EvanPhos. A New Ligand for ppm Level Pd-Catalyzed Suzuki-Miyaura Couplings in *Either* Organic Solvent or Water

Evan B. Landstrom[‡], Sachin Handa[!], Don Aue[‡], Fabrice Gallou[¥], and Bruce H. Lipshutz[‡]*

[‡]*Department of Chemistry & Biochemistry, University of California, Santa Barbara, CA 93106 USA
[!] Department of Chemistry, University of Lousiville, KY, 40292 USA
[¥] Novartis Pharma, Basel, Switzerland

PHONE: 805-893-2521
FAX: 805-893-8265
E MAIL: lipshutz@chem.ucsb.edu
WWW: http://www.chem.ucsb.edu/~lipshutzgroup/

Supporting Information

I. General Information

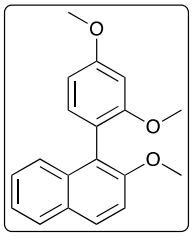
Unless otherwise noted, all reactions were performed under an atmosphere of argon. All commercially available reagents were used without further purification. A 2 wt % TPGS-750-M/H_2O solution was prepared by dissolving TPGS-750-M in water (degassed with argon prior to mixing, HPLC grade). A solution of TPGS-750-M can be purchased from Sigma Aldrich® (catalog numbers 733857 and 763918). TPGS- 750-M was made as previously described.[1] Tetrahydrofuran (THF) and toluene, obtained from Fisher Scientific, were degassed by sparging with argon and dried by pushing through a column of activated aluminum oxide. HPLC grade ethyl acetate (EtOAc), obtained from Fisher Scientific, was degassed by sparging with argon for a minimum of 2 h while stirring. All glassware and stir bars were cleaned with *aqua regia* prior to use to avoid trace metal contamination. Palladium catalysts were purchased from Spectrum Chemicals or were graciously donated by Johnson Matthey. The source of palladium acetate can have a dramatic effect on success of the reaction as noted by Colacot and co-workers.[2] Spectrum and Johnson Matthey branded palladium was found to be competent. Strem and Sigma-Aldrich palladium acetate was found to be inferior. Reagents were purchased from Sigma-Aldrich, Combi-Blocks, Alfa Aeser, or Acros Orgnaics. *n*-Butyllithium (nominally 2.5 M) was purchased from Sigma Aldrich and titrated with diphenylacetic acid prior to each use. Analytical thin layer chromatography (TLC) was performed using Silica Gel 60 F254 glass backed plates (Merck, 0.25 mm thick) or Aluminum Oxide 60 F254 polyester backed plates (Sigma-Aldrich, 0.2 mm thick). The developed chromatogram was analyzed by UV lamp (254 nm). UV inactive compounds were visualized using aqueous potassium permanganate ($KMnO_4$), aqueous dinitro-phenyl hydrazine, aqueous ceric ammoniumnitrate/ phosphomolybdic acid, or butanolic vanillin and developed with a heat gun. Flash chromatography was performed using Silicycle Siliaflash® P60 Unbounded Grade Silica: Particle size: 40-60 μm, Pore size: 60 Å. ^1H and ^{13}C NMR data were recorded at 297.8 K on an Agilent® Technologies 400 MHz or Varian Unity Inova® 500 MHz. ^{19}F and ^{31}P NMR were recorded at 297.8 K on an Agilent® Technologies 400 MHz. The FID was processed using MestReNova (release: 10.0). Chemical shifts in ^1H NMR spectra are reported in parts per million (ppm) on the δ scale with the residual ^1H resonance from deuterated chloroform set at 7.26 ppm, deuterated acetone set at 2.05 ppm, and deuterated dimethyl sulfoxide set at 2.50 ppm. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sext = sextet, sep = septet, m = multiplet, br = broad, dt = doublet of triplets, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets), coupling constant in hertz (Hz), and integration. Chemical shifts of ^{13}C NMR spectra were referenced through the chloroform ^{13}C resonance reported at 77.16 ppm from the central peak on the δ scale according to IUPAC recommended secondary referencing method[3] and the manufacturer's protocols. Reactions were deemed complete by TLC or via GCMS analyses. GCMS data were recorded on a 5975C Mass Selective Detector, coupled with a 7890A Gas Chromatograph (Agilent Technologies). A capillary column HP-5MS cross-linked 5% phenylmethylpolysiloxanediphenyl column (30 m x 0.250 mm, 0.25 micron, Agilent Technologies) was employed. Helium was used as carrier gas at a constant flow of 1 mL/min.

1) Lipshutz, B. H.; Ghorai, S.; Abela, A. R.; Moser, R.; Nishikata, T.; Duplais, C.; and Krasovskiy, A. *J. Org. Chem.* **2011**, *76*, 4379.

2) (a) Carole, W.A.; Bradley, J.; Sarwar, M.; Colacot, T.J. *Org. Lett.* **2015**, 17, 5472-5475. (b) Carole, W.A.; Colacot, T.J. *Chem. Eur. J.* **2016**, 22, 7686-7695.

3) (a) Harris, R. K.; Becker, E. D.; Cabral de Menezes, S. M.; Goodfellow, R.; Granger, P. *Pure Appl. Chem.* **2001**, *73*, 1795. (b) Harris, R. K.; Becker, E. D.; Cabral de Menezes, S. M.; Granger, P.; Hoffman, R. E.; Zilm, K. W. *Pure Appl. Chem.* **2008**, *80*, 59.

II. Experimental Procedures and Analytical Data for the Synthesis of EvanPhos (2) and its Pd Complexes

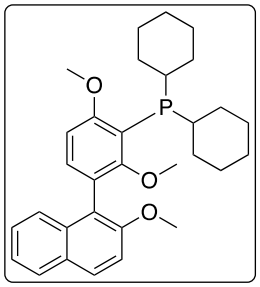


1-(2,4-Dimethoxyphenyl)-2-methoxynaphthalene. An oven-dried 5 mL conical microwave vial containing an oblong stir bar was charged with $Pd(OAc)_2$ (7.0 mg) and EvanPhos (29 mg) and sealed with a septum. The vial was evacuated and refilled 3x with argon. Toluene (0.64 mL) was added via syringe and the mixture was stirred for a minimum of 30 min under an inert atmosphere. A 4 mL dram vial containing an oblong stir bar was charged with 1-bromo-2-methoxynaphthalene (119 mg, 0.5 mmol), 2,4-dimethoxyphenylboronic acid (173 mg, 0.95 mmol) and tribasic potassium phosphate monohydrate (173 mg, 0.75 mmol). The vial was fitted with a rubber septum and then evacuated and refilled 3x with argon. A 2 wt % solution of TPGS-750-M/H_2O (0.9 mL) was added via syringe followed by the previously prepared catalyst solution (0.1 mL). The septum was removed and quickly replaced with a PTFE-lined threaded cap. The dram vial was placed in an aluminum reactor block containing a magnetic stir plate with a thermocouple set to 49 ^oC (NOTE: this yields a temperature of 45 ^oC within the reaction vial). The reaction was stirred rapidly for 3 h. The vial was removed from the reactor block and allowed to cool to rt. The reaction was extracted with EtOAc (3 x 1 mL) in flask and the combined organic layers were flushed through a Pasteur pipette plugged with cotton and 4 cm of silica gel into a 50 mL round-bottomed flask. Volatiles were removed in vacuo. The product was purified via flash chromatography on silica gel eluting with 20% diethyl ether/hexanes (R_f = 0.20 1:4 diethyl ether:hexanes). The column was flushed with 100% diethyl ether. The pure product was collected. The impure fractions were collected along with the ether flush, concentrated in vacuo, and the resulting crude sample was chromatographed over silica gel eluting with 20% diethyl ether/hexanes. The pure fractions were combined and volatiles removed in vacuo to yield the title compound as an off-white powder (combined 130 mg, 88%).

Gram scale synthesis of 1-(2,4-Dimethoxyphenyl)-2-methoxynaphthalene. A 100 mL Schlenk flask containing a an oblong football shaped magnetic stir bar was consecutively charged with $(EvanPhos)_2Pd(OAc)_2$ (60.3 mg, 0.05 mmol), 1-bromo-2-methoxynaphthalene (1.186 g, 5.0 mmol), 2,4-dimethoxyphenylboronic acid (1.592 g, 8.75 mmol), and tribasic potassium phosphate monohydrate (2.02 g, 8.75 mmol). The flask was sealed with a septum then subjected to 3 evacuation/argon refill cycles. The flask was charged with toluene (1.5 mL), and an aqueous solution of 2 wt % TPGS-750-M (8.5 mL). The flask was submerged in a heated oil bath (bath temperature 48 ^oC) and stirred vigorously for 5 h. After cooling to rt the mixture was diluted with EtOAc (40 mL) and stirred vigorously until all solids had dissolved. The mixture was transferred to a separatory funnel, washing with EtOAc to ensure complete transfer, and the phases were separated. The organic phase was dried over anhydrous Na_2SO_4 followed by solvent removal in vacuo. The crude material was chromatographed as before to yield the title compound as an off-white powder (1.251 g, 85%)

^1H NMR (500 MHz, chloroform-*d*) δ 7.87 (d, *J* = 9.0 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.44 – 7.40 (m, 1H), 7.37 (d, *J* = 9.0 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.67 – 6.63 (m, 2H), 3.90 (s, 3H), 3.85 (s, 3H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, chloroform-*d*) δ 160.38, 158.63,

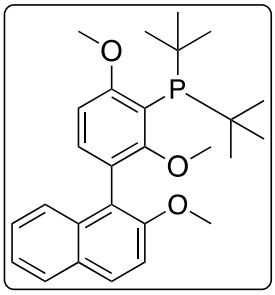
154.47, 133.97, 132.63, 129.04, 128.90, 127.80, 126.03, 125.31, 123.33, 121.77, 117.67, 114.10, 104.40, 99.03, 56.93, 55.66, 55.34.



EvanPhos (2); dicyclohexyl(2,6-dimethoxy-3-(2-methoxynaphthalen-1-yl)phenyl)phos-phane. A flame dried 250 mL 3-neck round bottomed flask containing a football shaped magnetic stir bar was charged with 1-(2,4-dimethoxyphenyl)-2-methoxynaphthalene (4.573 g, 15.53 mmol) under a flow of argon. The vessel was evacuated and back-filled with argon three times. The vessel was charged with anhydrous THF (75 mL) and stirred until dissolution of the biaryl was visually complete. The vessel was submerged in an ice bath and stirred for 20 min. *n*-Butyllithium ([2.23 M] in hexanes, 6.9 mL, 15.38 mmol) was added to the stirring solution dropwise via syringe over 20 min. Upon complete addition of *n*-butyllithium, the solution was allowed to stir in the ice bath for 30 min. Neat chlorodicyclohexylphosphine (3.35 mL, 15.16 mmol) was added dropwise via syringe over the course of 15 min. The solution was allowed to stir in the ice bath for 30 min. at which point the vessel was removed from the ice bath. Stirring was continued at rt for 1 h. The solution was quenched with water (25 mL) and diluted with diethyl ether (100 mL). The phases were separated and the aqueous phase was extracted with diethyl ether (2 x 50 mL). The combined organic phases were washed with a solution of 10% sulfuric acid/water (5 x 20 mL) and the acidic layers were collected into a 1 L beaker. Diethyl ether (150 mL) was added to the beaker that was then cooled in an ice bath. Solid sodium carbonate was slowly added while gently swirling until gas evolution had ceased [CAUTION: extremely exothermic. Add carbonate slowly and add more diethyl ether as needed to maintain approximately 100-150 mL of diethyl ether in the beaker]. The phases were separated and the aqueous phase was extracted with diethyl ether (3 x 50 mL). The ether was dried over anhydrous $MgSO_4$ and concentrated *in vacuo*. The mixture was chromatographed over basic aluminum oxide eluting with 30% diethyl ether/hexanes (R_f = 0.26 30% diethyl ether/hexanes) which yielded a flocculent white solid (5.73 g, 77%). **IMPORTANT NOTES CONCERNING ISOLATION**: this chromatographic purification must be run in 20 min or less. Extended time in contact with the aluminum oxide will result in oxidation of the ligand to the phosphine oxide. The less time spent during chromatography directly translates to a lower percentage of phosphine oxide in the final product. Silica gel is extremely useful for analytically determining purity of the fractions by TLC but results in rapid oxidation of the phosphine to the phosphine oxide during column chromatography. **DO NOT USE SILICA GEL FOR PURIFICATION AND RUN THE ALUMINUM OXIDE CHROMATOGRAPHIC PURIFICATION RAPIDLY**. Additionally, fractions should be collected and concentrated rapidly. Allowing the phosphine to sit in the chromatographic eluent exposed to atmosphere will result in oxidation of the phosphine to the phosphine oxide as well. Finally, once the last traces of solvent are removed in vacuo the product will foam vigorously and expand to consume the full headspace of the vessel and will likely end up in the rotary evaporator and/or hi-vac lines. To avoid this use a significantly larger vessel than one would normally pick for this scale of reaction. A batch synthesized on the scale presented here should use a 1 L round-bottomed flask or other appropriate vessel for concentration/solvent evaporation.

^{1}H NMR with ^{31}P decoupling (400 MHz, chloroform-*d*) δ 7.88 (d, *J* = 9.0 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.48 – 7.43 (m, 1H), 7.39 – 7.29 (m, 3H), 7.18 (d, *J* = 8.3 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H),

3.88 (s, 3H), 3.87 (s, 3H), 3.22 (s, 3H), 2.46 – 2.30 (m, 2H), 2.01 – 1.88 (m, 2H), 1.81 – 1.54 (m, 8H), 1.37 – 1.06 (m, 10H). ^{13}C NMR (101 MHz, chloroform-*d*) δ 164.78, 164.65, 163.30, 154.43, 134.41, 133.87, 129.17, 129.14, 127.95, 126.42, 125.39, 123.56, 122.56, 121.98, 113.93, 106.20, 61.05, 56.90, 55.58, 34.76 (d, *J* = 11.5 Hz), 34.32 (d, *J* = 11.7 Hz), 32.71 (d, *J* = 24.5 Hz), 32.34 (d, *J* = 22.2 Hz), 30.70 (dd, *J* = 8.8, 6.4 Hz), 27.64 – 27.15 (m), 26.67. ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.81, 164.71, 163.35, 154.49, 134.44, 133.93, 129.21, 129.18, 127.96, 126.42, 125.44, 123.58, 122.68, 122.04, 114.02, 106.24, 61.06, 61.03, 56.93, 55.59, 34.86, 34.76, 34.44, 34.35, 32.82, 32.63, 32.48, 32.30, 30.81, 30.74, 30.68, 27.64, 27.59, 27.57, 27.53, 27.42, 27.34, 27.31, 27.22, 26.71 (complexity due to phosphorus coupling). ^{31}P NMR (162 MHz, chloroform-*d*) δ -9.24 (phosphine oxide appears at 50.80). Chemical Formula: $C_{31}H_{39}O_3P$. EI-MS [M^{*+}] calcd: 490.2637; found: 490.2630.

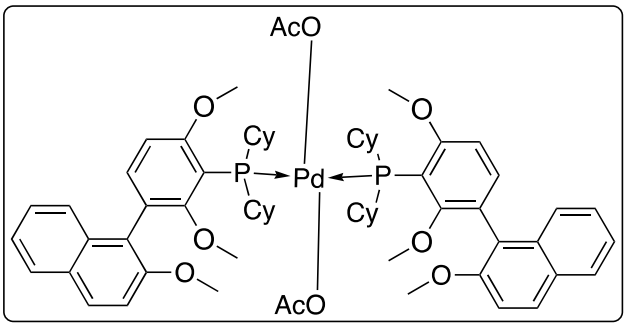


***t*-BuEvanPhos. Di-*t*-butyl(2,6-dimethoxy-3-(2-methoxynaphthalen-1-yl)phenyl)phosphane.** A flame dried 400 mL cylindrical pressure vessel with 24/40 jointed side arm and threaded screw cap (see page 6 for picture of the reaction apparatus) containing a football shaped magnetic stir bar was charged with 1-(2',4'-dimethoxyphenyl)-2-methoxynaphthalene (1.30 g, 4.42 mmol) under a flow of argon. The vessel was charged with anhydrous THF (25 mL) and sealed with a rubber septum. The mixture was stirred until dissolution of the biaryl was visually complete. The vessel was submerged in an ice bath and stirred for 20 min. *n*-Butyllithium (2.39 M in hexanes, 1.77 mL, 4.22 mmol) was added to the stirring solution dropwise via syringe over 20 min. Upon complete addition of *n*-butyllithium, the solution was allowed to stir in the ice bath for 30 min. Neat di-*t*-butylchlorophosphane (0.76 mL, 4.22 mmol) was added dropwise via syringe over the course of 15 min. The solution was allowed to stir in the ice bath for 30 min. at which point the vessel was removed from the ice bath. Stirring was continued at rt for 1 h. The rubber septum was removed and neat Cu(I)Cl (0.605 g, 4.22) was added to the vessel. Residual Cu(I)Cl was rinsed into the vessel with anhydrous THF (5 mL). The vessel was sealed with a threaded screw cap, placed in an oil bath set to 90 °C, and stirred for 18 h. The vessel was cooled to rt. The solution was quenched with water (25 mL) and diluted with diethyl ether (100 mL). The phases were separated and the aqueous phase was extracted with diethyl ether (2 x 50 mL). The combined organic phases were washed with a solution of 10% sulfuric acid/water (5 x 20 mL) and the acidic layers were collected into a 1 L beaker. Diethyl ether (150 mL) was added to the beaker that was then cooled in an ice bath. Solid sodium carbonate was slowly added while gently swirling until gas evolution had ceased [CAUTION: extremely exothermic. Add carbonate slowly and add more diethyl ether as needed to maintain approximately 100-150 mL of diethyl ether in the beaker]. The phases were separated and the aqueous phase was extracted with diethyl ether (3 x 50 mL). The ether was removed in vacuo and the resulting viscous oil was flushed through a plug of basic alumina with 30% ether/hexanes. The solvent was removed in vacuo yielding a white powder (0.833 g, 45%).

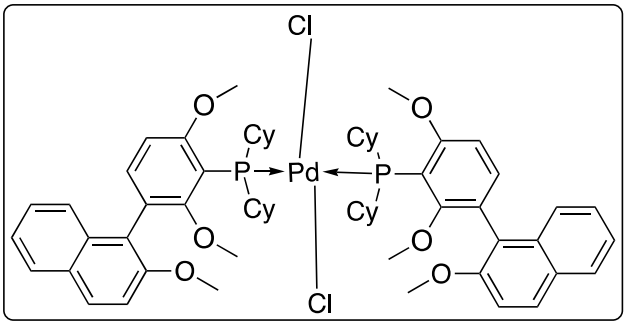
^{1}H NMR with ^{31}P decoupling (400 MHz, chloroform-*d*) δ 7.91 – 7.77 (m, 2H), 7.52 – 7.45 (m, 1H), 7.40 – 7.27 (m, 3H), 7.21 (d, *J* = 8.4 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 3.84 (s, 6H), 3.27 (s, 3H), 1.27 (d, *J* = 11.3 Hz, 18H). ^{31}P NMR (162 MHz, $cdcl_3$) δ 61.89, 24.75. Molecular formula: $C_{27}H_{35}O_3P$ ESI-MS [$M+H]^+$ calcd: 439.2402; found: 439.2389.

Figure S1: 400 mL threaded screwcap pressure flask.

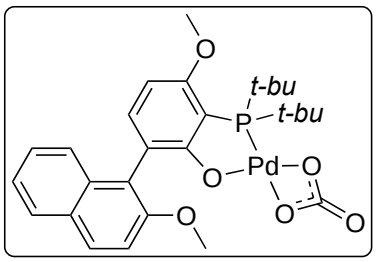
General procedure for the synthesis of (EvanPhos)$_2$Pd and related complexes. A dry 25 mL round-bottom flask containing a magnetic stir bar was charged with an appropriate palladium(II) salt under an argon atmosphere. Sufficient dry toluene was added to achieve [0.4 M] relative to the palladium(II) salt and the mixture was stirred until dissolution of the palladium was complete. A separate dry 25 mL round-bottom flask was charged the appropriate ligand (2.05:1 L:Pd) and dissolved in dry toluene to achieve [0.4 M]. The ligand solution was transferred to the palladium solution via syringe in a dropwise fashion over the course of 30 min. Upon complete addition the flask containing the ligand was rinsed with a small portion of dry toluene and this was subsequently transferred to the palladium-containing flask. The mixture was allowed to stir for 1-2h (EvanPhos) 24h (*t*-BuEvanPhos) under an argon atmosphere. A yellow powdery precipitate was observed in all cases. A 22 gauge vent needle was placed into the septum to halve the volume of toluene in the flask. The mixture was vacuum filtered and the resulting yellow powder was rinsed liberally with hexanes. The material was transferred to a vial and volatiles were removed in vacuo.



EvanPhos$_2$[Pd(OAc)$_2$]. Synthesized according to the general procedure utilizing $Pd(OAc)_2$ (86 mg, 0.38 mmol) and EvanPhos (383 mg, 0.781 mmol). Material was isolated as a yellow powder (366 mg, 85%). Chemical Formula: $C_{66}H_{84}O_{10}P_2Pd$. ESI-MS $[M+H-2(OAc)]^+$ calcd: 1087.4408; found: 1087.4413.



(EvanPhos)$_2$PdCl$_2$. Synthesized according to the general procedure utilizing $(MeCN)_2PdCl_2$ (52 mg, 0.2 mmol) and EvanPhos (202 mg, 0.411 mmol). Material was isolated as a yellow powder (154 mg, 67%). Chemical Formula: $C_{62}H_{78}Cl_2O_6P_2Pd$. ESI-MS $[M+H-2(Cl)]^+$ calcd: 1087.4408; found: 1087.4404.



(*t*-BuEvanPhos)Pd(OAc). Synthesized according to the general procedure utilizing $Pd(OAc)_2$ (60 mg, 0.27 mmol) and EvanPhos (234 mg, 0.53 mmol). Material was isolated as a yellow powder. Chemical Formula: $C_{58}H_{76}O_{10}P_2Pd$. ESI-MS $[M+2CH_3CN-(OAc)]^+$ calcd: 611.1167; found: 611.1642.

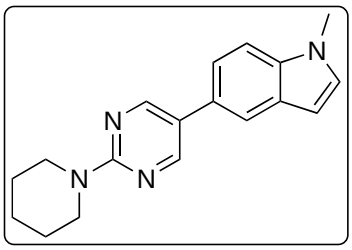
III. General Experimental Procedures and Analytical Data for Suzuki-Miyaura Products

General procedure for catalyst solution preparation and optional pre-reduction. $Pd(OAc)_2$ (3.0-11.0 mg) and EvanPhos (1.75-2.0 equiv EvanPhos : Pd) were added to a dry 5 mL microwave vial containing an oblong stir bar. The vial was sealed with a rubber septum and the vial was evactuated and refilled with argon 3x. Dry toluene was added to the vial to achieve a concentration of 0.56 mg

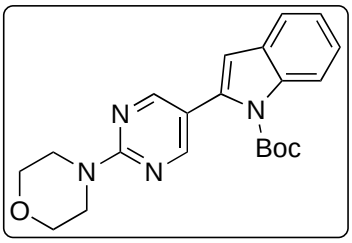
$Pd(OAc)_2$/0.1 mL toluene for a 0.5 mmol scale reaction (0.56 mg $Pd(OAc)_2$ in 0.1 mL toluene yields 0.5 mol % catalyst loading). To achieve lower catalyst loadings, e.g., 0.1-0.25 mol % Pd, dilute this mixture accordingly). The mixture was stirred at a moderate speed for a minimum of 30 min under an argon atmosphere. OPTIONAL: For reactions that may be slow to initiate pre-reduction of the catalyst with DIBAL may be beneficial. After 30 min DIBAL ([1.0 M] in toluene or DCM, 2.0-2.1 equiv relative to Pd) was added dropwise. Complete reduction is accompanied by the mixture turning brown/black. At this point the catalyst is ready and may be added to the reaction mixture. This procedure is exactly the same for the use of isolated $EvanPhos_2PdX_2$ catalysts in place of $Pd(OAc)_2$ + 2EvanPhos.

General procedure A for Suzuki-Miyaura reactions in EtOAc. A 4 mL dram vial containing an oblong magnetic stir bar was charged with solid halide (0.5 mmol), organoboron (0.75 mmol, though many reactions can be conducted effectively with 0.625 mmol) and potassium phosphate monohydrate (0.75 mmol). The vial was fitted with a rubber septum, and then evacuated and refilled with argon 3x. At this point liquid halides could be added via syringe. Degassed EtOAc (0.8 mL), DI water (0.1 mL), and the catalyst solution (0.1 mL = 0.1-0.5 mol % Pd) were added sequentially to the vial via syringe. Unless otherwise noted the catalyst was pre-reduced with DIBAL. The septum was removed and quickly replaced with a PTFE lined threaded cap. The vial was placed in an aluminum heating block over a stir plate with stir rate set to $\geq$ **1100** rpm and a thermocouple probe in the aluminum block set to 49 ^{o}C (NOTE: this yields a temperature of 45 ^{o}C within the reaction vial). Reactions were followed by TLC and/or GC/MS monitoring. When the reactions were judged complete (or continued progress was not observed for incomplete reactions) the vial was cooled to rt. The mixture was flushed through a Pasteur pipette containing a cottton plug and silica gel. If needed the vial was rinsed with additional EtOAc to remove any material remaining. Volatiles were removed in vacuo and the crude mixture purified via flash chromatography.

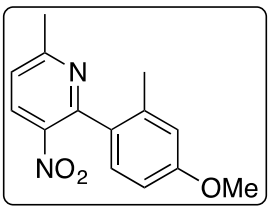
General procedure B for Suzuki-Miyaura reactions in aqueous TPGS-750-M. A 4 mL dram vial containing an oblong magnetic stir bar was charged with solid halide (0.5 mmol), organoboron (0.75 mmol, though many reactions can be conducted effectively with 0.625 mmol) and potassium phosphate monohydrate (0.75 mmol). The vial was fitted with a rubber septum and then evacuated and refilled with argon 3x. At this point liquid halides could be added via syringe. A solution of 2 wt % aq. TPGS-750-M (0.9 mL) and the catalyst solution (0.1 mL = 0.05-0.5 mol % Pd) were added sequentially to the vial. Unless otherwise noted the catalyst was pre-reduced with DIBAL. The septum was removed and quickly replaced with a PTFE lined threaded cap. The vial was placed in an aluminum heating block over a stir plate with stir rate set to $\geq$ **1100** rpm with a thermocouple probe in the aluminum block set to 49 ^{o}C (NOTE: this yields a temperature of 45 ^{o}C within the reaction vial). Reactions were followed by TLC and/or GC/MS monitoring. When the reactions were judged complete (or continued progress was not observed for incomplete reactions) the vial was cooled to rt. The mixture was extracted with EtOAc (3 x 1 mL) and the organic phase was flushed through a Pasteur pipette containing a cotton plug and silica gel. Volatiles were removed in vacuo and the crude mixture was purified via flash chromatography.



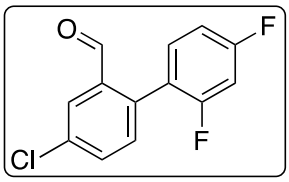
1-Methyl-5-(2-(piperidin-1-yl)pyrimidin-5-yl)-1*H*-indole. Synthesized utilizing 5-bromo-2-(piperidin-1-yl)pyrimidine and (1-methyl-1*H*-indol-5-yl)boronic acid according to general procedure A (3.5 h, 134 mg, 92% yield. 0.5 mol % Pd) and general procedure B (16 h, 127 mg, 87%. 0.1 mol % Pd) (1.5 h, 136 mg, 93%. 0.5 mol % Pd) (1.5 h, 132 mg, 90%. 0.5 mol % of isolated *t*-BuEvanPhosPd[OAc]). White solid, turns red over time when exposed to the atmosphere. R_f = 0.31 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.59 (s, 2H), 7.70 (d, *J* = 1.6 Hz, 1H), 7.43 – 7.29 (m, 2H), 7.09 (d, *J* = 3.1 Hz, 1H), 6.53 (d, *J* = 3.1 Hz, 1H), 3.83 (d, *J* = 5.8 Hz, 7H), 1.76 – 1.61 (m, 6H). ^{13}C NMR (101 MHz, chloroform-*d*) δ 160.92, 156.15, 136.23, 129.79, 129.26, 127.41, 123.83, 120.31, 118.24, 109.96, 101.32, 45.20, 33.08, 25.93, 25.07. Chemical Formula: $C_{18}H_{20}N_4$ ESI-MS $[M+H]^+$ calcd: 293.1766; found: 293.1767.



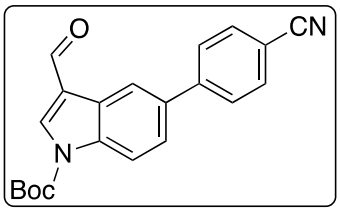
***t*-Butyl 2-(2-morpholinopyrimidin-5-yl)-1*H*-indole-1-carboxylate**: Synthesized utilizing 4-(5-bromopyrimidin-2-yl)morpholine and (1-(*t*-butoxycarbonyl)-1*H*-indol-2-yl)boronic acid according to general procedure A (3 h, 179 mg, 94% yield. 0.5 mol % Pd) and general procedure B (3 h, 185 mg, 97%, 0.5 mol % Pd). White solid. R_f = 0.23 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.39 (s, 2H), 8.18 (d, *J* = 8.3 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.38 – 7.21 (m, 2H), 6.55 (s, 1H), 3.90 – 3.82 (m, 4H), 3.83 – 3.75 (m, 4H), 1.50 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.84, 157.27, 150.23, 137.27, 135.08, 129.25, 124.67, 123.27, 120.56, 117.87, 115.85, 110.63, 84.28, 66.96, 44.49, 28.11. Chemical Formula: $C_{21}H_{24}N_4O_3$. ESI-MS $[M+Na]^+$ calcd: 403.1746; found: 403.1748.



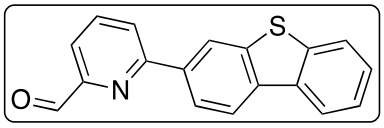
2-(4-Methoxy-2-methylphenyl)-6-methyl-3-nitropyridine. Synthesized utilizing 2-bromo-6-methyl-3-nitropyridine and (4-methoxy-2-methylphenyl)boronic acid according to general procedure A (10 h, 123 mg, 95% yield. 0.5 mol % Pd) and general procedure B (1.5 h, 121 mg, 94%. 0.1 mol % Pd) (1.5 h, 118 mg, 92%, 0.25 mol % of isolated *t*-BuEvanPhosPd[OAc]). Viscous yellow oil that slowly solidifies. R_f = 0.19 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.17 (d, *J* = 8.3 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 6.85 – 6.75 (m, 2H), 3.82 (s, 3H), 2.69 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.74, 160.10, 153.75, 144.58, 137.47, 132.55, 129.65, 129.46, 122.16, 116.08, 111.44, 55.38, 24.97, 19.90. Chemical Formula: $C_{14}H_{14}N_2O_3$ ESI-MS $[M+Na]^+$ calcd: 281.0902; found: 281.0902.



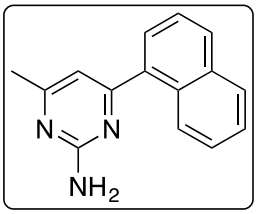
4-Chloro-2',4'-difluoro-[1,1'-biphenyl]-2-carbaldehyde. Synthesized utilizing 2-bromo-5-chloro-benzaldehyde and (2,4-difluorophenyl)boronic acid without DIBAL pre-reduction of the catalyst according to general procedure A (3 h, 120 mg, 95% yield, 0.5 mol % Pd) and general procedure B (2 h, 122 mg, 97 %, 0.5 mol % Pd). R_f = 0.53 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 9.84 (d, *J* = 3.0 Hz, 1H), 8.00 (d, *J* = 2.3 Hz, 1H), 7.64 (dd, *J* = 8.2, 2.3 Hz, 1H), 7.37 – 7.28 (m, 2H), 7.00 (dtd, *J* = 27.7, 9.1, 8.6, 2.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 190.01 (d, *J* = 2.3 Hz), 163.46 (dd, *J* = 251.5, 11.6 Hz), 159.80 (dd, *J* = 249.7, 12.2 Hz), 136.17, 135.43, 135.15, 133.87, 132.96, 132.68 (dd, *J* = 9.6, 4.1 Hz), 128.08, 120.84, 112.13 (dd, *J* = 21.4, 4.0 Hz), 104.50 (d, *J* = 25.8 Hz).^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.24 (p, *J* = 7.7 Hz, J^1 C-F= 251.5 Hz), -110.84 (q, *J* = 8.4 Hz, J^1 C-F= 249.7). Chemical Formula: $C_{13}H_7ClF_2O$ CI-MS [M$^+$] calcd: 252.0154; found: 252.0154.



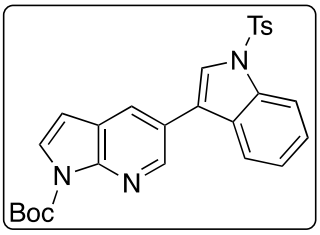
***t*-Butyl 5-(4-cyanophenyl)-3-formyl-1*H*-indole-1-carboxylate.** Synthesized utilizing *t*-butyl 5-bromo-3-formyl-1*H*-indole-1-carboxylate and (4-cyanophenyl)boronic acid according to general procedure A (14 h, 121 mg, 70% yield, 0.5 mol % Pd) R_f = 0.16 in 15% EtOAc/ hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 10.12 (s, 1H), 8.53 (s, 1H), 8.31 – 8.21 (m, 2H), 7.75 (q, *J* = 8.1 Hz, 4H), 7.64 (d, *J* = 8.7 Hz, 1H), 1.73 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.81, 148.67, 145.60, 137.44, 136.16, 135.97, 132.71, 128.15, 126.97, 125.48, 121.70, 121.04, 119.10, 115.91, 110.92, 86.27, 77.48, 77.16, 76.84, 28.22. Chemical Formula: $C_{21}H_{18}N_2O_3$ ESI-MS [M+Na]$^+$ calcd: 369.1215; found: 369.1208.



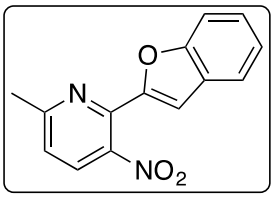
6-(Dibenzo[*b*,*d*]thiophen-3-yl)picolinaldehyde. Synthesized utilizing 6-bromopicolinaldehyde and dibenzo[*b*,*d*]thiophen-3-ylboronic acid according to general procedure A (14 h, 144 mg, quantitative) R_f = 0.24 in 10% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 10.22 (s, 1H), 8.84 (d, *J* = 1.7 Hz, 1H), 8.31 – 8.22 (m, 1H), 8.14 (dd, *J* = 8.5, 1.8 Hz, 1H), 8.01 (dd, *J* = 6.6, 2.3 Hz, 1H), 7.97 – 7.82 (m, 4H), 7.55 – 7.44 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.01, 157.74, 152.87, 141.07, 139.97, 137.92, 136.30, 135.53, 134.68, 127.21, 125.44, 124.71, 124.42, 123.24, 123.02, 121.96, 120.13, 119.79. Chemical Formula: $C_{18}H_{11}NOS$ ESI-MS [M+Na]$^+$ calcd: 312.0459; found: 312.0458.



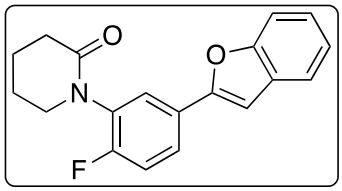
4-Methyl-6-(naphthalen-1-yl)pyrimidin-2-amine : Synthesized utilizing 4-chloro-6-methyl-pyrimidin-2-amine and naphthalene-1-boronic acid according to general procedure A (18 h, 118 mg, quantitative. 0.5 mol % Pd) R_f = 0.17 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.19 – 8.10 (m, 1H), 7.95 – 7.85 (m, 2H), 7.58 (dd, *J* = 7.1, 1.4 Hz, 1H), 7.57 – 7.45 (m, 3H), 6.79 (s, 1H), 5.24 (s, 2H), 2.44 (s, 3H), .^{13}C NMR (101 MHz, cdcl$_3$) δ 168.56, 167.80, 163.03, 136.86, 134.01, 130.72, 129.77, 128.55, 127.05, 126.77, 126.20, 125.54, 125.32, 112.23, 24.30. Chemical Formula: $C_{15}H_{13}N_3$ ESI-MS $[M+Na]^+$ calcd: 258.1007; found: 258.1011.



***t*-Butyl 5-(1-tosyl-1*H*-indol-3-yl)-1*H*-pyrrolo[2,3-*b*]pyridine-1-carboxylate** : Synthesized utilizing *tert*-butyl 5-bromo-1*H*-pyrrolo[2,3-*b*]pyridine-1-carboxylate and (1-tosyl-1*H*-indol-3-yl)boronic acid according to general procedure A (18 h, 224 mg, 92%, 0.5 mol % Pd) R_f = 0.35 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.73 (d, *J* = 2.1 Hz, 1H), 8.10 – 8.02 (m, 2H), 7.82 (d, *J* = 8.1 Hz, 2H), 7.77 – 7.66 (m, 3H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 6.55 (d, *J* = 4.0 Hz, 1H), 2.33 (s, 3H), 1.69 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.92, 147.73, 145.27, 144.57, 135.45, 135.11, 130.08, 129.38, 128.29, 127.49, 126.99, 125.19, 124.09, 123.83, 123.23, 123.18, 121.28, 120.15, 113.96, 104.58, 84.37, 28.19, 21.68. Chemical Formula: $C_{27}H_{25}N_3O_4S$ ESI-MS $[M+Na]^+$ calcd: 510.1463; found: 510.1476.

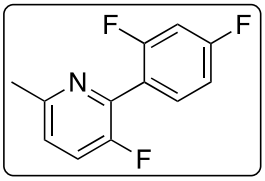


2-(Benzofuran-2-yl)-6-methyl-3-nitropyridine. Synthesized utilizing 2-bromo-6-methyl-3-nitro-pyridine and benzofuran-2-ylboronic acid according to general procedure B (4 h, 116 mg, 91%, 0.25 mol % Pd) R_f = in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 7.94 (d, *J* = 8.3 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.52 (d, *J* = 9.8 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.31 – 7.21 (m, 2H), 2.71 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.14, 155.82, 151.21, 141.12, 132.30, 128.02, 126.30, 123.61, 122.75, 122.17, 112.04, 109.38, 24.87. Chemical Formula: $C_{14}H_{10}N_2O_3$ CI-MS $[M]^+$ calcd: 254.0591; found: 254.0694.

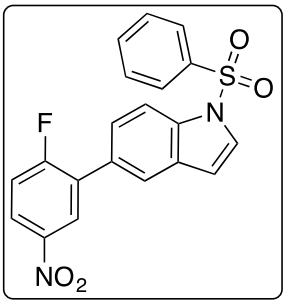


1-(5-(Benzofuran-2-yl)-2-fluorophenyl)piperidin-2-one. Synthesized utilizing 1-(5-bromo-2-fluorophenyl)piperidin-2-one and benzofuran-2-ylboronic acid according to general procedure B (16 h, 114 mg, 74%, 0.5 mol % Pd) (16 h, 118 mg, 76%, 0.5 mol % of isolated *t*-BuEvanPhosPd[OAc]) R_f = 0.22 in 40% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 7.80 – 7.71 (m, 1H), 7.57 (d, *J* = 7.4 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.17 (m, 3H), 6.96 (s, 1H), 3.65 (t, *J* = 5.3 Hz, 2H), 2.65 – 2.57 (m, 2H), 1.99 (p, *J* = 3.3 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.11, 157.90

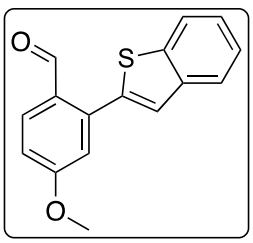
(d, *J* = 252.8 Hz), 154.95, 154.43 (d, *J* = 1.5 Hz), 131.27 (d, *J* = 13.9 Hz), 129.18, 127.74, 125.95 (d, *J* = 1.9 Hz), 125.58 (d, *J* = 8.1 Hz), 124.55 (d, *J* = 8.0 Hz), 123.16, 121.10, 117.32 (d, *J* = 21.3 Hz), 111.23 (d, *J* = 21.3 Hz), 101.63, 51.46 (d, *J* = 1.8 Hz), 32.71, 23.52, 21.52. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -120.24 – -120.31 (m, J^1 C-F= 252.8 Hz). Chemical Formula: $C_{19}H_{16}FNO_2$ ESI-MS $[M+Na]^+$ calcd: 332.1063; found: 332.1067.



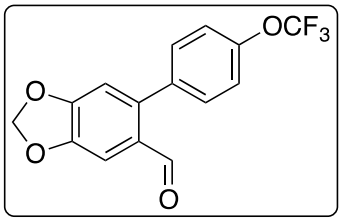
2-(2,4-Difluorophenyl)-3-fluoro-6-methylpyridine. Synthesized utilizing 2-bromo-3-fluoro-6-methylpyridine and (2,4-difluorophenyl)boronic acid according to general procedure B (20 h, 78 mg, 70%, 0.5 mol % Pd) R_f = 0.43 in 15% EtOAc/hexanes. ^{1}H NMR (500 MHz, chloroform-*d*) δ 7.58 (td, *J* = 8.4, 6.4 Hz, 1H), 7.38 (t, *J* = 8.8 Hz, 1H), 7.18 (dd, *J* = 8.4, 3.6 Hz, 1H), 7.01 (td, *J* = 8.3, 2.4 Hz, 1H), 6.96 – 6.87 (m, 1H), 2.60 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.72 (dd, *J* = 250.6, 11.8 Hz), 160.51 (dd, *J* = 253.2, 12.0 Hz), 155.86 (d, *J* = 256.8 Hz), 154.50 (d, *J* = 4.8 Hz), 140.94 (d, *J* = 15.4 Hz), 132.62 (ddd, *J* = 9.9, 5.0, 1.3 Hz), 124.13 – 124.05 (m), 123.88, 120.34 – 120.00 (m), 111.86 (dd, *J* = 21.4, 3.8 Hz), 104.25 (t, *J* = 25.7 Hz).^{19}F NMR (376 MHz, chloroform-*d*) δ -108.81 – -108.91 (m, J^1 C-F = 250.6 Hz), -109.95 (dq, *J* = 30.6, 8.9 Hz, J^1 C-F= 253.7 Hz), -126.82 (ddd, *J* = 30.5, 9.3, 3.6 Hz, J^1 C-F= 256.8 Hz). Chemical Formula: $C_{12}H_8F_3N$ CI-MS $[M]^+$ calcd: 223.0609; found: 223.0609.



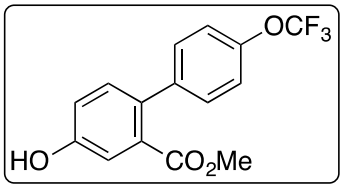
5-(2-Fluoro-5-nitrophenyl)-1-(phenylsulfonyl)-1*H*-indole. Synthesized utilizing 2-bromo-1-fluoro-4-nitrobenzene and (1-(phenylsulfonyl)-1*H*-indol-5-yl)boronic acid according to general procedure B (8 h, 168 mg, 85%, 0.5 mol % Pd) R_f = 0.28 in 20% EtOAc/hexanes. ^{1}H NMR (500 MHz, chloroform-*d*) δ 8.38 (dd, *J* = 6.6, 2.9 Hz, 1H), 8.25 – 8.18 (m, 1H), 8.11 (d, *J* = 8.7 Hz, 1H), 7.92 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.74 (d, *J* = 3.6 Hz, 1H), 7.65 (d, *J* = 3.7 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.45 (m, 3H), 7.30 (t, *J* = 9.2 Hz, 1H), 6.74 (d, *J* = 3.6 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 163.31 (d, *J* = 258.8 Hz), 144.62, 138.30, 134.97, 134.21, 131.25, 130.67, 130.55, 129.56, 128.80, 127.51, 126.96, 126.90 (d, *J* = 5.6 Hz), 125.59 (d, *J* = 3.0 Hz), 124.53 (d, *J* = 10.1 Hz), 122.23 (d, *J* = 3.2 Hz), 117.34 (d, *J* = 25.8 Hz), 113.99, 109.37.. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.04 (dt, *J* = 9.6, 4.7 Hz). Chemical Formula: $C_{20}H_{13}FN_2O_4S$ ESI-MS $[2M+Na]^+$ calcd: 815.1058; found: 815.1064.



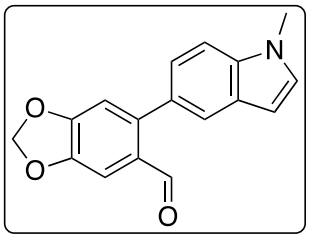
2-(Benzo[*b*]thiophen-2-yl)-4-methoxybenzaldehyde. Synthesized utilizing 2-bromo-4-methoxybenzaldehyde and benzo[*b*]thiophen-2-ylboronic acid MIDA ester according to general procedure B (48 h, 92%) R_f = 0.38 in 15% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 10.13 (s, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.86 (ddd, *J* = 18.0, 7.0, 2.1 Hz, 2H), 7.41 (tt, *J* = 7.3, 5.7 Hz, 2H), 7.31 (s, 1H), 7.10 – 7.00 (m, 2H), 3.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.61, 163.59, 140.62, 140.56, 139.90, 138.82, 130.42, 128.12, 126.33, 125.14, 125.06, 124.08, 122.28, 115.97, 115.06, 77.48, 77.16, 76.84, 55.88. Chemical Formula: $C_{16}H_{12}O_2S$ ESI-MS $[M+Na]^+$ calcd: 291.0456; found: 291.0462.



6-(4-(Trifluoromethoxy)phenyl)benzo[*d*][1,3]dioxole-5-carbaldehyde. Synthesized utilizing 6-bromopiperonal and 4-(trifluormethoxy)benzeneboronic acid according to general procedure B (20 h, 152 mg, 98%. 0.25 mol % Pd); R_f = 0.44 in 20% EtOAc/hexanes; ^{1}H NMR (400 MHz, chloroform-*d*) δ 9.73 (s, 1H), 7.47 (s, 1H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 6.82 (s, 1H), 6.11 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.15, 152.35, 149.36, 148.28, 142.05, 136.37, 131.62, 129.05, 120.96, 110.33, 106.65, 102.40. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.85 (J^1C-F= 287.7 Hz). Chemical Formula: $C_{15}H_9F_3O_4$ ESI-MS $[M-Na]^-$ calcd: 333.0351; found: 333.0355.

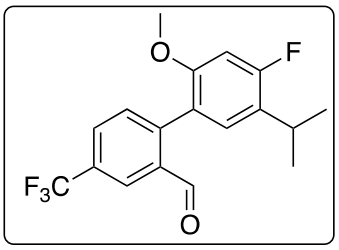


Methyl 4-hydroxy-4'-(trifluoromethoxy)-[1,1'-biphenyl]-2-carboxylate. Synthesized utilizing methyl 5-hydroxy-2-iodobenzoate and 4-(trifluoromethoxy)benzeneboronic acid according to general procedure B (10 h, 116 mg, 74%. 0.1 mol % Pd) R_f = 0.45 in 40% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 7.68 (d, *J* = 9.2 Hz, 2H), 7.58 (s, 1H), 7.56 (s, 1H), 7.33 (dd, *J* = 8.1, 4.3 Hz, 3H), 5.50 (s, 1H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.87, 152.63, 135.28, 131.68, 131.16, 130.75, 130.66, 122.36, 121.54, 117.42, 52.51. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.79 (J^1 C-F= 257.6 Hz). Chemical Formula: $C_{15}H_{11}F_3O_4$ ESI-MS $[M-H]^-$ calcd: 311.0531; found: 311.0537.

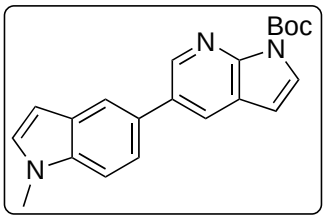


6-(1-Methyl-1*H*-indol-5-yl)benzo[*d*][1,3]dioxole-5-carbaldehyde. Synthesized utilizing 5-bromopiperonal and (1-methyl-1*H*-indol-5-yl)boronic acid according to general procedure A (20 h, 113 mg, 81%. 0.1 mol % Pd) without pre-reduction of the palladium acetate and utilizing toluene:water 9:1 as the reaction medium. R_f = 0.40 in 20% EtOAc/hexanes. ^{1}H NMR (500 MHz, chloroform-*d*) δ 9.78 (s, 1H), 7.58 (d, *J* = 1.7 Hz, 1H), 7.48 (s, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.20 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.14 (d, *J* = 3.1 Hz, 1H), 6.93 (s, 1H), 6.53 (d, *J* = 3.0 Hz, 1H), 6.09 (s, 2H), 3.85 (s, 3H). ^{13}C

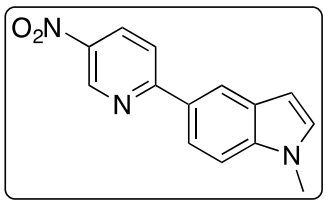
NMR (126 MHz, $CDCl_3$) δ 191.61, 152.00, 147.44, 145.39, 136.53, 130.19, 129.14, 128.84, 128.52, 124.07, 122.89, 110.88, 109.20, 106.26, 102.08, 101.46, 33.17. Chemical Formula: $C_{17}H_{13}NO_3$ ESI-MS $[M+Na]^+$ calcd: 302.0793; found: 302.0790.



4'-Fluoro-5'-isopropyl-2'-methoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-2-carbaldehyde. Synthesized utilizing 2-bromo-5-(trifluoromethyl)benzaldehyde and (4-fluoro-5-isopropyl-2-methoxyphenyl)boronic acid according to general procedure B (20 h, 155, 91%, 0.05 mol % Pd). R_f = 0.60 in 20% Et_2O/hexanes. **1**H NMR (400 MHz, chloroform-*d*) δ 9.77 (s, 1H), 8.25 (s, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.70 (d, *J* = 11.9 Hz, 1H), 3.72 (s, 3H), 3.24 (hept, *J* = 6.9 Hz, 1H), 1.27 (d, *J* = 7.2 Hz, 7H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 191.16, 161.78 (d, *J* = 248.3 Hz), 155.46 (d, *J* = 10.2 Hz), 144.54, 134.49, 132.21, 130.17, 129.96 (q, *J* = 3.4 Hz), 129.76 (d, *J* = 7.4 Hz), 127.94 (d, *J* = 15.6 Hz), 124.08 (q, *J* = 3.8 Hz), 121.12 (d, *J* = 3.5 Hz), 99.42 (d, *J* = 27.8 Hz), 55.92, 26.88, 22.91.^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.84 (J^1 C-F= 272.4 Hz), -114.25 (dd, *J* = 11.8, 8.4 Hz, J^1 C-F = 248.3 Hz).Chemical Formula: $C_{18}H_{16}F_4O_2$ ESI-MS $[M+Na+MeOH]^+$ calcd: 395.1246; found: 395.1236.

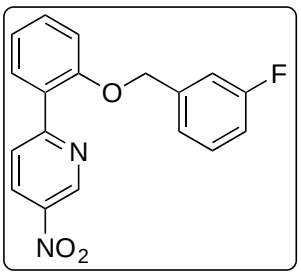


***t*-Butyl 5-(1-methyl-1*H*-indol-5-yl)-1*H*-pyrrolo[2,3-*b*]pyridine-1-carboxylate**. Synthesized utilizing *t*-butyl 5-bromo-1*H*-pyrrolo[2,3-*b*]pyridine-1-carboxylate and (1-methyl-1*H*-indol-5-yl)boronic acid according to general procedure B (3 h, 165 mg, 95%, 0.005 mol % Pd). R_f = 0.21 in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 8.79 (s, 1H), 8.08 (s, 1H), 7.85 (s, 1H), 7.66 (d, *J* = 3.9 Hz, 1H), 7.52 – 7.38 (m, 2H), 7.11 (d, *J* = 3.0 Hz, 1H), 6.55 (m, 2H), 3.83 (s, 3H), 1.69 (s, 9H). ^{13}C NMR (101 MHz, chloroform-*d*) δ 148.13, 147.41, 144.79, 136.40, 133.64, 130.28, 129.84, 129.19, 127.66, 127.03, 123.13, 121.64, 119.86, 109.84, 104.80, 101.44, 84.07, 33.10, 28.27. Chemical Formula: $C_{21}H_{21}N_3O_2$ ESI-MS $[M+Na]^+$ calcd: 370.1531; found: 370.1527.

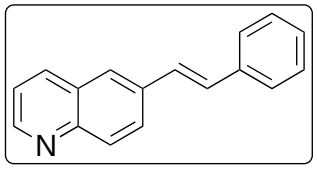


1-Methyl-5-(5-nitropyridin-2-yl)-1*H*-indole. Synthesized utilizing 2-bromo-5-nitropyridine and (1-methyl-1*H*-indol-5-yl)boronic acid according to general procedure A (20 h, 106 mg, 84%. 0.1 mol % Pd) without pre-reduction of the palladium acetate and utilizing toluene:water 9:1 as the reaction medium. R_f = 0.32 in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 9.48 (d, *J* = 2.7 Hz, 1H), 8.49 (dd, *J* = 8.9, 2.7 Hz, 1H), 8.41 (d, *J* = 1.7 Hz, 1H), 8.02 (dd, *J* = 8.7, 1.8 Hz, 1H), 7.95 (d, *J*

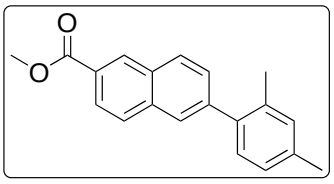
= 8.9 Hz, 1H), 7.44 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 3.1 Hz, 1H), 6.62 (d, *J* = 3.1 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, chloroform-*d*) δ 163.51, 144.87, 142.00, 138.30, 132.00, 130.45, 128.96, 128.00, 121.44, 121.39, 119.64, 109.96, 102.54, 33.07. Chemical Formula: $C_{14}H_{11}N_3O_2$ ESI-MS $[M+H]^+$ calcd: 254.0930; found: 254.0923.



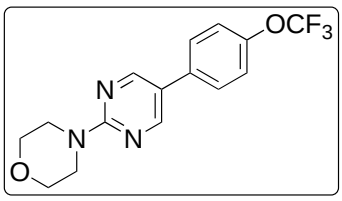
2-(2-((3-Fluorobenzyl)oxy)phenyl)-5-nitropyridine. Synthesized utilizing 2-chloro-5-nitropyridine and (2-((3-fluorobenzyl)oxy)phenyl)boronic acid according to general procedure B (3 h, 154 mg, 95%, 0.25 mol % Pd). R_f = 0.24 in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, chloroform-*d*) δ 9.51 (d, *J* = 2.6 Hz, 1H), 8.43 (dd, *J* = 8.8, 2.7 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.96 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.50 – 7.40 (m, 1H), 7.34 (td, *J* = 7.9, 5.7 Hz, 1H), 7.21 – 6.98 (m, 6H), 5.17 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.08 (d, *J* = 246.8 Hz), 161.38, 156.41, 144.97, 142.52, 138.99 (d, *J* = 7.4 Hz), 131.98 (d, *J* = 2.9 Hz), 130.85, 130.50, 130.41, 127.41, 125.07, 122.71 (d, *J* = 2.9 Hz), 122.05, 115.23 (d, *J* = 21.2 Hz), 114.23 (d, *J* = 22.1 Hz), 113.19, 70.14. ^{19}F NMR (376 MHz, chloroform-*d*) δ -112.35 (td, *J* = 9.0, 5.7 Hz, J^1 C-F= 246.8 Hz). Chemical Formula: $C_{18}H_{13}FN_2O_3$ ESI-MS $[M+H]^+$ calcd: 325.0988; found: 325.0977.



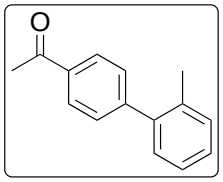
(*E*)-6-Styrylquinoline. Synthesized utilizing 5-bromoquinoline and (E)-phenethylboronic acid acid according to general procedure A with no DIBAL pre-reduction (8 h, 106 mg, 92%, 0.25 mol% Pd). R_f = 0.15 in 20% EtOAc/hexanes. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.95 (dd, *J* = 4.6, 1.3 Hz, 1H), 8.56 (dd, *J* = 8.6, 1.4 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.84 – 7.69 (m, 3H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.47 – 7.40 (m, 3H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.18 (d, *J* = 16.0 Hz, 1H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.46, 148.70, 137.32, 135.52, 133.00, 132.30, 129.41, 129.39, 128.96, 128.27, 126.89, 126.60, 124.36, 124.03, 121.08. Chemical Formula: $C_{17}H_{13}N$ EI-MS $[M\cdot]^+$ calcd: 231.1048; found: 231.1048



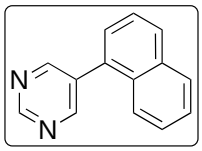
Methyl 6-(2,4-dimethylphenyl)-2-naphthoate. Synthesized utilizing methyl 6-bromo-2-naphthoateand (E)-phenethylboronic acid acid according to general procedure A with no DIBAL pre-reduction (6 h, 140 mg, 96%, 0.1 mol% Pd). R_f = 0.58 in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.65 (s, 1H), 8.08 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.6 Hz, 1H), 7.80 (s, 1H), 7.53 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 7.17 – 7.09 (m, 2H), 4.00 (s, 3H), 2.40 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, cdcl$_3$) δ 167.44, 142.18, 138.58, 137.56, 135.58, 135.39, 131.40, 131.36, 130.99, 129.99, 129.05, 128.89, 128.32, 127.80, 127.35, 126.78, 125.65, 52.41, 21.26, 20.59. Chemical Formula $C_{20}H_{18}O_2$. EI-MS $[M\cdot]^+$ calcd: 290.1307 found: 290.1314



4-(5-(4-(Trifluoromethoxy)phenyl)pyrimidin-2-yl)morpholine. Synthesized utilizing 4-(5-bromopyrimidin-2-yl)morpholine and 4-(trifluoromethoxy)phenylboronic acid acid according to general procedure A with no DIBAL pre-reduction (22h h, 130 mg, 80%, 0.1 mol% Pd). R_f = 0.58 in 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.53 (s, 2H), 7.51 – 7.46 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 3.89 – 3.77 (m, 8H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 161.30, 156.00, 148.76, 134.54, 127.36, 122.23, 121.86, 119.61, 66.96, 44.51. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.91 (J^1 C-F= 257.4 Hz). Chemical Formula $C_{15}H_{14}F_3N_3O_2$. EI-MS $[M\cdot]^+$ calcd: 325.1038 found: 325.1049

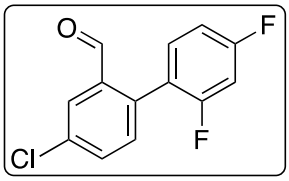


1-(2'-Methyl-[1,1'-biphenyl]-4-yl)ethan-1-one. Synthesized according to a modified general procedure B. EvanPhos$_2$Pd(OAc)$_2$ (1.5 mg, 0.0013 mmol), 4-bromoacetophenone (100 mg, 0.5 mmol), 2-methylphenylboronic acid (102 mg, 0.75 mmol), and potassium phosphate monohydrate (173 mg, 0.75 mmol) were added to a 4mL vial with an oblong stir bar. The vial was fitted with a septum and purged under a strong flow of argon for 5 minutes. Toluene (0.1 mL) then TPGS-750-M solution (0.9 mL) were added to the vial. The septum was removed and the vial was quickly sealed with a threaded screw-cap. The vial was placed in an alumnimum heating block and stirred for 1 hour. The reaction was cooled to r.t and extracted 3 x 1 mL EtOAc. The crude was purified by silica gel flash chromatography (104 mg, 99%, 0.25 mol% Pd). R_f = 0.43 in 20% 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 8.00 (m, 2H), 7.45 – 7.42 (m, 2H), 7.31 – 7.21 (m, 4H), 2.65 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 198.01, 147.09, 140.86, 135.70, 135.29, 130.66, 129.63, 129.59, 128.35, 128.03, 126.07, 26.83, 20.55. Chemical Formula $C_{15}H_{14}O$. EI-MS $[M\cdot]^+$ calcd: 210.1045 found: 210.1046



5-(Naphthalen-1-yl)pyrimidine. Synthesized according to a modified general procedure B. EvanPhos$_2$Pd(OAc)$_2$ (3.0 mg, 0.0025 mmol), 5-bromopyrimidine (79 mg, 0.5 mmol), naphthalene-1-boronic acid (129 mg, 0.75 mmol), and potassium phosphate monohydrate (173 mg, 0.75 mmol) were added to a 4mL vial with an oblong stir bar. The vial was fitted with a septum and purged under a strong flow of argon for 5 minutes. Toluene (0.1 mL) then TPGS-750-M solution (0.9 mL) were added to the vial. The septum was removed and the vial was quickly sealed with a threaded screw-cap. The vial was placed in an alumnimum heating block and stirred for 4.5 hours. The reaction was cooled to r.t and extracted 3 x 1 mL EtOAc. The crude was purified by silica gel flash chromatography (103 mg, quantitative, 0.5 mol % Pd). R_f = 0.14 in 20% 20% EtOAc/hexanes. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.31 (s, 1H), 8.90 (s, 2H), 7.96 (dd, *J* = 8.3, 3.8 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.49 (m, 3H), 7.43 (d, *J* = 7.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.78, 157.45, 134.48, 133.91, 132.54, 131.30, 129.57, 128.82, 127.89, 127.22, 126.58, 125.57, 124.69. Chemical Formula $C_{14}H_{10}N_2$. EI-MS $[M\cdot]^+$ calcd: 206.0844 found: 206.0849

IV. Catalyst Stability Study EvanPhos vs. SPhos.



Following the general procedure for catalyst stock solution preparation (no DIBAL pre-reduction) and general procedure A (0.5 mol % $Pd(OAc)_2$), three reactions for each ligand (SPhos and EvanPhos) based on stock solution age were set up utilizing 2-bromo-5-chloro-benzaldehyde and (2,4-difluorophenyl)boronic acid (1.1 equiv). Conversions were determined by GCMS at 1h (SPhos) or 2 h (EvanPhos) based on the relative ratio of starting bromide to product. SPhos catalyst age: 0.25 min 100%, 6 h 95%, 22 h 36%. EvanPhos catalyst age : 15 min 96%, 6 h 96%, 22 h 96%.

V. E Factor and Recycling Study

The initial reaction was set up according to the general procedure. After 2 h, the aqueous solution was extracted three times with MTBE (0.75 mL total), placed in a 10 mL round bottom flask, and the solvent was removed via rotary evaporation. The crude product was purified by flash column chromatography as described previously using EtOAc/hexane to provide the desired compound.

E Factor calculation:
Note: density of MTBE = 0.74 g/mL, toluene = (0.867 g/mL)

$$\textbf{E Factor} = \frac{\textbf{Waste (mg)}}{\textbf{Product (mg)}}$$

$$\frac{(\mathbf{0.75\ mL\ MTBE})\left(\mathbf{0.74}\,\frac{\mathbf{g}}{\mathbf{mL}}\right) + (\mathbf{0.10\ mL\ toluene})(\mathbf{0.867}\,\frac{\mathbf{g}}{\mathbf{mL}})}{\mathbf{0.136\ g}} = \mathbf{4.7}$$

Re-use of surfactant solution. The vial was sparged with argon and then sequentially charged with bromide (0.5 mmol), boronic acid (0.625 mmol), and tribasic potassium phosphate monohydrate (0.5 mmol), and catalyst solution (0.1 mL). The headspace of the vial was flushed with argon then capped, sealed, and stirred at 45 °C according to the general procedure.

First run: 93% yield
Second run: 95% yield
Third run: 90% yield

Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

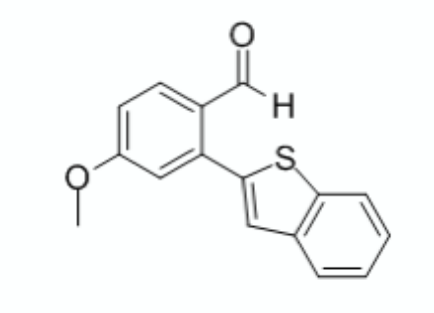
CIB001

Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILJO3-001-EXP088 **Test #:** 1 **Received:** 05/30/2017 **Completed:** 06/01/2017

ICP-OES: Palladium = 178 ppm

Services
ICP-OES Synthesized with 0.5 mol% Pd (5000 ppm)



Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

CIB001

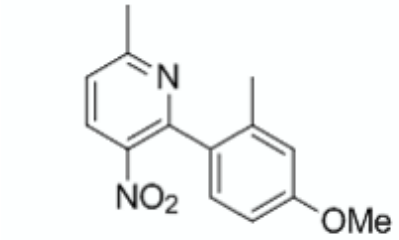
Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILLJO3-001-EXP093 **Test #:** 1 **Received:** 08/04/2017 **Completed:** 08/08/2017

ICP-OES: Palladium = 10 ppm

Services
ICP-OES

Synthesized with 0.1 mol % Pd (1000 ppm)



Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

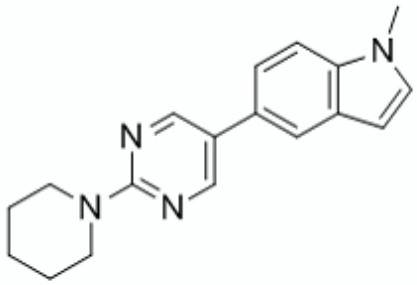
CIB001

Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILLJO3-001-EXP094 **Test #:** 1 **Received:** 08/04/2017 **Completed:** 08/08/2017

ICP-OES: Palladium = 2 ppm

Services
ICP-OES Synthesized with 0.1 mol% Palladium (1000 ppm)



Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

CIB001

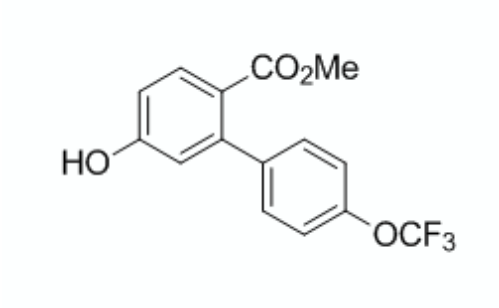
Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILLJO3-001-EXP095 **Test #:** 1 **Received:** 08/04/2017 **Completed:** 08/08/2017

ICP-OES: Palladium = < 1 ppm

Services
ICP-OES

Synthesized with 0.1 mol% Palladium (1000 ppm)



Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

CIB001

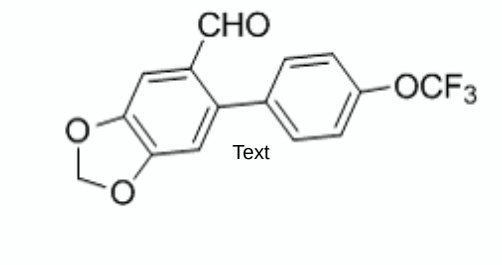
Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILLJO3-001-EXP096 **Test #:** 1 **Received:** 08/04/2017 **Completed:** 08/08/2017

ICP-OES: Palladium = 5 ppm

Services
ICP-OES

Synthesized with 0.25 mol% Palladium (2500 ppm)



Robertson Microlit Laboratories
1705 U.S. Highway 46 / Suite 1D / Ledgewood, NJ 07852 / (973) 966-6668 / Fax (973) 966-0136
www.robertson-microlit.com results@robertson-microlit.com

CIB001

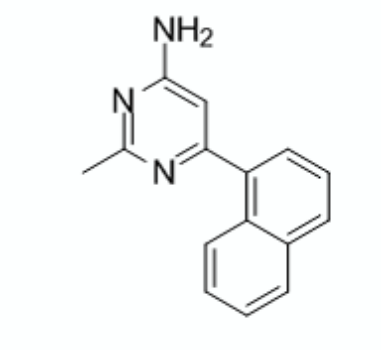
Min-Kyu Cho
Novartis Institute for Biomedical Research
250 Mass. Ave.
Cambridge, Massachusetts 02139

Sample #: REILJO3-001-EXP084 **Test #:** 1 **Received:** 05/30/2017 **Completed:** 06/01/2017

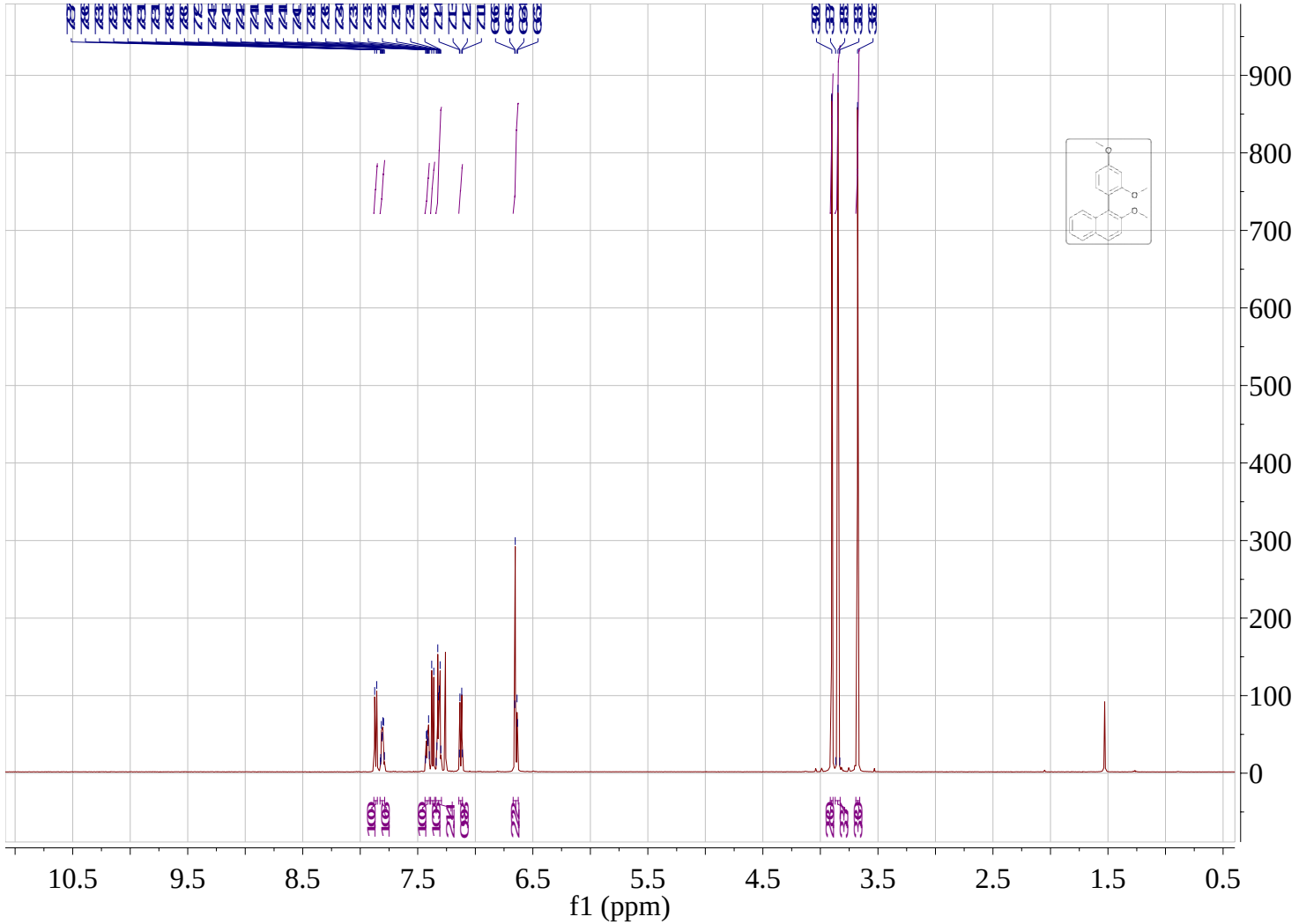
ICP-OES: Palladium = 211 ppm

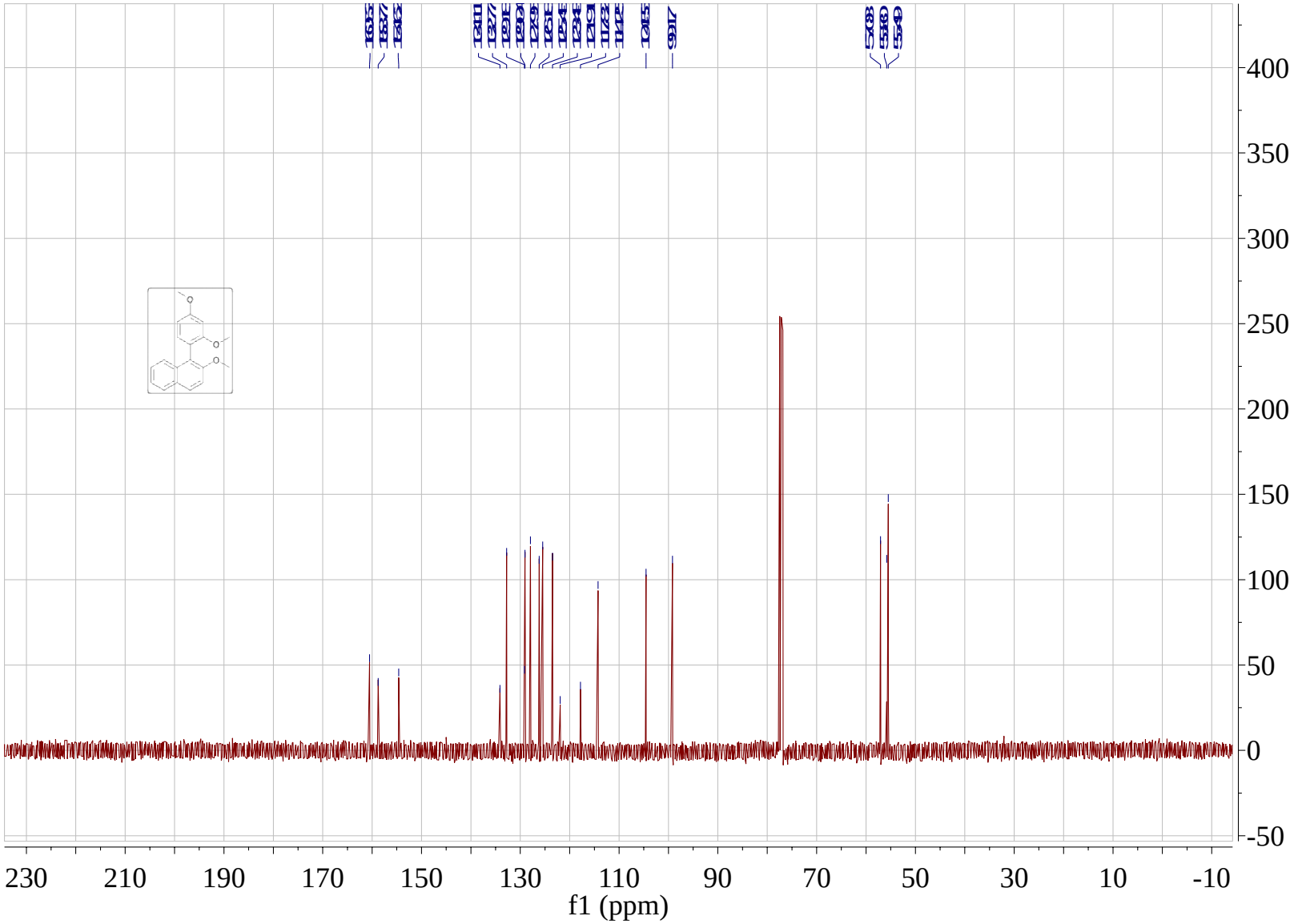
Services
ICP-OES

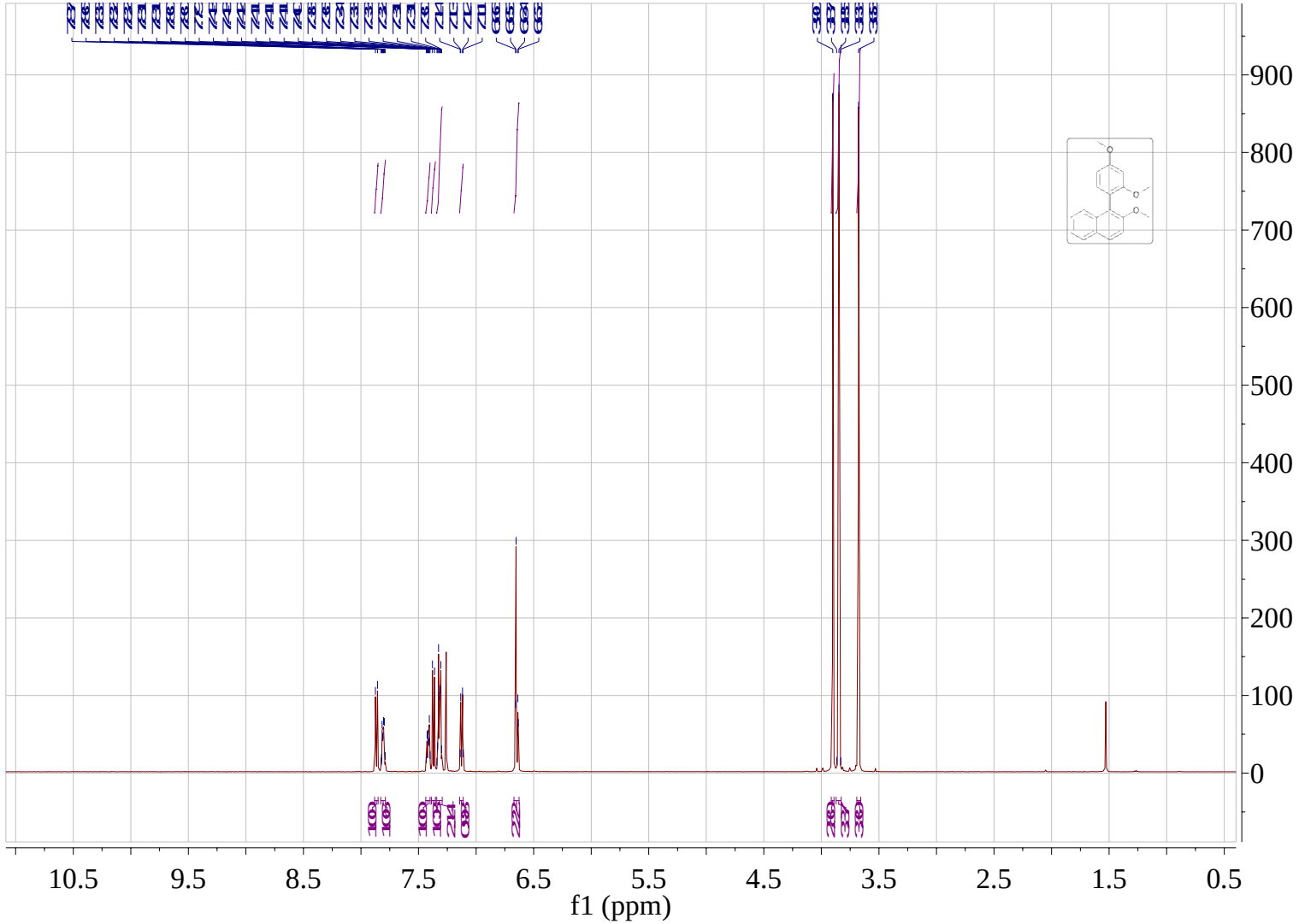
Synthesized with 0.5 mol% Palladium (5000 ppm)

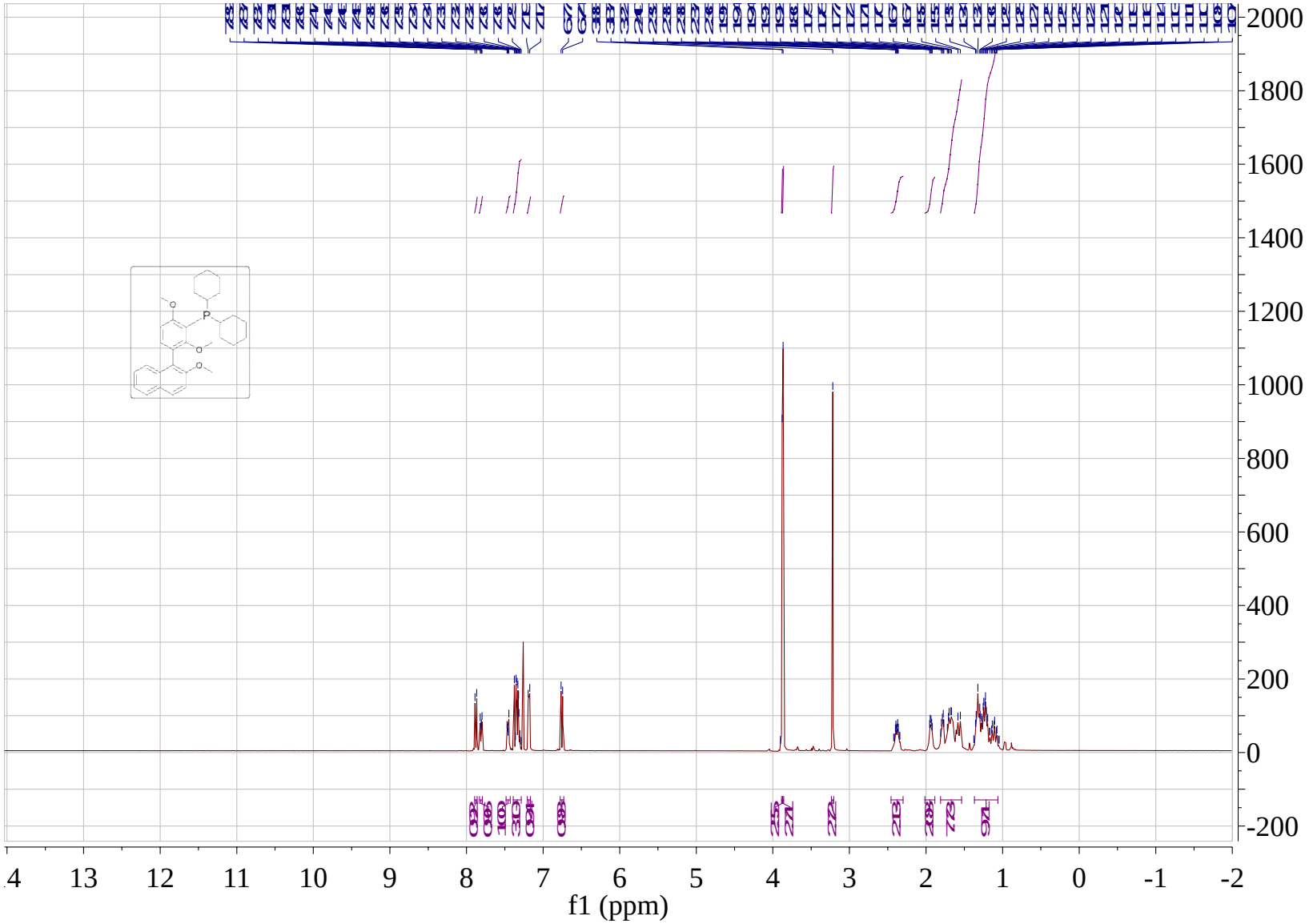


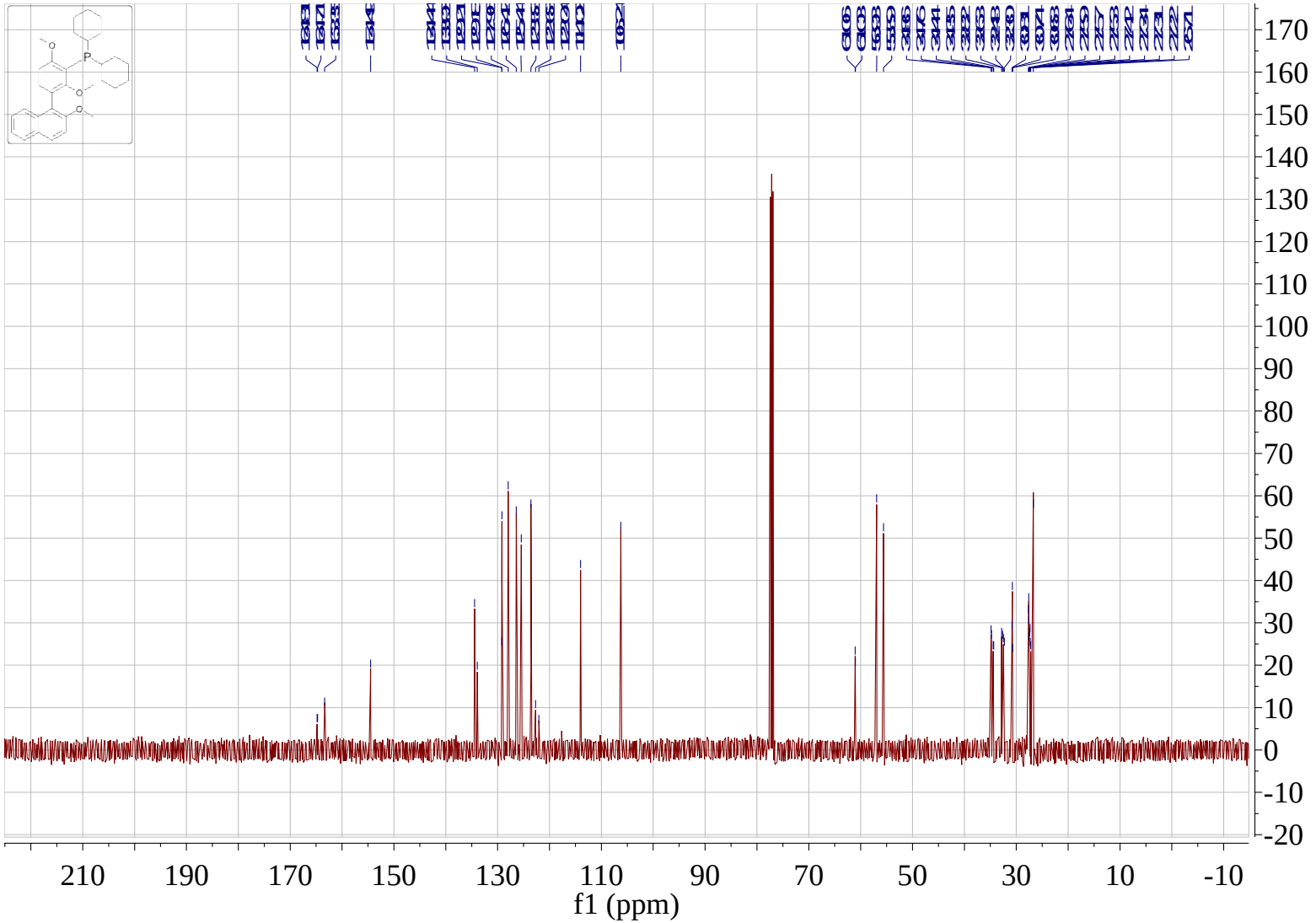
I. ^{1}H, ^{13}C, ^{31}P, and ^{19}F NMR of synthesized products

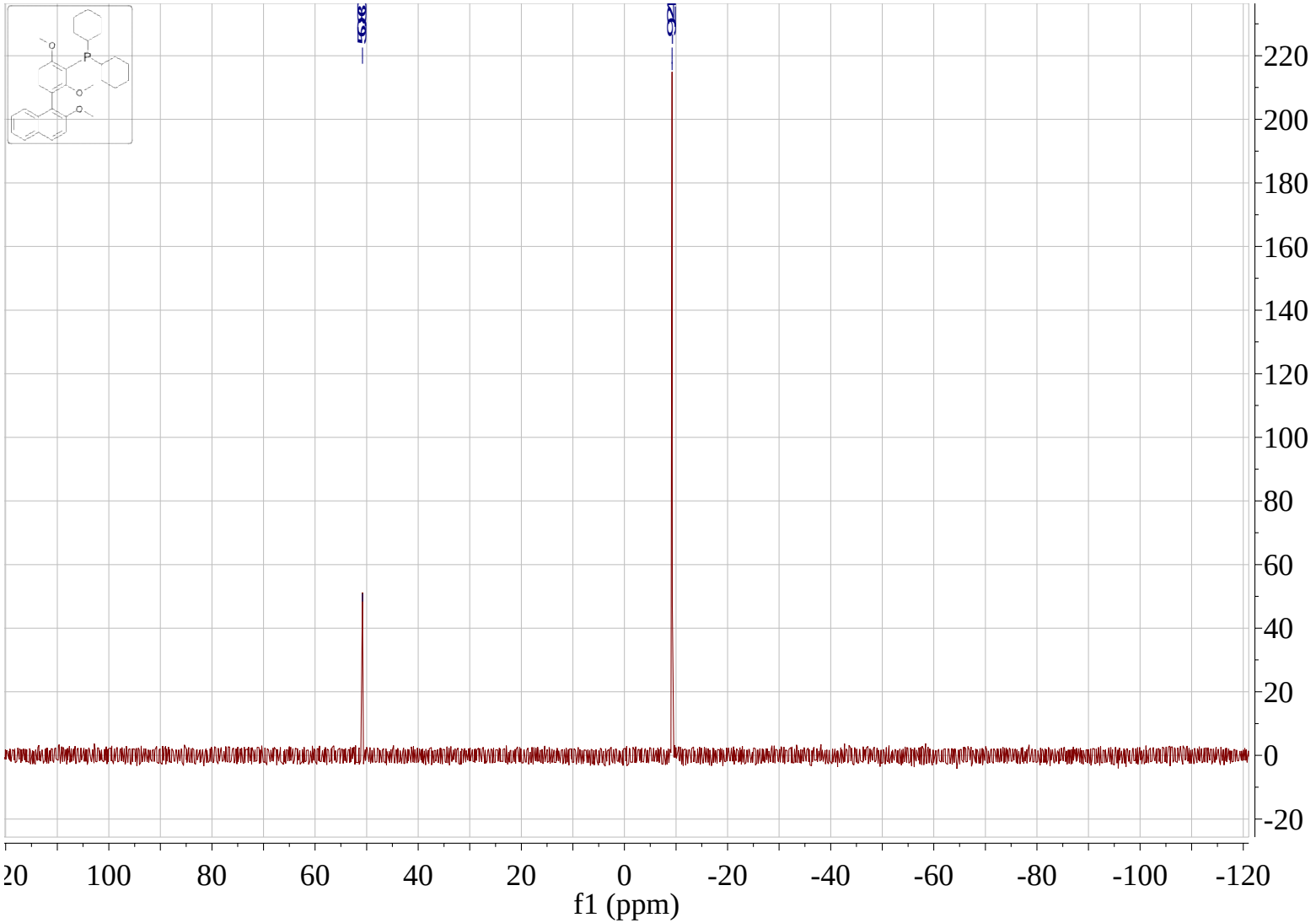


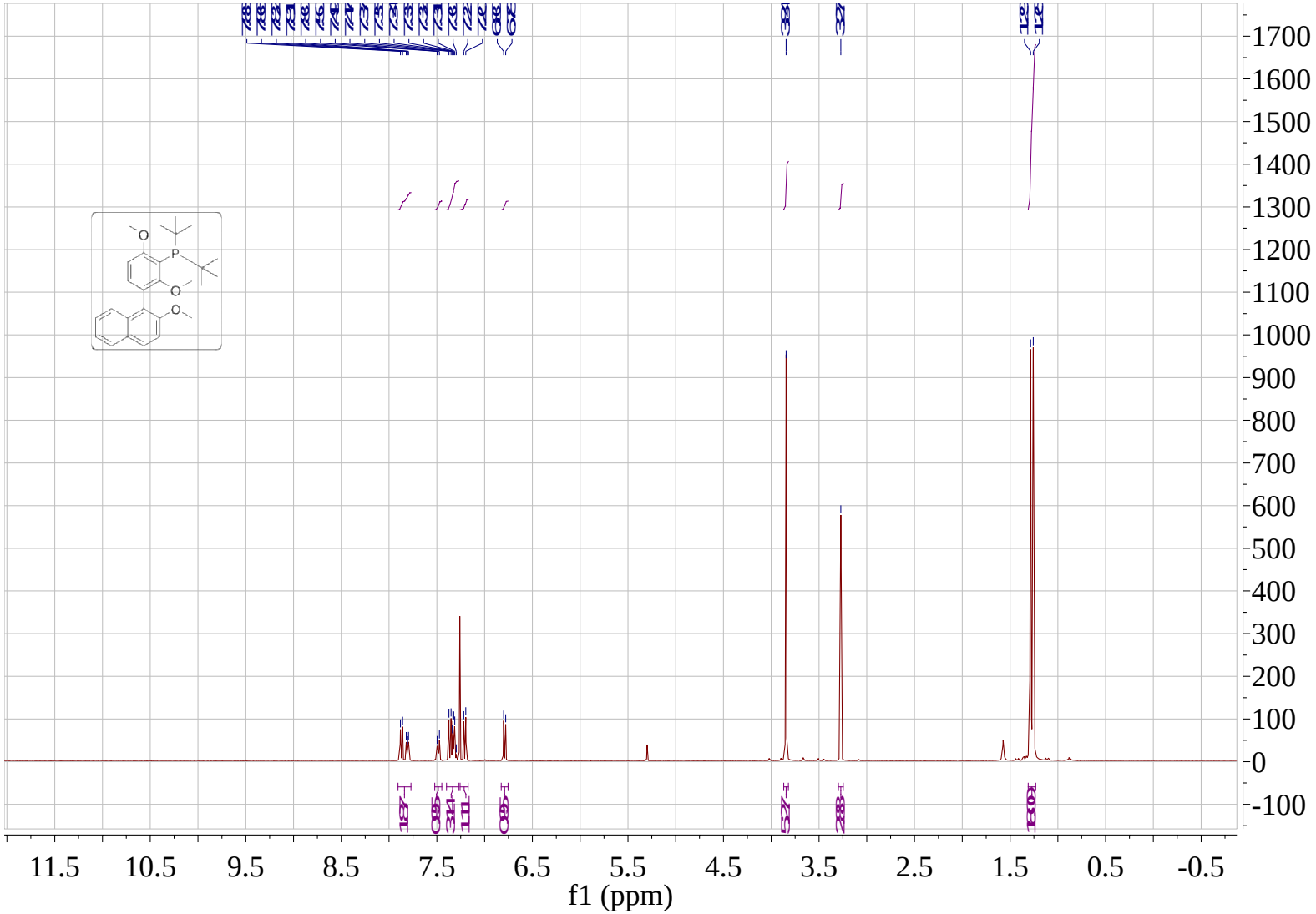

f1 (ppm)

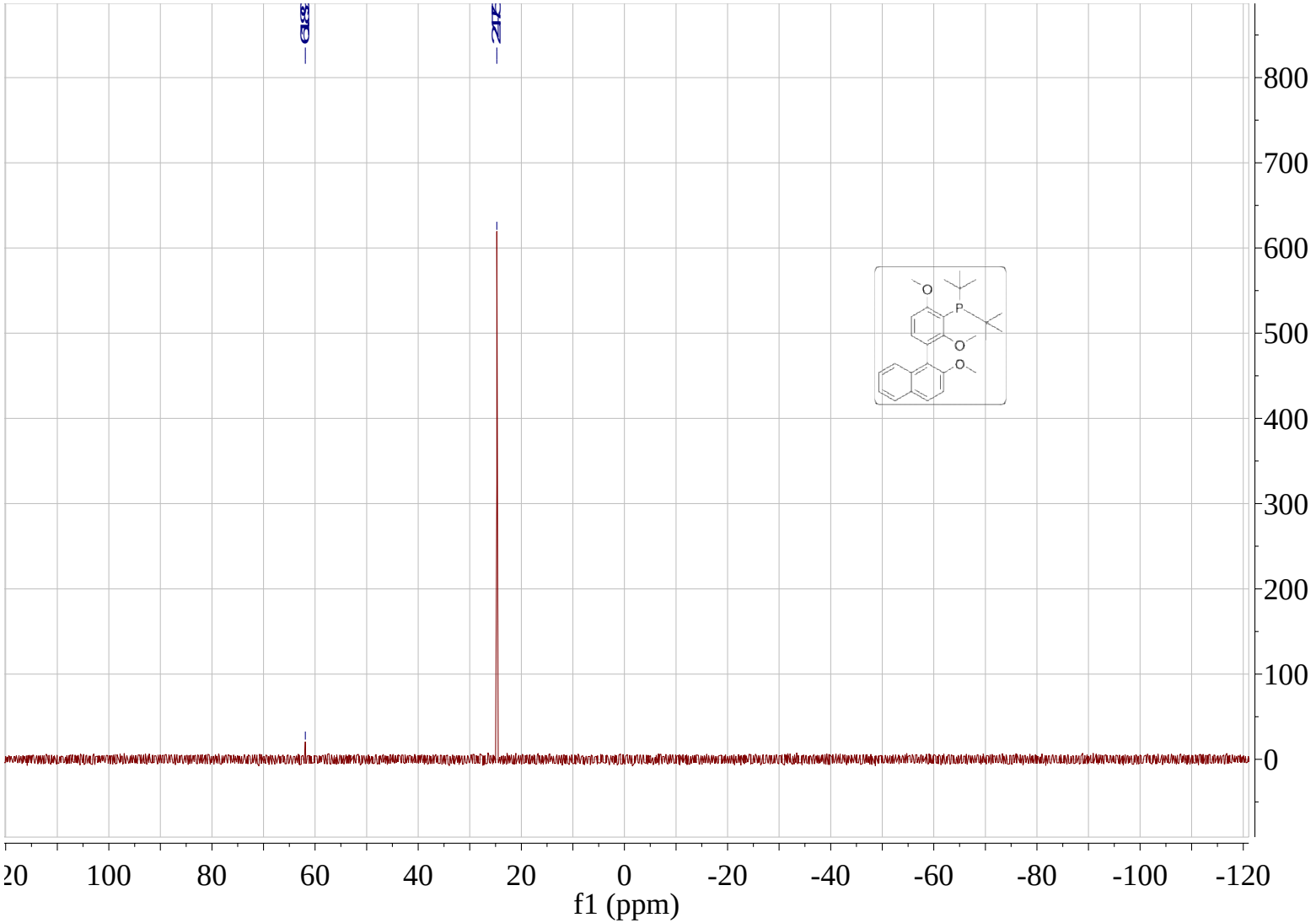

900
800
700
600
500
400
300
200
100
0
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

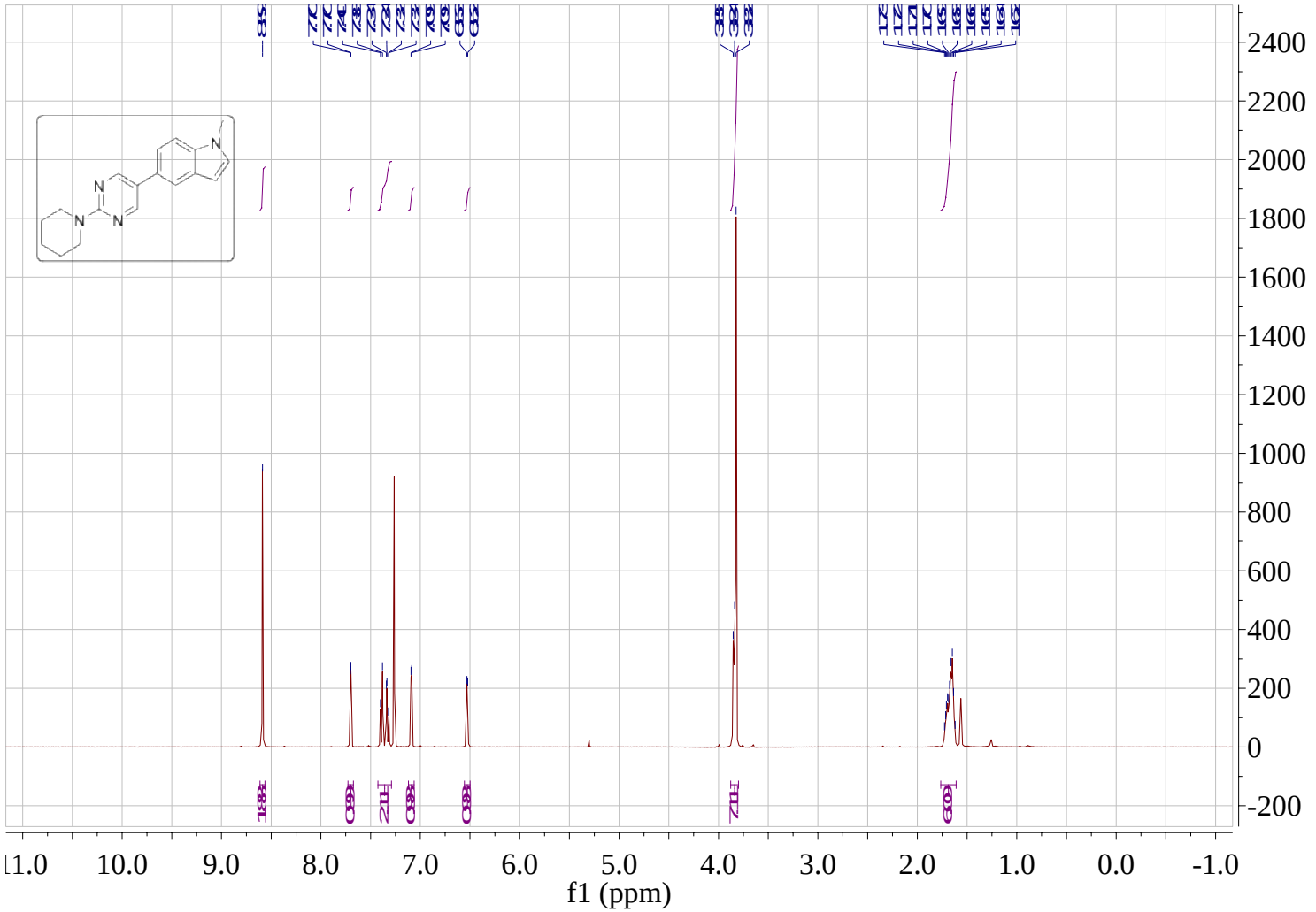

2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

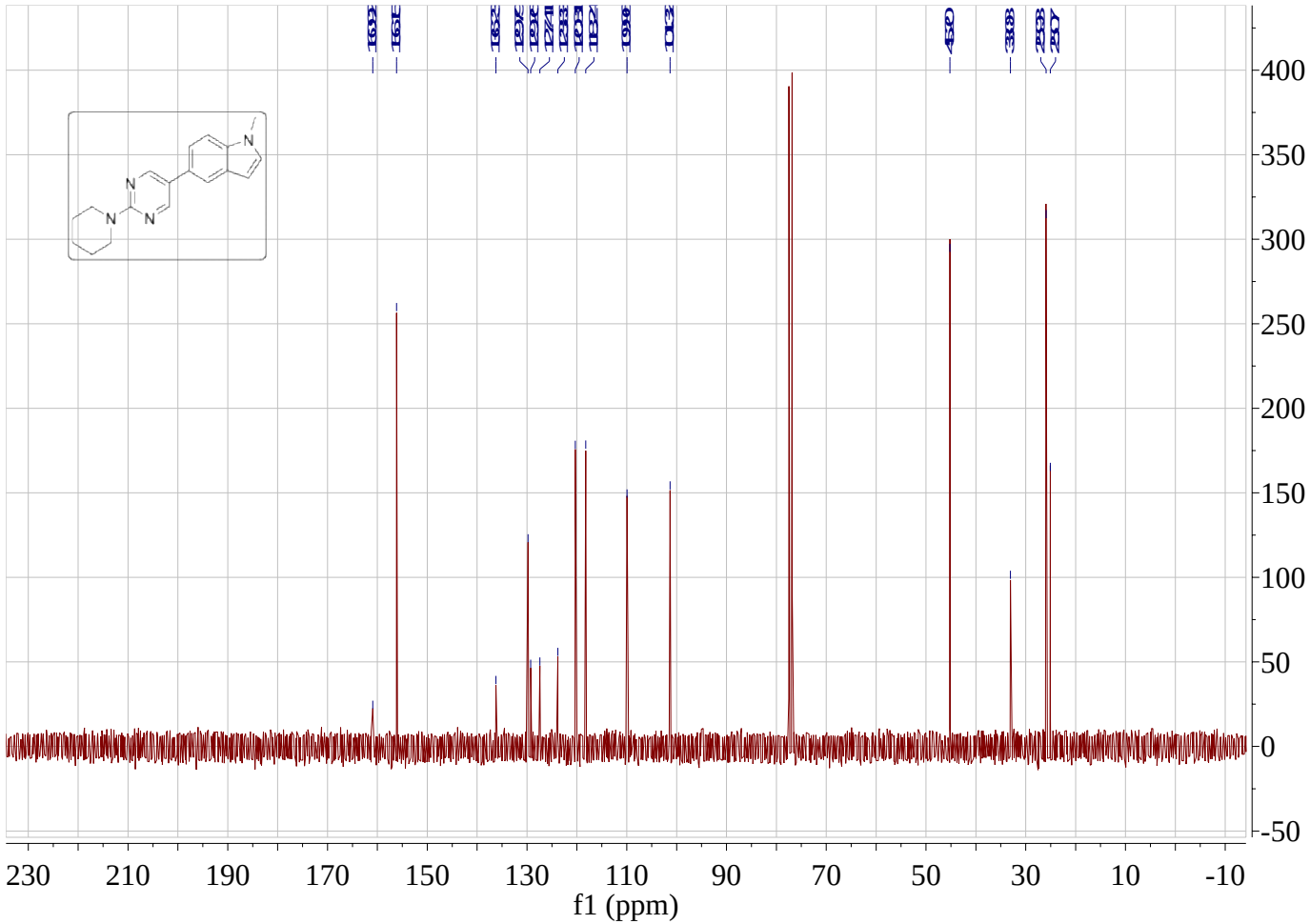

220
200
180
160
140
120
100
80
60
40
20
0
-20
20
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
f1 (ppm)

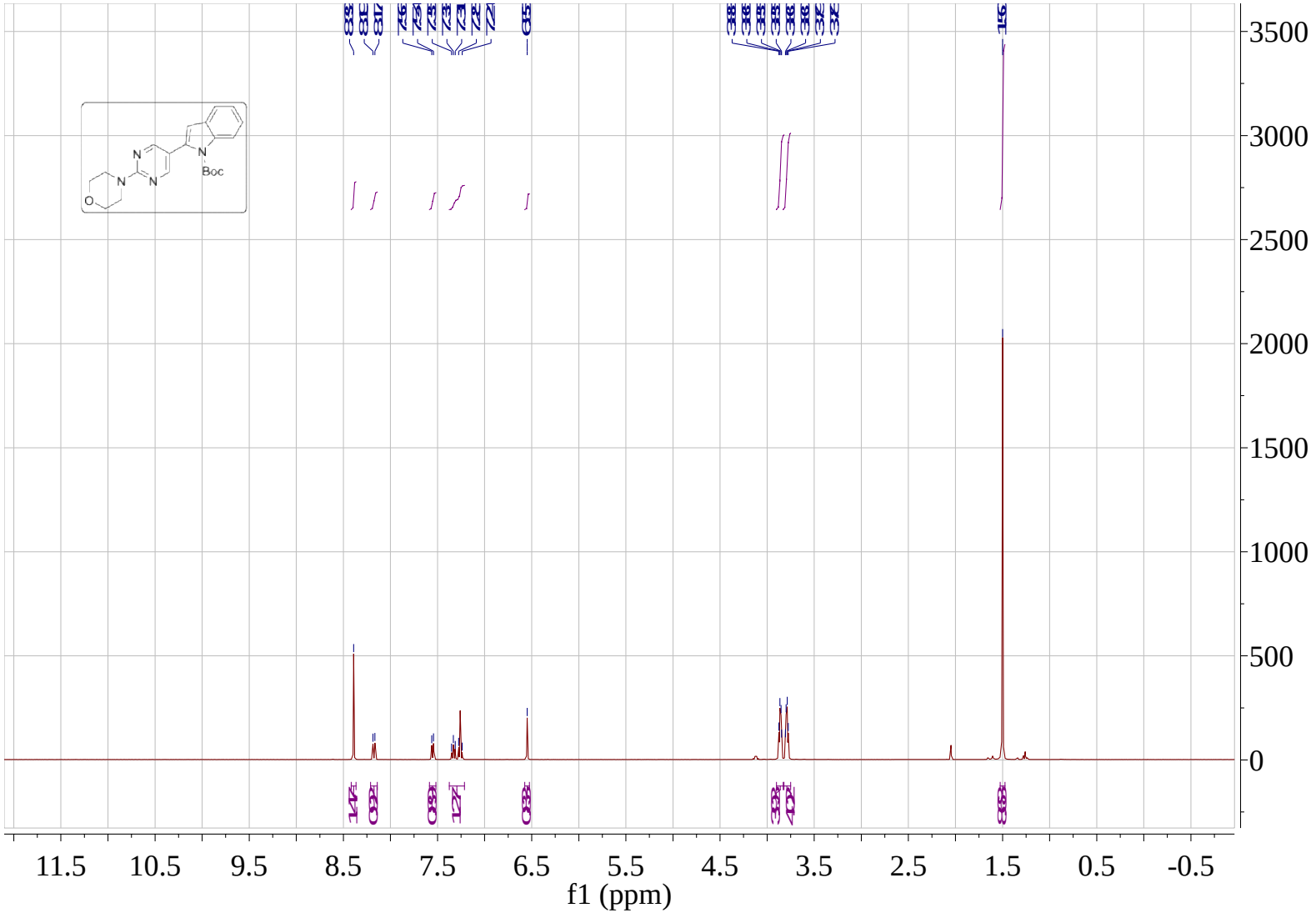

1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

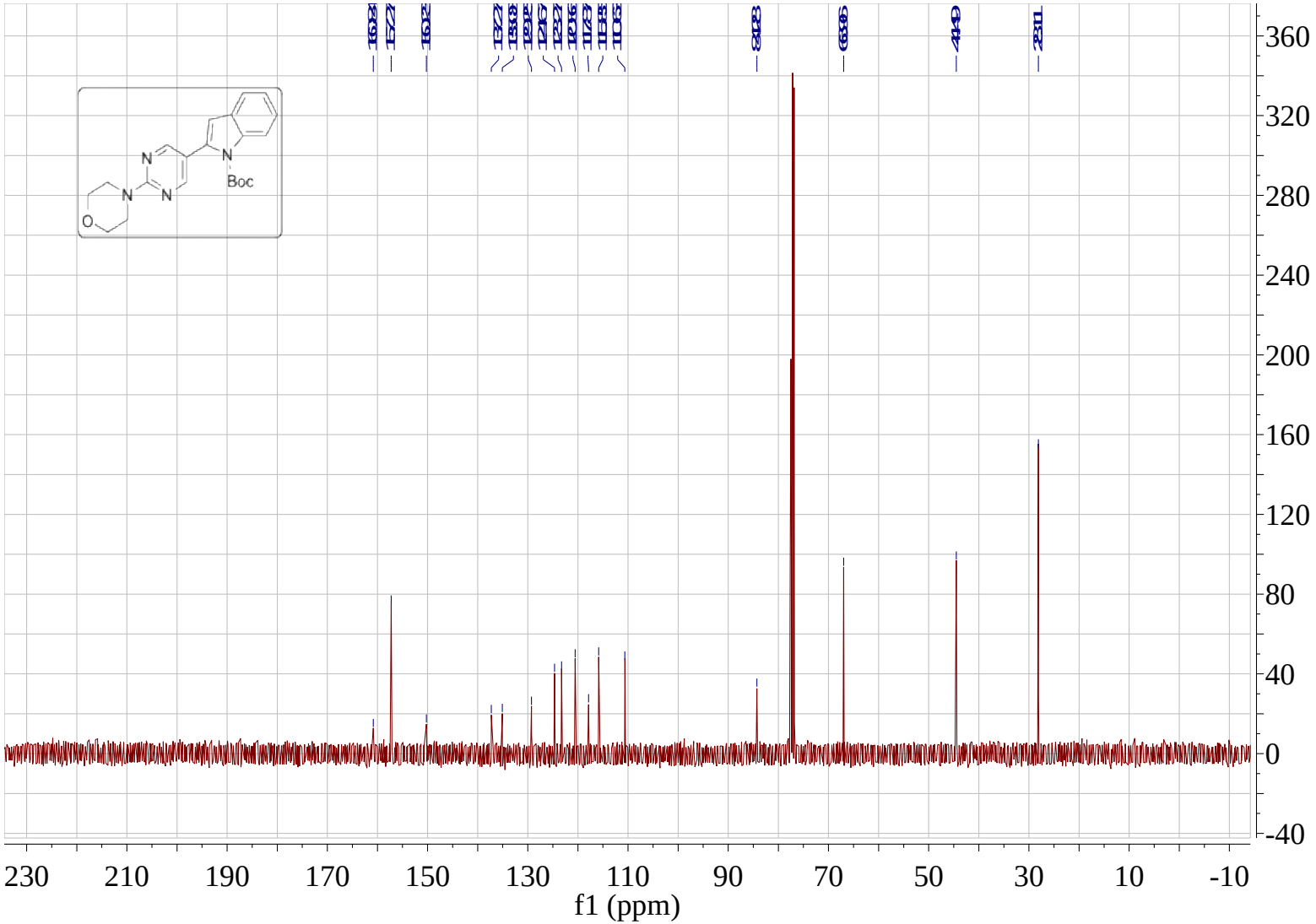

800
700
600
500
400
300
200
100
0
20
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
f1 (ppm)

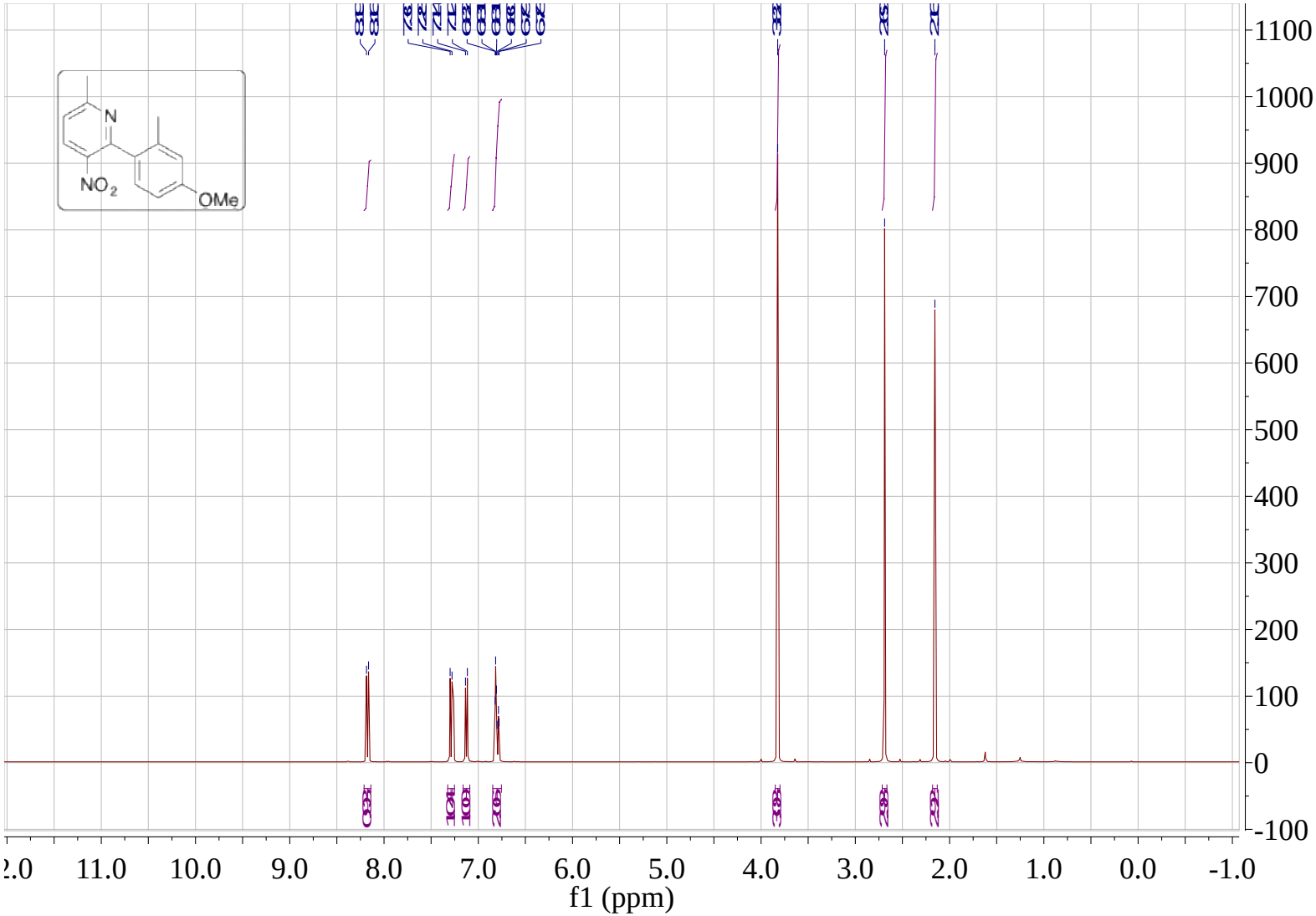

2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

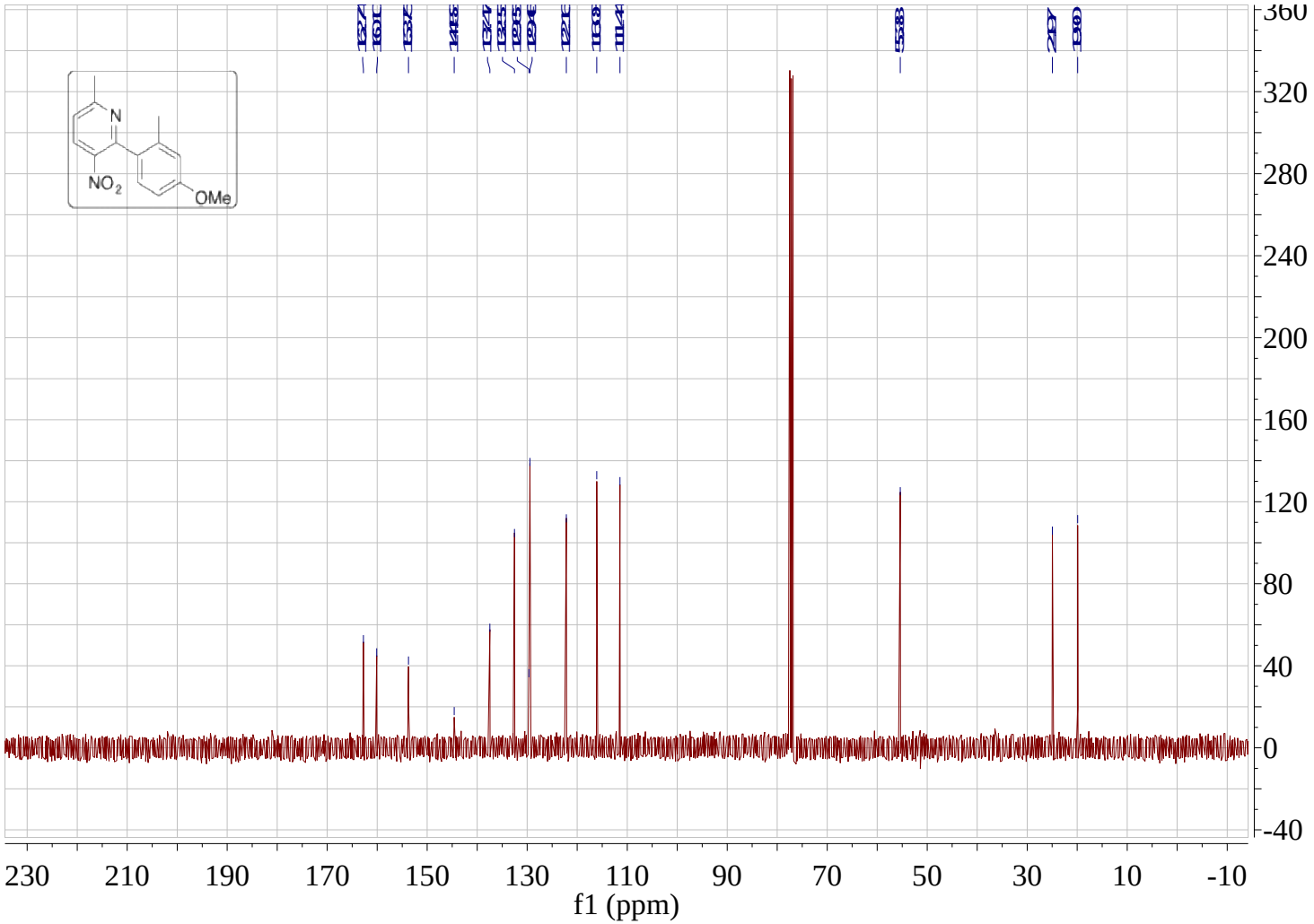
ts

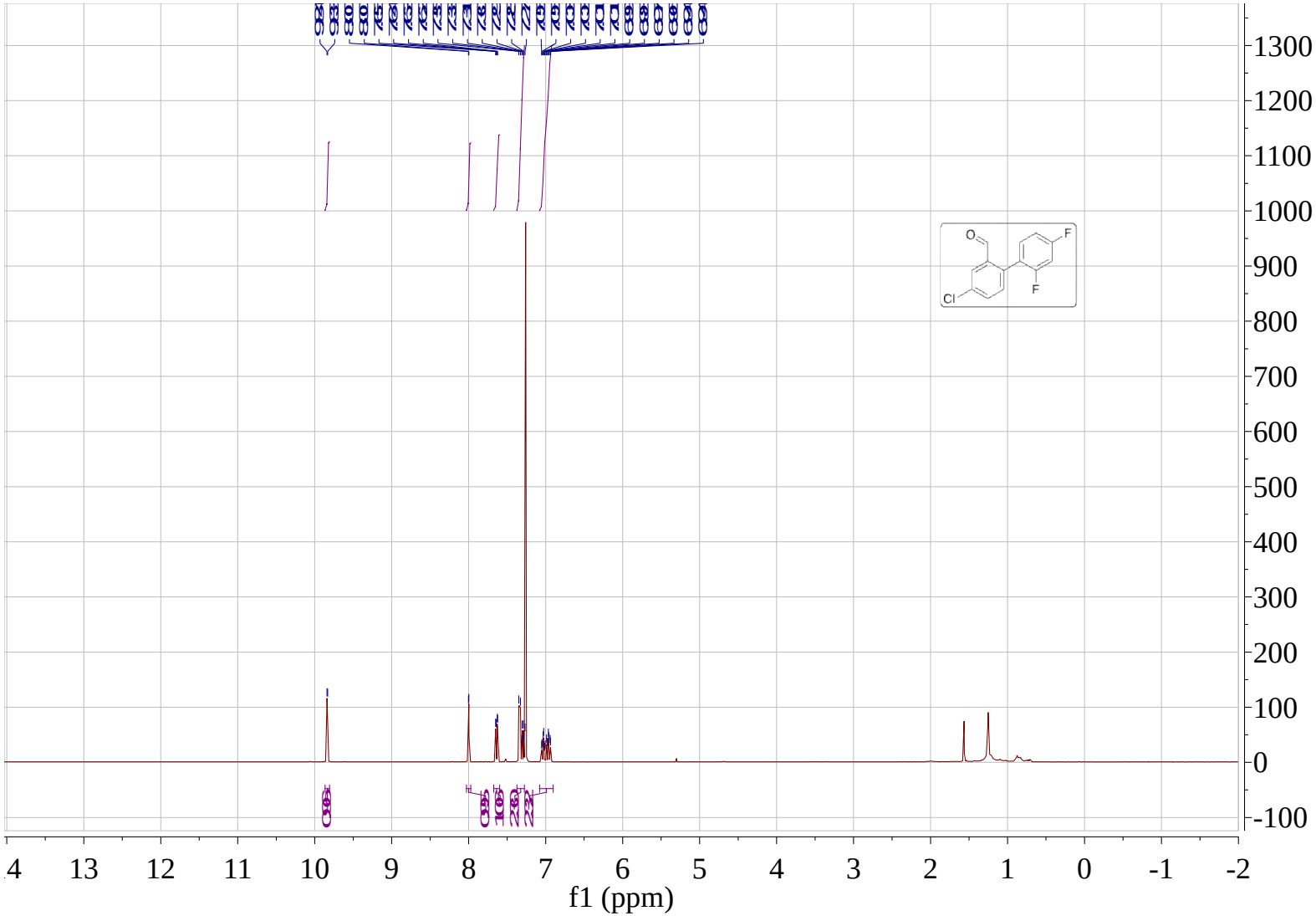

400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

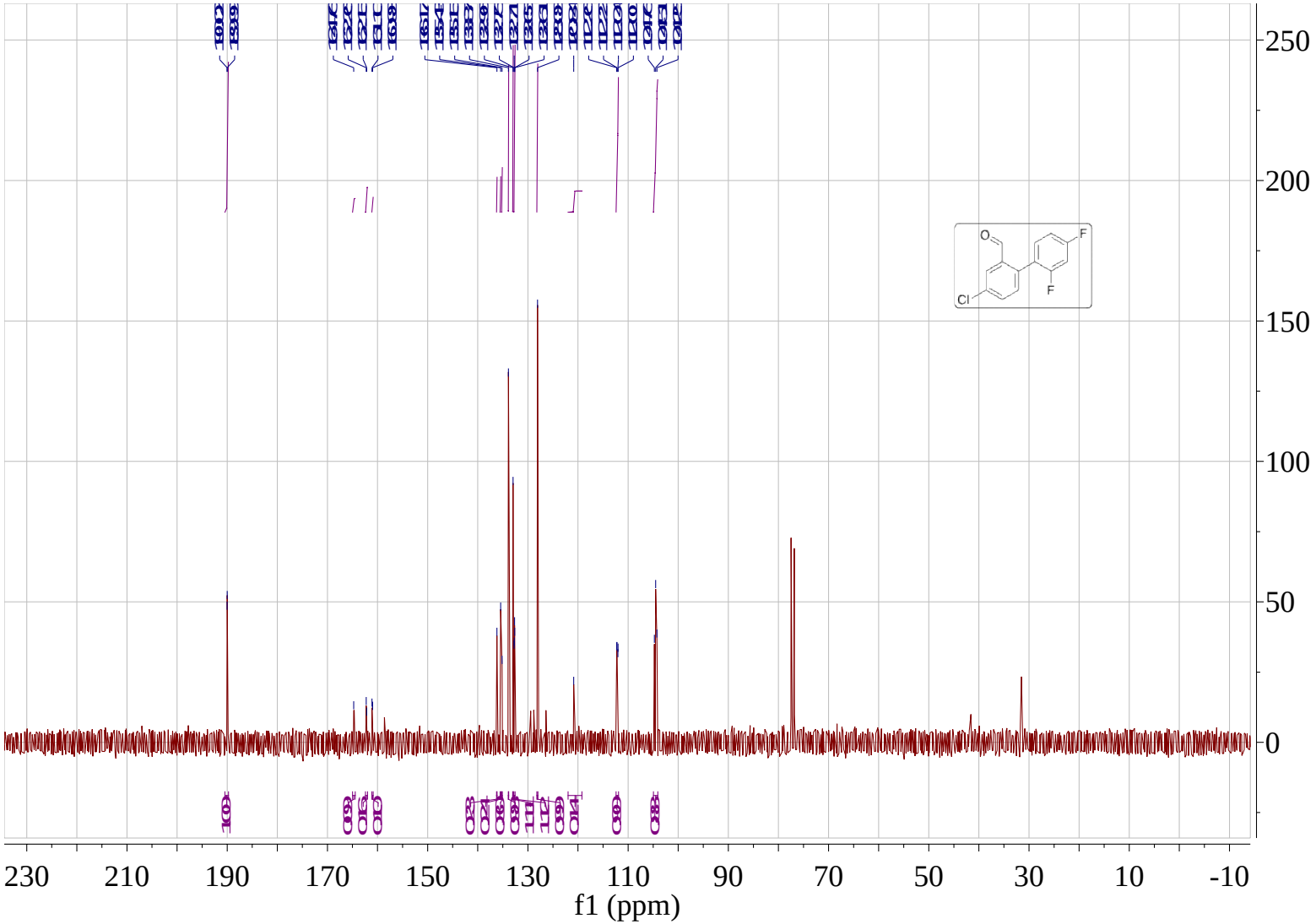

Boc
3500
3000
2500
2000
1500
1000
500
0
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

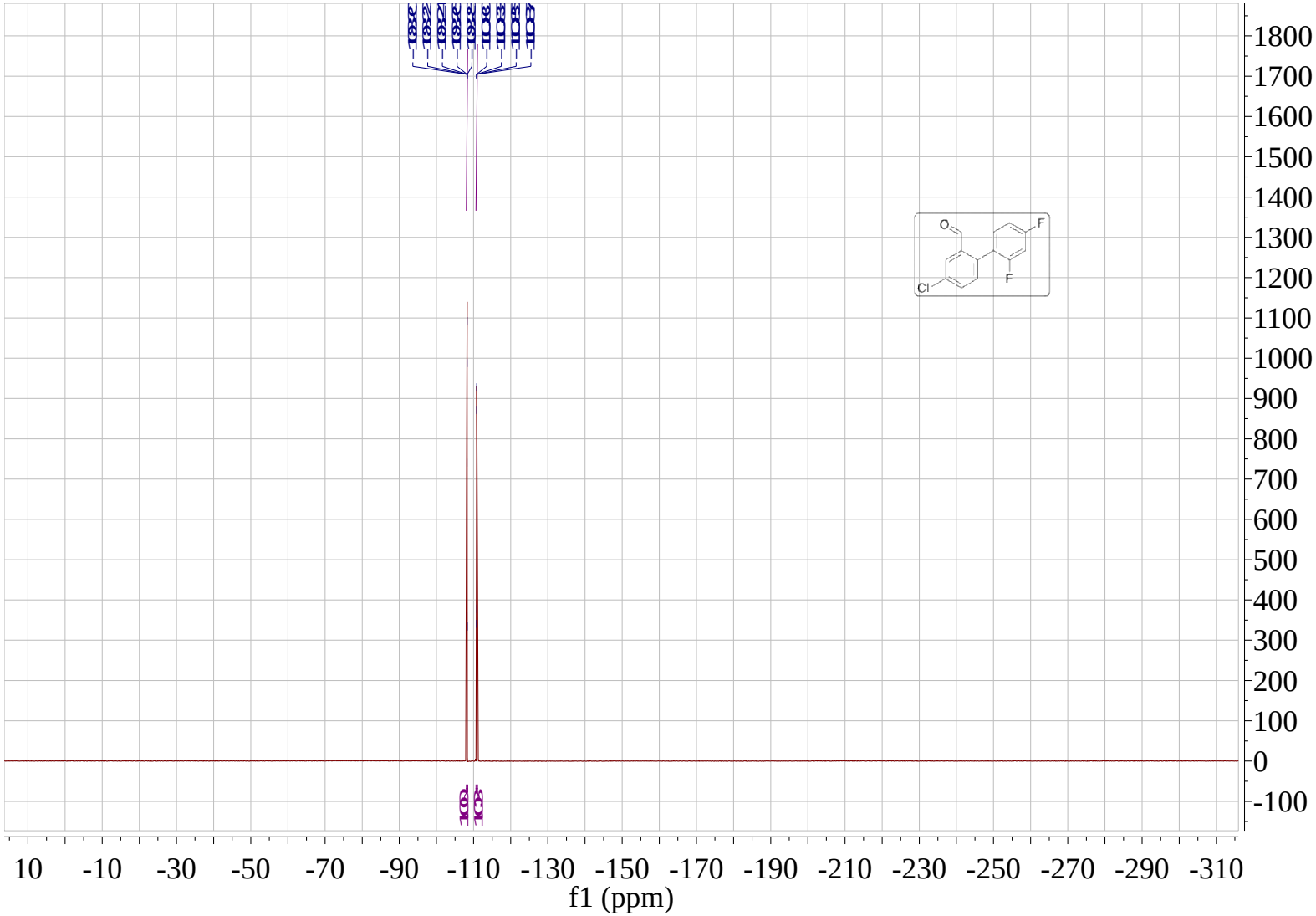

Boc
N
N
N
N
O
360
320
280
240
200
160
120
80
40
0
-40
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

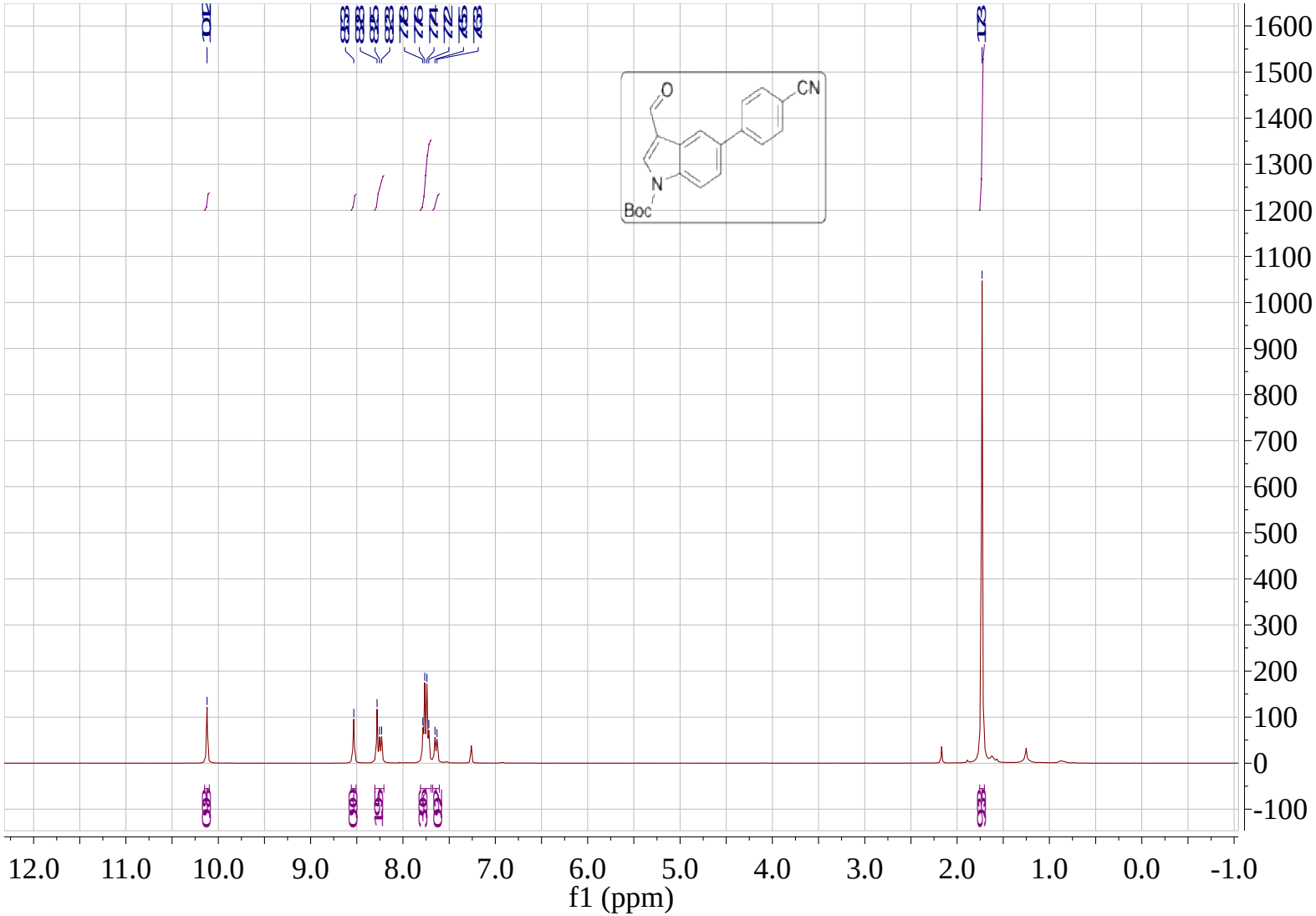

N
NO2
OMe
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

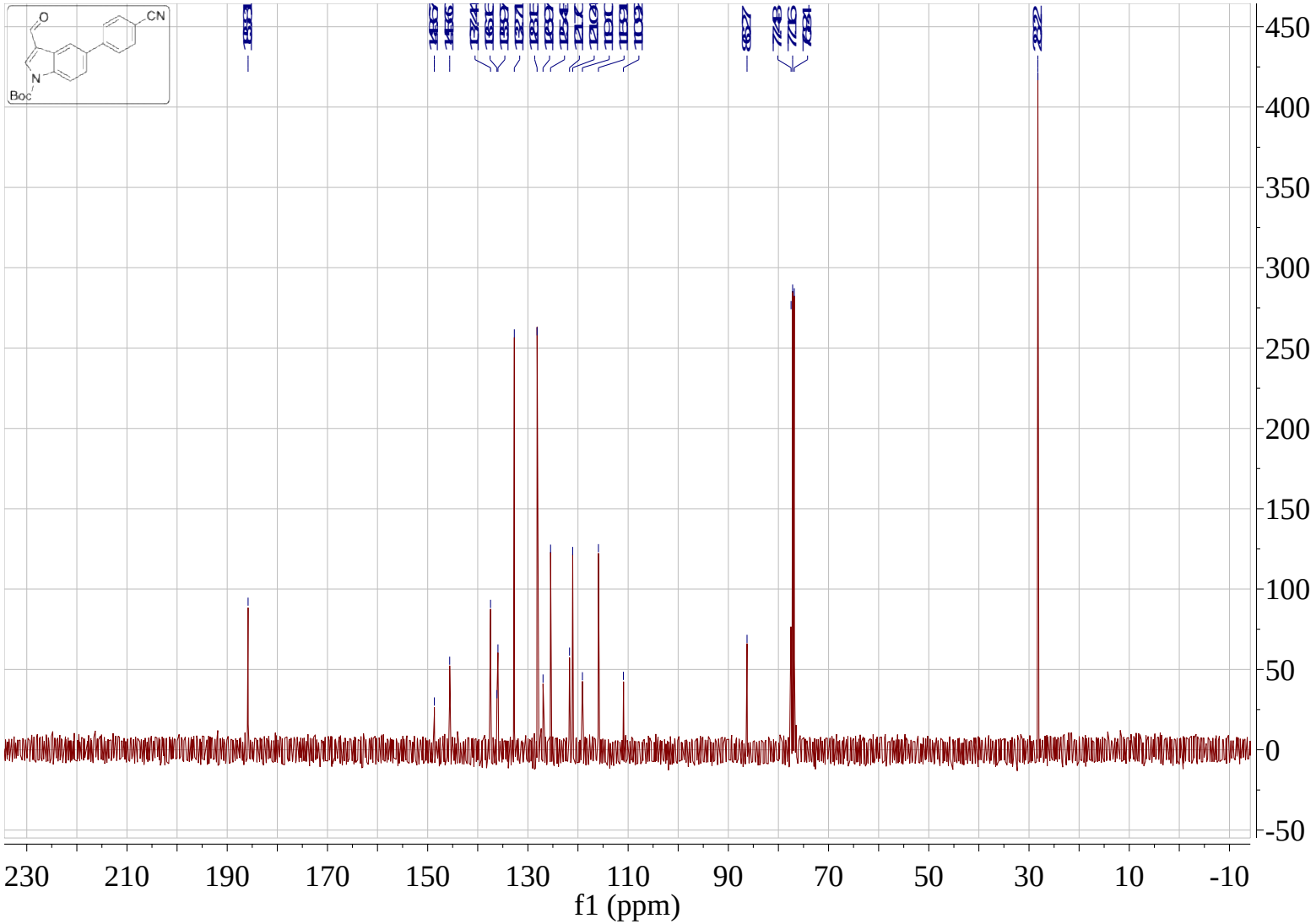

N
NO2
OMe
55.83
29.7
19.0
360
320
280
240
200
160
120
80
40
0
-40
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

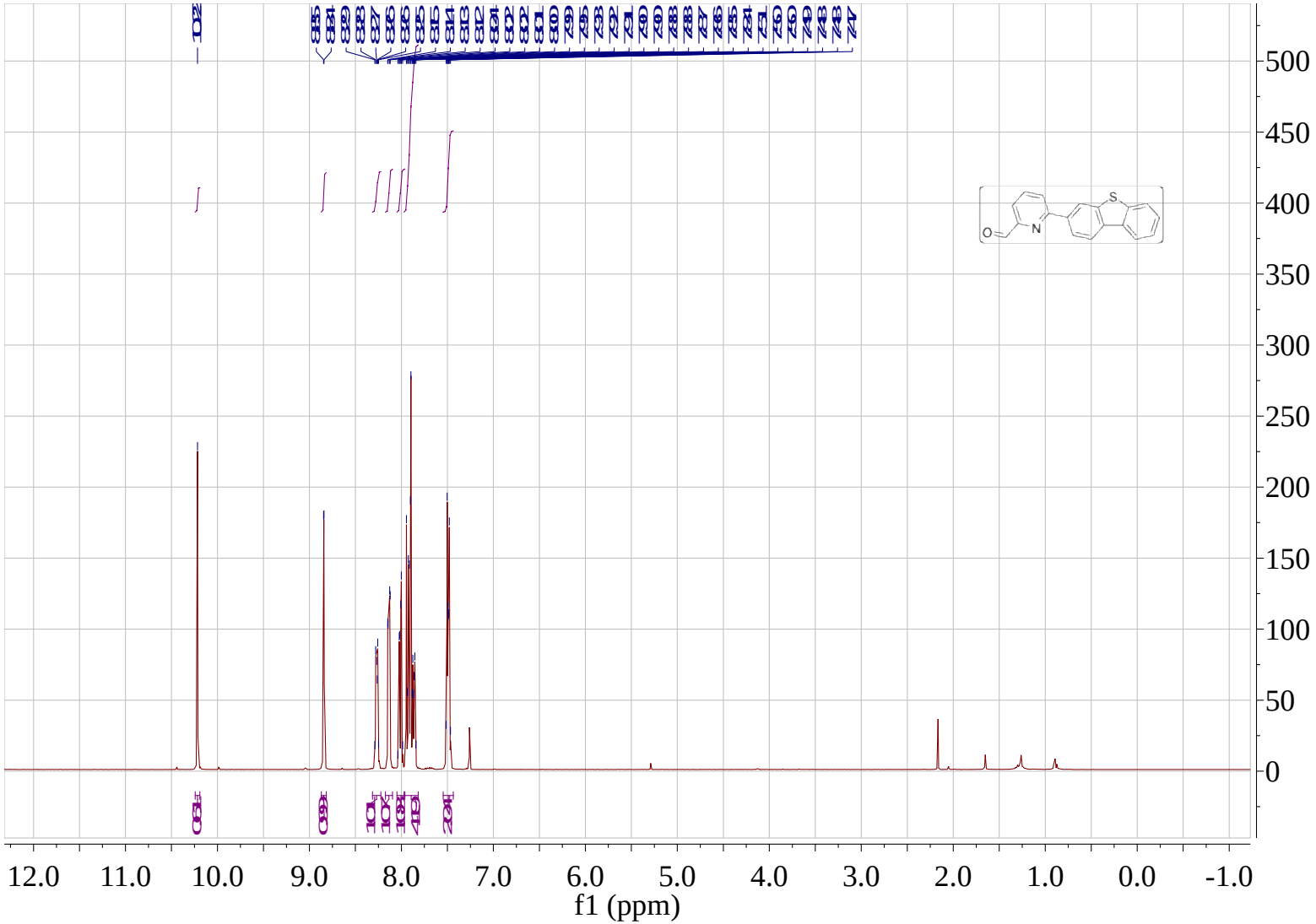

1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
O
F
Cl
F
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

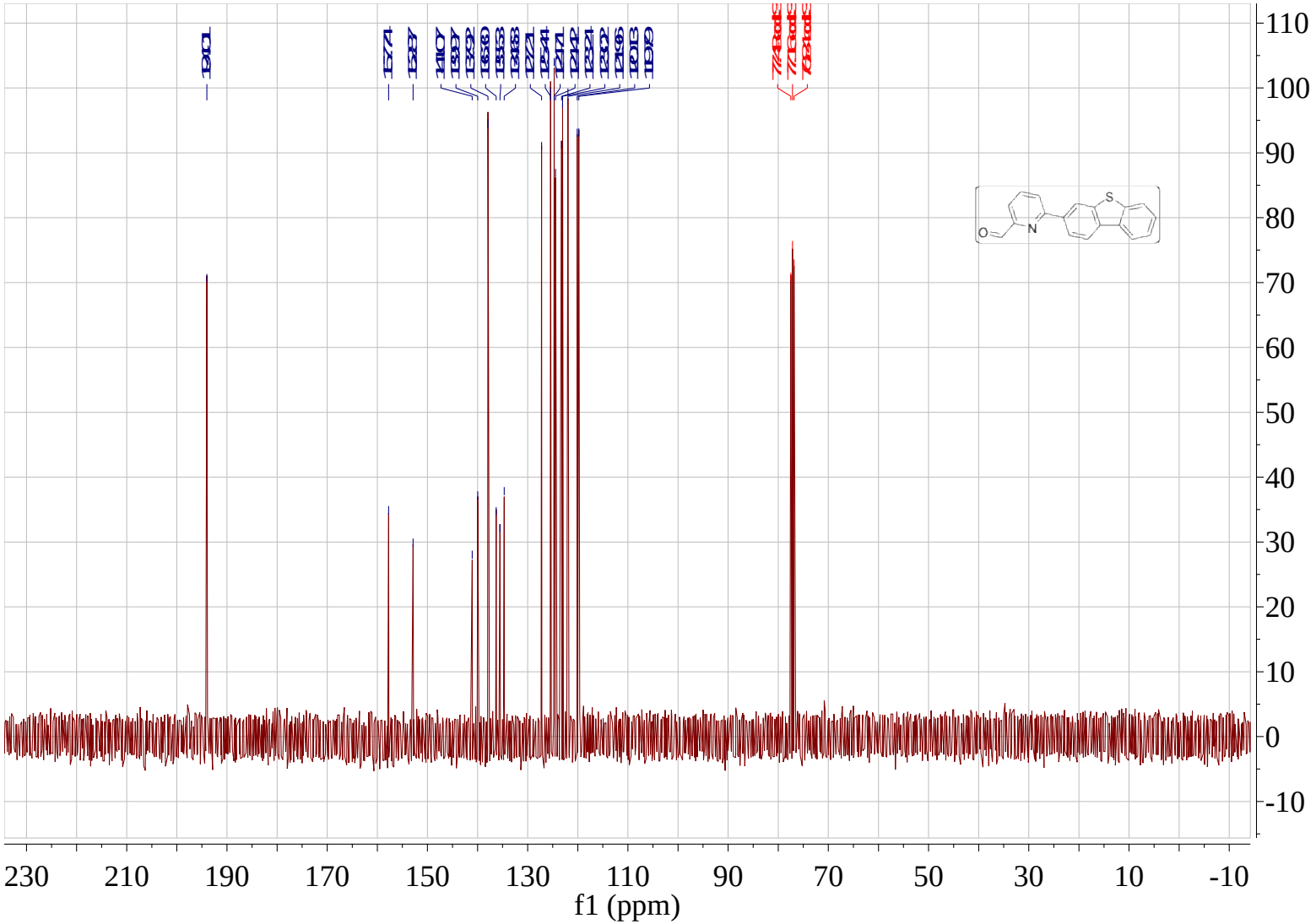

O
F
Cl
F
250
200
150
100
50
0
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

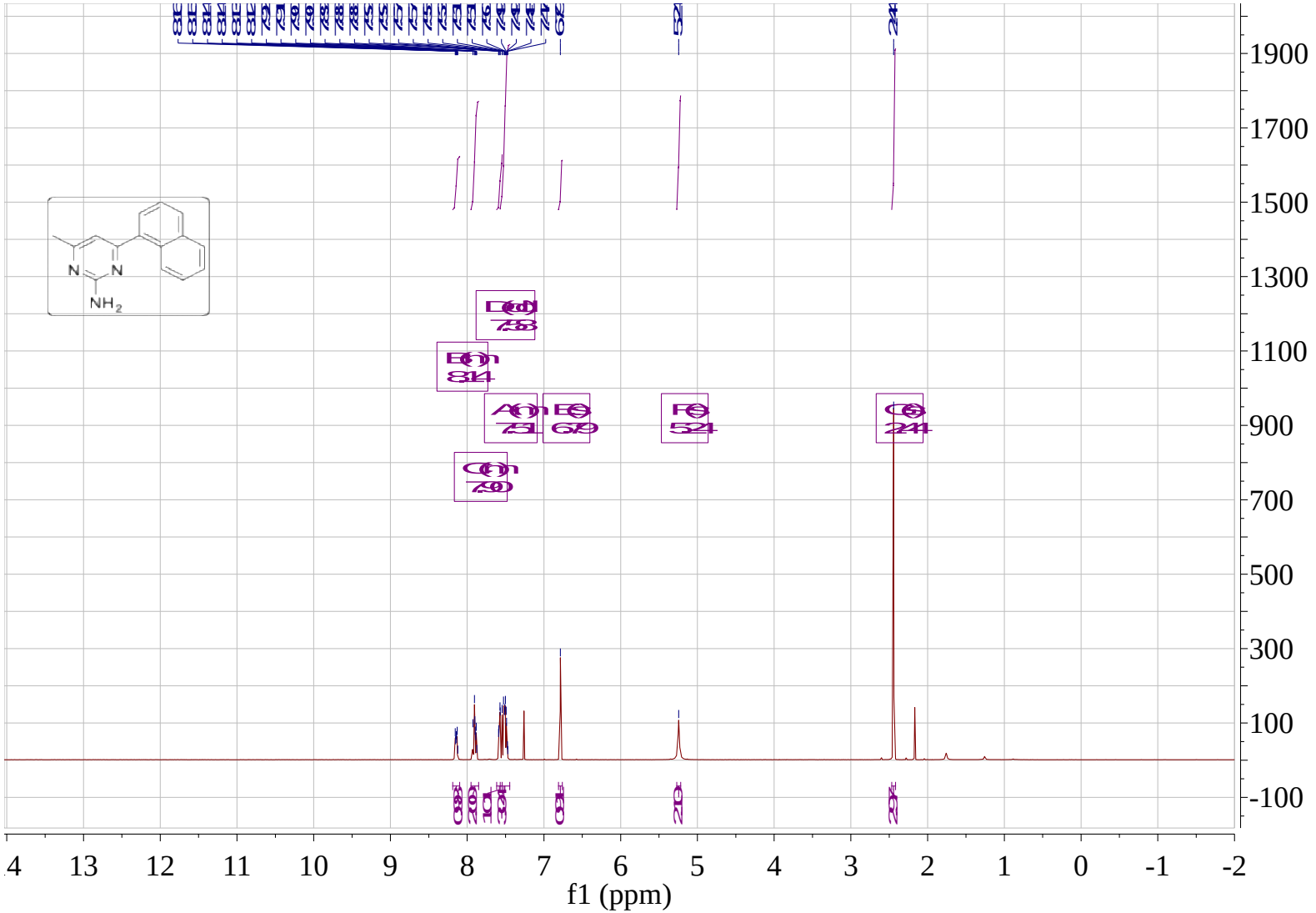

1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
-310
f1 (ppm)
O
F
Cl
F

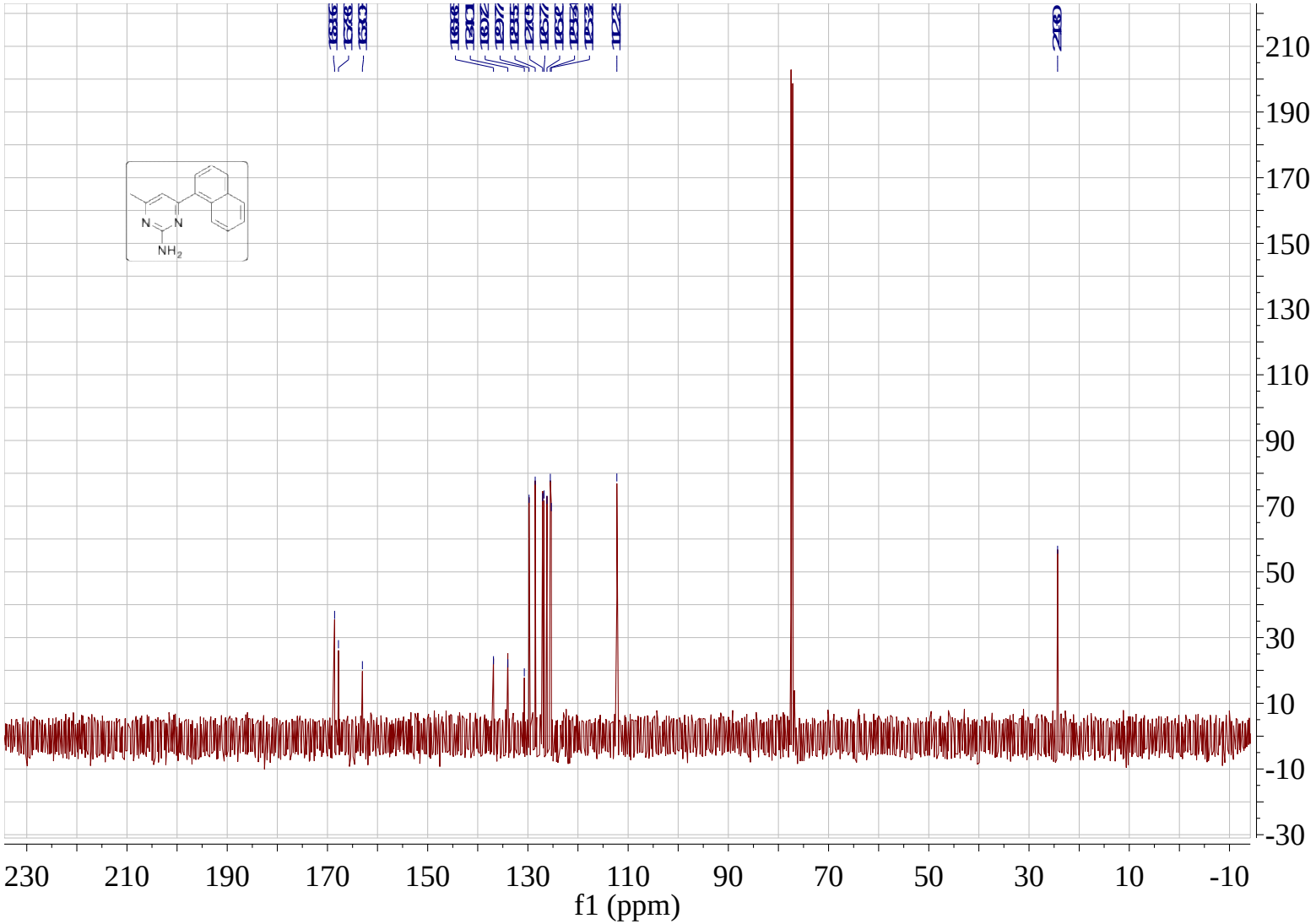

O
CN
N
Boc
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

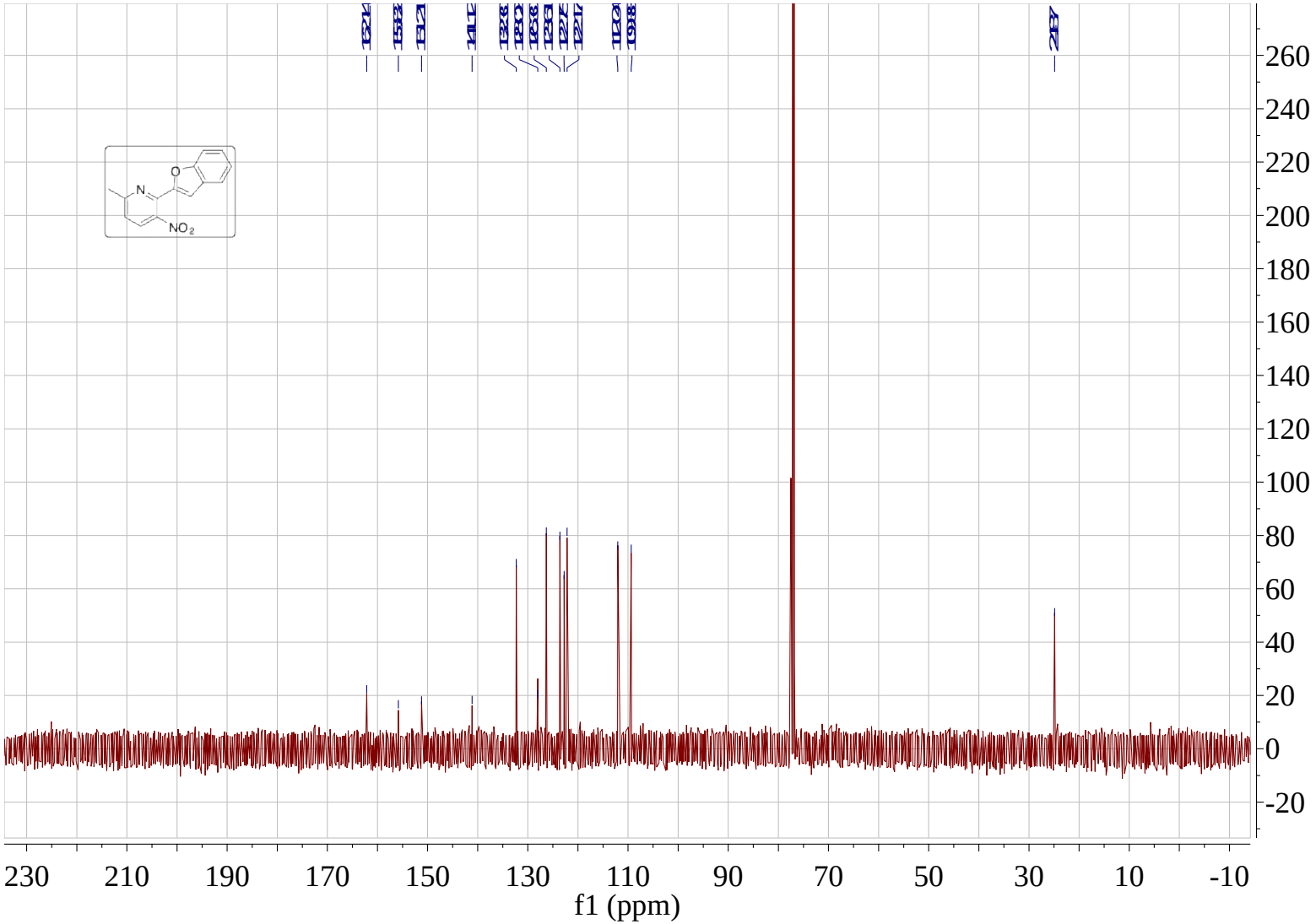

O
CN
N
Boc
450
400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

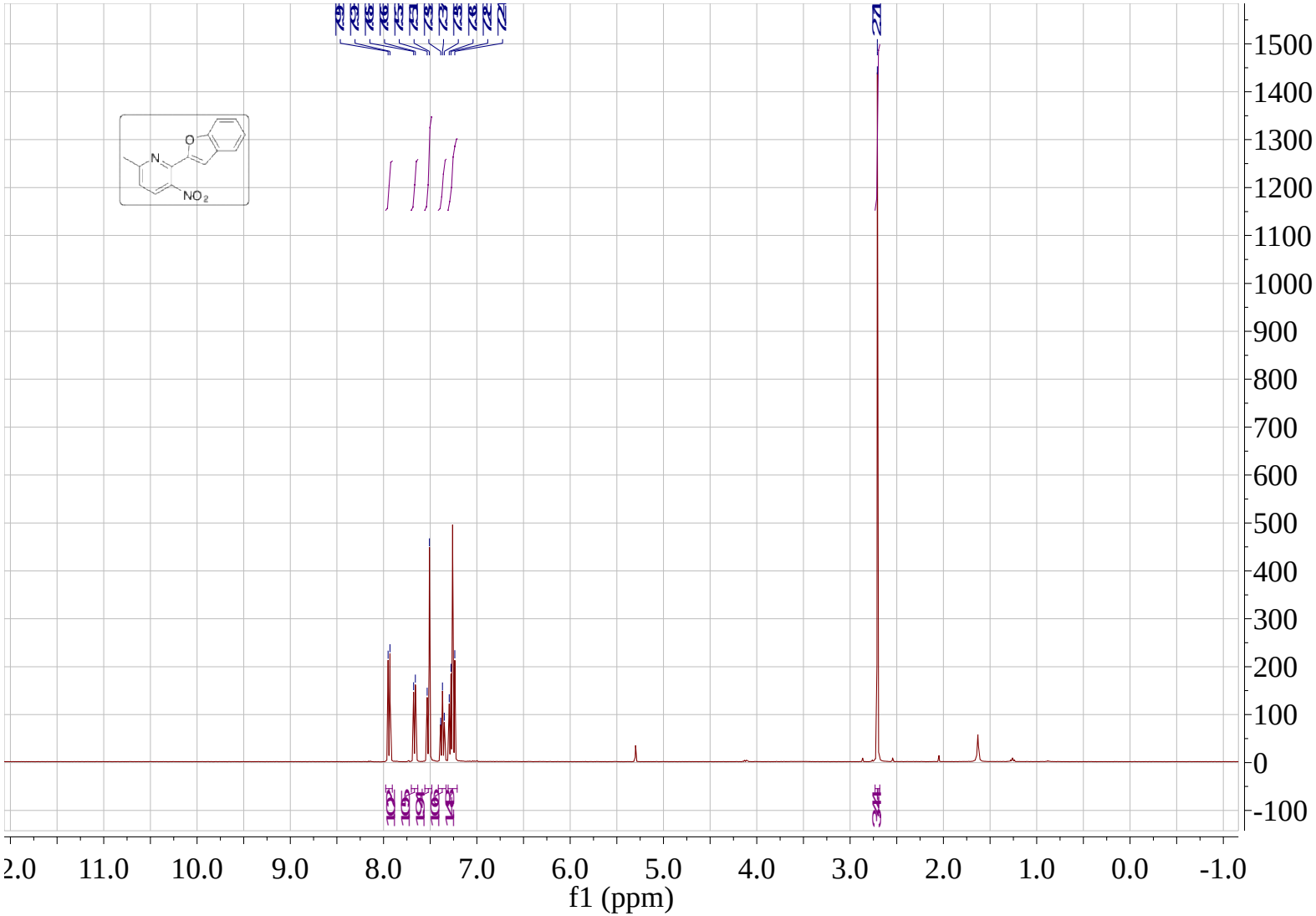

S
N
O
500
450
400
350
300
250
200
150
100
50
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

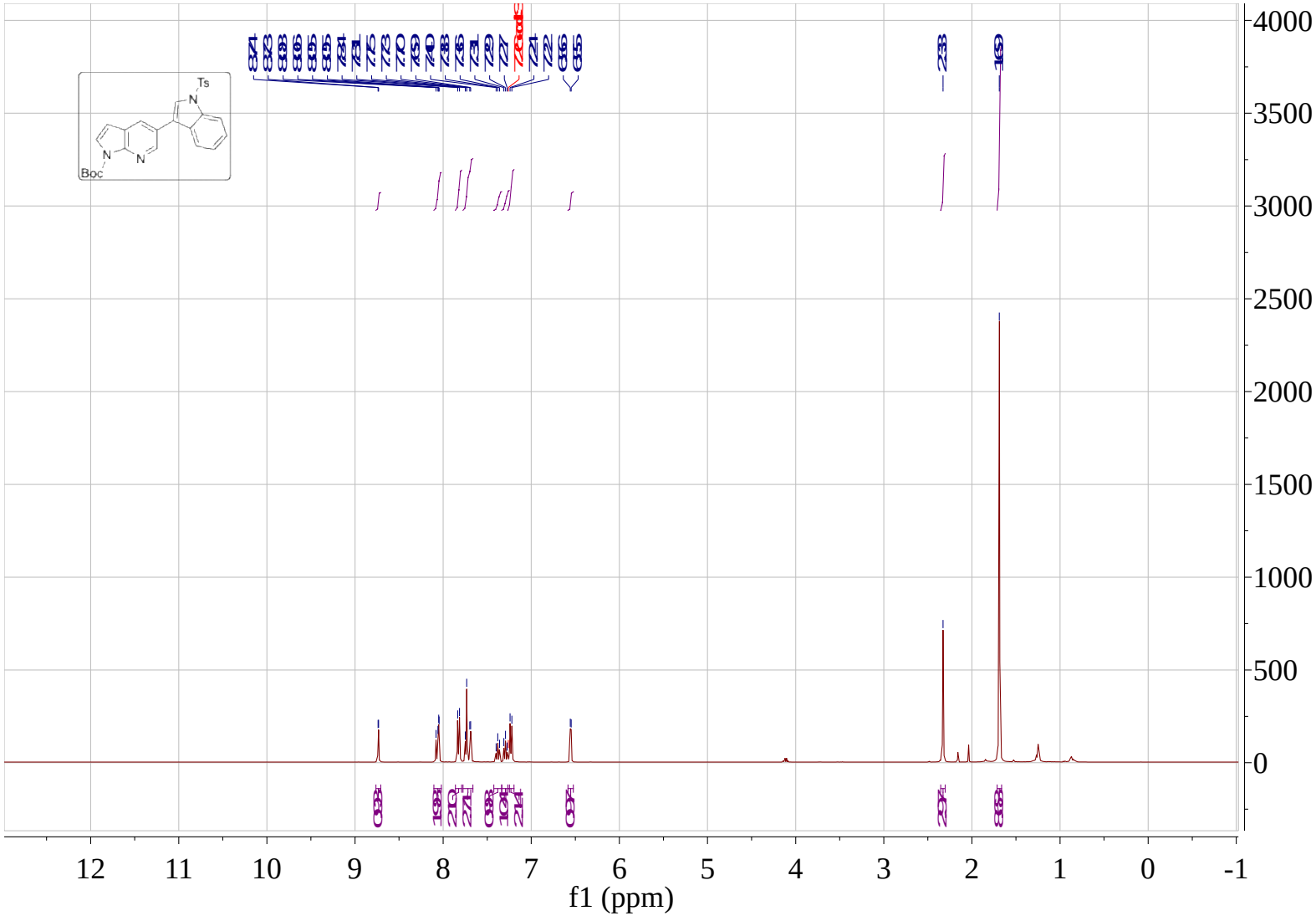

191.1
157.4
152.7
141.0
139.7
139.2
135.8
135.3
134.8
132.1
131.1
130.7
124.2
123.2
122.6
120.3
119.9
77.4
77.0
76.6
O
N
S
110
100
90
80
70
60
50
40
30
20
10
0
-10
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

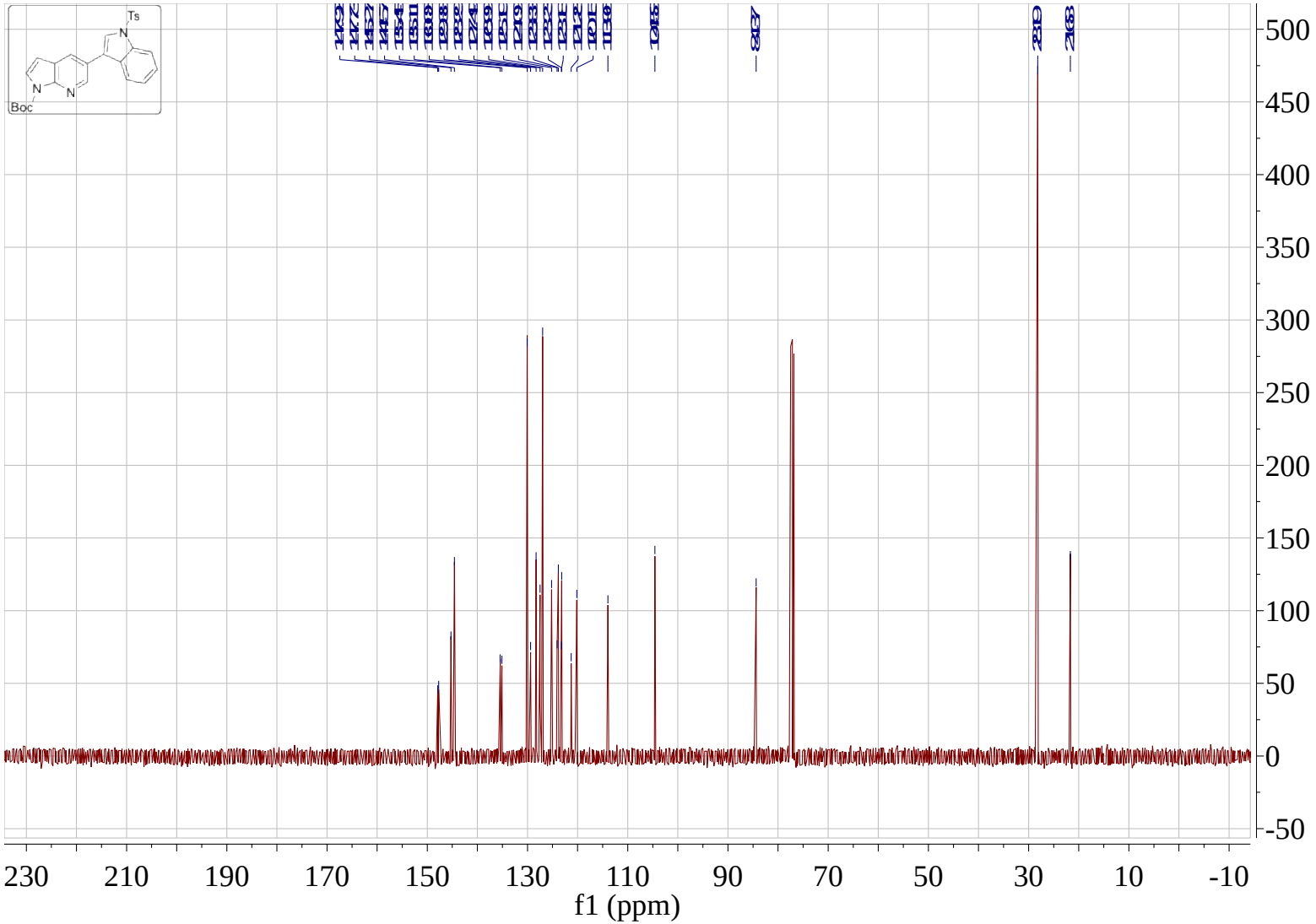

N
N
NH2
1900
1700
1500
1300
1100
900
700
500
300
100
-100
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

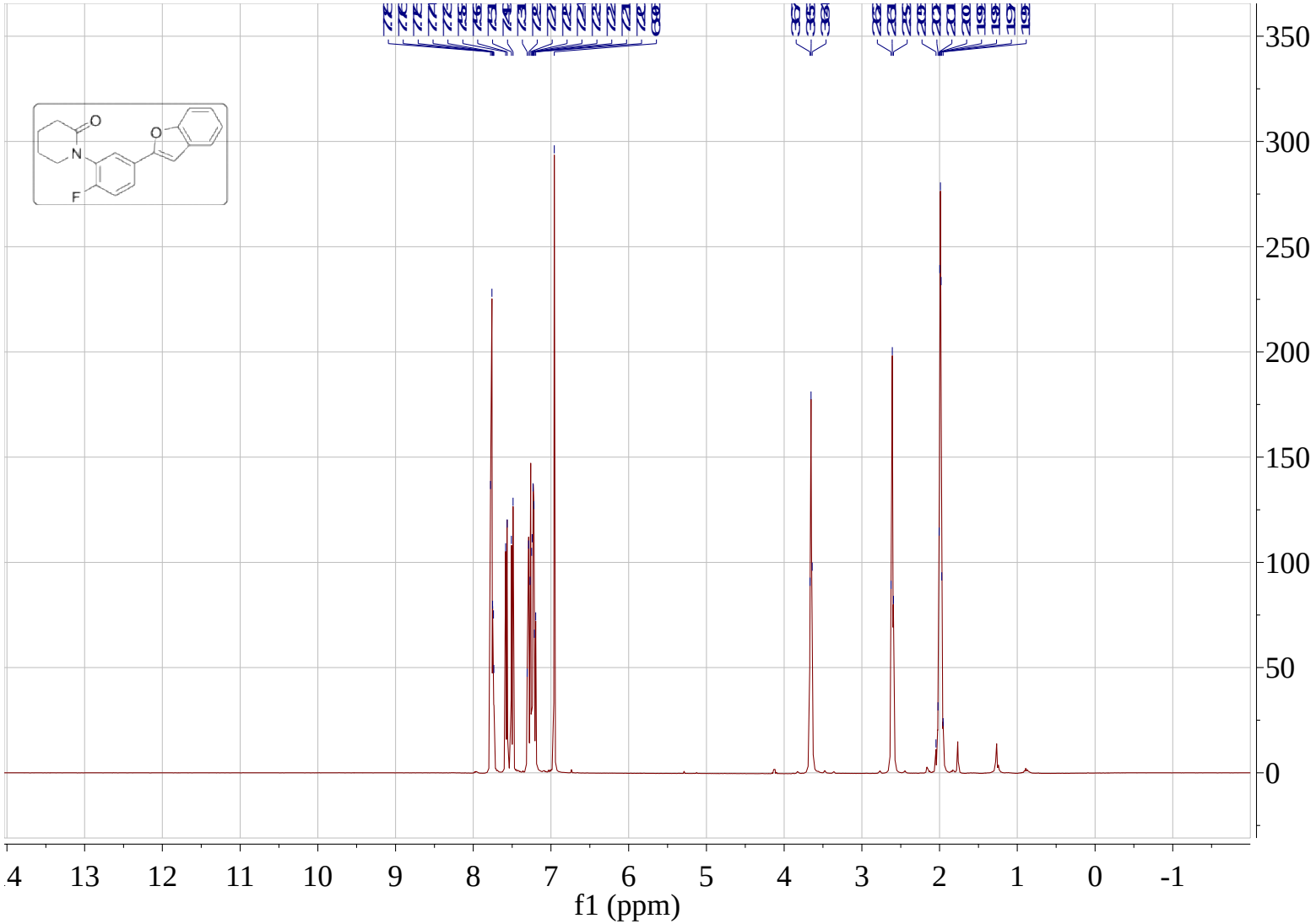

N
N
NH2
210
190
170
150
130
110
90
70
50
30
10
-10
-30
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

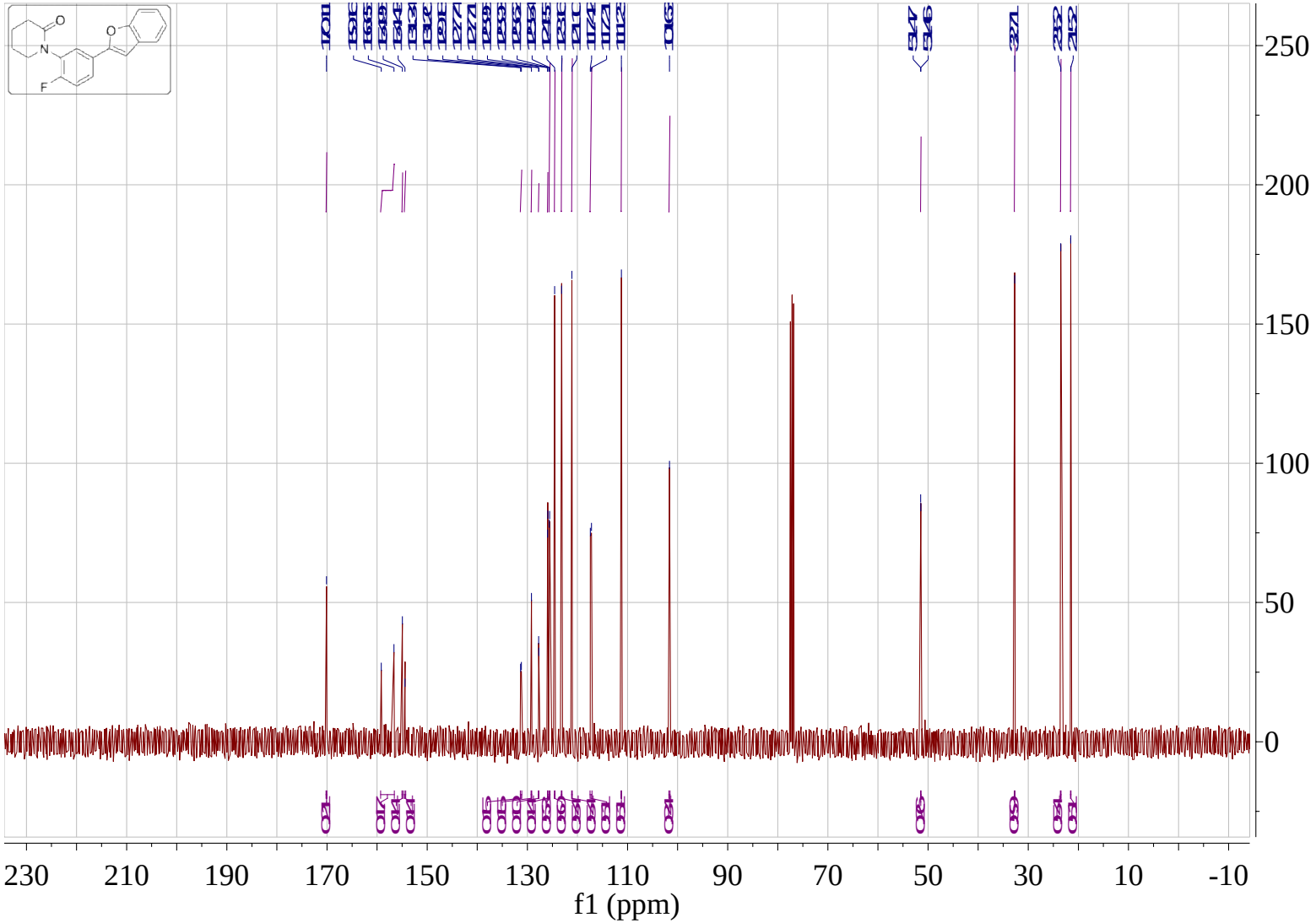

O
N
NO2
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

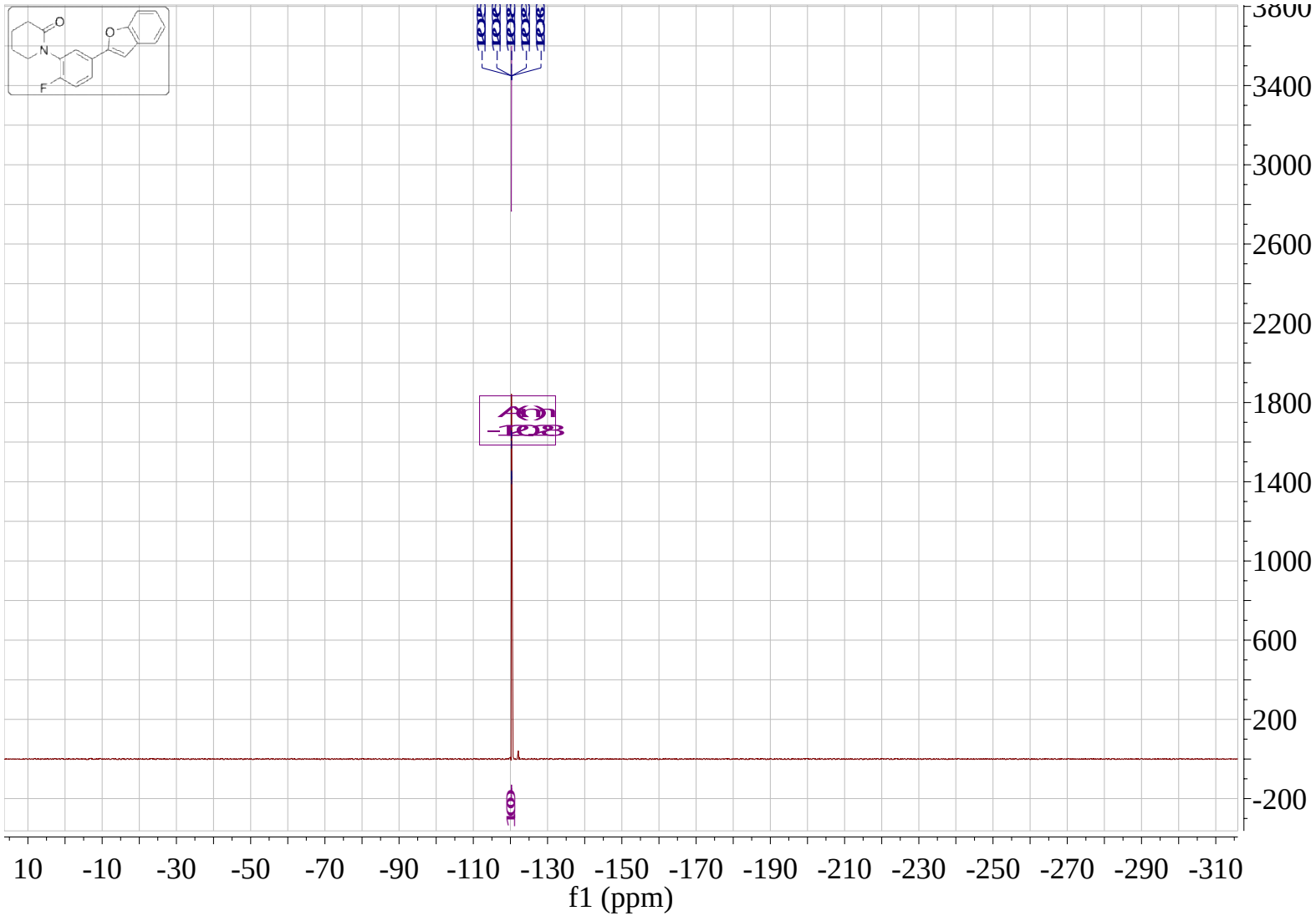

O
N
NO2
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

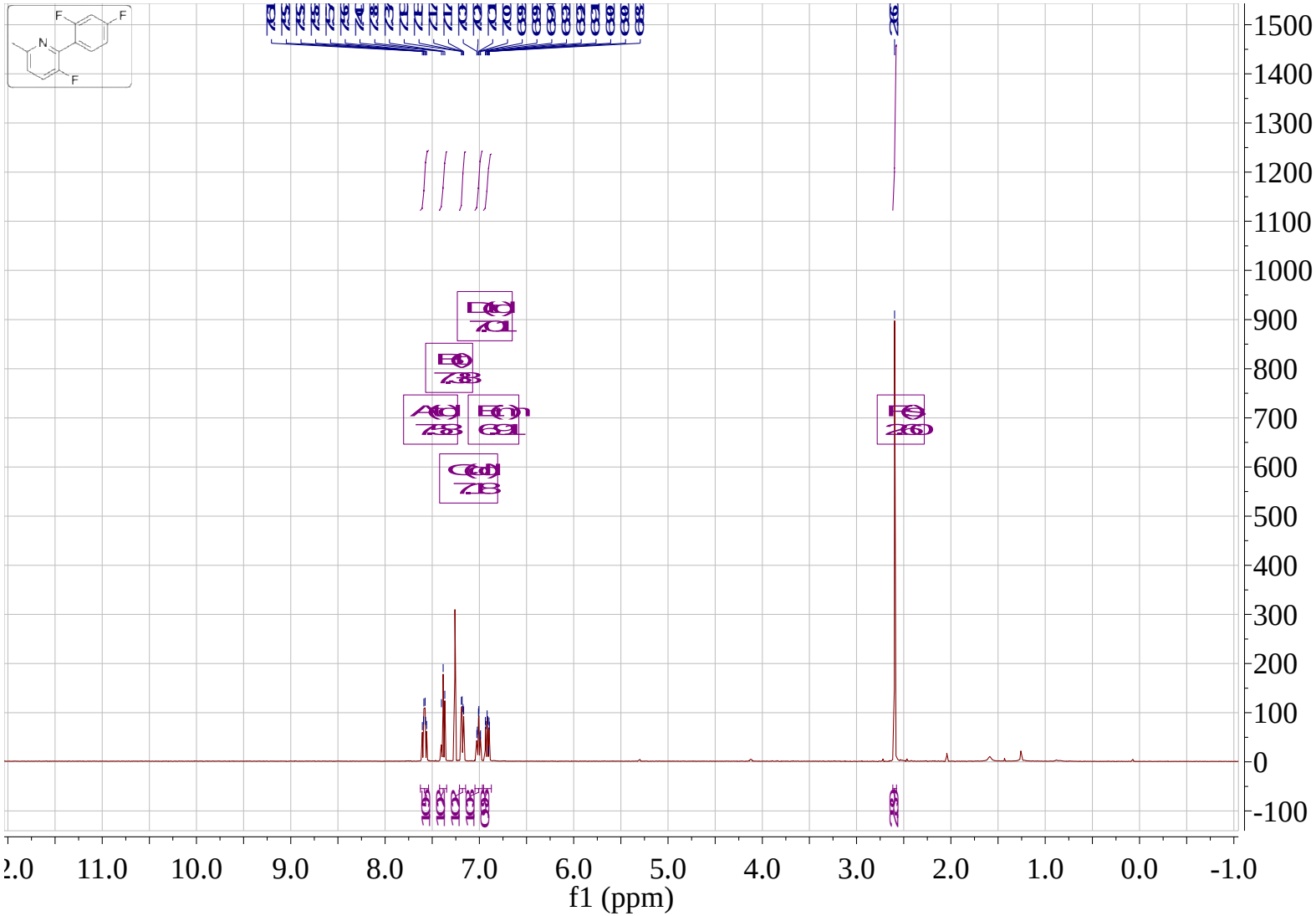

Ts
N
N
N
Boc
4000
3500
3000
2500
2000
1500
1000
500
0
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

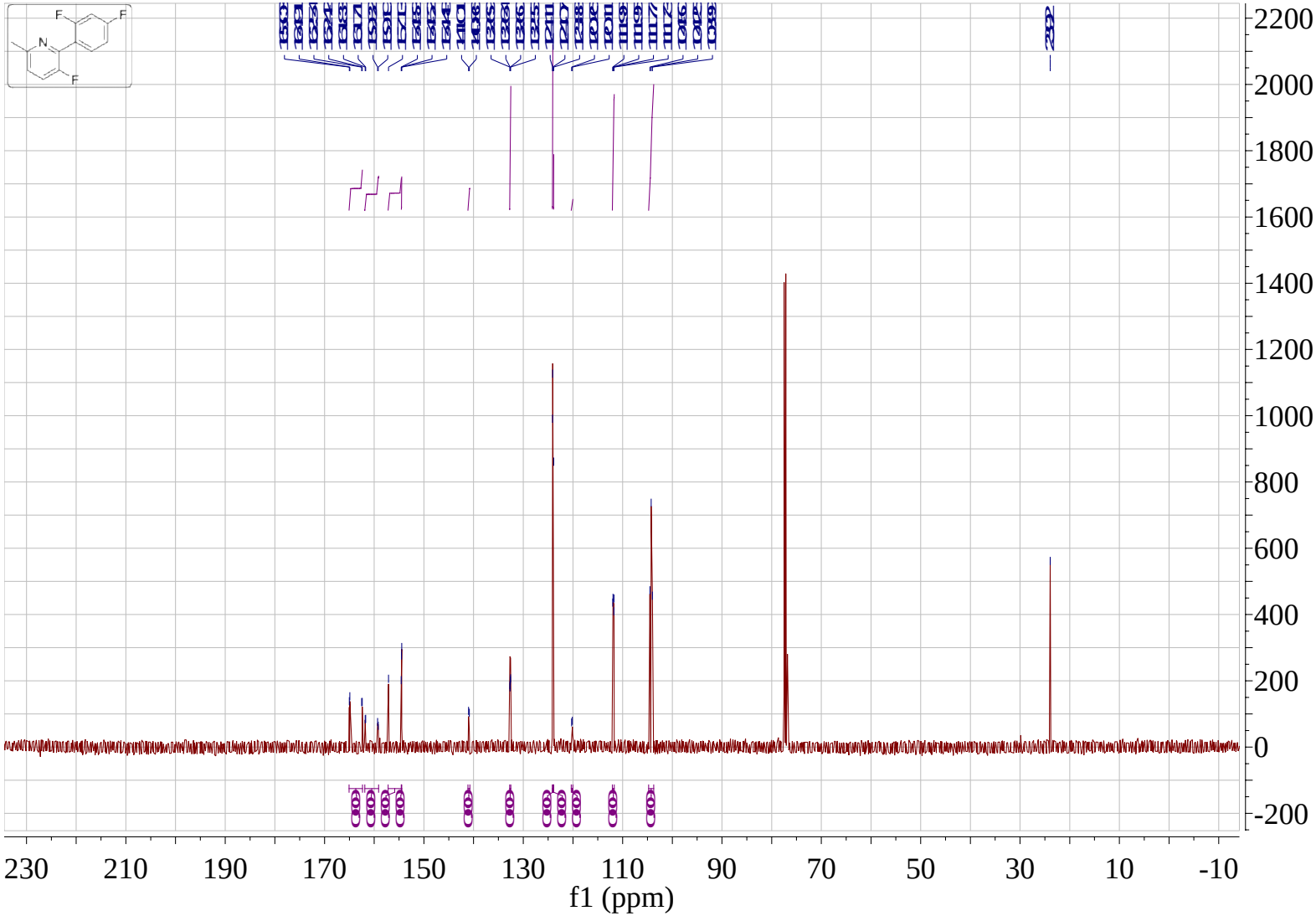

Ts
N
N
N
Boc
500
450
400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

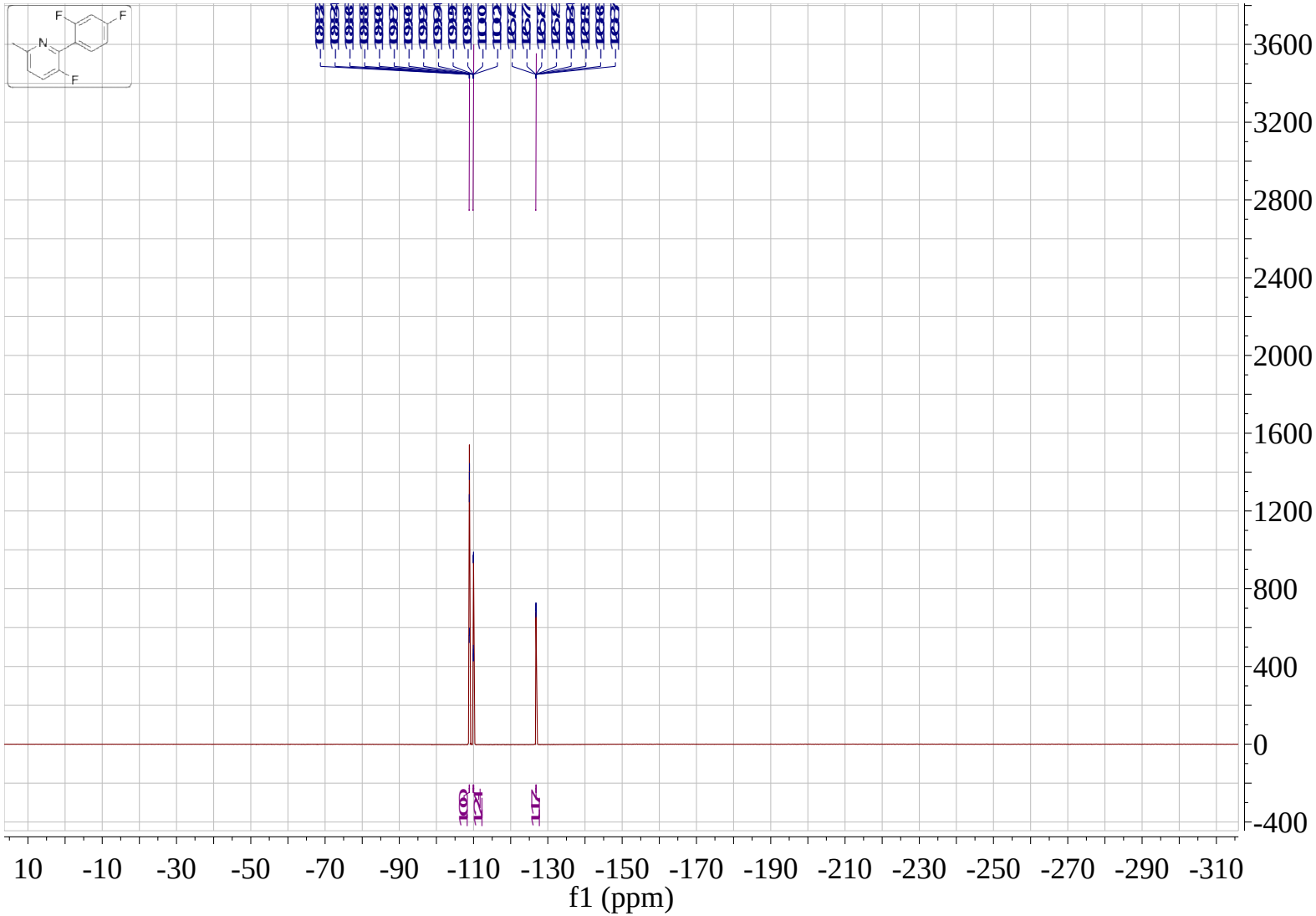

O
N
O
F
350
300
250
200
150
100
50
0
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

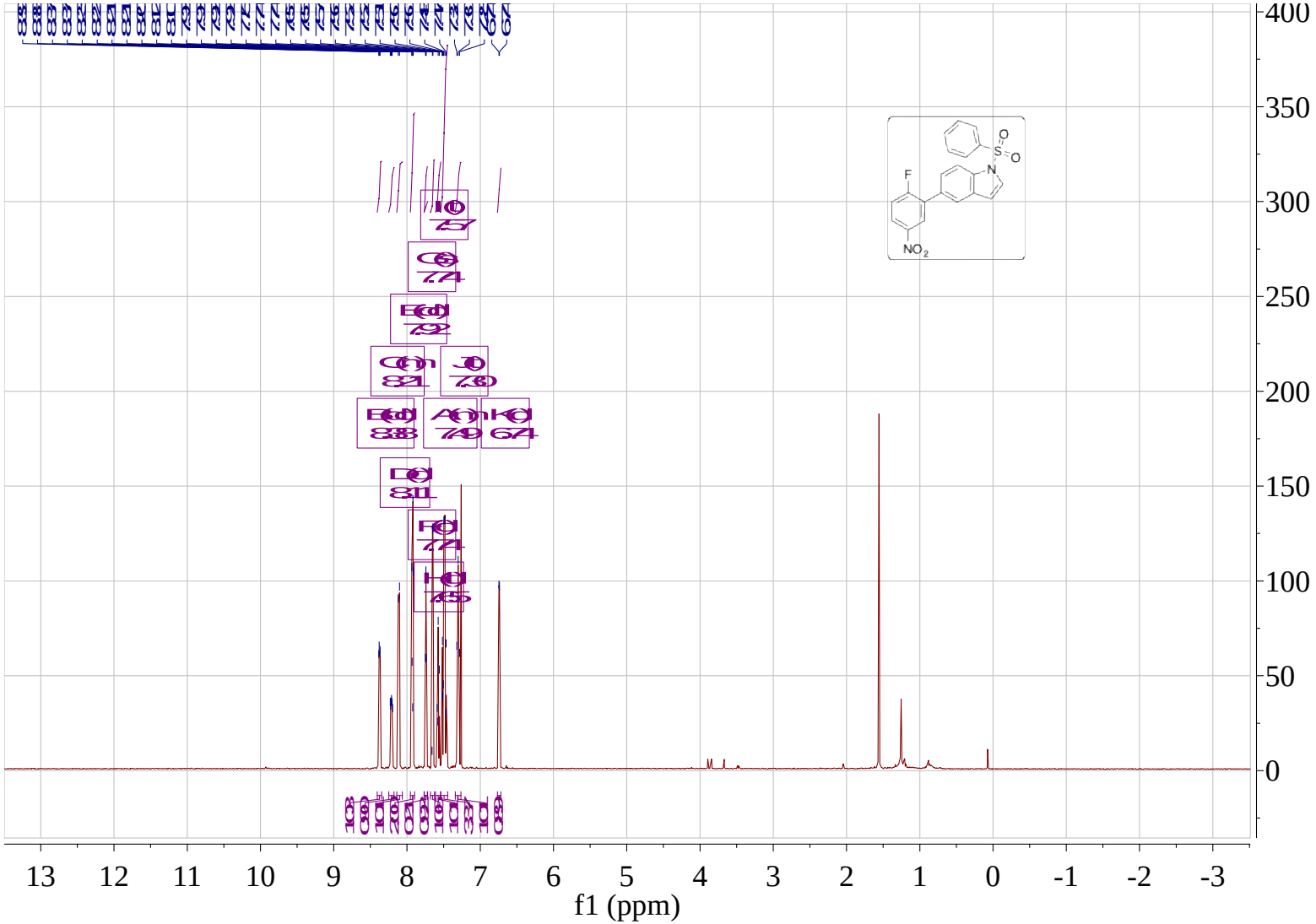

O
N
O
F
250
200
150
100
50
0
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

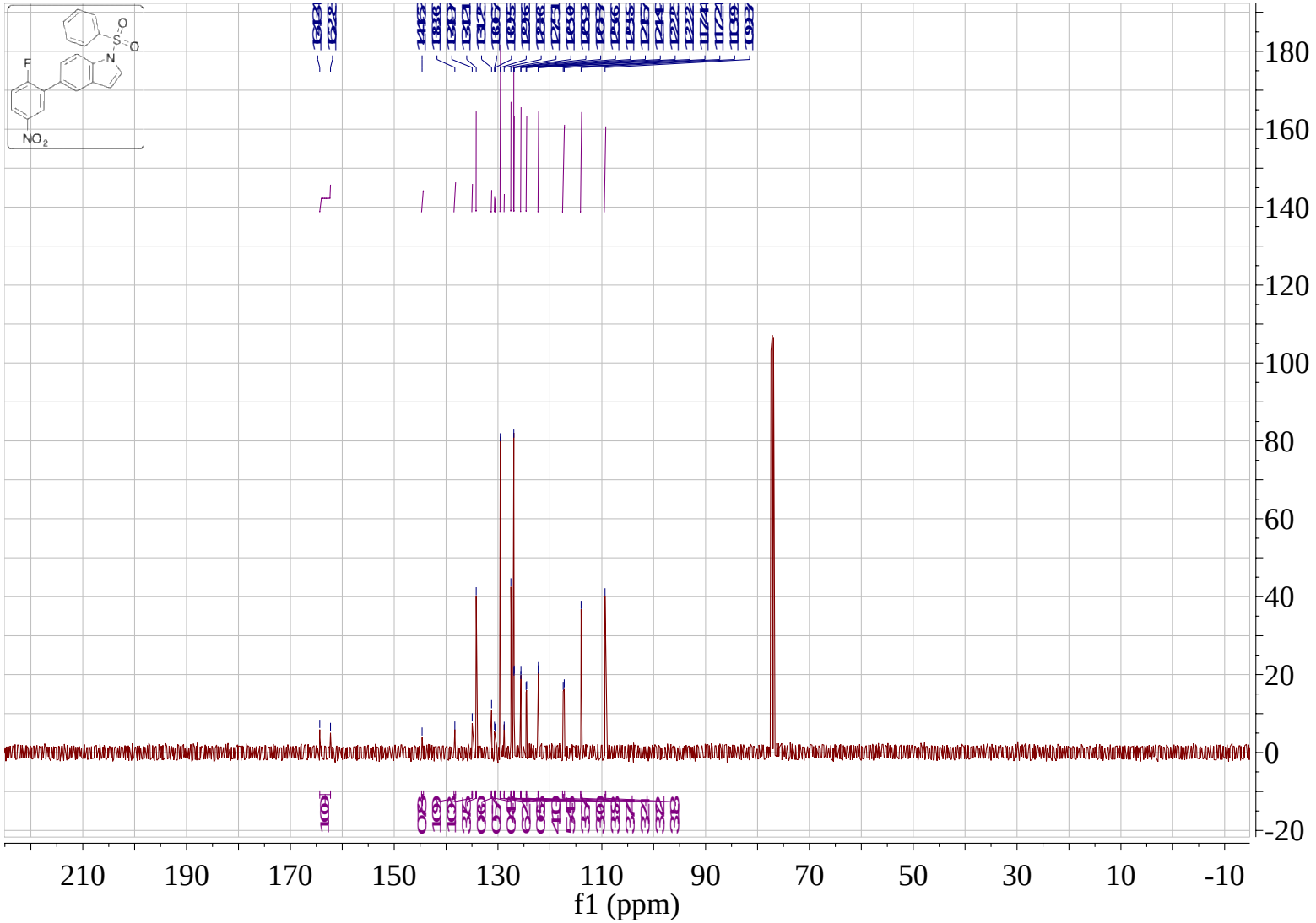

3800
3400
3000
2600
2200
1800
1400
1000
600
200
-200
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290 -310
f1 (ppm)

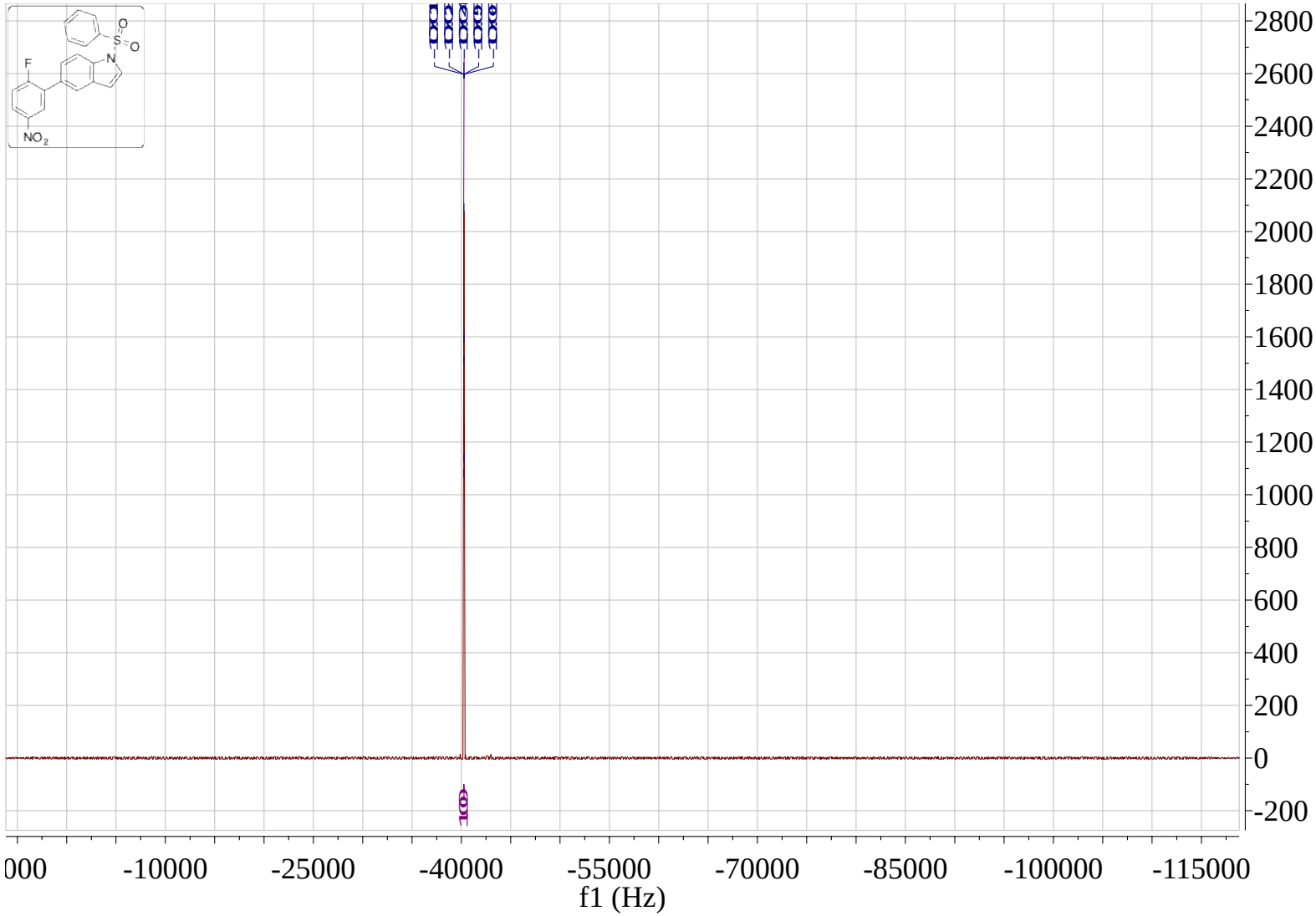

F
F
N
F
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
2.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

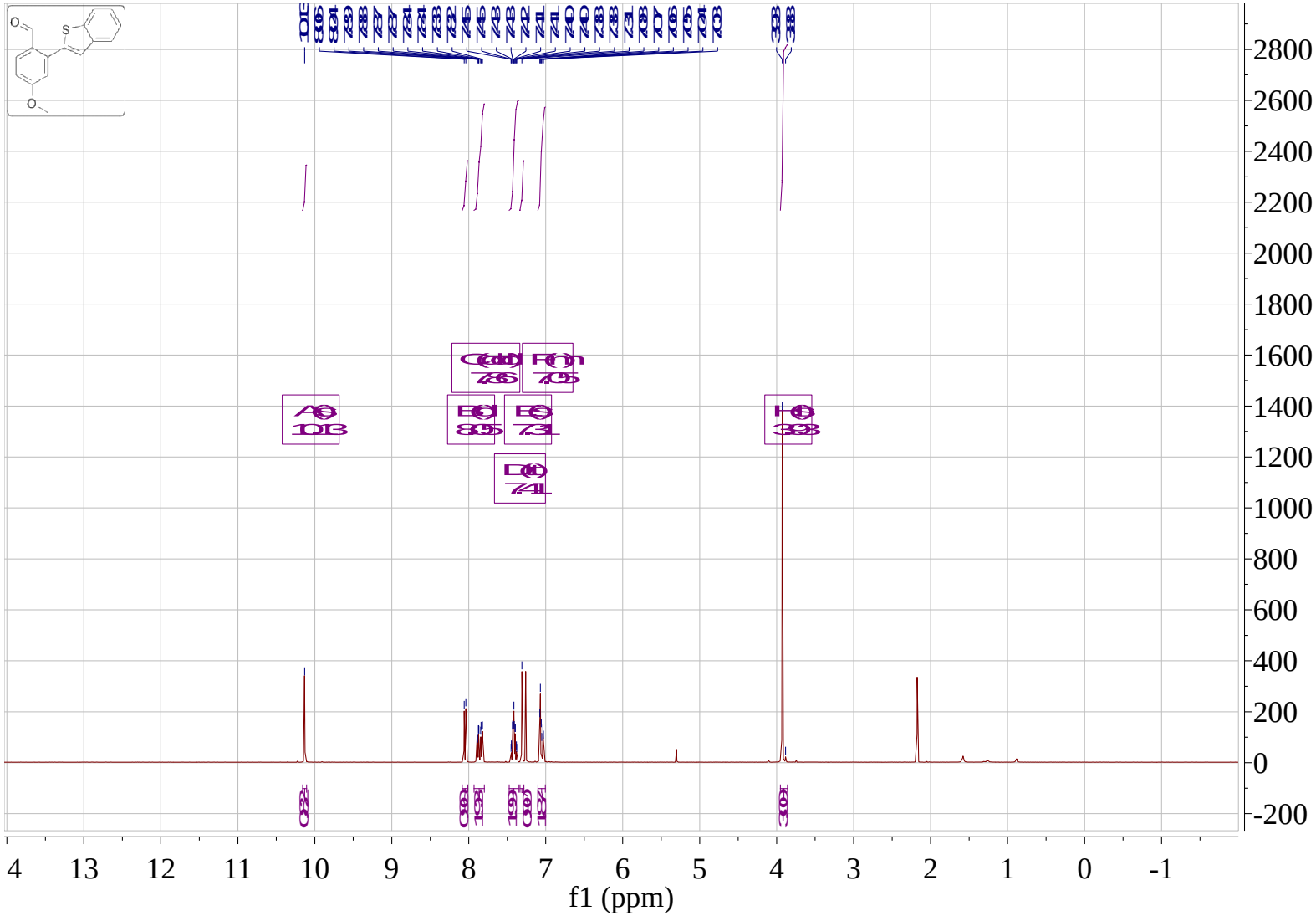

F
F
N
F
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

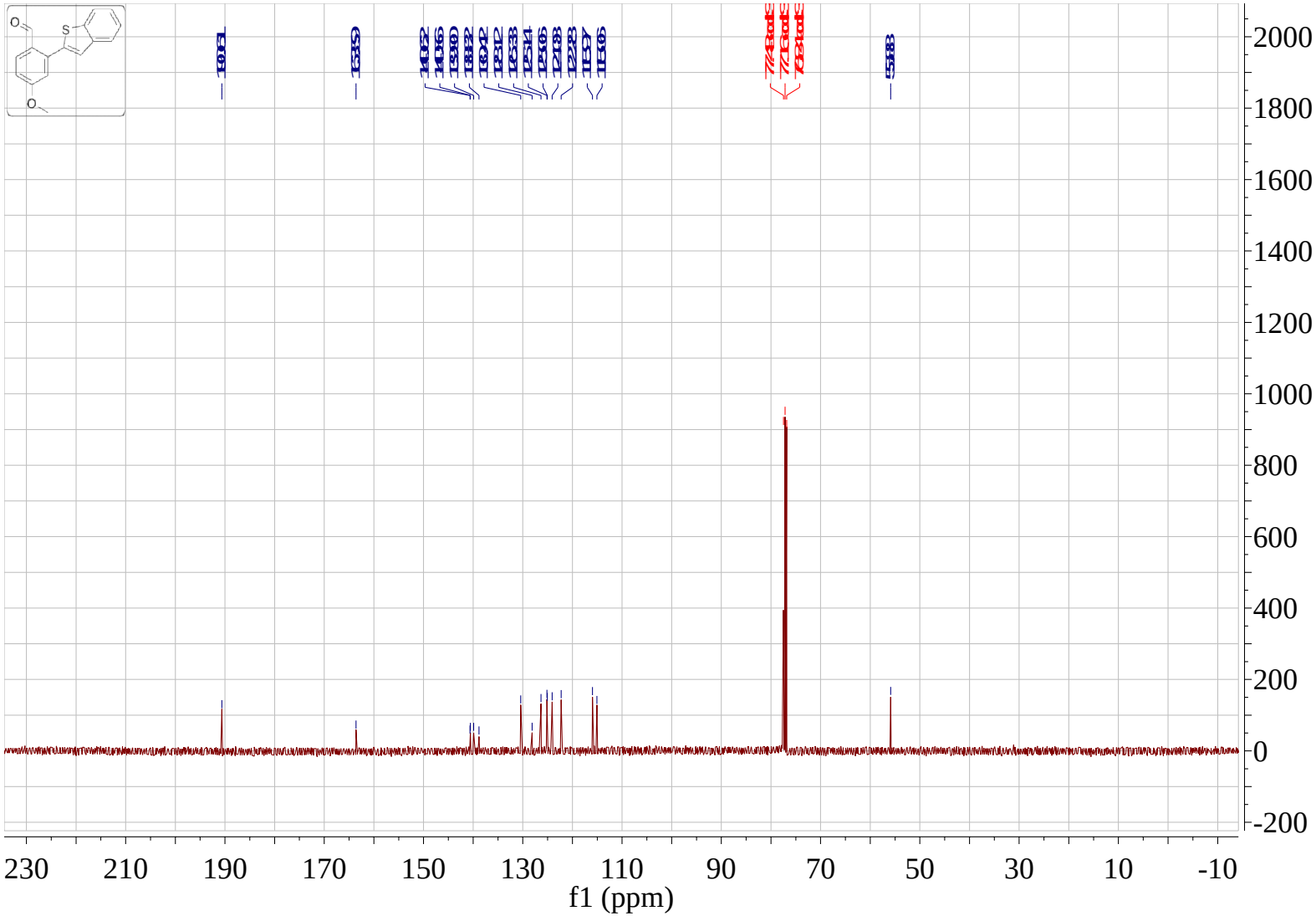

F
F
N
F
3600
3200
2800
2400
2000
1600
1200
800
400
0
-400
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
-310
f1 (ppm)

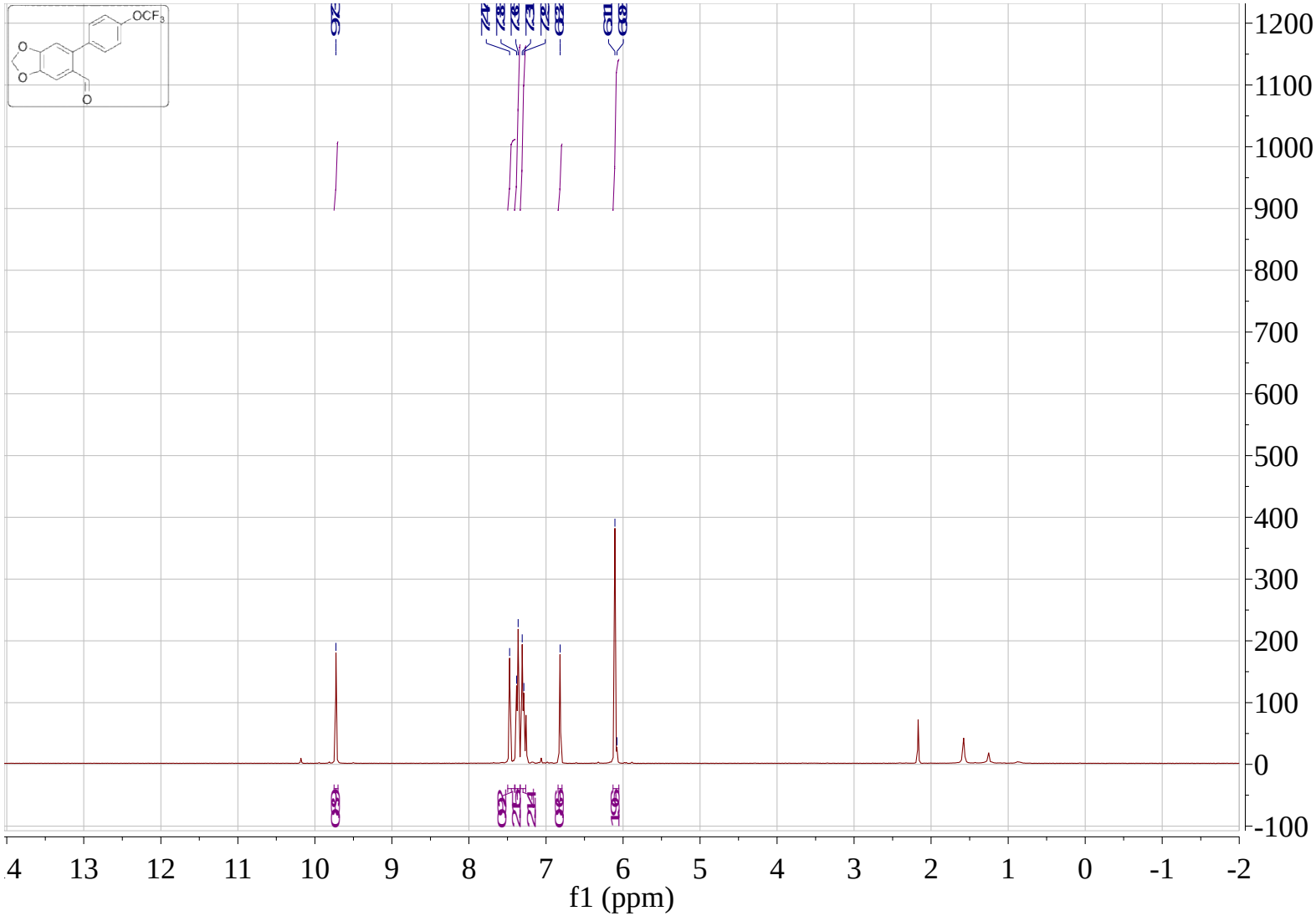

f1 (ppm)

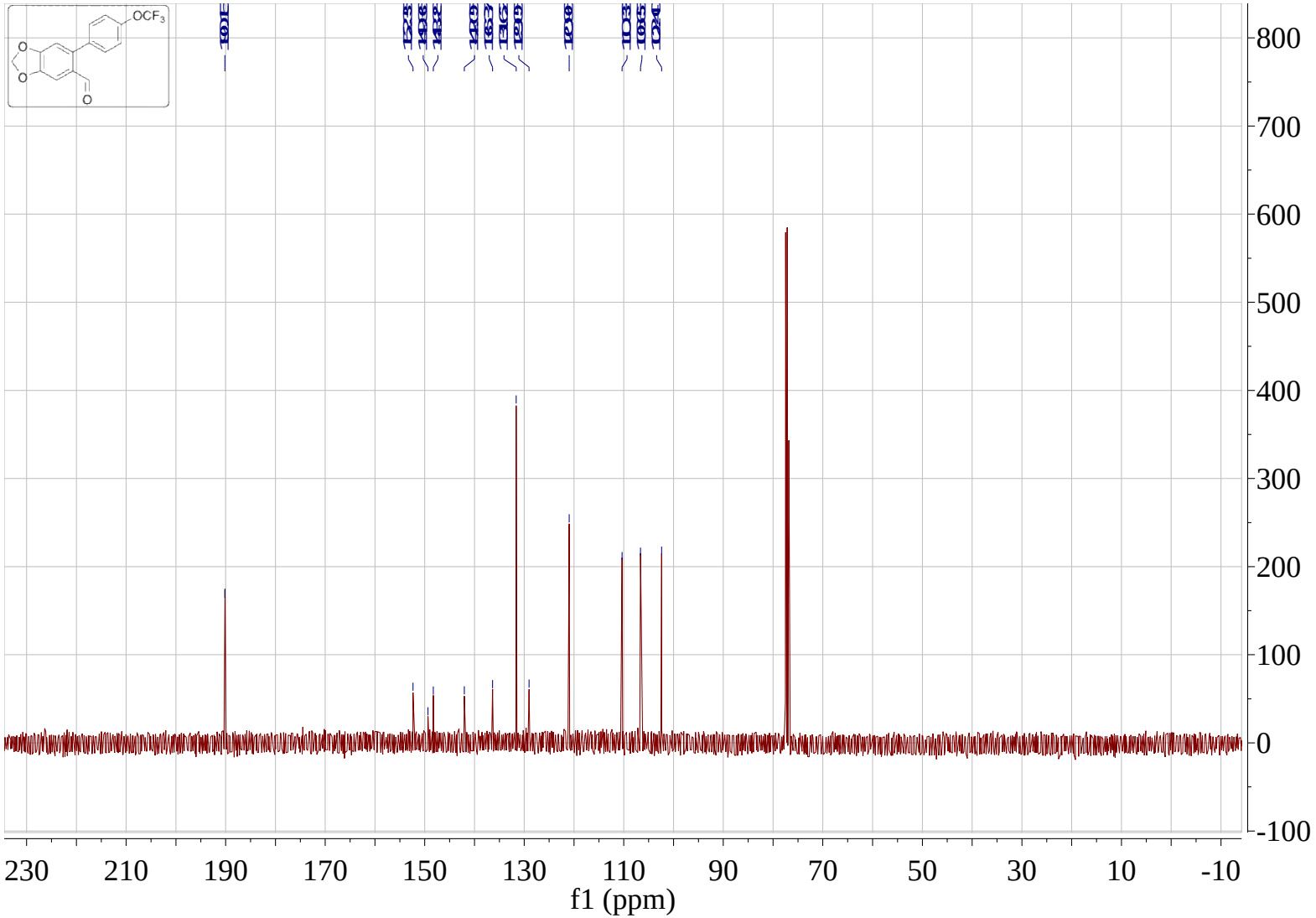

O
S
O
N
F
NO2
180
160
140
120
100
80
60
40
20
0
-20
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

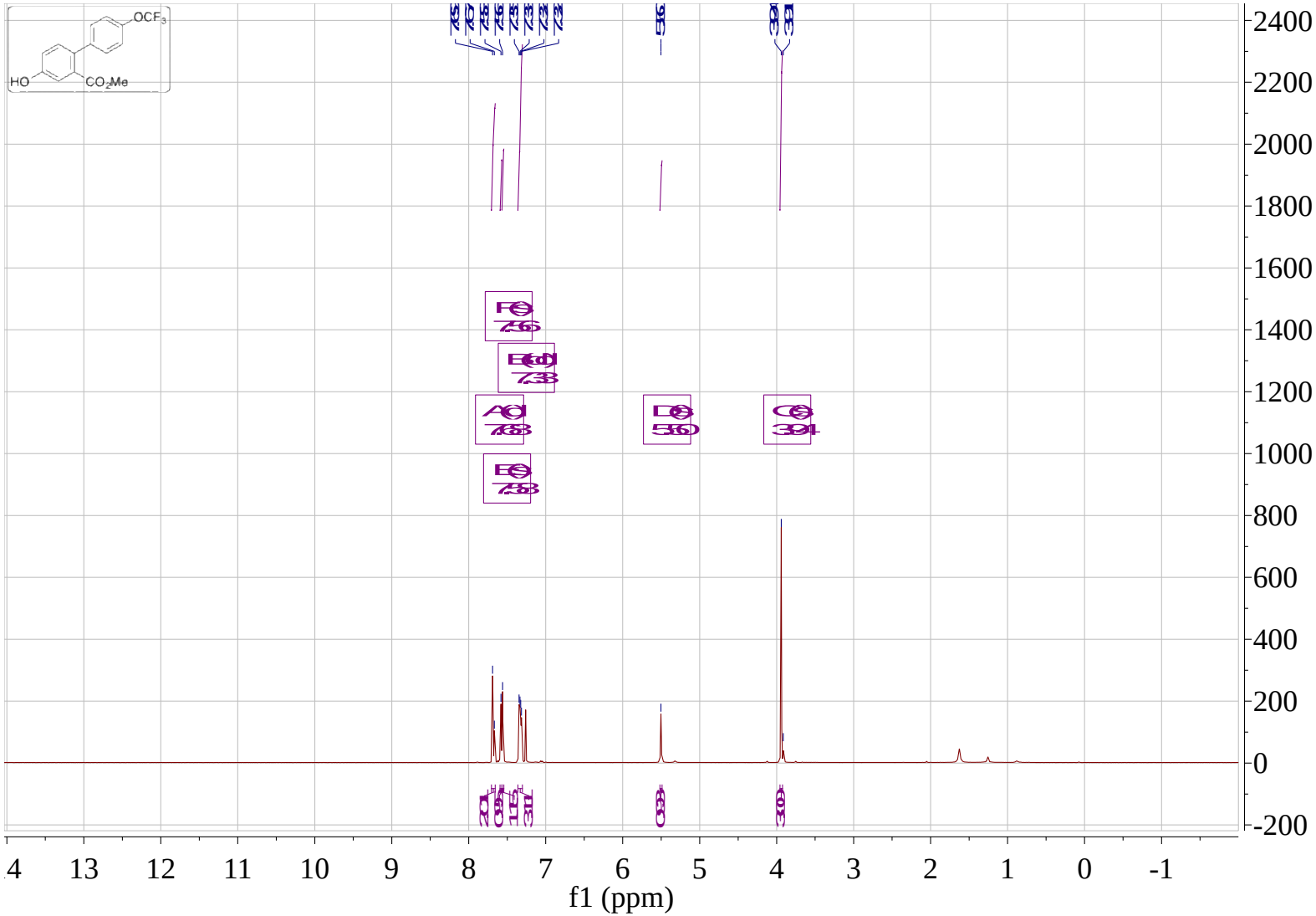

O
S
O
N
F
NO2
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
000
-10000
-25000
-40000
-55000
-70000
-85000
-100000
-115000
f1 (Hz)

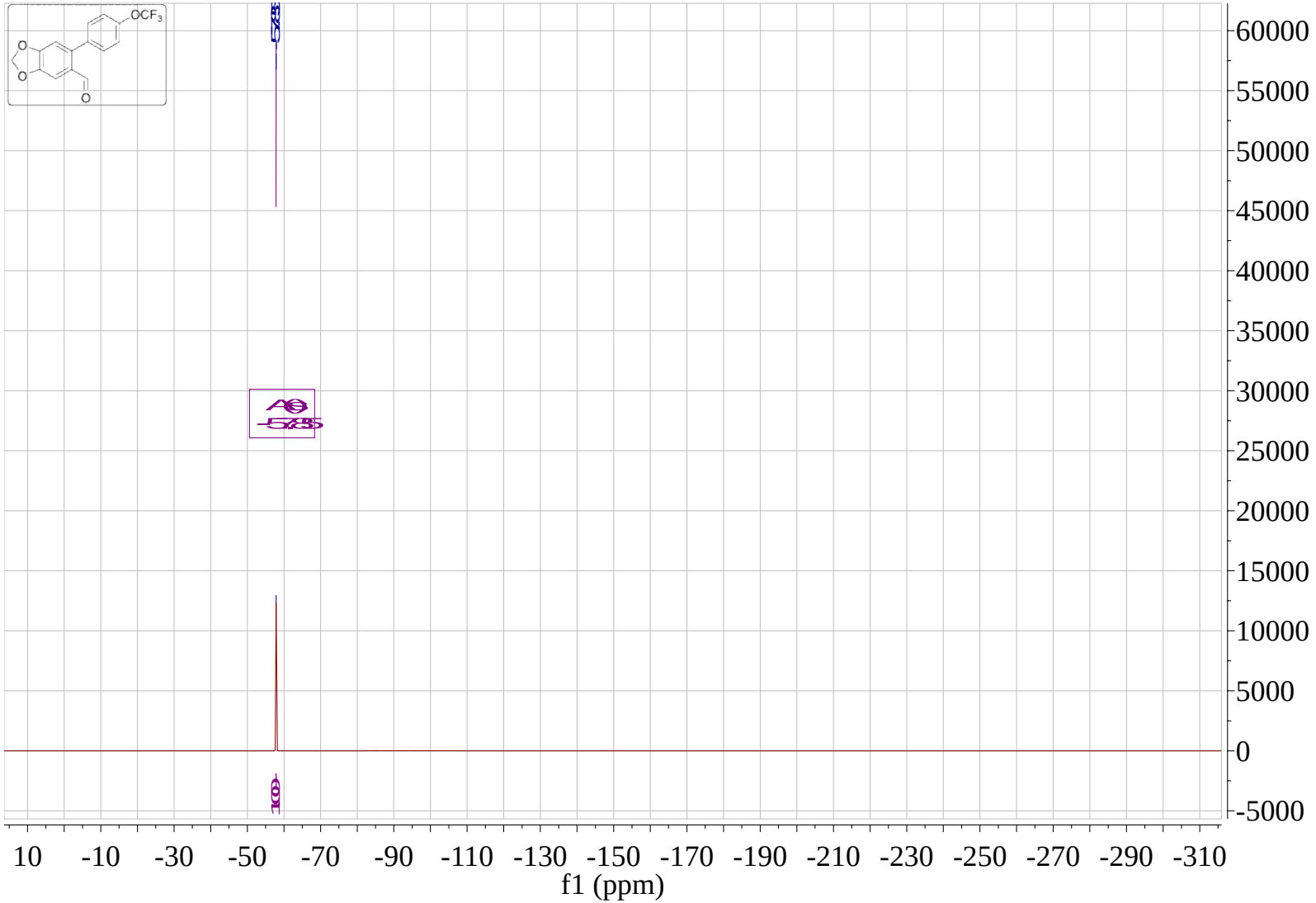

2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
4 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

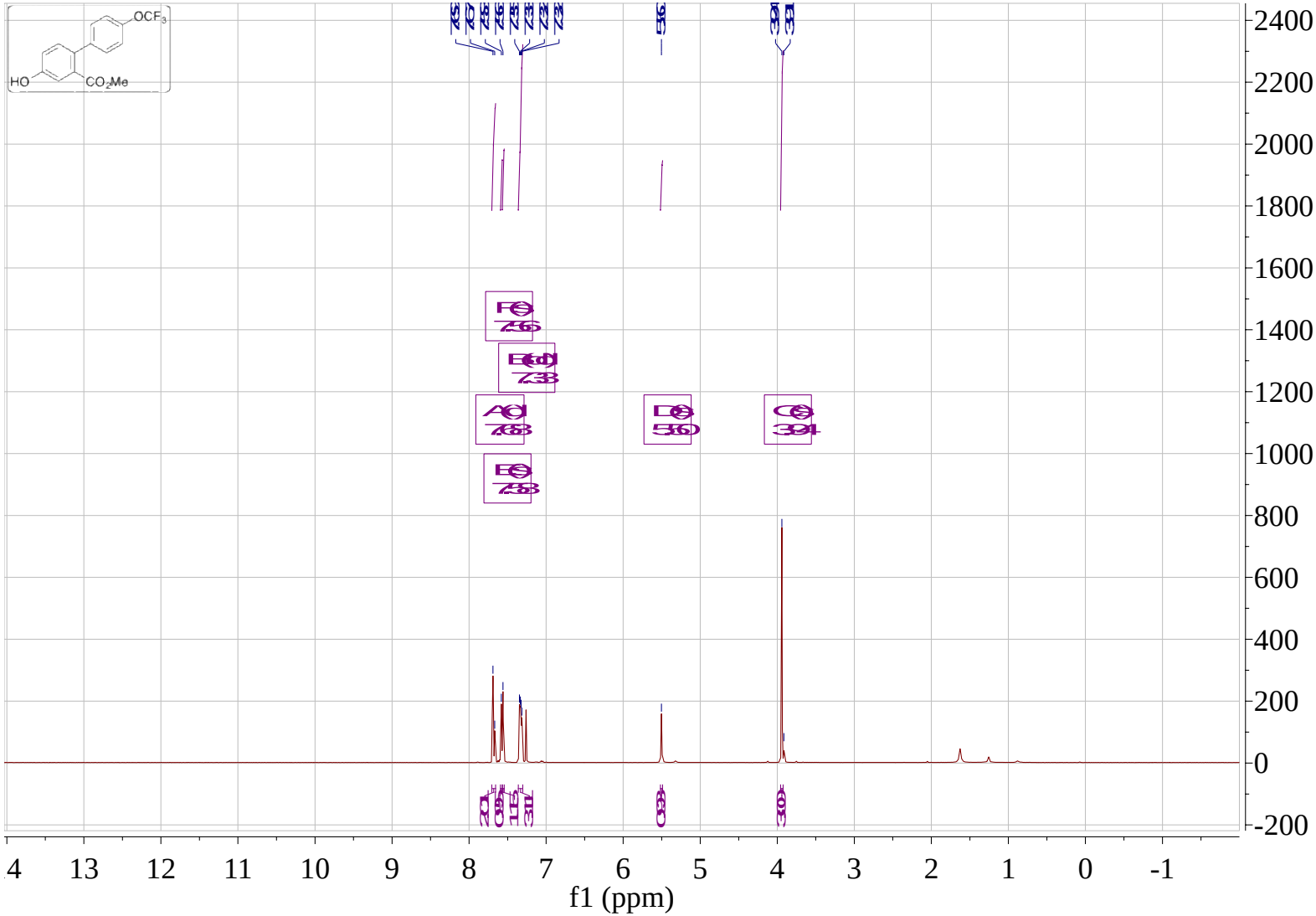

O
S
O
195.1
153.9
141.2
141.6
139.0
138.2
132.4
131.2
125.3
125.4
125.6
124.8
122.8
115.7
115.6
77.4
77.0
76.6
55.8
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

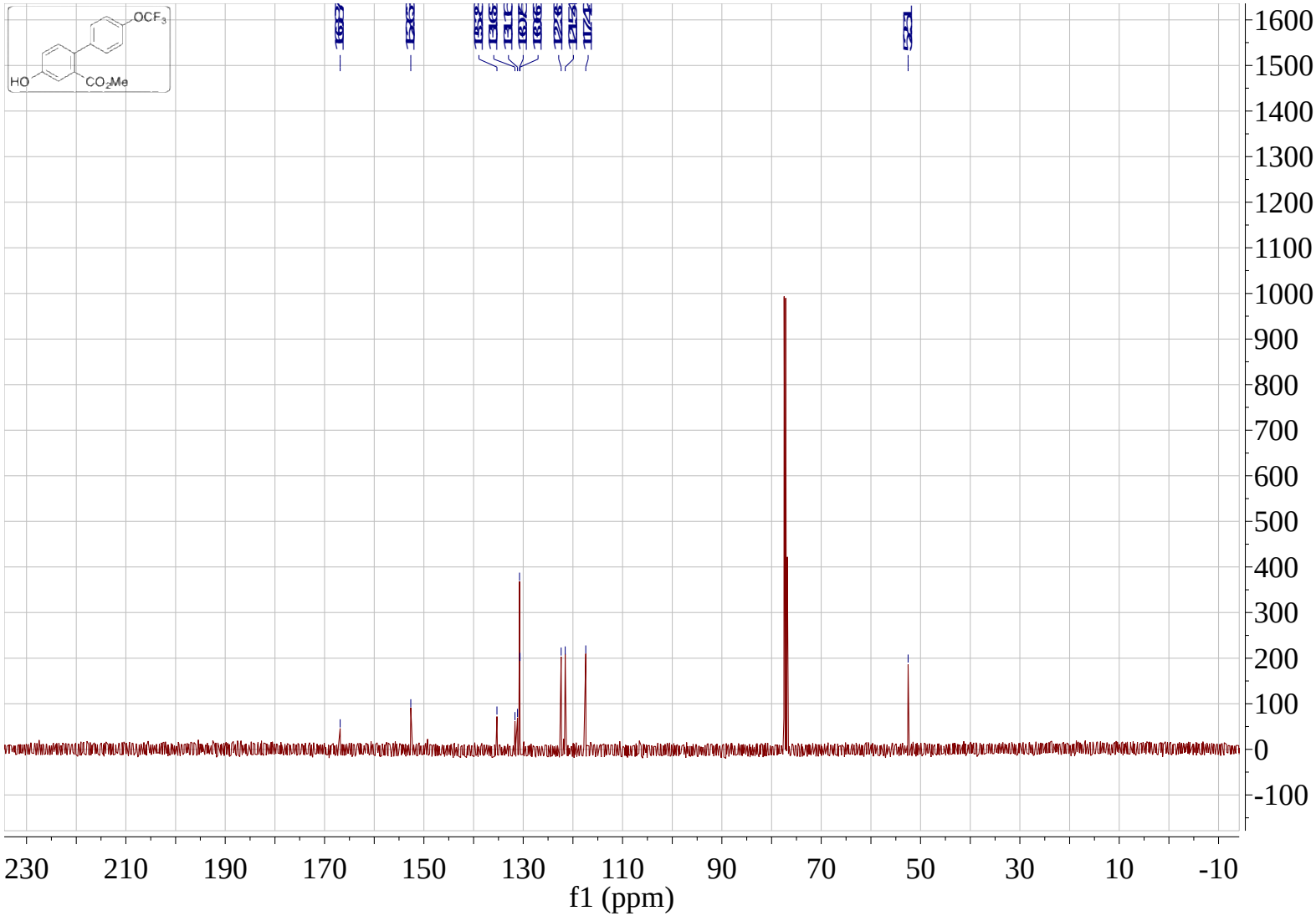

OCF3
O
O
O
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

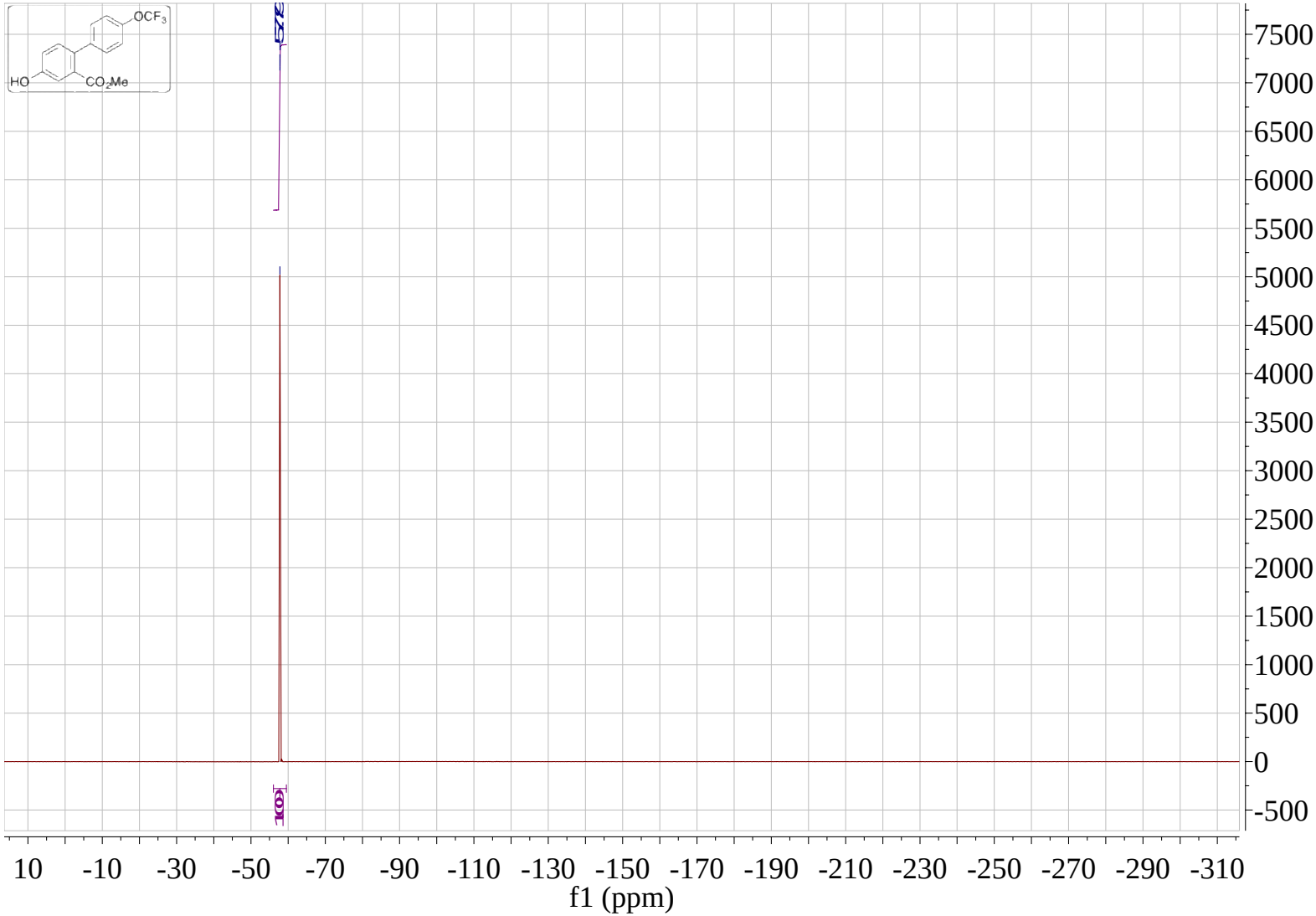

OCF3
O
O
O
800
700
600
500
400
300
200
100
0
-100
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

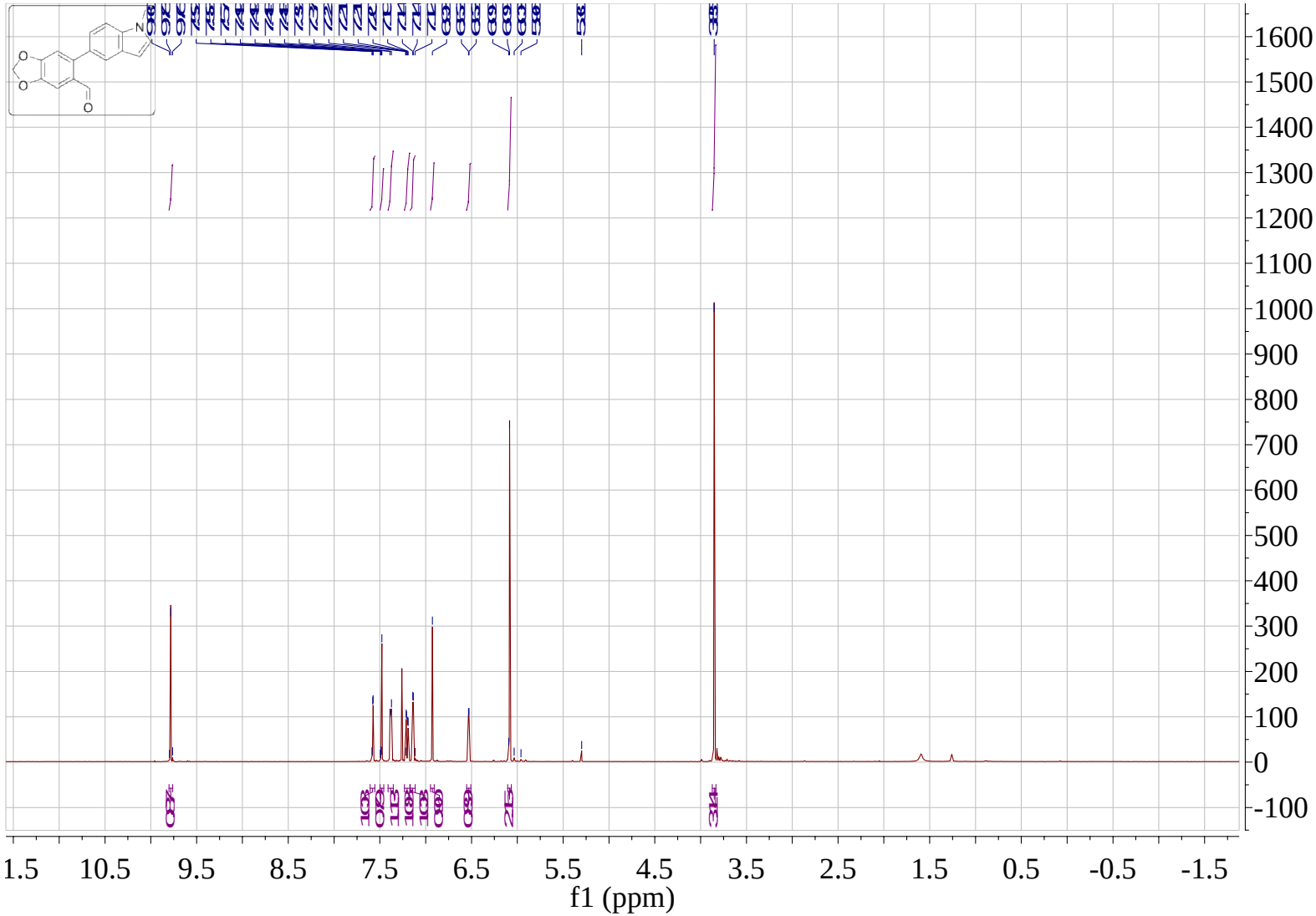

OCF3
HO
CO2Me
f1 (ppm)

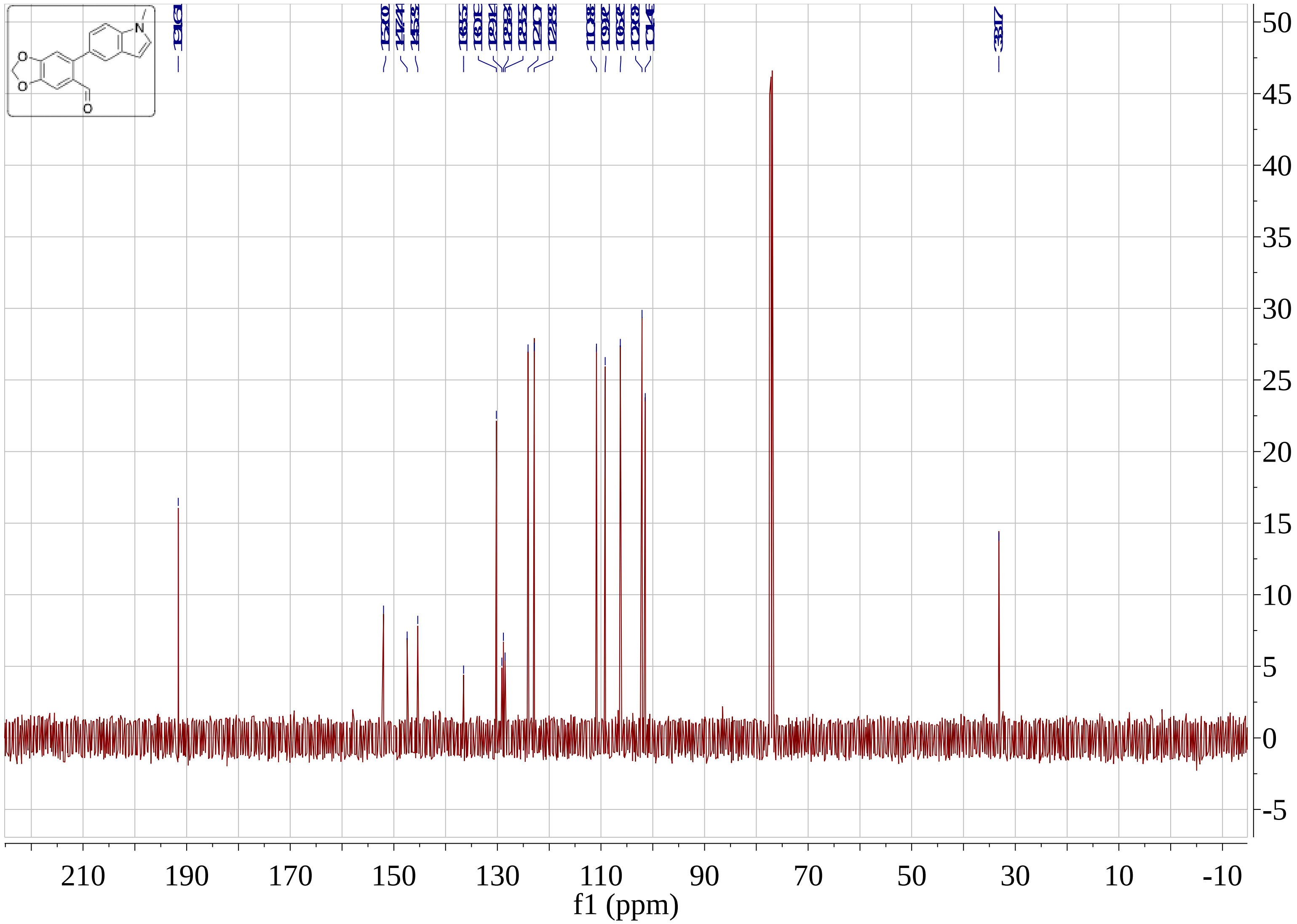

OCF3
O
O
O
-58.25
1.00
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
-310
f1 (ppm)

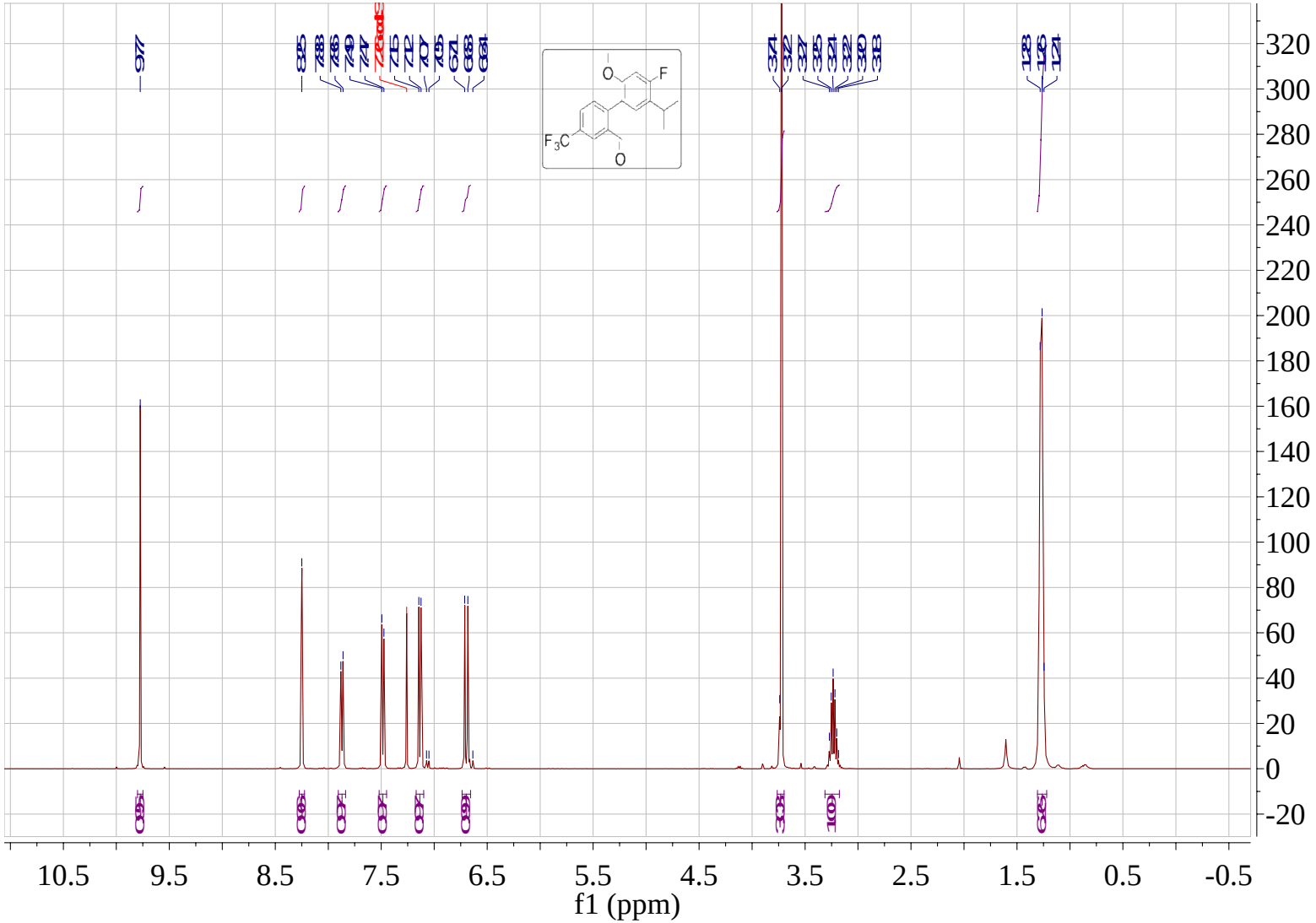

OCF3
HO
CO2Me
f1 (ppm)

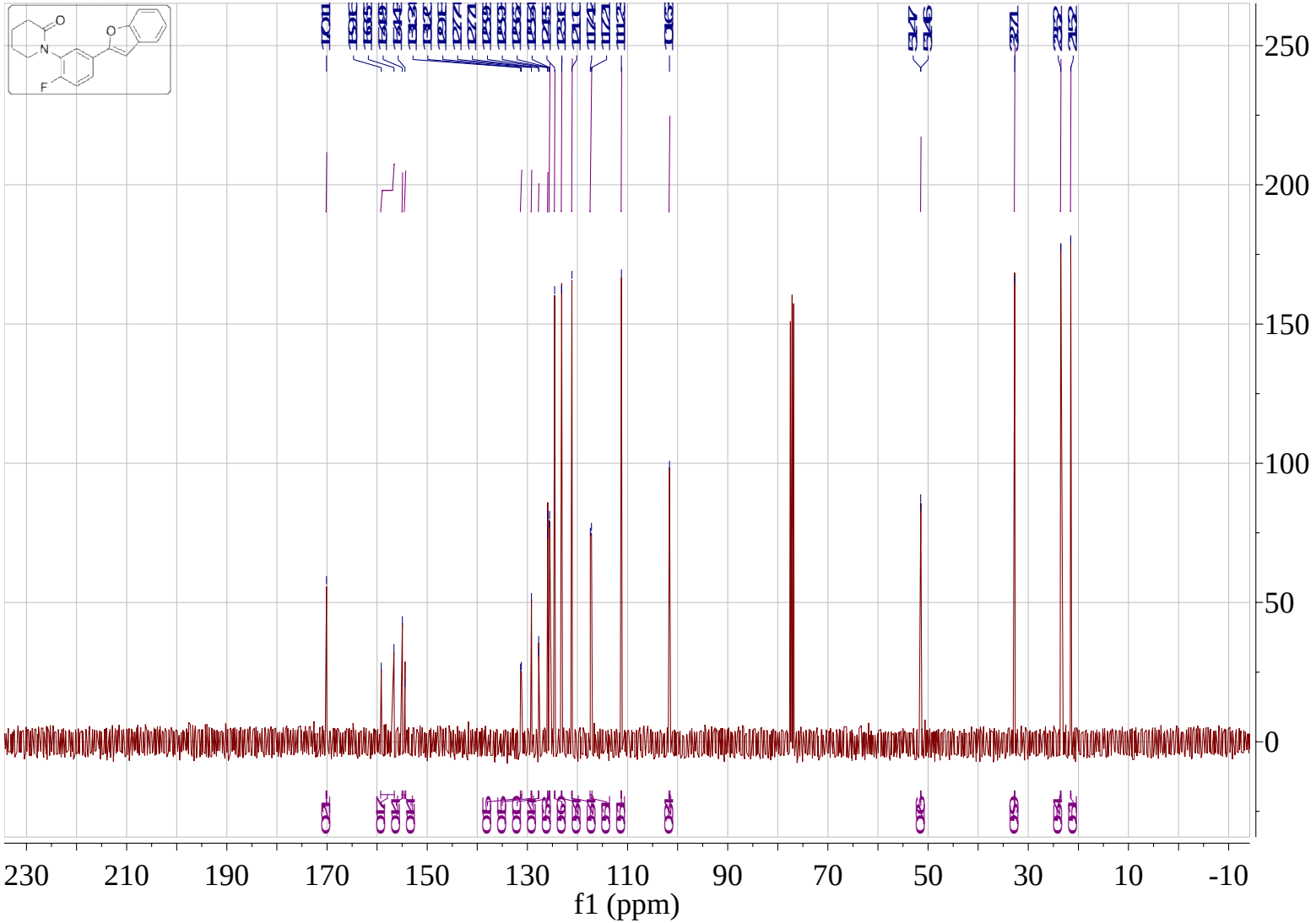

OCF3
HO
CO2Me
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

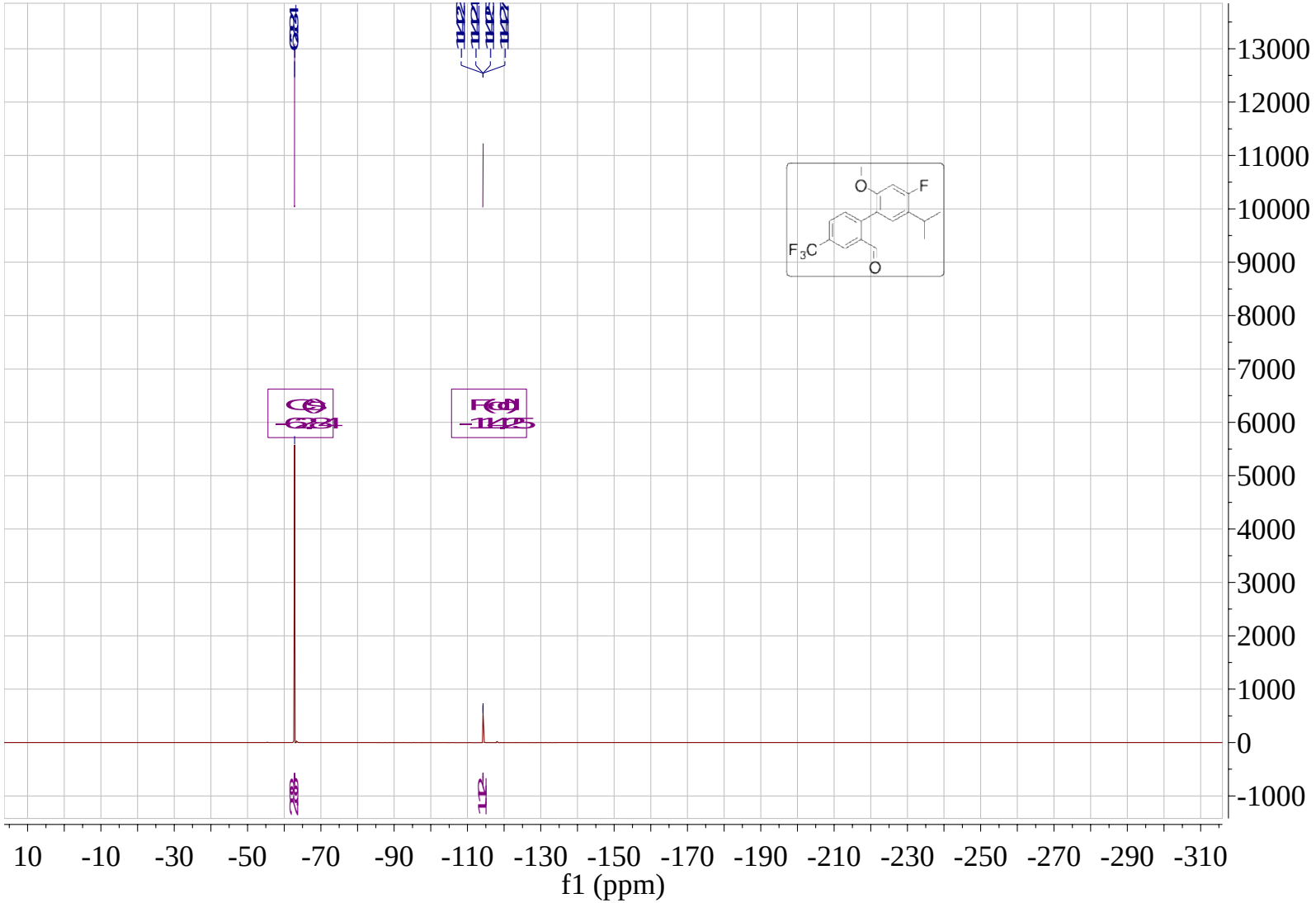

OCF3
HO
CO2Me
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
-310
f1 (ppm)

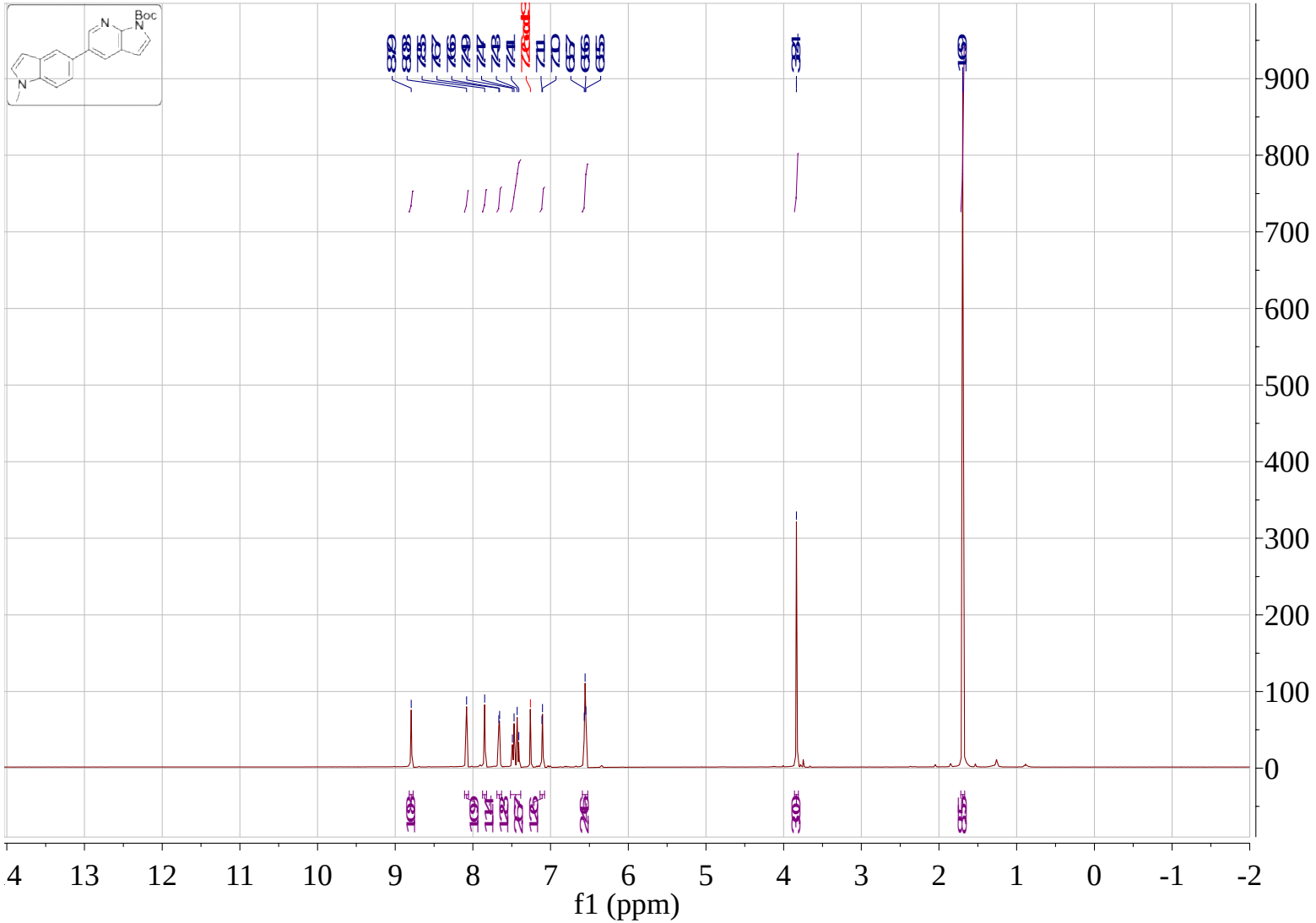

1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
1.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

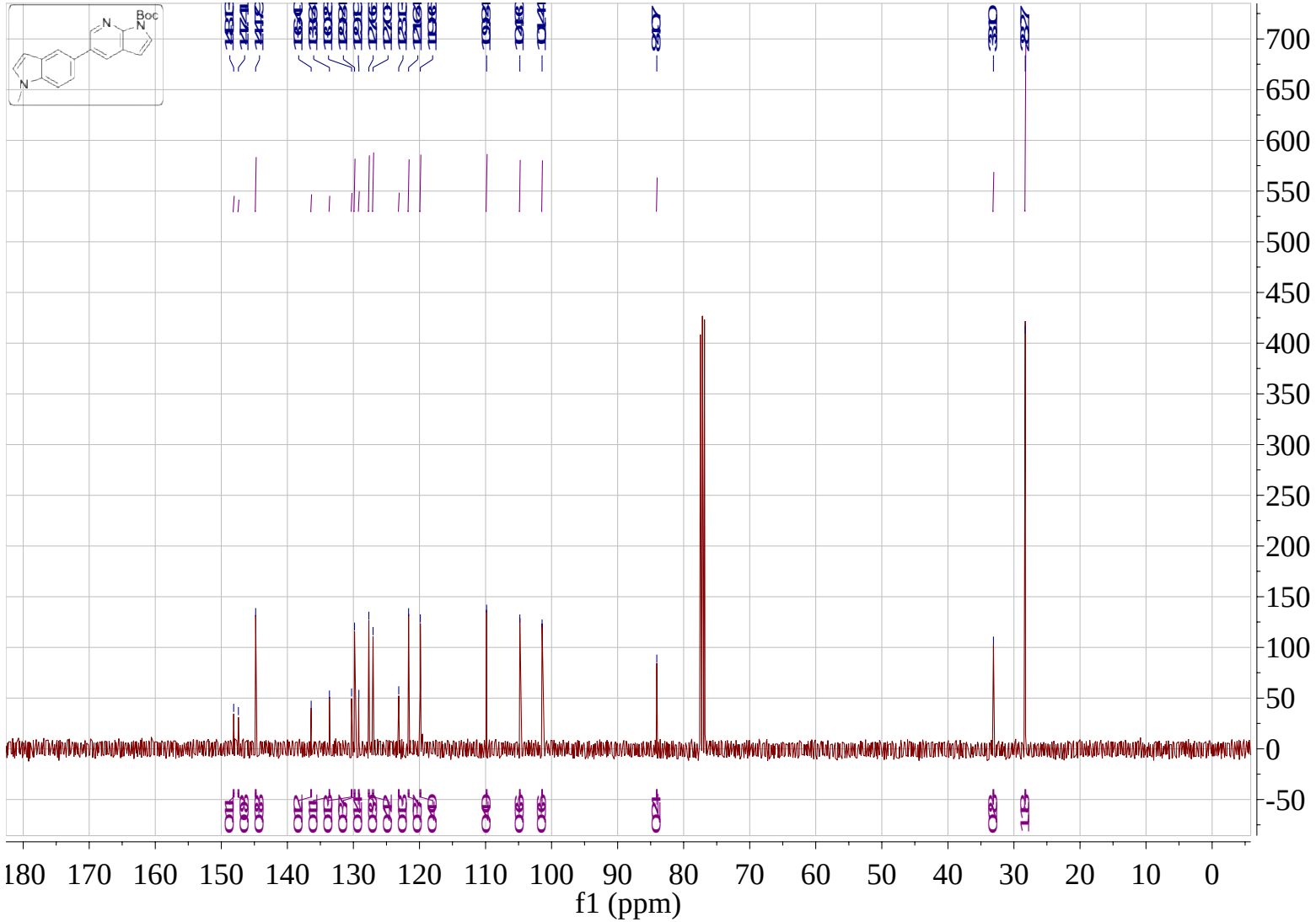


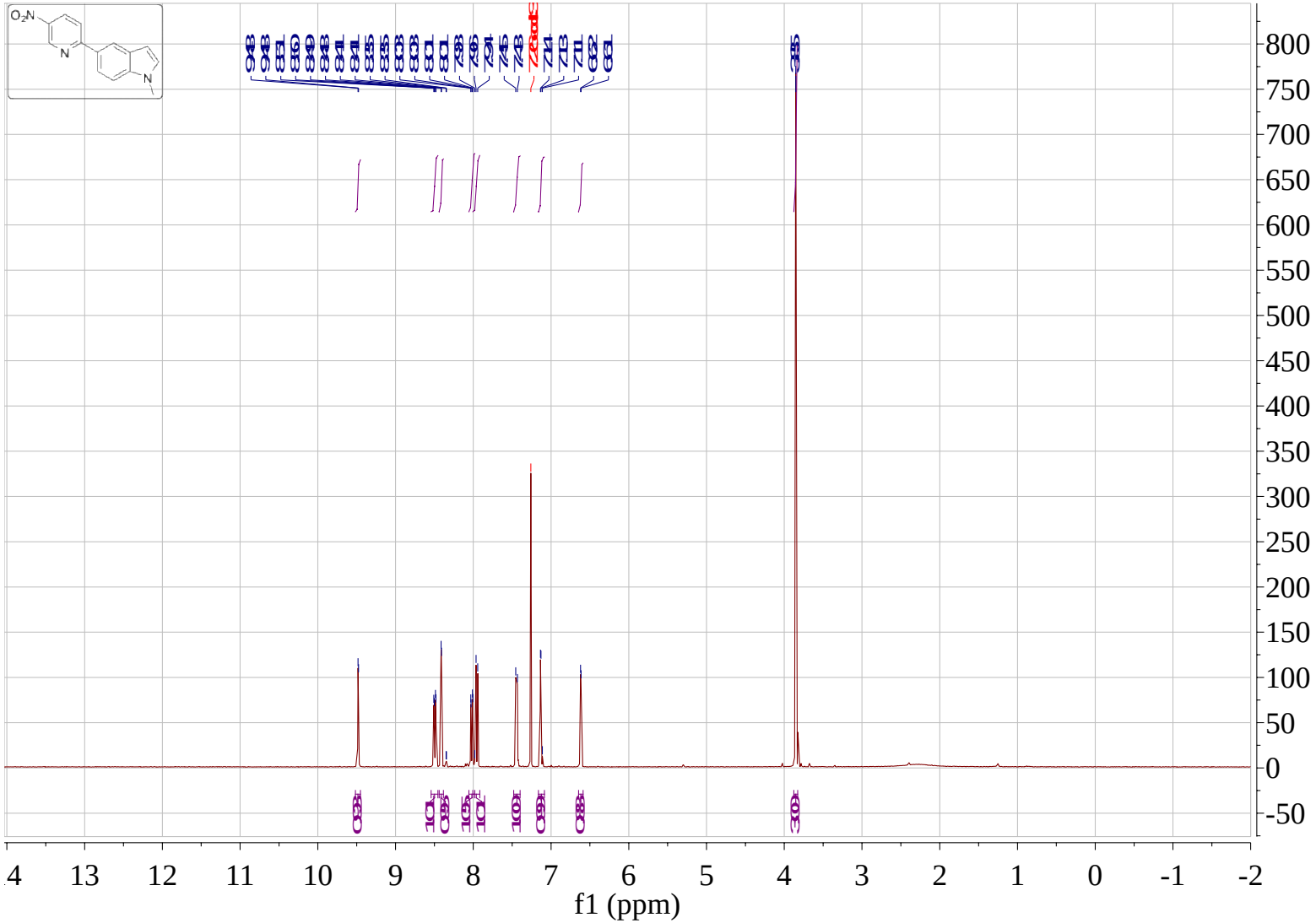

O
F
F3C
O
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

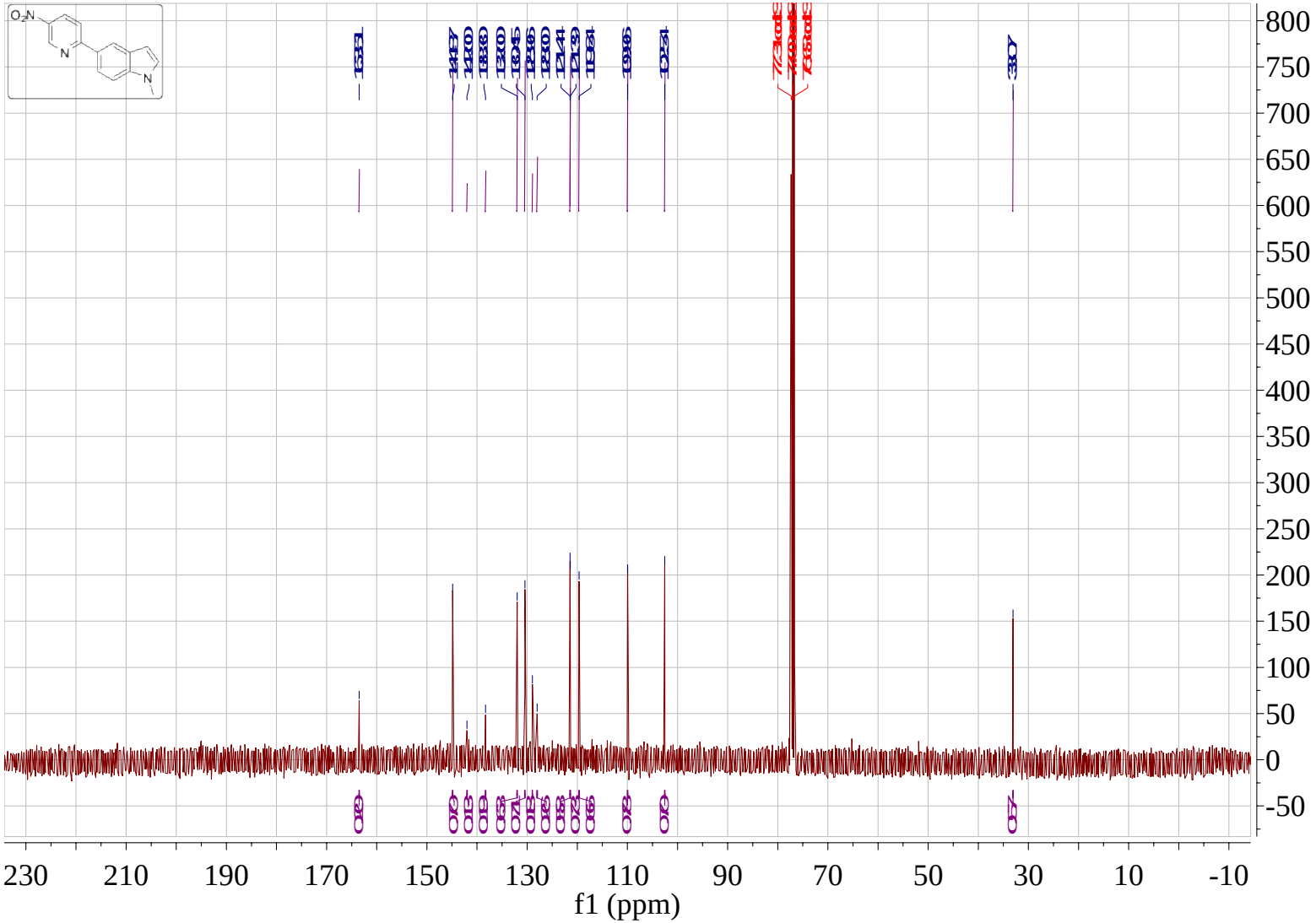

O
N
O
F
250
200
150
100
50
0
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

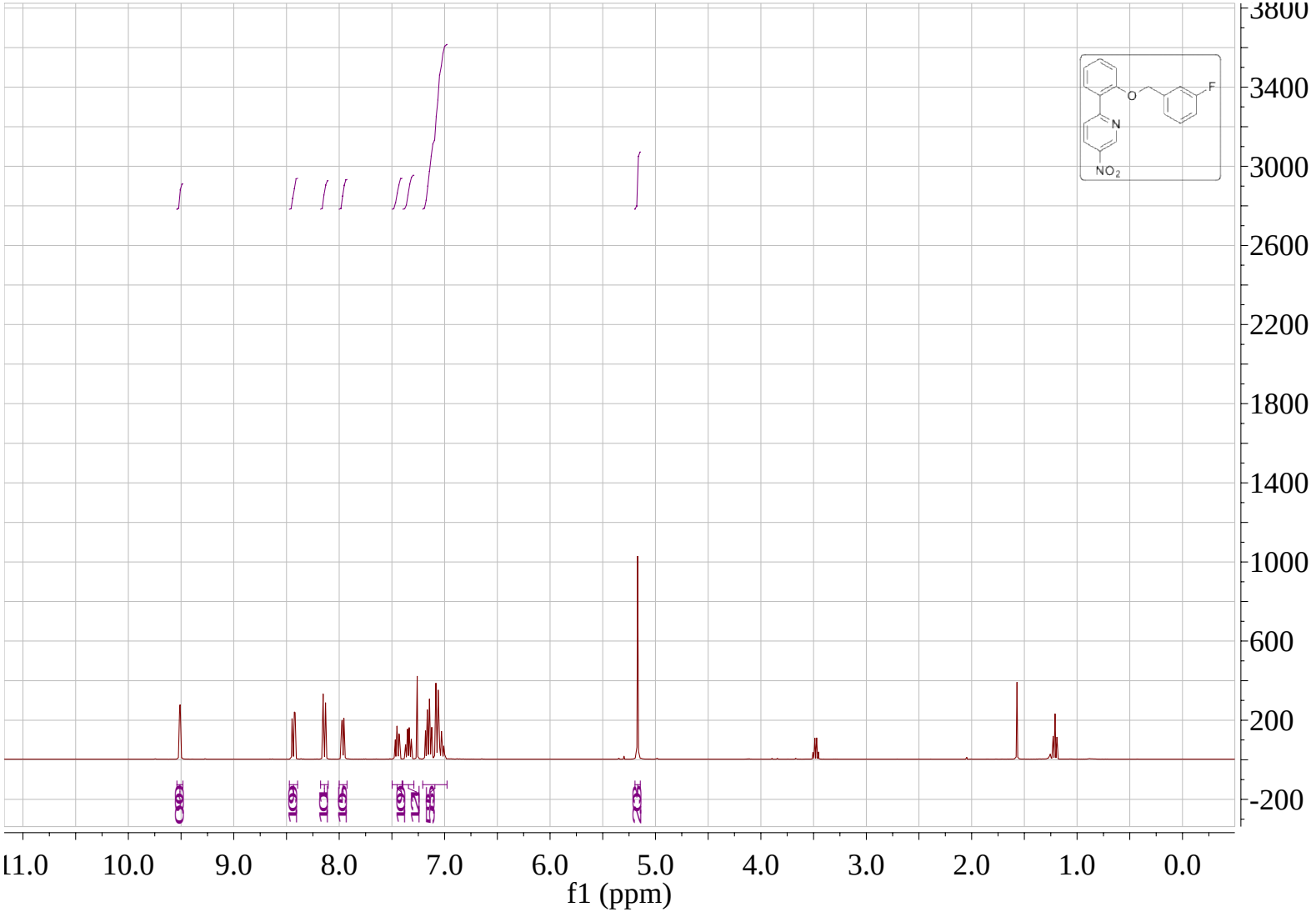

-63.4
-114.2
-114.2
-114.2
-114.2
-114.2
-114.2
-114.2
F
O
F3C
O
-63.4
-114.25
2.88
1.12
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290 -310
f1 (ppm)

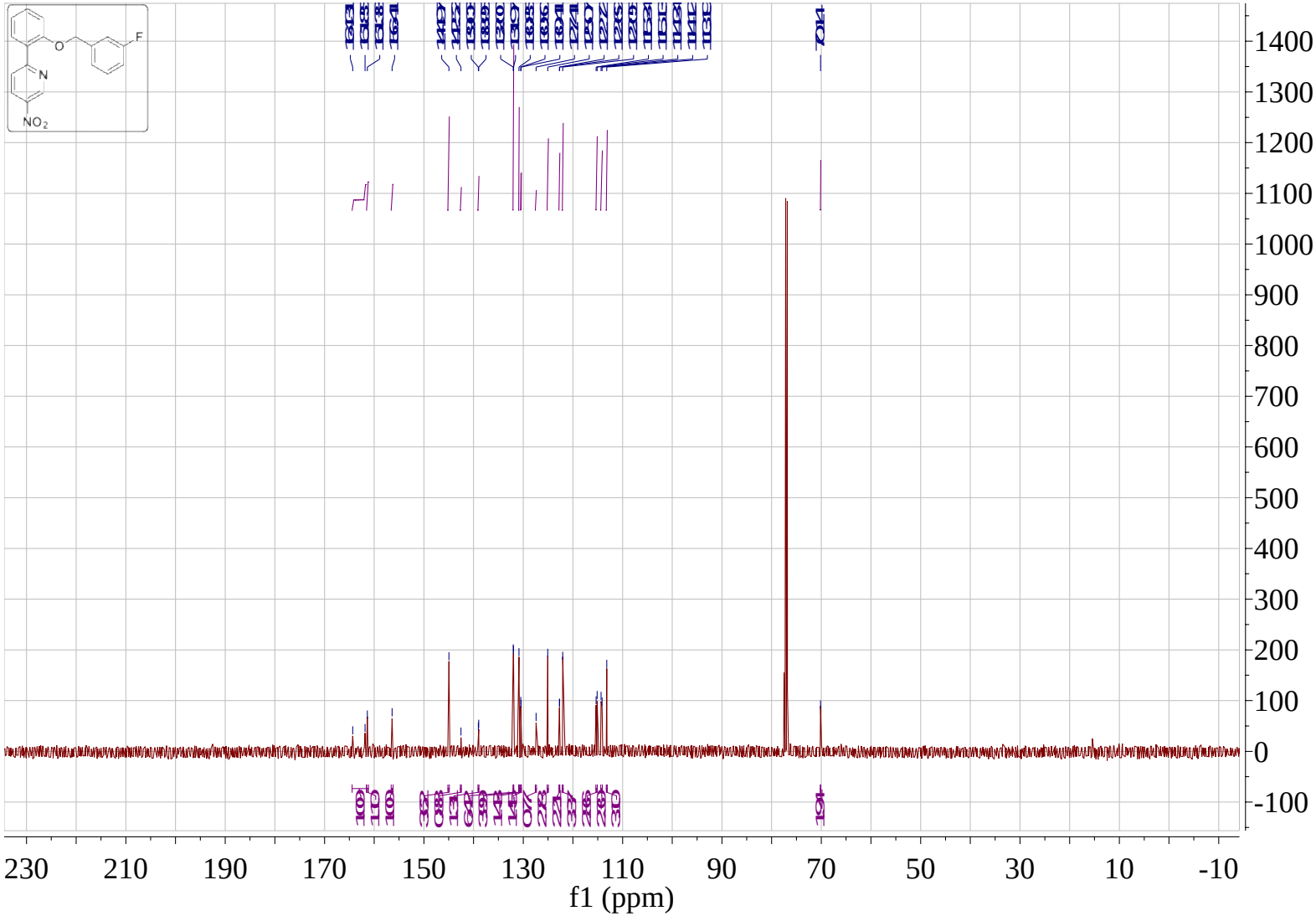

Boc
N
N
N
8.29
8.08
7.85
7.67
7.66
7.49
7.47
7.43
7.41
7.26
7.11
7.10
6.87
6.86
6.85
3.84
1.69
1.08
1.09
1.14
1.28
2.71
1.25
2.61
3.01
8.55
900
800
700
600
500
400
300
200
100
0
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

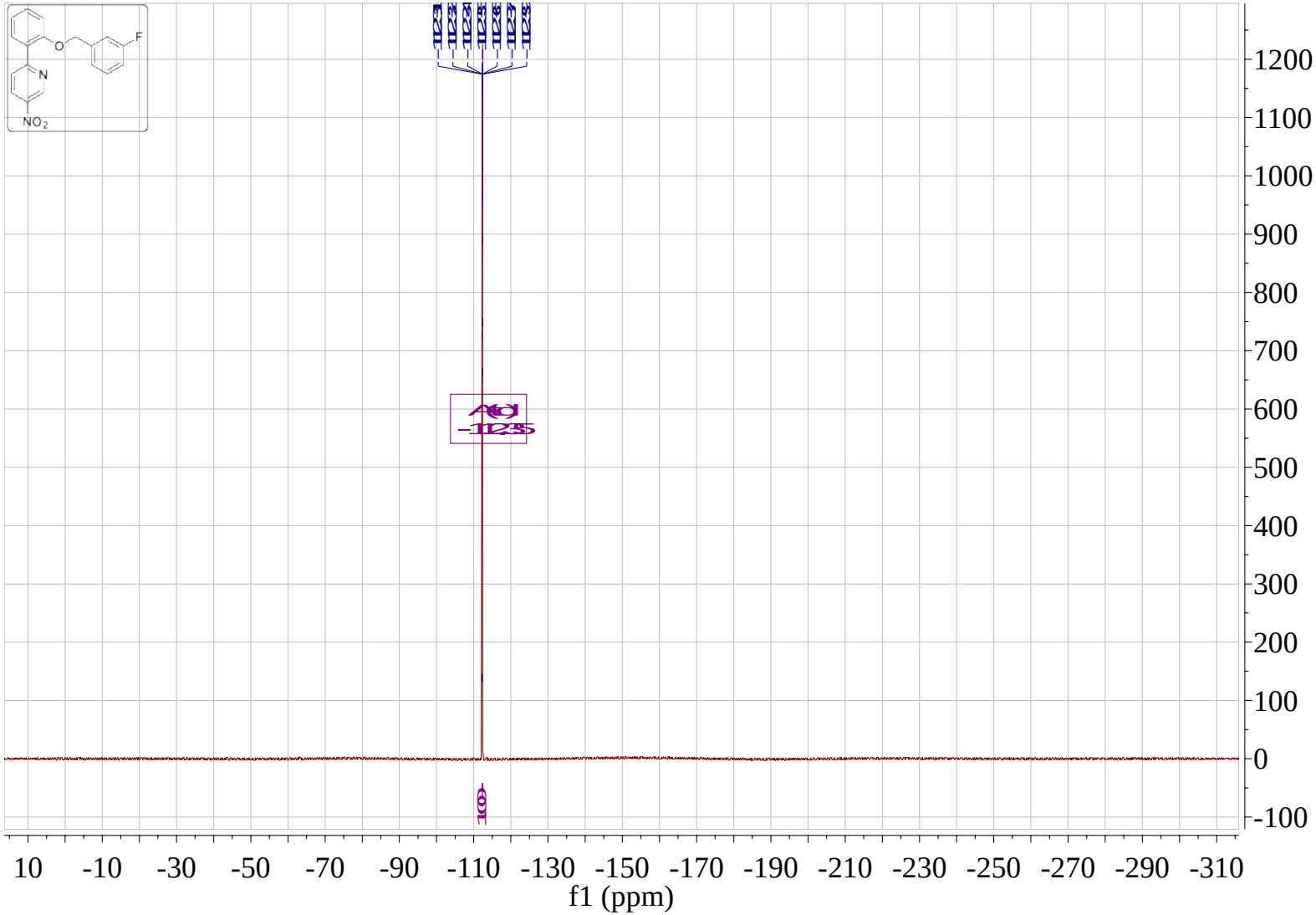

Boc
N
N
N
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

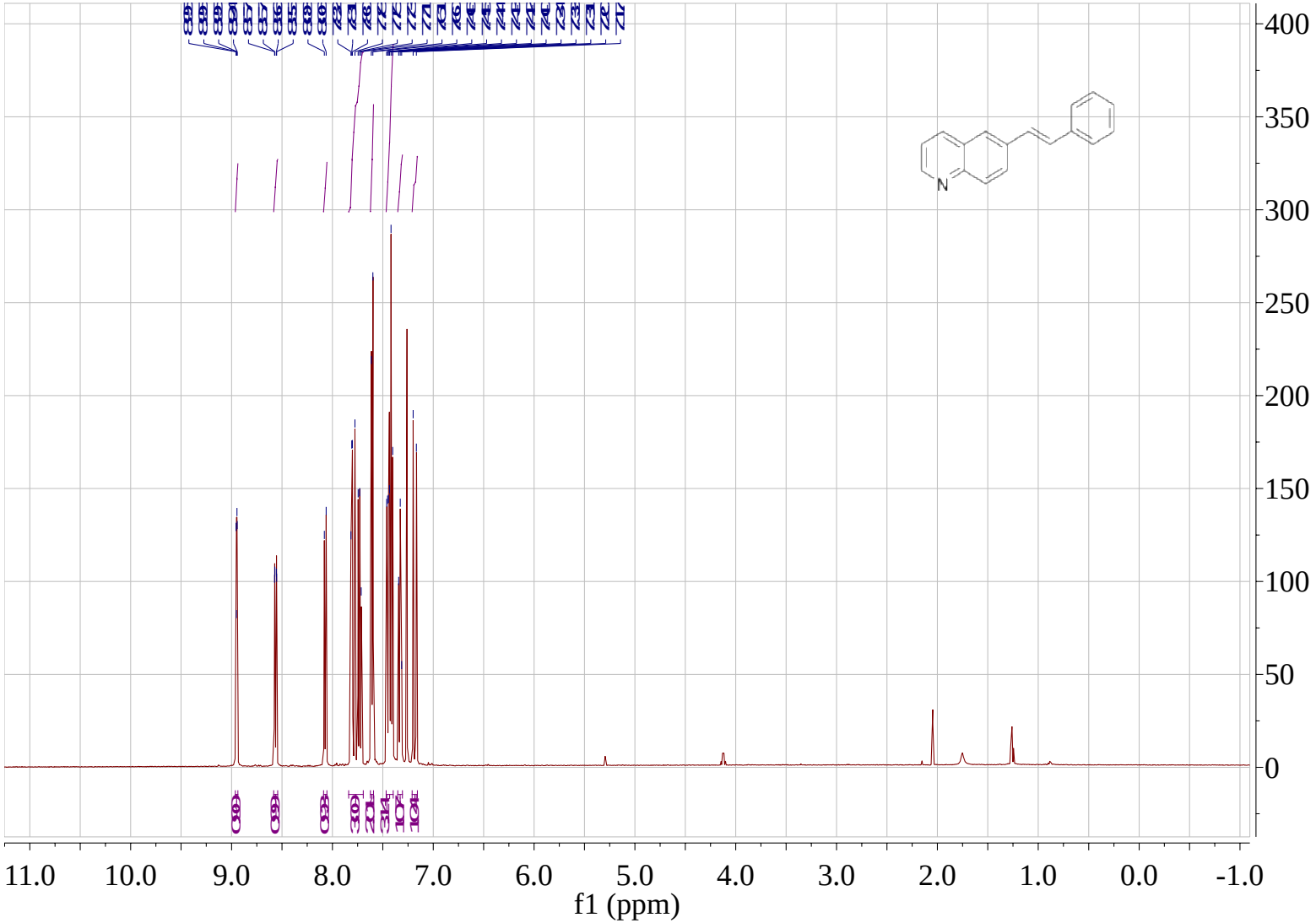

O2N
N
N
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

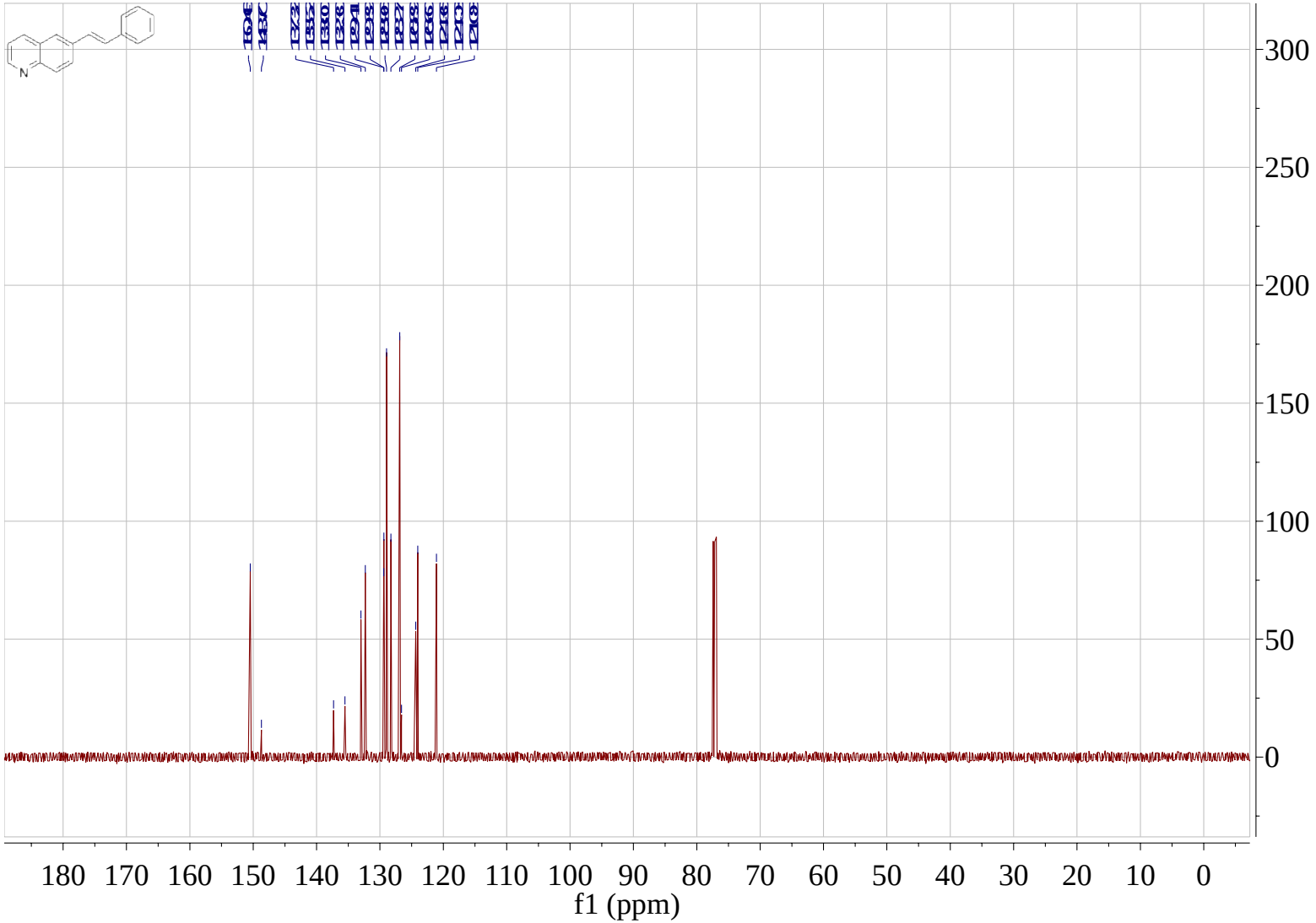

O2N
N
N
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

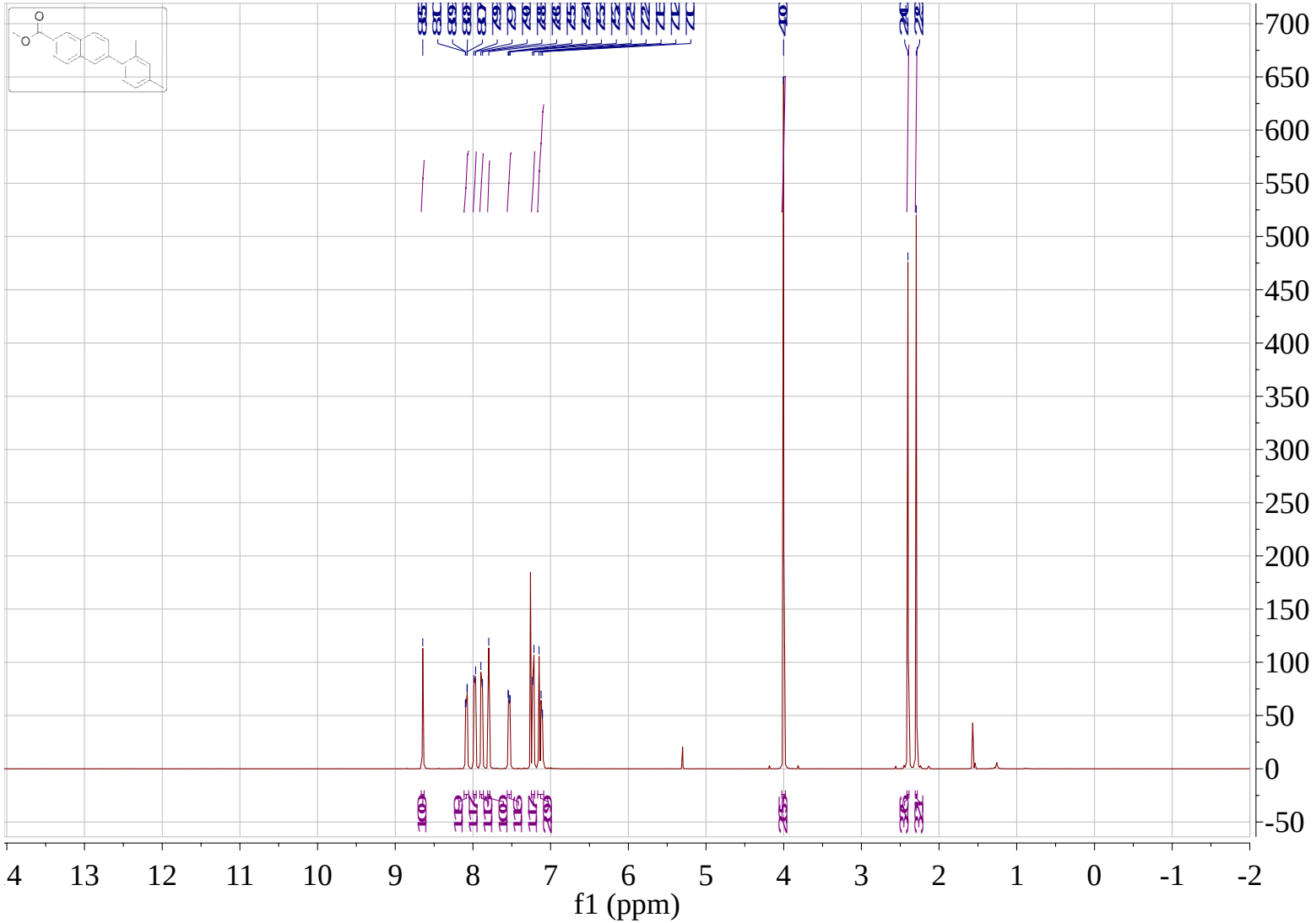

3800
3400
3000
2600
2200
1800
1400
1000
600
200
-200
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
O
F
N
NO2

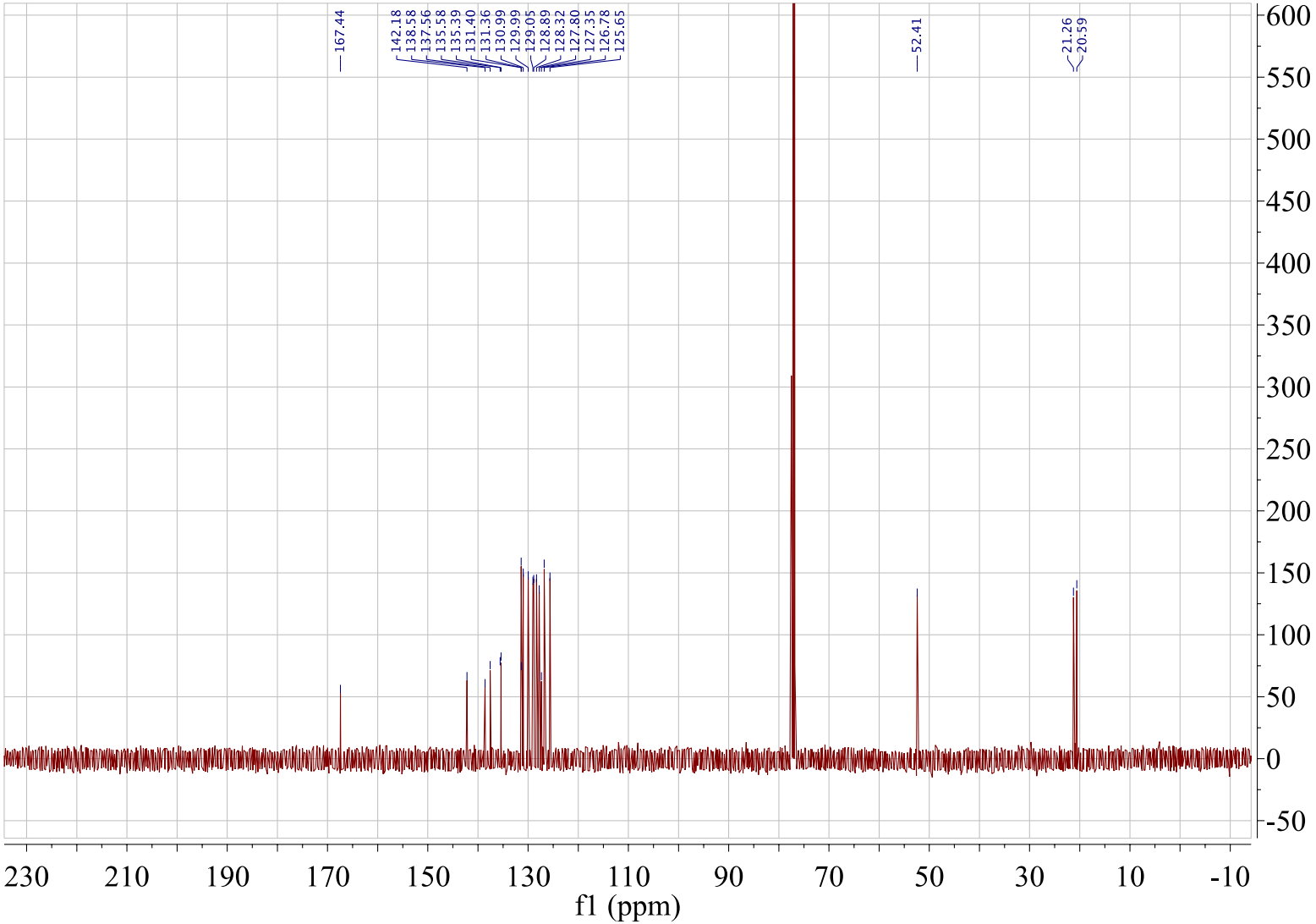

O
F
N
NO2
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

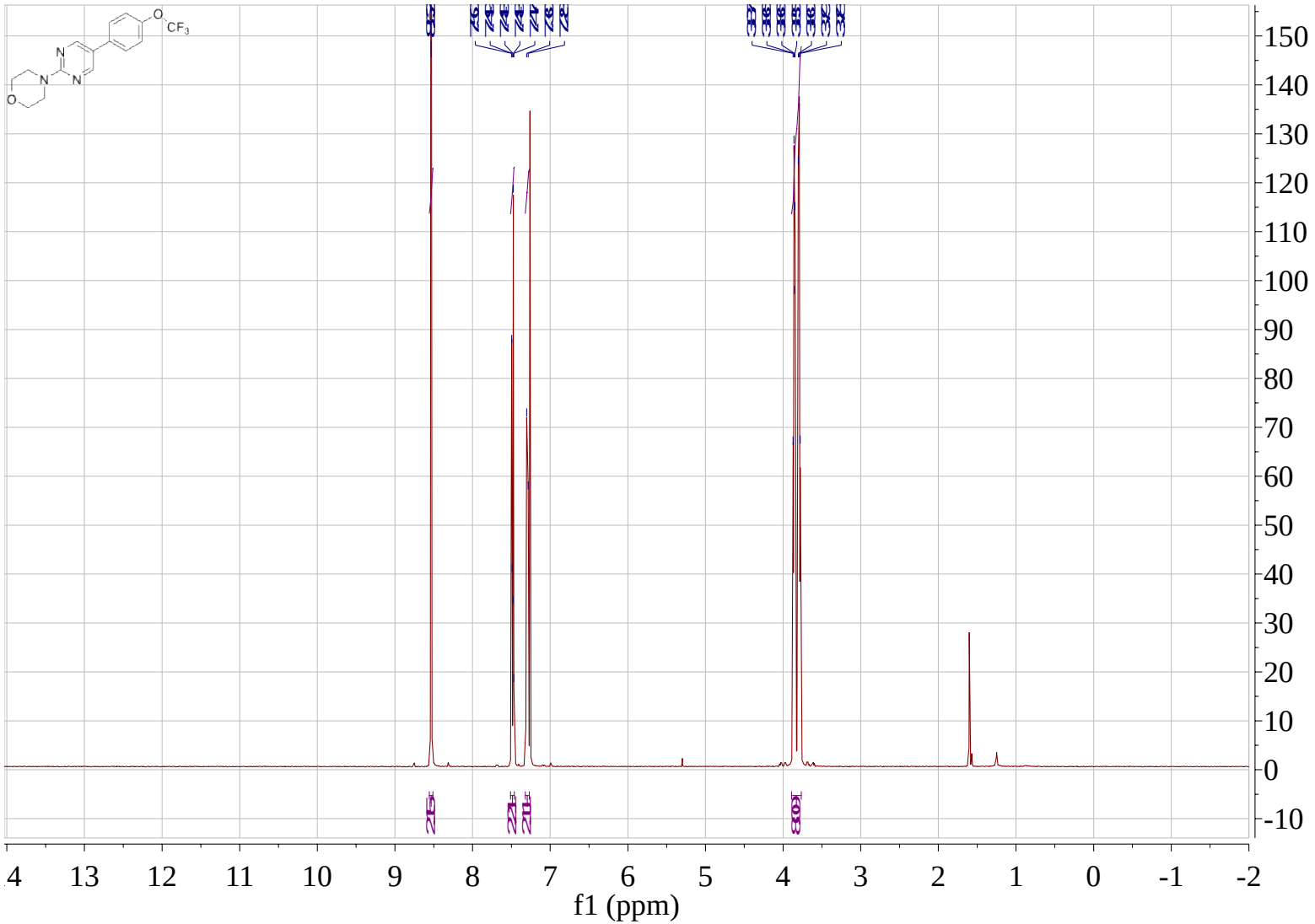

O
F
N
NO2
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
-230
-250
-270
-290
-310
f1 (ppm)

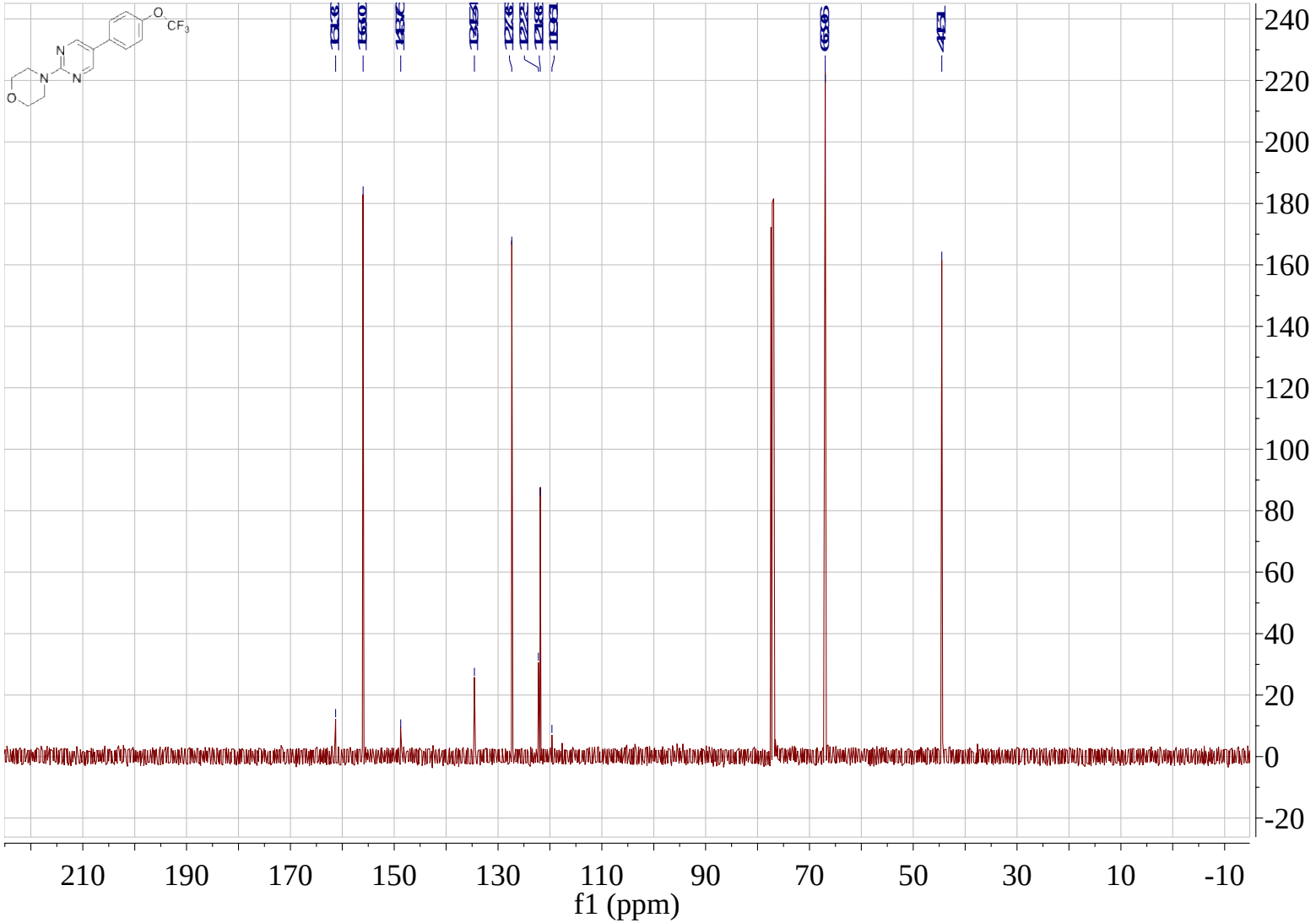

N
400
350
300
250
200
150
100
50
0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

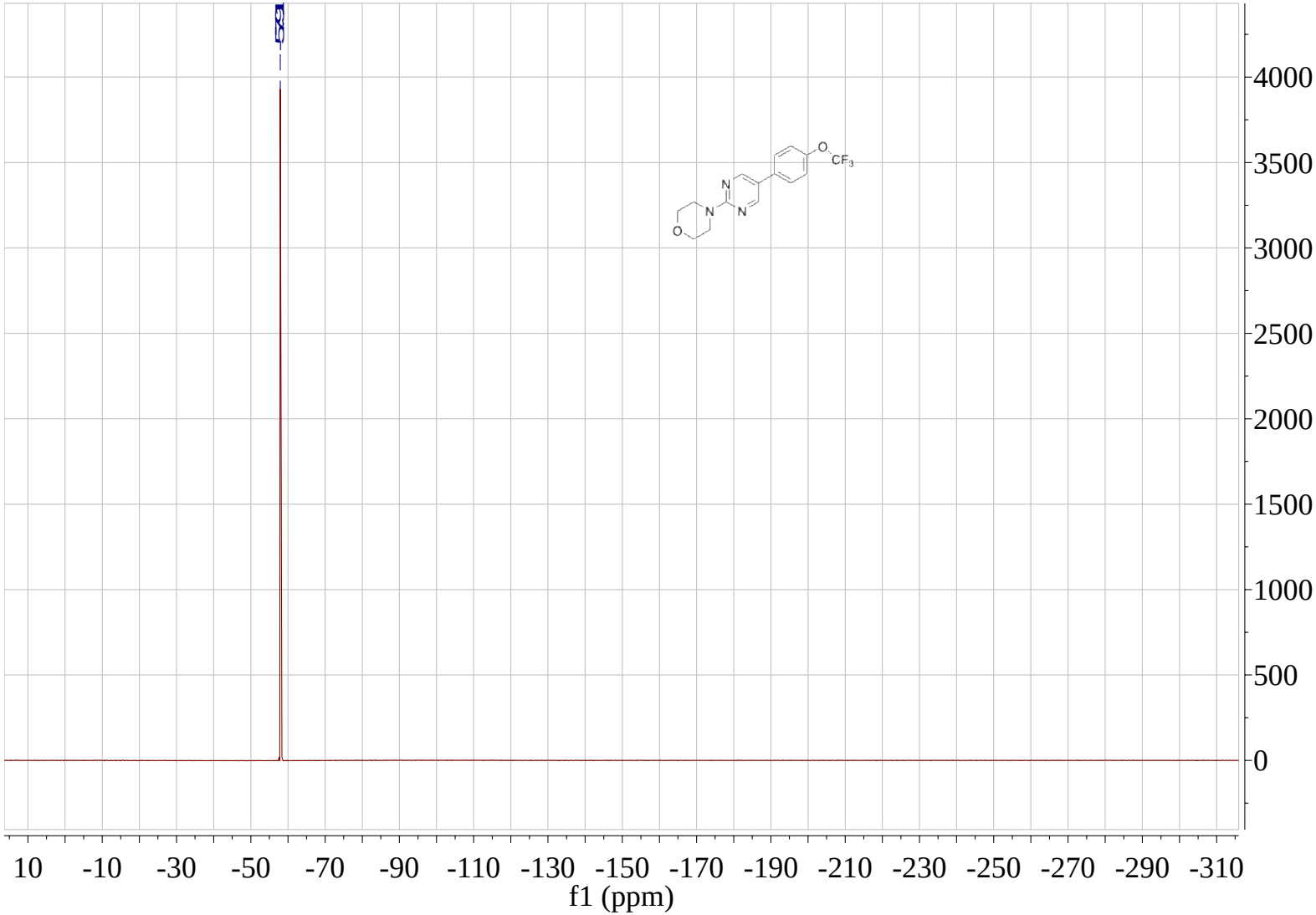

N
300
250
200
150
100
50
0
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

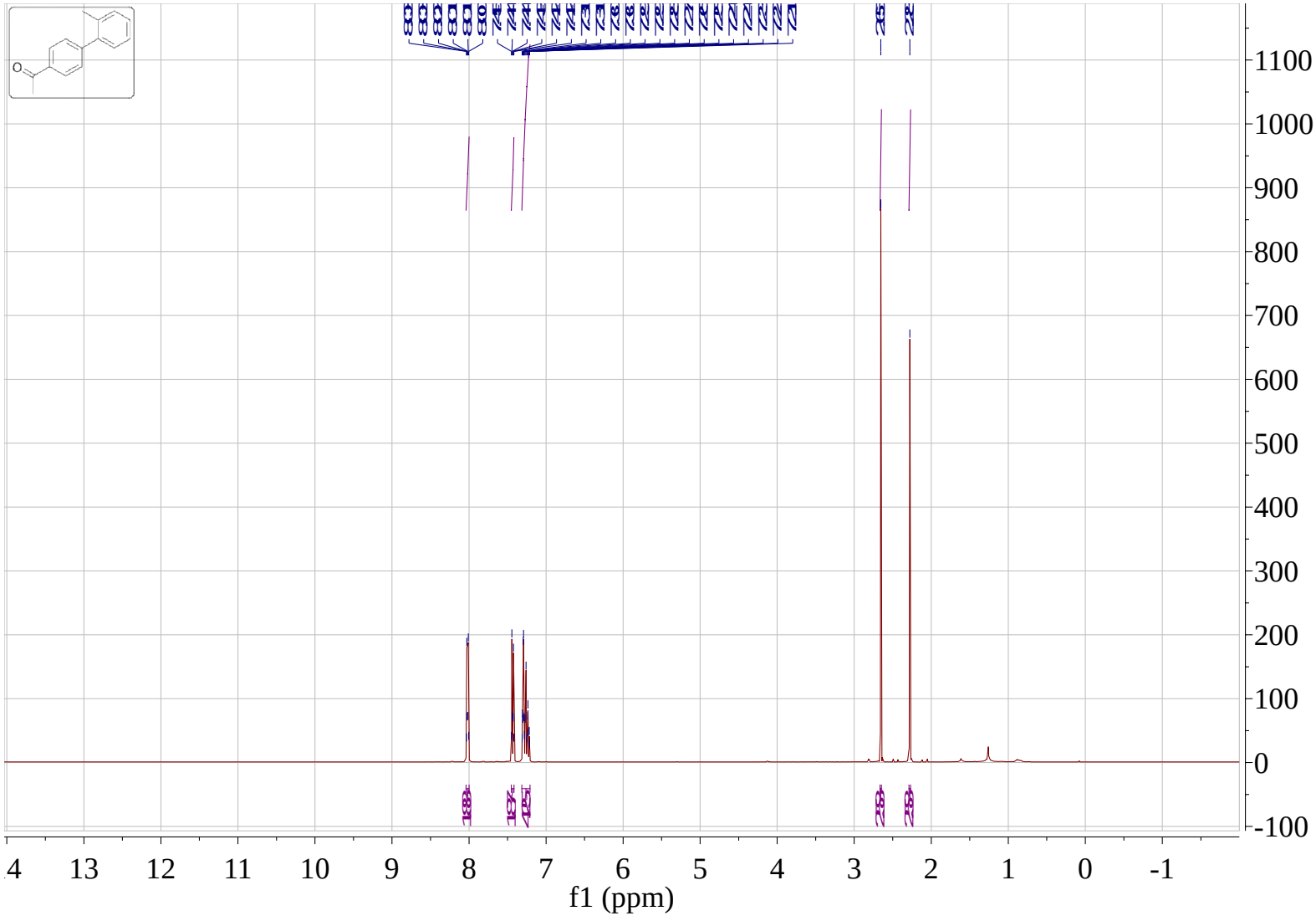

700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

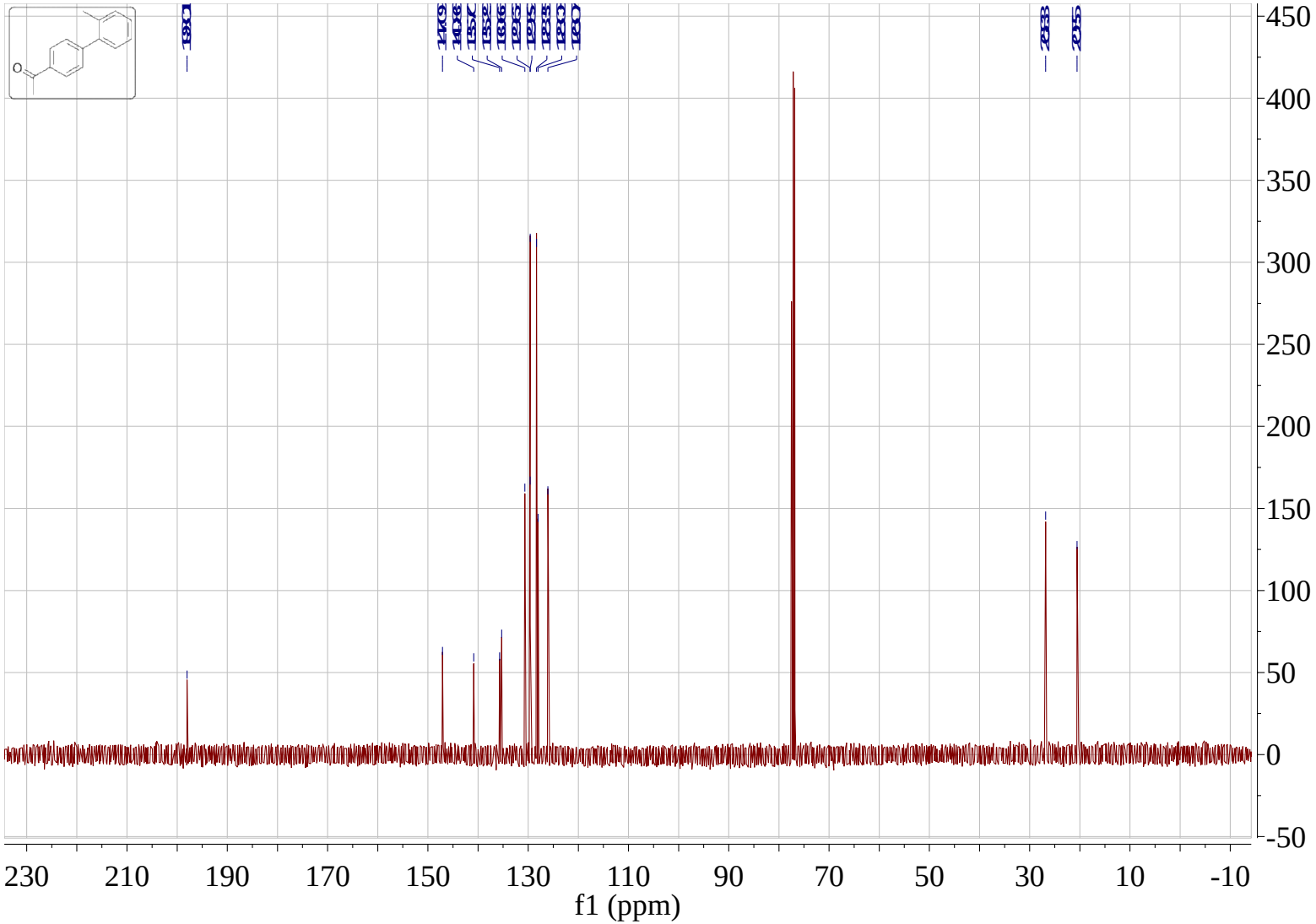

167.44
142.18
138.58
137.56
135.58
135.39
131.40
131.36
130.99
129.99
129.05
128.89
128.32
127.80
127.35
126.78
125.65
52.41
21.26
20.59
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

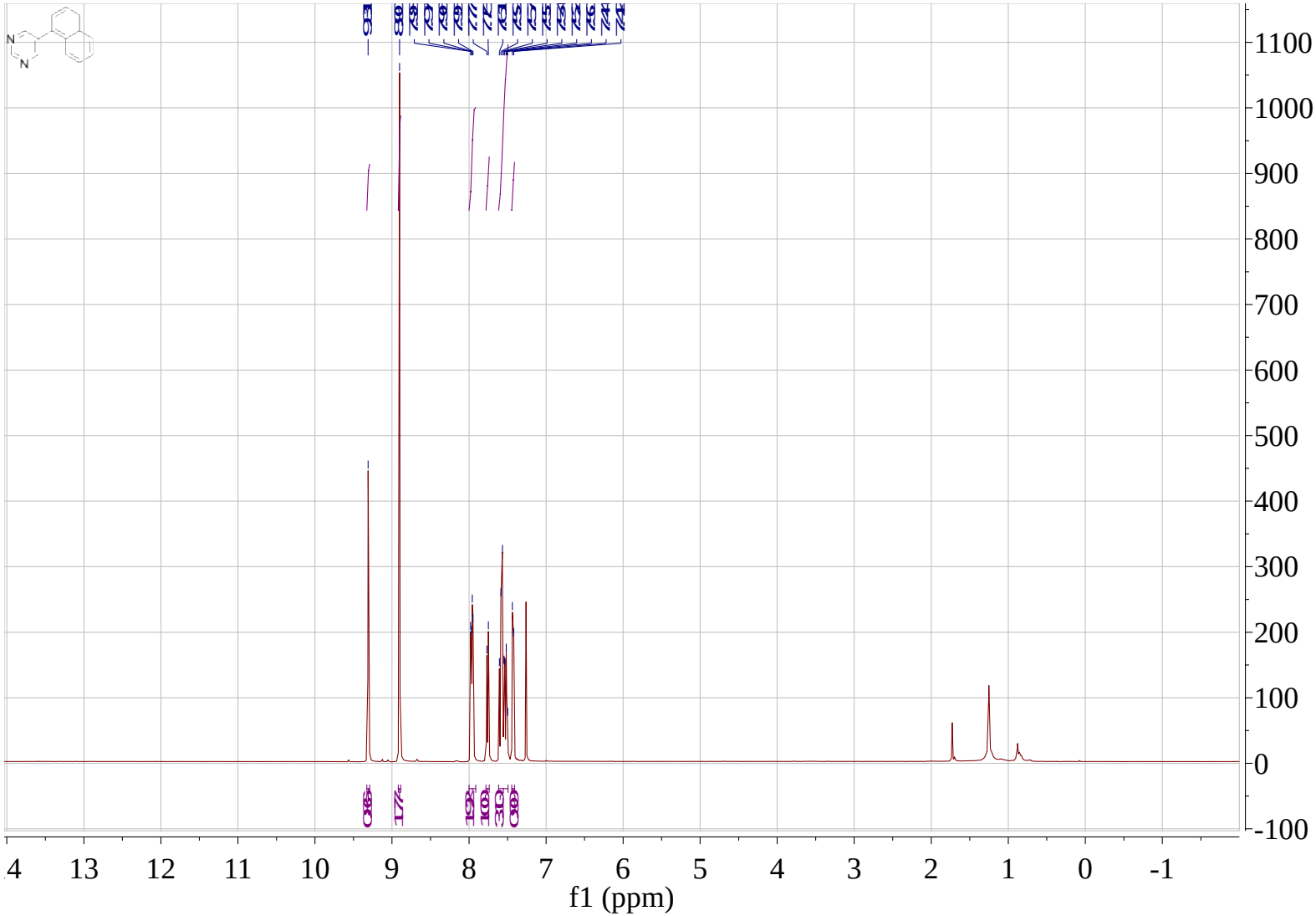

O
CF3
N
N
N
O
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

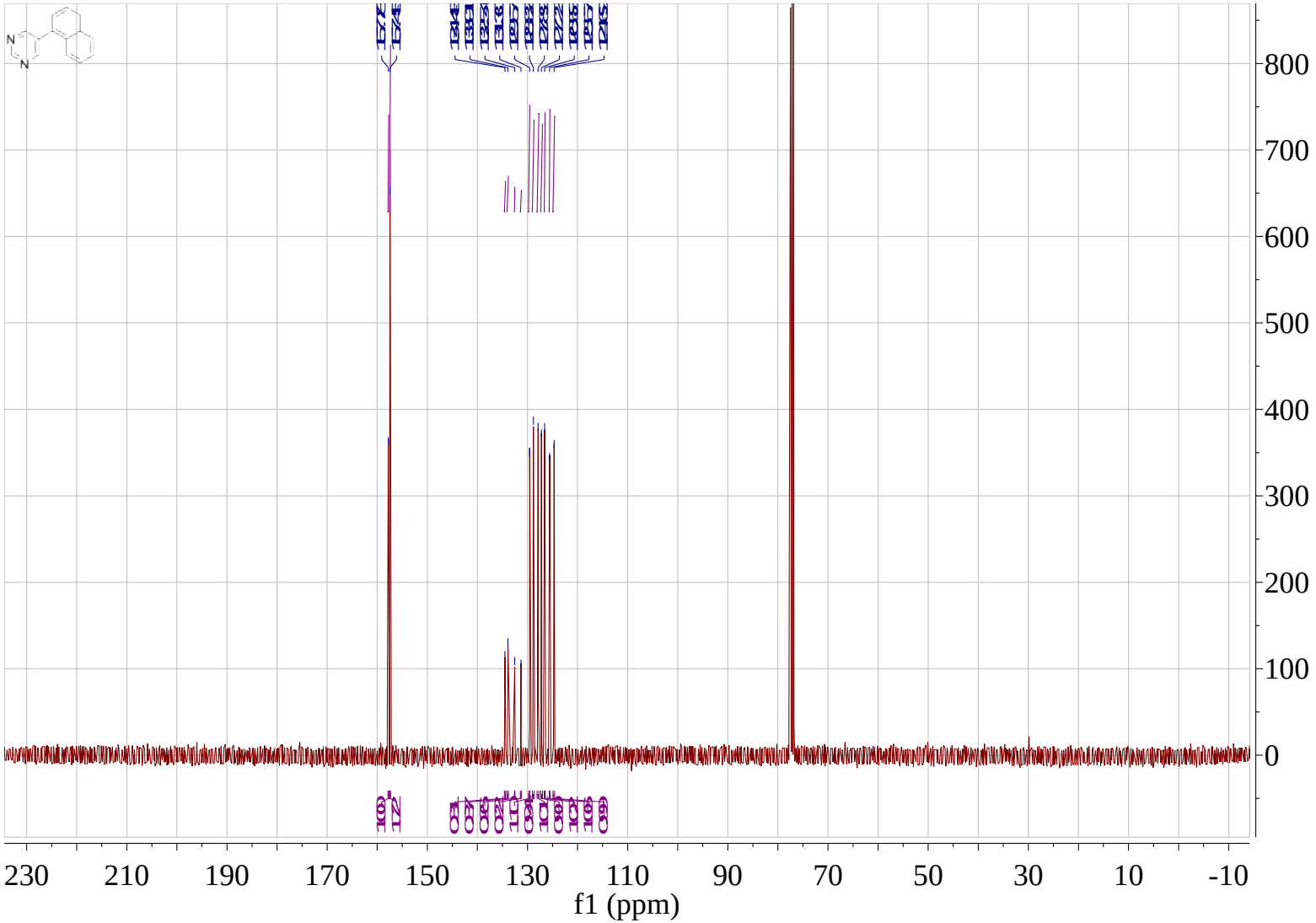

O
CF3
N
N
N
O
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


-59.1
4000
3500
3000
2500
2000
1500
1000
500
0
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290 -310
f1 (ppm)


1100
1000
900
800
700
600
500
400
300
200
100
0
-100
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


198.1
144.9
140.8
135.7
133.2
130.6
129.5
129.5
128.5
128.3
126.0
126.7
29.8
29.5
450
400
350
300
250
200
150
100
50
0
-50
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)


1100
1000
900
800
700
600
500
400
300
200
100
0
-100
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


800
700
600
500
400
300
200
100
0
230
210
190
170
150
130
110
90
70
50
30
10
-10
f1 (ppm)

Supporting Information II

EvanPhos. A New Ligand, Easily Made, Works in Organic Solvent or Water; Application to Suzuki-Miyaura Couplings

Evan Landstrom, Sachin Handa, Donald H. Aue*, Fabrice Gallou, and Bruce H. Lipshutz*

Department of Chemistry & Biochemistry, University of California,

Santa Barbara, California 93106, United States

COMPUTATIONAL RESULTS

Theoretical Methods. For molecules with no palladium, complete geometry optimizations were carried out using density functional theory (DFT) methods, at B3LYP/6-31G(d)[1] and M06/6-31G(d) [2], M06/6-31+G(d,p), and MN15/6-31+G(d,p)[3] levels. The basis set used for palladium was the SDD[4,5] effective core potential. M06/6-31G(d)(C,H,N,O,F,P)-SDD(Pd) level geometry optimizations and frequency calculations were carried out in order to verify that the stationary points thus obtained were true minima and to determine thermodynamic parameters for the determination of reaction energetics. MN15/6-31+G(d,p)(C,H,N,O,Cl,P)-SDD(Pd) single-point calculations, scf=tight, were done to get reaction energies. All M06 and MN15 calculations were done with the Gaussian 'int=ultrafine' option.

Thermochemical data were calculated with zero-point energy corrections from scaled frequencies using a scaling factor of 0.99 for zero-point energies.[6] A scaling factor of 1.00 for frequencies for the thermal and entropy terms was used. [6ab] The quasiharmonic approximation was used for low frequencies to calculate entropies to avoid the large distortions found when many low-frequency vibrations are present in organometallic compounds.[6c] Thus, frequencies below 100 cm^{-1} were treated as free rotors rather than by the harmonic approximation in calculating entropies. We have chosen a polarized continuum model in toluene (to mimic the interior of micelles) solvent for our calculations using the SMD method of Truhlar and Cramer.[7] Solvent effects by similar methods have been treated successfully for cases where quantitative comparison with experiment is possible.[8] All calculations were performed using the Gaussian 16 program suite.[9]

Solvation is expected to play a role for these polar species, generally favoring species with high charge densities.[10] It is not certain what polarity to expect for the medium in the interior of the micelles containing

these palladium complexes. Some experiments to probe this issue were carried out with the commercially available 2,6-di-t-butyl-4(2,4,6-triphenyl-1-pyridino) phenolate E_T dye[11] dissolved in the TPGS-750-M micelle used in this work. These experiments gave an E_T value similar to n-propanol. This is more polar than we would expect for the hydrophobic region of the micelle. Despite the t-butyl groups encumbering the phenoxy anion end of the dye, it appears that the phenoxy group is attracted to the polar interface of the micelle by hydrogen bonding to water in that region as seen to a greater extent for the less encumbered 2,6-di-t-butyl-4(2,4,6-triphenyl-1-pyridino) phenolate $E_T(30)$ dye.[12] It is likely that toluene solvent best mimics the micellar environment of our palladium complexes.

Theoretical Results. The structures and energies of the pre-reductive elimination intermediate and the reductive elimination transition state for the Suzuki reaction to form biphenyl as the coupling product were calculated using DFT methods to help understand how EvanPhos functions and how it might be improved and how stereochemical control might be achieved from the reductive elimination transition state where any stereochemistry in a coupling product would be determined.

In Scheme S1 and Tables S1 and S2 is a summary of the structures and free energies at 298K calculated for different conformations (in order of increasing free energy) for four basic structures, **A**-**F** (EvanPhos ligand), **G**-**H** and **G'**-**H'** (pre-reductive elimination intermediates), **TS1**-**TS2** (reductive elimination TS), and **I**-**J** $(EvanPhos)_2PdCl_2$). Table S1 compares bond distances and angles between the X-ray structure and the calculated structure **I**.

The energies of the two best conformations, **A** and **B**, for the ligand EvanPhos are nearly identical for the rotation of the naphthalene ring, with a slight preference for rotation of the majority of the naphthalene ring toward the out-of-plane (CO-C=C dihed angle 84.9º) methoxy methyl of the dimethoxybenzene ring and further away from the phosphine. The two cyclohexyl rings in **A** are oriented with the methine hydrogens at dihedral angles (H-C-P-C=, gauche, syn to the out-of-plane methoxyl) 41.7º and (H-C-P-C=, gauche, anti to the out-of-plane methoxyl) 57.2º. The aromatic rings are twisted with a dihedral angle (O)C=C-C=C(O) of 72.5º. Some conformers **C** to **F** have various alternative rotational arrangements of the cyclohexyl rings and methoxy groups, and are all higher in free energy.

For the diphenyl palladium pre-reductive elimination complexes, we did not do exhaustive conformational searches, but took advantage of what was learned about the preferred ligand conformations from the studies above of conformations of the free ligands. We also find that the optimized geometries of the ligand moiety here and in the transition states are similar to those found in the X-ray crystal structure discussed below for the ligand dimer, $(EvanPhos)_2PdCl_2$, **I .** In the diphenyl palladium complexes **G** and **H**, there is a clear preference for the conformer **G** with the majority of the naphthalene ring rotated away from the out-of-plane methoxy methyl of the dimethoxybenzene ring, toward the phosphine, and away from the Pd in the B3LYP/6-

31G(d)-SDD(Pd) geometries. The structure **G** is a square planar complex with a C-Pd-C angle of 87.68° and a short 2.330 Å Pd-O bond to a methoxy oxygen on the resorcinol ring. The two cyclohexyl rings in **G** are oriented with the methine hydrogens at dihedral angles (H-C-P-C=, gauche, syn to the out-of-plane methoxyl) 36.9º and (H-C-P-C=, gauche, anti to the out-of-plane methoxyl) 58.5º. The aromatic rings are twisted with a dihedral angle (O)C=C-C=C(O) of 70.5º, all similar to structure **A**. In the gas phase, structure **G** is more stable by 0.83 kcal/mol in electronic energy, 0.68 kcal/mol in enthalpy and 0.46 kcal/mol in free energy at 298K at the B3LYP/6-31G(d)-SDD(Pd) level. The MN15/6-31+G(d,p)-SDD(Pd) free energy difference, using the B3LYP structure and frequency data, is 1.07 kcal/mol, and the free energy difference in toluene solvent is 0.56 kcal/mol. In addition, we found two other structures **G'** and **H'**, with a palladium center that is within 0.14^{o} of planarity and has a T shape with a =C-Pd-C= angle of 162.0º. One methoxyl group in **G'** is twisted out of plane with a COC=C dihedral angle of 46.3º and appears to be weakly bound to Pd from above the C-Pd-C plane with a P-Pd-O angle of 65.1º and a Pd-O distance of 3.05 Å. **G'**, with the naphthyl group anti to Pd, is again lower in energy than **H',** with the naphthyl group syn, by 2.97 kcal/mol free energy at 298K at the B3LYP/6-31G(d)-SDD(Pd) level. This intermediate **G'** is 20.43 kcal/mol higher in free energy [B3LYP/6-31G(d)-SDD] than **G**, in part reflecting the strength of the increasing degree of methoxy coordination in **G**, which seems to have a remarkably large effect that might be further exploited in catalyst design.

The reductive elimination transition states are also roughly square planar in nature, but with a C-Pd-C angle of 60.25° and a longer 2.936 Å distance to the nearly coplanar methoxy oxygen in **TS1**. The free energy of activation for reductive elimination in toluene is calculated for **G** to **TS1** to be 14.1 kcal/mol [MN15/6-31+G(d,p)-SDD] at 298K in toluene continuum solvent to mimic a micellar environment. Without the methoxy group on the naphthyl ring the free energy of activation in toluene is predicted to be 12.7 kcal/mol. In the gas phase, structure **TS1** is more stable by 0.14 kcal/mol in electronic energy, 0.11 kcal/mol enthalpy and 0.05 kcal/mol free energy at 298K at the B3LYP/6-31G(d)-SDD(Pd) level. The MN15/6-31+G(d,p)-SDD(Pd) free energy difference, using the B3LYP structure and frequency data, is -0.09 kcal/mole, and the free energy difference in toluene with the SMD continuum model is -0.01 kcal/mol. The negative (imaginary) frequencies for **TS1** and **TS2** were -274 and -276 cm-1, respectively, and atomic vectors for each showed a clear motion toward C-C bond formation between the phenyl groups.

Comparison of theoretical structures for the ligand dimer, $(EvanPhos)_2PdCl_2$, with experimental X-ray crystal structure provides a valuable opportunity to test different DFT methods for accuracy and to confirm which conformational isomers are more stable. The two cyclohexyl rings in **I** are oriented with the methine hydrogens at dihedral angles (H-C-P-C=, gauche and syn to the out-of-plane methoxyl) 73.7º and (H-C-P-C=, gauche and distal to the out-of-plane methoxyl) 71.0º. The two aromatic rings are twisted with a dihedral angle (O)C=C-C=C(O) of 107.0º. An alternative conformer, **J**, has a B3LYP/6-31G(d)-SDD(Pd) geometry with the naphthyl ring rotated 180 º with the majority of the naphthyl ring away from the Pd. This conformer is,

however, 1.72 kcal/mol higher in free energy at 298K at the B3LYP/6-31+G(d,p)-SDD(Pd) level of theory. In **H**, the palladium center is within 0.4º of planarity and has a T shape with a =C-Pd-C= angle of 159.0º. One methoxyl group is twisted out of plane with a COC=C dihedral angle of 73.1º appears to be weakly bound to Pd from above the C-Pd-C plane with a P-Pd-O angle of 67.7º and a Pd-O distance of 3.080 Å. The two cyclohexyl rings in **I** are oriented with the methine hydrogens at dihedral angles (H-C-P-C=, gauche and syn to the out-of-plane methoxyl) 83.4º and (H-C-P-C=, gauche and distal to the out-of-plane methoxyl) 73.1º. The two aromatic rings are twisted with a dihedral angle (O)C=C-C=C(O) of 100.9º.

The calculated structure of the preferred gas-phase conformer of $(EvanPhos)_2PdCl_2$ **I** (C_2 symmetry) has the majority of the naphthalene ring rotated toward the phosphine and Pd and a somewhat different orientation of the cyclohexyl rings compared to **A** or **G**, fully consistent with the experimental X-ray structure. One methoxyl group is twisted out of plane with a COC=C dihedral angle of 40.6 º appears to be weakly bound to Pd from above the P-Pd-Cl plane with a P-Pd-O angle of 60.6º and a Pd-O distance of 3.171 Å. The corresponding C_2 conformer **J**, with the naphthylene ring rotated 180º, is 1.72 kcal/mol higher in free energy than **I** at 298K at the B3LYP/6-31G(d)-SDD(Pd) level, 2.07 kcal/mol optimized at the B3LYP/6-31+G(d,p)-SDD(Pd) level, and 3.91 kcal/mol optimized at the M06/6-31+G(d,p)-SDD(Pd) level, and 4.36 kcal/mol optimized at the MN15/6-31+G(d,p)-SDD(Pd) level using B3LYP/6-31G(d)-SDD(Pd) frequencies in all cases. Table S1 shows a comparison of selected geometry parameters for I at these levels of theory with all levels reasonably close to the experimental X-ray data. The M06 and MN15 methods are slightly closer to experiment, suggesting that these levels might also give better energies. Table S1 show that the B3LYP/6-31G(d)-SDD(Pd) level used elsewhere in this work gives a geometry close to that of the other levels of theory, especially to the B3LYP/6-31+G(d,p)-SDD(Pd) geometry.

These computational results suggest that the methoxy group does not have any large electronic or steric effect on the reductive elimination barrier and perhaps not for other reactions in the mechanism. The overall mechanism for Suzuki couplings is complicated, but experiments suggest that the rate-determining step is more likely in the transmetallation phase of the reaction than in the reductive elimination.[13] The rates for Suzuki reactions with the methoxy substituent don't appear to be much different experimentally from those with a hydrogen substituent. This is consistent with expectations from the DFT calculations suggesting any rate differences are likely to be the result of subtle, and perhaps relatively small, rate effects.

Acknowledgments. We are pleased to acknowledge support from the Center for Scientific Computing at the CNSI and MRL: NSF MRSEC (DMR-1121053) and NSF CNS-0960316, and the use of software for 3-D drawings from CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).

References:

[1] A. D. Becke *J. Chem. Phys*. **1993**, *98*, 5648.

[2] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.

[3] Yu, H. S.; He, X.; Li, S. L.; Truhlar, D. G. *Chem. Sci.* **2016**, *7*, 5032-5051.

[4] P. J. Hay and W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299.

[5] From EMSL Library of Basis Set Exchange: Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L. *J. Chem. Inf. Model*. **2007**, *47*, 1045-1052.

[6] (a) A. P. Scott, L. Radom *J. Phys. Chem*. **1996**, *100*, 16502. (b) I. M. Alecu, J. Zheng, Y. Zhao, and D. G. Truhlar,. *J. Chem. Theory Comput.* **2010,** *6,* 2872–2887. (c) R. F. Ribeiro, A. V. Marenich, C. J. Cramer, and D. G. Truhlar *J. Phys. Chem*. *A* **2011**, *115*, 14556-14562. (d) D. H. Aue, to be published. We have evaluated optimum scale factors for experimental fundamental frequencies for numerous organic molecules and find that the DFT scale factors differ with basis set between 0.96 for the B3LYP/6-31G(d) and 0.954 for M06-2X/ 6-311+G(d,p) levels to 0.967 for the B3LYP/ 6-311G(d,p) level. For thermal terms and entropies, such variation has little effect, and one may argue that a scaling factor close to 1.00 might be best for the dominant low frequencies (we get 1.005 for 111 frequencies below 150 cm^{-1})(see also ref. 6a). For zero point energies determined from experimental values and CCSD(T)-F12/cc-aug-pVDZ values, the scale factors 1.00 (B3LYP/6-311G(d,p)), 0.984 (M06-2X/6-311+G(d,p)), 0.991 (M06/6-31G(d)), 0.996 (M06/6-31+G(d,p)) give the best fit for large variety of organic molecules.

[7] A. V. Marenich, C. J. Cramer, and D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-96.

[8] a) K. S. Raymond, A. K. Grafton, R. A. Wheeler, *J. Phys. Chem. B* **1997**, *101*, 623 (and references therein); b) M. Namazian, P. Norouzi, *J. Electroanal. Chem*. **2004**, *573*, 49.

[9] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

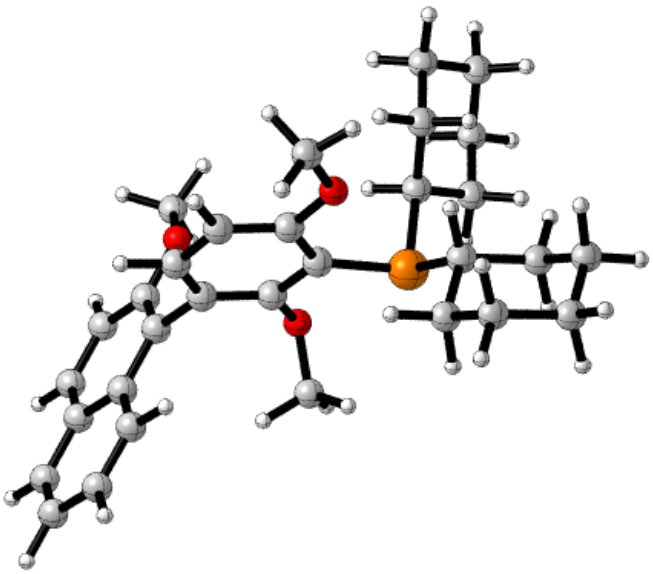
[10] (a) D. H. Aue, H. M. Webb, and M. T. Bowers, *J. Am. Chem. Soc*. **1976**, *98*, 318. (b) H. P. Hopkins Jr., D. V. Jahagirdar, S. P. Moulik, D. H. Aue, H. M. Webb, W. R. Davidson, and M. D. Pedley, *J. Am. Chem. Soc*. **1984**, *106*, 4341. (c) D. H. Aue, H. M. Webb, W. R. Davidson, P. Toure, H. P. Hopkins, Jr., S. P. Moulik, and D. V. Jahagirdar, *J. Am. Chem. Soc*. **1991**, *113*, 1770.

[11] C. Reichardt *Chem. Rev*. **1994**, *94,* 2319-2358.

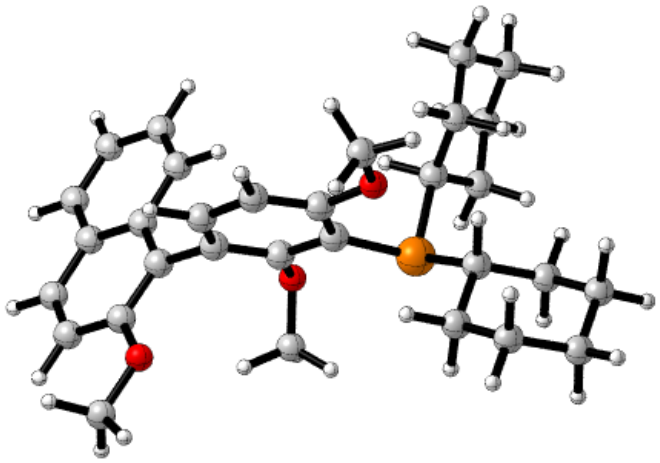
[12] P. K. Das, P. K., R. Pramanik, S. Bagchi *Spectrochimica Acta A* **2003**, *59*, 1681-1688.

[13] Carrow, B. P.; Hartwig, J. F. *J. Am. Chem. Soc*. **2014**, *133*, 2116-2119, and references therein.

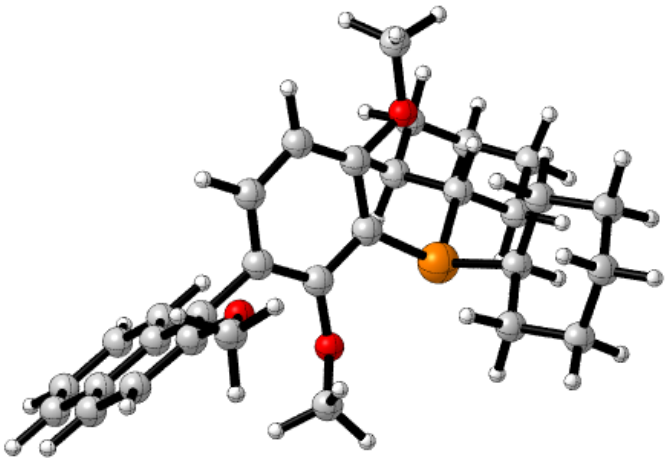
Scheme S1. B3LYP/6-31G(d)-SDD(Pd) structures and relative B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd) and MN15/6-31G+(d,p)-SDD(Pd) free energies in gas phase. (kcal/mol at 298K).



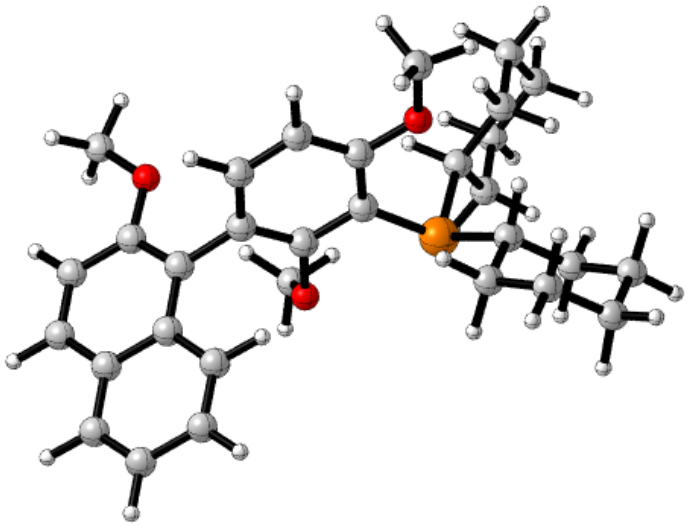
A (0.00, 0.00) [B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



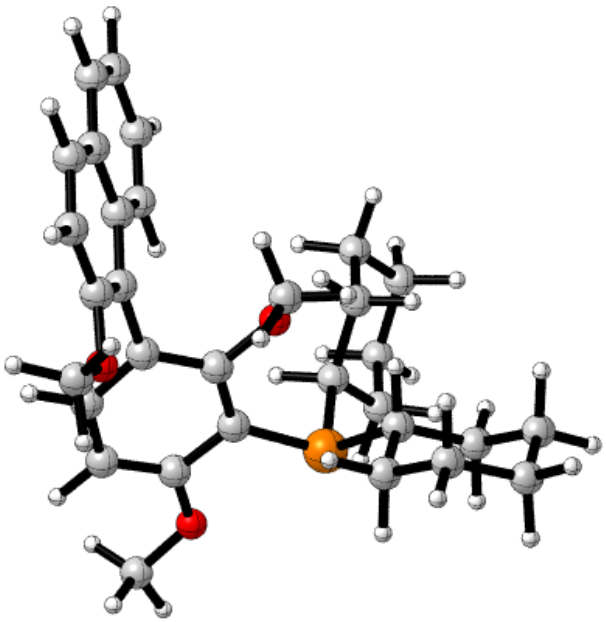
B (0.05, 0.02) [B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



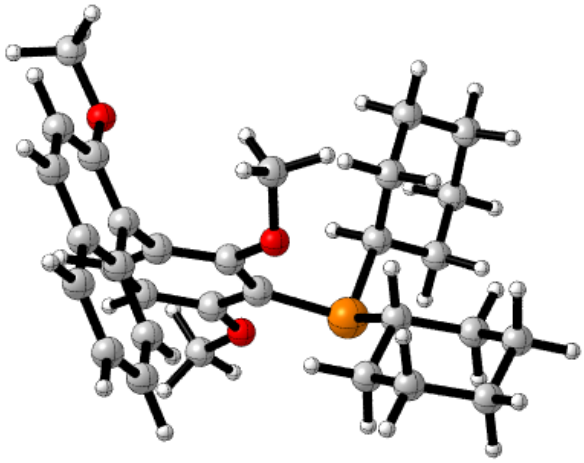
C (1.41, 1.54) [B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



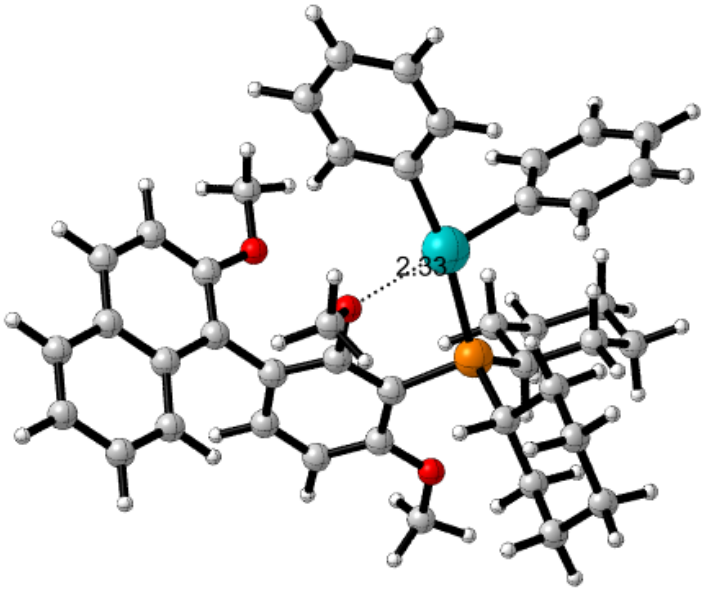
D (1.33) [B3LYP/6-31G(d)-SDD(Pd) level]



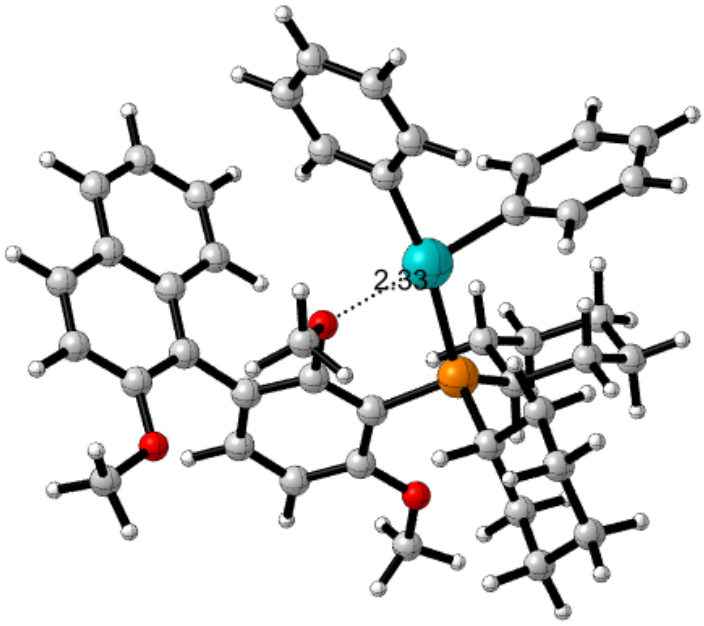
E (2.72) [B3LYP/6-31G(d)-SDD(Pd) level]



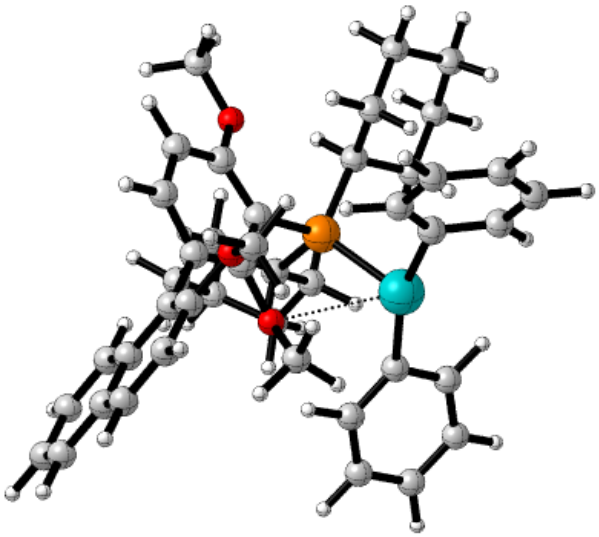
F (2.60) [B3LYP/6-31G(d)-SDD(Pd) level]



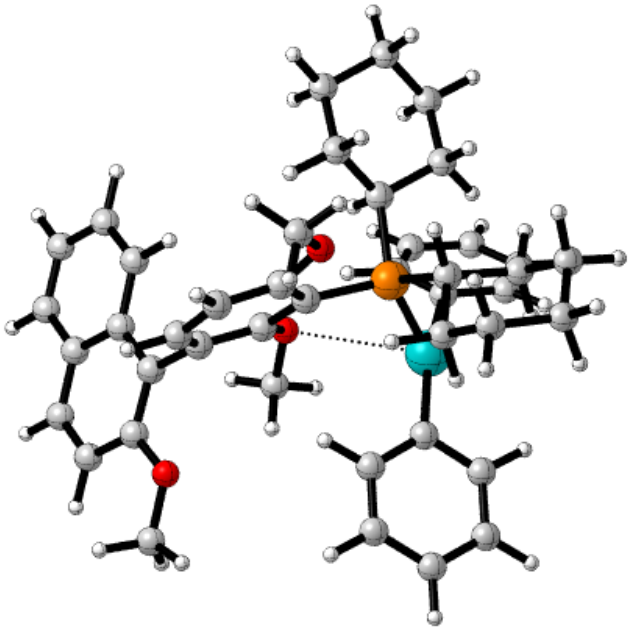
G (0.00, 0.00) [B3LYP/6-31G(d)-SDD(Pd) and MN15/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



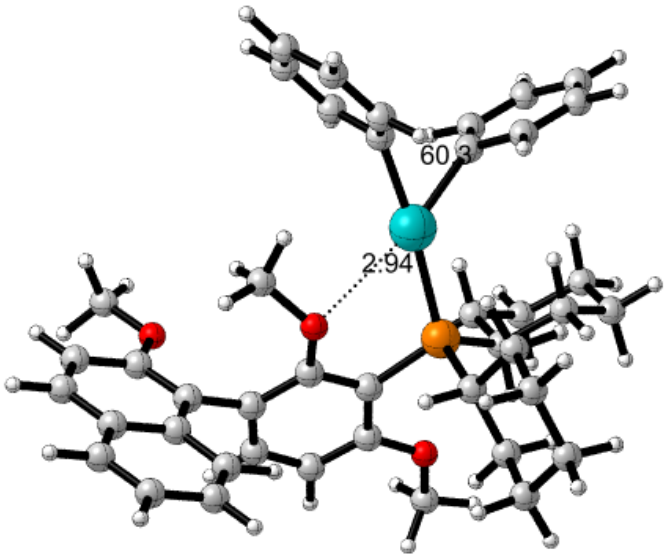
H (0.46, 1.07) [B3LYP/6-31G(d)-SDD(Pd) and MN15/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



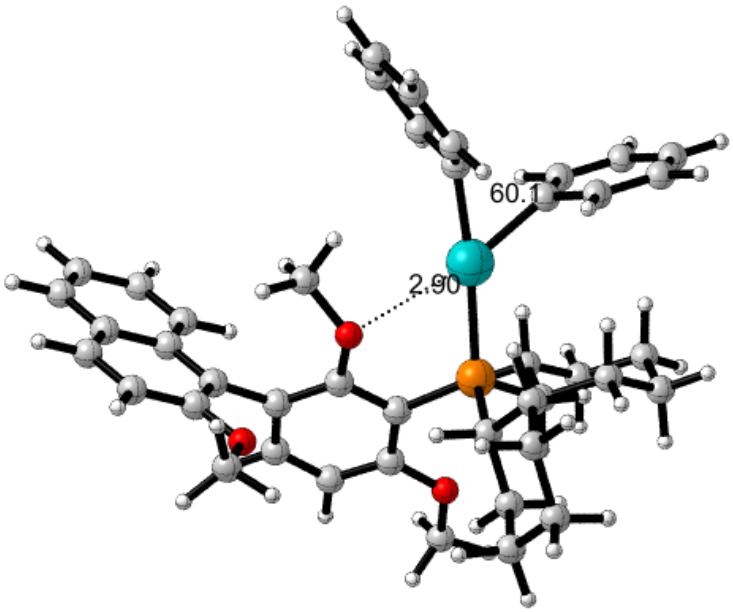
G' (0.00) [20.82 kcal/mol less stable than **G** at B3LYP/6-31G(d)-SDD electronic energy]



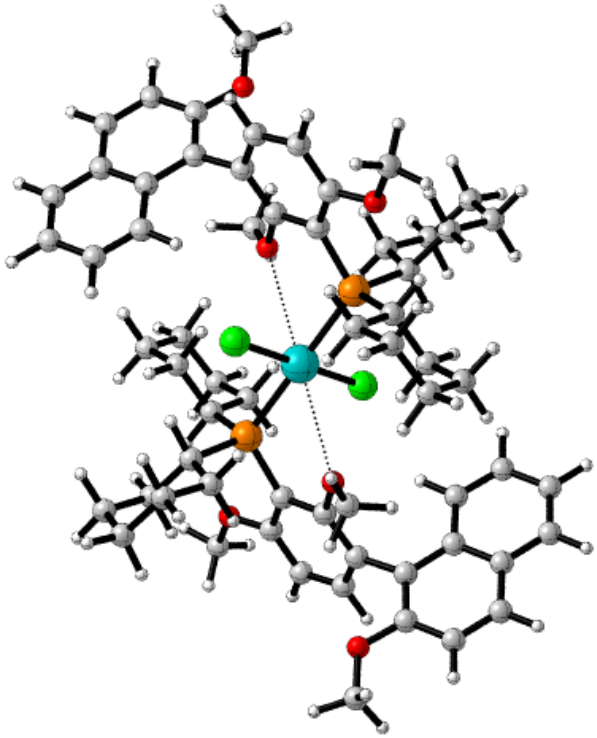
H' (2.97) [B3LYP/6-31G(d)-SDD(Pd) level]



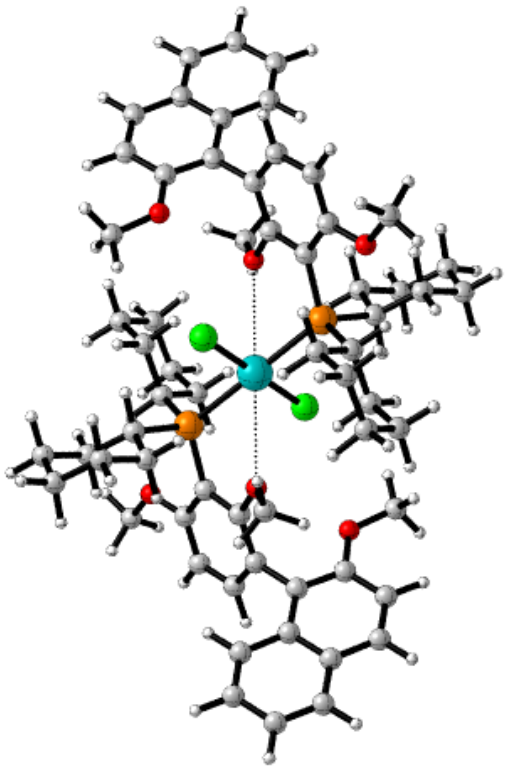
TS1 (0.00, 0.00) [B3LYP/6-31G(d)-SDD(Pd) and MN15/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



TS2 (0.05, -0.09) [B3LYP/6-31G(d)-SDD(Pd) and MN15/6-31G+(d,p)-SDD(Pd)//B3LYP/6-31G(d)-SDD(Pd) levels]



I (0.00, 0.00, 0.00) [B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd) and MN15/6-31+G(d,p)-SDD(Pd) levels with B3LYP/6-31G(d)-SDD(Pd)] frequencies]



J (1.72, 2.07, 4.36) [B3LYP/6-31G(d)-SDD(Pd) and B3LYP/6-31G+(d,p)-SDD(Pd) and MN15/6-31+G(d,p)-SDD(Pd) levels with B3LYP/6-31G(d)-SDD(Pd)] frequencies]

Table S1. Structural distances, angles and dihedral angles comparing values between the experimental X-ray structure and the corresponding optimized structures for **I** at various levels of theory.

	B3LYP/ 6-31+G(d,p)	M06/ 6-31+G(d,p)	MN15/ 6-31+G(d,p)	X-ray
d(Pd-P)	2.4134	2.3804	2.3418	2.3295
d(Pd-Cl)	2.3779	2.3750	2.3434	2.3216
d(=C-P)	1.8664	1.8428	1.8296	1.8420
for =C-C= bond between arom rings:				
d (=C-C=)	1.4975	1.4856	1.491	1.4815
dihed angle(OC=C-C=CO)	110.73	112.81	114.66	115.88
for OCH3 nearest Pd:				
d(Pd-O)	3.1706	3.0081	3.0083	3.0765
d(=C-O)	1.3651	1.3576	1.3603	1.3731
d(CH3-O)	1.4315	1.4180	1.4214	1.4376
dihed angle(C=C-O-CH3)	40.60	44.20	44.29	43.10
for cyclohexyl rings:				
d(C-P)(parallel to O--Pd)	1.8867	1.8628	1.8442	1.8333
dihed angle(C-C-P-C)(par to O--Pd)	178.08	174.27	178.54	174.08
d(C-P)(perp to O--Pd)	1.8846	1.8630	1.8463	1.8407
dihed angle (C'-C'-P-C)	-172.18	-170.38	-170.98	-176.33
for most distant O's:				
d(O-O)	14.6255	14.3834	14.4497	14.558

Table S1a. Structural distances, angles and dihedral angles comparing values between the experimental X-ray structure and the corresponding B3LYP/6-31G(d)-SDD(Pd) optimized and other levels for structure **I**.

	B3LYP/ 6-31G(d)	B3LYP/ 6-31+G(d,p)	MN15/ 6-31+G(d,p)	X-ray
d(Pd-P)	2.4111	2.4234	2.3418	2.3295
d(Pd-Cl)	2.3789	2.3779	2.3434	2.3216
d(=C-P)	1.8636	1.8664	1.8296	1.842
for =C-C= bond between arom rings:				
d(=C-C=)	1.4966	1.4975	1.491	1.4815
dihed angle(OC=C-C=CO)	112.31	110.73	114.66	115.88
for OCH3 nearest Pd:				
d(Pd-O)	3.1607	3.1706	3.0083	3.0765
d(=C-O)	1.3656	1.3651	1.3603	1.3731
d(CH3-O)	1.4297	1.4315	1.4214	1.4376
dihed angle(C=C-O-CH3)	42,24	40.60	44.29	43.1
for cyclohexyl rings:				
d(C-P)(parallel to O--Pd)	1.8861	1.8867	1.8442	1.8333
dihed angle(C-C-P-C)(par to O--Pd)	177.44	178.08	178.54	174.08
d(C-P)(perp to O--Pd)	1.8887	1.8846	1.8463	1.8407
dihed angle (C'-C'-P-C)	-172.31	-172.18	-170.98	-176.33
for most distant O's:				
d(O-O)	14.6455	14.6255	14.4497	14.558

Table S2. B3LYP/6-31G(d)/SDD(Pd) thermodynamic values and optimized structures.

A:

Processing: evanphos-a6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.8007513

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.88275	423.124	214.043	195.356	423.217	44.457	37.377

Processing: evanphos-a6dbe.log
74

C	-6.379382	-2.482111	-0.702788
C	-6.606486	-1.128326	-0.781072
C	-5.583132	-0.193384	-0.467198
C	-4.292516	-0.667645	-0.051163
C	-4.091915	-2.078774	0.006479
C	-5.104159	-2.956566	-0.308943
C	-3.260365	0.269097	0.267011
C	-3.527737	1.634103	0.165301
C	-4.798942	2.098538	-0.256943
C	-5.797307	1.202208	-0.560503
C	-1.916969	-0.180793	0.737943
C	-0.758688	-0.007986	-0.046091
C	0.530245	-0.369672	0.392463
C	0.635467	-0.900545	1.700453
C	-0.502907	-1.111889	2.485528
C	-1.758272	-0.750657	2.001618
P	1.888624	-0.060106	-0.859362
C	3.290590	-1.248417	-0.420048
C	4.482234	-1.008723	-1.374183
C	5.612793	-2.027103	-1.144145
C	5.110893	-3.472183	-1.266688
C	3.920680	-3.722374	-0.330527
C	2.793048	-2.703103	-0.563047
O	-0.880898	0.613399	-1.273190
C	-1.260323	-0.242234	-2.354665
O	1.895136	-1.185158	2.156670
C	2.047908	-1.737797	3.454052
O	-2.515959	2.477754	0.518544
C	-2.676665	3.871013	0.316343
C	2.450517	1.667858	-0.295211
C	3.310328	1.751315	0.979780
C	3.596522	3.212414	1.371973
C	4.241858	3.994446	0.218719

C	3.388809	3.910513	-1.055568
C	3.104007	2.452270	-1.454150
H	-0.421414	-1.528357	3.482299
H	-2.632195	-0.891096	2.631832
H	3.629479	-1.098255	0.608598
H	4.136412	-1.078558	-2.416133
H	4.879569	0.005088	-1.246738
H	6.428331	-1.844291	-1.856283
H	6.035974	-1.875355	-0.139880
H	4.798949	-3.659454	-2.305007
H	5.923524	-4.178591	-1.052166
H	3.536297	-4.742079	-0.466176
H	4.260276	-3.653010	0.713826
H	2.383891	-2.845741	-1.574776
H	1.972508	-2.893263	0.136626
H	1.487865	2.156916	-0.084211
H	4.048837	1.972864	-1.746715
H	2.454740	2.420469	-2.337216
H	3.885020	4.435759	-1.882407
H	2.433264	4.428926	-0.885135
H	5.239434	3.577510	0.013518
H	4.395782	5.042642	0.506814
H	4.241428	3.242477	2.260546
H	2.652008	3.700340	1.655786
H	4.267652	1.237134	0.811638
H	2.817411	1.227483	1.805226
H	-1.383576	0.405789	-3.225481
H	-0.473590	-0.978028	-2.558980
H	-2.206571	-0.752854	-2.142843
H	3.121371	-1.882954	3.589515
H	1.673529	-1.057958	4.230338
H	1.537341	-2.705289	3.544903
H	-4.993604	3.162041	-0.332396
H	-6.771843	1.565602	-0.878082
H	-3.119797	-2.457634	0.303206
H	-4.922527	-4.027087	-0.257556
H	-7.578033	-0.748060	-1.089304
H	-7.169349	-3.187411	-0.945830
H	-1.727037	4.323030	0.608819
H	-2.879281	4.107660	-0.736293
H	-3.478471	4.286260	0.941973

Processing: evanphos-a6pbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31+G(d,p)	0

HF Energy
-1771.8947952

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
399.40465	420.785	215.226	196.351	420.878	44.457	37.384

Processing: evanphos-a6pbe.log

74

C	-6.304896	-2.544386	-0.771991
C	-6.564930	-1.193763	-0.833037
C	-5.568483	-0.237927	-0.490403
C	-4.270970	-0.686715	-0.065912
C	-4.035809	-2.094217	-0.024456
C	-5.022571	-2.993437	-0.366531
C	-3.265465	0.269406	0.280753
C	-3.566446	1.628950	0.201996
C	-4.844183	2.070630	-0.228602
C	-5.816489	1.154555	-0.563458
C	-1.915739	-0.159221	0.755873
C	-0.761495	-0.006124	-0.038086
C	0.532226	-0.352159	0.406350
C	0.643714	-0.844158	1.729313
C	-0.491689	-1.031117	2.527376
C	-1.750779	-0.688844	2.036736
P	1.887418	-0.079263	-0.860372
C	3.290784	-1.255576	-0.394201
C	4.480890	-1.040081	-1.356297
C	5.612344	-2.053168	-1.104766
C	5.110677	-3.501743	-1.187764
C	3.922292	-3.727950	-0.242238
C	2.793657	-2.714068	-0.496425
O	-0.886612	0.585559	-1.279841
C	-1.266955	-0.286273	-2.352369
O	1.905291	-1.115336	2.189661
C	2.069664	-1.615448	3.510040
O	-2.581468	2.493102	0.585792
C	-2.774764	3.890540	0.415857
C	2.448766	1.665772	-0.353349
C	3.305878	1.791323	0.920286
C	3.591256	3.264637	1.266669
C	4.234612	4.013122	0.089602
C	3.382899	3.886738	-1.182778
C	3.101360	2.415647	-1.535869
H	-0.406347	-1.417080	3.535500
H	-2.621580	-0.813551	2.674069
H	3.629237	-1.075545	0.629686
H	4.132753	-1.135064	-2.395215
H	4.878493	-0.024484	-1.253937
H	6.423488	-1.888271	-1.825515
H	6.040385	-1.875685	-0.107132
H	4.796704	-3.716694	-2.219797

H	5.923831	-4.201294	-0.955996
H	3.536195	-4.749534	-0.352639
H	4.264980	-3.633889	0.798773
H	2.380620	-2.883136	-1.502059
H	1.976604	-2.885442	0.211671
H	1.484458	2.157665	-0.159095
H	4.047065	1.930064	-1.812885
H	2.451994	2.355235	-2.416787
H	3.879399	4.385155	-2.025236
H	2.426419	4.408322	-1.030482
H	5.233799	3.594216	-0.101810
H	4.383698	5.069881	0.345279
H	4.237149	3.321346	2.152661
H	2.646758	3.759486	1.536893
H	4.263065	1.271854	0.771798
H	2.809923	1.295639	1.760573
H	-1.358189	0.345801	-3.237833
H	-0.492090	-1.042072	-2.524385
H	-2.227977	-0.769164	-2.146421
H	3.144227	-1.750919	3.642542
H	1.698911	-0.903998	4.258487
H	1.563973	-2.580232	3.641331
H	-5.065708	3.129314	-0.288146
H	-6.794632	1.500369	-0.887788
H	-3.059619	-2.454576	0.280867
H	-4.814991	-4.059191	-0.327099
H	-7.541598	-0.834464	-1.148325
H	-7.073588	-3.264554	-1.036254
H	-1.842201	4.356929	0.736291
H	-2.964246	4.144761	-0.634371
H	-3.596444	4.265475	1.039537

B:

Processing: evanphos6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.8004862

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.82648	423.108	214.962	195.708	423.201	44.457	37.363

Processing: evanphos6dbe.log

74

C	2.936052	2.073314	1.033905
C	2.120557	1.866815	-0.256189
C	2.648990	2.767957	-1.393990
C	2.680461	4.246775	-0.971397
C	3.489481	4.451953	0.317753
C	2.967641	3.555319	1.449862
P	1.865717	0.078319	-0.853885
C	3.440039	-0.863651	-0.400978
C	4.590512	-0.414156	-1.329515
C	5.872375	-1.230804	-1.088361
C	5.623049	-2.737903	-1.235304
C	4.476319	-3.197113	-0.324380
C	3.197094	-2.379241	-0.567629
C	0.558612	-0.483143	0.364522
C	-0.766356	-0.360120	-0.101547
C	-1.889623	-0.751875	0.652392
C	-1.655940	-1.302505	1.913015
C	-0.367511	-1.430454	2.424337
C	0.730468	-1.002998	1.669073
O	-0.978311	0.247992	-1.323332
H	-0.232326	-1.840616	3.417913
H	-2.502226	-1.619222	2.515860
C	-3.287978	-0.565108	0.157154
H	3.730833	-0.671688	0.635464
H	4.279474	-0.527206	-2.378611
H	4.808836	0.650307	-1.183985
H	6.657520	-0.903929	-1.782871
H	6.246740	-1.023537	-0.074682
H	5.364647	-2.961063	-2.281229
H	6.539272	-3.300447	-1.012801
H	4.271586	-4.265108	-0.477585
H	4.781785	-3.085444	0.726832
H	2.834721	-2.575539	-1.588154
H	2.408546	-2.713936	0.114357
H	1.086771	2.185592	-0.055277
H	3.664398	2.457294	-1.677962
H	2.025731	2.642384	-2.287301
H	3.093734	4.860059	-1.783041
H	1.649548	4.595827	-0.810422
H	4.545589	4.210619	0.123949
H	3.461720	5.506436	0.622049
H	3.585542	3.678746	2.349500
H	1.950865	3.874258	1.723984
H	3.968294	1.729693	0.874309
H	2.527121	1.460713	1.843940
C	-1.171909	-0.645443	-2.423992
O	2.010480	-1.057401	2.153831

C 2.233706 -1.595367 3.447199
H -1.486690 -0.026306 -3.267089
H -0.232717 -1.153394 -2.673050
H -1.947658 -1.385398 -2.199439
H 3.312324 -1.543373 3.607292
H 1.723961 -1.009494 4.223027
H 1.907751 -2.641493 3.512547
C -4.035266 -1.672441 -0.238682
C -5.378837 -1.534645 -0.670457
C -5.966180 -0.291587 -0.706993
C -5.254057 0.867923 -0.317471
C -3.895465 0.728999 0.123571
O -3.392361 -2.882836 -0.205527
H -5.947412 -2.404870 -0.976993
H -6.996540 -0.190397 -1.039824
C -5.853960 2.156287 -0.346845
C -3.203409 1.906578 0.527225
C -3.814031 3.138924 0.488714
H -2.178236 1.819873 0.869489
H -3.262933 4.022136 0.801282
C -5.153072 3.271757 0.045624
H -6.884113 2.240902 -0.686112
H -5.620656 4.252270 0.019505
C -4.107722 -4.051825 -0.567718
H -3.403357 -4.877513 -0.448962
H -4.973436 -4.219966 0.086725
H -4.447451 -4.017339 -1.611526

Processing: evanphos6pbe.log
PG=C01

Method BasisSet Imaginary Freqs
RB3LYP 6-31+G(d,p) 0

HF Energy
-1771.8945788

ZPE E298 S298 Squasihar Equasihar Strans Srot
399.32803 420.755 216.273 196.732 420.849 44.457 37.369

Processing: evanphos6pbe.log
74
C 2.901974 2.110516 1.001561
C 2.110950 1.867238 -0.297547
C 2.648131 2.749167 -1.446526
C 2.656574 4.237634 -1.056075
C 3.442174 4.480949 0.241624
C 2.913769 3.602081 1.385303

P	1.877541	0.063902	-0.854661
C	3.455839	-0.858261	-0.376295
C	4.611453	-0.410832	-1.299752
C	5.897917	-1.215238	-1.039283
C	5.662227	-2.726742	-1.168294
C	4.510577	-3.183903	-0.261546
C	3.226797	-2.378255	-0.524523
C	0.565193	-0.479522	0.369485
C	-0.759832	-0.364845	-0.104098
C	-1.885504	-0.747254	0.651344
C	-1.656450	-1.278238	1.921891
C	-0.369144	-1.395211	2.441795
C	0.732603	-0.980466	1.682488
O	-0.961971	0.236705	-1.331324
H	-0.238903	-1.789965	3.441686
H	-2.504413	-1.586972	2.526123
C	-3.283907	-0.576977	0.149017
H	3.732840	-0.648642	0.660355
H	4.310344	-0.537679	-2.349923
H	4.820622	0.655771	-1.163664
H	6.683889	-0.890850	-1.733282
H	6.264239	-0.991913	-0.026407
H	5.415600	-2.965977	-2.213212
H	6.580555	-3.278096	-0.929497
H	4.313838	-4.254218	-0.405318
H	4.806709	-3.058956	0.790452
H	2.874002	-2.590349	-1.544822
H	2.436193	-2.709930	0.156033
H	1.070810	2.178259	-0.121014
H	3.670857	2.444407	-1.707339
H	2.039955	2.597239	-2.345565
H	3.077028	4.836192	-1.874317
H	1.619693	4.578510	-0.920241
H	4.504100	4.249938	0.069832
H	3.395359	5.540747	0.522459
H	3.518231	3.749830	2.289827
H	1.890566	3.916170	1.638990
H	3.939225	1.772121	0.868678
H	2.482674	1.513868	1.817740
C	-1.160474	-0.649288	-2.440725
O	2.010540	-1.028196	2.174432
C	2.231488	-1.533603	3.484460
H	-1.401169	-0.013881	-3.295134
H	-0.241879	-1.209829	-2.648516
H	-1.987691	-1.340143	-2.249424
H	3.309033	-1.474333	3.645676
H	1.718017	-0.927523	4.241320
H	1.908760	-2.578475	3.572922

C -4.009448 -1.688575 -0.275774
C -5.352223 -1.564224 -0.717745
C -5.961350 -0.329415 -0.733389
C -5.272924 0.833426 -0.308461
C -3.915479 0.706742 0.141708
O -3.350131 -2.891415 -0.259403
H -5.903909 -2.435687 -1.048768
H -6.989535 -0.239712 -1.074459
C -5.895269 2.112946 -0.311546
C -3.246551 1.886105 0.581779
C -3.878401 3.110157 0.569323
H -2.222289 1.809459 0.928364
H -3.345135 3.993809 0.908563
C -5.216654 3.231447 0.116437
H -6.922998 2.189964 -0.658198
H -5.701029 4.203482 0.110390
C -4.046710 -4.072212 -0.634764
H -3.329490 -4.885753 -0.516585
H -4.911450 -4.254834 0.015630
H -4.377936 -4.033404 -1.680304

C:

Processing: evanphos-d6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.7982240

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.74902	423.052	215.319	195.721	423.149	44.457	37.339

Processing: evanphos-d6dbe.log
74
C -4.963689 -3.826347 -0.265308
C -5.543613 -2.474014 -0.702468
C -4.447688 -1.527227 -1.222365
C -3.325091 -1.323425 -0.180382
C -2.747328 -2.689569 0.243941
C -3.840334 -3.638150 0.763857
P -1.966020 -0.260075 -0.953141
C -2.772162 1.456415 -1.072252
C -1.788871 2.446208 -1.732723
C -2.452235 3.800742 -2.034249

C	-3.087359	4.413801	-0.778136
C	-4.065234	3.431460	-0.118134
C	-3.392260	2.081456	0.190783
C	-0.668403	-0.041323	0.382878
C	0.671698	0.040055	-0.068043
C	1.767795	0.139339	0.817269
C	1.487986	0.211758	2.183230
C	0.188379	0.155190	2.672650
C	-0.880887	0.018829	1.779898
C	3.193773	0.104685	0.369717
C	3.985430	1.246446	0.480363
C	5.353815	1.229393	0.110358
C	5.922296	0.073605	-0.372662
C	5.166093	-1.115241	-0.508406
C	3.781991	-1.101501	-0.127065
C	3.043267	-2.312633	-0.258836
C	3.635504	-3.456901	-0.742162
C	5.000162	-3.463727	-1.121834
C	5.745761	-2.314892	-1.003659
O	3.359134	2.378000	0.933455
C	4.118004	3.563838	1.101862
O	0.860786	-0.045547	-1.422371
C	1.664644	0.931570	-2.084645
O	-2.177020	-0.051069	2.211662
C	-2.445413	0.023377	3.601887
H	6.971771	0.065900	-0.657530
H	6.795961	-2.304792	-1.287177
H	5.956862	2.125418	0.200030
H	4.536556	3.920716	0.151316
H	4.933028	3.427369	1.824975
H	5.452253	-4.375580	-1.502352
H	3.419135	4.309298	1.486302
H	2.672687	0.549233	-2.271210
H	1.172741	1.137390	-3.040314
H	1.729432	1.856200	-1.501632
H	-1.714784	4.491262	-2.464963
H	3.048912	-4.367212	-0.833983
H	-3.229798	3.658524	-2.799654
H	-1.383346	2.012502	-2.655074
H	-3.597554	5.353461	-1.027533
H	-2.293658	4.669272	-0.060037
H	-0.935435	2.606835	-1.057867
H	1.998562	-2.324709	0.030125
H	2.315821	0.295861	2.881440
H	-3.584693	1.282665	-1.796242
H	-4.920331	3.265855	-0.790874
H	-4.475574	3.864549	0.804123
H	-2.605307	2.233949	0.940280

H 0.021070 0.205715 3.741590
H -4.121159 1.398625 0.641165
H -4.899543 -0.565406 -1.496334
H -2.107499 0.976397 4.029321
H -4.017051 -1.942886 -2.145255
H -3.752292 -0.842505 0.704145
H -1.979225 -2.552187 1.013026
H -2.247568 -3.154309 -0.619327
H -1.977277 -0.804116 4.150581
H -3.530440 -0.049474 3.698216
H -6.051042 -2.004287 0.153446
H -6.308721 -2.618980 -1.476651
H -4.264986 -3.225593 1.691442
H -4.562069 -4.348450 -1.146533
H -3.398925 -4.608381 1.028031
H -5.755583 -4.467377 0.143951

Processing: evanphos-d6pbe.log
PG=C01

Method BasisSet Imaginary Freqs
RB3LYP 6-31+G(d,p) 0

HF Energy
-1771.8920655

ZPE E298 S298 Squasihar Equasihar Strans Srot
399.26419 420.697 216.380 196.585 420.795 44.457 37.348

Processing: evanphos-d6pbe.log
74
C -4.964903 -3.836485 -0.304462
C -5.550193 -2.478509 -0.718205
C -4.459615 -1.519789 -1.229105
C -3.329941 -1.329530 -0.191662
C -2.747126 -2.700895 0.209562
C -3.834734 -3.661560 0.720396
P -1.977202 -0.251077 -0.954871
C -2.784468 1.465944 -1.047577
C -1.817910 2.460646 -1.725638
C -2.490939 3.815355 -2.007446
C -3.101928 4.422811 -0.735985
C -4.061625 3.434744 -0.056658
C -3.379334 2.084108 0.230815
C -0.671178 -0.049522 0.379095
C 0.668625 0.038621 -0.076935
C 1.768676 0.129730 0.804939
C 1.494320 0.183829 2.173510

C	0.196222	0.116588	2.668820
C	-0.877765	-0.007012	1.777894
C	3.195534	0.111945	0.357116
C	3.973831	1.264231	0.458869
C	5.343380	1.260849	0.088737
C	5.927687	0.106422	-0.383090
C	5.186396	-1.094794	-0.503432
C	3.801241	-1.092983	-0.123600
C	3.077226	-2.316032	-0.238813
C	3.684691	-3.461554	-0.704780
C	5.051044	-3.456687	-1.083187
C	5.782469	-2.295021	-0.981455
O	3.337459	2.394444	0.904138
C	4.085953	3.589608	1.084439
O	0.847734	-0.040280	-1.433887
C	1.659517	0.925215	-2.108849
O	-2.171605	-0.084386	2.216909
C	-2.438190	-0.019311	3.611103
H	6.976709	0.110530	-0.667740
H	6.832134	-2.276886	-1.264528
H	5.935817	2.164228	0.168272
H	4.502416	3.954781	0.137093
H	4.896650	3.452382	1.811023
H	5.515332	-4.367473	-1.449742
H	3.377410	4.323832	1.470550
H	2.674647	0.548334	-2.262042
H	1.184976	1.092570	-3.079764
H	1.698536	1.867932	-1.553996
H	-1.763772	4.508534	-2.449950
H	3.109159	-4.379389	-0.784638
H	-3.283337	3.674193	-2.757223
H	-1.432685	2.031233	-2.657889
H	-3.621544	5.360091	-0.972364
H	-2.294315	4.680275	-0.034736
H	-0.950314	2.621444	-1.069899
H	2.031436	-2.336864	0.045008
H	2.324498	0.260911	2.869421
H	-3.610591	1.291565	-1.755131
H	-4.932216	3.270233	-0.708958
H	-4.449811	3.862398	0.877099
H	-2.576960	2.234255	0.964004
H	0.035176	0.152386	3.738780
H	-4.096421	1.397695	0.693064
H	-4.916310	-0.555622	-1.483117
H	-2.098871	0.931188	4.041644
H	-4.034014	-1.918640	-2.161381
H	-3.750073	-0.859563	0.702058
H	-1.976201	-2.573174	0.976890

H -2.250515 -3.150453 -0.663060
H -1.970712 -0.852297 4.150758
H -3.522700 -0.091569 3.707710
H -6.055357 -2.023795 0.146711
H -6.317167 -2.613356 -1.491687
H -4.254485 -3.266671 1.657436
H -4.568456 -4.344970 -1.195579
H -3.387760 -4.633994 0.964326
H -5.752763 -4.484103 0.100874

D:

Processing: evanphos-b6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.7981110

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.67156	423.008	217.321	196.063	423.101	44.457	37.406

Processing: evanphos-b6dbe.log
74
C 3.335188 1.915042 -2.035671
C 2.820073 1.490937 -0.640089
C 3.957148 1.576467 0.396759
C 4.602004 2.974693 0.418683
C 5.108555 3.392445 -0.968472
C 3.986186 3.308015 -2.012096
P 1.843981 -0.147012 -0.813459
C 2.977188 -1.490399 -0.116197
C 4.073389 -1.809021 -1.157418
C 4.986698 -2.956538 -0.692970
C 4.179473 -4.219677 -0.363004
C 3.076294 -3.918013 0.661009
C 2.168010 -2.765584 0.199237
C 0.494690 0.048287 0.468800
C -0.824869 0.151174 -0.020733
C -1.946524 0.288393 0.823432
C -1.722472 0.329332 2.198278
C -0.439199 0.226085 2.730278
C 0.657388 0.081425 1.875316
C -3.338616 0.359132 0.281596
C -4.015905 -0.815743 -0.170595

C	-5.368897	-0.722774	-0.639636
C	-6.003790	0.542343	-0.641621
C	-5.347047	1.670321	-0.208077
C	-4.009332	1.579102	0.253577
C	-3.398206	-2.098984	-0.167720
C	-4.075278	-3.214430	-0.604246
C	-5.409977	-3.117293	-1.069077
C	-6.038967	-1.894989	-1.083831
O	-3.298317	2.673846	0.675402
C	-3.942094	3.936184	0.717563
O	-1.063592	0.050189	-1.373953
C	-1.105663	1.286141	-2.083698
O	1.936103	-0.043565	2.348518
C	2.150214	-0.065054	3.751091
H	-0.308599	0.252362	3.805412
H	-2.570529	0.434297	2.869113
H	3.454745	-1.149879	0.808119
H	3.596683	-2.086898	-2.108654
H	4.680463	-0.919059	-1.365462
H	5.735895	-3.173049	-1.465905
H	5.543394	-2.637956	0.201062
H	3.720389	-4.605259	-1.285435
H	4.842681	-5.010848	0.010599
H	2.472915	-4.816424	0.846973
H	3.539426	-3.648849	1.622245
H	1.616767	-3.077620	-0.700475
H	1.416246	-2.556267	0.968155
H	2.044804	2.214195	-0.344561
H	4.071657	1.179418	-2.391946
H	2.512945	1.895341	-2.761318
H	4.370927	3.558779	-3.009511
H	3.217576	4.059622	-1.776284
H	5.932009	2.726826	-1.268104
H	5.524608	4.407898	-0.935171
H	5.424564	2.993621	1.146420
H	3.860220	3.708521	0.768517
H	4.733409	0.837200	0.153045
H	3.579120	1.321058	1.389200
H	-1.487500	1.054662	-3.080667
H	-1.769475	2.005891	-1.590503
H	-0.100500	1.719086	-2.175027
H	3.226315	-0.190671	3.884742
H	1.834272	0.873949	4.223751
H	1.624693	-0.903213	4.226364
H	-5.856904	2.626541	-0.224638
H	-7.029688	0.616703	-0.994738
H	-2.376187	-2.187816	0.183626
H	-3.580179	-4.181988	-0.594461

H -7.064099 -1.804291 -1.436495
H -5.930715 -4.007472 -1.411364
H -3.197116 4.634976 1.103307
H -4.261592 4.266995 -0.279760
H -4.810868 3.928918 1.389189

E:

Processing: evanphos-c6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.7965716

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.90773	423.106	213.563	194.941	423.195	44.457	37.252

Processing: evanphos-c6dbe.log
74
C -4.232219 1.810093 0.636630
C -2.751987 1.418790 0.426605
C -2.211267 2.008587 -0.890208
C -2.417446 3.533278 -0.952588
C -3.887935 3.920329 -0.741015
C -4.431678 3.333763 0.569714
P -2.505193 -0.444778 0.745116
C -2.538604 -1.280388 -0.948954
C -3.986369 -1.274314 -1.489620
C -4.108171 -2.053258 -2.810978
C -3.600990 -3.494685 -2.668435
C -2.165710 -3.521329 -2.125046
C -2.043385 -2.736047 -0.808420
C -0.710329 -0.460650 1.290016
C 0.444808 -0.378482 0.480910
C 1.750445 -0.395648 1.024284
C 1.876611 -0.556404 2.406200
C 0.770962 -0.642547 3.242935
C -0.511284 -0.566334 2.689750
C 2.990137 -0.163147 0.219956
C 3.303606 1.137075 -0.288356
C 4.522968 1.343419 -1.017816
C 5.398634 0.247058 -1.205013
C 5.097071 -0.999465 -0.707245
C 3.888637 -1.206434 0.004519
C 2.444755 2.257830 -0.096923

C	2.768889	3.496223	-0.602315
C	3.969836	3.692661	-1.327399
C	4.826415	2.635838	-1.525796
O	3.518435	-2.434172	0.486547
C	4.408800	-3.528519	0.340884
O	0.241531	-0.208803	-0.866834
C	0.988384	-0.989274	-1.803749
O	-1.640231	-0.582973	3.457604
C	-1.518066	-0.758125	4.858363
H	0.915614	-0.739945	4.311919
H	2.873477	-0.579637	2.837109
H	-1.897109	-0.753949	-1.661190
H	-4.656523	-1.722300	-0.741209
H	-4.335475	-0.246265	-1.642514
H	-5.152200	-2.047897	-3.151032
H	-3.524223	-1.539167	-3.589034
H	-4.258672	-4.042183	-1.976998
H	-3.655956	-4.017227	-3.632458
H	-1.834088	-4.557282	-1.973656
H	-1.489001	-3.084505	-2.874983
H	-2.638444	-3.242323	-0.033565
H	-1.005471	-2.754297	-0.457276
H	-2.183052	1.870963	1.253545
H	-4.855318	1.334967	-0.134570
H	-4.586913	1.423058	1.599378
H	-5.495928	3.578480	0.685725
H	-3.909827	3.801806	1.418087
H	-4.486195	3.539770	-1.582688
H	-4.001408	5.012424	-0.746819
H	-2.055862	3.919430	-1.915067
H	-1.803240	4.012078	-0.174828
H	-2.736412	1.548415	-1.739812
H	-1.152293	1.764207	-1.012064
H	0.301013	-1.229295	-2.620926
H	1.835275	-0.422338	-2.199980
H	1.349598	-1.916569	-1.348752
H	-2.539363	-0.773929	5.243406
H	-1.022232	-1.705787	5.106668
H	-0.967434	0.069530	5.325318
H	5.785199	-1.821071	-0.868652
H	6.325211	0.400260	-1.753232
H	1.525872	2.124419	0.462842
H	2.096204	4.334689	-0.441951
H	5.755096	2.771921	-2.075718
H	4.210830	4.676592	-1.720337
H	3.914414	-4.376390	0.818835
H	4.593193	-3.768699	-0.714742
H	5.368537	-3.342074	0.840580

F:

Processing: evanphos-f6dbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	6-31G(d)	0

HF Energy
-1771.7963475

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
401.80650	423.087	214.011	195.781	423.177	44.457	37.255

Processing: evanphos-f6dbe.log
74

C	4.829342	-0.768966	-0.026061
C	3.297133	-0.892299	-0.171952
C	2.881078	-0.936137	-1.652973
C	3.621811	-2.048284	-2.418101
C	5.145056	-1.921923	-2.270447
C	5.558476	-1.886525	-0.791715
P	2.374356	0.340943	0.947147
C	2.076533	1.892645	-0.089743
C	3.427014	2.590912	-0.368308
C	3.237670	3.934512	-1.094913
C	2.299734	4.873426	-0.325011
C	0.957038	4.189521	-0.035549
C	1.148480	2.848798	0.692075
C	0.735355	-0.561760	1.081917
C	-0.444889	-0.381215	0.330200
C	-1.652220	-1.047103	0.649999
C	-1.629396	-1.980122	1.687880
C	-0.473276	-2.239694	2.415850
C	0.691367	-1.528766	2.118038
C	-2.952013	-0.753843	-0.028837
C	-3.643431	0.476331	0.207950
C	-4.905803	0.720318	-0.430778
C	-5.446499	-0.279035	-1.274908
C	-4.783818	-1.465120	-1.490861
C	-3.532180	-1.702647	-0.868994
C	-3.128923	1.485785	1.071918
C	-3.813491	2.661652	1.278328
C	-5.053443	2.901832	0.636828
C	-5.585330	1.946737	-0.196650
O	-2.810411	-2.848051	-1.081072

C	-3.363639	-3.869796	-1.894069
O	-0.400803	0.523313	-0.703333
C	-0.878386	0.132603	-1.992382
O	1.871978	-1.739325	2.775271
C	1.898260	-2.630736	3.876911
H	-0.492456	-2.978017	3.208323
H	-2.546162	-2.507261	1.935630
H	1.601920	1.653253	-1.044924
H	3.954706	2.762698	0.581645
H	4.076466	1.947551	-0.972736
H	4.214210	4.411968	-1.250992
H	2.819061	3.746745	-2.095029
H	2.773959	5.157169	0.626454
H	2.145113	5.803810	-0.887246
H	0.314089	4.848872	0.562592
H	0.425983	4.011936	-0.982203
H	1.582920	3.036519	1.685597
H	0.173249	2.380040	0.851811
H	3.016948	-1.854483	0.281150
H	5.169599	0.202397	-0.409563
H	5.102932	-0.794503	1.035615
H	6.645080	-1.755870	-0.702429
H	5.321226	-2.855686	-0.327589
H	5.480444	-0.995972	-2.761568
H	5.648212	-2.748988	-2.788266
H	3.338277	-2.027309	-3.479078
H	3.301860	-3.026432	-2.028854
H	3.101160	0.029888	-2.129377
H	1.798499	-1.086586	-1.732727
H	-0.184011	0.559031	-2.723875
H	-0.893383	-0.956896	-2.097395
H	-1.881684	0.528677	-2.174532
H	2.918067	-2.592548	4.264219
H	1.198858	-2.320096	4.663840
H	1.664480	-3.659551	3.572015
H	-5.221406	-2.211267	-2.143822
H	-6.404452	-0.099765	-1.757382
H	-2.186318	1.311570	1.578613
H	-3.399049	3.414782	1.943333
H	-6.540077	2.113049	-0.690815
H	-5.580782	3.836071	0.809244
H	-2.628688	-4.677075	-1.894071
H	-4.311815	-4.245657	-1.487478
H	-3.524160	-3.530327	-2.926116

G:

Processing: pddiphevanphos-b6dsdbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	0

HF Energy
-2363.0072496

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
516.71651	545.940	274.116	245.954	546.082	45.725	38.880

Processing: pddiphevanphos-b6dsdbe.log
97

C	-4.949951	-2.001858	0.989159
C	-4.925624	-0.874117	0.116343
C	-6.087187	-0.030327	0.081619
C	-7.209141	-0.347925	0.893726
C	-7.199743	-1.448608	1.718851
C	-6.053600	-2.279261	1.765017
C	-6.079373	1.104155	-0.765763
C	-4.991167	1.401420	-1.552572
C	-3.845298	0.565486	-1.529008
C	-3.795209	-0.555290	-0.699139
C	-2.589936	-1.436400	-0.747183
C	-1.331498	-1.045059	-0.249424
C	-0.161177	-1.806413	-0.431601
C	-0.301983	-3.061280	-1.073190
C	-1.547517	-3.494267	-1.536742
C	-2.664152	-2.677531	-1.382722
P	1.438725	-1.026895	0.129368
C	2.757770	-1.545721	-1.102171
C	2.377658	-1.055172	-2.516634
C	3.460751	-1.416044	-3.547607
C	4.837214	-0.877851	-3.132656
C	5.215784	-1.367382	-1.728179
C	4.142199	-0.993620	-0.690605
O	-1.231747	0.177927	0.413606
C	-1.809459	0.214468	1.740450
O	0.828278	-3.816105	-1.206042
C	0.753096	-5.058192	-1.892217
O	-2.752674	0.790614	-2.312015
C	-2.766995	1.870147	-3.237990
Pd	0.800436	1.312715	0.314632
C	-0.041631	3.159750	0.588950
C	0.471549	4.197463	1.388932
C	-0.257186	5.367242	1.629408
C	-1.521476	5.542639	1.063082
C	-2.050278	4.532238	0.258316
C	-1.319327	3.360843	0.027435
C	2.555818	2.237807	0.079240

C	2.929813	2.731063	-1.184058
C	4.190081	3.301458	-1.395315
C	5.104289	3.407469	-0.344512
C	4.739209	2.944563	0.920964
C	3.479536	2.370862	1.130157
C	1.785755	-1.911793	1.770297
C	2.582769	-1.013297	2.741541
C	2.717310	-1.668488	4.126625
C	3.335539	-3.071096	4.036544
C	2.543030	-3.962514	3.070053
C	2.409755	-3.319214	1.677488
H	-1.654476	-4.450428	-2.034095
H	-3.620489	-3.003259	-1.781632
H	2.806431	-2.638096	-1.115907
H	4.094952	0.096359	-0.593683
H	4.435492	-1.385703	0.290441
H	6.180379	-0.942617	-1.423032
H	5.344400	-2.460584	-1.746057
H	4.812570	0.221085	-3.134059
H	5.600604	-1.179663	-3.861489
H	3.176112	-1.023266	-4.532414
H	3.514297	-2.510623	-3.650705
H	2.246901	0.034786	-2.494632
H	1.416104	-1.483949	-2.822508
H	0.774765	-2.024691	2.191647
H	3.583860	-0.819764	2.333702
H	2.091385	-0.037572	2.827949
H	3.318653	-1.026199	4.782515
H	1.721402	-1.741597	4.589364
H	4.373843	-2.987057	3.682562
H	3.380848	-3.533139	5.031014
H	3.020948	-4.946645	2.977716
H	1.538676	-4.141347	3.482646
H	3.407764	-3.247292	1.223621
H	1.812340	-3.958350	1.021039
H	-1.759347	2.582648	-0.590898
H	-3.036546	4.651519	-0.188238
H	-2.085918	6.454192	1.245931
H	0.168953	6.146665	2.258651
H	1.459998	4.099949	1.829459
H	2.228931	2.680420	-2.013410
H	4.450913	3.675163	-2.383776
H	6.082034	3.854171	-0.507245
H	5.434600	3.030352	1.753975
H	3.222340	2.021681	2.127115
H	-1.773892	1.259613	2.045244
H	-2.841556	-0.139008	1.715653
H	-1.213413	-0.400502	2.424146
H	1.769160	-5.456185	-1.893608
H	0.088106	-5.762814	-1.377183
H	0.412267	-4.925093	-2.926383

H	-6.954789	1.748525	-0.790142
H	-5.015035	2.274623	-2.193618
H	-4.079986	-2.648830	1.036327
H	-6.044759	-3.145240	2.421846
H	-8.079673	0.302735	0.851168
H	-8.063036	-1.680792	2.336024
H	-1.815343	1.812435	-3.768086
H	-3.591739	1.771397	-3.955551
H	-2.831898	2.838939	-2.728833

Processing: pddiphevanphos-b6dsdbe.log
Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3236.6316	11.4681	181.9355	0.2192	0.3596	8.6769
A	3233.2844	9.1935	116.1055	0.2247	0.3670	
A	3216.1874	15.6152	229.0090	0.1211	0.2161	
A	3207.1148	36.5146	209.2228	0.2947	0.4552	
A	3202.9080	9.8202	79.8368	0.4162	0.5878	
A	3199.5336	1.4509	51.8226	0.7499	0.8571	
A	3198.0602	45.9713	435.8537	0.0966	0.1762	
A	3197.4401	36.9041	231.7223	0.1974	0.3297	
A	3194.1076	36.6845	21.9814	0.2668	0.4212	
A	3189.9142	21.4211	219.5326	0.6206	0.7659	
A	3188.3838	41.0697	14.7914	0.7425	0.8522	
A	3187.9656	2.9152	52.2484	0.3212	0.4863	
A	3186.5164	36.2907	176.2236	0.4782	0.6470	
A	3184.3986	13.2373	75.4397	0.7500	0.8571	
A	3179.9671	2.3902	30.3447	0.4920	0.6595	
A	3167.2163	10.6299	136.2602	0.7499	0.8571	
A	3167.0025	14.6899	60.4404	0.5887	0.7411	
A	3164.5919	19.5939	138.4589	0.7037	0.8261	
A	3163.0453	16.5655	78.9476	0.5321	0.6946	
A	3161.1566	8.2046	32.5746	0.3165	0.4808	
A	3153.6196	20.8994	90.1084	0.3287	0.4948	
A	3153.3426	6.5279	35.4339	0.6580	0.7937	
A	3119.2059	11.9089	21.3874	0.6601	0.7953	
A	3117.6110	22.8010	37.9141	0.3276	0.4935	
A	3102.4900	37.1795	55.7956	0.7485	0.8561	
A	3099.7826	16.4575	49.5892	0.1744	0.2971	
A	3099.0948	25.1313	80.1172	0.6318	0.7743	
A	3093.1706	29.7707	36.8157	0.6282	0.7717	
A	3086.1809	24.3703	53.2702	0.6897	0.8163	
A	3077.3287	36.8858	90.1861	0.4260	0.5975	
A	3076.0872	63.1799	78.9911	0.4025	0.5740	
A	3072.6998	70.3511	225.6510	0.1064	0.1924	
A	3071.8839	54.2923	184.8031	0.3718	0.5420	
A	3068.2217	65.8357	187.3303	0.3642	0.5339	
A	3067.8893	61.7239	144.4229	0.2050	0.3403	
A	3061.2838	17.7526	57.2391	0.2981	0.4593	
A	3060.7088	25.6975	75.4062	0.0746	0.1388	

A	3046.9025	29.0914	37.4824	0.5600	0.7179
A	3046.2664	26.0200	51.5136	0.3033	0.4655
A	3042.7279	3.5363	32.1271	0.7299	0.8439
A	3035.5987	50.6330	241.6355	0.0229	0.0447
A	3035.3824	76.0026	28.8178	0.5869	0.7397
A	3032.5634	18.6897	76.1902	0.3188	0.4835
A	3025.7924	28.3582	22.5628	0.7384	0.8495
A	3019.6744	24.4316	141.5333	0.1223	0.2180
A	3018.1621	17.0629	50.7228	0.2773	0.4341
A	3016.9178	44.8100	117.7054	0.1751	0.2980
A	3014.2941	17.7627	24.3293	0.6167	0.7629
A	3006.5603	6.7892	23.5547	0.4011	0.5725
A	1677.3388	25.7468	11.3233	0.6188	0.7645
A	1652.2674	50.9374	8.8927	0.6812	0.8104
A	1640.9032	70.0872	135.0732	0.4788	0.6475
A	1628.0671	20.7161	17.9892	0.6805	0.8099
A	1624.7651	42.8756	12.7781	0.7421	0.8520
A	1621.9025	15.0505	118.0528	0.4909	0.6585
A	1619.3820	0.8262	12.5734	0.7444	0.8535
A	1618.4542	3.5822	11.9744	0.7442	0.8533
A	1607.3085	43.8265	25.6963	0.7031	0.8257
A	1564.3478	53.0210	7.1898	0.2975	0.4586
A	1537.9714	5.9963	9.2956	0.7431	0.8526
A	1537.2143	4.6819	13.5040	0.6619	0.7965
A	1535.4069	1.1066	1.8096	0.6471	0.7858
A	1531.2093	13.2052	17.0348	0.4749	0.6440
A	1524.9980	38.5216	27.4914	0.4807	0.6493
A	1524.0599	2.7529	6.3842	0.0485	0.0925
A	1522.9627	10.0757	11.3737	0.5804	0.7345
A	1522.5630	13.2751	17.9088	0.7499	0.8571
A	1521.9249	18.3995	11.7186	0.1689	0.2889
A	1521.1058	12.7644	8.8625	0.7339	0.8466
A	1519.4477	6.4863	13.2234	0.0619	0.1165
A	1518.7731	9.1032	3.6354	0.5806	0.7346
A	1518.0266	5.7798	7.4749	0.4639	0.6338
A	1517.1236	5.4444	7.6854	0.5782	0.7327
A	1516.5016	43.6217	22.7497	0.5720	0.7277
A	1515.3739	12.4414	18.4587	0.7443	0.8534
A	1514.8168	4.5562	20.0337	0.6966	0.8212
A	1513.4696	23.4067	7.2525	0.4473	0.6181
A	1512.1571	3.2624	20.8192	0.7180	0.8359
A	1511.9206	2.1805	12.7819	0.7500	0.8571
A	1499.4389	16.7659	17.4411	0.5696	0.7258
A	1496.9506	18.9894	8.4573	0.7341	0.8467
A	1487.8732	46.5334	11.5445	0.5988	0.7490
A	1476.6008	14.3653	36.3910	0.5083	0.6740
A	1470.0909	2.3190	1.7983	0.7500	0.8571
A	1468.2130	2.2647	0.6546	0.7465	0.8549
A	1424.6357	28.9377	27.2616	0.7271	0.8420
A	1410.5717	48.0790	5.8572	0.3803	0.5511
A	1408.6553	57.1422	17.7808	0.2510	0.4013

A	1408.3796	2.2171	226.1373	0.1846	0.3117
A	1406.5588	13.3844	4.4166	0.0856	0.1577
A	1404.2919	3.9546	2.9481	0.6347	0.7766
A	1399.5776	0.4359	5.1629	0.7470	0.8552
A	1399.0228	2.3209	6.8133	0.7361	0.8480
A	1396.2008	2.1640	11.9013	0.5471	0.7073
A	1391.9810	4.8735	4.3177	0.5789	0.7333
A	1386.3869	0.6264	1.0576	0.3539	0.5228
A	1381.0244	2.3826	5.9032	0.6908	0.8171
A	1378.2101	2.9620	3.5972	0.7027	0.8254
A	1374.9721	52.2419	8.0329	0.3049	0.4673
A	1361.9442	1.2142	3.2032	0.7128	0.8323
A	1352.0136	0.2232	3.4424	0.7428	0.8524
A	1348.8134	1.3269	11.3888	0.7487	0.8563
A	1342.3863	0.3886	14.0182	0.7500	0.8571
A	1320.1193	76.5116	19.7637	0.1869	0.3149
A	1317.9480	44.1632	18.3276	0.4217	0.5932
A	1315.3896	146.7178	5.9665	0.7083	0.8293
A	1313.7466	2.5370	5.6193	0.4946	0.6618
A	1313.2724	8.4300	2.9972	0.7471	0.8552
A	1309.7539	4.0534	2.2225	0.5187	0.6831
A	1309.5403	1.6405	11.5814	0.6746	0.8057
A	1308.0268	6.4626	15.8756	0.6834	0.8119
A	1305.0819	25.2660	10.0180	0.3885	0.5596
A	1304.5920	46.5988	22.4996	0.0497	0.0947
A	1301.1383	75.1479	3.8212	0.7256	0.8410
A	1298.2158	1.3119	2.7763	0.7410	0.8512
A	1272.6515	23.2788	32.5225	0.1469	0.2562
A	1252.3742	10.6946	3.7292	0.4810	0.6495
A	1245.5806	3.9529	15.8262	0.2607	0.4136
A	1241.4904	34.7546	14.5575	0.5764	0.7313
A	1237.8022	4.9278	9.5949	0.4957	0.6628
A	1221.6163	1.7132	10.9031	0.3419	0.5095
A	1217.6636	0.3648	9.4435	0.4234	0.5949
A	1215.2916	6.8185	10.4565	0.6629	0.7973
A	1211.8691	4.4128	2.5920	0.5157	0.6804
A	1209.1551	0.4816	3.5916	0.5746	0.7299
A	1207.6146	2.2754	0.8081	0.6315	0.7741
A	1203.6363	6.3169	0.7254	0.7414	0.8515
A	1192.6285	2.0729	7.4273	0.5708	0.7268
A	1189.9804	10.6688	3.8246	0.6298	0.7728
A	1186.3317	0.2095	7.0329	0.6879	0.8151
A	1186.1656	0.0679	5.0394	0.7428	0.8524
A	1183.9344	0.4347	7.3668	0.6910	0.8173
A	1183.6587	0.8533	5.1752	0.7455	0.8542
A	1181.6075	1.0841	6.9525	0.6181	0.7640
A	1175.0744	11.0207	4.8562	0.4352	0.6064
A	1150.6590	9.2340	4.3083	0.7295	0.8436
A	1144.1698	42.2921	6.7221	0.1260	0.2238
A	1142.7250	16.4446	3.0299	0.5015	0.6680
A	1119.5000	182.4771	3.5175	0.0688	0.1287

A	1108.5330	70.1145	3.3151	0.0400	0.0770
A	1107.4352	6.5500	0.6166	0.1973	0.3296
A	1100.8290	0.4110	0.2308	0.5705	0.7265
A	1099.0399	0.5185	0.7870	0.7406	0.8510
A	1097.6761	0.2966	1.3882	0.7305	0.8442
A	1095.3590	2.4251	1.3124	0.5497	0.7094
A	1093.1733	2.3022	0.6119	0.7097	0.8302
A	1091.5283	6.1885	1.4710	0.7464	0.8548
A	1083.9749	7.8649	0.5088	0.1130	0.2030
A	1065.0429	1.4555	5.4529	0.7232	0.8394
A	1061.8880	2.4581	7.1386	0.7490	0.8565
A	1055.8328	9.8568	28.6108	0.1948	0.3261
A	1045.9592	5.5566	22.4247	0.1125	0.2022
A	1044.5519	4.5568	15.5435	0.2986	0.4599
A	1042.9886	3.3966	14.5014	0.7499	0.8571
A	1039.3303	23.6490	6.0893	0.4532	0.6237
A	1034.2730	35.6534	9.9847	0.3422	0.5099
A	1026.1903	5.8179	10.7829	0.7424	0.8522
A	1020.7060	6.2085	13.1748	0.1207	0.2154
A	1011.6641	5.3981	77.7458	0.0792	0.1468
A	1009.3244	6.2403	28.4282	0.5381	0.6997
A	1007.7654	5.3920	11.2822	0.7185	0.8362
A	990.5851	0.0365	0.2904	0.6803	0.8097
A	985.0966	0.3281	1.0919	0.4635	0.6334
A	979.2315	0.9330	0.7959	0.6431	0.7828
A	969.6094	0.2967	1.8622	0.3976	0.5690
A	962.9763	0.9978	0.5565	0.6992	0.8230
A	960.2306	0.0372	0.9586	0.6784	0.8084
A	954.2633	3.1206	1.1975	0.7114	0.8314
A	948.4922	0.3073	0.6057	0.1704	0.2912
A	939.3821	4.0104	0.6683	0.7324	0.8455
A	934.7712	9.5035	2.4243	0.7496	0.8569
A	933.7024	3.3758	0.4036	0.7312	0.8447
A	917.2976	10.1660	4.5452	0.2893	0.4488
A	913.4299	2.4783	0.4983	0.5190	0.6833
A	906.7987	1.7150	0.4224	0.5018	0.6682
A	903.8515	0.3086	0.6744	0.4856	0.6537
A	901.4334	5.1279	0.9977	0.7455	0.8542
A	900.5799	4.0223	1.2692	0.5482	0.7081
A	897.9713	4.0364	0.1077	0.3758	0.5463
A	882.0956	1.4190	2.0736	0.7492	0.8566
A	866.3980	8.8353	4.2777	0.7264	0.8415
A	863.1598	3.7582	9.4453	0.0621	0.1170
A	859.1961	0.3696	1.8417	0.7013	0.8244
A	849.9798	1.4281	12.3059	0.2153	0.3543
A	849.5609	0.0925	3.0619	0.4402	0.6113
A	830.5576	57.2955	1.8326	0.6407	0.7810
A	826.4127	2.6711	3.3726	0.5936	0.7449
A	824.1271	15.5090	2.3672	0.3258	0.4915
A	822.3396	1.8029	6.1750	0.0851	0.1568
A	803.6398	0.2018	0.7758	0.7469	0.8551

A	802.0386	0.5187	0.6275	0.2527	0.4034
A	799.2098	2.9396	3.6209	0.3932	0.5644
A	787.5448	3.9873	1.9129	0.3084	0.4715
A	777.1599	13.6252	38.1446	0.1191	0.2128
A	766.4416	14.7482	4.0097	0.7445	0.8536
A	756.7922	11.2680	5.3398	0.7496	0.8569
A	746.5770	55.4067	2.7906	0.5014	0.6679
A	740.9058	29.6924	2.0297	0.7387	0.8497
A	722.0512	5.1234	1.5481	0.5645	0.7216
A	713.8817	4.6968	17.2644	0.0550	0.1043
A	711.2576	17.9690	6.2186	0.4738	0.6430
A	708.9684	12.7508	6.3505	0.6841	0.8124
A	703.9411	1.0357	3.5248	0.7237	0.8397
A	693.8711	4.0497	2.7793	0.3993	0.5707
A	672.0345	6.4911	12.2044	0.0048	0.0095
A	669.9429	0.5585	1.0961	0.4844	0.6526
A	662.8502	3.8877	7.9350	0.1165	0.2087
A	642.9551	8.5070	2.7330	0.0671	0.1257
A	635.1905	12.1316	4.7685	0.1032	0.1871
A	631.1421	0.6115	3.4429	0.7088	0.8296
A	628.6373	0.0337	2.7370	0.7496	0.8569
A	617.6985	3.3599	3.5520	0.4946	0.6618
A	581.6075	6.0599	4.5093	0.0480	0.0916
A	558.9409	8.6403	3.4389	0.6915	0.8176
A	544.2409	0.5210	4.1190	0.4269	0.5983
A	541.9631	6.7709	1.4998	0.5916	0.7434
A	529.8560	0.9918	6.6114	0.5256	0.6890
A	513.9139	7.2065	2.4366	0.0807	0.1493
A	510.8603	8.7991	4.2712	0.1580	0.2728
A	495.5492	1.5484	3.5711	0.4160	0.5876
A	477.2751	11.8069	1.3174	0.2380	0.3845
A	474.3119	27.3956	0.9185	0.6471	0.7857
A	458.3918	14.0985	2.9374	0.5147	0.6796
A	445.0649	0.6045	1.0476	0.4541	0.6245
A	442.4384	0.5204	0.7772	0.6692	0.8018
A	441.2768	1.8071	1.2671	0.2942	0.4546
A	436.3232	3.5127	2.0980	0.4220	0.5935
A	419.0961	7.6654	1.4233	0.4441	0.6151
A	408.8546	0.1709	0.8313	0.3672	0.5371
A	407.6201	0.0264	0.2996	0.7400	0.8506
A	405.5403	2.6465	1.1237	0.6843	0.8125
A	396.5398	8.2972	2.5964	0.4783	0.6471
A	391.2852	5.9403	2.1705	0.5891	0.7414
A	384.5352	0.6588	2.9243	0.7299	0.8439
A	375.8112	7.2023	11.6092	0.1222	0.2178
A	352.8163	0.9827	0.8423	0.5972	0.7478
A	349.2452	2.4049	3.8869	0.4310	0.6024
A	323.9278	0.8468	0.5348	0.7385	0.8496
A	319.3168	0.1776	1.1898	0.1599	0.2758
A	308.9627	3.4639	0.4086	0.7448	0.8537
A	290.4151	4.3100	3.3463	0.2366	0.3826

A	277.7452	0.3660	1.3735	0.4526	0.6232
A	266.5549	1.3198	2.8662	0.1785	0.3030
A	261.2326	0.8019	2.0304	0.2976	0.4587
A	257.7353	3.4736	0.9858	0.3072	0.4700
A	255.1990	3.9489	3.0290	0.1079	0.1947
A	248.1450	1.0051	1.2142	0.2165	0.3559
A	238.0313	0.1647	0.0726	0.3530	0.5218
A	228.8434	0.6271	0.5179	0.7133	0.8327
A	222.8353	1.6788	2.0782	0.5498	0.7095
A	217.2854	0.2198	2.6318	0.5166	0.6813
A	214.0782	0.1221	3.8273	0.7254	0.8408
A	207.0808	1.8750	7.2002	0.4068	0.5783
A	202.3188	1.3941	5.9896	0.0838	0.1547
A	184.6600	0.0796	1.9662	0.6939	0.8193
A	177.9954	0.4701	1.1767	0.7397	0.8504
A	175.7394	2.0346	0.4965	0.2445	0.3929
A	172.4779	1.0077	0.3034	0.1118	0.2011
A	159.6813	0.3202	1.5940	0.3466	0.5148
A	156.7380	0.6943	1.2263	0.5549	0.7137
A	149.6118	1.0657	1.6785	0.3986	0.5700
A	147.6486	1.9611	4.3271	0.3667	0.5366
A	138.4251	4.2560	0.6134	0.4759	0.6449
A	133.1327	0.8654	3.0891	0.4502	0.6209
A	119.9334	2.7966	0.7091	0.7411	0.8513
A	113.4871	1.1654	1.5348	0.6682	0.8011
A	103.7502	1.2908	1.4824	0.7447	0.8537
A	91.7528	2.5315	0.7796	0.7130	0.8325
A	85.3242	0.5217	1.3652	0.7120	0.8318
A	79.7753	0.0972	1.3904	0.7439	0.8532
A	76.0639	0.4655	0.8216	0.7492	0.8566
A	63.3634	0.6636	2.7574	0.7447	0.8537
A	62.2937	0.0738	2.9544	0.7475	0.8555
A	57.1105	0.1050	2.1729	0.7294	0.8435
A	55.4287	0.7110	4.3295	0.6900	0.8165
A	50.7366	0.0404	4.0162	0.7500	0.8571
A	49.0350	0.4368	0.4945	0.7475	0.8555
A	46.4896	0.1549	5.9652	0.7493	0.8567
A	44.5013	0.0380	5.0611	0.6163	0.7626
A	41.4980	0.1595	4.4410	0.7407	0.8510
A	34.0646	0.1520	3.4235	0.7500	0.8571
A	24.7470	0.3276	2.7566	0.6848	0.8129
A	23.7085	0.2657	8.6113	0.7237	0.8397
A	17.2534	0.1298	2.7755	0.7304	0.8442
A	14.2067	0.2017	2.0346	0.7225	0.8389

H:

Processing: pddiphevanphos-c6dsdbe.log
PG=C01

Method BasisSet Imaginary Freqs
RB3LYP GenECP 0

HF Energy
-2363.0059294

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
516.39894	545.785	277.301	246.670	545.936	45.725	38.833

auelinux:/aue/chem126/aue/ark/pj/pd> gtg pddiphevanphos-c6dsdbe.log
Processing: pddiphevanphos-c6dsdbe.log
97
C -3.389610 0.356949 -2.109664
C -4.196517 -0.147694 -1.049772
C -5.487863 0.444694 -0.848020
C -5.908326 1.512511 -1.686839
C -5.099016 1.980554 -2.695402
C -3.828834 1.389960 -2.907323
C -6.317358 -0.061125 0.181874
C -5.908934 -1.102561 0.982438
C -4.631694 -1.686105 0.787151
C -3.772157 -1.221080 -0.204925
C -2.455908 -1.894345 -0.433391
C -1.221867 -1.328655 -0.058624
C 0.021835 -1.898030 -0.398654
C -0.003567 -3.139577 -1.078702
C -1.216022 -3.744336 -1.423904
C -2.416643 -3.114954 -1.109971
P 1.544151 -0.909082 0.035090
C 2.781034 -1.170816 -1.352918
C 2.174322 -0.698193 -2.692409
C 3.181108 -0.834790 -3.847349
C 4.490278 -0.091995 -3.546519
C 5.095488 -0.565987 -2.218134
C 4.097189 -0.415230 -1.056599
O -1.236516 -0.118056 0.632807
C -1.633640 -0.198554 2.023314
O 1.203944 -3.706502 -1.371440
C 1.236381 -4.926319 -2.099507
O -4.158464 -2.709634 1.567943
C -5.003575 -3.260966 2.566007
Pd 0.599637 1.302973 0.399390
C -0.464954 2.990317 0.828476
C -0.145418 3.890658 1.860986
C -1.011891 4.929152 2.219306
C -2.217690 5.107987 1.537659
C -2.548109 4.237230 0.497506
C -1.682205 3.193871 0.149576
C 2.157923 2.516223 0.078568
C 2.341656 3.117173 -1.180184
C 3.475601 3.889014 -1.456356

C	4.448273	4.094288	-0.475034
C	4.267899	3.526410	0.787393
C	3.134675	2.751535	1.060985
C	2.195798	-1.797406	1.578788
C	2.948724	-0.825579	2.514162
C	3.331229	-1.507268	3.838903
C	4.141242	-2.790887	3.607083
C	3.392415	-3.755174	2.676472
C	3.012639	-3.084361	1.343575
H	-1.235333	-4.691575	-1.948765
H	-3.353387	-3.576043	-1.408617
H	2.998612	-2.239892	-1.428851
H	3.886832	0.647439	-0.893695
H	4.555578	-0.791418	-0.134254
H	6.007094	0.000573	-1.990286
H	5.395084	-1.621304	-2.310581
H	4.289404	0.986867	-3.483692
H	5.206779	-0.234735	-4.365831
H	2.730109	-0.457707	-4.774443
H	3.398422	-1.900627	-4.015732
H	1.870917	0.353051	-2.597671
H	1.267877	-1.270982	-2.921517
H	1.265114	-2.084389	2.092405
H	3.858260	-0.460667	2.018547
H	2.328099	0.057076	2.705711
H	3.896142	-0.805808	4.465964
H	2.414287	-1.754458	4.395270
H	5.110107	-2.530955	3.155259
H	4.363913	-3.280149	4.563966
H	4.000918	-4.647758	2.480216
H	2.477551	-4.105706	3.177597
H	3.933147	-2.838067	0.796521
H	2.451612	-3.782059	0.715406
H	-1.972156	2.527884	-0.659761
H	-3.481767	4.364541	-0.047526
H	-2.888412	5.919817	1.810138
H	-0.737925	5.605633	3.027091
H	0.799324	3.791317	2.390321
H	1.588599	2.992189	-1.954153
H	3.589883	4.341769	-2.439570
H	5.327507	4.697445	-0.687722
H	5.009294	3.687188	1.568045
H	3.020579	2.324936	2.054715
H	-1.846414	0.825728	2.327267
H	-2.516663	-0.829467	2.129014
H	-0.809212	-0.604938	2.619927
H	2.293467	-5.163135	-2.230975
H	0.748595	-5.738510	-1.546007
H	0.761953	-4.819404	-3.082850
H	-7.296193	0.386240	0.336565
H	-6.565715	-1.468633	1.762744

H	-2.414080	-0.083413	-2.285878
H	-3.192578	1.758765	-3.707325
H	-6.888089	1.952222	-1.514717
H	-5.428888	2.797592	-3.330758
H	-4.428500	-4.065313	3.028654
H	-5.267252	-2.520556	3.332541
H	-5.923265	-3.676834	2.134418

Processing: pddiphevanphos-c6dsdbe.log
Population analysis using the SCF density.

Label	Frequencies	IR Inten	Raman Activ	Depolar (P)	Depolar (U)	Dipole
A	3236.2615	12.6077	192.0945	0.2201	0.3609	10.3984
A	3231.2405	15.3572	186.5402	0.2465	0.3955	
A	3221.8180	12.2963	139.1788	0.1273	0.2259	
A	3208.9442	31.0764	196.2702	0.2469	0.3960	
A	3205.1017	6.7608	68.5001	0.4346	0.6059	
A	3204.0448	3.1723	48.6699	0.7341	0.8467	
A	3197.2936	45.9640	363.1253	0.1282	0.2273	
A	3193.5126	57.2028	359.0238	0.1392	0.2444	
A	3192.5905	13.6709	130.5629	0.6584	0.7940	
A	3188.3659	8.1397	102.2546	0.3990	0.5704	
A	3186.6814	34.7700	24.5591	0.6915	0.8176	
A	3185.5315	52.1537	31.0748	0.6981	0.8222	
A	3182.2544	15.0661	70.9296	0.7199	0.8371	
A	3180.3073	3.7679	38.5427	0.5418	0.7028	
A	3180.0320	14.1730	96.2606	0.7493	0.8567	
A	3166.2217	8.4369	127.1825	0.7473	0.8553	
A	3164.9436	11.3510	118.1687	0.7144	0.8334	
A	3162.9691	16.5265	77.7474	0.5339	0.6962	
A	3160.1500	8.7710	32.6086	0.3474	0.5157	
A	3158.4509	14.6238	51.7312	0.3826	0.5535	
A	3157.3907	4.3806	28.3220	0.5483	0.7083	
A	3156.9622	20.0225	91.1097	0.5219	0.6858	
A	3119.4205	11.9105	42.9076	0.3893	0.5604	
A	3116.6982	23.7456	15.2433	0.4604	0.6305	
A	3099.1127	24.8126	42.1522	0.4765	0.6454	
A	3098.5388	16.4038	96.7838	0.3966	0.5679	
A	3092.6232	30.3686	37.6327	0.6309	0.7737	
A	3089.2079	35.1058	74.7419	0.7226	0.8390	
A	3084.7009	28.2330	49.9324	0.7192	0.8367	
A	3077.3071	34.8975	86.5891	0.5002	0.6669	
A	3075.8340	64.6127	82.7782	0.3794	0.5501	
A	3072.6928	66.3521	207.2944	0.1326	0.2342	
A	3071.5942	57.9577	199.4230	0.3235	0.4889	
A	3067.9777	62.6156	127.7800	0.2364	0.3824	
A	3067.8658	65.7744	198.2566	0.3332	0.4999	
A	3063.0147	31.6785	83.6672	0.0668	0.1253	
A	3059.4656	10.7990	55.7960	0.2758	0.4324	
A	3046.1865	46.1557	27.9488	0.6117	0.7591	
A	3044.3270	10.6255	58.0305	0.2999	0.4614	
A	3042.5545	3.2857	32.4461	0.7245	0.8403	

A	3035.3715	66.1145	132.5610	0.0480	0.0916
A	3032.8221	18.5874	75.8134	0.3090	0.4721
A	3028.4358	81.3851	137.9419	0.0497	0.0947
A	3025.7178	27.7153	23.5130	0.7467	0.8550
A	3019.5272	25.4393	144.6774	0.1207	0.2154
A	3017.3684	17.1481	48.1397	0.2911	0.4510
A	3016.8733	44.1487	116.5113	0.1835	0.3100
A	3014.0323	18.6546	26.8948	0.5379	0.6995
A	3006.3136	6.4209	21.7888	0.4080	0.5796
A	1678.7450	17.4331	9.6423	0.5899	0.7421
A	1653.2688	51.6743	4.4301	0.6804	0.8098
A	1641.1087	61.2798	118.1042	0.5088	0.6745
A	1627.4693	19.7652	19.9190	0.6204	0.7658
A	1624.5058	34.3896	16.1564	0.7016	0.8246
A	1623.9782	18.5572	96.5238	0.4946	0.6618
A	1619.9072	0.5068	13.2096	0.7478	0.8557
A	1619.2622	4.3350	9.1209	0.7496	0.8569
A	1608.3678	49.5327	24.4011	0.5905	0.7425
A	1564.3177	45.4280	3.5335	0.4965	0.6635
A	1538.0051	4.5667	12.1173	0.7278	0.8424
A	1537.3582	8.0611	17.9353	0.5787	0.7331
A	1536.5913	23.0561	8.4823	0.6008	0.7506
A	1535.3852	1.6246	2.0851	0.7221	0.8386
A	1525.4754	31.1868	21.8377	0.4724	0.6417
A	1524.0445	6.4555	11.3204	0.0309	0.0599
A	1523.6715	13.6672	8.0050	0.1786	0.3031
A	1523.2556	5.9328	19.4205	0.7498	0.8570
A	1522.3901	6.5367	18.8177	0.5921	0.7438
A	1520.9881	11.6988	9.5249	0.7069	0.8283
A	1518.7239	17.6721	8.5451	0.1746	0.2973
A	1517.5772	3.9060	3.4123	0.7156	0.8342
A	1517.1908	1.2470	5.8940	0.0634	0.1192
A	1516.2282	37.8247	24.8822	0.7160	0.8345
A	1515.6056	9.3892	24.5640	0.6997	0.8233
A	1514.9915	13.1043	12.3177	0.5225	0.6864
A	1514.2266	5.6303	9.8829	0.3651	0.5349
A	1513.7398	28.9098	5.0652	0.6147	0.7614
A	1511.9361	1.9078	23.4303	0.7276	0.8423
A	1511.6722	2.2974	12.7023	0.7412	0.8514
A	1500.8450	15.3209	13.5822	0.6665	0.7999
A	1496.7953	21.8274	7.8402	0.6457	0.7847
A	1487.6987	55.2697	11.5853	0.6673	0.8004
A	1477.5223	6.7189	27.5615	0.4980	0.6649
A	1470.2178	1.7300	1.7666	0.7488	0.8564
A	1467.7665	3.5048	0.8158	0.7481	0.8559
A	1426.0646	33.9539	19.6267	0.7228	0.8391
A	1410.5963	0.4699	139.0162	0.1378	0.2422
A	1409.8994	11.2269	7.2892	0.1713	0.2925
A	1407.4283	44.1203	3.4418	0.4032	0.5747
A	1406.2012	49.5107	1.3141	0.4557	0.6261
A	1403.8797	7.0739	2.9959	0.6727	0.8043

A	1399.5323	0.5152	5.1312	0.7443	0.8534
A	1399.0886	1.6204	6.4323	0.7336	0.8463
A	1395.5041	2.5208	13.7052	0.5772	0.7319
A	1391.2487	4.5772	2.8575	0.5968	0.7475
A	1385.8539	0.4396	1.0060	0.3878	0.5589
A	1380.9010	1.4309	5.4539	0.7331	0.8460
A	1377.8789	1.1670	4.2743	0.7499	0.8571
A	1372.8962	42.0633	5.8218	0.3825	0.5533
A	1358.2303	0.3833	2.6080	0.7347	0.8471
A	1352.0965	0.1565	3.1964	0.7474	0.8554
A	1348.9914	1.2671	11.1892	0.7485	0.8562
A	1342.7221	0.4732	14.4477	0.7496	0.8569
A	1319.5384	69.6350	9.3690	0.3155	0.4797
A	1317.4924	39.4483	17.8125	0.4385	0.6097
A	1313.3394	2.0658	5.9300	0.4003	0.5717
A	1312.7585	0.0386	1.0147	0.7249	0.8405
A	1309.7851	4.5611	0.9148	0.5968	0.7475
A	1309.5363	87.5067	4.3993	0.7400	0.8506
A	1309.2568	37.5705	13.6501	0.5870	0.7398
A	1308.1116	27.0706	21.6969	0.5688	0.7252
A	1306.1450	58.3227	21.4093	0.2444	0.3928
A	1303.7102	18.7877	7.7035	0.0183	0.0359
A	1298.4147	72.3831	7.4794	0.1323	0.2338
A	1297.9638	33.3718	4.1264	0.3425	0.5103
A	1272.7305	40.2771	26.4243	0.1086	0.1959
A	1254.0071	13.9994	1.9790	0.6312	0.7739
A	1245.1297	5.3457	14.0866	0.2791	0.4365
A	1242.7948	30.3909	14.2703	0.5190	0.6833
A	1237.3471	5.4260	8.8533	0.5294	0.6923
A	1221.3468	1.4469	13.2947	0.3938	0.5651
A	1214.9043	8.6039	10.1889	0.7032	0.8257
A	1214.2348	2.0887	7.2067	0.4202	0.5917
A	1211.7782	4.2502	2.7128	0.5149	0.6798
A	1209.1198	0.4713	3.0053	0.6172	0.7633
A	1207.5472	2.2563	0.6808	0.6859	0.8137
A	1202.8578	7.6768	0.7858	0.7462	0.8546
A	1193.6951	0.4071	2.7248	0.4216	0.5931
A	1189.8823	16.2989	7.4836	0.7211	0.8380
A	1186.0429	0.0428	4.8715	0.7500	0.8571
A	1185.7616	0.3641	7.3584	0.7247	0.8404
A	1183.5864	0.5144	5.8313	0.7473	0.8553
A	1183.1106	1.1819	6.0048	0.7451	0.8539
A	1182.2572	1.7149	2.7428	0.6860	0.8138
A	1177.0681	12.8367	4.6229	0.5514	0.7108
A	1150.3693	7.0284	4.6402	0.7211	0.8379
A	1145.6186	46.0727	5.0815	0.1423	0.2491
A	1142.7677	8.9322	1.8446	0.6685	0.8013
A	1118.9273	188.3485	2.3640	0.0568	0.1075
A	1110.1496	98.8672	4.8440	0.0769	0.1428
A	1106.8824	2.8756	0.2393	0.4215	0.5930
A	1100.5678	1.1025	0.2934	0.6355	0.7771

A	1098.9093	0.5228	0.7217	0.7410	0.8513
A	1097.6942	0.4212	1.4502	0.7314	0.8448
A	1095.1267	3.2129	0.7303	0.6671	0.8003
A	1093.5347	2.1163	0.4948	0.7080	0.8290
A	1091.3870	7.0166	1.5896	0.7497	0.8569
A	1083.3167	9.2274	0.3467	0.1710	0.2921
A	1064.8494	1.4856	5.4457	0.7229	0.8392
A	1061.7805	2.5851	7.0359	0.7489	0.8564
A	1055.8182	6.3599	17.1041	0.1219	0.2173
A	1045.9645	5.3151	21.2669	0.1349	0.2377
A	1044.4739	6.1423	15.6816	0.2436	0.3918
A	1043.2486	3.1788	15.1394	0.7466	0.8549
A	1039.7697	22.2072	5.5409	0.5864	0.7393
A	1033.3689	27.7322	9.6245	0.3949	0.5662
A	1026.3256	6.2239	10.0554	0.7392	0.8501
A	1020.7651	6.1126	13.2671	0.1261	0.2240
A	1011.3846	5.6138	71.8770	0.0451	0.0864
A	1008.6465	10.8051	31.0457	0.7299	0.8439
A	1007.3168	5.2896	9.8014	0.4980	0.6649
A	992.3955	0.0670	0.6251	0.5905	0.7426
A	983.1291	0.5546	0.7782	0.4900	0.6577
A	978.7842	0.9250	0.8964	0.6764	0.8070
A	966.0467	0.2650	2.3084	0.4456	0.6165
A	962.3125	1.7751	0.7680	0.6308	0.7736
A	959.7218	0.0487	1.0254	0.6018	0.7514
A	953.4637	0.7319	1.8979	0.5535	0.7126
A	946.7425	0.0977	0.1011	0.6528	0.7900
A	939.2836	4.2377	0.7754	0.7494	0.8568
A	934.8085	7.6960	3.0593	0.3474	0.5157
A	933.7505	3.0596	0.3983	0.7241	0.8400
A	915.8378	12.3218	4.2375	0.5010	0.6676
A	908.7536	3.7777	0.8297	0.4668	0.6365
A	906.3842	1.8865	0.5156	0.4669	0.6366
A	903.7601	0.8723	0.4900	0.4924	0.6599
A	901.3338	2.6790	0.7421	0.7001	0.8236
A	899.3787	4.6862	1.4239	0.5881	0.7407
A	897.8965	5.0151	0.2090	0.4668	0.6365
A	881.5169	0.2062	1.5257	0.5932	0.7447
A	866.5063	8.6787	4.4873	0.7127	0.8322
A	863.2497	3.7179	9.3195	0.0669	0.1254
A	856.2964	0.9181	1.2669	0.6814	0.8105
A	850.4128	2.9319	11.6710	0.1632	0.2806
A	848.7209	0.0052	2.1861	0.5101	0.6756
A	826.3684	7.0066	4.0926	0.6817	0.8107
A	826.0827	52.1115	2.4226	0.3501	0.5186
A	822.8812	9.8951	2.4246	0.1187	0.2122
A	822.2710	6.4208	6.0882	0.1468	0.2561
A	803.2209	0.1807	0.8395	0.7118	0.8316
A	801.9275	0.3428	0.3418	0.4811	0.6496
A	798.4415	2.9742	2.8135	0.6991	0.8229
A	793.1009	8.2675	4.7362	0.0546	0.1035

A	773.7155	7.5260	26.7587	0.1072	0.1936
A	764.5589	20.5911	3.4774	0.7341	0.8466
A	757.3519	9.9988	5.9696	0.6940	0.8193
A	746.1171	55.0035	3.1959	0.5035	0.6698
A	740.4871	31.3694	0.9726	0.7493	0.8567
A	723.9980	4.5679	2.6633	0.6979	0.8220
A	713.2567	7.5187	17.0818	0.0507	0.0965
A	710.3266	23.2823	8.2911	0.5005	0.6671
A	707.2824	9.2243	4.8611	0.7478	0.8557
A	701.8327	2.2758	4.1235	0.1741	0.2966
A	695.6551	7.3912	4.1891	0.2243	0.3664
A	671.8590	5.3882	14.4190	0.0094	0.0186
A	669.6113	1.2916	1.8765	0.7452	0.8540
A	664.7141	5.9576	5.8727	0.1316	0.2325
A	648.6058	3.8064	3.2783	0.1617	0.2784
A	636.1783	10.1831	1.2832	0.3427	0.5105
A	629.9851	0.6669	3.0770	0.6537	0.7906
A	628.5894	0.0907	2.5356	0.7409	0.8511
A	606.4403	1.7340	2.4981	0.2815	0.4393
A	580.8116	7.7586	3.4984	0.2356	0.3814
A	560.1438	11.3682	1.9741	0.7305	0.8443
A	543.0597	2.4450	0.2866	0.7352	0.8474
A	539.4143	5.6030	3.1205	0.1254	0.2228
A	529.9201	0.9741	9.0672	0.5634	0.7208
A	514.1121	5.1894	2.5389	0.1657	0.2844
A	510.4963	11.8601	4.5727	0.0612	0.1154
A	494.0626	1.2459	3.6092	0.3980	0.5694
A	479.4281	7.9300	0.9800	0.3764	0.5469
A	472.9504	28.3776	0.8698	0.6730	0.8046
A	457.5870	15.1064	2.4511	0.6609	0.7958
A	444.4047	2.1905	1.3285	0.7125	0.8321
A	441.9533	0.5017	0.4718	0.6808	0.8101
A	440.4605	0.9245	1.0324	0.5673	0.7240
A	436.6443	2.6856	2.6878	0.3377	0.5048
A	419.0726	6.8238	1.1474	0.0359	0.0694
A	407.6239	0.0217	0.3678	0.7413	0.8514
A	405.0045	0.1403	1.1271	0.4212	0.5927
A	404.0291	2.8880	0.6183	0.6107	0.7583
A	396.0490	8.1594	2.7262	0.4691	0.6386
A	390.2393	4.6736	3.0515	0.5568	0.7153
A	383.9257	0.4714	6.7697	0.2038	0.3387
A	373.2064	6.2729	2.1374	0.6694	0.8020
A	353.7547	0.6736	0.9600	0.6425	0.7823
A	347.4629	0.7010	4.5319	0.1926	0.3230
A	324.7163	0.5027	0.6810	0.7315	0.8450
A	319.0140	0.3292	1.4107	0.1648	0.2830
A	307.5404	2.2879	0.7222	0.4117	0.5832
A	289.4342	5.6585	2.8970	0.3037	0.4659
A	279.0783	0.2556	2.6051	0.1528	0.2650
A	267.2316	1.5657	1.1331	0.3736	0.5440
A	263.7179	0.7188	0.7746	0.3069	0.4697

A	259.0073	5.0370	0.8457	0.3198	0.4846
A	253.5735	2.5237	4.4669	0.1425	0.2495
A	247.1116	0.9264	2.5002	0.0504	0.0959
A	236.0669	0.2096	0.2220	0.1886	0.3174
A	228.2921	0.5448	0.6120	0.6442	0.7836
A	221.0756	1.6834	3.6166	0.3885	0.5596
A	215.6491	0.0313	0.9744	0.2188	0.3590
A	211.3036	0.1421	3.2271	0.7431	0.8526
A	205.6635	2.1340	1.0286	0.6842	0.8125
A	200.4578	1.4211	11.9048	0.3101	0.4734
A	182.7717	0.1559	2.1005	0.4718	0.6411
A	177.3798	1.3327	0.6474	0.7489	0.8564
A	174.7987	1.4975	1.7747	0.3456	0.5137
A	169.9035	1.2206	0.2124	0.7488	0.8564
A	157.9791	0.4900	2.0410	0.3617	0.5312
A	149.9259	0.3025	1.7377	0.4313	0.6026
A	146.8594	1.7440	0.1546	0.7479	0.8558
A	144.8729	1.1399	2.4207	0.3888	0.5599
A	134.6732	1.5462	0.8905	0.6183	0.7642
A	129.4267	0.6123	3.4776	0.4202	0.5917
A	113.0665	1.3368	0.3687	0.7272	0.8420
A	110.4535	0.9414	2.3353	0.6353	0.7770
A	97.3907	1.8202	1.1745	0.6740	0.8053
A	83.2366	1.3004	1.7355	0.7457	0.8543
A	77.7683	0.6359	1.4923	0.7353	0.8475
A	74.5440	0.5902	0.1015	0.6183	0.7641
A	65.1842	1.1832	3.5727	0.7396	0.8503
A	62.1332	0.9390	2.0569	0.7195	0.8369
A	59.3012	0.0945	2.4950	0.7238	0.8397
A	55.1990	0.2572	1.4911	0.6815	0.8106
A	52.0837	0.2001	7.2942	0.7156	0.8342
A	47.4936	0.7014	1.3868	0.7426	0.8523
A	44.6161	0.0509	4.5938	0.7244	0.8402
A	43.1060	0.3663	3.7787	0.6537	0.7906
A	42.5345	0.0258	6.6405	0.7321	0.8453
A	32.3550	0.0584	3.5121	0.7450	0.8539
A	28.5682	0.0910	4.6172	0.7029	0.8255
A	27.9793	0.0295	3.9570	0.7205	0.8376
A	23.0786	0.0736	5.0698	0.7122	0.8319
A	16.3898	0.0100	2.4985	0.7312	0.8447
A	14.4278	0.0630	0.3113	0.6993	0.8230

TS1

Processing: pddiphevanphosts-ab6dsdbe.log
PG=C01

WARNING: Imaginary frequencies

Method BasisSet Imaginary Freqs
RB3LYP GenECP 1

HF Energy
-2362.9861437

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
515.64060	544.812	280.096	245.362	544.964	45.725	39.004

Processing: pddiphevanphosts-ab6dsdbe.log
97

C	1.476732	3.696387	1.809499
C	1.626604	3.183402	0.506055
C	1.241360	4.002447	-0.573049
C	0.686777	5.265501	-0.355359
C	0.521895	5.749726	0.945210
C	0.920617	4.959446	2.026360
Pd	1.451221	1.154458	0.280711
C	3.307331	2.036207	0.179687
C	4.163278	1.932388	1.293302
C	5.550985	1.961288	1.139539
C	6.122213	2.114853	-0.126305
C	5.285015	2.245573	-1.237295
C	3.896612	2.217185	-1.086623
P	0.996973	-1.196831	0.053704
C	2.355355	-2.100464	-0.884019
C	3.702661	-1.962859	-0.138872
C	4.847918	-2.621775	-0.928925
C	4.959805	-2.052568	-2.349660
C	3.624194	-2.179155	-3.095338
C	2.476010	-1.522018	-2.310966
C	0.701738	-2.117619	1.681731
C	1.561236	-1.581627	2.846144
C	1.156531	-2.237081	4.177989
C	1.222489	-3.769909	4.100558
C	0.377455	-4.305108	2.935113
C	0.776211	-3.654993	1.597648
C	-0.631680	-1.521588	-0.803786
C	-1.678411	-0.599965	-0.531542
C	-2.957315	-0.723124	-1.120330
C	-3.146668	-1.765521	-2.032363
C	-2.157967	-2.698447	-2.313233
C	-0.919349	-2.600152	-1.670424
O	-1.371916	0.356378	0.400033
C	-1.927624	1.681087	0.323983
C	-4.153027	0.110350	-0.777183
C	-4.896972	-0.137431	0.418629
C	-6.076645	0.632615	0.696258
C	-6.482669	1.616229	-0.238055
C	-5.768952	1.842312	-1.392557
C	-4.599458	1.087561	-1.664096

C	-6.808060	0.388276	1.890351
C	-6.402255	-0.574959	2.784221
C	-5.241098	-1.340140	2.513152
C	-4.510267	-1.129934	1.365427
O	0.056410	-3.541994	-1.843169
C	-0.163310	-4.607453	-2.754340
O	-3.830839	1.290239	-2.777509
C	-4.241297	2.254810	-3.733642
H	-2.369282	-3.508722	-2.999659
H	-4.120414	-1.866903	-2.502824
H	2.101840	-3.160540	-0.955189
H	3.930842	-0.901653	0.019852
H	3.640831	-2.424736	0.853291
H	5.792157	-2.483144	-0.386861
H	4.674767	-3.707446	-0.985302
H	5.242201	-0.991821	-2.289959
H	5.758168	-2.563314	-2.904022
H	3.697426	-1.724629	-4.092227
H	3.395121	-3.244261	-3.253416
H	2.659460	-0.441240	-2.239913
H	1.533561	-1.650442	-2.854031
H	-0.339894	-1.843543	1.905639
H	2.623773	-1.783056	2.655593
H	1.458450	-0.491755	2.907903
H	1.801784	-1.868049	4.985756
H	0.130656	-1.931262	4.432639
H	2.268891	-4.079910	3.959950
H	0.889937	-4.214673	5.047427
H	0.474565	-5.396431	2.862309
H	-0.684976	-4.098637	3.133187
H	1.802172	-3.959470	1.347222
H	0.134630	-4.026161	0.790966
H	1.378841	3.653239	-1.593172
H	0.390138	5.876500	-1.205326
H	0.100035	6.737198	1.113725
H	0.806011	5.329204	3.043018
H	1.800393	3.107008	2.663611
H	3.268057	2.334847	-1.964952
H	5.712352	2.378068	-2.229118
H	7.202210	2.144788	-0.243581
H	6.187643	1.868369	2.016906
H	3.744466	1.824787	2.290019
H	-1.210603	2.324670	0.835122
H	-2.026667	1.998650	-0.717479
H	-2.895265	1.726742	0.827336
H	0.751908	-5.202149	-2.739028
H	-1.008722	-5.235383	-2.445403
H	-0.338835	-4.238118	-3.772594
H	-7.376793	2.200081	-0.033044
H	-6.102988	2.603613	-2.087764
H	-3.628261	-1.729061	1.166145

H	-4.925522	-2.103634	3.219368
H	-7.699358	0.981216	2.083192
H	-6.967901	-0.752952	3.694571
H	-3.490268	2.223256	-4.525052
H	-5.224386	2.012964	-4.158702
H	-4.271117	3.265806	-3.306550

Processing: pddiphevanphosts-ab6dsdbe.log
Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3238.1294	13.0204	5.8734
A	3230.2363	14.9263	
A	3222.1087	11.8919	
A	3207.1395	38.0786	
A	3203.8703	35.5575	
A	3202.4510	50.0090	
A	3200.4047	9.1091	
A	3194.7868	52.3575	
A	3191.1824	7.8669	
A	3190.8233	8.5966	
A	3190.2243	19.7798	
A	3186.8432	7.2036	
A	3186.5647	7.7350	
A	3178.4376	2.5336	
A	3174.3071	19.1089	
A	3172.9265	0.4982	
A	3172.8224	9.2172	
A	3168.1935	5.4999	
A	3167.3380	13.4839	
A	3158.8083	23.0476	
A	3158.6762	14.0405	
A	3157.8288	18.3964	
A	3118.4205	29.6562	
A	3098.5368	53.2044	
A	3096.5516	12.2541	
A	3094.5767	10.1084	
A	3094.2945	36.1101	
A	3087.0761	26.2352	
A	3086.8887	36.6829	
A	3075.2733	57.4535	
A	3074.5309	22.5544	
A	3073.2090	55.8353	
A	3069.2907	76.6201	
A	3068.4550	47.9720	
A	3066.1535	69.2971	
A	3064.3829	65.1587	
A	3055.3502	7.4976	
A	3043.9467	40.6479	
A	3042.9733	8.2438	
A	3036.3855	10.5441	
A	3032.2310	70.6437	

A	3030.5889	18.2361
A	3026.7208	75.5162
A	3024.3370	26.6283
A	3020.4310	7.2500
A	3019.8356	22.5567
A	3017.2804	14.8486
A	3015.7152	43.0696
A	3012.9481	19.4446
A	1678.2592	17.1727
A	1652.8234	50.3670
A	1640.9368	78.1328
A	1626.2874	44.9789
A	1622.5323	3.3848
A	1622.1772	21.1730
A	1619.2852	0.3386
A	1616.5253	5.5416
A	1604.4559	54.8062
A	1564.2262	44.8435
A	1538.0639	6.3409
A	1537.6687	1.6310
A	1535.5899	23.1737
A	1534.1162	1.3010
A	1531.4467	28.1595
A	1524.8667	56.4853
A	1523.6988	4.0767
A	1523.4346	1.4329
A	1521.8573	2.7623
A	1520.3036	26.5766
A	1518.7749	9.3072
A	1517.2491	20.6206
A	1516.2612	6.7086
A	1515.9896	3.9583
A	1515.1434	16.4478
A	1513.9090	7.0686
A	1511.3084	5.3874
A	1510.9525	16.5188
A	1510.2760	15.5461
A	1509.8590	14.8611
A	1505.6669	5.6473
A	1499.2923	12.7751
A	1489.2398	67.7048
A	1477.1926	11.0468
A	1476.2355	0.2677
A	1468.5770	6.2198
A	1425.6164	41.7861
A	1409.7132	3.6865
A	1409.0982	3.1312
A	1405.2299	3.9695
A	1403.9197	33.0035
A	1402.6797	98.9454
A	1398.4639	9.6115

A	1395.6800	1.3628
A	1394.6458	3.4494
A	1387.7498	1.2051
A	1385.9640	1.3034
A	1379.7681	2.2063
A	1378.6101	1.0245
A	1371.3112	49.3275
A	1362.4656	1.0819
A	1348.1446	0.2632
A	1347.4561	2.2117
A	1340.6486	0.5558
A	1321.2074	33.3367
A	1320.0145	0.4795
A	1317.2788	43.3347
A	1315.6486	77.5538
A	1313.8849	21.9576
A	1312.9697	3.2710
A	1309.6223	149.5590
A	1308.5177	18.1093
A	1306.9130	4.7194
A	1302.8597	1.1053
A	1298.5279	2.1821
A	1296.1742	48.6322
A	1274.6911	83.3935
A	1257.0281	38.6675
A	1250.1644	5.3941
A	1248.9550	14.7218
A	1235.4486	5.2487
A	1221.3728	5.3198
A	1215.1732	7.0567
A	1214.2354	0.8138
A	1209.6539	4.7379
A	1206.7250	1.2130
A	1206.4125	0.6223
A	1205.0059	3.1739
A	1193.4503	1.9345
A	1189.4538	12.3096
A	1188.5359	0.0460
A	1186.2102	0.0119
A	1183.8437	1.8544
A	1183.1132	1.0372
A	1180.9558	8.3804
A	1177.5691	6.4411
A	1151.8732	4.8751
A	1150.4014	111.9172
A	1142.2113	10.3331
A	1133.7758	119.2370
A	1110.2665	85.6124
A	1105.2991	2.5724
A	1101.4207	2.2318
A	1100.8314	4.8215

A	1098.7958	0.2806
A	1097.6533	0.0421
A	1097.0110	0.3071
A	1068.6151	1.8388
A	1065.9268	1.6664
A	1062.9533	2.0310
A	1061.4832	2.5945
A	1055.5585	10.1190
A	1054.6812	18.7992
A	1045.6893	1.4101
A	1042.0903	3.0509
A	1029.6750	12.9875
A	1026.3069	6.1694
A	1021.0850	11.7761
A	1017.5486	34.1362
A	1011.2104	3.8796
A	1008.1114	0.0824
A	1003.7171	6.9560
A	990.9061	0.2072
A	983.7761	0.2983
A	978.2662	0.2077
A	963.3648	0.1591
A	961.1621	1.4395
A	953.9682	0.0021
A	946.7826	0.9814
A	946.1677	0.6003
A	939.0931	3.1173
A	933.4404	1.9751
A	933.0355	1.9135
A	915.9643	12.5127
A	907.5677	1.9073
A	902.9107	1.4134
A	901.7407	0.6309
A	901.0877	6.3473
A	898.1318	2.1308
A	892.1460	7.5825
A	881.2357	0.8720
A	867.1143	7.7342
A	863.6103	3.5124
A	851.0934	0.1241
A	847.7848	0.6369
A	835.8187	0.0703
A	828.2592	49.9805
A	825.6627	1.6628
A	821.5954	0.8217
A	808.3512	17.2069
A	803.2496	0.3575
A	800.6773	0.1214
A	798.9593	4.4299
A	773.5400	8.9775
A	772.8908	5.0829

A	765.7957	15.3757
A	754.1775	8.8273
A	745.1311	8.0893
A	726.7644	138.4921
A	725.0838	24.4642
A	716.9019	14.1161
A	708.0279	0.8971
A	704.6842	3.0753
A	698.6680	6.2890
A	698.2636	6.7696
A	657.8616	3.6211
A	656.4042	0.8639
A	652.9617	2.4056
A	642.6326	28.0306
A	636.2918	10.5670
A	627.9360	0.0048
A	623.3537	0.0030
A	606.9714	6.6650
A	575.7585	11.9349
A	562.1601	6.4591
A	545.0381	2.5162
A	541.6088	9.0556
A	527.3617	0.8955
A	514.1771	7.2400
A	508.5404	5.9247
A	484.9555	4.3279
A	473.4748	34.8753
A	461.8553	12.4453
A	443.2735	0.7625
A	442.2861	0.9479
A	440.3652	1.8867
A	436.6366	2.3771
A	419.1651	0.0098
A	410.7525	4.5158
A	407.9520	1.3895
A	407.0439	4.7918
A	399.5080	15.7900
A	390.3110	3.8633
A	385.8069	5.4978
A	377.8561	0.9252
A	362.3733	0.1351
A	346.5893	0.9866
A	340.1837	0.9363
A	330.2081	0.0788
A	323.2055	0.7380
A	302.2768	3.2537
A	287.3161	3.4940
A	275.1314	0.1252
A	-273.8623	65.8899
A	272.0847	1.4373
A	266.9436	0.1158

A	258.2242	0.2030
A	255.6906	0.4342
A	253.5955	0.4688
A	245.0275	0.7274
A	234.7179	0.0846
A	233.9583	0.5531
A	218.0006	0.7778
A	216.8644	0.7308
A	193.8195	1.5277
A	189.9956	0.8628
A	180.4410	0.7436
A	174.3339	0.2745
A	166.4973	1.9035
A	161.1098	0.4430
A	151.2822	2.1245
A	142.6482	1.8903
A	136.4252	1.9437
A	128.1432	2.1212
A	119.0418	3.5248
A	111.1866	0.4530
A	106.1512	0.8725
A	104.1028	0.6368
A	82.3292	0.0577
A	74.3542	0.3412
A	69.2377	1.2050
A	64.5601	1.8686
A	62.7227	0.5345
A	60.0782	0.3645
A	56.3532	0.1646
A	53.7091	0.5298
A	50.3756	0.7444
A	47.4240	0.2086
A	43.5386	0.2570
A	38.7538	0.3059
A	36.4266	0.5394
A	28.0400	0.1163
A	20.2660	0.0060
A	10.8890	0.0376
A	10.6475	0.0707
A	7.4775	0.1622

TS2

Processing: pddiphevanphosts6dsdbe.log
PG=C01

WARNING: Imaginary frequencies

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	1

HF Energy
-2362.9859283

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
515.60010	544.791	280.313	245.585	544.943	45.725	39.026

Processing: pddiphevanphosts6dsdbe.log
97

C	-4.659490	0.771970	-2.242080
C	-5.011509	0.440400	-0.900772
C	-6.223405	0.997823	-0.368998
C	-7.030075	1.833011	-1.188860
C	-6.663321	2.123985	-2.482104
C	-5.461629	1.588690	-3.007614
C	-6.579010	0.702033	0.968956
C	-5.787892	-0.103026	1.756247
C	-4.593685	-0.659548	1.231509
C	-4.194382	-0.396900	-0.079031
C	-2.976890	-1.076363	-0.621549
C	-1.645981	-0.811433	-0.222980
C	-0.559456	-1.623151	-0.645771
C	-0.851660	-2.727029	-1.478727
C	-2.150379	-2.957198	-1.943898
C	-3.182861	-2.137431	-1.508944
P	1.128452	-1.151637	0.003932
C	1.133535	-2.125536	1.628268
C	2.076941	-1.524136	2.691463
C	1.910083	-2.237001	4.044658
C	2.115519	-3.754050	3.917480
C	1.187444	-4.353444	2.850674
C	1.348501	-3.645879	1.492796
O	-1.310645	0.191668	0.645636
C	-2.018865	1.442262	0.658617
O	0.184188	-3.558881	-1.801115
C	-0.049470	-4.646435	-2.682221
O	-3.772554	-1.468743	1.964172
C	-4.122290	-1.778491	3.303118
Pd	1.372619	1.225347	0.255084
C	3.113402	2.285841	-0.027879
C	4.101873	2.236605	0.974384
C	5.452790	2.402709	0.662193
C	5.853196	2.642208	-0.654851
C	4.881496	2.719532	-1.655900
C	3.529466	2.553987	-1.346621
C	1.386913	3.256696	0.528660
C	1.346894	3.722888	1.857528
C	0.704058	4.920104	2.181446
C	0.104429	5.691532	1.182545
C	0.156076	5.255279	-0.144169
C	0.798128	4.058338	-0.468750

C	2.435341	-1.898261	-1.124976
C	3.847786	-1.633050	-0.555681
C	4.940414	-2.158899	-1.504111
C	4.807482	-1.560804	-2.911130
C	3.405670	-1.814839	-3.482341
C	2.309079	-1.291434	-2.539510
H	-2.370322	-3.786801	-2.603980
H	-4.198796	-2.350612	-1.829342
H	2.282159	-2.977668	-1.191520
H	3.987214	-0.556466	-0.398288
H	3.962402	-2.112887	0.423282
H	5.928589	-1.930928	-1.084403
H	4.871657	-3.255750	-1.567794
H	4.986521	-0.477424	-2.858670
H	5.574078	-1.977697	-3.577514
H	3.301868	-1.341541	-4.467694
H	3.266760	-2.895679	-3.638415
H	2.389057	-0.198316	-2.464072
H	1.321697	-1.510929	-2.959917
H	0.106006	-1.962788	1.986155
H	3.121418	-1.615333	2.364800
H	1.877683	-0.450985	2.795769
H	2.612557	-1.817007	4.776248
H	0.899297	-2.040021	4.432863
H	3.161252	-3.954721	3.640166
H	1.950068	-4.244569	4.885540
H	1.381172	-5.428203	2.736122
H	0.142992	-4.258329	3.183731
H	2.359863	-3.840687	1.108968
H	0.650026	-4.068055	0.762443
H	0.843356	3.747581	-1.509360
H	-0.299020	5.852209	-0.931618
H	-0.386291	6.628435	1.433184
H	0.678738	5.253986	3.216547
H	1.825636	3.148857	2.646803
H	2.793103	2.632952	-2.141558
H	5.173890	2.917395	-2.685096
H	6.904195	2.778866	-0.895206
H	6.194927	2.349303	1.456023
H	3.816515	2.063605	2.008361
H	-1.301977	2.177702	1.025313
H	-2.342209	1.719226	-0.348590
H	-2.882301	1.397368	1.324889
H	0.916210	-5.140752	-2.803195
H	-0.771250	-5.358601	-2.262393
H	-0.406248	-4.303177	-3.661492
H	-7.495187	1.122903	1.376147
H	-6.086911	-0.313546	2.776384
H	-3.741255	0.370459	-2.657392
H	-5.168313	1.827824	-4.026465
H	-7.946249	2.242278	-0.768955

H	-7.286524	2.765190	-3.099182
H	-3.328655	-2.430817	3.671787
H	-4.168603	-0.879027	3.931064
H	-5.081543	-2.309908	3.360707

Processing: pddiphevanphosts6dsdbe.log
Population analysis using the SCF density.

Label	Frequencies	IR Inten	Dipole
A	3238.3824	12.3247	6.2467
A	3230.9564	14.0197	
A	3220.3583	10.8618	
A	3207.1065	39.2139	
A	3203.8307	34.7553	
A	3202.7285	49.9430	
A	3198.6951	9.8976	
A	3194.6189	54.5373	
A	3191.1097	6.3852	
A	3190.7306	8.6776	
A	3190.2791	18.5575	
A	3187.0704	6.8437	
A	3186.4490	7.7076	
A	3178.5323	2.7059	
A	3174.7243	9.0947	
A	3174.3343	16.8741	
A	3172.8069	1.6201	
A	3168.4807	5.4117	
A	3167.3510	13.6495	
A	3158.3074	20.8227	
A	3157.7812	18.0308	
A	3156.6458	17.4404	
A	3118.6750	29.6938	
A	3100.9428	36.2042	
A	3097.0202	24.2730	
A	3094.5035	19.6928	
A	3093.7243	28.5523	
A	3087.0140	27.3283	
A	3086.0185	36.5978	
A	3075.2171	58.5936	
A	3074.7756	23.3207	
A	3072.6271	61.2987	
A	3069.3375	67.1788	
A	3067.8498	58.5011	
A	3065.5746	71.0325	
A	3064.4471	65.3485	
A	3055.5262	7.9156	
A	3043.6998	41.4348	
A	3041.4964	7.3766	
A	3036.3864	10.1158	
A	3032.2237	69.5463	
A	3030.5138	17.9467	
A	3026.0416	73.7618	

A	3023.5702	27.0463
A	3020.2451	7.2701
A	3018.2297	21.6771
A	3016.7338	14.9457
A	3015.6954	43.9640
A	3013.0368	18.7031
A	1677.5309	19.8619
A	1651.8465	49.4282
A	1639.5138	83.5481
A	1626.3843	44.7277
A	1622.2982	20.5253
A	1620.9560	5.0586
A	1619.1832	0.3381
A	1616.3791	5.5390
A	1603.8040	53.6109
A	1564.2405	48.3145
A	1537.8623	8.9442
A	1537.4982	1.3894
A	1535.3426	25.8096
A	1534.1513	0.6547
A	1529.9749	46.8155
A	1523.7462	9.3583
A	1523.3331	0.8199
A	1523.1214	25.3525
A	1521.8499	8.7581
A	1520.4271	32.6723
A	1518.8687	12.8175
A	1517.2891	12.3153
A	1516.1461	3.1376
A	1515.4281	1.8911
A	1513.8676	3.3221
A	1512.8514	21.4417
A	1511.0392	7.2062
A	1510.8010	18.9353
A	1510.2238	8.6543
A	1509.8239	18.0547
A	1506.2377	2.2792
A	1499.5211	11.9060
A	1489.1174	71.5111
A	1476.5146	9.9595
A	1476.2630	0.3017
A	1468.5632	6.2098
A	1424.7980	41.6719
A	1409.8890	4.5309
A	1408.2733	15.6080
A	1405.2701	6.9464
A	1404.4633	88.2051
A	1403.2720	46.6020
A	1398.4468	6.5098
A	1395.8719	1.7257
A	1394.3404	3.5428

A	1387.3751	1.6576
A	1385.7336	1.4563
A	1379.8080	3.7536
A	1378.6027	1.5395
A	1372.0678	47.6695
A	1362.5975	1.0469
A	1348.2533	0.3221
A	1347.7414	2.0145
A	1340.9058	0.7317
A	1321.8000	62.2824
A	1320.0954	0.3961
A	1316.8677	52.3516
A	1315.4236	71.3000
A	1314.1400	10.1986
A	1313.0326	4.9401
A	1311.1011	153.3251
A	1308.7987	3.7102
A	1306.9767	0.8212
A	1302.8249	0.8575
A	1299.2616	13.6867
A	1298.6537	14.0562
A	1274.5191	89.6618
A	1256.2133	45.2988
A	1250.9804	1.7777
A	1250.0631	9.8705
A	1234.7924	5.3582
A	1220.9088	5.2677
A	1215.6407	7.6466
A	1214.4179	0.7427
A	1209.7321	4.7347
A	1206.7772	1.1139
A	1206.5771	0.8829
A	1204.7979	1.5827
A	1193.0504	4.0580
A	1189.7812	11.1261
A	1188.5997	0.0379
A	1186.2091	0.0105
A	1183.7722	0.8567
A	1183.0766	0.8661
A	1178.7981	14.5632
A	1173.2980	2.6093
A	1152.1488	4.0642
A	1149.6091	119.9396
A	1142.1655	7.5400
A	1134.6720	116.3344
A	1112.0130	68.7122
A	1104.9567	3.0927
A	1101.3272	1.8052
A	1100.8747	5.5559
A	1098.7902	0.3450
A	1097.8428	0.0754

A	1096.9218	0.3744
A	1068.7055	1.9057
A	1065.9703	1.7051
A	1063.0515	2.0055
A	1061.7190	2.8220
A	1055.7628	22.6295
A	1055.4503	10.5081
A	1045.8640	1.3676
A	1042.3378	3.1866
A	1029.5069	12.9559
A	1026.4406	6.3861
A	1021.2765	11.8372
A	1017.5510	35.0631
A	1011.1956	3.7281
A	1008.0208	0.1002
A	1003.7275	6.5364
A	992.4256	0.0029
A	984.2680	0.2637
A	978.0259	0.2345
A	963.7325	0.1641
A	962.4829	1.2058
A	953.8877	0.0029
A	949.1586	1.9791
A	945.9857	0.0945
A	938.8273	3.4027
A	935.0358	1.2024
A	933.1609	2.9232
A	914.4123	16.3312
A	907.6039	1.9919
A	903.1423	1.5696
A	901.8498	0.6024
A	901.5147	6.0784
A	898.2029	2.1910
A	891.4684	7.7884
A	882.9211	0.7744
A	867.3941	7.6167
A	863.6236	3.4701
A	851.1086	0.1342
A	846.1694	0.9785
A	835.5085	0.0855
A	827.7796	49.7918
A	825.8211	1.8024
A	821.8189	0.6859
A	810.7730	14.0834
A	802.9764	0.3618
A	800.7704	0.0696
A	797.3164	7.1047
A	780.5034	6.4072
A	766.1724	15.5981
A	764.2149	9.2225
A	755.6324	9.1826

A	745.2792	7.7383
A	726.5822	146.8717
A	722.9074	15.1555
A	716.7378	16.7078
A	707.1328	0.1484
A	704.9273	3.4856
A	698.4279	7.4328
A	696.2190	4.4391
A	659.3374	5.3106
A	656.2330	0.4165
A	648.6897	3.6745
A	642.5697	27.6300
A	636.2568	12.5501
A	627.9831	0.0055
A	623.3652	0.0028
A	616.6664	4.3064
A	579.2359	4.7018
A	555.6192	7.1512
A	544.5456	3.3199
A	544.0324	13.3434
A	527.7161	1.9255
A	514.5095	5.6062
A	508.2211	7.8700
A	485.2696	4.1106
A	473.1744	33.0521
A	461.9851	13.7837
A	443.5528	0.8283
A	442.1852	0.9690
A	440.3180	1.3206
A	436.2149	2.9689
A	419.3207	0.0125
A	410.2093	4.8648
A	408.2683	4.4623
A	407.4322	2.2602
A	399.6274	15.5018
A	390.8326	3.9961
A	387.1295	5.8261
A	378.0979	1.4748
A	361.1055	0.0344
A	350.7160	0.8865
A	341.0229	1.7436
A	332.2593	0.2116
A	323.1093	1.2450
A	305.5697	2.3515
A	279.9799	2.8825
A	-275.7173	66.0159
A	274.7799	0.6935
A	271.6477	1.1781
A	268.2877	0.3368
A	258.7807	0.0748
A	254.3615	0.0965

A	253.0030	1.1063
A	240.0100	0.6967
A	234.8285	0.8447
A	228.5419	0.4709
A	218.4792	0.6492
A	215.0537	0.3955
A	191.3129	2.0354
A	190.3382	0.5937
A	180.4218	0.6256
A	173.0527	0.3382
A	167.7450	1.3988
A	158.2925	0.1014
A	151.1813	1.7269
A	144.7177	1.5383
A	135.1459	1.6034
A	127.1353	0.7357
A	117.3451	3.4115
A	111.0593	0.7404
A	106.2020	0.2527
A	102.4445	0.8451
A	81.4456	0.0850
A	74.8668	0.3298
A	69.2868	0.8321
A	65.6399	1.2286
A	60.4609	0.4595
A	59.2510	0.6072
A	57.0769	0.7212
A	53.0703	1.6796
A	51.7002	0.7742
A	48.4603	0.1126
A	40.8623	0.5299
A	40.0623	0.4227
A	34.4117	0.0508
A	27.5670	0.0600
A	23.2224	0.0309
A	11.3398	0.0775
A	10.1024	0.0136
A	7.2622	0.0159

G':

Processing: pddiphevanphos-a6dsdbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	0

HF Energy
-2362.9740743

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
516.27189	545.665	278.377	246.856	545.816	45.725	38.834

Processing: pddiphevanphos-a6dsdbe.log
97

C	6.019855	-3.232583	0.165668
C	6.561937	-2.108670	-0.412629
C	5.888722	-0.858178	-0.352361
C	4.624790	-0.766864	0.322469
C	4.096725	-1.950988	0.913574
C	4.774394	-3.146841	0.835698
C	6.433515	0.310568	-0.937893
C	5.774978	1.517029	-0.872288
C	4.522848	1.607158	-0.212505
C	3.941620	0.487474	0.378737
C	2.646211	0.624862	1.114647
C	1.398931	0.187196	0.614567
C	0.211853	0.274163	1.386708
C	0.333653	0.697936	2.731949
C	1.550883	1.176468	3.224689
C	2.675871	1.148920	2.408606
P	-1.400432	-0.236232	0.604976
C	-2.838419	0.600491	1.500383
C	-4.161656	0.377033	0.727306
C	-5.358064	0.966560	1.496421
C	-5.168098	2.460204	1.790999
C	-3.830581	2.714190	2.499160
C	-2.649153	2.118598	1.713036
O	1.270859	-0.431221	-0.593107
C	1.918522	0.082728	-1.769519
O	-0.775874	0.588603	3.519447
C	-0.718289	1.044368	4.863456
O	3.806006	2.769476	-0.140424
C	4.331684	3.944102	-0.739681
Pd	-1.517995	0.275101	-1.595328
C	-1.281864	2.329886	-1.471601
C	-2.240171	2.997567	-2.267278
C	-2.106621	4.345879	-2.621491
C	-1.014308	5.081332	-2.159039
C	-0.064468	4.455359	-1.347303
C	-0.200969	3.105439	-1.007801
C	-1.789740	-1.624461	-2.358240
C	-0.772952	-2.590589	-2.506618
C	-0.932308	-3.710043	-3.330330
C	-2.126566	-3.904633	-4.029623
C	-3.157765	-2.973229	-3.894335
C	-2.991715	-1.859590	-3.061820
C	-1.446408	-2.086631	1.013788

C	-0.971133	-2.462467	2.434530
C	-0.846989	-3.991196	2.580722
C	-2.154336	-4.715501	2.233292
C	-2.657152	-4.307585	0.841894
C	-2.791198	-2.779831	0.716123
H	1.638506	1.535315	4.242479
H	3.625738	1.497632	2.803391
H	-2.910132	0.110479	2.478674
H	-4.077368	0.863472	-0.253764
H	-4.342025	-0.682335	0.532822
H	-6.277405	0.804362	0.919008
H	-5.484741	0.420051	2.443329
H	-5.183604	3.019024	0.844170
H	-6.002303	2.840460	2.394877
H	-3.671238	3.791608	2.635526
H	-3.861555	2.271896	3.507068
H	-2.580714	2.605966	0.734916
H	-1.715462	2.332309	2.235746
H	-0.710537	-2.476607	0.297870
H	-3.546235	-2.435526	1.436558
H	-3.141654	-2.521598	-0.286611
H	-3.625986	-4.778598	0.632286
H	-1.960788	-4.668234	0.071905
H	-2.918994	-4.461156	2.982824
H	-2.012887	-5.802614	2.288204
H	-0.532625	-4.236513	3.603813
H	-0.047651	-4.347883	1.914491
H	-1.683345	-2.080066	3.178198
H	-0.004460	-2.000795	2.655626
H	-3.118549	2.457912	-2.627913
H	-2.860938	4.821303	-3.245740
H	-0.909064	6.131834	-2.419937
H	0.786248	5.023284	-0.973063
H	0.556706	2.657913	-0.368033
H	-3.823147	-1.160782	-2.962264
H	-4.095435	-3.117033	-4.428198
H	-2.253527	-4.775644	-4.668209
H	-0.122427	-4.431079	-3.428358
H	0.168134	-2.465818	-1.972921
H	1.261813	-0.183371	-2.600359
H	2.017495	1.169138	-1.716427
H	2.896715	-0.384003	-1.905737
H	-1.712905	0.869714	5.277175
H	0.021876	0.481839	5.446042
H	-0.486304	2.115335	4.915820
H	7.391772	0.246132	-1.447747
H	6.216245	2.393753	-1.331628
H	3.147780	-1.898213	1.436379

H 4.350521 -4.036082 1.294798
H 7.518688 -2.158464 -0.927649
H 6.541910 -4.183882 0.112821
H 3.587822 4.722753 -0.562787
H 5.283941 4.242015 -0.281523
H 4.471993 3.820965 -1.821246

H':

Processing: pddiphevanphos6dsdbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	0

HF Energy
-2362.9693424

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
516.43345	545.803	276.661	247.298	545.949	45.725	38.869

Processing: pddiphevanphos6dsdbe.log
97
C 2.059943 -1.413988 3.254110
C 2.491171 -0.252608 2.581145
C 3.709942 0.308468 3.026371
C 4.434301 -0.231558 4.095833
C 3.970635 -1.376695 4.745920
C 2.778762 -1.967519 4.319423
Pd 1.394753 1.004307 1.348457
C 0.406231 2.698570 0.721436
C 1.162523 3.872200 0.505693
C 0.586262 5.146019 0.571990
C -0.776851 5.282903 0.840449
C -1.552722 4.138608 1.040616
C -0.971568 2.867396 0.969532
P 1.398117 -0.192565 -0.581708
C -0.276859 -0.574671 -1.326826
C -1.432649 -0.637904 -0.513475
C -2.714528 -0.906136 -1.042908
C -2.816604 -1.154511 -2.410668
C -1.700753 -1.152774 -3.239928
C -0.440163 -0.880632 -2.704253
O -1.307598 -0.378966 0.829032
C 2.141891 -1.932559 -0.365236
C 1.757467 -2.999076 -1.412565

C	2.262896	-4.389780	-0.984227
C	3.777545	-4.401113	-0.739915
C	4.179561	-3.312246	0.263258
C	3.671951	-1.924575	-0.166838
C	2.412433	0.728391	-1.886458
C	3.701762	1.322421	-1.271486
C	4.557961	2.020219	-2.344280
C	3.772034	3.110166	-3.084345
C	2.467329	2.546674	-3.662716
C	1.616578	1.854127	-2.583355
O	0.689620	-0.921651	-3.469865
H	-1.820416	-1.369858	-4.293961
H	-3.795229	-1.361139	-2.834110
C	-3.964105	-0.919243	-0.217087
H	2.693095	-0.020516	-2.635367
H	3.422507	2.044170	-0.493680
H	4.298078	0.552715	-0.776492
H	5.454060	2.445622	-1.874315
H	4.912382	1.271028	-3.068532
H	3.532954	3.922927	-2.383484
H	4.386399	3.551471	-3.879870
H	1.880478	3.347454	-4.130789
H	2.704672	1.825270	-4.459941
H	1.309234	2.591247	-1.833640
H	0.701948	1.465059	-3.035391
H	1.696668	-2.231500	0.593222
H	4.159239	-1.645239	-1.111825
H	3.955173	-1.186845	0.588165
H	5.270543	-3.281824	0.378435
H	3.767491	-3.547269	1.254558
H	4.298249	-4.226033	-1.693546
H	4.099493	-5.388661	-0.385058
H	1.991626	-5.128786	-1.749752
H	1.744520	-4.691799	-0.061948
H	2.191985	-2.737390	-2.385178
H	0.672405	-3.036362	-1.548791
H	2.228367	3.802054	0.291754
H	1.202428	6.028924	0.411355
H	-1.229776	6.270445	0.890612
H	-2.615454	4.231238	1.255036
H	-1.597895	1.994244	1.128899
H	4.110029	1.193697	2.529842
H	5.363946	0.237057	4.413611
H	4.532532	-1.806186	5.571916
H	2.406175	-2.859991	4.819726
H	1.133859	-1.901146	2.954638
C	-1.401373	-1.499930	1.713244
H	-1.177890	-1.110379	2.707291

H -2.401301 -1.939474 1.700580
H -0.664172 -2.267246 1.446653
C 0.579882 -1.208663 -4.856333
H 1.598780 -1.174750 -5.245865
H 0.158082 -2.206909 -5.027747
H -0.031694 -0.460049 -5.374904
C -4.669947 0.289685 0.072765
C -5.907309 0.233573 0.798940
C -6.401171 -1.028329 1.208371
C -5.726021 -2.189898 0.912526
C -4.506815 -2.136312 0.190381
C -4.204514 1.566093 -0.354586
C -6.613673 1.435914 1.074937
H -7.336660 -1.073691 1.760817
H -6.131743 -3.142164 1.233393
O -3.788771 -3.258742 -0.131070
C -4.918307 2.710837 -0.078130
H -3.272436 1.631613 -0.904819
H -4.540732 3.670950 -0.418527
C -6.134508 2.651400 0.646122
H -7.547240 1.373300 1.629604
H -6.683544 3.564500 0.858689
C -4.307851 -4.531326 0.219240
H -3.586312 -5.258882 -0.157507
H -4.402235 -4.649581 1.306896
H -5.283663 -4.715811 -0.248971

I:

Processing: pdevanphos-x6dsdbe.log
PG=CI

Method BasisSet Imaginary Freqs
RB3LYP GenECP 0

HF Energy
-4592.0167284

ZPE E298 S298 Squasihar Equasihar Strans Srot
809.16230 855.838 399.009 354.580 856.054 47.015 41.134

Processing: pdevanphos-x6dsdbe.log
151
C -7.634552 2.468743 -0.242482
C -7.883829 1.204026 -0.723969
C -2.231056 3.822639 -3.133589

C	-6.236072	4.042270	1.062789
C	-0.814503	3.605199	-3.684619
C	-8.327243	-1.413604	-1.678013
C	-6.502356	2.737911	0.563679
C	-2.192820	4.299884	-1.674871
C	-5.131990	4.286122	1.846265
C	-6.999397	0.140388	-0.414233
C	3.249269	5.014144	-2.950477
C	-5.607802	1.660418	0.883848
C	-3.829991	0.279165	-1.753027
C	0.003611	2.657024	-2.790932
C	-5.871908	0.347135	0.379311
C	-4.246683	3.225996	2.162563
C	-1.358042	3.364787	-0.780733
C	0.070405	3.196339	-1.348361
C	-4.475180	1.949667	1.698117
C	-1.970890	-3.351222	-3.797597
C	-5.005961	-0.815965	0.749560
C	-2.039982	-2.540524	-2.492427
C	-2.386514	-4.812361	-3.581313
C	3.461848	3.000709	-1.657008
C	-3.684202	-1.012123	0.293235
C	1.606234	4.649497	1.160138
C	4.782124	2.840655	-2.091796
C	-5.522772	-1.755494	1.645685
C	1.549493	5.458468	2.469607
C	2.869459	2.070191	-0.773544
C	1.177844	3.183863	1.389251
C	-1.549493	-5.458468	-2.469607
C	-1.177844	-3.183863	-1.389251
C	-2.869459	-2.070191	0.773544
C	5.522772	1.755494	-1.645685
C	-4.782124	-2.840655	2.091796
C	-1.606234	-4.649497	-1.160138
C	-3.461848	-3.000709	1.657008
C	2.386514	4.812361	3.581313
C	3.684202	1.012123	-0.293235
C	5.005961	0.815965	-0.749560
C	2.039982	2.540524	2.492427
C	1.970890	3.351222	3.797597
C	4.475180	-1.949667	-1.698117
C	-0.070405	-3.196339	1.348361
C	4.246683	-3.225996	-2.162563
C	5.871908	-0.347135	-0.379311
C	1.358042	-3.364787	0.780733
C	-3.249269	-5.014144	2.950477
C	5.607802	-1.660418	-0.883848
C	3.829991	-0.279165	1.753027

C	-0.003611	-2.657024	2.790932
C	6.999397	-0.140388	0.414233
C	5.131990	-4.286122	-1.846265
C	8.327243	1.413604	1.678013
C	6.502356	-2.737911	-0.563679
C	2.192820	-4.299884	1.674871
C	6.236072	-4.042270	-1.062789
C	7.883829	-1.204026	0.723969
C	0.814503	-3.605199	3.684619
C	7.634552	-2.468743	0.242482
C	2.231056	-3.822639	3.133589
H	-8.315198	3.282017	-0.483433
H	-2.779981	4.542016	-3.755818
H	-6.926418	4.844768	0.811866
H	-8.755610	1.029311	-1.343670
H	-8.342980	-0.831421	-2.609194
H	-0.859909	3.202754	-4.705210
H	-0.300398	4.576475	-3.754737
H	-2.785670	2.874844	-3.188395
H	-9.255717	-1.226777	-1.122065
H	-1.761442	5.312148	-1.639105
H	-3.209042	4.379764	-1.268423
H	-4.937276	5.286558	2.223532
H	-8.263907	-2.475801	-1.922690
H	2.462184	5.752120	-3.116435
H	-4.299089	1.245134	-1.552209
H	3.511838	4.543234	-3.906041
H	-3.096202	0.389435	-2.554771
H	-4.593535	-0.446264	-2.051048
H	-2.609616	-2.881006	-4.557077
H	4.134089	5.514794	-2.536777
H	1.008826	2.528943	-3.202108
H	-0.453748	1.661939	-2.790101
H	0.544818	4.179502	-1.383027
H	-1.843119	2.384252	-0.705205
H	-1.336470	3.770734	0.236373
H	-3.371755	3.415976	2.778041
H	-0.943652	-3.315354	-4.187801
H	-1.697945	-1.518792	-2.672871
H	-2.287469	-5.383656	-4.513645
H	0.967820	5.134781	0.414885
H	-3.450250	-4.849696	-3.301498
H	-3.085098	-2.493350	-2.157455
H	-3.772628	1.161950	1.945277
H	5.233181	3.549616	-2.774487
H	-6.539719	-1.623899	2.003210
H	1.888405	6.485912	2.281011
H	2.629317	4.673168	0.761117

H	0.503104	5.530932	2.801392
H	0.140484	3.164132	1.744655
H	-0.140484	-3.164132	-1.744655
H	-0.503104	-5.530932	-2.801392
H	-1.888405	-6.485912	-2.281011
H	-2.629317	-4.673168	-0.761117
H	6.539719	1.623899	-2.003210
H	-5.233181	-3.549616	2.774487
H	3.450250	4.849696	3.301498
H	2.287469	5.383656	4.513645
H	3.772628	-1.161950	-1.945277
H	3.085098	2.493350	2.157455
H	-0.967820	-5.134781	-0.414885
H	0.943652	3.315354	4.187801
H	1.697945	1.518792	2.672871
H	3.371755	-3.415976	-2.778041
H	1.336470	-3.770734	-0.236373
H	-4.134089	-5.514794	2.536777
H	1.843119	-2.384252	0.705205
H	-0.544818	-4.179502	1.383027
H	2.609616	2.881006	4.557077
H	-1.008826	-2.528943	3.202108
H	0.453748	-1.661939	2.790101
H	-3.511838	-4.543234	3.906041
H	8.263907	2.475801	1.922690
H	4.593535	0.446264	2.051048
H	3.096202	-0.389435	2.554771
H	-2.462184	-5.752120	3.116435
H	4.299089	-1.245134	1.552209
H	9.255717	1.226777	1.122065
H	4.937276	-5.286558	-2.223532
H	1.761442	-5.312148	1.639105
H	3.209042	-4.379764	1.268423
H	8.342980	0.831421	2.609194
H	0.300398	-4.576475	3.754737
H	2.785670	-2.874844	3.188395
H	8.755610	-1.029311	1.343670
H	0.859909	-3.202754	4.705210
H	6.926418	-4.844768	-0.811866
H	8.315198	-3.282017	0.483433
H	2.779981	-4.542016	3.755818
O	-7.179222	-1.130477	-0.896526
O	2.706793	4.074203	-2.037017
O	-3.094256	-0.183515	-0.617896
O	3.094256	0.183515	0.617896
O	-2.706793	-4.074203	2.037017
O	7.179222	1.130477	0.896526
P	1.104038	2.135926	-0.180312

P -1.104038 -2.135926 0.180312
Cl 0.976084 -0.640905 -2.072550
Cl -0.976084 0.640905 2.072550
Pd 0.000000 0.000000 0.000000

Processing: pdevanphos-x6psdbe.log
Method Basis Set Imaginary Freqs
RB3LYP GenECP Geometry optimized, no freq

HF
-4592.20124650

Processing: pdevanphos-x6psdbe.log
Frequency job incomplete: pdevanphos-x6psdbe.log
151
C -7.690078 2.457239 -0.193503
C -7.906346 1.203143 -0.721102
C -2.180762 3.815861 -3.195482
C -6.352849 4.008849 1.203225
C -0.760444 3.576673 -3.729337
C -8.310635 -1.405562 -1.735476
C -6.579942 2.718790 0.647265
C -2.155145 4.300548 -1.737988
C -5.270082 4.244853 2.021097
C -7.009809 0.144356 -0.424440
C 3.271788 5.012870 -2.978381
C -5.670130 1.647349 0.946651
C -3.838828 0.313641 -1.725114
C 0.037790 2.628363 -2.817545
C -5.900258 0.345399 0.395646
C -4.366035 3.192005 2.312033
C -1.338815 3.364429 -0.826883
C 0.093515 3.180864 -1.379046
C -4.557968 1.929416 1.793082
C -1.960040 -3.347365 -3.782267
C -5.027360 -0.814588 0.762929
C -2.037073 -2.532254 -2.479665
C -2.390446 -4.805261 -3.567354
C 3.480690 2.996678 -1.676960
C -3.704164 -1.010118 0.309362
C 1.639658 4.641001 1.135649
C 4.802968 2.837457 -2.110213
C -5.544594 -1.753314 1.660362
C 1.574729 5.456252 2.441527
C 2.887072 2.066571 -0.793387
C 1.192536 3.181336 1.365633
C -1.574729 -5.456252 -2.441527

C	-1.192536	-3.181336	-1.365633
C	-2.887072	-2.066571	0.793387
C	5.544594	1.753314	-1.660362
C	-4.802968	-2.837457	2.110213
C	-1.639658	-4.641001	-1.135649
C	-3.480690	-2.996678	1.676960
C	2.390446	4.805261	3.567354
C	3.704164	1.010118	-0.309362
C	5.027360	0.814588	-0.762929
C	2.037073	2.532254	2.479665
C	1.960040	3.347365	3.782267
C	4.557968	-1.929416	-1.793082
C	-0.093515	-3.180864	1.379046
C	4.366035	-3.192005	-2.312033
C	5.900258	-0.345399	-0.395646
C	1.338815	-3.364429	0.826883
C	-3.271788	-5.012870	2.978381
C	5.670130	-1.647349	-0.946651
C	3.838828	-0.313641	1.725114
C	-0.037790	-2.628363	2.817545
C	7.009809	-0.144356	0.424440
C	5.270082	-4.244853	-2.021097
C	8.310635	1.405562	1.735476
C	6.579942	-2.718790	-0.647265
C	2.155145	-4.300548	1.737988
C	6.352849	-4.008849	-1.203225
C	7.906346	-1.203143	0.721102
C	0.760444	-3.576673	3.729337
C	7.690078	-2.457239	0.193503
C	2.180762	-3.815861	3.195482
H	-8.381135	3.264760	-0.422302
H	-2.712006	4.539584	-3.827166
H	-7.053783	4.806718	0.968976
H	-8.762057	1.034801	-1.363877
H	-8.331467	-0.808226	-2.656063
H	-0.800268	3.163886	-4.745559
H	-0.234579	4.540703	-3.804106
H	-2.747454	2.875998	-3.253296
H	-9.239569	-1.243281	-1.174049
H	-1.716930	5.309408	-1.702187
H	-3.175697	4.391285	-1.346135
H	-5.105249	5.233282	2.440857
H	-8.227742	-2.461881	-1.996390
H	2.484223	5.749901	-3.143733
H	-4.308186	1.273707	-1.498440
H	3.534038	4.541672	-3.933511
H	-3.099859	0.447115	-2.517863
H	-4.599284	-0.402649	-2.050202

H	-2.586275	-2.873828	-4.549453
H	4.154241	5.512995	-2.560338
H	1.045419	2.484922	-3.216241
H	-0.429591	1.638256	-2.812709
H	0.574000	4.160683	-1.416792
H	-1.833054	2.389198	-0.748912
H	-1.323628	3.777800	0.186698
H	-3.504655	3.377658	2.947084
H	-0.928601	-3.320340	-4.160825
H	-1.684827	-1.514173	-2.658526
H	-2.282570	-5.379347	-4.496489
H	1.017156	5.129413	0.379815
H	-3.458105	-4.833195	-3.302773
H	-3.084785	-2.475481	-2.156585
H	-3.839369	1.149471	2.017753
H	5.254632	3.544094	-2.794215
H	-6.561714	-1.621776	2.017566
H	1.928390	6.478312	2.253012
H	2.668065	4.651597	0.751116
H	0.525375	5.542213	2.759250
H	0.151352	3.173595	1.709938
H	-0.151352	-3.173595	-1.709938
H	-0.525375	-5.542213	-2.759250
H	-1.928390	-6.478312	-2.253012
H	-2.668065	-4.651597	-0.751116
H	6.561714	1.621776	-2.017566
H	-5.254632	-3.544094	2.794215
H	3.458105	4.833195	3.302773
H	2.282570	5.379347	4.496489
H	3.839369	-1.149471	-2.017753
H	3.084785	2.475481	2.156585
H	-1.017156	-5.129413	-0.379815
H	0.928601	3.320340	4.160825
H	1.684827	1.514173	2.658526
H	3.504655	-3.377658	-2.947084
H	1.323628	-3.777800	-0.186698
H	-4.154241	-5.512995	2.560338
H	1.833054	-2.389198	0.748912
H	-0.574000	-4.160683	1.416792
H	2.586275	2.873828	4.549453
H	-1.045419	-2.484922	3.216241
H	0.429591	-1.638256	2.812709
H	-3.534038	-4.541672	3.933511
H	8.227742	2.461881	1.996390
H	4.599284	0.402649	2.050202
H	3.099859	-0.447115	2.517863
H	-2.484223	-5.749901	3.143733
H	4.308186	-1.273707	1.498440

H 9.239569 1.243281 1.174049
H 5.105249 -5.233282 -2.440857
H 1.716930 -5.309408 1.702187
H 3.175697 -4.391285 1.346135
H 8.331467 0.808226 2.656063
H 0.234579 -4.540703 3.804106
H 2.747454 -2.875998 3.253296
H 8.762057 -1.034801 1.363877
H 0.800268 -3.163886 4.745559
H 7.053783 -4.806718 -0.968976
H 8.381135 -3.264760 0.422302
H 2.712006 -4.539584 3.827166
O -7.165036 -1.115511 -0.945605
O 2.727187 4.069307 -2.064921
O -3.107949 -0.184508 -0.599629
O 3.107949 0.184508 0.599629
O -2.727187 -4.069307 2.064921
O 7.165036 1.115511 0.945605
P 1.119119 2.128993 -0.198572
P -1.119119 -2.128993 0.198572
Cl 0.999941 -0.674814 -2.049204
Cl -0.999941 0.674814 2.049204
Pd 0.000000 0.000000 0.000000

J:
Processing: pdevanphos-xaci6dsdbe.log
PG=CI

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	0

HF Energy
-4592.0133217

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
808.94547	855.709	400.848	355.551	855.926	47.015	41.237

Processing: pdevanphos-xaci6dsdbe.log
151
C -2.223224 -4.257407 -2.503318
C -2.161771 -4.501214 -0.988680
C -1.317029 -3.438240 -0.261318
C 0.100798 -3.355876 -0.872252
C 0.009834 -3.048439 -2.380141
C -0.815757 -4.126752 -3.102429
P 1.150447 -2.123709 0.096279
Pd 0.000000 0.000000 0.000000

Cl	0.888963	0.345099	-2.177147
C	1.276454	-2.920719	1.804841
C	2.164804	-2.110383	2.769118
C	2.138521	-2.707271	4.186285
C	2.556581	-4.183652	4.189027
C	1.693406	-4.997146	3.215801
C	1.709978	-4.402443	1.795036
C	2.903571	-2.157804	-0.538708
C	3.726637	-1.039827	-0.248068
C	5.054282	-0.941303	-0.725539
C	5.562005	-2.027656	-1.442336
C	4.809705	-3.166432	-1.697647
C	3.485679	-3.231456	-1.252015
C	5.909684	0.279244	-0.603408
C	5.572011	1.415297	-1.342201
C	6.391367	2.573801	-1.312811
C	7.541706	2.587305	-0.558084
C	7.933562	1.460274	0.204747
C	7.104234	0.287335	0.181126
C	7.506733	-0.825210	0.977521
C	8.658022	-0.783618	1.732136
C	9.479025	0.370701	1.739615
C	9.117358	1.466766	0.991203
O	4.434903	1.331803	-2.077420
C	3.967094	2.463472	-2.794010
O	3.140517	-0.070380	0.509838
C	3.878351	0.612329	1.523556
O	2.717196	-4.343416	-1.452320
C	3.252163	-5.432255	-2.187632
P	-1.150447	2.123709	-0.096279
C	-1.276454	2.920719	-1.804841
C	-1.709978	4.402443	-1.795036
C	-1.693406	4.997146	-3.215801
C	-2.556581	4.183652	-4.189027
C	-2.138521	2.707271	-4.186285
C	-2.164804	2.110383	-2.769118
C	-0.100798	3.355876	0.872252
C	-0.009834	3.048439	2.380141
C	0.815757	4.126752	3.102429
C	2.223224	4.257407	2.503318
C	2.161771	4.501214	0.988680
C	1.317029	3.438240	0.261318
C	-2.903571	2.157804	0.538708
C	-3.485679	3.231456	1.252015
C	-4.809705	3.166432	1.697647
C	-5.562005	2.027656	1.442336
C	-5.054282	0.941303	0.725539
C	-3.726637	1.039827	0.248068

O	-2.717196	4.343416	1.452320
C	-3.252163	5.432255	2.187632
O	-3.140517	0.070380	-0.509838
C	-3.878351	-0.612329	-1.523556
C	-5.909684	-0.279244	0.603408
C	-7.104234	-0.287335	-0.181126
C	-7.933562	-1.460274	-0.204747
C	-7.541706	-2.587305	0.558084
C	-6.391367	-2.573801	1.312811
C	-5.572011	-1.415297	1.342201
C	-9.117358	-1.466766	-0.991203
C	-9.479025	-0.370701	-1.739615
C	-8.658022	0.783618	-1.732136
C	-7.506733	0.825210	-0.977521
O	-4.434903	-1.331803	2.077420
C	-3.967094	-2.463472	2.794010
Cl	-0.888963	-0.345099	2.177147
H	8.168069	3.476212	-0.543122
H	2.778868	5.066140	2.996123
H	9.733734	2.363172	0.991379
H	6.118723	3.446249	-1.895304
H	4.657819	2.741921	-3.601818
H	0.878712	3.889039	4.172383
H	0.298592	5.096006	3.027729
H	2.782164	3.330832	2.697307
H	3.817093	3.325963	-2.131365
H	1.728047	5.495409	0.801497
H	3.174938	4.519951	0.564841
H	10.385803	0.387829	2.337854
H	3.006155	2.159142	-3.208845
H	-2.455671	6.177418	2.232603
H	4.334934	1.526889	1.137982
H	-3.527736	5.134316	3.206924
H	3.149423	0.865543	2.296824
H	4.656426	-0.027452	1.951793
H	2.795926	-2.123222	4.843800
H	-4.126914	5.866715	1.686903
H	-1.008862	2.983682	2.820117
H	0.452220	2.066688	2.528257
H	-0.578031	4.331686	0.760625
H	1.803901	2.457536	0.325764
H	1.270819	3.686047	-0.805394
H	8.939807	-1.646121	2.330742
H	1.122623	-2.612041	4.595861
H	1.821147	-1.073816	2.797945
H	2.487042	-4.602437	5.201490
H	-1.057083	5.000678	-1.151123
H	3.612364	-4.262538	3.888668

H	3.199697	-2.113342	2.400400
H	6.887862	-1.716248	0.982670
H	-5.253453	3.986239	2.248064
H	6.577985	-1.967070	-1.822263
H	-2.033250	6.040845	-3.180783
H	-2.722779	4.484753	-1.378268
H	-0.656836	5.018686	-3.584051
H	-0.250022	2.849386	-2.184290
H	0.250022	-2.849386	2.184290
H	0.656836	-5.018686	3.584051
H	2.033250	-6.040845	3.180783
H	2.722779	-4.484753	1.378268
H	-6.577985	1.967070	1.822263
H	5.253453	-3.986239	-2.248064
H	-3.612364	4.262538	-3.888668
H	-2.487042	4.602437	-5.201490
H	-6.887862	1.716248	-0.982670
H	-3.199697	2.113342	-2.400400
H	1.057083	-5.000678	1.151123
H	-1.122623	2.612041	-4.595861
H	-1.821147	1.073816	-2.797945
H	-8.939807	1.646121	-2.330742
H	-1.270819	-3.686047	0.805394
H	4.126914	-5.866715	-1.686903
H	-1.803901	-2.457536	-0.325764
H	0.578031	-4.331686	-0.760625
H	-2.795926	2.123222	-4.843800
H	1.008862	-2.983682	-2.820117
H	-0.452220	-2.066688	-2.528257
H	3.527736	-5.134316	-3.206924
H	-3.006155	-2.159142	3.208845
H	-4.656426	0.027452	-1.951793
H	-3.149423	-0.865543	-2.296824
H	2.455671	-6.177418	-2.232603
H	-4.334934	-1.526889	-1.137982
H	-3.817093	-3.325963	2.131365
H	-10.385803	-0.387829	-2.337854
H	-1.728047	-5.495409	-0.801497
H	-3.174938	-4.519951	-0.564841
H	-4.657819	-2.741921	3.601818
H	-0.298592	-5.096006	-3.027729
H	-2.782164	-3.330832	-2.697307
H	-6.118723	-3.446249	1.895304
H	-0.878712	-3.889039	-4.172383
H	-9.733734	-2.363172	-0.991379
H	-8.168069	-3.476212	0.543122
H	-2.778868	-5.066140	-2.996123

Processing: pdevanphos-xaci6psdbe.log

Method	Basis Set	Imaginary Freqs
RB3LYP	GenECP	Geometry optimized, no freq

HF
-4592.19728700

Processing: pdevanphos-xaci6psdbe.log
151

C	-2.208484	-4.262604	-2.528737
C	-2.145689	-4.513795	-1.014486
C	-1.311514	-3.447067	-0.279404
C	0.105672	-3.349952	-0.889227
C	0.013307	-3.030427	-2.394847
C	-0.802219	-4.110039	-3.127360
P	1.155934	-2.123168	0.082855
Pd	0.000000	0.000000	0.000000
Cl	0.911953	0.373362	-2.161713
C	1.286442	-2.920776	1.788591
C	2.159160	-2.101690	2.760101
C	2.127053	-2.700745	4.176785
C	2.560038	-4.173619	4.181861
C	1.716117	-4.995893	3.197805
C	1.737772	-4.396949	1.778216
C	2.908936	-2.163892	-0.560951
C	3.736928	-1.047446	-0.271330
C	5.064330	-0.950885	-0.750690
C	5.567991	-2.036419	-1.472243
C	4.811662	-3.173318	-1.728905
C	3.487489	-3.236761	-1.278650
C	5.924762	0.267809	-0.633477
C	5.616839	1.387178	-1.409958
C	6.441286	2.543141	-1.385312
C	7.569180	2.570120	-0.595056
C	7.933232	1.457423	0.204315
C	7.097970	0.287928	0.183096
C	7.473252	-0.811093	1.012888
C	8.605543	-0.759963	1.798204
C	9.432584	0.391845	1.804834
C	9.096252	1.475241	1.023499
O	4.503878	1.289460	-2.181687
C	4.048271	2.409839	-2.929744
O	3.150468	-0.078731	0.486932
C	3.889159	0.624639	1.489023
O	2.717890	-4.347709	-1.484612
C	3.249225	-5.439461	-2.224461
P	-1.155934	2.123168	-0.082855
C	-1.286442	2.920776	-1.788591

C	-1.737772	4.396949	-1.778216
C	-1.716117	4.995893	-3.197805
C	-2.560038	4.173619	-4.181861
C	-2.127053	2.700745	-4.176785
C	-2.159160	2.101690	-2.760101
C	-0.105672	3.349952	0.889227
C	-0.013307	3.030427	2.394847
C	0.802219	4.110039	3.127360
C	2.208484	4.262604	2.528737
C	2.145689	4.513795	1.014486
C	1.311514	3.447067	0.279404
C	-2.908936	2.163892	0.560951
C	-3.487489	3.236761	1.278650
C	-4.811662	3.173318	1.728905
C	-5.567991	2.036419	1.472243
C	-5.064330	0.950885	0.750690
C	-3.736928	1.047446	0.271330
O	-2.717890	4.347709	1.484612
C	-3.249225	5.439461	2.224461
O	-3.150468	0.078731	-0.486932
C	-3.889159	-0.624639	-1.489023
C	-5.924762	-0.267809	0.633477
C	-7.097970	-0.287928	-0.183096
C	-7.933232	-1.457423	-0.204315
C	-7.569180	-2.570120	0.595056
C	-6.441286	-2.543141	1.385312
C	-5.616839	-1.387178	1.409958
C	-9.096252	-1.475241	-1.023499
C	-9.432584	-0.391845	-1.804834
C	-8.605543	0.759963	-1.798204
C	-7.473252	0.811093	-1.012888
O	-4.503878	-1.289460	2.181687
C	-4.048271	-2.409839	2.929744
Cl	-0.911953	-0.373362	2.161713
H	8.198639	3.456462	-0.582823
H	2.752135	5.076311	3.025777
H	9.717678	2.367725	1.022548
H	6.191237	3.403031	-1.995459
H	4.759344	2.677133	-3.722473
H	0.868744	3.861480	4.194205
H	0.274516	5.073804	3.063377
H	2.780016	3.343611	2.719116
H	3.873687	3.278486	-2.282637
H	1.703404	5.504736	0.832161
H	3.158462	4.544056	0.592111
H	10.322816	0.417453	2.426480
H	3.101132	2.093166	-3.366468
H	-2.450716	6.182050	2.266700

H	4.348024	1.529806	1.084939
H	-3.519830	5.139299	3.244082
H	3.158766	0.895223	2.254228
H	4.662848	-0.008709	1.932928
H	2.773096	-2.111030	4.839769
H	-4.123385	5.875370	1.725048
H	-1.011373	2.952179	2.833690
H	0.456722	2.051523	2.534902
H	-0.589197	4.323215	0.784176
H	1.807185	2.471096	0.338943
H	1.264331	3.700159	-0.785312
H	8.866619	-1.611632	2.420586
H	1.107238	-2.615400	4.577678
H	1.805217	-1.068999	2.786896
H	2.483459	-4.593932	5.192722
H	-1.098459	5.000718	-1.126789
H	3.619625	-4.241268	3.893296
H	3.196380	-2.094100	2.400088
H	6.851655	-1.700027	1.019458
H	-5.252472	3.991519	2.283267
H	6.582854	-1.977747	-1.855435
H	-2.070693	6.034264	-3.162769
H	-2.755099	4.465605	-1.370970
H	-0.676987	5.032436	-3.556501
H	-0.256782	2.861978	-2.161165
H	0.256782	-2.861978	2.161165
H	0.676987	-5.032436	3.556501
H	2.070693	-6.034264	3.162769
H	2.755099	-4.465605	1.370970
H	-6.582854	1.977747	1.855435
H	5.252472	-3.991519	-2.283267
H	-3.619625	4.241268	-3.893296
H	-2.483459	4.593932	-5.192722
H	-6.851655	1.700027	-1.019458
H	-3.196380	2.094100	-2.400088
H	1.098459	-5.000718	1.126789
H	-1.107238	2.615400	-4.577678
H	-1.805217	1.068999	-2.786896
H	-8.866619	1.611632	-2.420586
H	-1.264331	-3.700159	0.785312
H	4.123385	-5.875370	-1.725048
H	-1.807185	-2.471096	-0.338943
H	0.589197	-4.323215	-0.784176
H	-2.773096	2.111030	-4.839769
H	1.011373	-2.952179	-2.833690
H	-0.456722	-2.051523	-2.534902
H	3.519830	-5.139299	-3.244082
H	-3.101132	-2.093166	3.366468

H -4.662848 0.008709 -1.932928
H -3.158766 -0.895223 -2.254228
H 2.450716 -6.182050 -2.266700
H -4.348024 -1.529806 -1.084939
H -3.873687 -3.278486 2.282637
H -10.322816 -0.417453 -2.426480
H -1.703404 -5.504736 -0.832161
H -3.158462 -4.544056 -0.592111
H -4.759344 -2.677133 3.722473
H -0.274516 -5.073804 -3.063377
H -2.780016 -3.343611 -2.719116
H -6.191237 -3.403031 1.995459
H -0.868744 -3.861480 -4.194205
H -9.717678 -2.367725 -1.022548
H -8.198639 -3.456462 0.5828238
H -2.752135 -5.076311 -3.025777

K:

Processing: pdevanphos-xbci6dsdbe.log
PG=C01

Method	BasisSet	Imaginary Freqs
RB3LYP	GenECP	0

HF Energy
-4592.0099339

ZPE	E298	S298	Squasihar	Equasihar	Strans	Srot
809.10118	855.917	405.362	355.577	856.136	47.015	41.483

Processing: pdevanphos-xbci6dsdbe.log
151
C -1.253075 -2.138380 1.462233
C -1.656784 -2.239219 -0.024086
C -0.703618 -3.193152 -0.780699
C -0.644211 -4.572732 -0.097116
C -0.261020 -4.479666 1.385850
C -1.198729 -3.521812 2.132545
P -1.722941 -0.531287 -0.834191
C -3.279454 0.358505 -0.306498
C -4.403965 -0.193950 0.352470
C -5.537540 0.587726 0.677201
C -5.501337 1.951731 0.383816
C -4.420410 2.533904 -0.262749
C -3.332821 1.737671 -0.627002
O -4.396158 -1.542282 0.595558
C -4.786659 -2.031161 1.883968

C	-6.801602	0.025090	1.247046
C	-7.147929	0.301403	2.569115
C	-8.365883	-0.170448	3.121291
C	-9.227472	-0.918326	2.351988
C	-8.927470	-1.227680	1.003158
C	-7.698940	-0.742221	0.439784
C	-7.424779	-1.049996	-0.924300
C	-8.304717	-1.795082	-1.676173
C	-9.512084	-2.277856	-1.113320
C	-9.813121	-1.995214	0.198393
O	-2.273866	2.235127	-1.321146
C	-2.381429	3.525495	-1.899404
O	-6.236121	1.015827	3.295741
C	-6.534222	1.356479	4.639920
Pd	0.339193	0.634832	-0.304629
Cl	1.329800	-0.148579	-2.310436
P	2.356783	1.881353	0.241776
C	2.122911	3.591317	-0.518293
C	1.990839	3.538557	-2.054317
C	1.953080	4.961517	-2.638091
C	0.824320	5.804563	-2.026118
C	0.867319	5.782780	-0.490386
C	0.920690	4.352229	0.080894
C	2.615217	2.262597	2.071650
C	2.722018	1.008008	2.962325
C	2.774945	1.399399	4.448795
C	3.935678	2.360500	4.741286
C	3.863810	3.599722	3.838818
C	3.793000	3.221909	2.347319
C	4.013435	1.231073	-0.336976
C	5.048226	1.988619	-0.939863
C	6.205740	1.367283	-1.420989
C	6.381801	0.002630	-1.240522
C	5.443259	-0.783547	-0.570944
C	4.254836	-0.152211	-0.141957
O	4.889741	3.342916	-1.021647
C	5.890230	4.123641	-1.655253
C	5.801138	-2.207864	-0.284670
C	6.255714	-2.604902	1.011243
C	6.633543	-3.970082	1.246905
C	6.559597	-4.891322	0.173979
C	6.135585	-4.500003	-1.075322
C	5.754705	-3.153573	-1.307630
C	7.075737	-4.361466	2.540001
C	7.148015	-3.451714	3.568922
C	6.781562	-2.102259	3.340196
C	6.349325	-1.689876	2.099863
O	3.296645	-0.800368	0.575809

C	2.885315	-2.125837	0.227865
O	5.302478	-2.711457	-2.518012
C	5.192287	-3.627526	-3.594754
Cl	-0.664911	1.400280	1.704305
C	-2.029131	-0.945866	-2.650453
C	-2.058034	0.268327	-3.599960
C	-2.143494	-0.193095	-5.065238
C	-3.369827	-1.083660	-5.309831
C	-3.387645	-2.274876	-4.342199
C	-3.280083	-1.824006	-2.873619
H	-10.158637	-1.280853	2.780990
H	0.878149	6.838671	-2.391748
H	-10.738791	-2.353875	0.643161
H	-8.620939	0.049461	4.151436
H	-6.657612	0.465120	5.269400
H	1.842645	4.915376	-3.729593
H	2.917919	5.454033	-2.443599
H	-0.142317	5.408387	-2.365610
H	-7.437854	1.976237	4.711582
H	1.755782	6.334998	-0.148495
H	-0.001960	6.313045	-0.079129
H	-10.195901	-2.865237	-1.719884
H	-5.675809	1.929313	4.995097
H	5.532601	5.154051	-1.609126
H	-5.833023	-2.346380	1.881867
H	6.025050	3.834059	-2.704939
H	-4.150020	-2.895935	2.087604
H	-4.630079	-1.272546	2.656538
H	-2.172486	0.683364	-5.726076
H	6.851766	4.049939	-1.131385
H	2.815356	2.974952	-2.499348
H	1.074784	2.996526	-2.320704
H	3.024304	4.158561	-0.281265
H	-0.008985	3.814391	-0.137162
H	0.989119	4.408888	1.172251
H	-8.072071	-2.014786	-2.714883
H	-1.229031	-0.747161	-5.321722
H	-1.162694	0.876499	-3.449539
H	-3.388293	-1.437468	-6.348981
H	3.709328	4.135060	1.748124
H	-4.283755	-0.487781	-5.165444
H	-2.929866	0.894677	-3.372816
H	-6.508271	-0.679997	-1.370452
H	6.982781	1.942746	-1.907418
H	-6.360982	2.562495	0.643571
H	4.729870	4.252474	4.012263
H	4.732922	2.736758	2.049620
H	2.971922	4.187231	4.102587

H	1.677227	2.760818	2.344321
H	-1.132385	-1.520136	-2.912904
H	-2.544893	-2.942752	-4.574883
H	-4.301800	-2.867639	-4.479174
H	-4.175764	-1.248034	-2.602768
H	7.297200	-0.466177	-1.589922
H	-4.433817	3.592916	-0.487358
H	4.889506	1.840320	4.565054
H	3.932998	2.659510	5.797785
H	6.080929	-0.651877	1.936014
H	3.624785	0.441506	2.705761
H	-3.272424	-2.705194	-2.223681
H	1.824731	1.875646	4.730857
H	1.867041	0.352503	2.777752
H	6.844244	-1.384327	4.153816
H	-1.036136	-3.334944	-1.813947
H	-2.376025	4.311770	-1.134835
H	0.299481	-2.757084	-0.839073
H	-2.665960	-2.650838	-0.079816
H	2.865990	0.494529	5.063872
H	-1.939426	-1.479110	2.002335
H	-0.269866	-1.658312	1.538817
H	-3.289840	3.613234	-2.509080
H	4.796244	-3.050151	-4.431776
H	3.508990	-2.874362	0.722812
H	1.861509	-2.205238	0.590955
H	-1.503568	3.635232	-2.535903
H	2.897853	-2.261722	-0.856056
H	4.498866	-4.446701	-3.363095
H	7.486668	-3.761649	4.553705
H	-1.629536	-5.055449	-0.182190
H	0.063623	-5.215802	-0.636482
H	6.168013	-4.048055	-3.873288
H	-2.206927	-3.962401	2.158680
H	0.773407	-4.119220	1.476520
H	6.089932	-5.227106	-1.877776
H	-0.880744	-3.410364	3.177239
H	7.358116	-5.399882	2.699212
H	6.846964	-5.925718	0.347368
H	-0.283879	-5.475872	1.846705