-7.24 (m, 5H), 7.06 (d, J = 8.4 Hz, 2H), 6.92 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 153.1 (d, J = 13 Hz), 141.2 (d, J = 12 Hz), 139.3 (d, J = 12 Hz), 134.7, 133.2 (d, J = 106 Hz), 131.6 (d, J = 10 Hz), 131.5 (d, J = 3 Hz), 131.3 (d, J = 3 Hz), 131.1, 128.4, 128.3, 127.6, 125.9, 125.0 (d, J = 3 Hz), 123.7 (d, J = 103 Hz), 121.5. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 21.41. HRMS *m/z* Calcd for $C_{26}H_{18}ClNaOPS$: $[M+Na]^+$ = 467.0397. Found: 467.0396.

Synthesis and Characterization Data of 4a



Diphenyl(2-phenylbenzofuran-3-yl)phosphane **4a**. The compound **3a** (0.2 mmol) was placed with a magnetic stir bar in a schlenk tube under an argon atmosphere. Then, toluene (1 mL) and $HSiCl_3$ (2.0 equiv) were then added by a syringe. The resulting solution was stirred at 80 ℃ for 12 h. After cooling, the resulting solution was quenched slowly by addition of 10% aq. NaOH (5 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were washed with water, brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude material was purified by flash column chromatography (petroleum ether/EtOAc = 20/1) to give **4a** in 64% yield. White solid (48.4 mg, 64%), mp: 84-86 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.99 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.4 Hz, 1H), 7.48-7.40 (m, 7H), 7.32-7.30 (m, 6H), 7.24-7.20 (m,1H), 6.91 (t, J = 7.6 Hz, 1H), 6.69 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 162.1 (d, J = 40 Hz), 154.8 (d, J = 3 Hz), 135.9 (d, J = 8 Hz), 132.6 (d, J = 18 Hz), 130.7 (d, J = 5 Hz), 130.3, 129.4, 129.0 (d, J = 10 Hz), 128.5 (d, J = 8 Hz), 128.4, 128.3, 124.4, 122.7, 122.5, 111.3, 107.7 (d, J = 16 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ -28.96. HRMS *m/z* Calcd for $C_{26}H_{20}OP$: $[M+H]^+$ = 379.1246. Found: 379.1246.

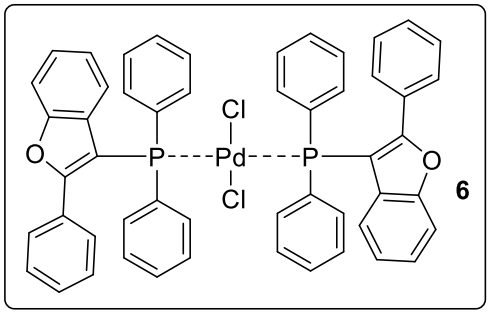
Synthesis and Characterization Data of 5



[$RuCl_2$(p-cymene)(2-phenylbenzofuran-3-yldiphenylphosphine)] **5**. To a solution of [$RuCl_2$(p-cymene)]$_2$ (0.1 mmol) in CH_2Cl_2 (1 mL) was added phosphine **4a** (0.15 mmol). The reaction was stirred for 6 h at room temperature. Then, the solvent was concentrated in vacuo and the residue was washed with ethyl ether to afford complex **5** (62.0 mg, 85% yield) as a red solid. mp: 206-208 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.72-7.68 (m, 4H), 7.62 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 7.6 Hz, 2H), 7.39-7.34 (m, 2H), 7.19-7.12 (m, 4H), 7.10-7.03 (m, 6H), 5.45 (d, J = 6.4 Hz, 2H), 5.20 (d, J = 5.0 Hz, 2H), 2.89-7.2.80 (m, 1H), 1.93 (m, 3H), 1.10 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 159.5 (d, J = 8 Hz), 153.8 (d, J = 10 Hz), 134.9 (d, J = 10 Hz), 130.3 (d, J = 11 Hz), 130.1 (d, J = 3 Hz), 129.5, 129.4, 128.8, 127.6, 127.2 (d, J = 10 Hz), 125.4, 124.1, 123.1, 111.1, 108.8 (d, J = 46 Hz), 108.8 (d, J = 2 Hz), 98.3,

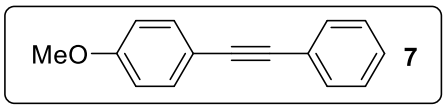
88.0, 87.5 (d, J = 4 Hz), 80.8 (d, J = 78 Hz), 30.0, 21.9, 17.8. ^{31}P NMR ($CDCl_3$, 162 MHz): δ 10.35. HRMS *m/z* Calcd for $C_{36}H_{33}ClOPRu$: $[M\text{-}Cl]^+$ = 649.0996. Found: 649.1004.

Synthesis and Characterization Data of 6

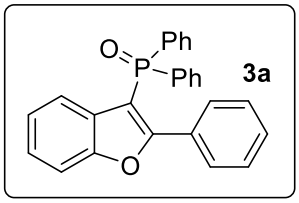


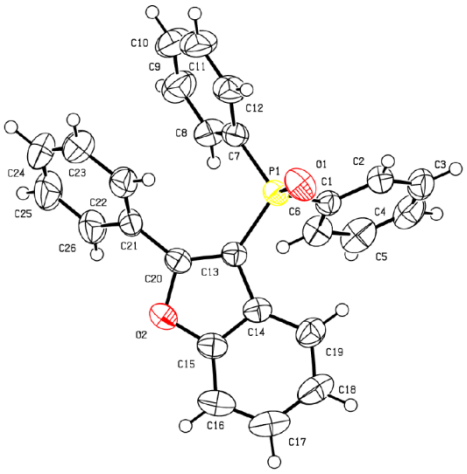
Dichlorobis(2-phenylbenzofuran-3-yldiphenylphosphine)palladium(II) **6**. To a soluton of $PdCl_2$ (0.4 mmol) in MeOH (4 mL) was added NaCl (0.8 mmol) and the reaction was stirred at room temperature overnight to form a dark red solution. Then, the phosphine **4a** was added into the dark red solution and the reaction was heated reflux for 4 h to produce yellow precipitation. After cooling, the mixture was filtered and the solid was washed with diethyl ether for three times to afford yield solid complex **6** (272.4 mg) in 73% yield. mp: 231-233 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.69-7.66 (m, 4H), 7.57-7.53 (m, 10H), 7.33-7.28 (m, 6H), 7.15 (t, J = 7.6 Hz, 8H), 7.09-7.05 (m, 8H), 6.94 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 161.4 (t, J = 8 Hz), 154.1 (t, J = 5 Hz), 135.3 (t, J = 6 Hz), 130.6, 130.5, 130.5, 130.0 (t, J = 41 Hz), 129.2, 128.2 (t, J = 26 Hz), 127.8, 127.6 (t, J = 6 Hz), 124.7, 123.1, 122.5, 111.1, 103.0 (t, J = 28 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 2.73. HRMS *m/z* Calcd for $C_{52}H_{38}ClO_2P_2Pd$: $[M\text{-}Cl]^+$ = 897.1065. Found: 897.1069.

Synthesis and Characterization Data of 7



1-Methoxy-4-(phenylethynyl)benzene **7**. The compound **7** was synthised from 1-ethynyl-4-methoxybenzene (1 mmol) and iodobenzene (1.5 mmol) by the use of Pd-catalyst **6** through Sonagashira coupling. White solid (183.0 mg, 88%), mp: 54-56 ℃ ^{1}H NMR (400 MHz, $CDCl_3$) δ ppm 7.52-7.49 (m, 2H), 7.47-7.45 (m, 2H), 7.33-7.28 (m, 3H), 6.85 (d, J = 8.8 Hz, 2H), 3.78 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm 159.5, 133.0, 131.4, 128.3, 127.9, 123.5, 115.3, 113.9, 89.4, 88.0, 55.2. HRMS *m/z* Calcd for $C_{15}H_{13}O$: $[M+H]^+$ = 209.0961. Found: 209.0959.





structure of **3a**, **CCDC：1960259**

Datablock

Bond precision: C-C = 0.0029 A Wavelength=0.71073

Cell: a=16.620(3) b=8.0600(16) c=16.710(3)
alpha=90 beta=106.98(3) gamma=90

Temperature: 293 K

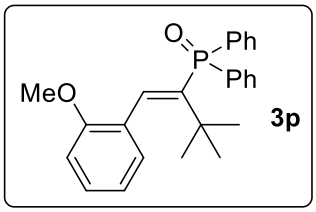
	Calculated	Reported
Volume	2140.8(8)	2140.8(8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H19 O2 P, H2 O	C26 H19 O2 P, H2 O
Sum formula	C26 H21 O3 P	C26 H21 O3 P
Mr	412.40	412.40
Dx,g cm-3	1.280	1.279
Z	4	4
Mu (mm-1)	0.153	0.153
F000	864.0	864.0
F000'	864.78	
h,k,lmax	21,10,21	21,10,21
Nref	4948	4916
Tmin,Tmax	0.962,0.983	0.675,0.733
Tmin'	0.961	

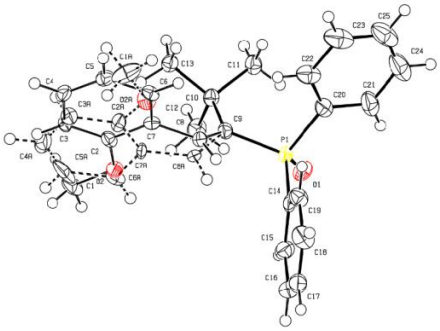
Correction method= # Reported T Limits: Tmin=0.675 Tmax=0.733
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.542

R(reflections)= 0.0458(3941) wR2(reflections)= 0.1256(4916)

S = 1.048 Npar= 281





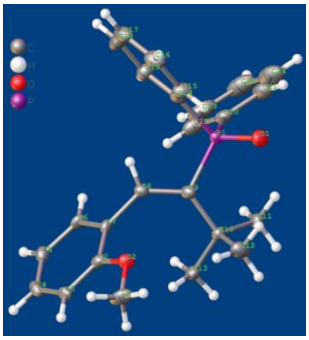


Figure 1 Figure 2

structure of **3p**, **CCDC：1978107**

As shown in the Figure 1, the benzene ring (C2-C7) and the atoms on the benzene ring (C1, O2, and C8) are disordered into two positions.

In the Figure 2, the disordered component is omitted for clarity.

Datablock:

Bond precision: C-C = 0.0028 A Wavelength=1.54184

Cell: a=10.4061(2) b=10.0093(2) c=20.3835(4)
alpha=90 beta=90.910(2) gamma=90

Temperature: 100 K

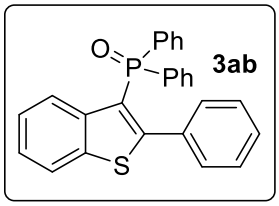
	Calculated	Reported
Volume	2122.83(7)	2122.83(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H27 O2 P	C25 H27 O2 P
Sum formula	C25 H27 O2 P	C25 H27 O2 P
Mr	390.44	390.43
Dx,g cm-3	1.222	1.222
Z	4	4
Mu (mm-1)	1.272	1.272
F000	832.0	832.0
F000'	835.30	
h,k,lmax	12,11,23	12,11,23
Nref	3595	3521
Tmin,Tmax	0.795,0.881	0.869,1.000
Tmin'	0.795	

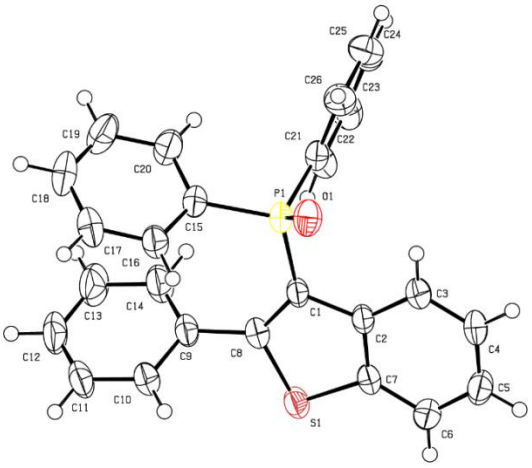
Correction method= # Reported T Limits: Tmin=0.869 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.979 Theta(max)= 64.830

R(reflections)= 0.0502(3079) wR2(reflections)= 0.1344(3521)

S = 1.030 Npar= 328





structure of **3ab**, **CCDC: 1960412**

Datablock

Bond precision: C-C = 0.0033 A Wavelength=0.71073

Cell: a=9.6323(13) b=13.6973(19) c=15.454(2)
alpha=90 beta=93.272(4) gamma=90

Temperature: 293 K

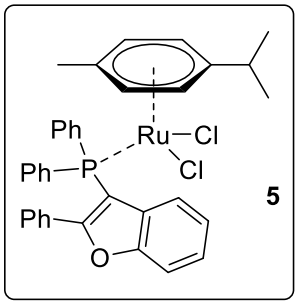
	Calculated	Reported
Volume	2035.6(5)	2035.6(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H19 O P S	C26 H19 O P S
Sum formula	C26 H19 O P S	C26 H19 O P S
Mr	410.44	410.44
Dx,g cm-3	1.339	1.339
Z	4	4
Mu (mm-1)	0.253	0.253
F000	856.0	856.0
F000'	857.20	
h,k,lmax	12,17,20	12,17,20
Nref	4776	4739
Tmin,Tmax	0.939,0.951	0.528,0.746
Tmin'	0.939	

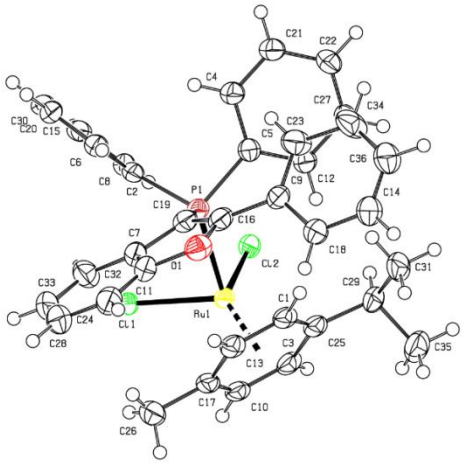
Correction method= # Reported T Limits: Tmin=0.528 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 27.722

R(reflections)= 0.0500(3583) wR2(reflections)= 0.1405(4739)

S = 1.017 Npar= 262





structure of **complex 5**, **CCDC: 1960413**

Datablock

Bond precision: C-C = 0.0058 A Wavelength=1.54184

Cell: a=11.0690(6) b=11.1524(5) c=13.6440(4)
alpha=94.062(3) beta=94.936(3) gamma=116.856(5)

Temperature: 100 K

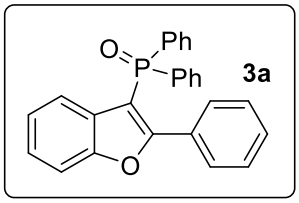
	Calculated	Reported
Volume	1485.62(13)	1485.62(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H33 C12 O P Ru	C36 H33 C12 O P Ru
Sum formula	C36 H33 C12 O P Ru	C36 H33 C12 O P Ru
Mr	684.56	684.56
Dx,g cm-3	1.530	1.530
Z	2	2
Mu (mm-1)	6.653	6.653
F000	700.0	700.0
F000'	703.57	
h,k,lmax	12,12,15	12,12,15
Nref	4733	4730
Tmin,Tmax	0.554,0.717	0.672,1.000
Tmin'	0.490	

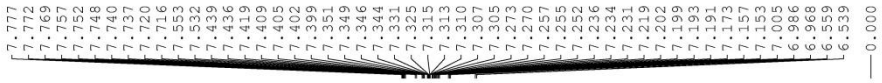
Correction method= # Reported T Limits: Tmin=0.672 Tmax=1.000
AbsCorr = MULTI-SCAN

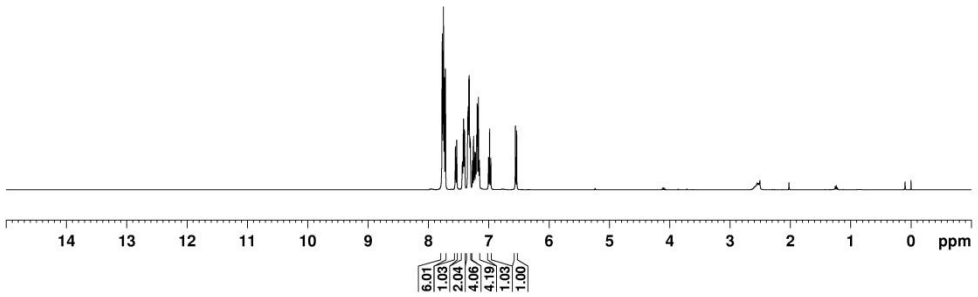
Data completeness= 0.999 Theta(max)= 62.500

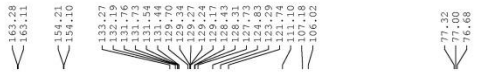
R(reflections)= 0.0366(4465) wR2(reflections)= 0.0959(4730)

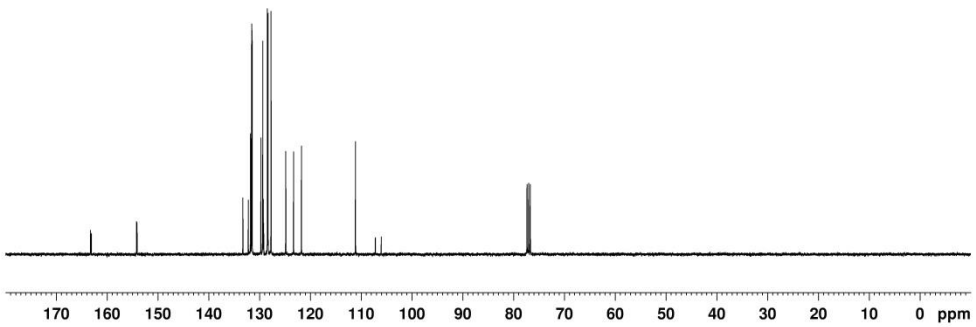
S = 1.060 Npar= 373

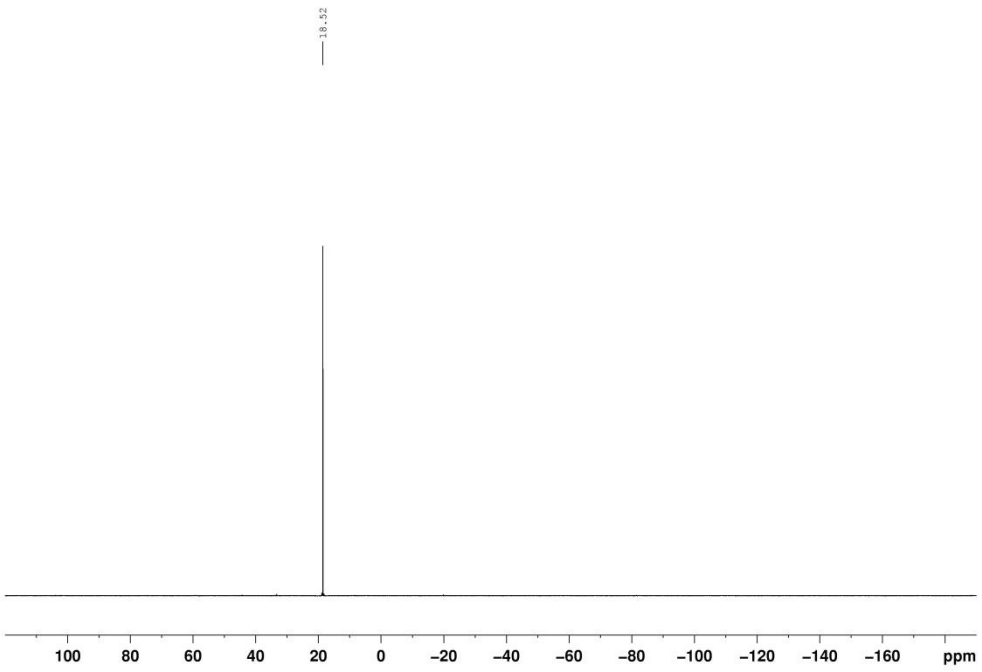

O
P
Ph
Ph
3a
O

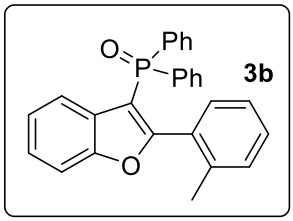

7.777
7.772
7.769
7.757
7.752
7.748
7.740
7.737
7.720
7.716
7.553
7.532
7.439
7.436
7.419
7.409
7.405
7.402
7.399
7.351
7.349
7.346
7.344
7.331
7.325
7.315
7.313
7.310
7.307
7.305
7.273
7.270
7.257
7.255
7.252
7.236
7.234
7.231
7.219
7.202
7.199
7.193
7.191
7.173
7.157
7.153
7.005
6.986
6.968
6.559
6.539
0.000

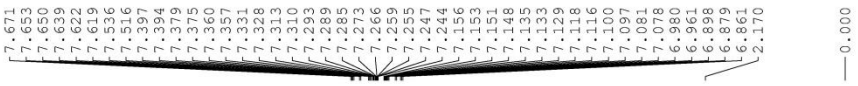

14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.01
1.03
2.04
4.06
4.19
1.03
1.00

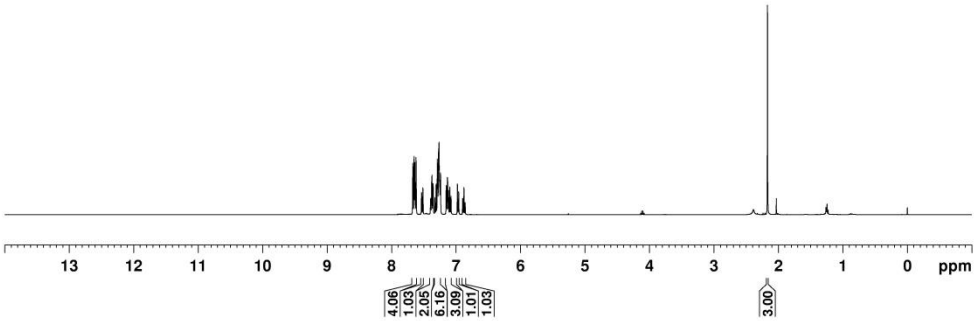

163.28
163.11
154.21
154.10
133.27
132.19
131.76
131.73
131.54
131.44
129.70
129.34
129.27
129.24
129.17
128.43
128.31
127.73
124.83
123.29
121.74
111.10
111.08
106.02
77.32
77.00
76.68

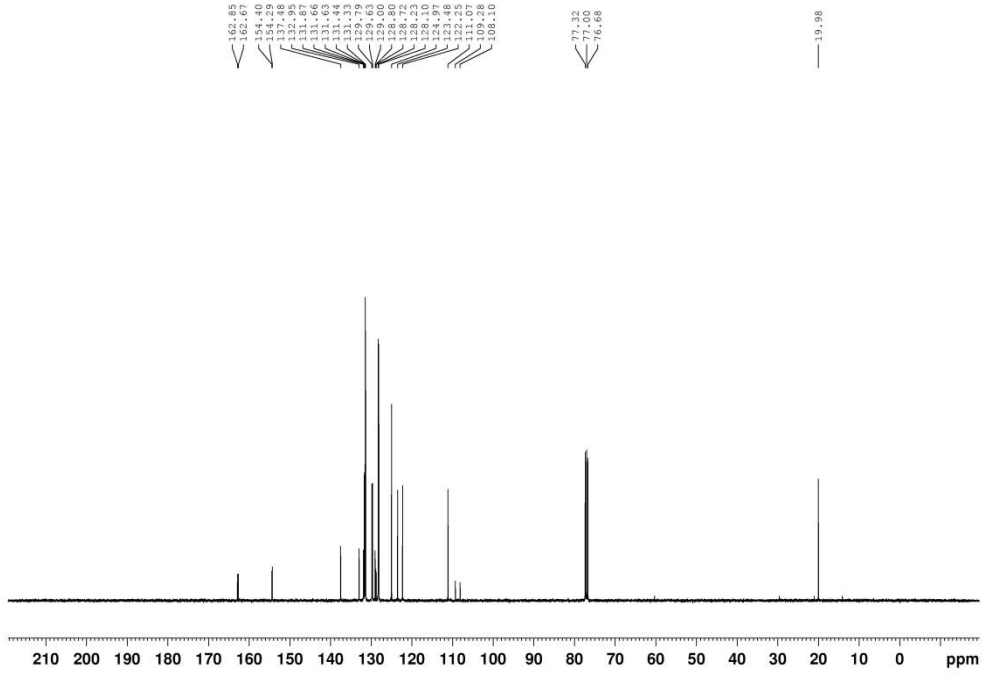

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

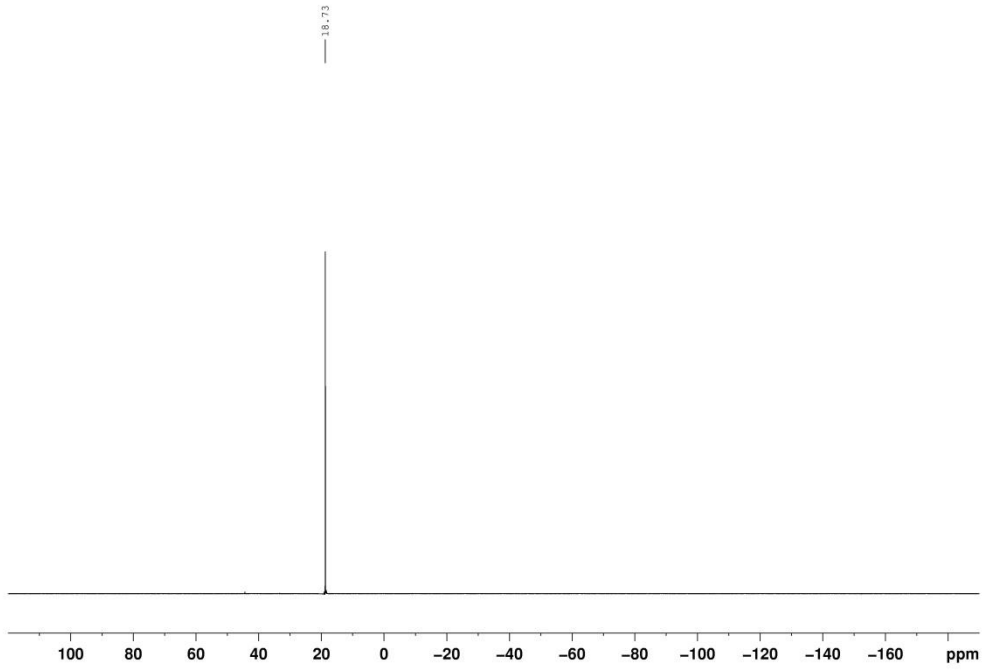

18.52
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

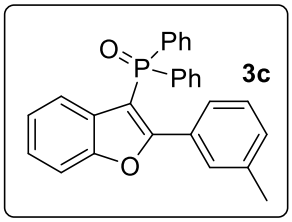

O
P
Ph
Ph
O
3b

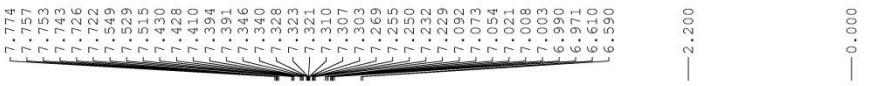

7.671
7.653
7.650
7.639
7.622
7.619
7.536
7.516
7.397
7.394
7.379
7.375
7.360
7.357
7.331
7.328
7.313
7.310
7.293
7.289
7.285
7.273
7.266
7.259
7.255
7.247
7.244
7.156
7.153
7.151
7.148
7.135
7.133
7.129
7.118
7.116
7.100
7.097
7.081
7.078
6.980
6.961
6.898
6.879
6.861
2.170
0.000

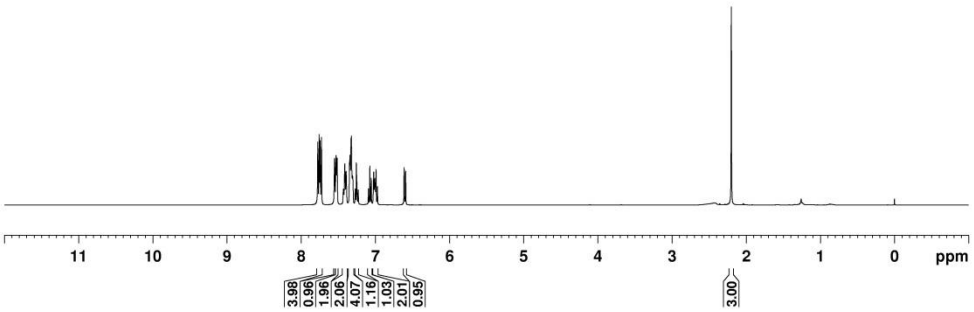

13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.06
1.03
2.05
6.16
3.09
1.01
1.03
3.00


162.85
162.67
154.40
154.29
137.48
132.95
131.87
131.66
131.63
131.44
131.33
129.79
129.45
129.00
128.80
128.72
128.13
128.10
124.97
123.48
122.25
111.07
109.28
108.10
77.32
77.00
76.68
19.98
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

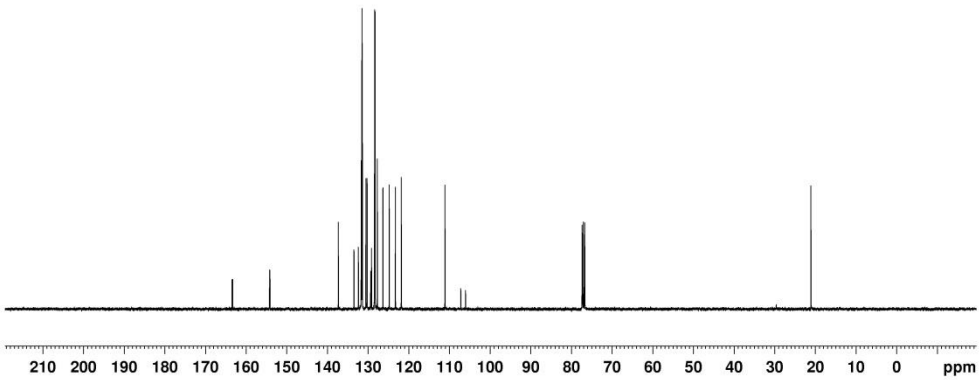

18.73
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

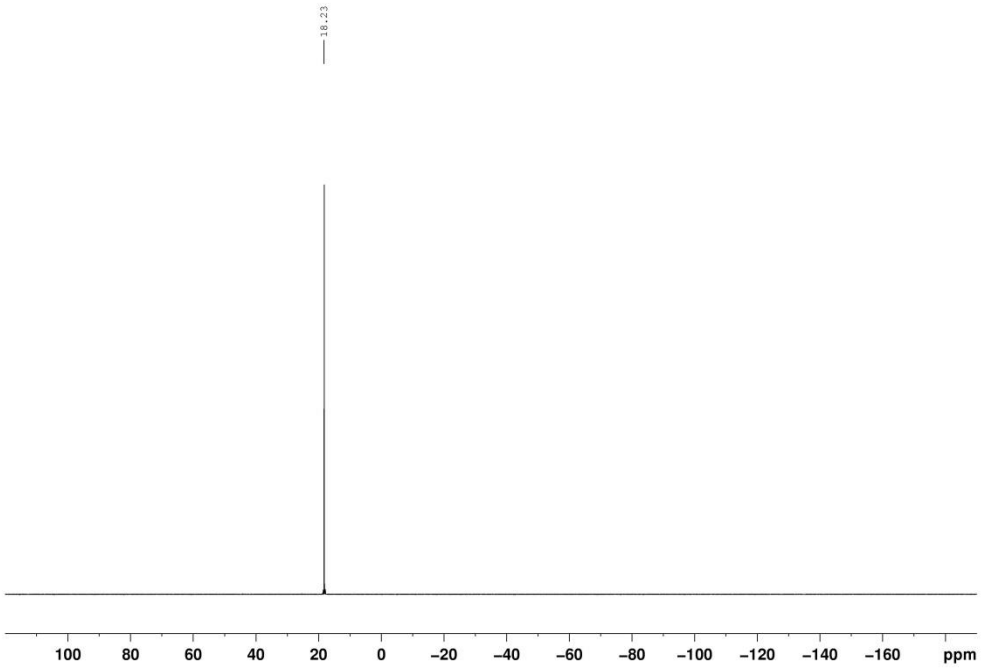

Ph
O
P
Ph
3c
O

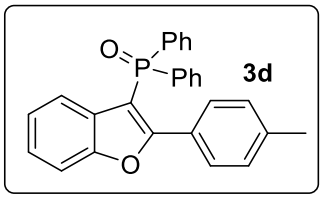

7.774
7.757
7.753
7.743
7.726
7.722
7.549
7.529
7.515
7.430
7.428
7.410
7.394
7.391
7.346
7.340
7.328
7.323
7.321
7.310
7.307
7.303
7.269
7.255
7.250
7.232
7.229
7.092
7.073
7.054
7.021
7.008
7.003
6.990
6.971
6.610
6.590
2.200
0.000

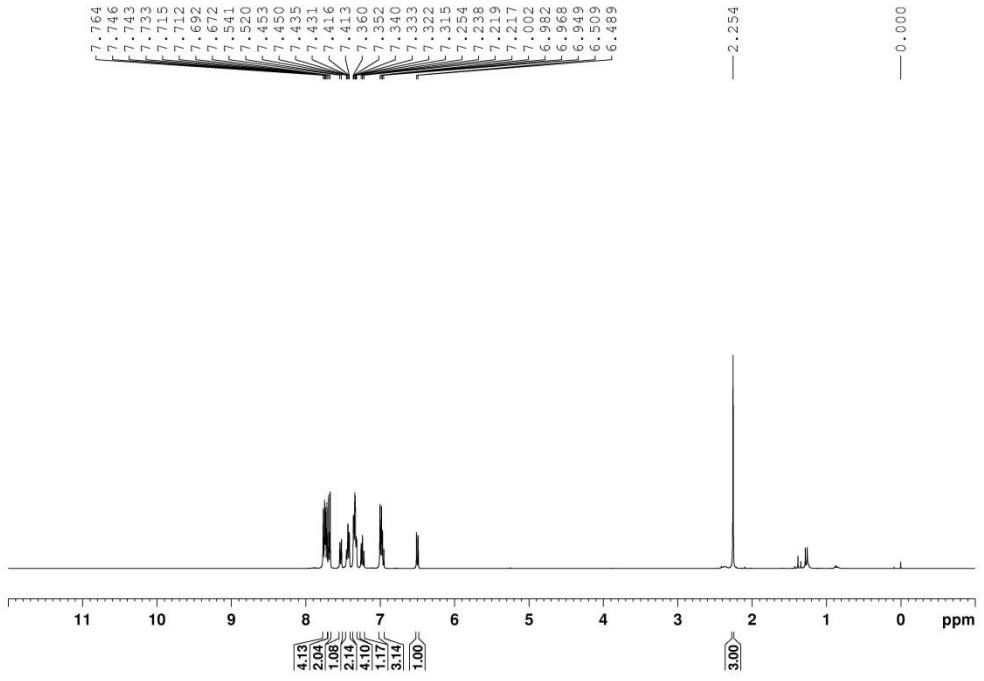

11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.98
0.96
1.96
2.06
4.07
1.16
1.03
2.01
0.95
3.00

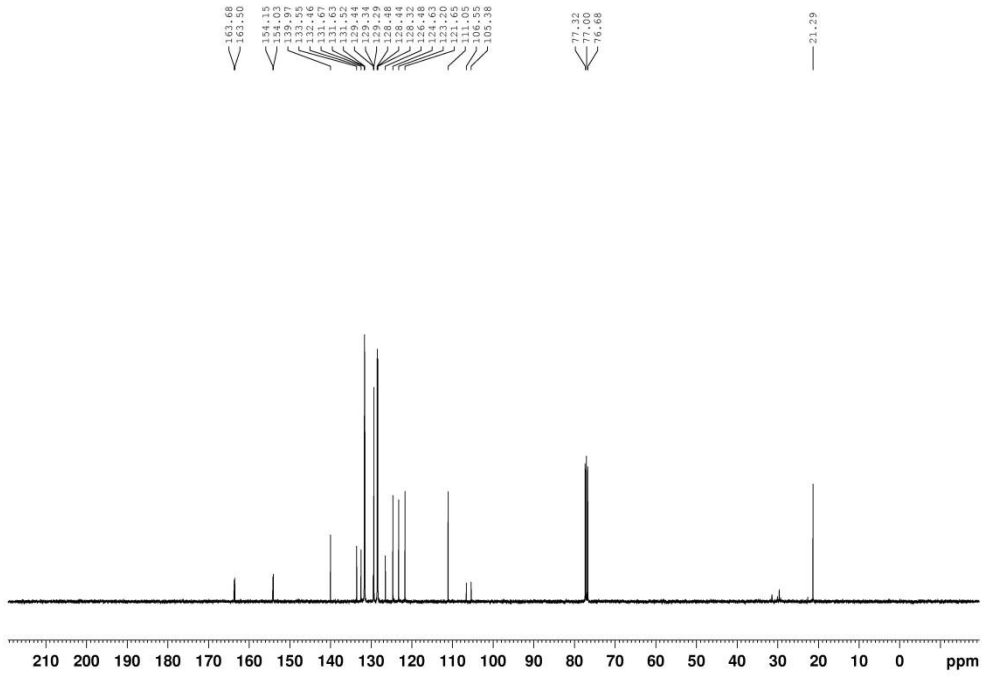

163.44
163.26
154.22
154.11
137.10
133.45
132.36
131.68
131.55
131.50
131.40
130.52
130.21
129.34
129.24
129.12
128.37
128.25
127.70
126.33
124.77
123.25
111.87
111.67
107.16
106.00
77.32
77.00
76.68
21.06

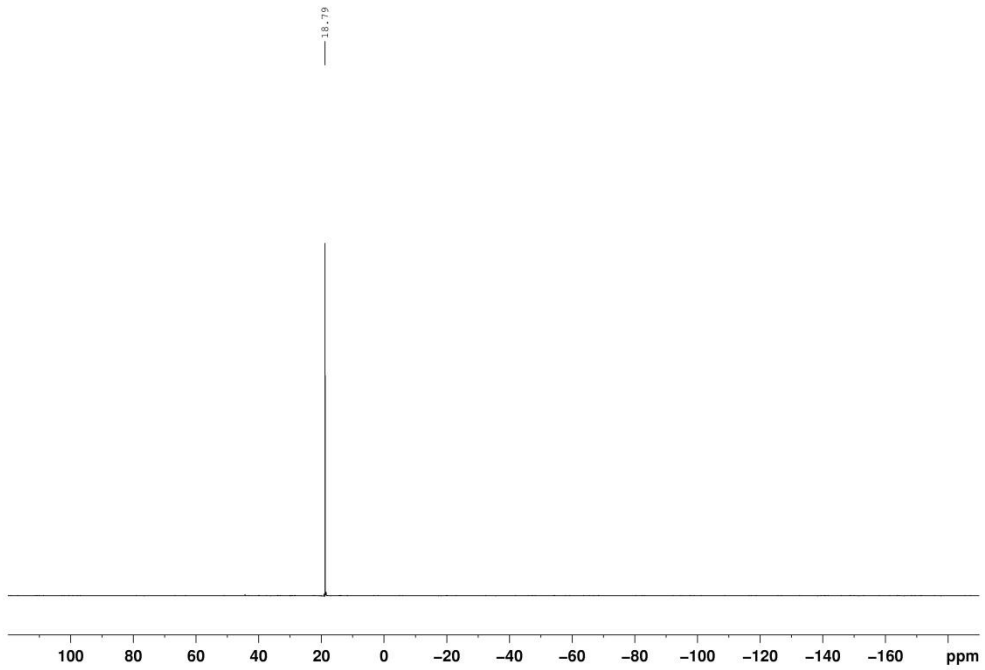

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

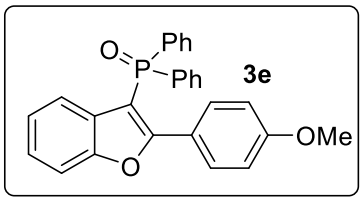

18.23
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

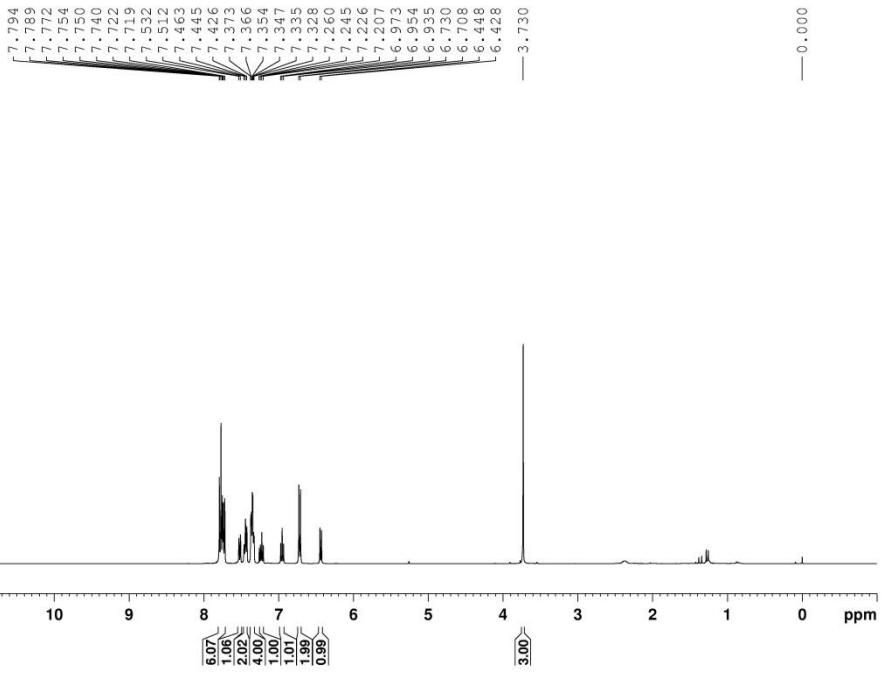

O
P
Ph
Ph
3d
O

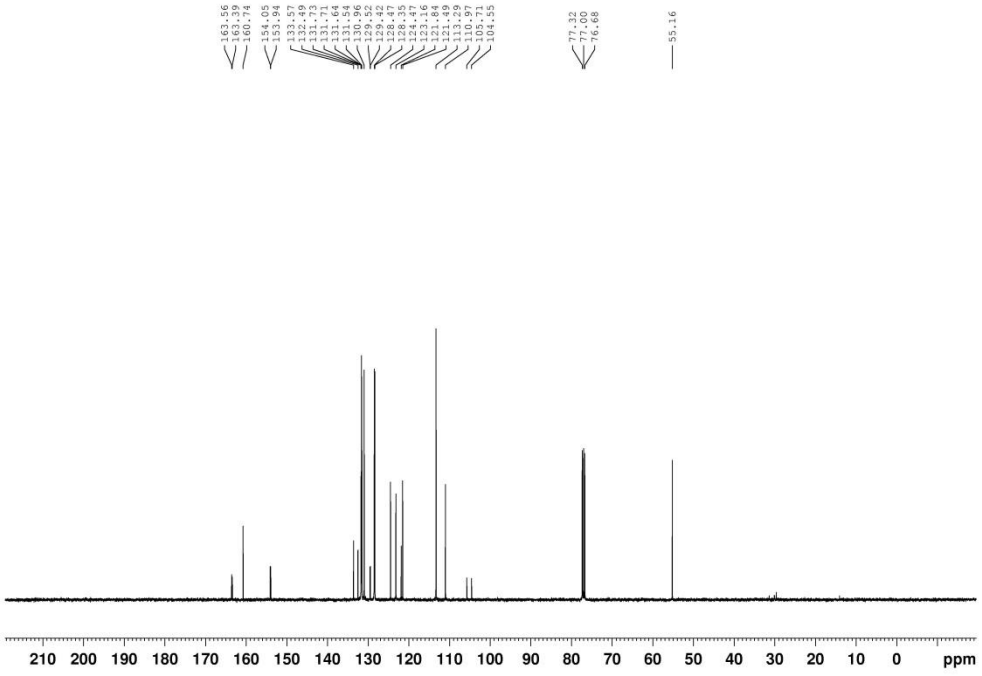

7.764
7.746
7.743
7.733
7.715
7.712
7.692
7.672
7.541
7.520
7.453
7.450
7.435
7.431
7.416
7.413
7.360
7.352
7.340
7.333
7.322
7.315
7.254
7.238
7.219
7.217
7.002
6.982
6.968
6.949
6.509
6.489
2.254
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.13
2.04
1.08
2.14
4.10
1.17
3.14
1.00
3.00

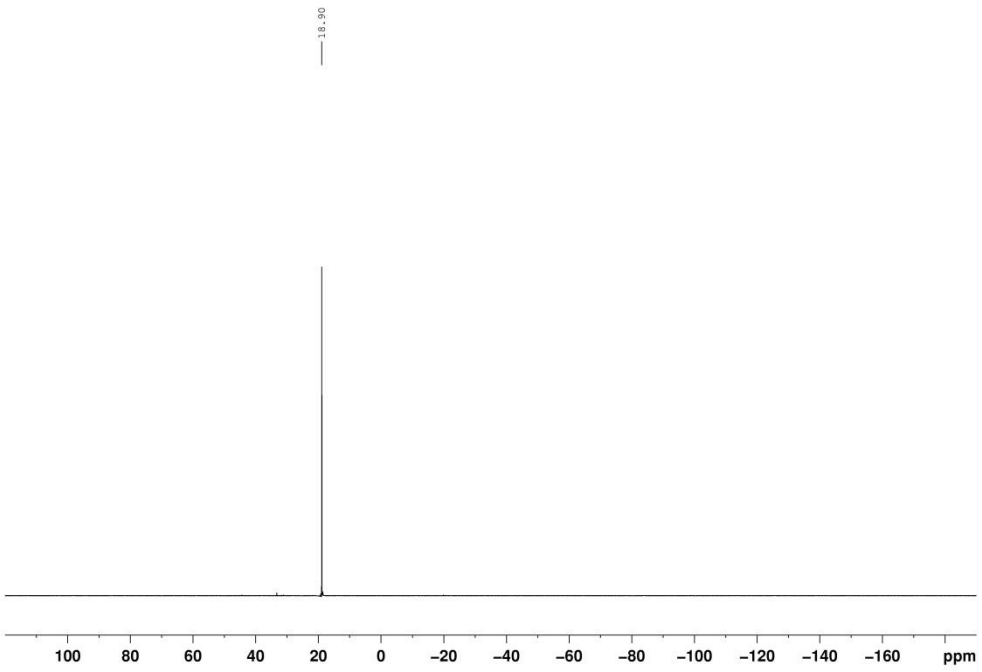

163.68
163.50
154.15
154.03
139.07
138.55
132.46
131.67
131.63
131.22
129.44
129.34
129.29
128.48
128.44
128.32
126.48
124.63
123.60
121.65
111.05
106.55
105.38
77.32
77.00
76.68
21.29
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

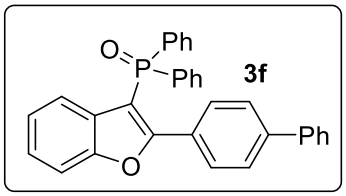

18.79
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

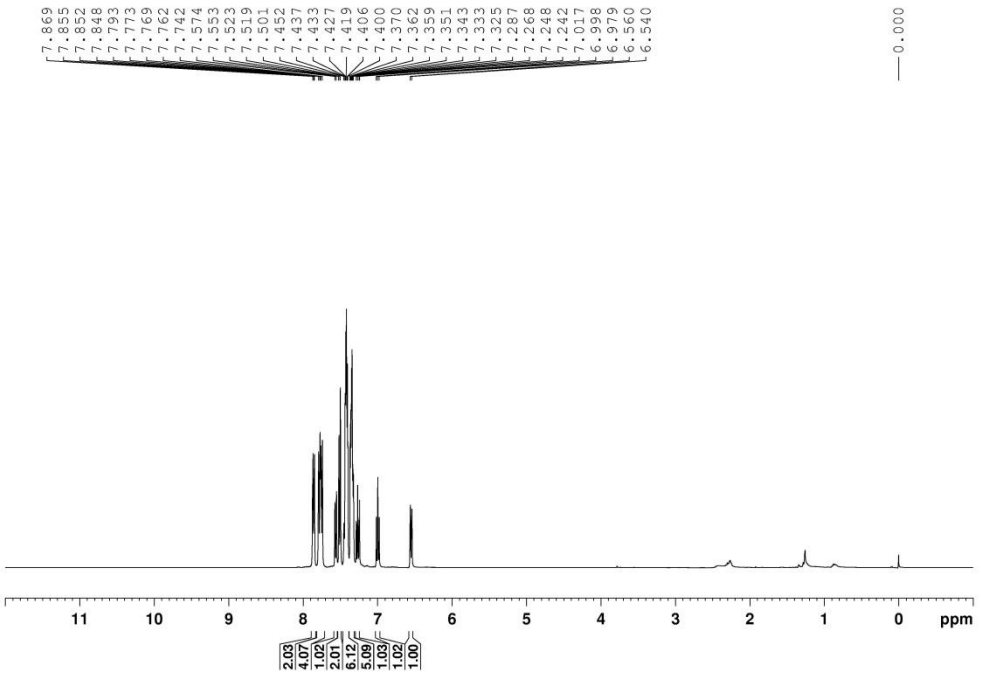

O
P
Ph
Ph
3e
OMe
O

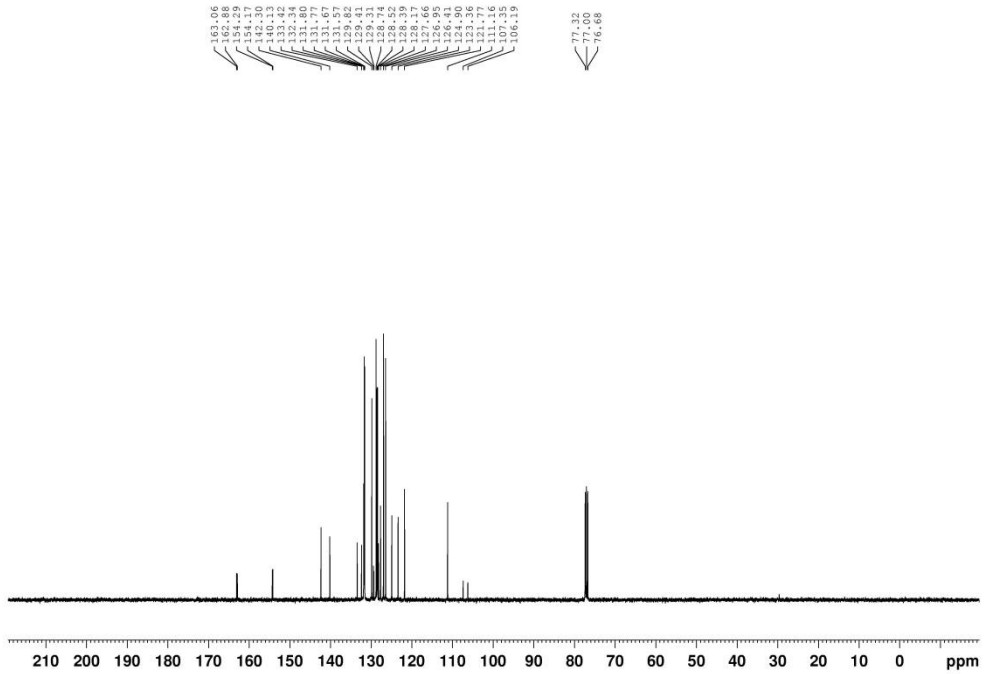

7.794
7.789
7.772
7.754
7.750
7.740
7.722
7.719
7.532
7.512
7.463
7.445
7.426
7.373
7.366
7.354
7.347
7.335
7.328
7.260
7.245
7.226
7.207
6.973
6.954
6.935
6.730
6.708
6.448
6.428
3.730
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.07
1.06
2.02
4.00
1.00
1.01
1.99
0.99
3.00

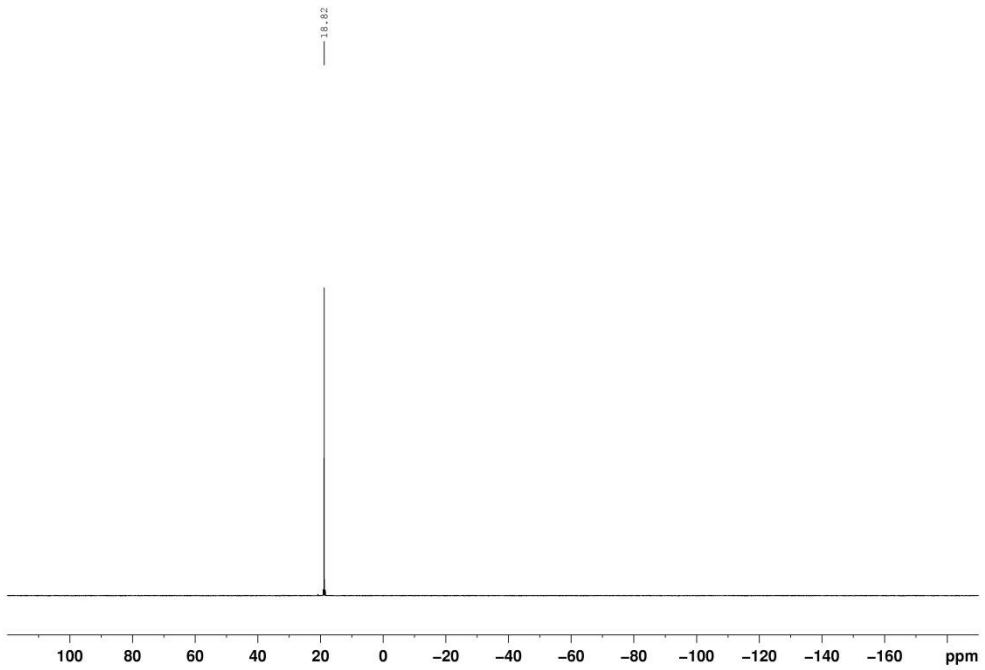

163.56
163.39
160.74
154.05
153.94
133.57
132.49
131.73
131.71
131.64
131.54
130.96
130.52
129.42
128.47
128.35
124.47
123.16
121.84
121.49
113.29
110.97
110.71
104.55
77.32
77.00
76.68
55.16
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

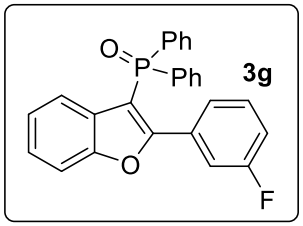

18.90
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

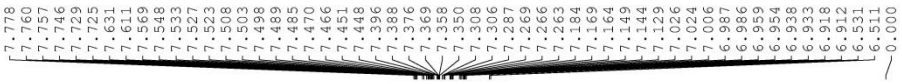

O
P
Ph
Ph
Ph
O
3f

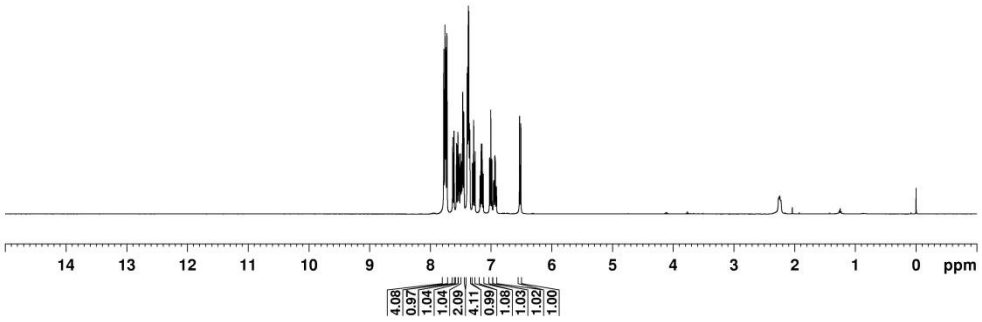

7.869
7.855
7.852
7.848
7.793
7.773
7.769
7.762
7.742
7.574
7.553
7.523
7.519
7.501
7.452
7.437
7.433
7.427
7.419
7.406
7.400
7.370
7.362
7.359
7.351
7.343
7.333
7.325
7.287
7.268
7.248
7.242
7.017
6.998
6.979
6.560
6.540
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
4.07
1.02
2.01
6.12
5.09
1.09
1.02
1.00

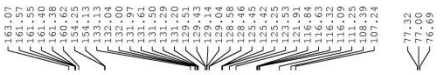

163.06
162.88
154.29
154.17
142.00
140.13
133.42
132.34
131.90
131.77
131.67
131.57
129.82
129.31
129.11
128.74
128.52
128.39
128.27
127.66
126.95
126.41
124.90
123.96
121.77
111.16
107.35
106.19
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


18.62
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm


O
P
Ph
Ph
3g
O
F


7.778
7.760
7.757
7.746
7.729
7.725
7.631
7.611
7.569
7.548
7.533
7.527
7.523
7.508
7.503
7.498
7.489
7.485
7.470
7.466
7.451
7.448
7.396
7.388
7.376
7.369
7.358
7.350
7.308
7.306
7.287
7.269
7.266
7.263
7.184
7.169
7.164
7.149
7.144
7.129
7.026
7.024
7.006
6.987
6.986
6.959
6.954
6.938
6.933
6.918
6.912
6.531
6.511
0.000


14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.08
0.97
1.04
1.04
2.09
4.11
0.99
1.08
1.03
1.02
1.00


163.07
161.57
161.55
161.40
161.38
160.22
154.25
154.13
133.13
132.04
132.00
131.97
131.61
131.50
131.29
131.00
129.51
129.43
129.14
129.04
128.68
128.46
125.45
125.42
123.55
123.53
121.91
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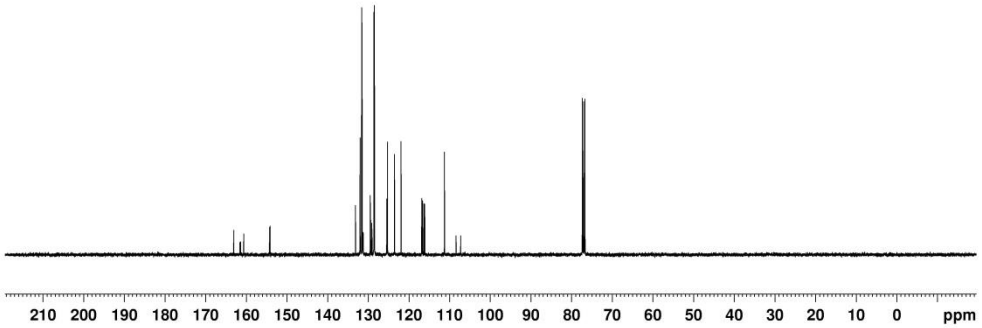
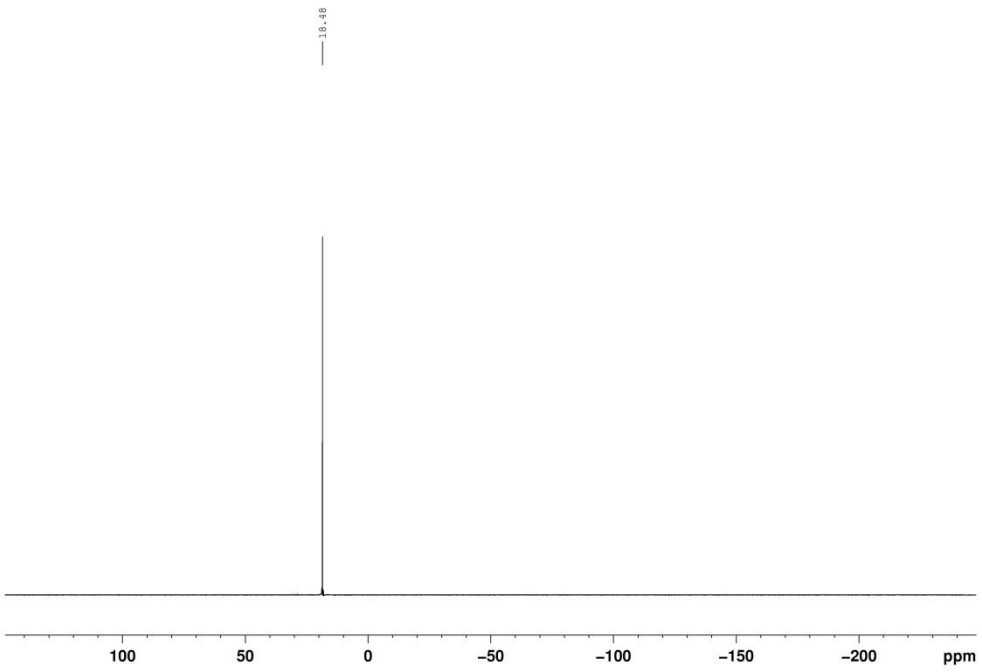
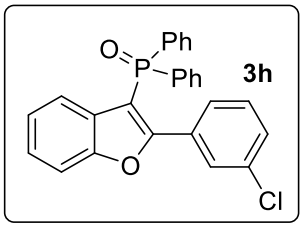
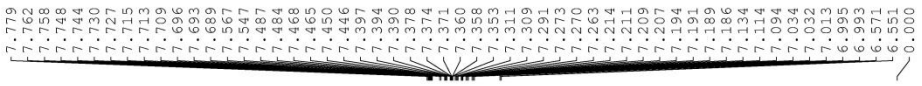
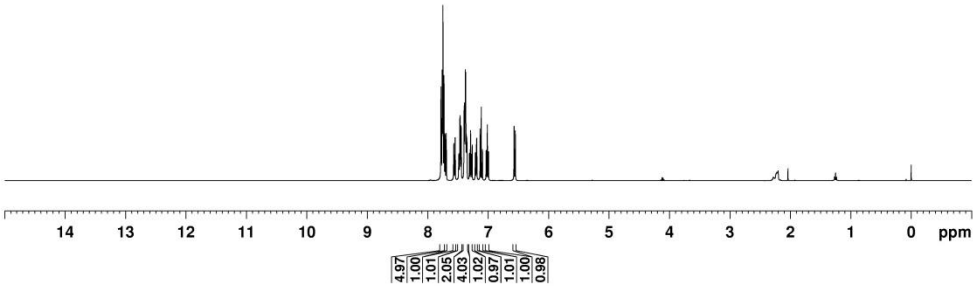
116.63
116.32
116.09
111.25
108.39
107.24
77.32
77.00
76.69

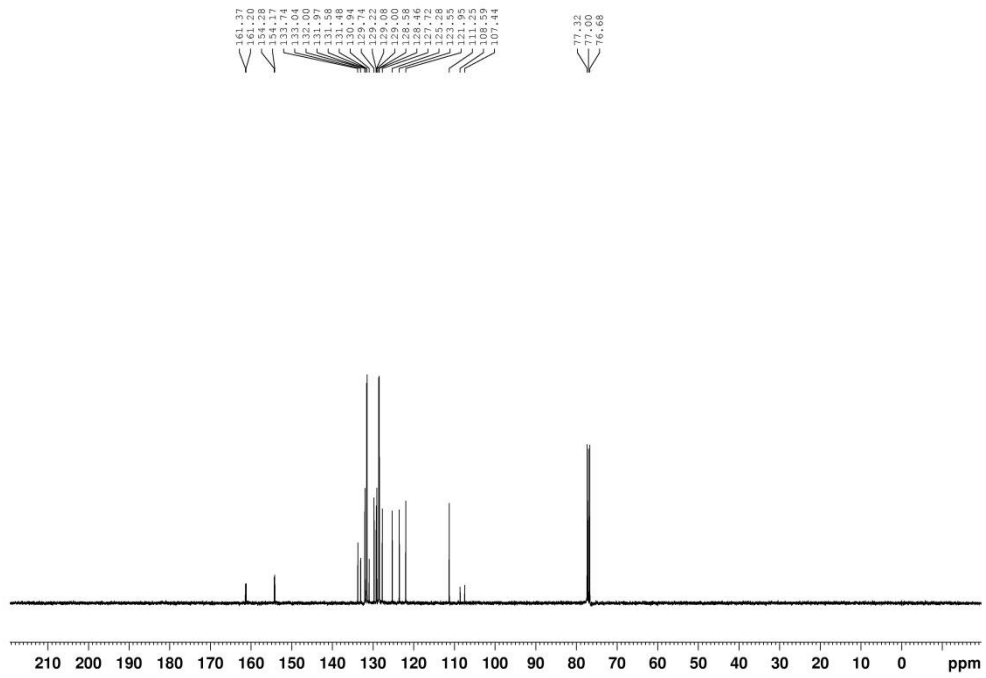

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

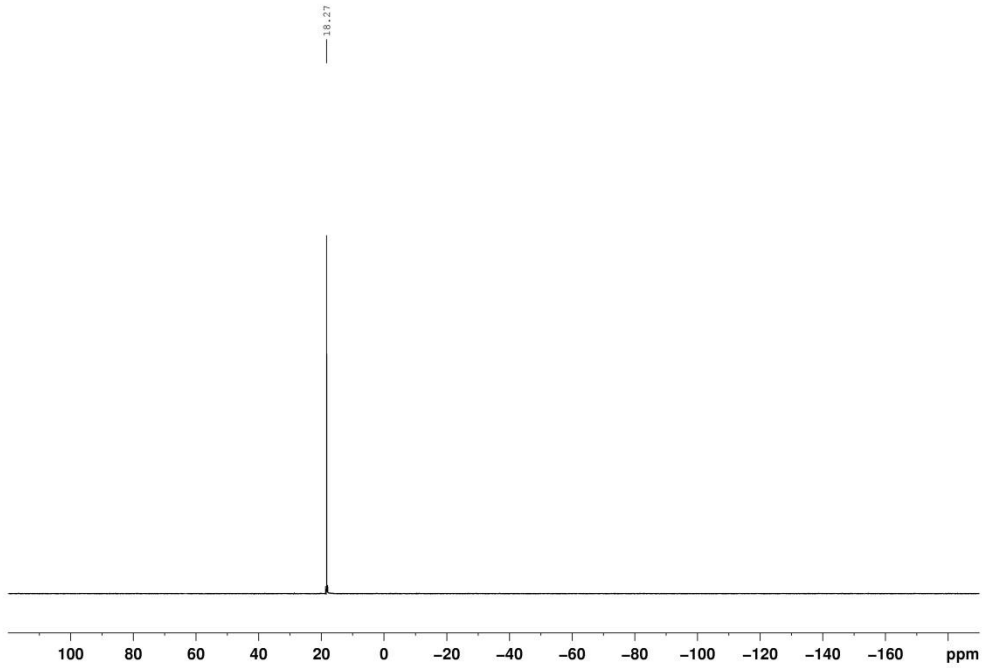

18.48
100
50
0
−50
−100
−150
−200
ppm

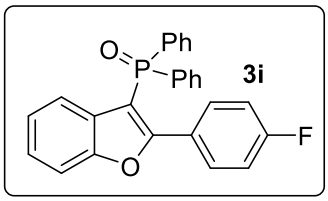

O
P
Ph
Ph
3h
O
Cl

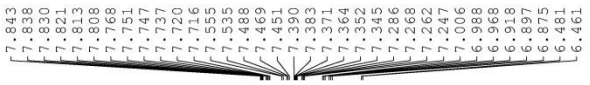

7.779
7.762
7.758
7.748
7.744
7.730
7.727
7.715
7.713
7.709
7.696
7.693
7.689
7.567
7.547
7.487
7.484
7.468
7.465
7.450
7.446
7.397
7.394
7.390
7.378
7.374
7.371
7.360
7.358
7.353
7.311
7.309
7.291
7.273
7.270
7.263
7.214
7.211
7.209
7.207
7.194
7.191
7.189
7.186
7.134
7.114
7.094
7.034
7.032
7.013
6.995
6.993
6.571
6.551
0.000

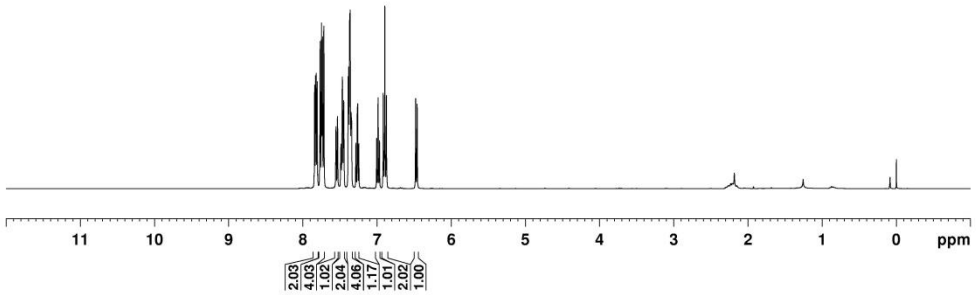

14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.97
1.00
1.01
2.05
4.03
1.02
0.97
1.01
1.00
0.98

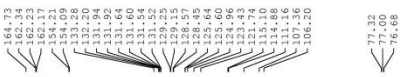

161.37
161.20
154.28
154.17
133.74
133.04
132.00
131.97
131.88
131.48
130.94
129.74
129.72
129.06
129.00
128.58
128.46
127.72
125.28
123.55
121.95
111.25
108.59
107.44
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

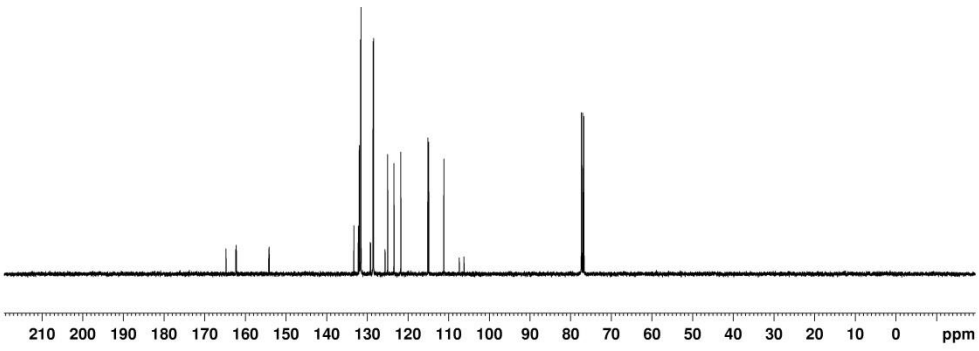

18.27
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

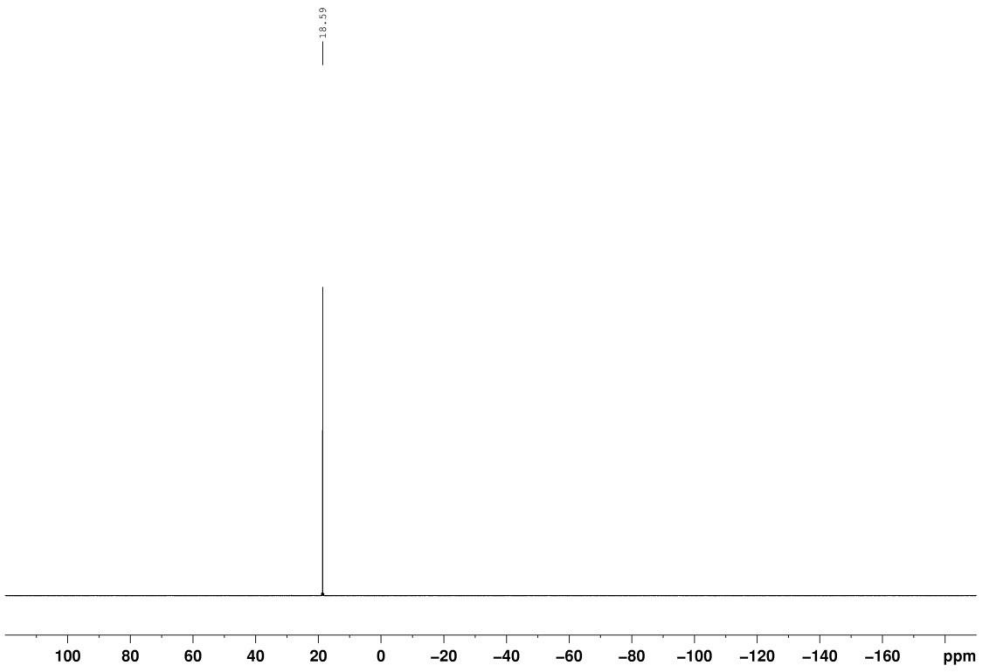

O
P
Ph
Ph
3i
O
F

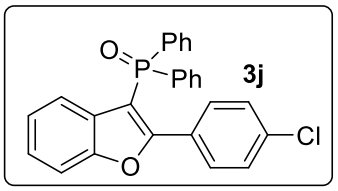

7.843
7.838
7.830
7.821
7.813
7.808
7.768
7.751
7.747
7.737
7.720
7.716
7.555
7.535
7.488
7.469
7.451
7.390
7.383
7.371
7.364
7.352
7.345
7.286
7.268
7.262
7.247
7.006
6.988
6.968
6.918
6.897
6.875
6.481
6.461
0.000

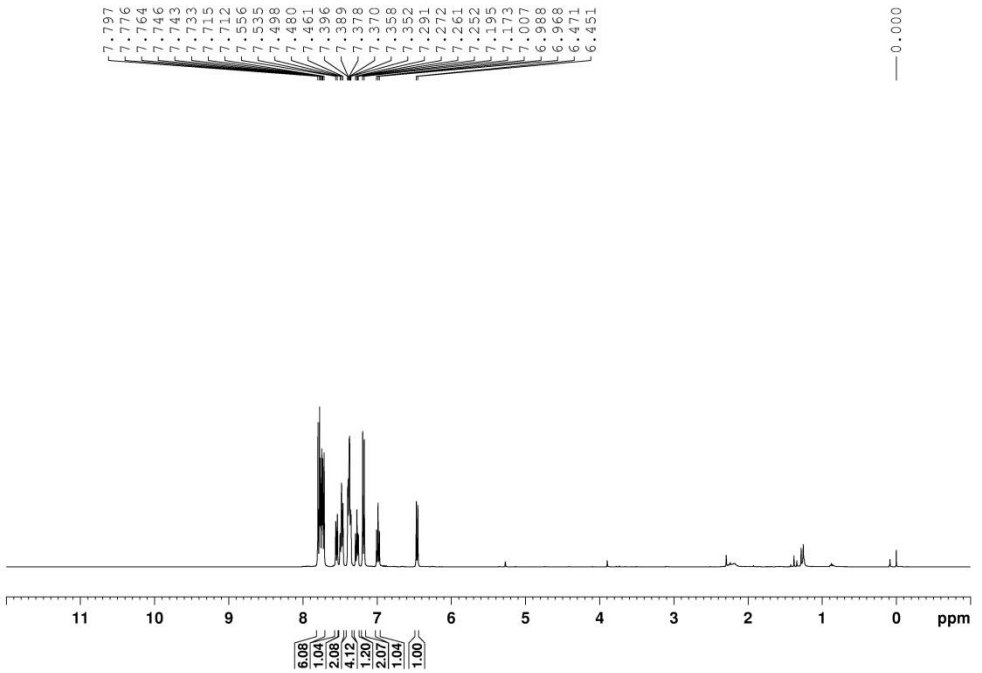

11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
4.03
1.02
2.04
4.06
1.17
1.01
2.02
1.00

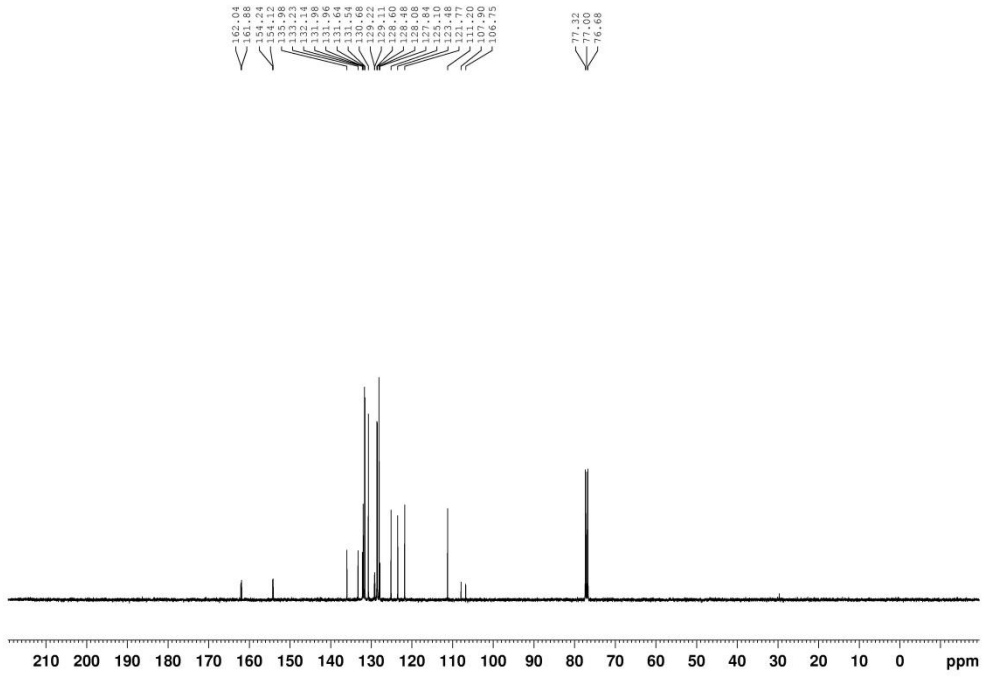

164.73
162.34
162.23
161.77
154.21
154.09
133.28
132.20
131.94
131.92
131.64
131.60
131.54
131.52
129.25
129.15
128.57
128.45
125.64
125.60
124.96
123.43
123.34
115.10
114.88
111.16
107.36
106.20
77.32
77.00
76.68

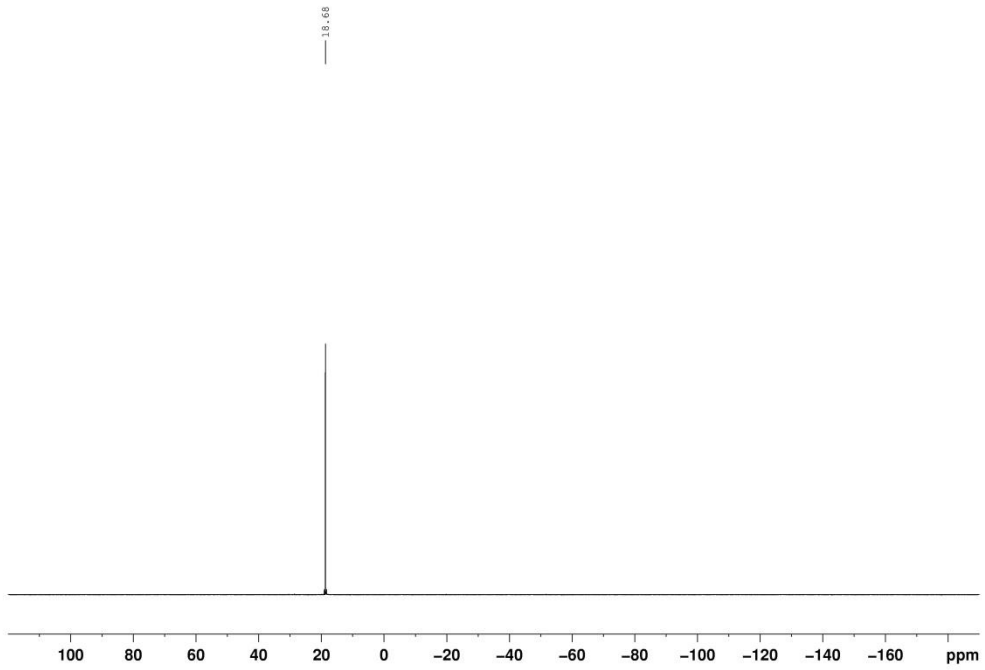

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

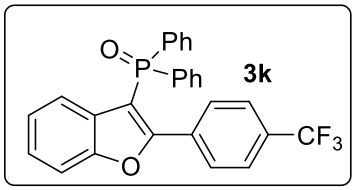

18.59
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

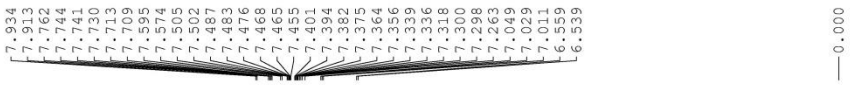

O
P
Ph
Ph
3j
Cl
O

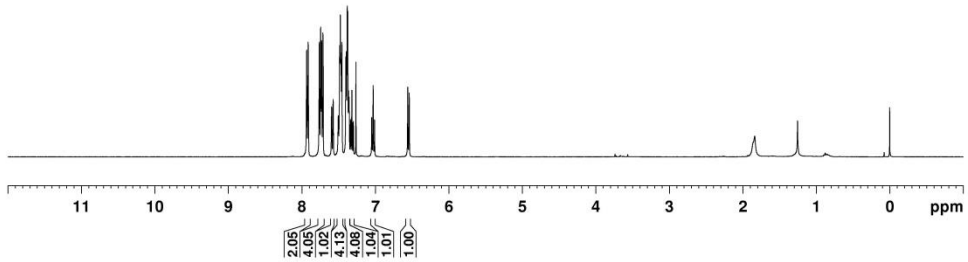

7.797
7.776
7.764
7.746
7.743
7.733
7.715
7.712
7.556
7.535
7.498
7.480
7.461
7.396
7.389
7.378
7.370
7.358
7.352
7.291
7.272
7.261
7.252
7.195
7.173
7.007
6.988
6.968
6.471
6.451
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.08
1.04
2.08
4.12
1.20
2.07
1.04
1.00

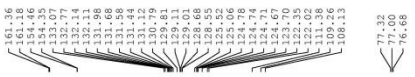

162.04
161.88
154.44
154.12
135.98
133.23
132.14
131.98
131.96
131.64
131.54
130.68
130.22
129.11
128.60
128.48
128.08
127.84
125.10
123.48
121.77
111.70
107.90
106.75
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

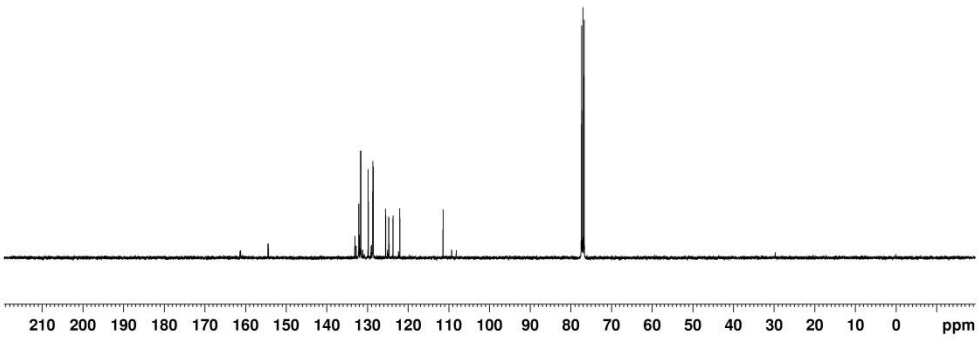

18.68
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

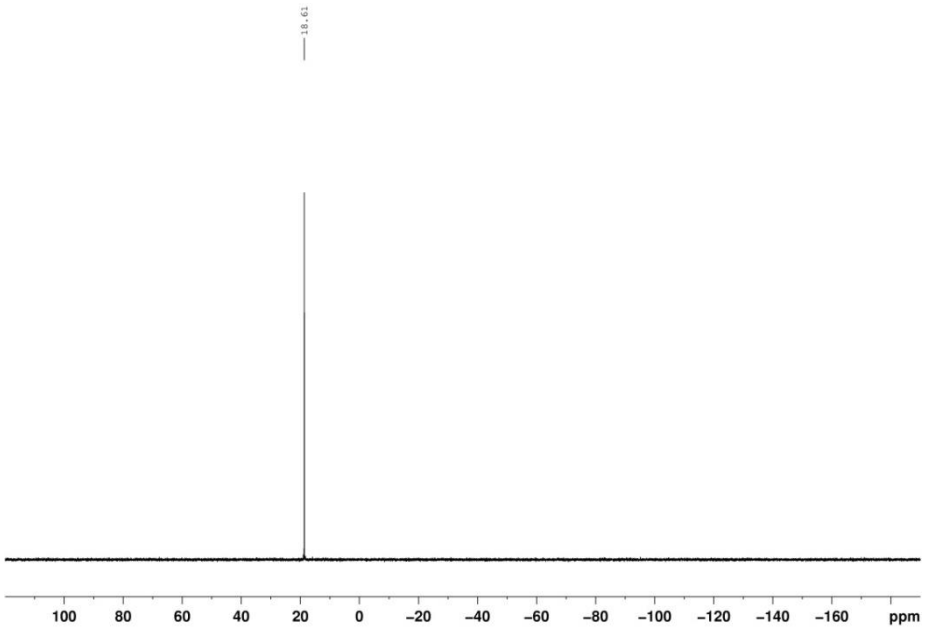

O
P
Ph
Ph
3k
O
CF3

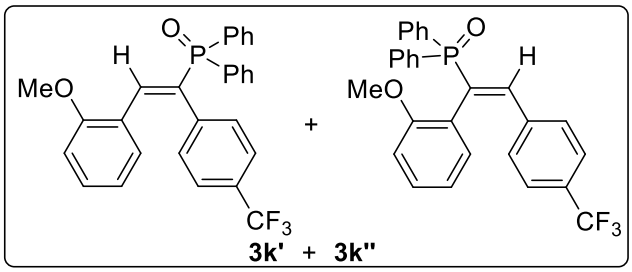

7.934
7.913
7.762
7.744
7.741
7.730
7.713
7.709
7.595
7.574
7.505
7.502
7.487
7.483
7.476
7.468
7.465
7.455
7.401
7.394
7.382
7.375
7.364
7.356
7.339
7.336
7.318
7.300
7.298
7.263
7.049
7.029
7.011
6.559
6.539
0.000

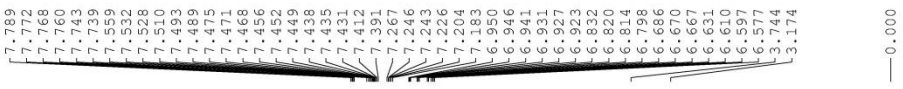

11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.05
4.05
1.02
4.13
4.08
1.04
1.01
1.00

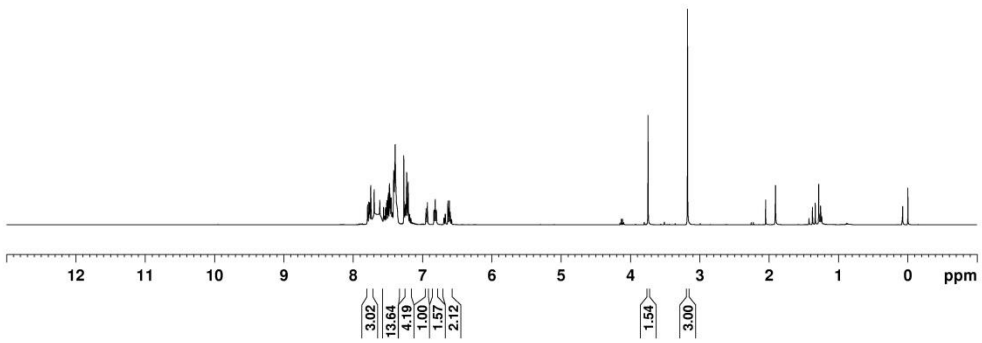

161.36
161.18
154.46
154.35
133.07
132.77
132.14
132.11
131.98
131.68
131.58
131.44
131.12
130.79
129.81
129.31
129.01
128.68
128.55
125.53
125.06
124.78
124.74
124.71
124.67
123.70
122.35
122.02
111.38
110.26
108.13
77.32
77.00
76.68

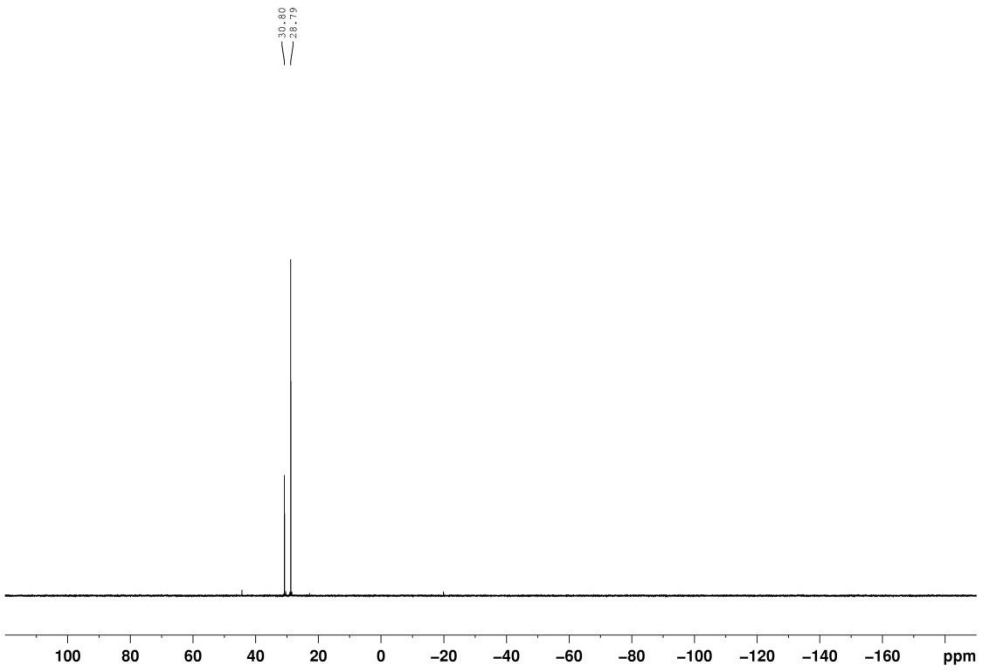

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

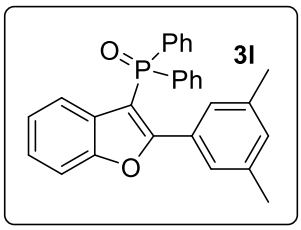

18.61
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
ppm


MeO
H
O
P
Ph
Ph
CF3
+
Ph
Ph
P
O
MeO
H
CF3
3k' + 3k''

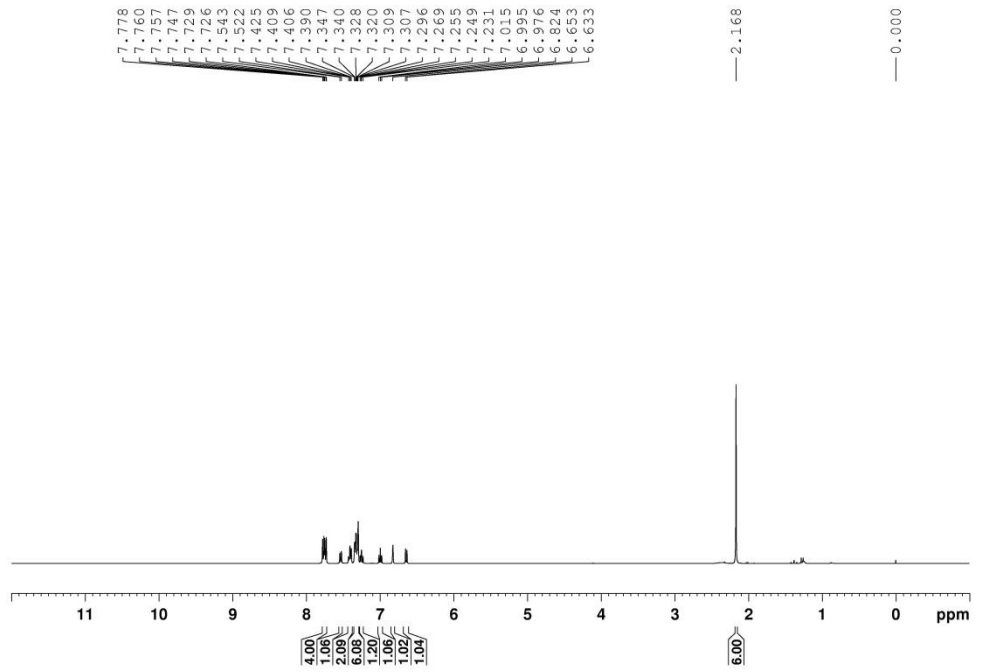

7.789
7.772
7.768
7.760
7.743
7.739
7.559
7.532
7.528
7.510
7.493
7.489
7.475
7.471
7.468
7.456
7.452
7.449
7.438
7.435
7.431
7.412
7.391
7.267
7.246
7.243
7.226
7.204
7.183
6.950
6.946
6.941
6.931
6.927
6.923
6.832
6.820
6.814
6.798
6.686
6.670
6.667
6.631
6.610
6.597
6.577
3.744
3.174
0.000

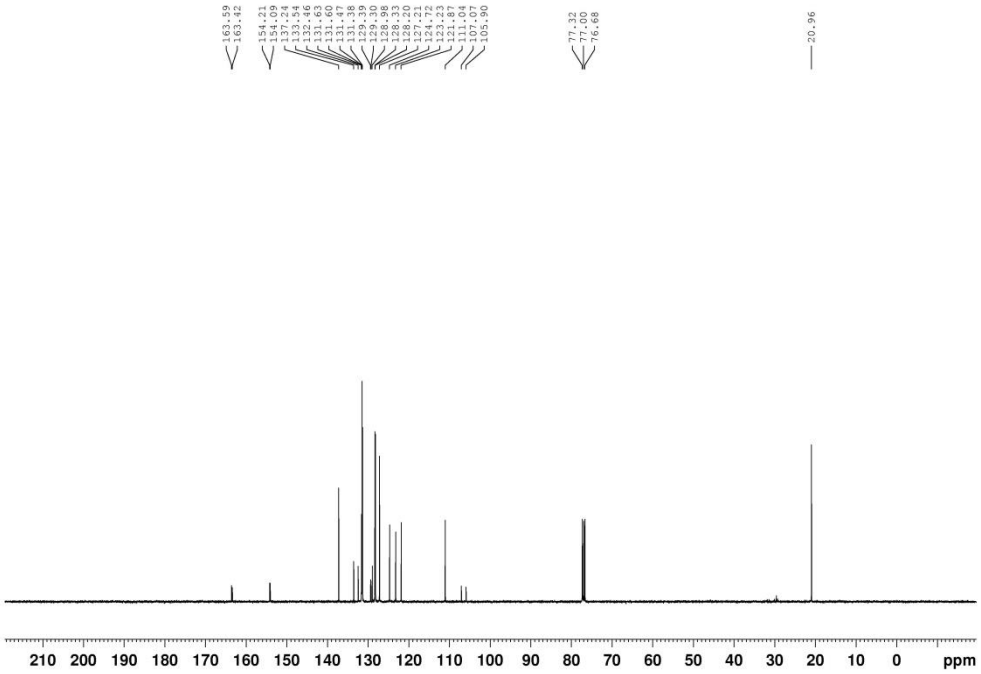

12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.02
13.64
4.19
1.00
1.57
2.12
1.54
3.00

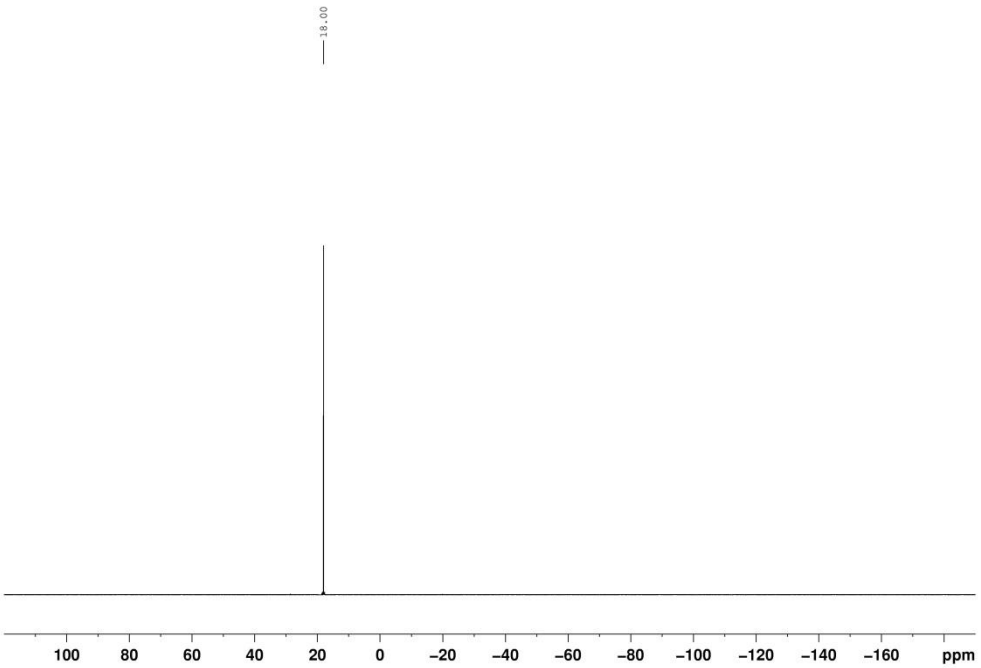

30.80
28.79
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

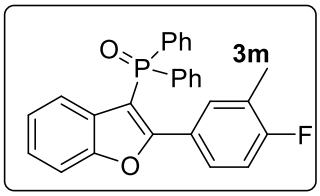

O
P
Ph
Ph
O

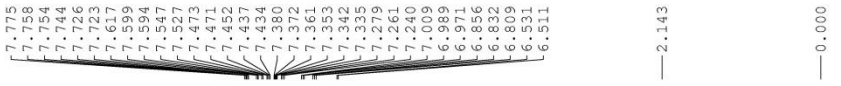
3l

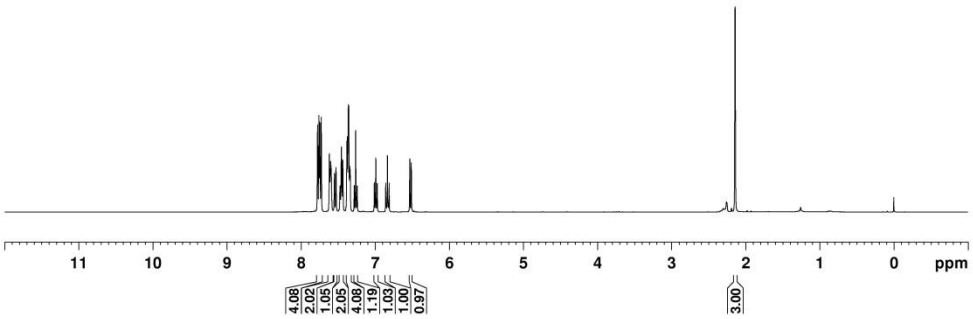

7.778
7.760
7.757
7.747
7.729
7.726
7.543
7.522
7.425
7.409
7.406
7.390
7.347
7.340
7.328
7.320
7.309
7.307
7.296
7.269
7.255
7.249
7.231
7.015
6.995
6.976
6.824
6.653
6.633
2.168
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
1.06
2.09
6.08
1.20
1.06
1.02
1.04
6.00


163.59
163.42
154.21
154.09
153.54
133.24
132.46
131.63
131.60
131.47
131.38
129.39
129.30
128.98
128.33
128.20
127.21
124.72
123.33
121.87
111.04
107.07
105.90
77.32
77.00
76.68
20.96
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

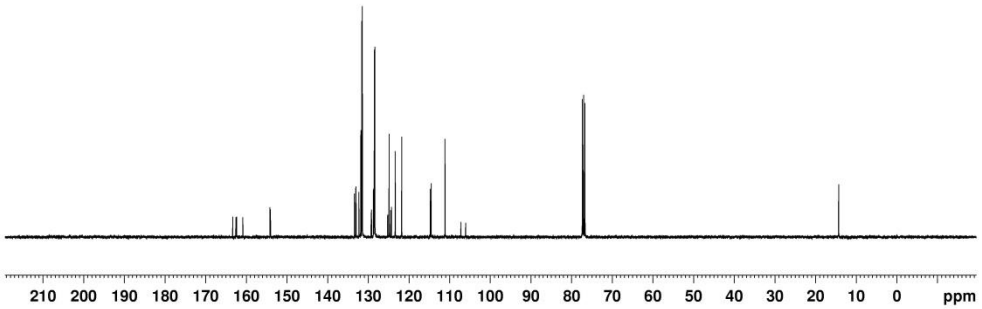

18.00
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

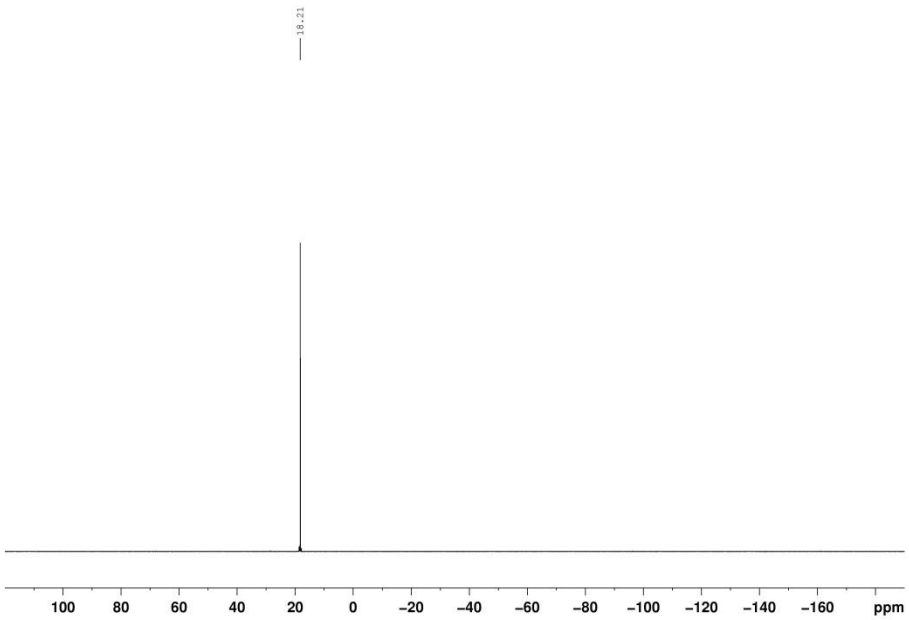

O
P
Ph
Ph
3m
O
F

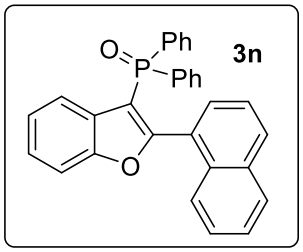

7.775
7.758
7.754
7.744
7.726
7.723
7.617
7.599
7.594
7.547
7.527
7.473
7.471
7.452
7.437
7.434
7.380
7.372
7.361
7.353
7.342
7.335
7.279
7.261
7.240
7.009
6.989
6.971
6.856
6.832
6.809
6.531
6.511
2.143
0.000

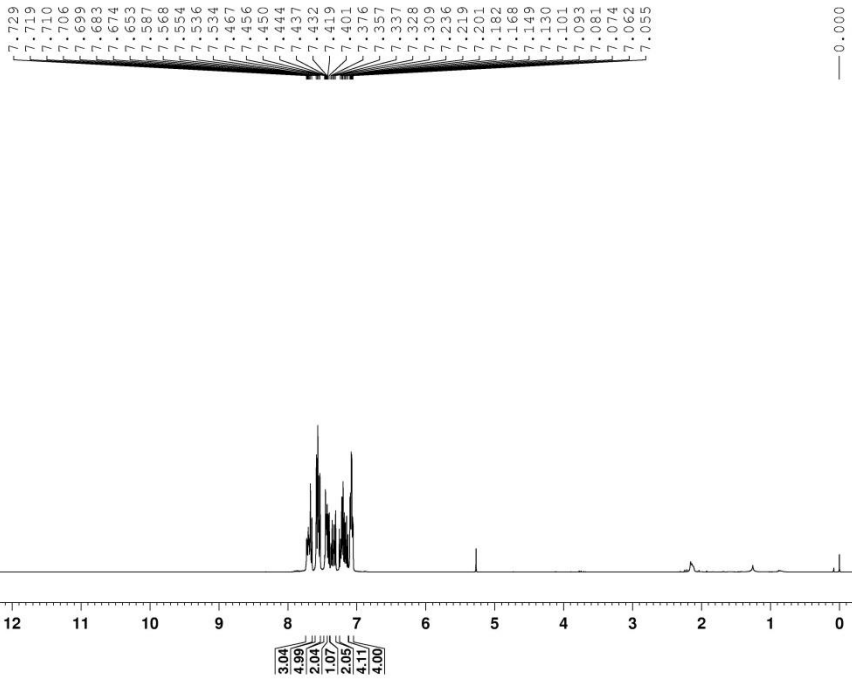

11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.08
2.02
1.05
2.05
4.08
1.19
1.03
1.00
0.97
3.00

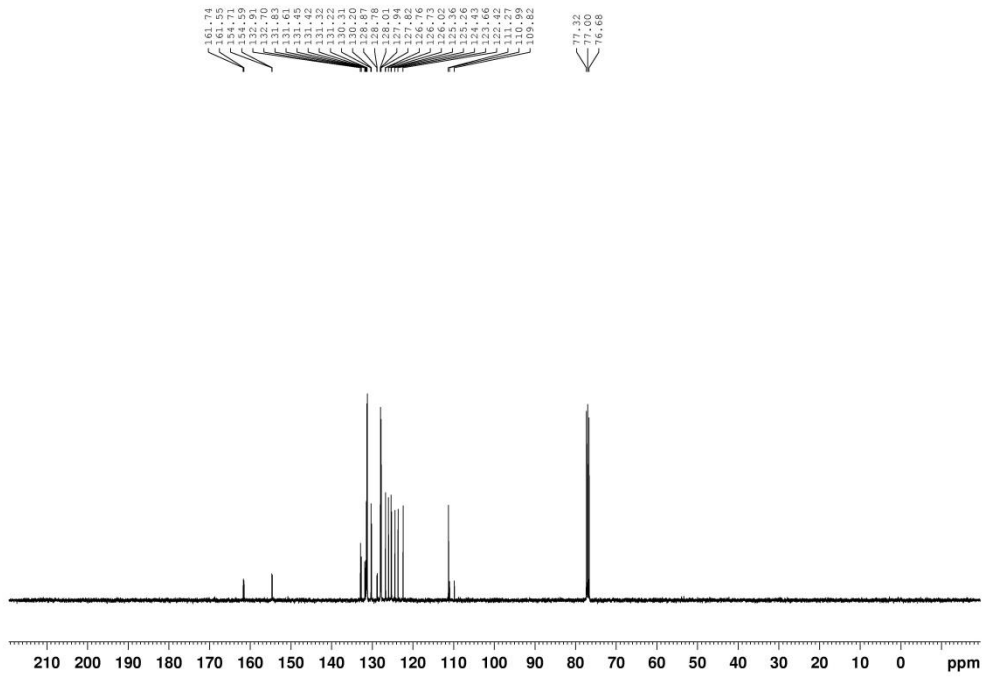

163.32
162.94
162.37
160.84
154.18
154.06
133.37
133.05
133.00
132.29
131.83
131.81
131.56
131.46
129.28
129.18
128.73
128.64
128.49
128.36
125.71
125.18
124.87
124.48
124.30
124.26
121.76
114.73
114.50
111.10
111.19
106.04
77.32
77.00
76.68
14.25

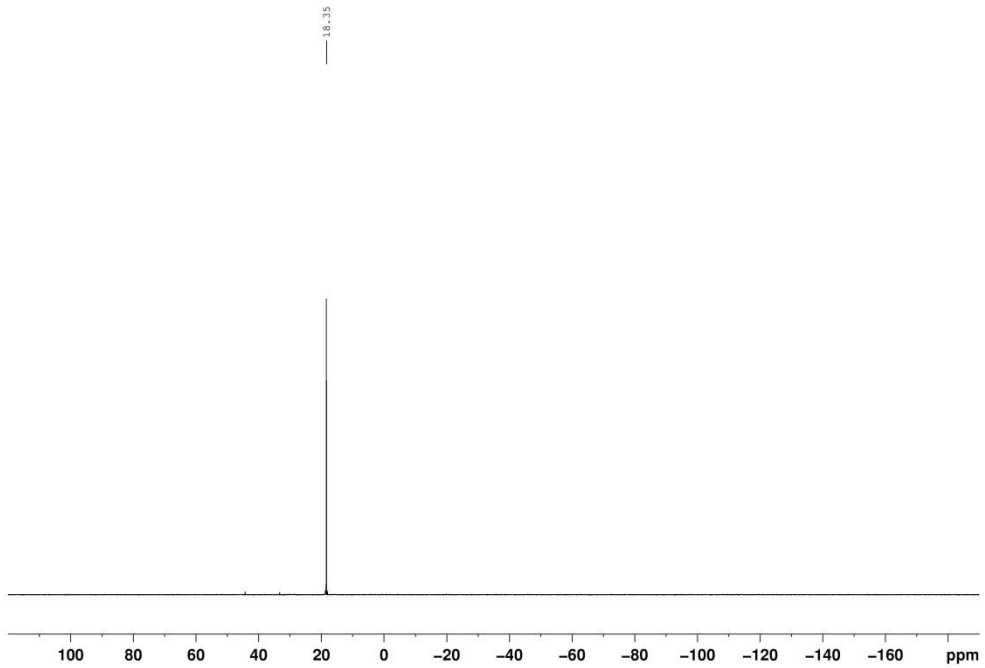

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

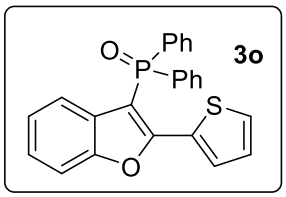

18.21
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

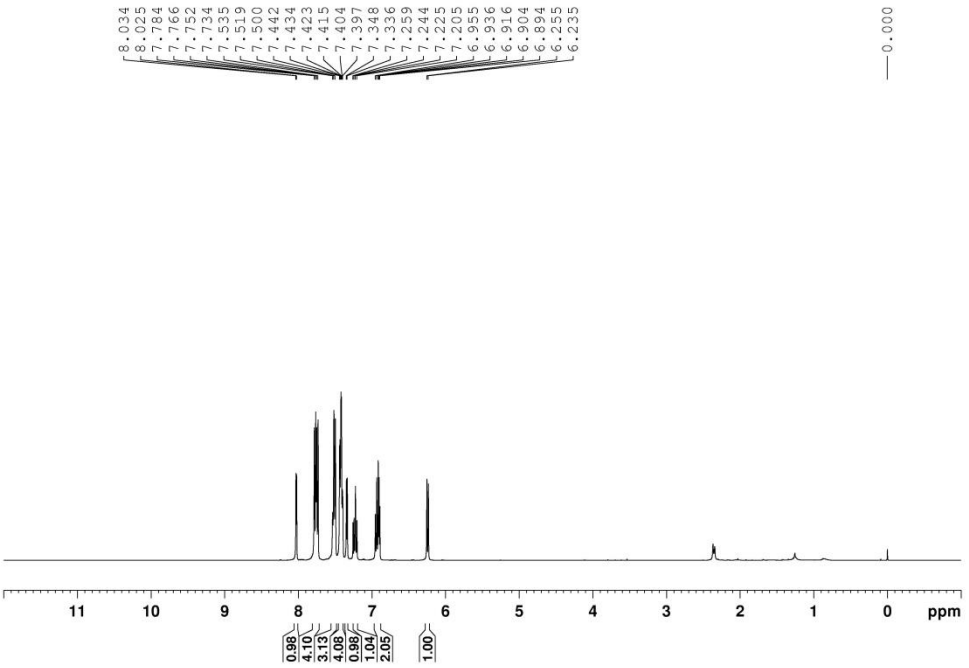

O
P
Ph
Ph
O
3n

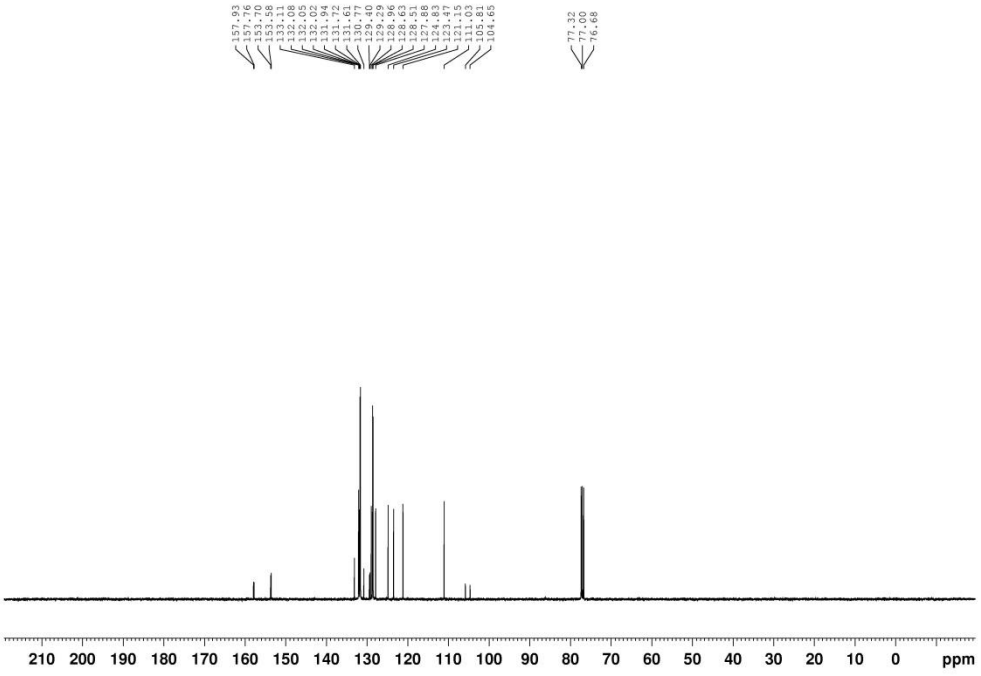

7.729
7.719
7.710
7.706
7.699
7.683
7.674
7.653
7.587
7.568
7.554
7.536
7.534
7.467
7.456
7.450
7.444
7.437
7.432
7.419
7.401
7.376
7.357
7.337
7.328
7.309
7.236
7.219
7.201
7.182
7.168
7.149
7.130
7.101
7.093
7.081
7.074
7.062
7.055
0.000
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.04
4.99
2.04
1.07
2.05
4.11
4.00

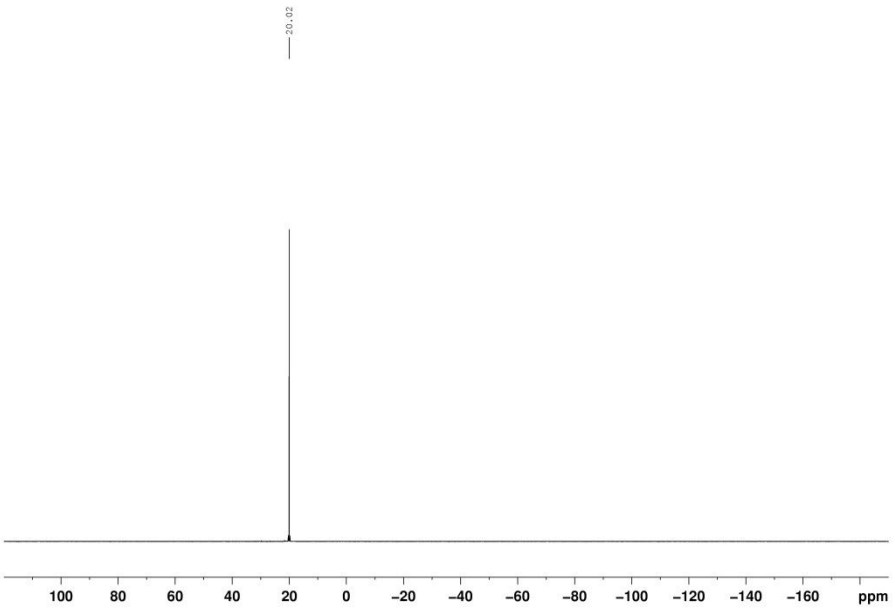

161.74
161.55
154.71
154.59
132.91
132.70
131.83
131.61
131.45
131.42
131.32
131.22
130.31
130.20
128.87
128.78
128.01
127.94
127.82
126.76
126.73
126.02
125.36
125.26
124.43
123.66
122.62
111.27
110.99
109.82
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

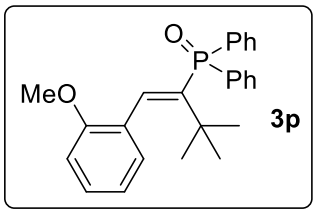

18.35
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

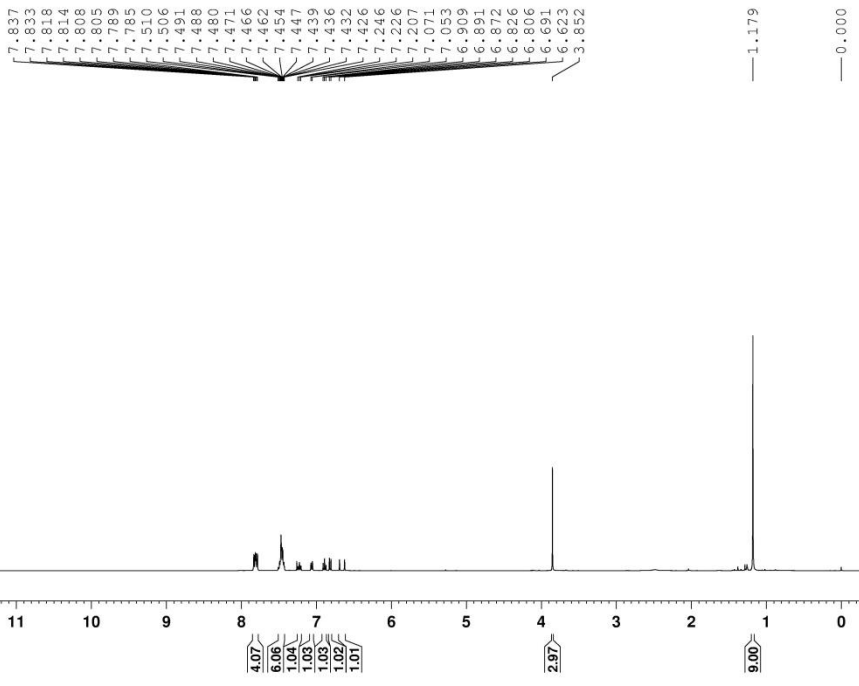

O
P
Ph
Ph
S
O
3o

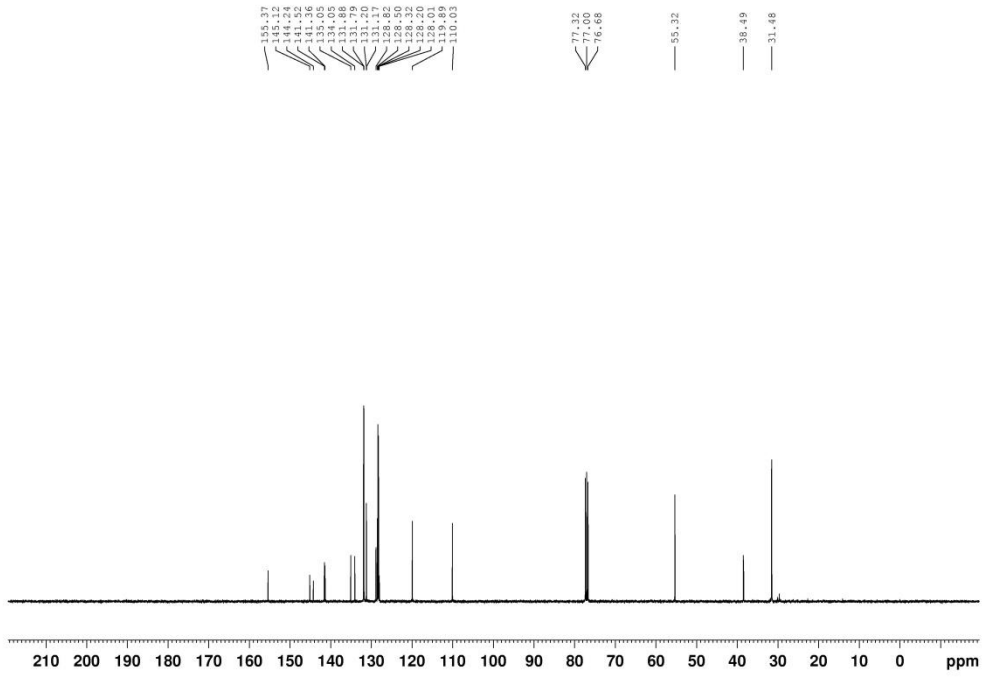

8.034
8.025
7.784
7.766
7.752
7.734
7.535
7.519
7.500
7.442
7.434
7.423
7.415
7.404
7.397
7.348
7.336
7.259
7.244
7.225
7.205
6.955
6.936
6.916
6.904
6.894
6.255
6.235
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
4.10
3.13
4.08
0.98
1.04
2.05
1.00

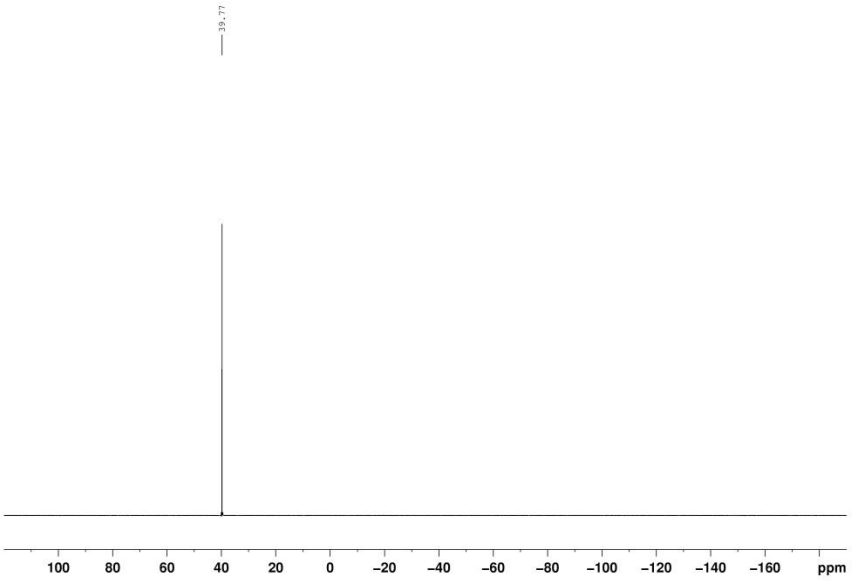

157.93
157.76
153.70
153.58
133.11
132.08
132.05
132.02
131.94
131.72
131.61
130.77
129.40
129.29
128.96
128.63
128.51
128.38
127.88
123.47
121.15
111.03
104.81
104.65
77.32
77.00
76.68
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

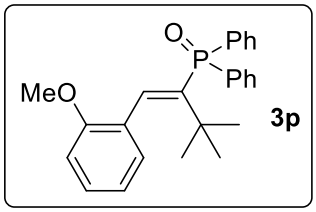

20.02
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm


O
P
Ph
Ph
MeO
3p

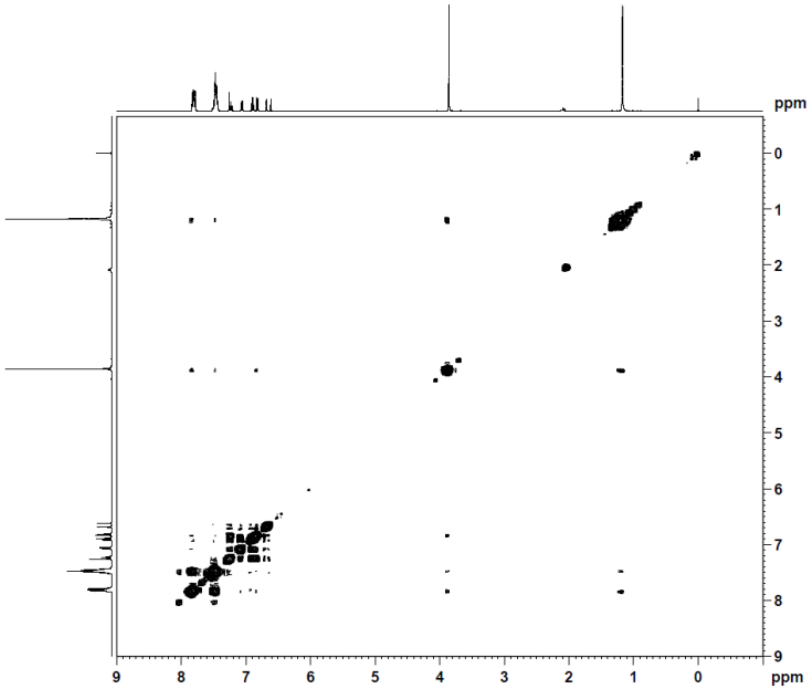

7.837
7.833
7.818
7.814
7.808
7.805
7.789
7.785
7.510
7.506
7.491
7.488
7.480
7.471
7.466
7.462
7.454
7.447
7.439
7.436
7.432
7.426
7.246
7.226
7.207
7.071
7.053
6.909
6.891
6.872
6.826
6.806
6.691
6.623
3.852
1.179
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.07
6.06
1.04
1.03
1.03
1.02
1.01
2.97
9.00

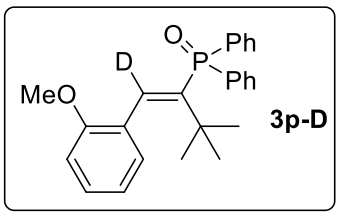

155.37
145.12
144.84
141.52
141.36
135.05
134.65
133.88
131.79
131.20
131.17
128.62
128.50
128.32
128.20
128.01
119.89
110.03
77.32
77.00
76.68
55.32
38.49
31.48
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

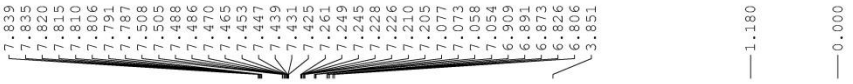

39.77
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

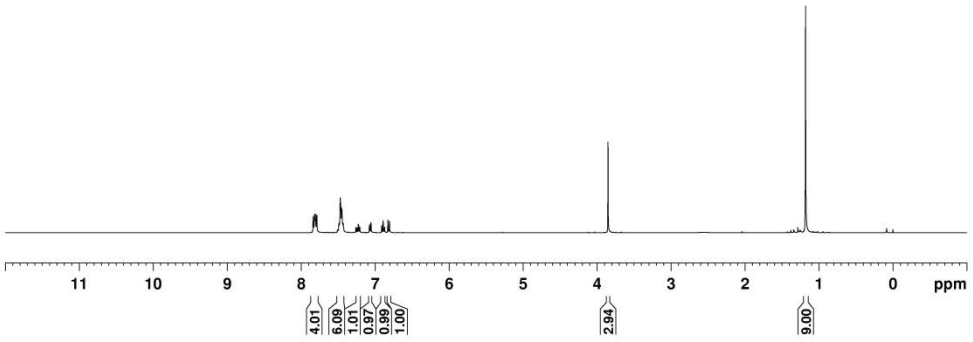


The COSY spectrum correlations from δ_H 1.18 (s, 9H) to δ_H 3.85 (s, 3H) confirms that the tert-butyl group is on the same side with methoxy group. Moreover, spectrum correlations from δ_H 1.18 (m, 9H) to 7.84-7.79 (m, 4H), from δ_H 1.18 (m, 9H) to 7.51-7.43 (m, 6H) confirms that the tert-butyl group is attached to the same carbon with the diphenyl phosphoxide group. Thus, we determine the structure of **3p** through COSY spectrum.

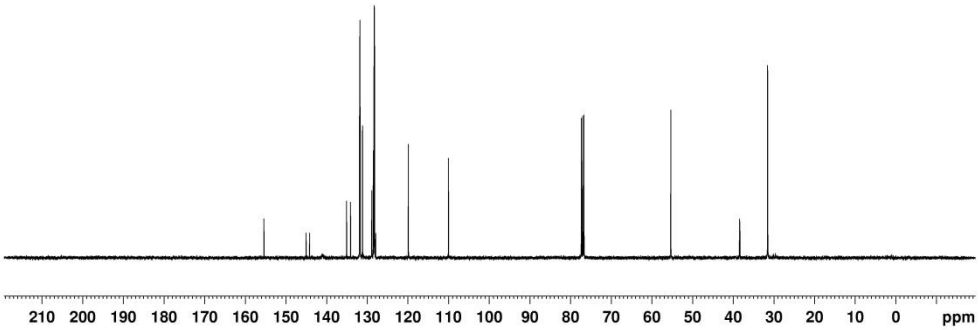


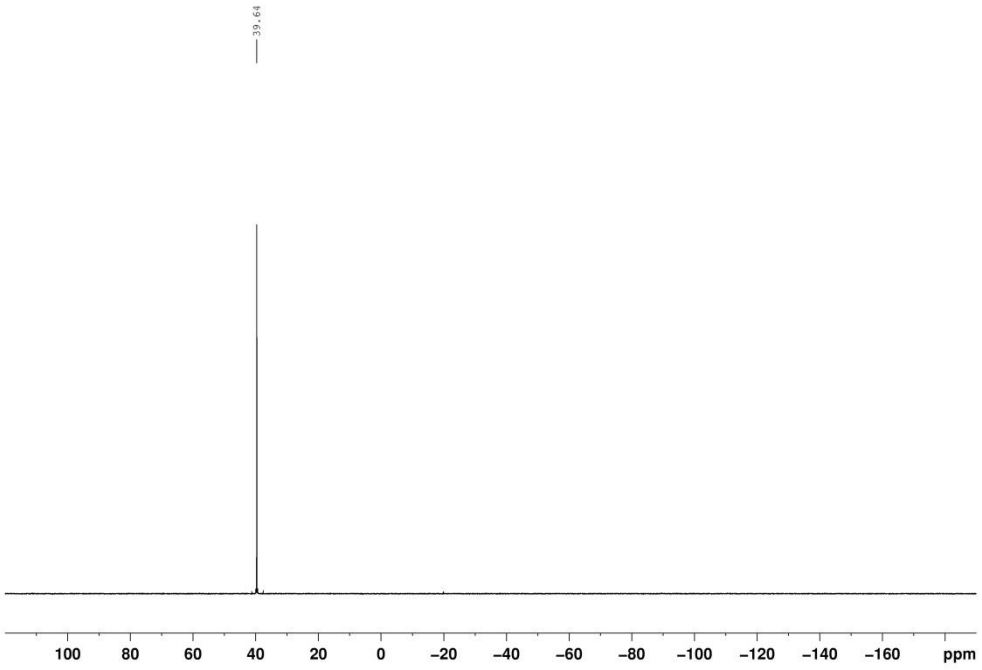

O
P
Ph
Ph
D
MeO
3p-D

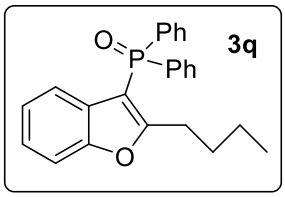

7.839
7.835
7.820
7.815
7.810
7.806
7.791
7.787
7.508
7.505
7.488
7.486
7.470
7.465
7.453
7.447
7.439
7.431
7.425
7.261
7.249
7.245
7.228
7.226
7.210
7.205
7.077
7.073
7.058
7.054
6.909
6.891
6.873
6.826
6.806
3.851
1.180
0.000

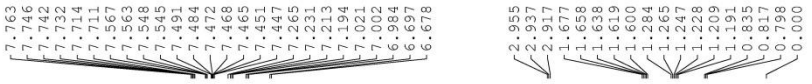

11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.01
6.09
1.01
0.97
0.99
1.00
2.94
9.00

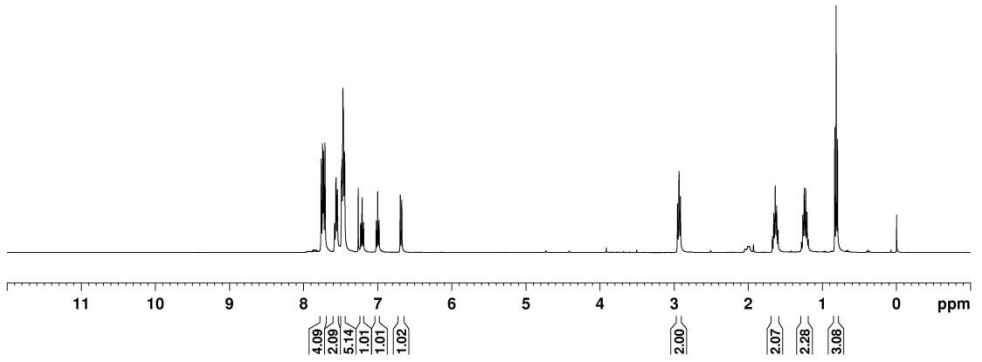

155.39
145.03
144.16
135.08
134.88
131.86
131.77
131.17
131.15
128.88
128.66
128.50
128.30
128.18
128.12
127.91
119.87
110.00
77.32
77.00
76.68
55.31
38.42
38.32
31.52
31.48

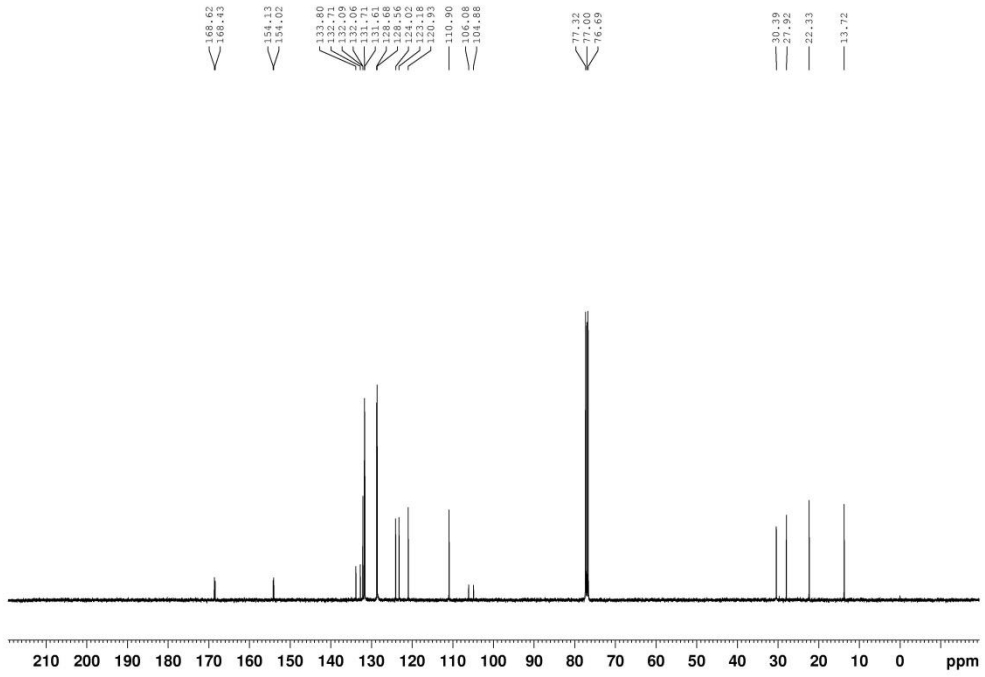

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

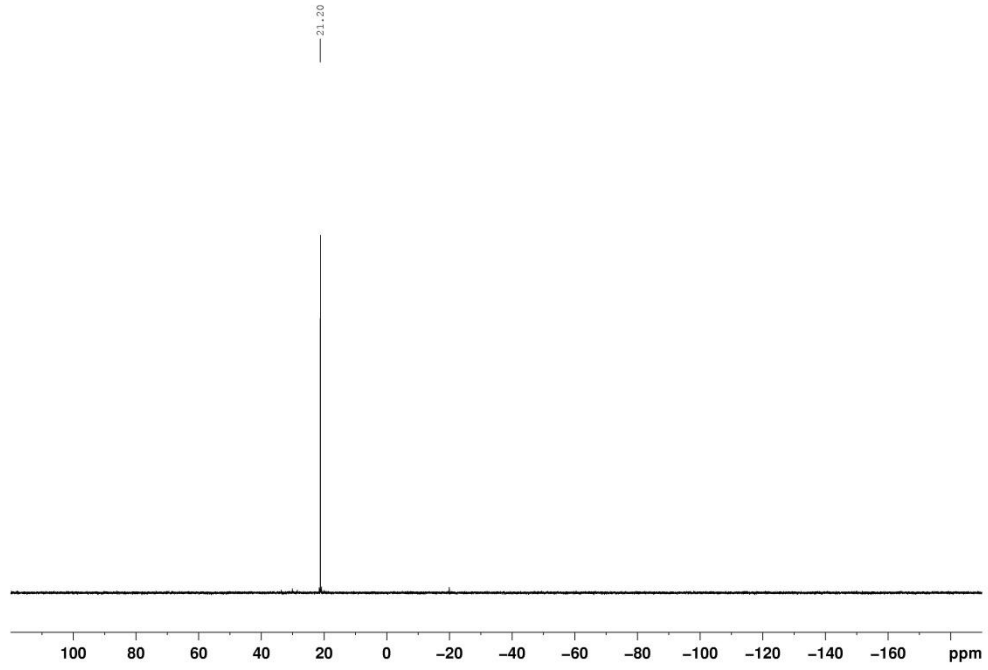

39.64
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

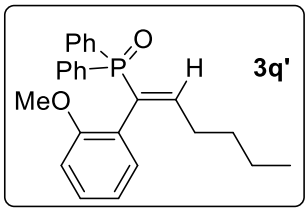

O
P
Ph
Ph
O
3q

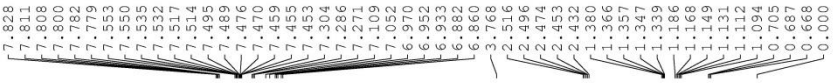

7.763
7.746
7.742
7.732
7.714
7.711
7.567
7.563
7.548
7.545
7.491
7.484
7.472
7.468
7.465
7.451
7.447
7.265
7.231
7.213
7.194
7.021
7.002
6.984
6.697
6.678
2.955
2.937
2.917
1.677
1.658
1.638
1.619
1.600
1.284
1.265
1.247
1.228
1.209
1.191
0.835
0.817
0.798
0.000

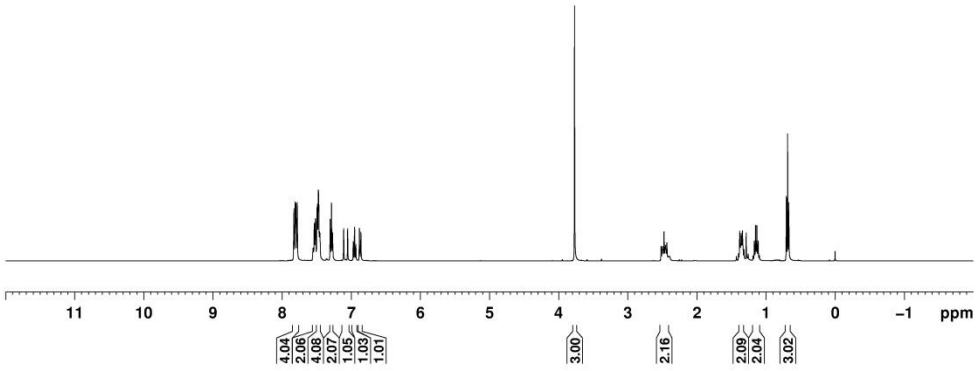

11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.09
2.09
5.14
1.01
1.01
1.02
2.00
2.07
2.28
3.08


168.62
168.43
154.13
154.02
133.80
132.71
132.09
132.06
131.71
131.61
128.68
128.56
124.02
123.18
120.93
110.90
106.08
104.88
77.32
77.00
76.69
30.39
27.92
22.33
13.72
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

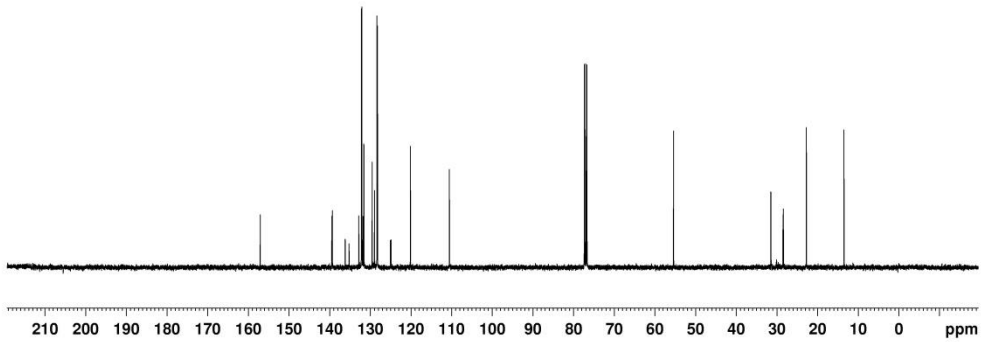

21.20
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

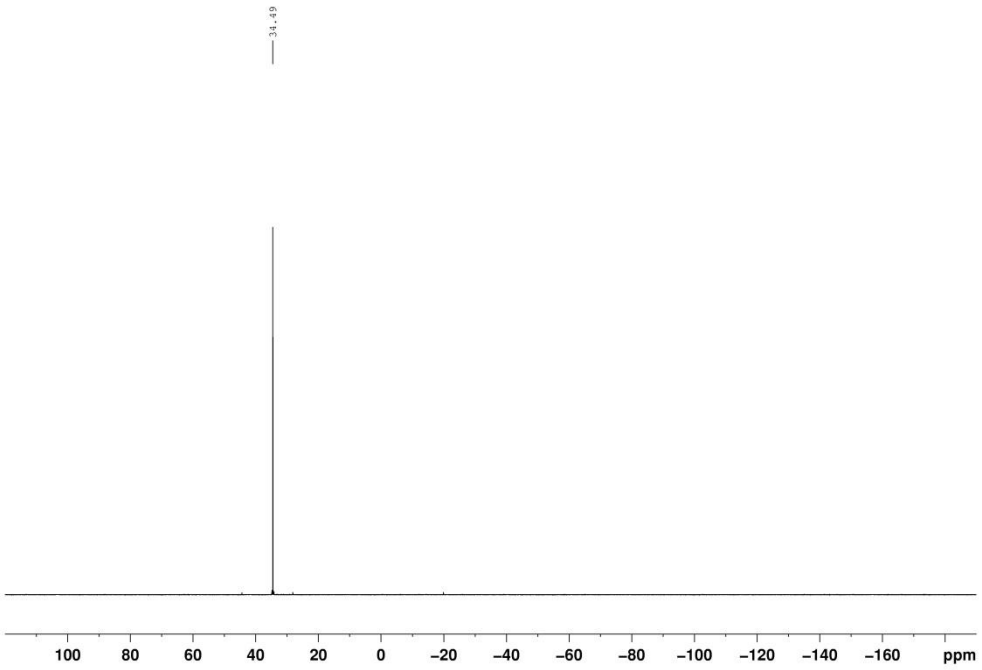

Ph
O
Ph
P
H
MeO
3q'

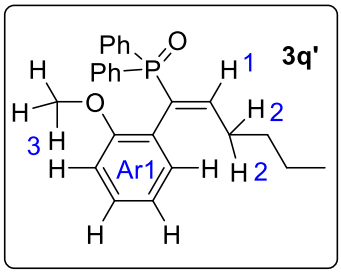

7.828
7.811
7.808
7.800
7.782
7.779
7.553
7.550
7.535
7.532
7.517
7.514
7.495
7.489
7.476
7.470
7.459
7.455
7.453
7.304
7.286
7.271
7.109
7.052
6.970
6.952
6.933
6.882
6.860
3.768
2.516
2.496
2.474
2.453
2.432
1.380
1.366
1.357
1.347
1.339
1.186
1.168
1.149
1.131
1.112
1.094
0.705
0.687
0.668
0.000


11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
4.04
2.06
4.08
2.07
1.05
1.03
1.01
3.00
2.16
2.09
2.04
3.02


157.03
139.44
139.30
136.15
135.20
132.61
132.54
132.05
131.80
131.57
131.54
129.52
128.94
128.93
128.33
128.21
125.05
124.85
120.12
110.52
77.32
77.00
76.68
55.38
31.46
31.45
28.47
28.37
22.72
13.47

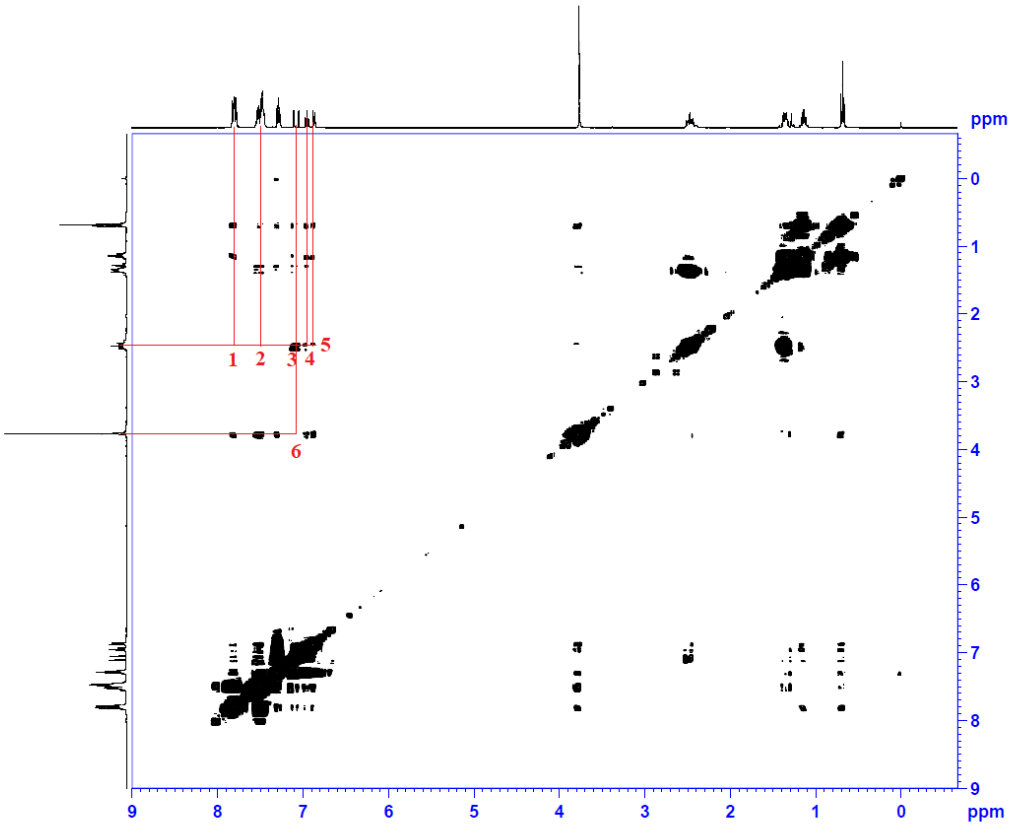

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

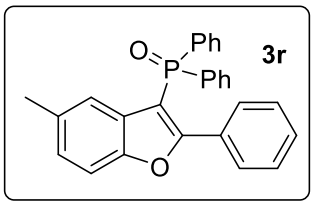

34.49
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

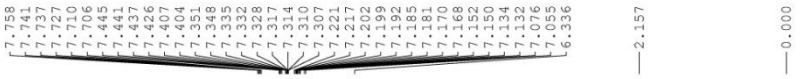


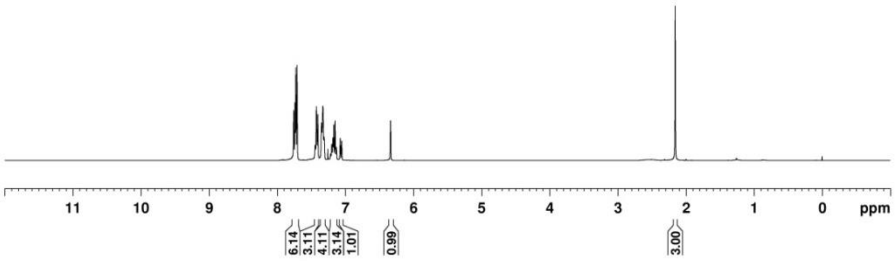
According to the literatures by Miura,[17] Breslow[19] and the crystal structure of **3p**, the phosphine oxide group is on the same side as alkenyl hydrogen in the hydrophosphinylated products. Thus, the phosphine oxide group is on the same side as alkenyl hydrogen of product **3q'**.

According to the COSY spectrum, the δ_H 2.52-2.43 (m, 2H) (H-2) has no connection with hydrogen of phosphine oxide group at positions 1 and 2. The results confirm that the n-butyl group is neither on the same side nor attached to the same carbon with phosphine oxide group. Meanwhile, the (H-2) has a connection with the δ_H 6.95 (t, J = 7.6 Hz, 1H), 6.87 (d, J = 8.8 Hz, 1H) of Ar1 at positions 4 and 5. The results confirm that the n-butyl group is indeed on the same side with aromatic ring 1 and the phosphine oxide group is on the same side with alkenyl hydrogen, which is in accord with reported work. The δ_H 7.08 (d, J = 22.8 Hz, 1H) (H-1) has a strong connection with δ_H 2.52-2.43 (m, 2H) (H-2) at position 3 and the (H-1) has no connection with (H-3) at position 6. The results confirm that the (H-1) is attached to the same carbon as the n-butyl group. Thus, we determined the structure of **3q'** through COSY spectrum and reported work.




O
P
Ph
Ph
3r
O


7.758
7.741
7.737
7.727
7.710
7.706
7.445
7.441
7.437
7.426
7.407
7.404
7.351
7.348
7.335
7.332
7.328
7.317
7.314
7.310
7.307
7.221
7.217
7.202
7.199
7.192
7.185
7.181
7.170
7.168
7.152
7.150
7.134
7.132
7.076
7.055
6.336
2.157
0.000


11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.14
3.11
4.11
3.14
1.01
0.99
3.00


163.16
162.98
152.66
152.55
133.36
132.73
132.27
131.69
131.66
131.63
131.53
129.55
129.32
129.38
129.32
129.26
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126.06
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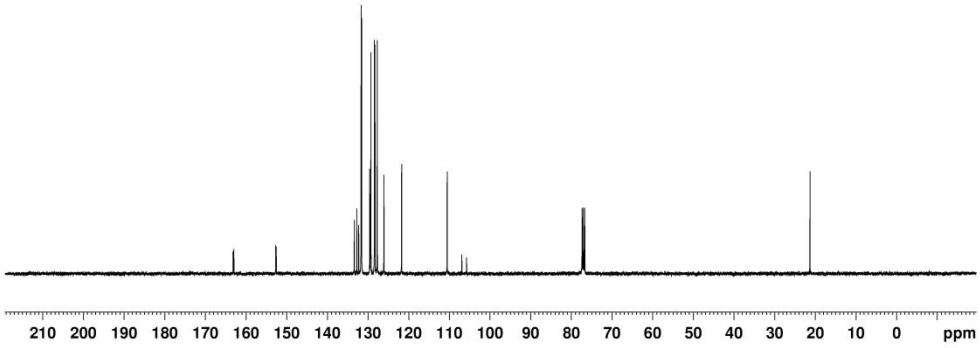
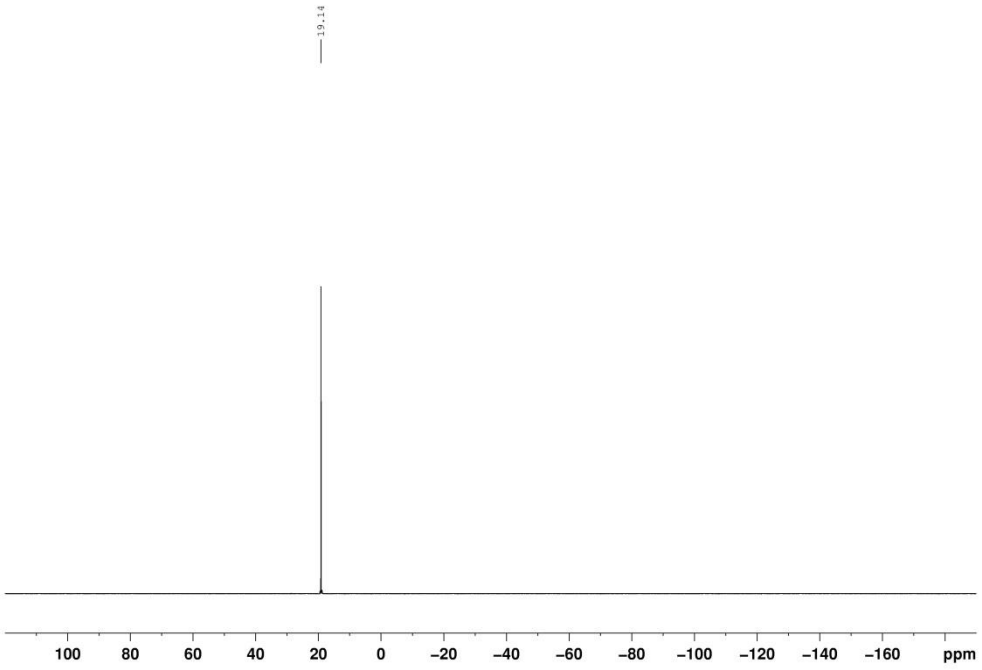
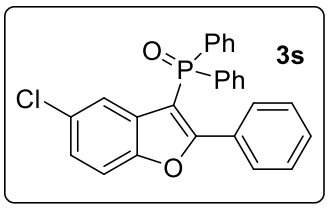
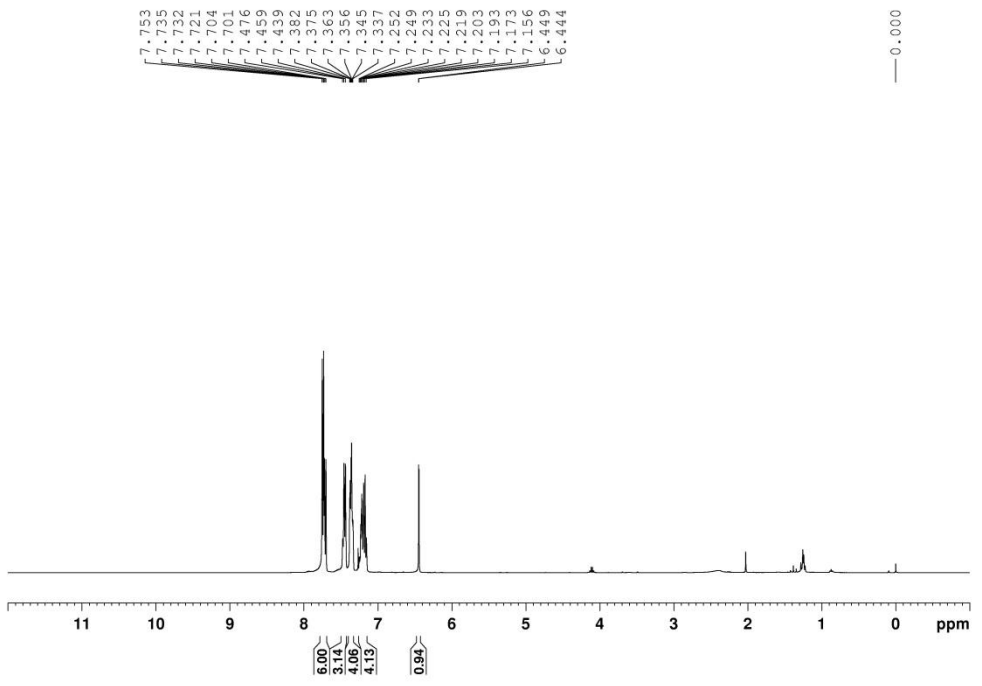
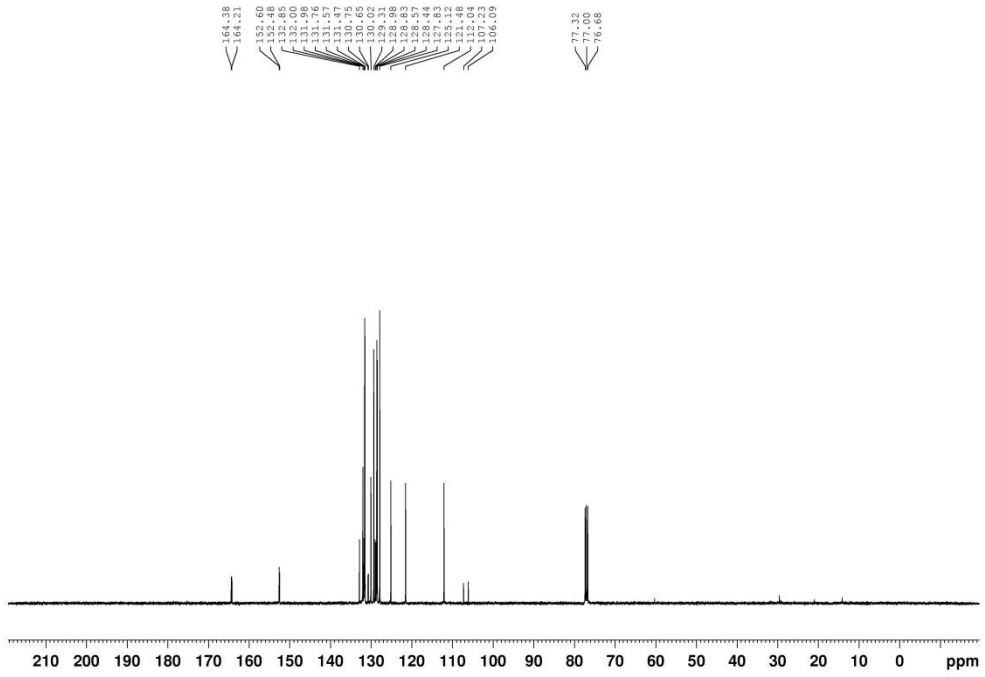
110.90
105.74
77.32
77.00
76.68
21.27

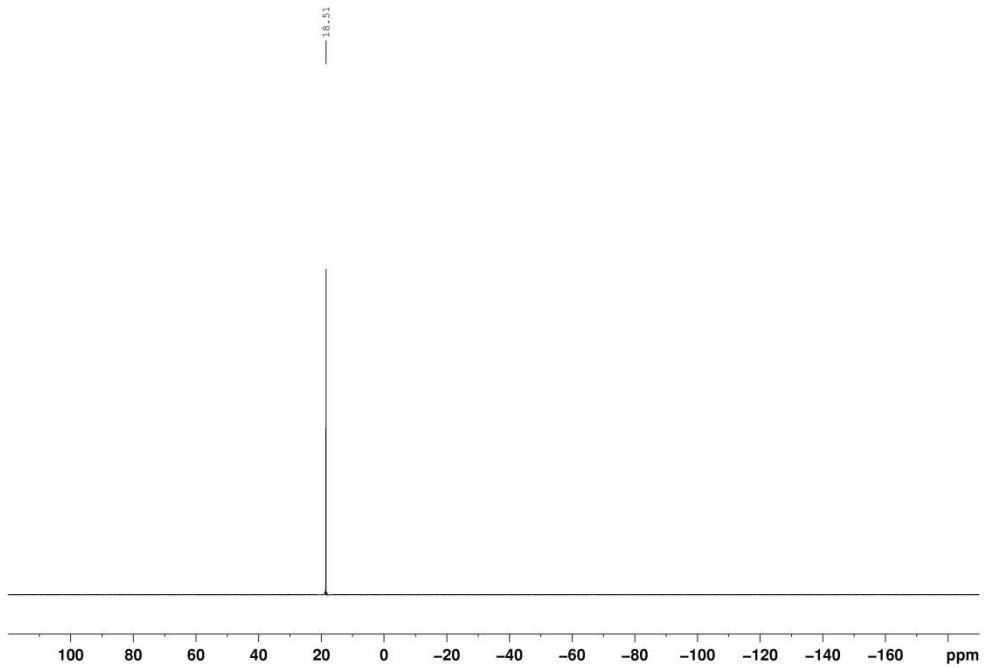

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

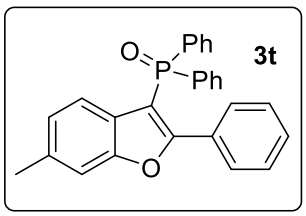

19.14
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

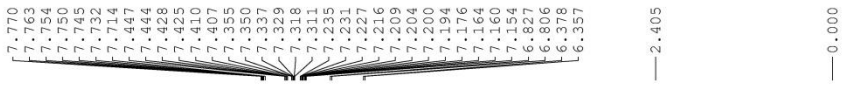

O
P
Ph
Ph
3s
Cl
O

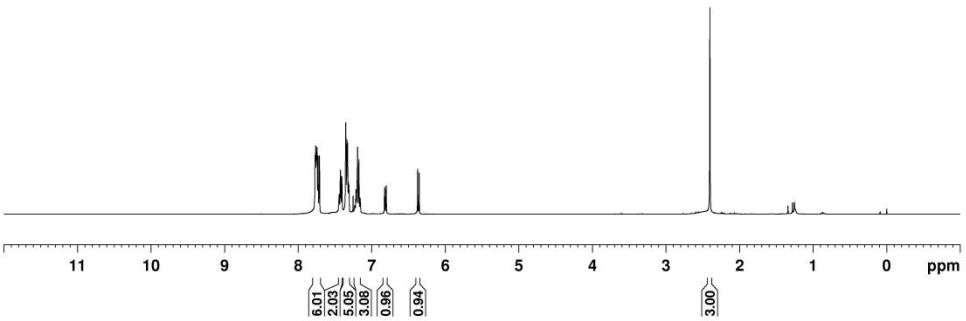

7.753
7.735
7.732
7.721
7.704
7.701
7.476
7.459
7.439
7.382
7.375
7.363
7.356
7.345
7.337
7.252
7.249
7.233
7.225
7.219
7.203
7.193
7.173
7.156
6.449
6.444
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.00
3.14
4.06
4.13
0.94


164.38
164.21
152.60
152.48
152.48
132.85
132.00
131.98
131.76
131.57
131.47
130.75
130.65
130.02
129.31
128.98
128.83
128.37
128.34
127.83
125.12
121.48
119.04
107.33
106.09
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

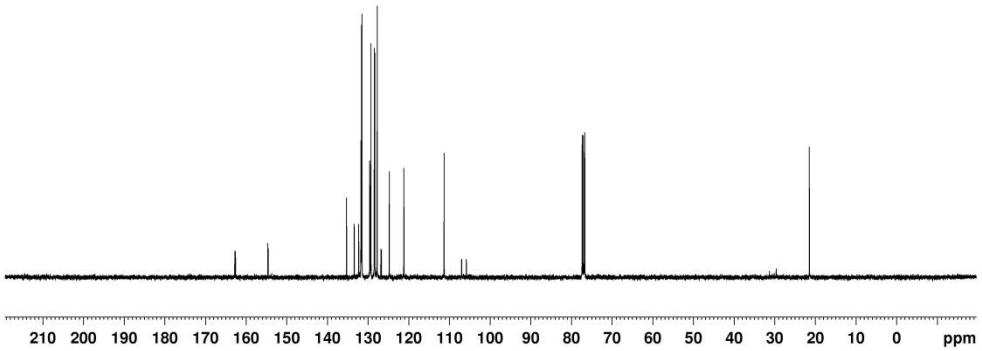

18.51
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

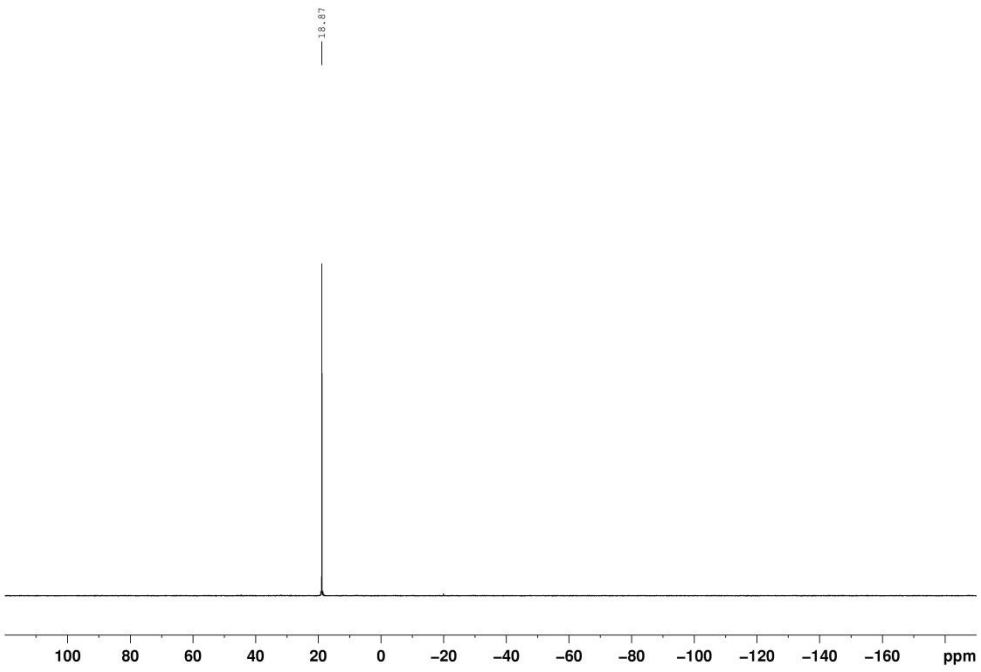

Ph
O
P
Ph
3t
O

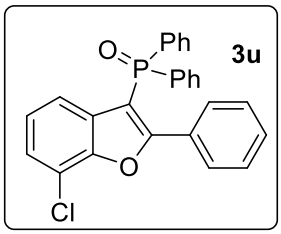

7.770
7.763
7.754
7.750
7.745
7.732
7.714
7.447
7.444
7.428
7.425
7.410
7.407
7.355
7.350
7.337
7.329
7.318
7.311
7.235
7.231
7.227
7.216
7.209
7.204
7.200
7.194
7.176
7.164
7.160
7.154
6.827
6.806
6.378
6.357
2.405
0.000

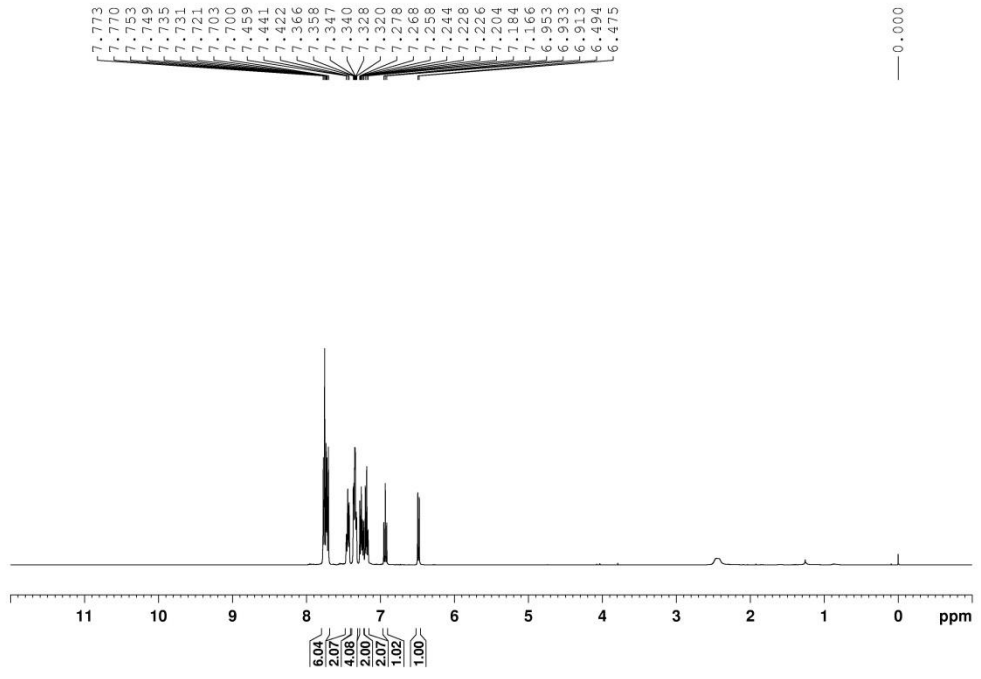

11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.01
2.03
5.05
3.08
0.96
0.94
3.00

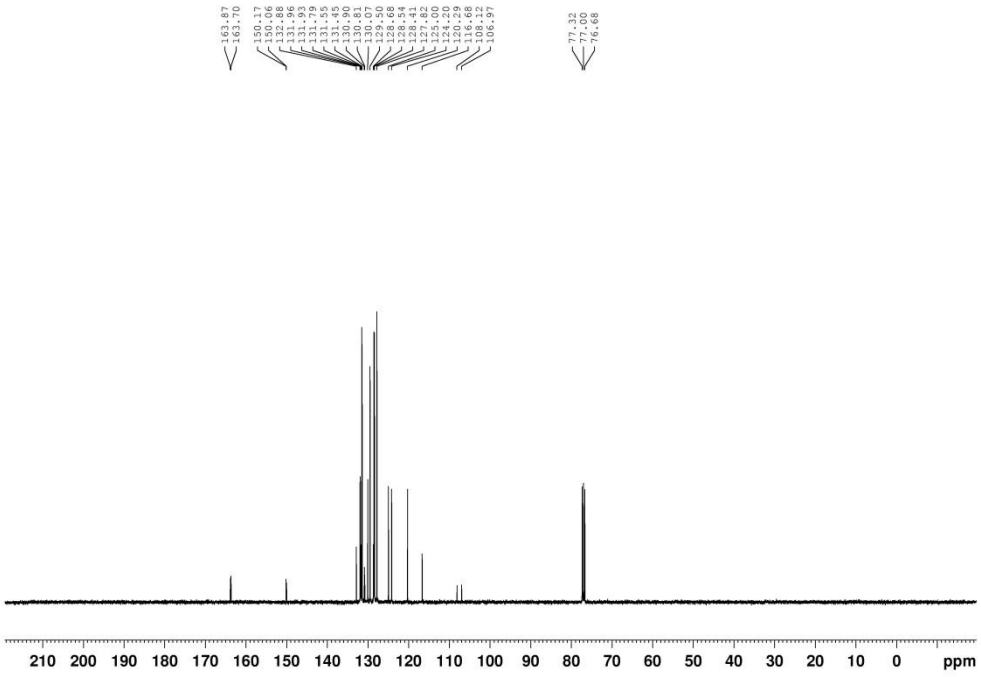

162.77
162.59
154.66
154.54
135.28
133.39
132.30
131.74
131.72
131.59
131.49
129.57
129.42
129.28
128.44
128.31
128.24
126.80
126.71
124.77
121.17
111.88
106.97
105.81
77.31
77.00
76.68
21.45

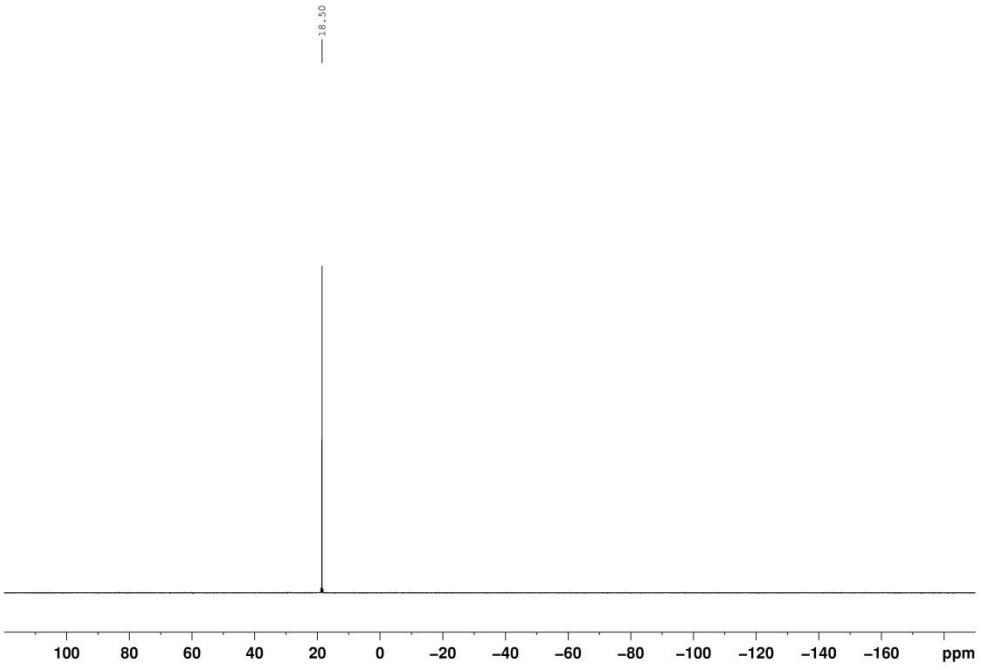

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

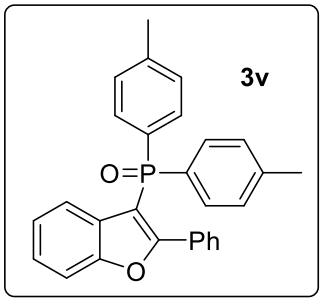

18.87
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

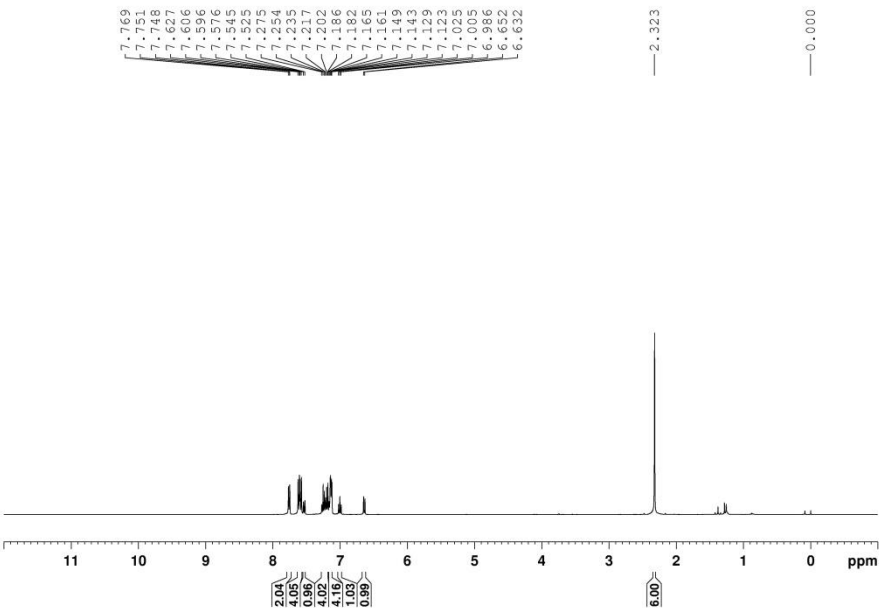

O
P
Ph
Ph
3u
O
Cl

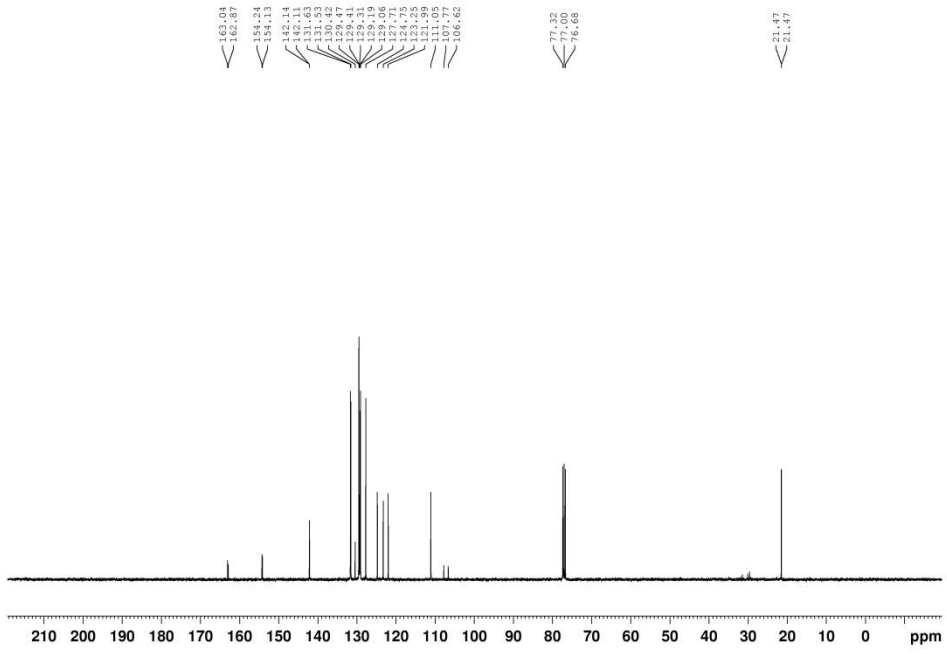

7.773
7.770
7.753
7.749
7.735
7.731
7.721
7.703
7.700
7.459
7.441
7.422
7.366
7.358
7.347
7.340
7.328
7.320
7.278
7.268
7.258
7.244
7.228
7.226
7.204
7.184
7.166
6.953
6.933
6.913
6.494
6.475
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.04
2.07
4.08
2.00
2.07
1.02
1.00

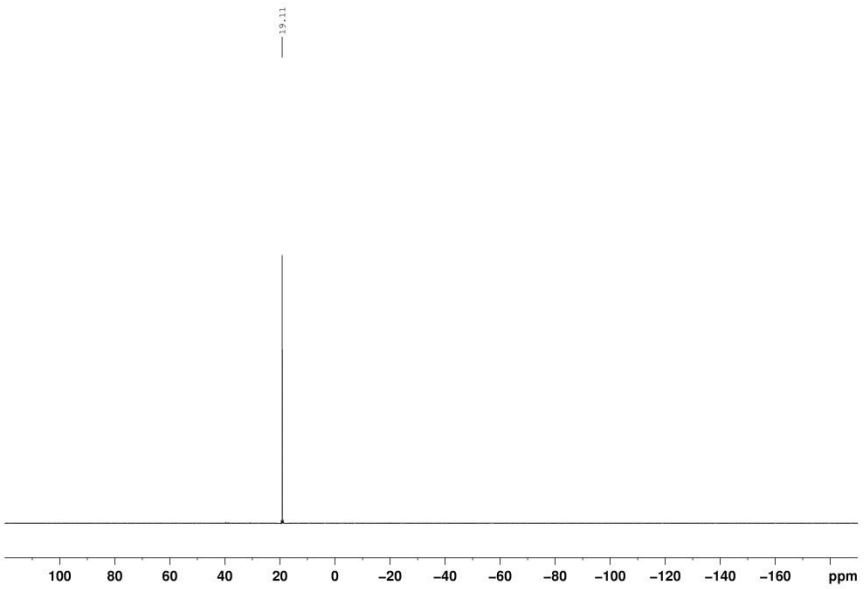

163.87
163.70
150.17
150.06
132.88
131.96
131.93
131.79
131.55
131.45
130.90
130.81
130.77
129.50
128.68
128.54
128.41
127.82
127.00
124.20
120.29
116.68
108.22
106.97
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

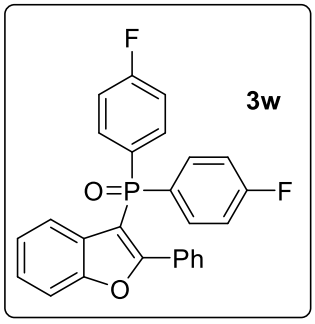

18.50
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

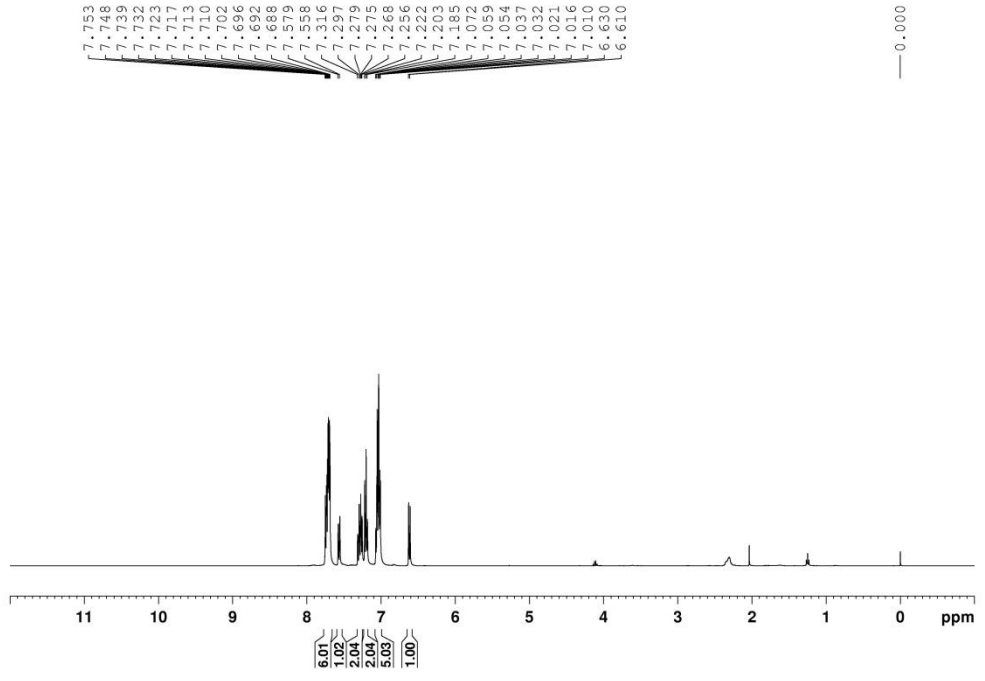

3v
O=P
Ph
O

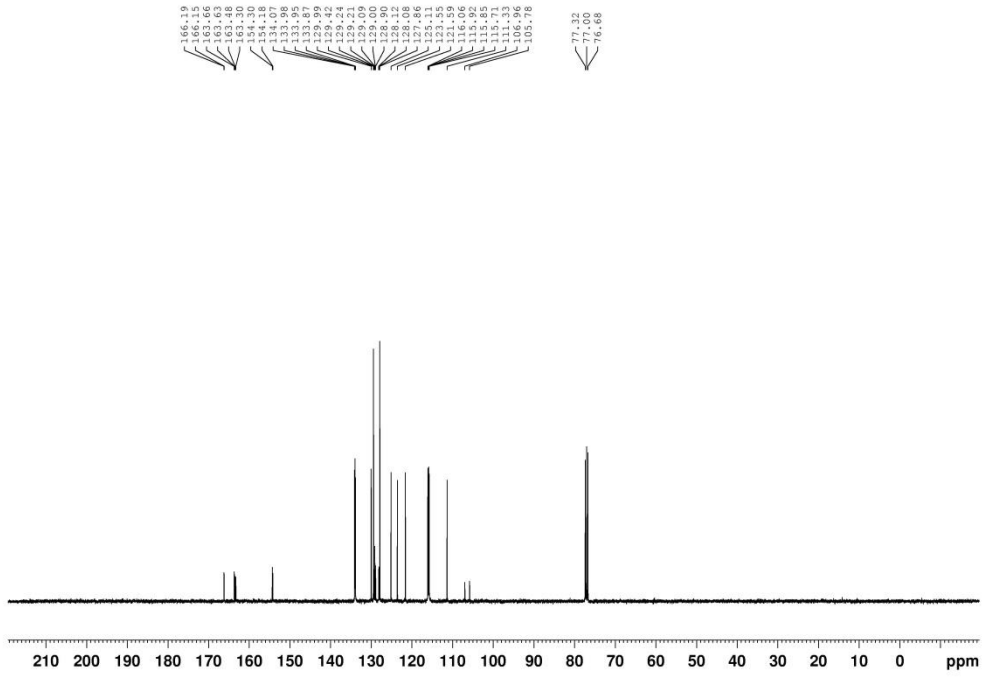

7.769
7.751
7.748
7.627
7.606
7.596
7.576
7.545
7.525
7.275
7.254
7.235
7.217
7.202
7.186
7.182
7.165
7.161
7.149
7.143
7.129
7.123
7.025
7.005
6.986
6.652
6.632
2.323
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
4.05
0.96
4.02
4.16
1.03
0.99
6.00

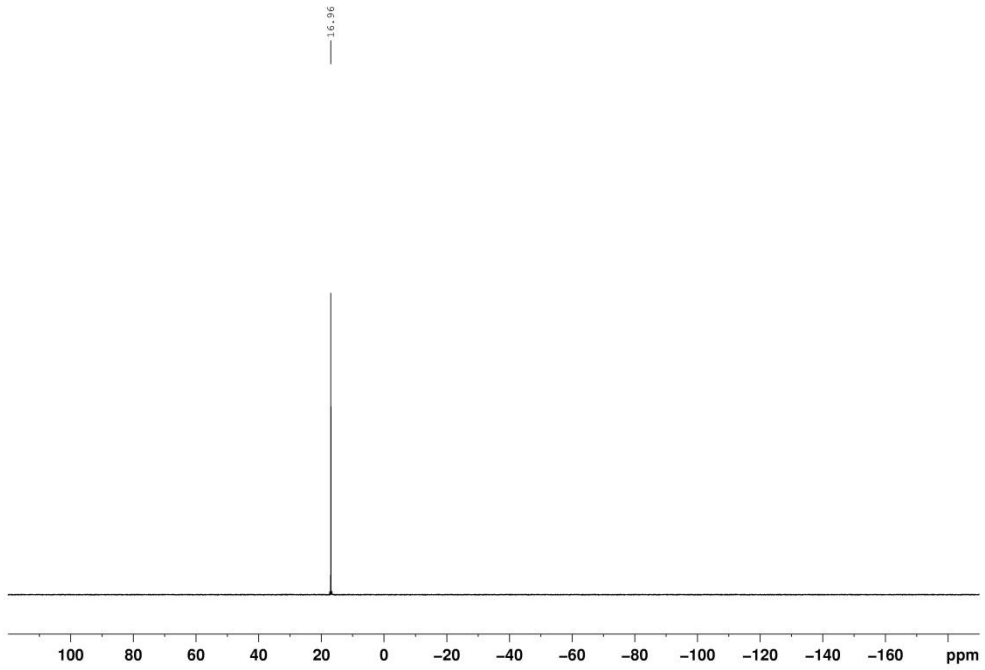

163.04
162.87
154.24
154.13
142.14
142.11
131.63
131.43
130.42
129.47
129.41
129.31
129.19
129.06
127.71
124.75
123.25
121.99
111.05
107.77
106.62
77.32
77.00
76.68
21.47
21.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

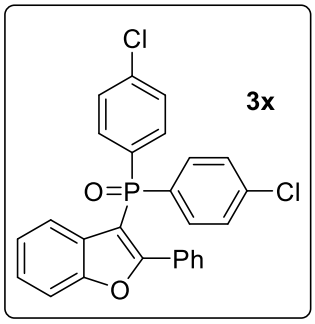

19.11
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

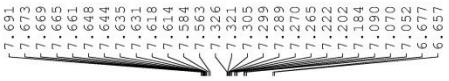

F
3w
O=P
F
Ph
O

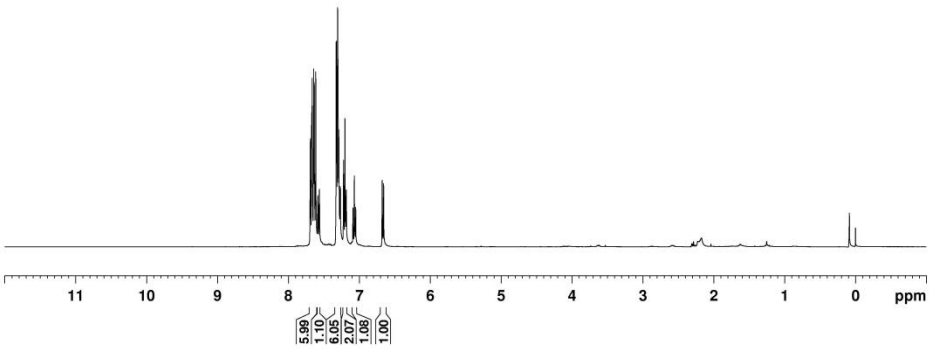

7.753
7.748
7.739
7.732
7.723
7.717
7.713
7.710
7.702
7.696
7.692
7.688
7.579
7.558
7.316
7.297
7.279
7.275
7.268
7.256
7.222
7.203
7.185
7.072
7.059
7.054
7.037
7.032
7.021
7.016
7.010
6.630
6.610
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.01
1.02
2.04
2.04
5.03
1.00

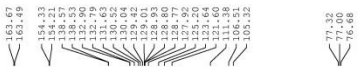

166.19
166.15
163.66
163.63
163.48
163.30
154.30
154.18
154.07
133.98
133.95
133.87
129.99
129.92
129.24
129.21
129.09
129.00
128.90
128.12
128.08
127.86
125.11
125.05
121.59
116.06
115.92
115.85
115.71
111.33
106.96
105.78
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

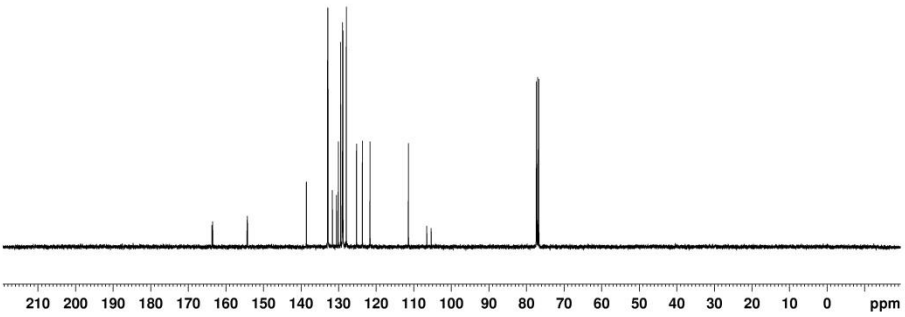

16.96
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

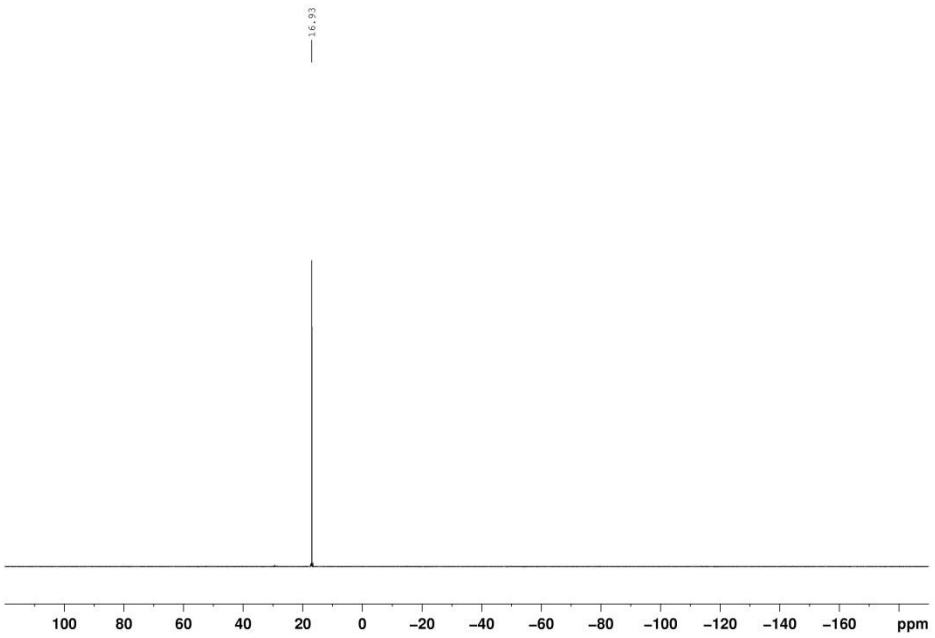

Cl
3x
O=P
Cl
Ph
O

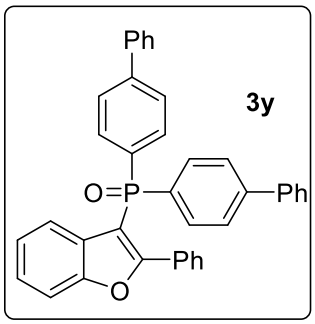

7.691
7.673
7.669
7.665
7.661
7.648
7.644
7.635
7.631
7.618
7.614
7.584
7.563
7.326
7.321
7.305
7.299
7.289
7.270
7.265
7.222
7.202
7.184
7.090
7.070
7.052
6.677
6.657
0.000

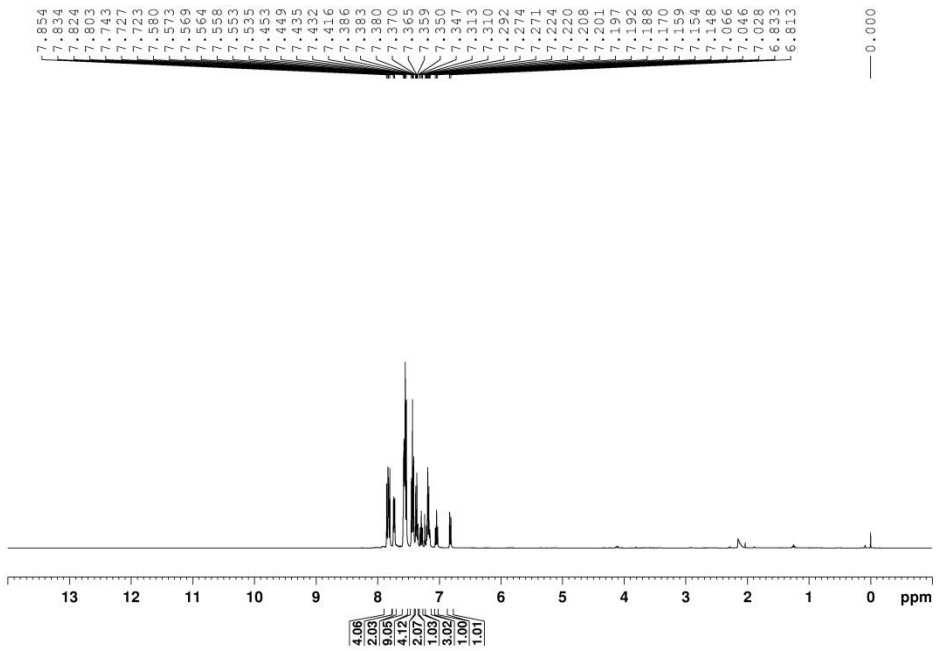

11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.99
1.10
6.05
2.07
1.06
1.00


163.67
161.49
154.33
154.21
138.57
138.53
132.90
132.79
131.68
130.52
130.04
129.42
129.01
128.93
128.80
128.77
127.92
125.20
123.64
121.60
111.38
106.51
105.32
77.32
77.00
76.68


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


16.93
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm


Ph
3y
O=P
Ph
Ph
O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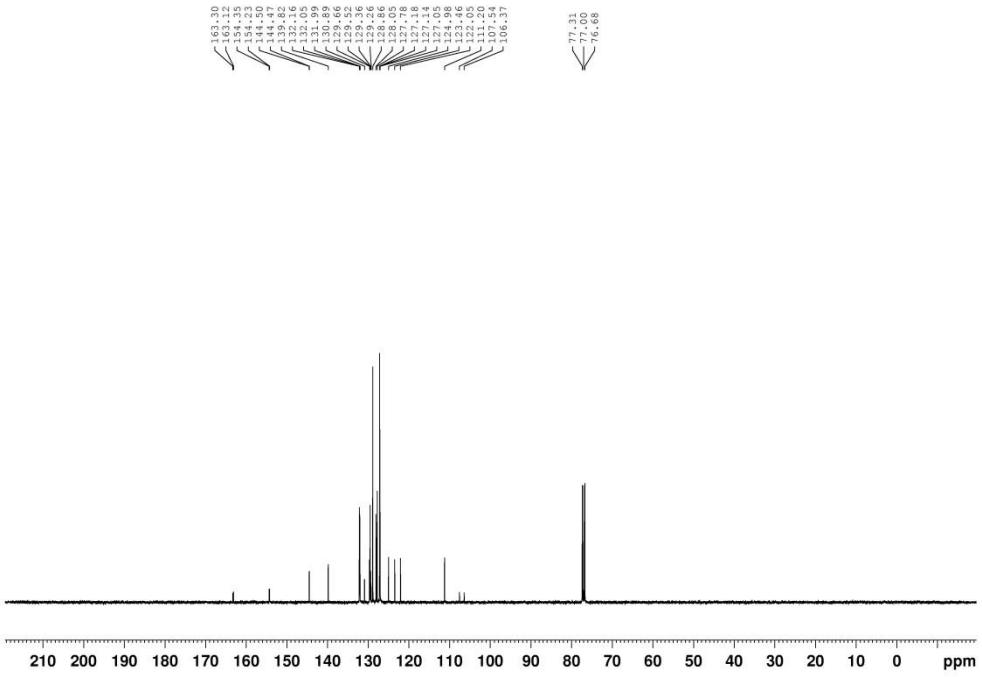
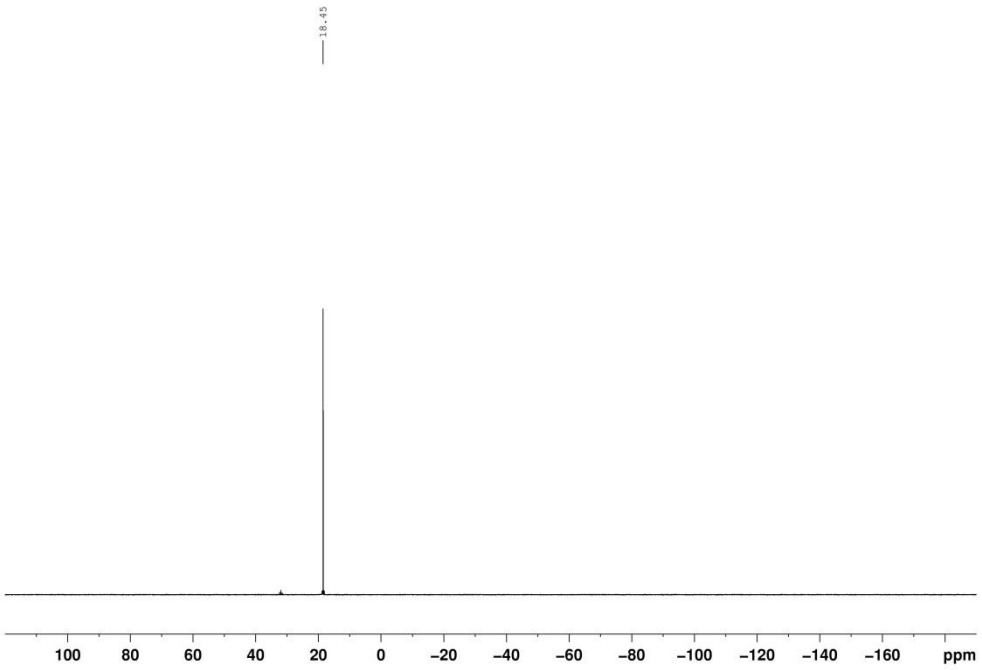
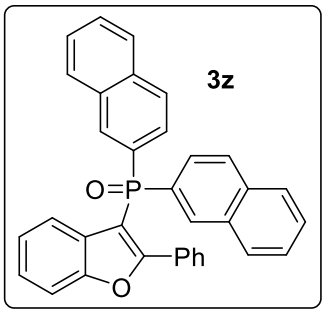
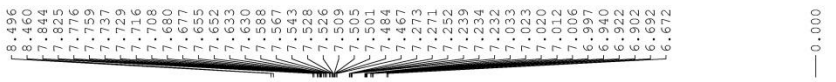
7.834
7.824
7.803
7.743
7.727
7.723
7.580
7.573
7.569
7.564
7.558
7.553
7.535
7.453
7.449
7.435
7.432
7.416
7.386
7.383
7.380
7.370
7.365
7.359
7.350
7.347
7.313
7.310
7.292
7.274
7.271
7.224
7.220
7.208
7.201
7.197
7.192
7.188
7.170
7.159
7.154
7.148
7.066
7.046
7.028
6.833
6.813
0.000
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.06
2.03
9.05
4.12
2.07
1.03
3.02
1.00
1.01


163.30
163.12
154.35
154.23
144.90
144.77
139.82
132.16
132.05
131.99
130.89
129.66
129.52
129.36
129.26
128.86
128.05
127.78
127.18
127.14
127.05
124.98
123.46
122.05
111.20
107.54
106.37
77.31
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


18.45
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm


3z
O=P
Ph
O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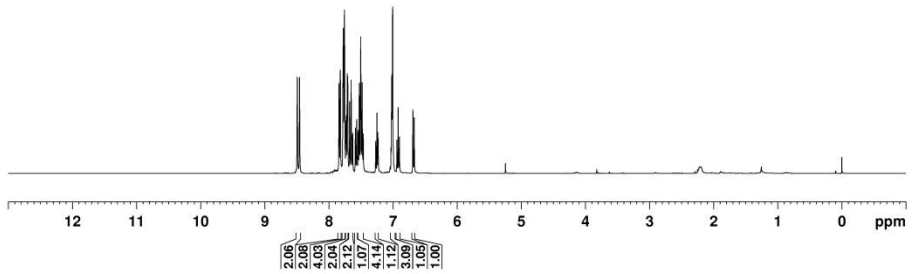
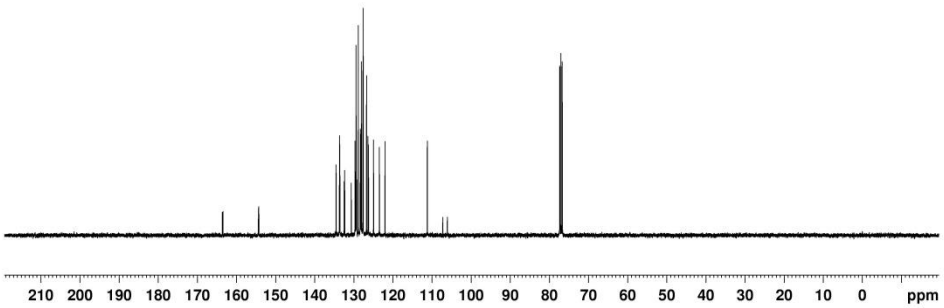
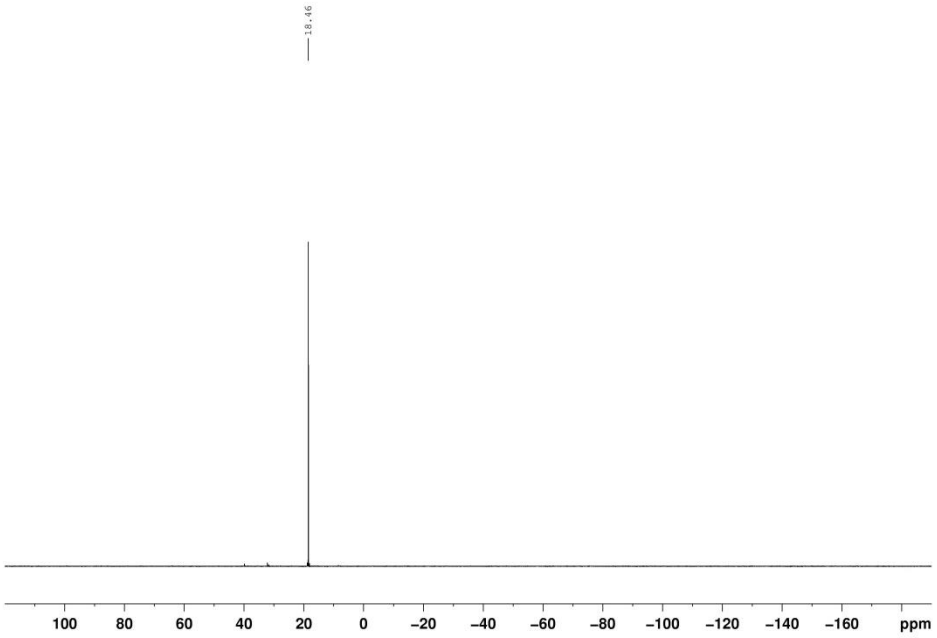
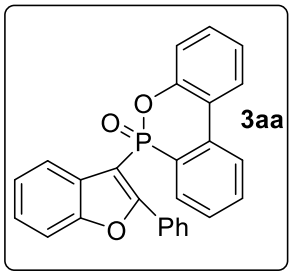
8.460
7.844
7.825
7.776
7.759
7.737
7.729
7.716
7.708
7.680
7.677
7.655
7.652
7.633
7.630
7.588
7.567
7.543
7.528
7.526
7.509
7.505
7.501
7.484
7.467
7.273
7.271
7.252
7.239
7.234
7.232
7.033
7.023
7.020
7.012
7.006
6.997
6.940
6.922
6.902
6.692
6.672
0.000

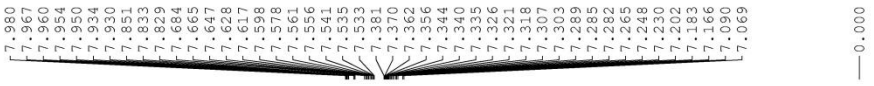

12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
2.08
4.03
2.04
2.12
1.07
4.14
1.12
3.09
1.05
1.00

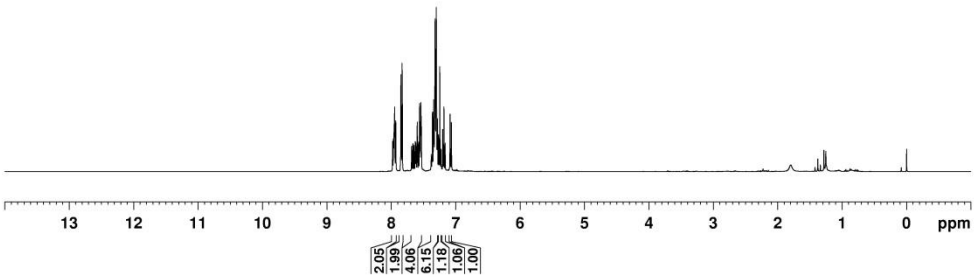

163.58
163.41
154.37
154.25
134.52
134.50
133.63
133.44
132.44
132.30
130.63
129.66
129.34
129.41
129.30
129.23
129.21
128.84
128.32
128.20
128.05
127.65
127.57
126.72
126.55
126.23
124.93
123.44
111.99
111.18
107.23
106.06
77.32
77.00
76.68

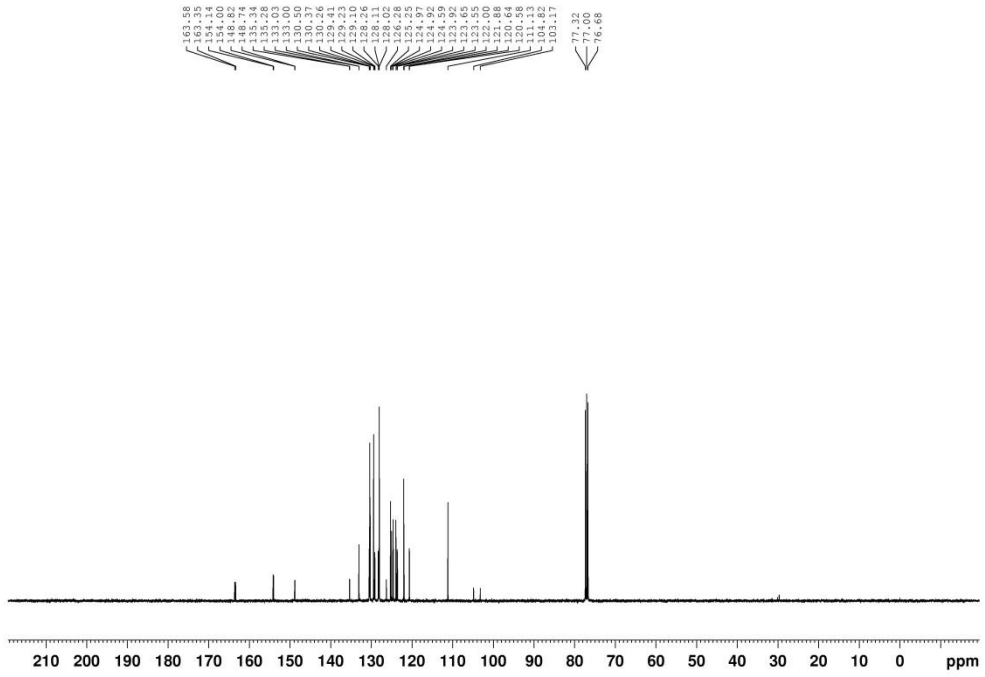

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

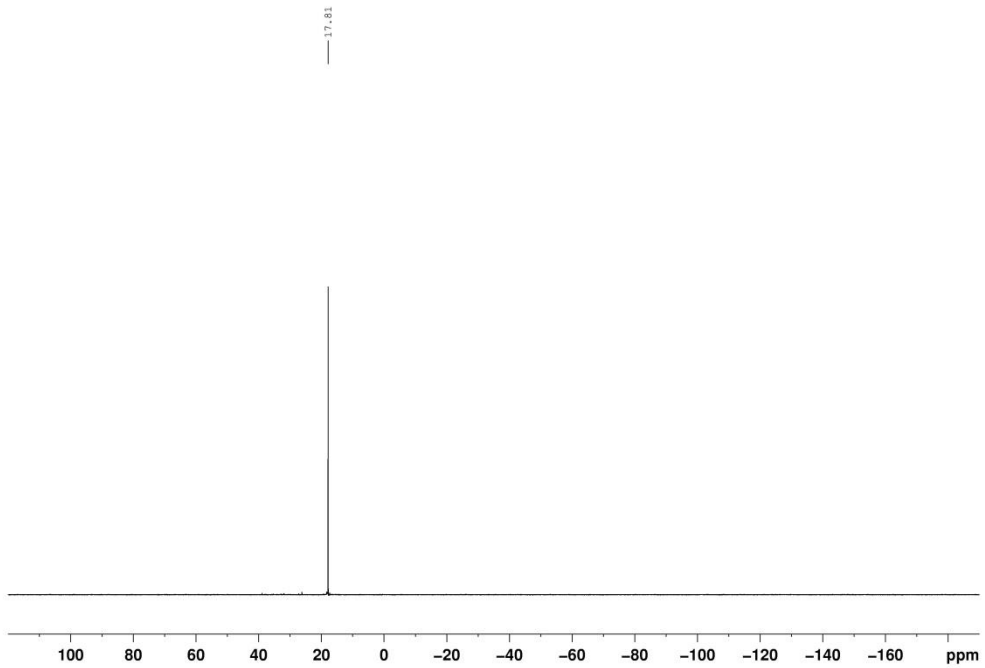

18.46
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm

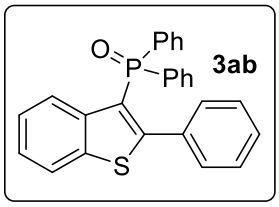

O
O
P
O
Ph
3aa

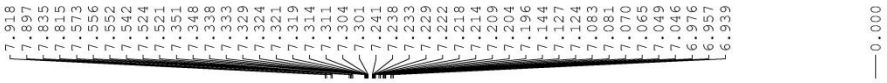

7.980
7.967
7.960
7.954
7.950
7.934
7.930
7.851
7.833
7.829
7.684
7.665
7.647
7.628
7.617
7.598
7.578
7.561
7.556
7.541
7.535
7.533
7.381
7.370
7.362
7.356
7.344
7.340
7.335
7.326
7.321
7.318
7.307
7.303
7.289
7.285
7.282
7.265
7.248
7.230
7.202
7.183
7.166
7.090
7.069
0.000

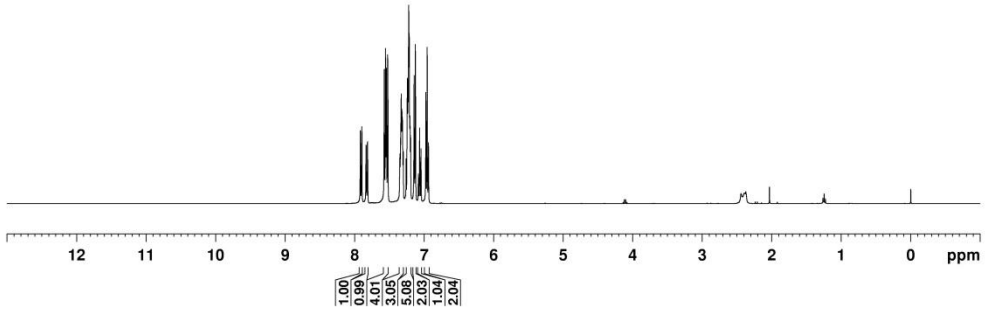

13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.05
1.99
4.06
6.15
1.18
1.06
1.00

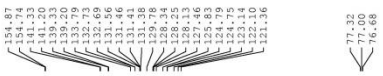

163.58
163.35
154.14
154.00
148.82
148.74
135.34
135.28
133.03
133.00
130.50
130.37
130.26
129.41
129.33
129.10
128.26
128.11
128.02
126.26
125.25
124.97
124.92
124.69
123.92
123.65
123.55
122.00
121.88
120.64
120.58
111.13
104.92
103.17
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

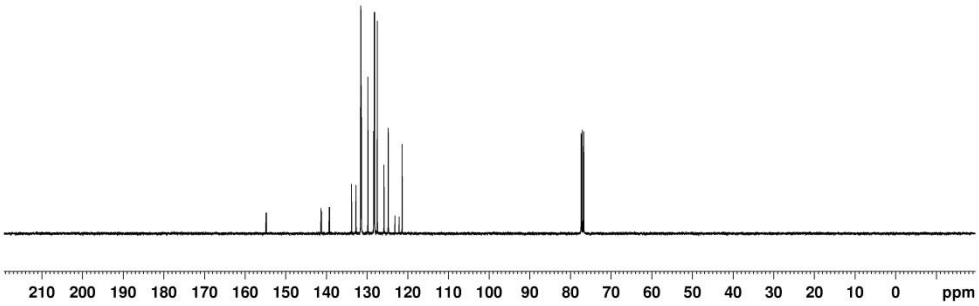

17.81
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

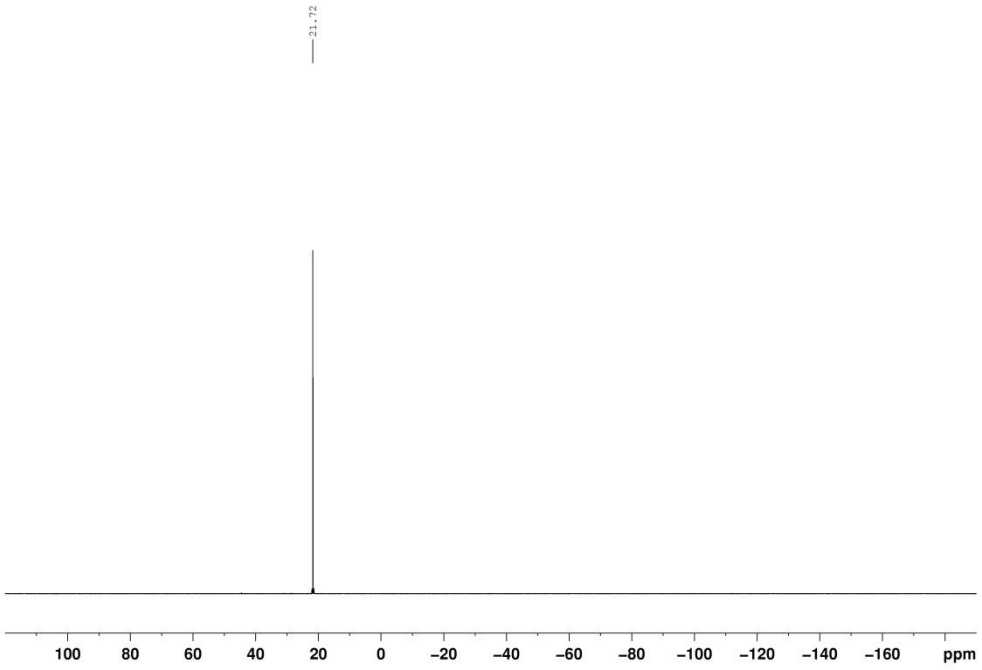

O
P
Ph
Ph
S
3ab

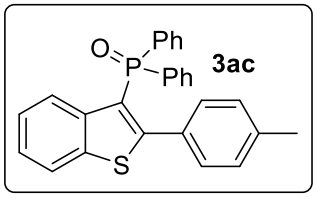

7.918
7.897
7.835
7.815
7.573
7.556
7.552
7.542
7.524
7.521
7.351
7.348
7.338
7.333
7.329
7.324
7.321
7.319
7.314
7.311
7.304
7.301
7.241
7.238
7.233
7.229
7.222
7.218
7.214
7.209
7.204
7.196
7.144
7.127
7.124
7.083
7.081
7.070
7.065
7.049
7.046
6.976
6.957
6.939
0.000

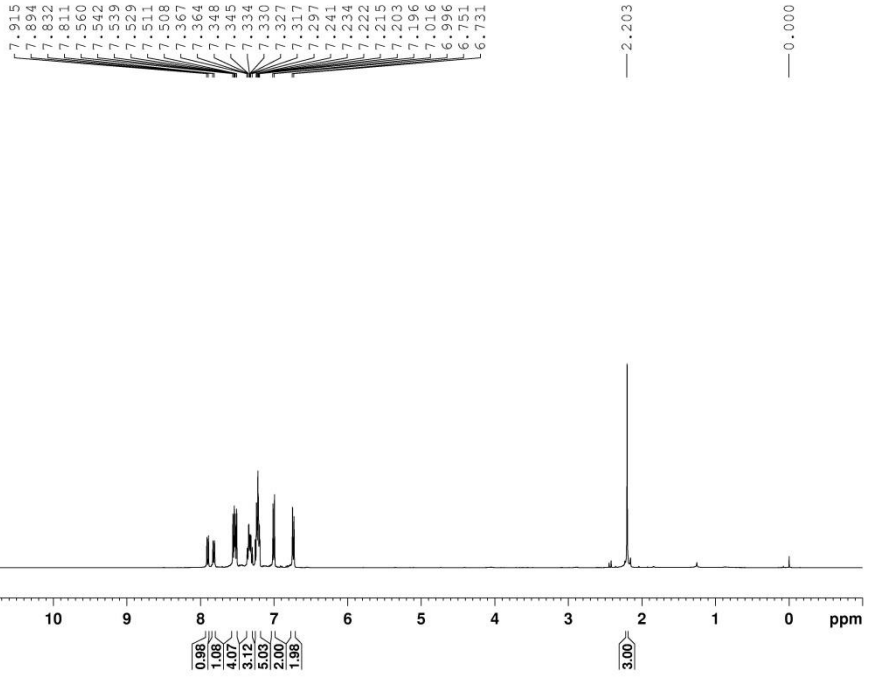

12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.99
4.01
3.05
5.08
2.03
1.04
2.04

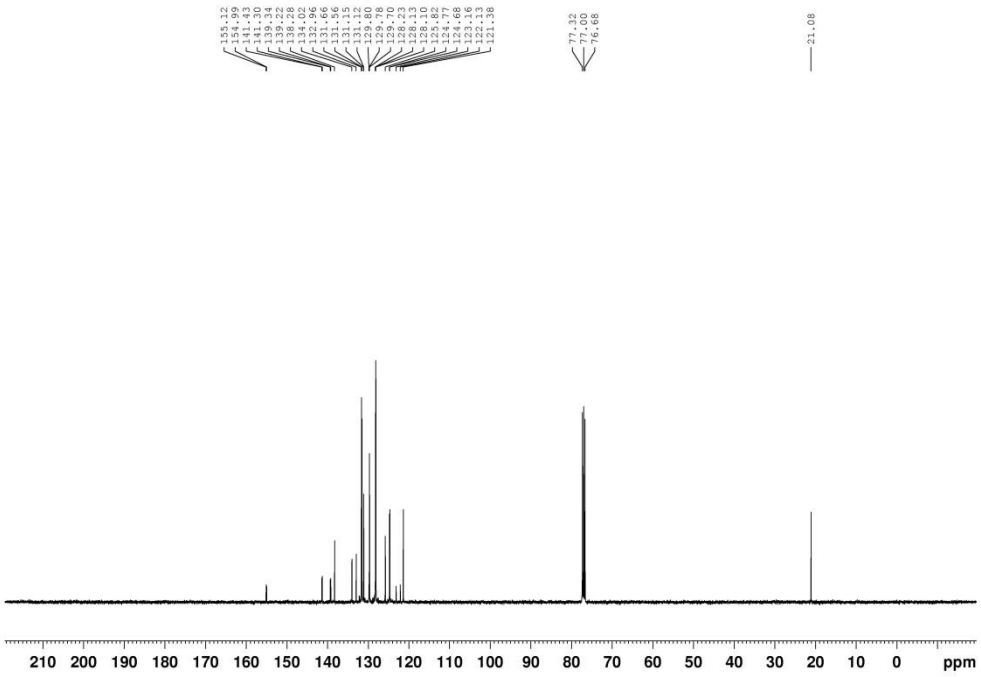

154.87
154.74
141.33
141.20
139.33
139.20
139.09
132.73
132.69
131.56
131.46
131.41
131.38
129.78
128.34
128.25
128.13
127.46
125.83
124.79
124.75
123.14
122.10
121.36
77.32
77.00
76.68

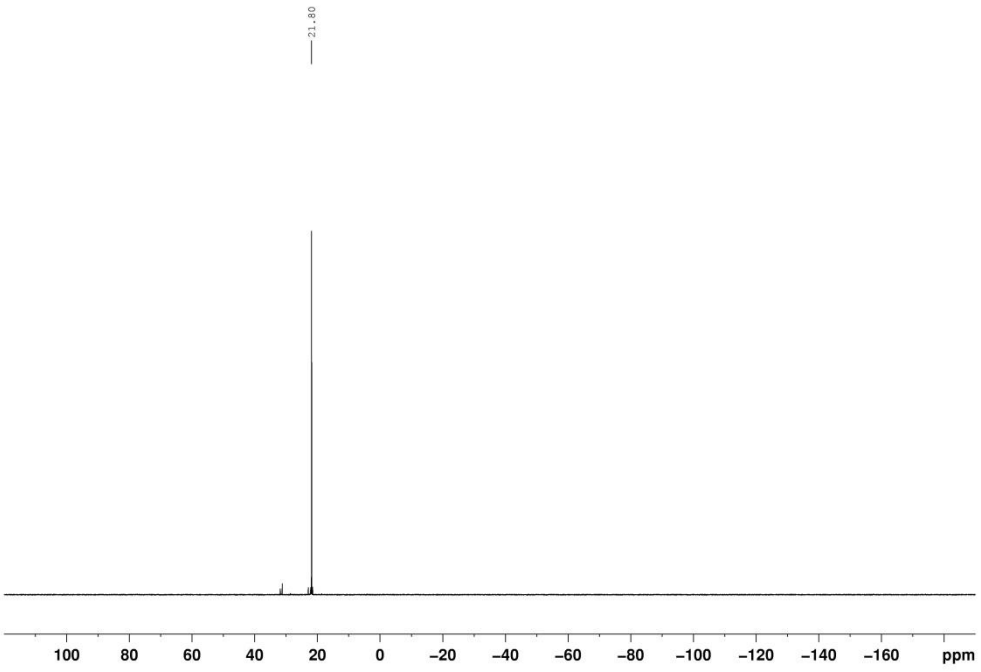

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

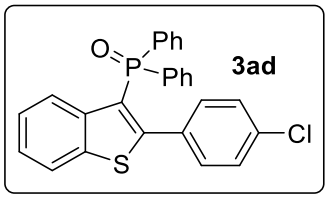

21.72
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
ppm

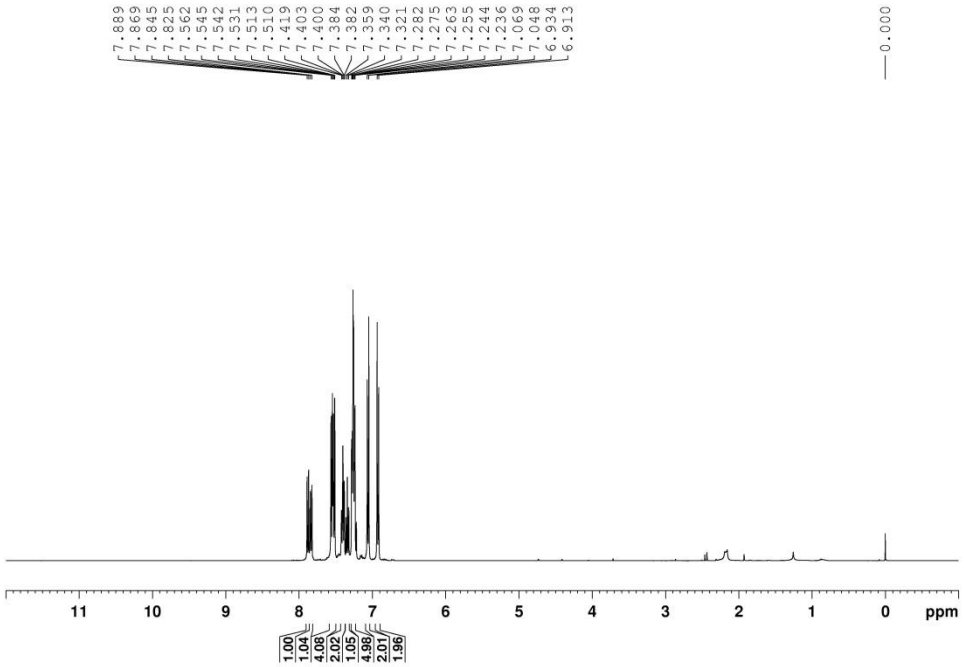

O
P
Ph
Ph
S
3ac

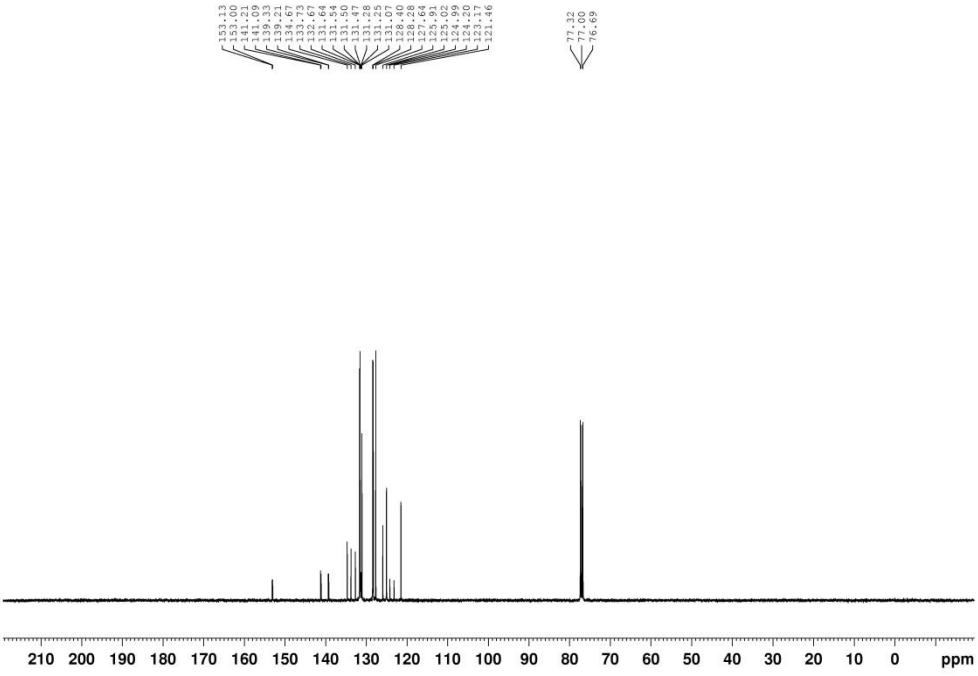

7.915
7.894
7.832
7.811
7.560
7.542
7.539
7.529
7.511
7.508
7.367
7.364
7.348
7.345
7.334
7.330
7.327
7.317
7.297
7.241
7.234
7.222
7.215
7.203
7.196
7.016
6.996
6.751
6.731
2.203
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.08
4.07
3.12
5.03
2.00
1.98
3.00

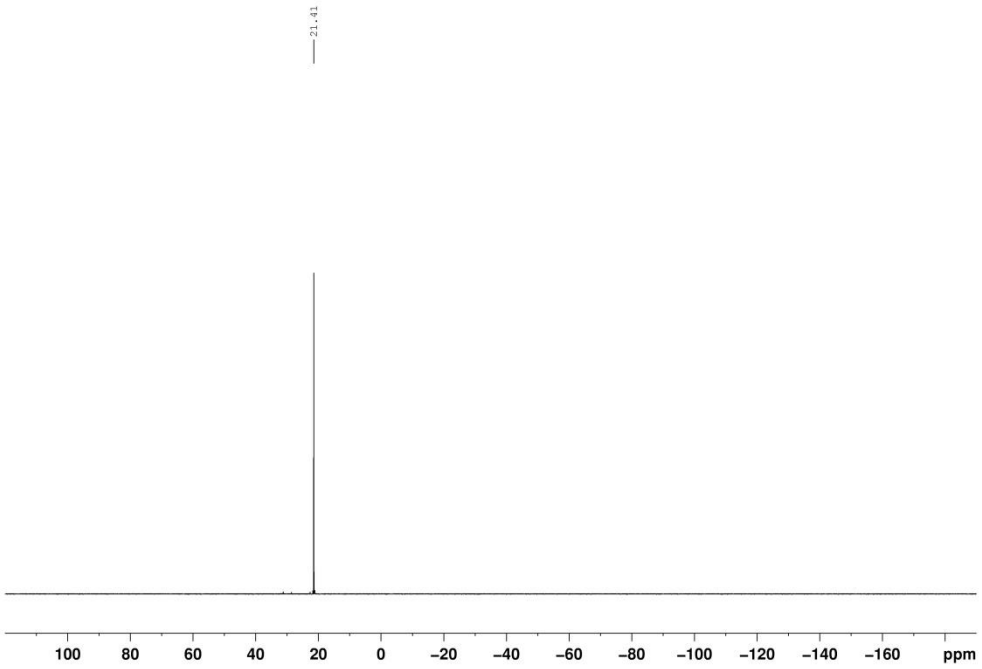

155.12
154.99
141.43
141.30
139.34
139.22
138.28
134.02
132.86
132.66
131.56
131.15
131.12
130.00
129.78
129.70
128.23
128.13
128.10
125.82
124.77
124.68
123.16
121.13
121.38
77.32
77.00
76.68
21.08
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

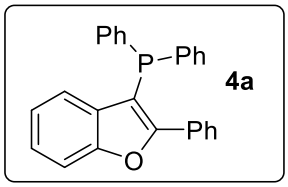

21.80
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm

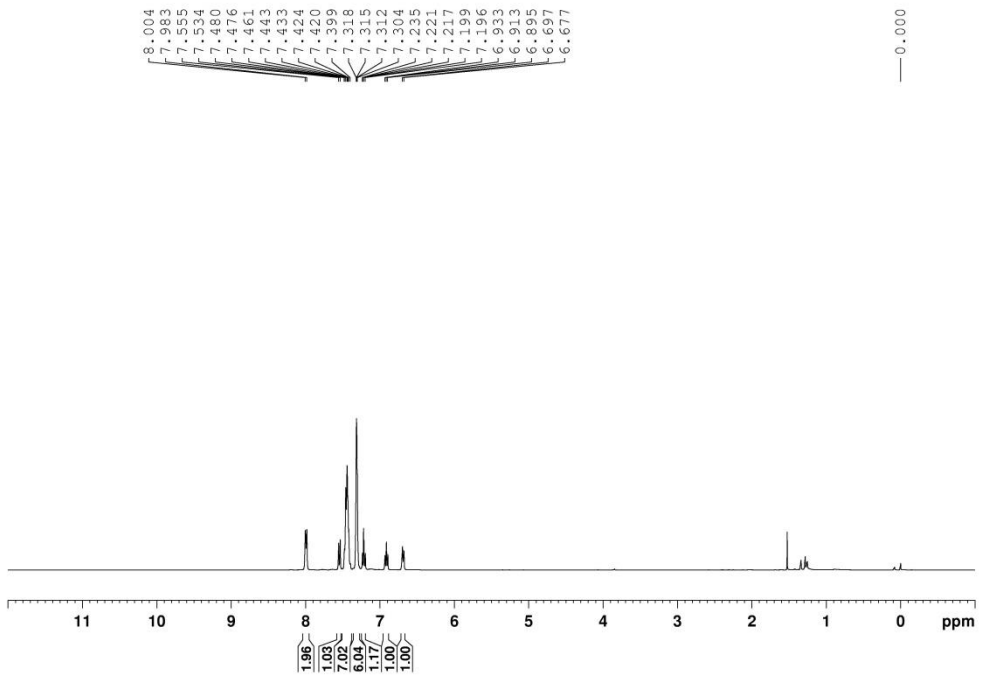

O
P
Ph
Ph
3ad
S
Cl

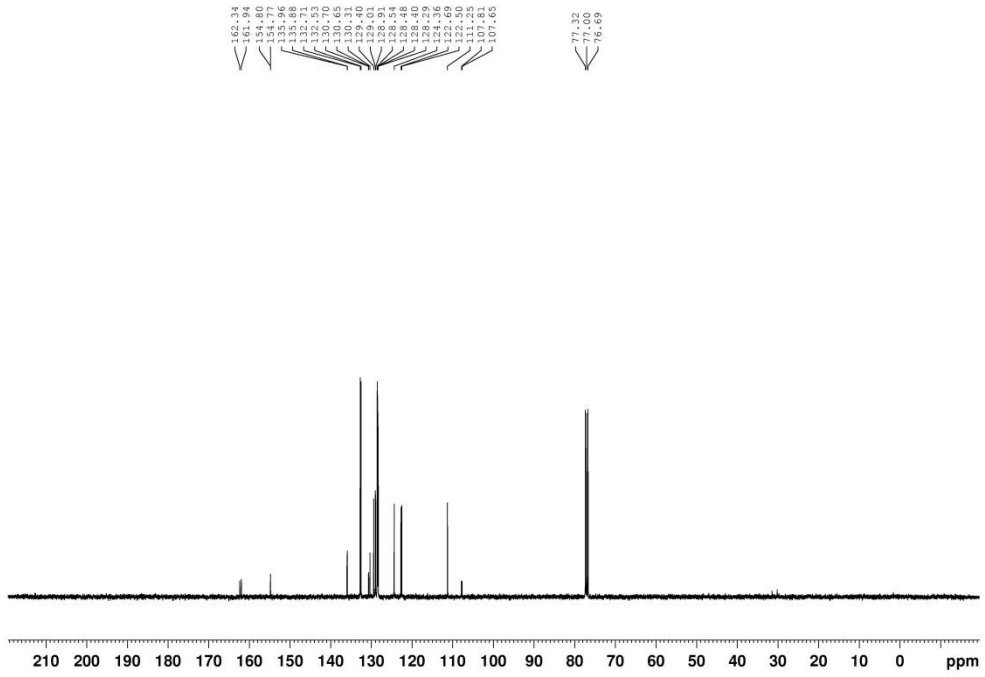

7.889
7.869
7.845
7.825
7.562
7.545
7.542
7.531
7.513
7.510
7.419
7.403
7.400
7.384
7.382
7.359
7.340
7.321
7.282
7.275
7.263
7.255
7.244
7.236
7.069
7.048
6.934
6.913
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
4.08
2.02
1.05
4.98
2.01
1.96

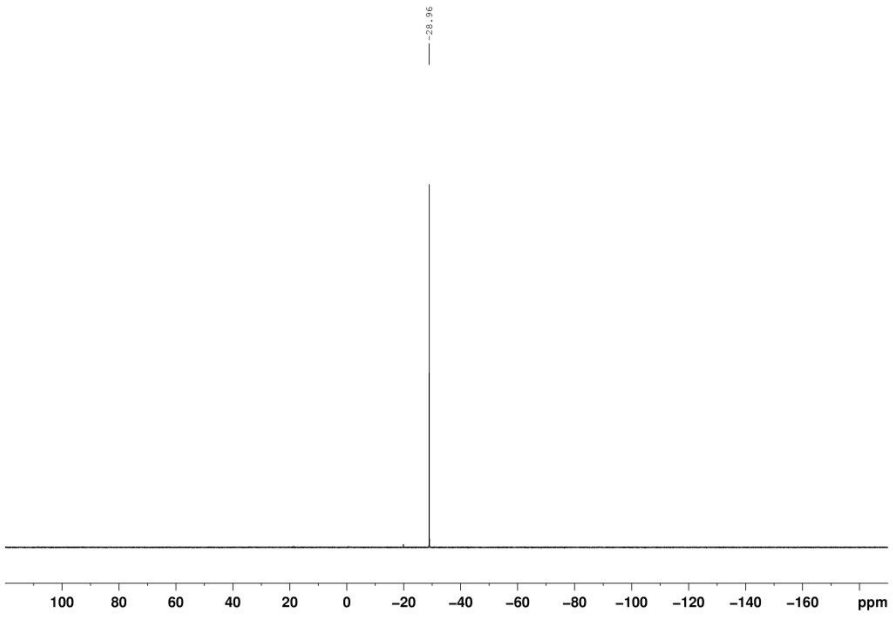

153.13
153.00
141.21
141.09
139.35
139.21
134.67
133.73
133.67
131.64
131.54
131.50
131.47
131.28
131.25
131.07
128.40
128.28
127.64
125.91
125.02
124.99
123.20
123.17
121.46
77.32
77.00
76.69
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

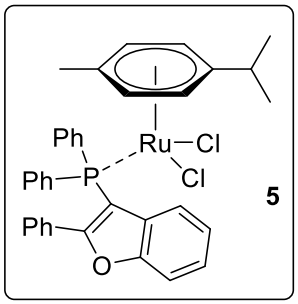

21.41
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm


Ph
P
Ph
Ph
O
4a

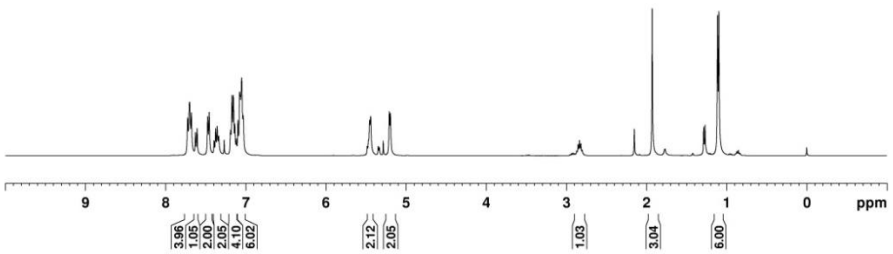

8.004
7.983
7.555
7.534
7.480
7.476
7.461
7.443
7.433
7.424
7.420
7.399
7.318
7.315
7.312
7.304
7.235
7.221
7.217
7.199
7.196
6.933
6.913
6.895
6.697
6.677
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.96
1.03
7.02
6.04
1.17
1.00
1.00

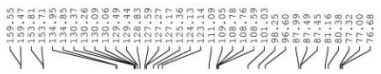

162.34
161.94
154.60
154.77
135.96
135.88
132.71
132.53
130.70
130.65
130.31
129.40
129.01
128.91
128.54
128.48
128.40
128.29
124.36
122.69
122.50
115.95
107.81
107.65
77.32
77.00
76.69
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

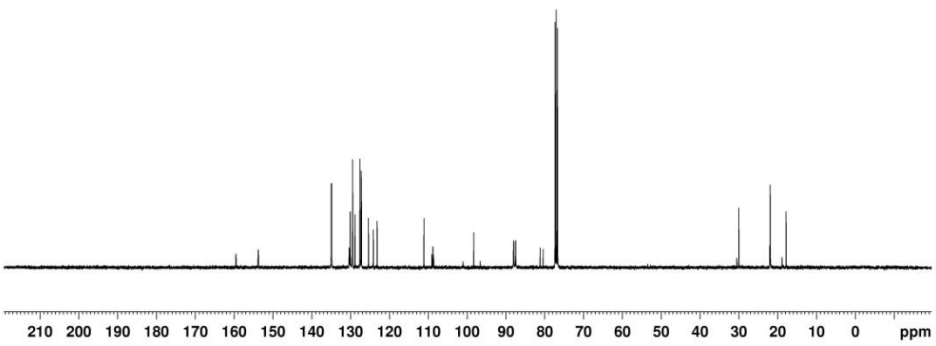

-28.96
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 ppm

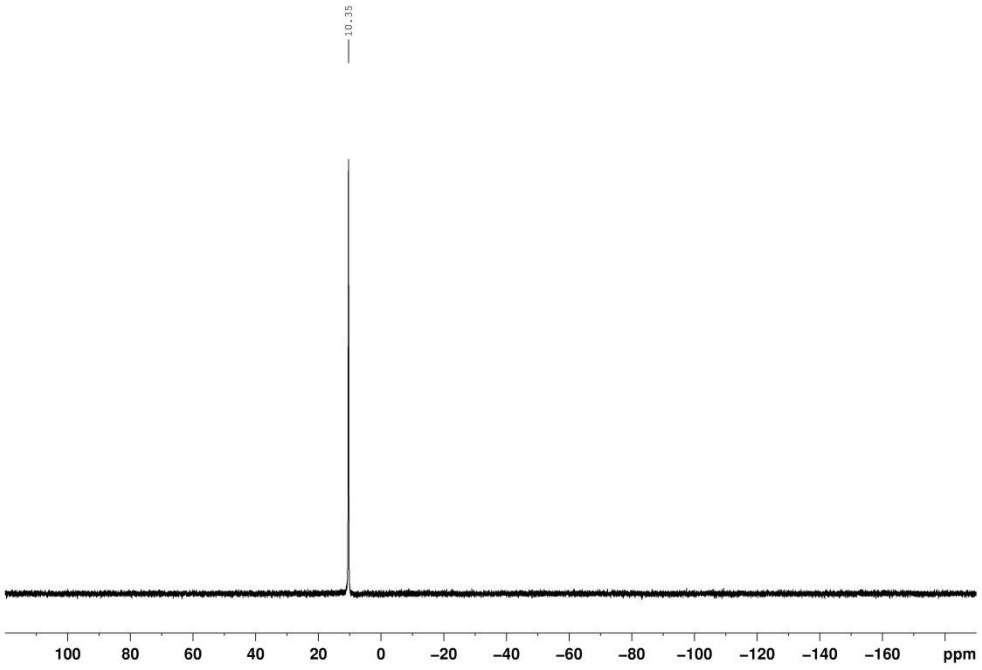

Ph
Ru—Cl
Ph—P
Cl
Ph
O
5

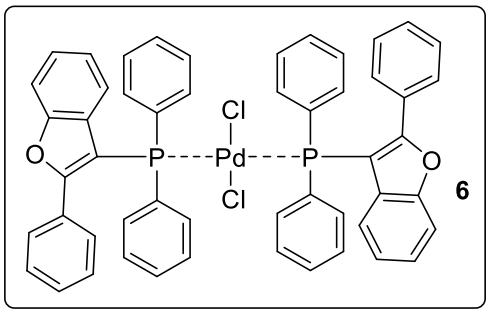

7.723
7.698
7.677
7.625
7.605
7.473
7.454
7.393
7.374
7.355
7.336
7.188
7.169
7.152
7.135
7.116
7.095
7.075
7.065
7.049
7.032
5.453
5.439
5.208
5.193
2.886
2.869
2.852
2.835
2.818
2.801
1.928
1.113
1.096
0.000

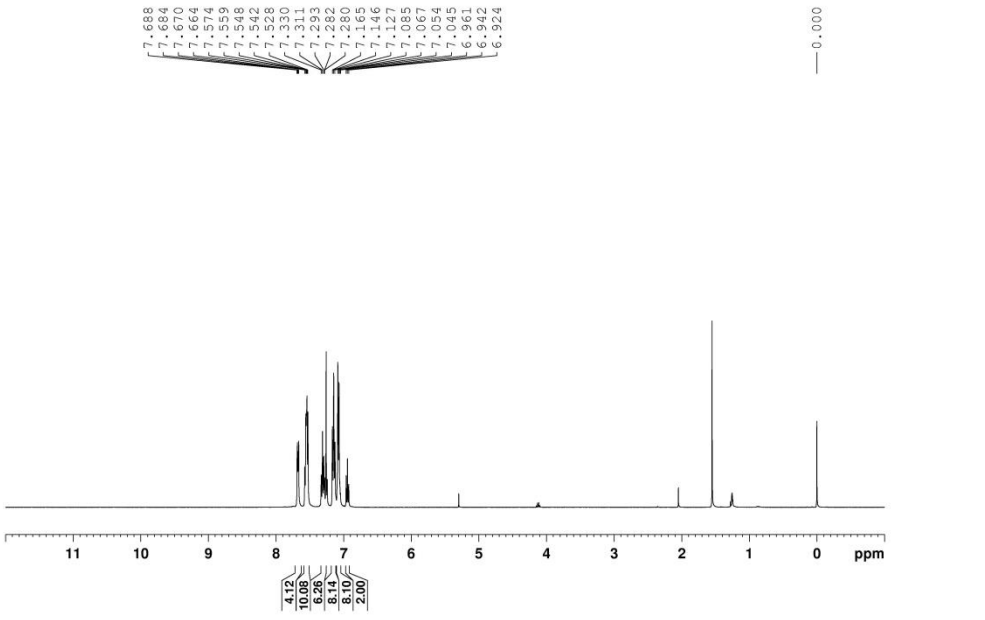

9
8
7
6
5
4
3
2
1
0
ppm
3.96
1.05
2.00
2.05
4.10
6.02
2.12
2.05
1.03
3.04
6.00


159.55
159.47
153.81
153.71
134.95
134.85
130.37
130.26
130.09
130.06
129.49
129.44
128.83
127.59
127.27
127.11
125.36
124.13
123.14
111.00
109.05
108.78
108.76
108.59
101.03
98.25
96.60
87.69
87.49
87.45
81.16
80.98
77.32
77.00
76.68
30.00
21.87
17.80


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


10.35
100
80
60
40
20
0
−20
−40
−60
−80
−100
−120
−140
−160
ppm


Cl
Pd
Cl
P
P
O
O
6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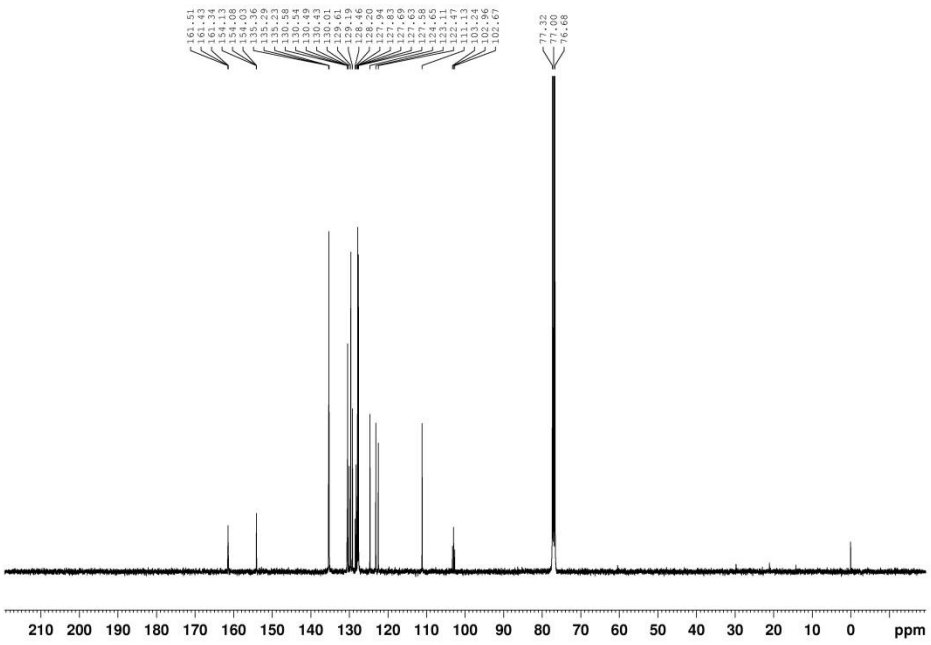
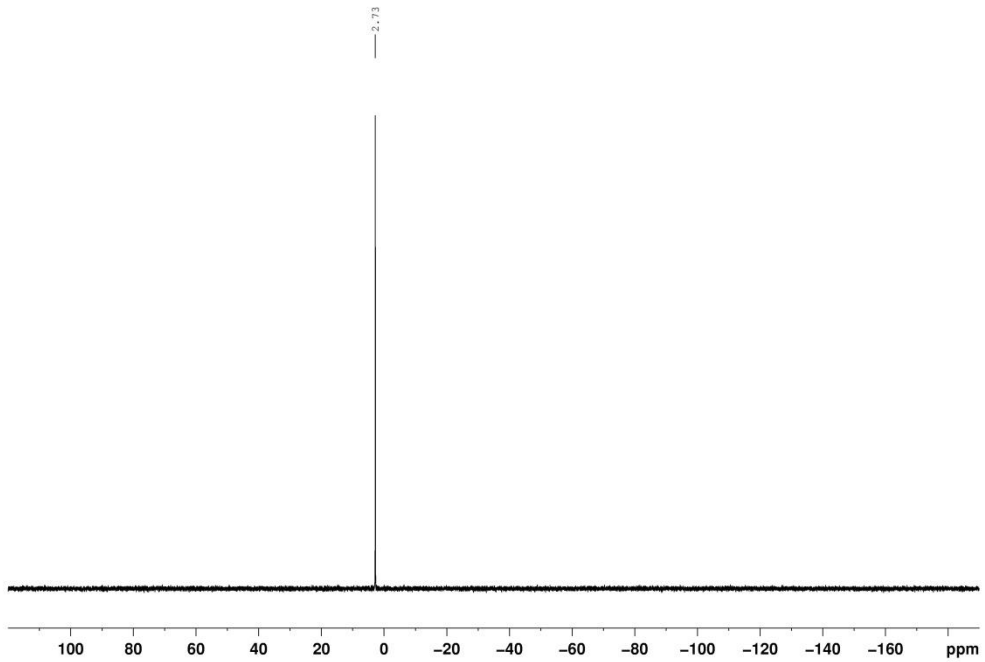
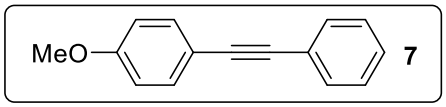
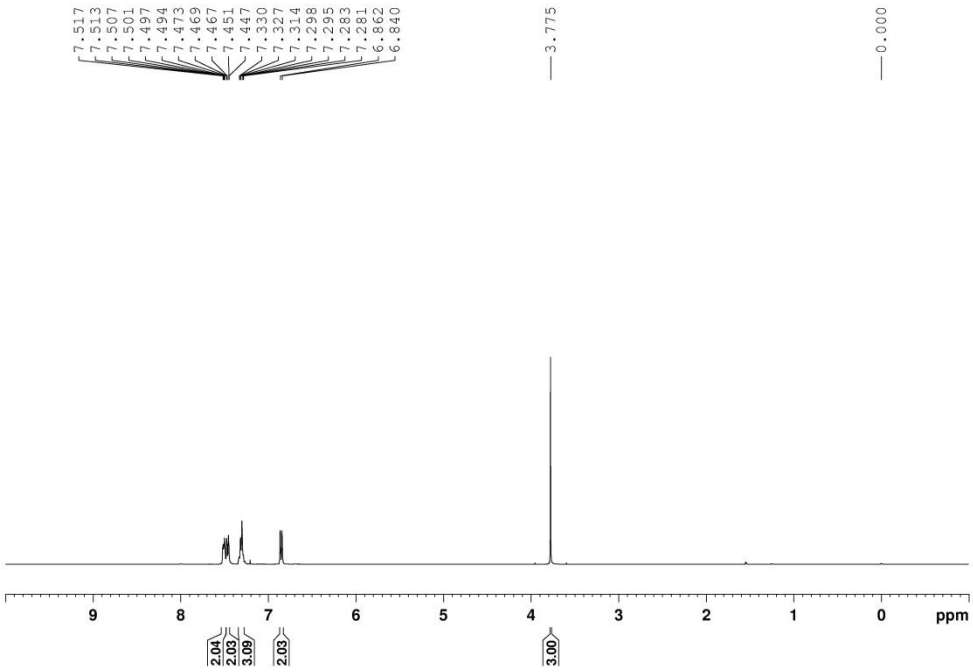
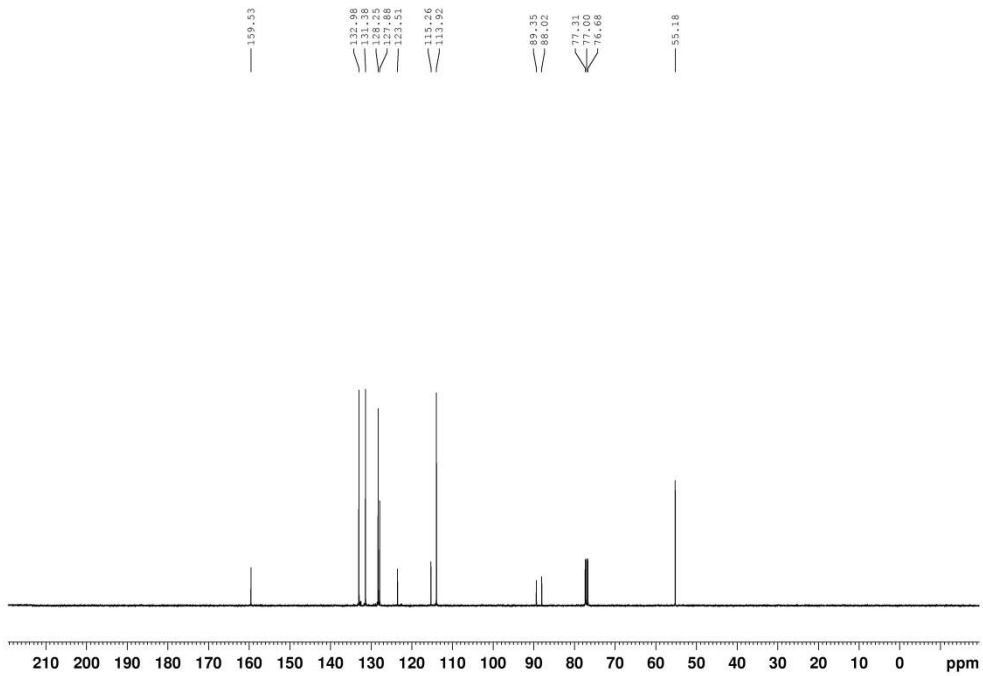
7.684
7.670
7.664
7.574
7.559
7.548
7.542
7.528
7.330
7.311
7.293
7.282
7.280
7.165
7.146
7.127
7.085
7.067
7.054
7.045
6.961
6.942
6.924
0.000
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.12
10.08
6.26
8.14
8.10
2.00


161.51
161.43
161.34
154.13
154.08
154.03
135.36
135.29
135.23
130.58
130.54
130.49
130.43
130.01
129.61
129.19
128.46
128.20
127.94
127.83
127.69
127.63
127.58
124.65
122.41
122.37
111.13
103.24
102.96
102.67
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


2.73
100 80 60 40 20 0 −20 −40 −60 −80 −100 −120 −140 −160 ppm


MeO
7


7.517
7.513
7.507
7.501
7.497
7.494
7.473
7.469
7.467
7.451
7.447
7.330
7.327
7.314
7.298
7.295
7.283
7.281
6.862
6.840
3.775
0.000
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.03
3.09
2.03
3.00


159.53
132.98
131.38
128.25
123.88
123.31
115.26
113.92
89.35
88.02
77.31
77.00
76.68
55.18
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm