Pd-Catalyzed N-Arylation of Secondary Acyclic Amides: Catalyst Development, Scope, and Computational Study

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Supporting Information

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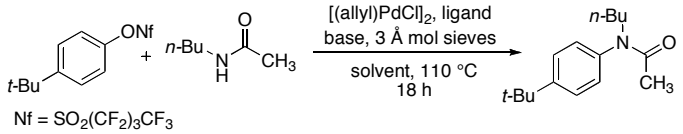
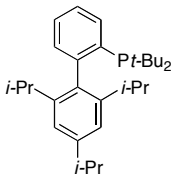
Reaction Optimization

Table SI-1. Ligand Investigation and Reaction Optimization[a]

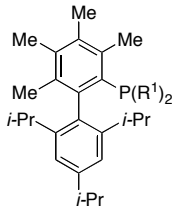


Nf = $SO_2(CF_2)_3CF_3$

entry	ligand	base	solvent	conversion (%)	yield (%)
1	**L1**	K_2CO_3	toluene	13	5
2	**LSI-1**	K_2CO_3	toluene	6	0
3	**L2**	K_2CO_3	toluene	41	27
4	**LSI-2**	K_2CO_3	toluene	1	0
5	**L3**	K_2CO_3	toluene	49	21
6	**LSI-3**	K_2CO_3	toluene	29	6
7	**L4**	K_2CO_3	toluene	16	0
8	**L5**	K_2CO_3	toluene	34	24
9	**L6**	K_2CO_3	toluene	100	87
10	**L6**	K_2CO_3	*t*-BuOH	100	23
11	**L6**	K_2CO_3	DME	45	18
12	**L6**	NaO*t*-Bu	toluene	100	0
13[b]	**L6**	K_2CO_3, No Sieves	toluene	100	69
14[c]	**L6**	K_2CO_3,	toluene	100	90

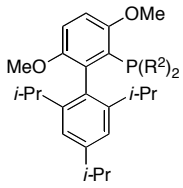


LSI-1, *t*-Bu_2XPhos



LSI-2, Me_4XPhos, R^1= Cy

LSI-3, Me_4*t*-Bu_2XPhos, R^1= *t*-Bu

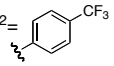


L2, BrettPhos, R^2= Cy

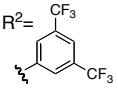
L3, *t*-Bu_2BrettPhos, R^2 = *t*-Bu

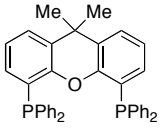
L4, R^2= Ph

L5, R^2=



L6, JackiePhos R^2=





L1, Xantphos

[a] ArONf (1 equiv), amide (2.5 equiv), $[(allyl)PdCl]_2$ (1 mol%), ligand (5 mol%), base (2.0 equiv), 3 Å mol sieves (50 mg/mL), solvent (0.25 M), 110 °C, 18 h. [b] 4,4'-oxybis(*tert*-butylbenzene) was observed as minor product. [c] $Pd(OAc)_2/H_2O$ activation was used in place of $[(allyl)PdCl]_2$.

General Information

All reactions were carried out in resealable test tubes with teflon septum under a dry argon atmosphere. $[Pd(allyl)Cl]_2$ and xantphos (**L1**) were purchased from Strem. *t*-Bu_2XPhos and Me_4*t*-Bu_2XPhos were purchased from Aldrich. Anhydrous K_2CO_3 (99%, Aldrich), K_3PO_4 (Riedel-de Haën), and Cs_2CO_3 (Chemetall) were stored under nitrogen in a Vacuum Atmospheres glovebox. Small portions (~5 g) were removed from the glovebox in glass vials, stored in a desiccator filled with anhydrous calcium sulfate, and weighed in the air. Chlorophosphines were purchased from Alfa Aesar. Amides were purchased from commercial sources and used without further purification. Aryl halides and phenols were purchased from commercial sources and, when necessary, filtered through neutral alumina. 3 Å powered molecular sieves were purchased from Avocado. Anhydrous toluene was purchased from J. T. Baker in CYCLE-TAINER® solvent delivery kegs and vigorously purged with argon for 2 h. The solvent was further purified by passing it through two packed columns of neutral alumina under argon. Flash column chromatography was performed using a Biotage SP4 Flash Purification System using KP-Sil flash cartridges.

All new compounds were characterized by ^{1}H NMR, ^{13}C NMR, IR spectroscopy, and elemental analysis (Atlantic Microlab, Inc., Norcross, GA). Nuclear Magnetic Resonance spectra were recorded on a Bruker 400 MHz or Varian 300 MHz instrument. Infrared spectra were recorded using a Perkin–Elmer 2000 FT-IR. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm) downfield from tetramethylsilane and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvents. All ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (77.0 ppm). Melting points (uncorrected) were obtained on a Mel-Temp capillary melting point apparatus. Gas chromatographic analyses were performed on a Hewlett-Packard 6890 gas chromatography instrument with an FID detector using DB1 (10 m x 0.20 mm) capillary. *In situ* monitoring of reactions using infrared spectroscopy was performed with a Mettler-Toledo iC10 ReactIR instrument equipped with a C1Fiber with a diamond-tipped probe.

General procedure A – For Chart 1 and Table SI-1: An oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_2CO_3 (69 mg, 0.5 mmol) and 3 Å mol sieves (100 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. After cooling to rt, the vessel was then charged with the ligand (5 mol%) and evacuated and backfilled with argon (this process was repeated a total of three times). *N*-Butylacetamide (72 mg, 0.63 mmol), 4-*t*-butylphenyl nonaflate (108 mg, 0.25 mmol), and a solution of $[Pd(allyl)Cl]_2$ in toluene (2 mol% Pd, 0.005 M) were added via syringe. The solution was heated to 110 °C for 17 h, cooled to room temperature, and diluted with ethyl acetate. Dodecane was then added as an internal standard and the reaction mixture was analyzed by GC.

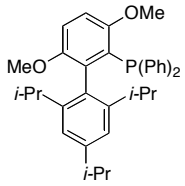
General procedure B – For Table SI-1, Entry 14, Water Activation: An oven-dried test tube, equipped with a magnetic stir bar and fitted with a teflon septum, was charged with $Pd(OAc)_2$ (2 mol%) and **L6** (5 mol%). The vessel was evacuated and backfilled with argon (this process was repeated a total of three times), then toluene (1 mL) and degassed H_2O (8 mol%) were added via syringe. After addition of the water, the solution was heated to 110 °C for 1 min. A second oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_2CO_3 (69 mg, 0.5 mmol) and 3 Å mol sieves (100 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. *N*-Butylacetamide (72 mg, 0.63 mmol), 4-*t*-butylphenyl nonaflate (108 mg, 0.25 mmol), and a solution of the catalyst prepared above were added via syringe. The solution was heated to 110 °C for 17 h, cooled to room temperature, and diluted with ethyl acetate. Dodecane was then added as an internal standard and the reaction mixture was analyzed by GC

Ligand Synthesis

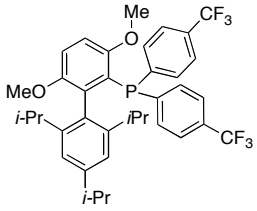
Known ligands: BrettPhos (**L2**),[1] *t*-Bu_2BrettPhos (**L3**),[2] and Me_4XPhos (**LSI-2**),[1] were synthesized according to literature procedures.

General procedure C – Synthesis of Triarylphosphines in Chart 1 and Table 6: To a sealable Schlenk tube containing a -78 °C solution of biaryl iodide (1 equiv) in THF was added *n*-BuLi (1.05 equiv) dropwise via syringe. The solution was stirred for 1 h at -78 °C and CuCl (1 equiv) was added quickly by opening the Schlenk tube under a stream of Ar. The reaction mixture was allowed to warm to rt (the CuCl dissolved) and a solution of chlorophosphine (1 equiv) was added. The Schlenk tube was sealed and heated to 70 °C for 18 h. The reaction mixture was cooled to rt, diluted with EtOAc, and washed with 30% NH_4OH (3x), sat. $NaHCO_3$ (aq), and brine; then dried over Na_2SO_4, filtered and concentrated. The resulting solid was crystallized from acetone to yield a white solid.

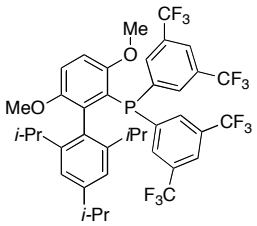
[1] Fors, B. P.; Watson, D. A.; Biscoe, M. R.; Buchwald, S. L. *J. Am. Chem. Soc.* **2008**, *130*, 13552.
[2] Fors, B. P.; Dooleweerdt, K. ; Zeng, Q.; Buchwald, S. L. *Tetrahedron,* **2009**, *65,* 6576.



Diphenyl(2',4',6'-triisopropyl-3,6-dimethoxybiphenyl-2-yl)phosphine (**L4**). Following general procedure A, a mixture of 2-iodo-2',4',6'-triisopropyl-3,6-dimethoxybiphenyl[1] (0.5 g, 1.07 mmol) in THF (6 mL) was treated with *n*-BuLi (480 μL, 2.5 M in hexane, 1.15 mmol), CuCl (106 mg, 1.07 mmol), and Ph_2PCl (196 μL, 1.07 mmol). The crude product was crystallized from acetone (58 mg, 10%): mp 200–202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.25–7.18 (m, 10H), 7.01 (d, J = 8.8 Hz, 1H), 6.93 (s, 2H), 6.86 (d, J = 8.8 Hz, 1H), 3.66 (s, 3H), 3.17 (s, 3H), 2.93 (septet, J = 7.2 Hz, 1H), 2.48 (septet, J = 7.2 Hz, 2H), 1.29 (d, J = 7.2 Hz, 6H), 0.97 (d, J = 6.8 Hz, 6H), 0.81 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.9, 152.2, 152.1, 147.4, 146.2, 139.0, 138.6, 138.3, 138.1, 132.5, 132.4, 132.3, 132.1, 127.61, 127.55, 127.0, 126.3, 126.1, 120.2, 112.6, 111.4, 55.1, 33.9, 30.9, 24.9, 23.9, 22.6 (Observed complexity due to P–C splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -16.17; IR (thin film) 2957, 1579, 1256 cm^{-1}; Anal. Calcd. for $C_{35}H_{41}O_2P$: C, 80.12; H, 7.88. Found: C, 80.11; H, 7.84.

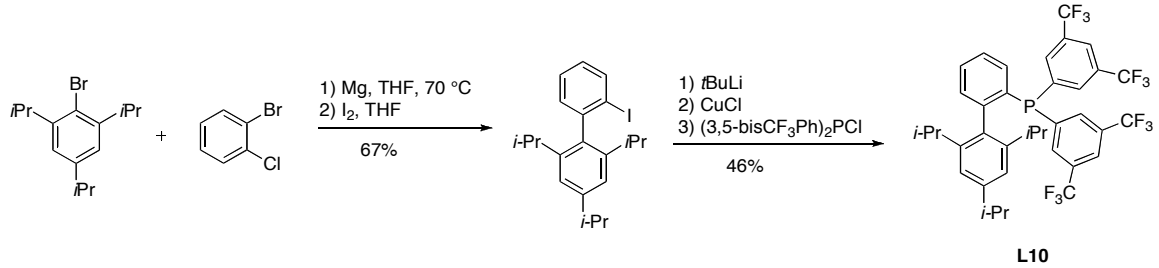


bis(4-(trifluoromethyl)phenyl)(2',4',6'-triisopropyl-3,6-dimethoxybiphenyl-2-yl)phosphine (**L5**). Following general procedure A, a mixture of 2-iodo-2',4',6'-triisopropyl-3,6-dimethoxybiphenyl[1] (300 mg, 0.64 mmol) in THF (4 mL) was treated with *t*-BuLi (780 μL, 1.8 M in pentane, 1.3 mmol), CuCl (64 mg, 0.64 mmol), and (4-CF_3Ph)$_2$PCl (227 mL, 0.64 mmol). The crude product was crystallized from acetone (181 mg, 45%): mp 202–204 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.27–7.17 (m, 10H), 6.64 (d, J = 8.8 Hz, 1H), 6.45 (d, J = 9.2 Hz, 1H), 3.13 (s, 3H), 2.84 (septet, J = 6.8 Hz, 1H), 2.77 (s, 3H), 2.72 (septet, J = 6.8 Hz, 2H), 1.26 (d, J = 6.8 Hz, 6H), 1.22 (d, J = 7.2 Hz, 6H), 1.03 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.50, 155.48, 152.6, 152.4, 148.6, 146.7, 147.6, 143.0, 139.8, 139.4, 132.7, 132.6, 132.4, 129.6, 129.3, 128.0, 127.9, 127.8, 127.7, 127.6, 126.1, 124.62, 124.58, 124.57, 124.5, 124.3, 123.4, 120.7, 113.44, 113.42, 111.3, 54.4, 54.3, 34.5, 31.3, 25.1, 24.0, 22.8 (Observed complexity due to P–C and C–F splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -16.97; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.90; IR (thin film) 2956, 2361, 1123 cm^{-1}; Anal. Calcd. for $C_{37}H_{40}F_6O_2P$: C, 67.26; H, 5.95. Found: C, 67.45; H, 6.01.



bis(3,5-bis(trifluoromethyl)phenyl)(2',4',6'-triisopropyl-3,6-dimethoxybiphenyl-2-yl)phosphine (**L6**). Following general procedure A, a mixture of 2-iodo-2',4',6'-triisopropyl-3,6-dimethoxybiphenyl[1] (1.0 g, 2.1 mmol) in THF (13 mL) was treated with *n*-BuLi (880 μL, 2.5 M in hexane, 2.2 mmol), CuCl (208 mg, 2.1 mmol), and (3,5-bisCF_3Ph)$_2$PCl (1.03 g, 1.07 mmol). The crude product was crystallized from acetone (1.17 g, 70%): mp 185–190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.76 (s, 2H), 7.64 (d, J = 6.0 Hz, 4H), 7.13 (d, J = 8.8 Hz, 1H), 7.00 (s, 2H), 6.90 (d, J = 9.2 Hz, 1H), 3.71 (s, 3H), 3.33 (s, 3H), 2.95 (septet, J = 6.8 Hz, 1H), 2.39 (septet, J = 6.8 Hz, 2H), 1.30 (d, J = 6.8 Hz, 6H), 1.00 (d, J = 6.8 Hz, 6H), 0.83 (d, J = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.0,

154.97, 152.6, 152.5, 148.4, 146.3, 146.2, 140.5, 140.3, 139.8, 139.4, 132.4, 132.2, 131.7, 131.6, 131.5, 131.30, 131.25, 131.0, 130.9, 130.6, 127.3, 124.6, 121.9, 121.7, 121.1, 120.5, 119.2, 114.7, 111.0, 55.2, 54.5, 34.0, 31.0, 24.8, 23.9, 22.6 (Observed complexity due to P–C and C–F splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -15.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.0–(-63.7); IR (thin film) 2962, 1278 cm^{-1}; Anal. Calcd. for $C_{39}H_{37}F_{12}O_2P$: C, 58.80; H, 4.68. Found: C, 58.58; H, 4.87.



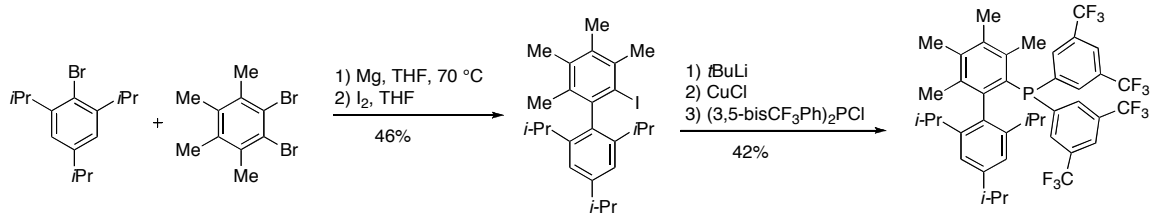
L10

bis(3,5-bis(trifluoromethyl)phenyl)(2',4',6'-triisopropylbiphenyl-2-yl)phosphine (**L7**). An oven-dried 100 mL round bottom flask was equipped with a magnetic stir bar, charged with magnesium shavings (1.15 g, 48 mmol) and fitted with a reflux condenser. The flask was purged with argon and then THF (28 mL) and 2,4,6-triisopropylbromobenzene (7.15 mL, 20 mmol) were added via syringe. The reaction mixture was heated to reflux and 1,2-dibromoethane (50 μL) was added via syringe. After heating to reflux for 1 h, 2-bromochlorobenzene (2.58 mL, 22 mmol) was added dropwise via syringe over 0.5 h. After an additional 1 h at reflux, the reaction mixture was cooled to rt and a solution of I_2 (5.56 g, 22 mmol) in THF (10 mL) was added via cannula until a deep purple color persisted. The reaction mixture was then quenched with MeOH and filtered. The filtrate was then washed with $Na_2S_2O_3$ and brine, then dried over Na_2SO_4, filtered and concentrated. The resulting solid was crystallized from acetone to yield a white powder (5.4 g, 67%)[3]: mp 148 °C (lit. 150–152 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (d, J = 8.0 Hz, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.05–7.01 (m, 3H), 2.95 (septet, J = 6.8 Hz, 1H), 2.38 (septet, J = 7.2 Hz, 2H), 1.30 (d, J = 7.2 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H), 1.01 (d, J = 6.8 Hz, 6H).

Following general procedure A, a mixture of 2'-iodo-2,4,6-triisopropylbiphenyl (300 mg, 0.73 mmol) in THF (3 mL) was treated with *t*-BuLi (880 μL, 1.7 M in pentane, 1.49 mmol), CuCl (73 mg, 0.73 mmol), and (3,5-bisCF_3Ph)$_2$PCl (353 mg, 0.72 mmol). The crude product was crystallized from acetone (247 mg, 46%): mp 125–126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85 (s, 2H), 7.56–7.52 (m, 5H), 7.44 (t, J = 7.6 Hz, 1H), 7.33 (t, J = 5.2 Hz, 1H), 7.14 (dd, J = 7.6, 3.6 Hz, 1H), 6.99 (s, 2H), 2.94 (septet, J = 6.8 Hz, 1H), 2.26 (septet, J = 6.8 Hz, 2H), 1.29 (d, J = 6.8 Hz, 6H), 0.98 (d, J = 6.8 Hz, 6H), 0.80 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.0, 148.6, 148.3, 146.20, 146.19, 140.4, 140.2, 134.8, 134.7, 134.51, 134.49, 133.0, 132.7, 132.6, 132.5, 132.24, 132.19, 131.91, 131.85, 131.7, 131.6, 131.5, 130.6, 128.2, 127.0, 124.3, 123.0, 122.91, 122.88, 121.6, 120.7, 34.1, 30.8, 25.4, 24.0, 22.12, 22,10 (Observed complexity due to P–C and C–F splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ:

[3] Hartmann, N.; Niemeyer, M. *Synthetic Commun.* **2001**, *31*, 3839.

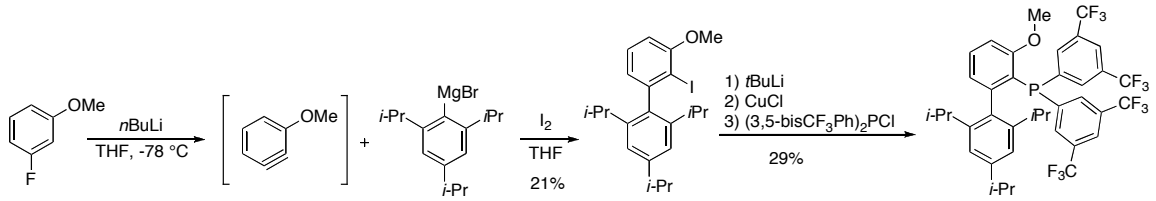
-63.0–(-63.2); IR (thin film) 2964, 2361, 1278 cm^{-1}; Anal. Calcd. for $C_{37}H_{33}F_{12}P$: C, 60.33; H, 4.52. Found: C, 60.49; H, 4.58.



L11

bis(3,5-bis(trifluoromethyl)phenyl)(2',4',6'-triisopropyl-3,4,5,6-tetramethylbiphenyl-2-yl)phosphine (**L8**). An oven-dried 100 mL round bottom flask equipped with a magnetic stir bar was charged with magnesium shavings (0.55 g, 23 mmol) and fitted with a reflux condenser. The flask was purged with argon and then THF (12 mL) and 2,4,6-triisopropylbromobenzene (2.53 mL, 10 mmol) were added via syringe. The reaction mixture was heated to reflux and 1,2-dibromethane (50 μL) was added via syringe. The reaction mixture heated to reflux for 1 h, then 1,2-dibromo-3,4,5,6-tetramethylbenzene (2.92 g, 10 mmol) was added portionwise. After an additional 1 h at reflux the reaction mixture was cooled to rt and a solution of I_2 (2.5 g, 10 mmol) in THF (10 mL) was added via cannula until a deep purple color persisted. The reaction mixture was then quenched with MeOH and filtered. The filtrate was then washed with $Na_2S_2O_3$ and brine, then dried over Na_2SO_4, filtered and concentrated. The resulting solid was crystallized from acetone to yield a white powder (2.1 g, 46%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.03 (s, 2H), 2.95 (septet, J = 7.2 Hz, 1H), 2.58 (s, 3H), 2.38–2.32 (m, 4H), 2.18 (s, 3H), 1.98 (s, 3H), 1.30 (d, J = 6.8 Hz, 6H), 1.19 (d, J = 6.8 Hz, 6H), 0.99 (d, J = 6.8 Hz, 6H).

Following general procedure A, a mixture of 2-iodo-2',4',6'-triisopropyl-3,4,5,6-tetramethylbiphenyl (300 mg, 0.64 mmol) in THF (3 mL) was treated with *t*-BuLi (780 μL, 1.7 M in pentane, 1.33 mmol), CuI (121 mg, 0.64 mmol), and (3,5-bisCF_3Ph)$_2$PCl (314 mg, 0.64 mmol). The crude product was crystallized from acetone (206 mg, 42%): mp 189–190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.66 (d, J = 4.4 Hz, 4H), 7.60 (s, 2H), 7.16 (s, 2H), 2.81 (septet, J = 6.8 Hz, 1H), 2.66 (septet, J = 6.8 Hz, H), 1.91 (s, 3H), 1.86 (s, 3H), 1.78 (s, 3H), 1.71 (s, 3H), 1.21 (d, J = 6.8 Hz, 6H), 1.13 (d, J = 6.8 Hz, 6H), 0.89 (d, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.2, 147.9, 147.4, 145.9, 145.8, 141.3, 141.0, 140.8, 138.9, 138.8, 136.9, 136.8, 135.1, 135.0, 131.9, 131.8, 131.54, 131.51, 130.4, 130.3, 126.41, 126.4, 124.5, 121.8, 121.4, 120.9, 34.0, 30.7, 34.8, 24.0, 23.2, 22.9, 19.70, 19.66, 17.6, 17.1 (Observed complexity due to P–C and C–F splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -9.50; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.1–(-63.3); IR (thin film) 2963, 1277 cm^{-1}; Anal. Calcd. for $C_{41}H_{41}F_{12}P$: C, 62.12; H, 5.21. Found: C, 62.03; H, 5.19.



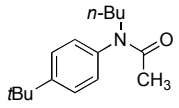
L12

bis(3,5-bis(trifluoromethyl)phenyl)(2',4',6'-triisopropyl-3-methoxybiphenyl-2-yl)phosphine (**L9**). An oven-dried 500 mL bottom flask equipped with a magnetic stir bar was charged with magnesium shavings (750 mg, 31.2 mmol) and fitted with a reflux condenser. The flask was purged with argon and then THF (35 mL) and 2,4,6-triisopropylbromobenzene (6.5 mL, 26 mmol) were added via syringe. The reaction mixture was heated to reflux and 1,2-dibromethane (50 μL) was added via syringe. The reaction mixture was allowed to stir at reflux for 1 h and was then cooled to room temperature. A separate oven-dried 1 L round bottom flask equipped with a magnetic stir bar was purged with argon and THF (320 mL) and 3-fluoroanisole (1.5 mL, 13 mmol) were added to the flask via syringe. The reaction vessel was cooled to -78 °C and *n*-BuLi (2.5 M in hexane, 13.7 mL, 1.05 mmol) was added dropwise. The solution was stirred for an additional 30 min and the Grignard reagent, which was prepared in the first reaction vessel, was added via cannula and the reaction was allowed to warm to rt overnight. A solution of iodine (6.5 g, 26 mmol) in THF (10 mL) was added cannula until a deep purple color persisted. The solvent was removed *in vacuo* and the remaining dark brown oil was taken up in CH_2Cl_2, washed with a saturated solution of sodium sulfite, and then brine. The organic layer was then dried over Na_2SO_4, filtered, and the solvent was removed *in vacuo*. The crude material was recrystallized from MeOH/EtOAc to yield the product as white crystals (1.2 g, 21%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31 (t, J = 8.4 Hz, 1H), 7.04 (s, 2H), 6.82 (dd, J = 7.6, 1.6 Hz, 1H), 6.78 (dd, J = 8.0, 1.2 Hz, 1H), 3.95 (s, 3H), 2.95 (septet, J = 6.8 Hz, 1H), 2.40 (septet, J = 6.8 Hz, 2H), 1.30 (d, J = 7.2 Hz, 6H), 1.19 (d, J = 6.8 Hz, 6H), 1.01 (d, J = 6.8 Hz, 6H).

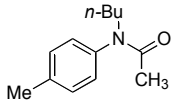
Following general procedure A, a mixture of 2-iodo-2',4',6'-triisopropyl-3-methoxybiphenyl (400 mg, 0.91 mmol) in THF (5 mL) was treated with *n*-BuLi (382 μL, 2.5 M in hexane, 0.95 mmol), CuI (90 mg, 0.91 mmol), and (3,5-bisCF$_3$Ph)$_2$PCl (450 mg, 0.91 mmol). The crude product was crystallized from MeOH (224 mg, 29%): mp 113–115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.93 (d, J = 5.2 Hz, 4H), 7.83 (s, 2H), 7.39 (s, 2H), 7.20 (t, J = 7.2 Hz, 1H), 7.06 (ddd, J = 7.6, 4.8, 0.8 Hz, 1H), 6.40 (d, J = 8.4 Hz, 1H) 3.04–2.98 (m, 4H), 2.89 (septet, J = 6.8 Hz, 2H), 1.42 (d, J = 6.8, 6H), 1.34 (d, J = 6.8 Hz, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.71, 161.68, 152.0, 151.6, 149.3, 146.48, 146.46, 140.9, 140.7, 136.7, 136.6, 133.4, 132.4, 131.63, 131.58, 131.30, 131.25, 128.3, 128.2, 128.1, 128.0, 127.9, 127.8, 125.1, 124.7, 122.4, 121.0, 110.6, 54.1, 34.7, 31.3, 25.7, 24.2, 22.9 (Observed complexity due to P–C and C–F splitting); ^{31}P NMR (161 MHz, $CDCl_3$) δ: -15.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -63.0–(-63.2); IR (thin film) 2963, 1277 cm^{-1}; Anal. Calcd. for $C_{38}H_{35}F_{12}OP$: C, 59.53; H, 4.60. Found: C, 59.34; H, 4.57.

Experimental Procedures for Table 1

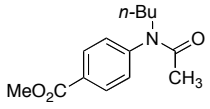
General procedure D: An oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_2CO_3 (276 mg, 2.0 mmol) and 3 Å mol sieves (200 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. The vessel was then charged with **L6** (40 mg, 5 mol%) and $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%). Next, the aryl nonaflate/triflate (1.0 mmol), amide (2.5 mmol), and toluene (4 mL) were added via syringe (aryl nonaflates/triflates or amides that were solids were added with the ligand and [Pd]). The solution was heated to 110 °C for 17 h, cooled to room temperature, diluted with ethyl acetate, filtered through celite, concentrated *in vacuo* and purified by column chromatography.



***N*-butyl-*N*-(4-tert-butylphenyl)acetamide** (Table 1, Entry 1) Following general procedure D, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), 4-*t*-butylphenyl nonaflate[4] (432 mg, 1.0 mmol), K_2CO_3 (192 mg, 14 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 6-40% EtOAc/hexanes) to provide the title compound as an oil (199 mg, 86%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 (d, J = 6.4 Hz, 2H), 7.06 (d, J = 6.4 Hz, 2H), 3.66 (t, J = 7.6 Hz, 2H), 1.81 (s, 3H), 1.5–1.45 (m, 2H), 1.36–1.27 (m, 11H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.3, 150.7, 140.4, 127.4, 126.4, 48.7, 34.5, 31.3, 29.8, 22.8, 20.0, 13.8; IR (thin film) 2961, 1663, 1511 cm^{-1}; Anal. Calcd. for $C_{16}H_{25}NO$: C, 77.68; H, 10.19; N, 5.66. Found: C, 77.39; H, 10.30; N, 5.74.



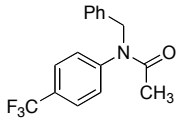
***N*-butyl-*N*-*p*-tolylacetamide** (Table 1, Entry 2) Following general procedure D, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), 4-methylphenyl nonaflate[5] (390 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 2-40% EtOAc/hexanes) to provide the title compound as an oil (167 mg, 82%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.20 (d, J = 8.4 Hz, 2H), 7.03 (d, J = 8.8 Hz, 2H), 3.65 (t, J = 7.6 Hz, 2H), 2.38 (s, 3H), 1.81 (s, 3H), 1.48–1.43 (m, 2H), 1.32–1.26 (m, 2H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.2, 140.5, 137.6, 130.1, 127.8, 48.7, 29.8, 22.7, 21.0, 20.0, 13.7; IR (thin film) 1653, 1506 cm^{-1}; Anal. Calcd. for $C_{13}H_{19}NO$: C, 76.06; H, 9.33. Found: C, 75.78; H, 9.34.



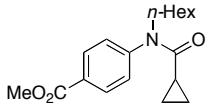
Methyl 4-(*N*-butylacetamido)benzoate (Table 1, Entry 3) Following general procedure D, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), methyl 4-(perfluorobutylsulfonyloxy)benzoate[4] (434 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 4-50% EtOAc/hexanes) to provide the

[4] Anderson, K. W.; Mendez-Perez, M.; Priego, J.; Buchwald, S. L**.** *J. Org. Chem.* **2003**, *68*, 9563.
[5] Meadows, R. E.; Woodward, S. *Tetrahedron* **2008**, *64*, 1218.

title compound as an oil (219 mg, 88%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.09 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 3.93 (s, 3H), 3.71 (t, J = 7.6 Hz, 2H), 1.85 (br s, 3H), 1.46 (pentet, J = 8.0 Hz, 2H), 1.29 (sextet, J = 7.2 Hz, 2H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.5, 166.1, 147.2, 130.9, 129.3, 127.9, 52.2, 48.7, 29.8, 22.8, 19.9, 13.6; IR (thin film) 2931, 1718, 1653 cm^{-1}; Anal. Calcd. for $C_{14}H_{19}NO_3$: C, 67.45; H, 7.68; N, 5.62. Found: C, 67.43; H, 7.77; N, 5.58.

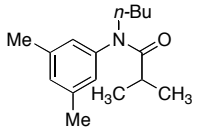


***N*-benzyl-*N*-(4-(trifluoromethyl)phenyl)acetamide** (Table 1, Entry 4) An oven-dried test tube, equipped with a magnetic stir bar and fitted with a teflon septum, was charged with $Pd(OAc)_2$ (4.4 mg, 2 mol%) and **L6** (40 mg, 5 mol%). The vessel was evacuated and backfilled with argon (this process was repeated a total of three times) and the toluene (4 mL) and degassed H_2O (8 mol%) were added via syringe. After addition of the water, the solution was heated to 110 °C for 1 min. A second oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_2CO_3 (276 mg, 2.0 mmol) and 3 Å mol sieves (200 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. *N*-benzylacetamide (372 mg, 2.5 mmol), 4-(trifluoromethyl)phenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate[6] (444 mg, 1.0 mmol), and a solution of the catalyst prepared above were added via syringe. The solution was heated to 110 °C for 17 h, cooled to room temperature, diluted with ethyl acetate, filtered through celite and concentrated *in vacuo*. The crude product was purified using a Biotage SP4 (silica-packed 25M; 10-50% EtOAc/hexanes) to provide the title compound as a tan solid (240 mg, 82%): mp 78–80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.60 (d, J = 8.0 Hz, 2H), 7.28–7.26 (m, 3H), 7.19–7.11 (m, 4H), 4.91 (d, 2H), 1.91 (br s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.0, 136.9, 128.6, 128.5, 127.6, 126.7, 125.0, 122.3, 52.7, 22.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.7; IR (thin film) 1655, 1559, 1272 cm^{-1}; Anal. Calcd. for $C_{16}H_{14}F_3NO$: C, 65.52; H, 4.81. Found: C, 65.32; H, 4.83.

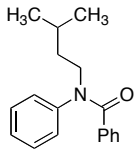


Methyl 4-(*N*-hexylcyclopropanecarboxamido)benzoate (Table 1, Entry 5) Following general procedure D, a mixture of *N*-hexylcyclopropanecarboxamide (423 mg, 2.5 mmol), methyl 4-(perfluorobutylsulfonyloxy)benzoate[4] (434 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 4-50% EtOAc/hexanes) to provide the title compound as an oil (247 mg, 82%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.09 (d, J = 6.4 Hz, 2H), 7.33 (d, J = 6.8 Hz, 2H), 3.94 (s, 3H), 3.73 (t, J = 8.0 Hz, 2H), 1.50–1.46 (m, 2H), 1.29–1.23 (m, 7H), 1.04–1.23 (m, 2H), 0.84 (t, J = 7.2 Hz, 3H), 0.64–0.61 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.8, 166.2, 147.1, 130.8, 128.9, 128.0, 52.2, 49.4, 31.4, 27.8, 26.4, 22.4, 13.9, 13.0, 8.6; IR (thin film) 1750, 1654, 1604 cm^{-1}; Anal. Calcd. for $C_{18}H_{25}NO_3$: C, 71.26; H, 8.31; N, 4.62. Found: C, 71.13; H, 8.22; N, 4.60.

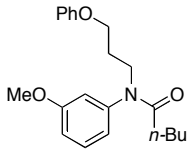
[6] Prepared via general procedure G. Niederpruem, H.; Voss, P.; Beyl, V. *Justus Liebigs Annalen der Chemie* **1973**, 20.



***N*-butyl-*N*-(3,5-dimethylphenyl)isobutyramide** (Table 1, Entry 6) An oven-dried test tube, equipped with a magnetic stir bar and fitted with a teflon septum, was charged with $Pd(OAc)_2$ (4.4 mg, 2 mol%) and **L6** (40 mg, 5 mol%). The vessel was evacuated and backfilled with argon (this process was repeated a total of three times) and the toluene (4 mL) and degassed H_2O (8 mol%) were added via syringe. After addition of the water, the solution was heated to 110 °C for 1 min. A second oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_2CO_3 (276 mg, 2.0 mmol) and 3 Å mol sieves (200 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. *N*-butylisobutyramide (358 mg, 2.5 mmol), 3,5-dimethylphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (404 mg, 1.0 mmol), and a solution of the catalyst prepared above were added via syringe. The solution was heated to 110 °C for 17 h, cooled to room temperature, diluted with ethyl acetate, filtered through celite and concentrated *in vacuo*. The crude product was purified using a Biotage SP4 (silica-packed 25M; 10-50% EtOAc/hexanes) to provide the title compound as an oil (194 mg, 78%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.97 (s, 1H), 6.75 (s, 2H), 3.62 (t, J = 7.6 Hz, 2H), 2.43 (septet, J = 6.4 Hz, 1H), 2.33 (s, 6H), 1.48–1.45 (m, 2H), 1.29 (sextet, J = 7.2 Hz, 2H), 1.00 (d, J = 6.4 Hz, 6H), 0.89 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 177.0, 142.7, 139.2, 129.3, 125.8, 49.0, 31.2, 29.9, 21.2, 20.0, 19.7, 13.8; IR (thin film) 2962, 1660 cm^{-1}; Anal. Calcd. for $C_{18}H_{25}NO_3$: C, 77.68; H, 10.19. Found: C, 77.47; H, 9.99.



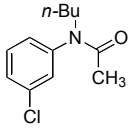
***N*-isopentyl-*N*-phenylbenzamide** (Table 1, Entry 7) Following general procedure D, a mixture of *N*-isopentylbenzamide (478 mg, 2.5 mmol), phenyl trifluoromethanesulfonate (163 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 5-40% EtOAc/hexanes) to provide the title compound as a white solid (206 mg, 77%): mp 54–55 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.27 (d, J = 7.2 Hz, 2H), 7.23–7.18 (m, 3H), 7.16–7.11 (m, 3H), 7.01 (d, J = 7.6 Hz, 2H), 3.93 (t, J = 8.0 Hz, 2H), 1.63 (septet, J = 6.8 Hz, 1H), 1.55–1.49 (m, 2H), 0.90 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.1, 143.4, 136.3, 129.3, 129.0, 128.5, 127.7, 127.6, 126.4, 48.9, 36.3, 26.1, 22.5; IR (thin film) 2956, 1645, 1493 cm^{-1}.



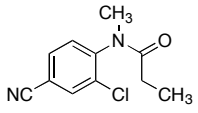
***N*-(3-methoxyphenyl)-*N*-(3-phenoxypropyl)pentanamide** (Table 1, Entry 8) Following general procedure D, a mixture of *N*-(3-phenoxypropyl)pentanamide (587 mg, 2.5 mmol), 3-methoxyphenyl trifluoromethanesulfonate[7] (356 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 5-40% EtOAc/hexanes) to provide the title compound as an oil (259 mg, 76%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.30–7.16 (m, 3H), 6.87 (t, J = 7.3 Hz, 2H), 6.80 (d, J = 8.0 Hz, 2H), 6.72–6.64 (m, 2H), 3.90 (t, J = 6.0 Hz, 2H), 3.74

[7] Lee, D.-Y.; Hartwig, J. F. *Org. Lett.* **2005**, *7*, 1169.

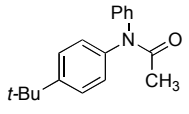
(s, 3H), 3.71–3.64 (m, 2H), 2.25 (t, J = 7.1 Hz, 2H), 2.12–2.00 (m, 2H), 1.54–1.52 (m, 2H), 1.32–1.25 (m, 2H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 171.7, 160.2, 158.6, 143.5, 130.1, 129.1, 120.4, 120.2, 114.2, 113.8, 112.9, 66.5, 55.1, 48.7, 30.5, 29.7, 24.9, 19.8, 13.6; IR (thin film) 2931, 2863, 1653, 1601, 1456, 1404, 1288, 1245, 1047, 754, 692 cm^{-1}; Anal. Calcd. for $C_{21}H_{27}NO_3$: C, 73.87; H, 7.97. Found: C, 73.82; H, 8.12.



***N*-butyl-*N*-(3-chlorophenyl)acetamide** (Table 1, Entry 9) Following general procedure D, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), 3-chlorophenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (410 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 5-40% EtOAc/hexanes) to provide the title compound as an oil (155 mg, 69%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.30–7.16 (m, 2H), 7.10–7.06 (m, 1H), 7.00–6.94 (m, 1H), 3.60–3.52 (m, 2H), 1.73 (s. 3H), 1.42–1.30 (m, 2H), 1.22–1.14 (m, 2H), 0.76 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 169.4, 144.1, 134.7, 130.3, 128.0, 127.8, 126.2, 48.5, 29.5, 22.5, 19.7, 13.5; IR (thin film) 2931, 1710, 1590, 1473, 1394, 1301 cm^{-1}.

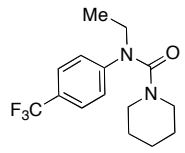


***N*-(2-chloro-4-cyanophenyl)-*N*-methylpropionamide** (Table 1, Entry 10) Following general procedure D, a mixture of *N*-methylpropionamide (216 mg, 2.5 mmol), 2-chloro-4-cyanophenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (436 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 4-50% EtOAc/hexanes) to provide the title compound as an oil (153 mg, 70%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81 (d, J = 2.0 Hz, 1H), 7.64 (dd, J = 8.0, 2.0 Hz, 1H), 7.40 (d, J = 8.0 Hz, 1H), 3.17 (s, 3H), 1.97–1.91 (m, 2H), 1.03 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.9, 145.6, 134.5, 134.2, 132.0, 130.9, 116.6, 113.5, 35.6, 30.2, 27.4; IR (thin film) 2985, 1683, 1388 cm^{-1}; Anal. Calcd. for $C_{11}H_{11}ClN_2O$: C, 59.33; H, 4.98. Found: C, 59.56; H, 5.00.

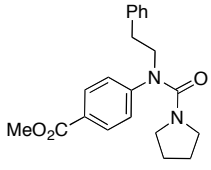


***N*-(4-*tert*-butylphenyl)-*N*-phenylacetamide** (Table 1, Entry 11) Following general procedure D, a mixture of *N*-phenylacetamide (336 mg, 2.5 mmol), 4-*t*-butylphenyl nonaflate[4] (432 mg, 1.0 mmol), K_3PO_4 (424 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 4-50% EtOAc/hexanes) to provide the title compound as a white solid (209 mg, 78%): mp 108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37–7.26 (m, 7H), 7.18 (d, J = 6.4 Hz, 2H), 2.06 (s, 3H), 1.30 (br s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.3, 129.4, 128.6, 128.2, 127.6, 126.3, 125.6, 34.3, 31.3, 23.6; IR (thin film) 2962, 1669, 1371 cm^{-1}.

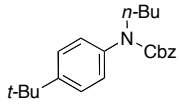
Experimental Procedures for Table 2



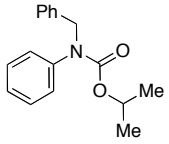
***N*-ethyl-*N*-(4-(trifluoromethyl)phenyl)piperidine-1-carboxamide** (Table 2, Entry 1) Following general procedure D, a mixture of *N*-ethylpiperidine-1-carboxamide (390 mg, 2.5 mmol), 4-(trifluoromethyl)phenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate[6] (444 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as a oil (192 mg, 64%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55 (d, J = 8.4 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 3.73 (q, J = 6.8 Hz, 2H), 3.17 (t, J = 5.6 Hz, 4H), 1.52–1.48 (m, 2H), 1.42–1.36 (m, 4H), 1.16 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.9, 148.5, 126.5, 126.42, 126.38, 126.3, 125.5, 125.2, 124.9, 122.8, 122.4, 46.6, 45.8, 25.4, 24.4, 13.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.6; IR (thin film) 2938, 1653, 1615, 1418 cm^{-1}; Anal. Calcd. for $C_{15}H_{19}F_3N_2O$: C, 59.99; H, 6.38. Found: C, 60.12; H, 6.32.



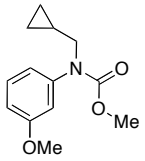
methyl 4-(*N*-phenethylpyrrolidine-1-carboxamido)benzoate (Table 2, Entry 2) Following general procedure D, a mixture of *N*-phenethylpyrrolidine-1-carboxamide (545 mg, 2.5 mmol), methyl 4-(perfluorobutylsulfonyloxy)benzoate[4] (434 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as an oil (211 mg, 60%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.92 (d, J = 8.7 Hz, 2H), 7.28–7.12 (m, 5H), 6.94 (d, J = 8.7 Hz, 2H), 3.88 (t, J = 7.4 Hz, 2H), 3.86 (s, 3H), 3.08–2.98 (m, 4H), 2.94–2.85 (m, 2H), 1.70–1.63 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 166.3, 158.2, 149.1, 139.2, 130.7, 128.8, 128.2, 126.1, 125.1, 123.1, 53.2, 51.9, 47.6, 34.9, 25.1; IR (thin film) 2957, 1717, 1653, 1603, 1558, 1496,1399, 1279, 1173, 1105 cm^{-1}; Anal. Calcd. for $C_{21}H_{24}N_2O$: C, 71.57; H, 6.86. Found: C, 71.87; H, 6.88.



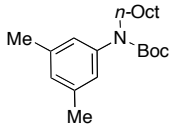
benzyl butyl(4-*tert*-butylphenyl)carbamate (Table 2, Entry 3) Following general procedure D, a mixture of benzyl butylcarbamate (518 mg, 2.5 mmol), 4-*t*-butylphenyl nonaflate[4] (432 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as an oil (335 mg, 98%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, J = 6.8 Hz, 2H), 7.35–7.20 (m, 5H), 7.10 (br s, 2H), 5.14 (s, 2H), 3.64 (t, J = 7.6 Hz, 2H), 1.57–1.48 (m, 2H), 1.33–1.25 (m, 11H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.4, 149.3 (br s), 139.1 (br s), 136.8, 128.2, 127.6, 127.3 (br s), 126.6 (br s), 125.7, 66.7 (br s), 50.2 (br s), 34.3, 31.2, 30.3 (br s), 19.7, 13.7; IR (thin film) 2960, 1700, 1516, 1296 cm^{-1}; Anal. Calcd. for $C_{22}H_{29}NO_2$: C, 77.84; H, 8.61. Found: C, 77.94; H, 8.42.



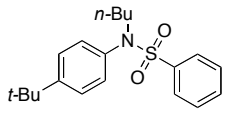
isopropyl benzyl(phenyl)carbamate (Table 2, Entry 4) Following general procedure D, a mixture of isopropyl benzylcarbamate (482 mg, 2.5 mmol), phenyl trifluoromethanesulfonate (163 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as an oil (239 mg, 88%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.37–7.15 (m, 10H), 5.08 (septet, J = 6.3 Hz, 1H), 4.92 (s, 2H), 1.25 (d, J = 6.2 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 155.1, 142.1, 137.9, 128.4, 128.1, 127.3, 126.9, 126.4, 125.8, 68.9, 53.7, 21.7; IR (thin film) 3031, 2980, 2933, 1700, 1597, 1496, 1456, 1398, 1276, 1225, 1179, 1111, 1018, 697 cm^{-1}; Anal. Calcd. for $C_{17}H_{19}NO_2$: C, 75.81; H, 7.11. Found: C, 75.60; H, 7.22.



methyl cyclopropylmethyl(3-methoxyphenyl)carbamate (Table 2, Entry 5) Following general procedure D, a mixture of methyl cyclopropylmethylcarbamate (323 mg, 2.5 mmol), 3-methoxyphenyl trifluoromethanesulfonate[7] (256 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as an oil (212 mg, 90%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.22 (t, J = 7.8 Hz, 1H), 6.81–6.76 (m, 3H), 3.75 (s, 3H), 3.63 (s, 3H), 3.48 (d, J = 7.2 Hz, 2H), 1.01–0.95 (m, 1H), 0.43–0.37 (m, 2H), 0.14–0.09 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 159.7, 155.8, 143.0, 129.3, 119.8, 113.5, 112.0, 55.0, 54.8, 52.5, 10.1, 3.3; IR (thin film) 2954, 1706, 1604, 1491 cm^{-1}; Anal. Calcd. for $C_{13}H_{17}NO_3$: C, 66.36; H, 7.28. Found: C, 66.55; H, 7.31.

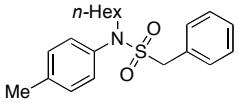


***tert*-butyl 3,5-dimethylphenyl(octyl)carbamate** (Table 2, Entry 6) Following general procedure D, a mixture of *tert*-butyl octylcarbamate (572 mg, 2.5 mmol), 3,5-dimethylphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (404 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 100 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 7-70% EtOAc/hexanes) to provide the title compound as an oil (289 mg, 87%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.83 (s, 1H), 6.80 (s, 2H), 3.55 (t, J = 7.6 Hz, 2H), 2.30 (s, 6H), 1.52–1.50 (m, 2H), 1.44 (br s, 9H), 1.30–1.21 (m, 10 H), 0.87 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 154.8, 142.4, 138.1, 127.6, 124.8, 79.7, 50.1, 31.8, 29.2, 28.5, 28.3, 28.2, 26.7, 22.6, 21.2, 14.1; IR (thin film) 2926, 1699, 1599, 1456 cm^{-1}; Anal. Calcd. for $C_{21}H_{35}NO_2$: C, 75.63; H, 10.58. Found: C, 75.54; H, 10.42.

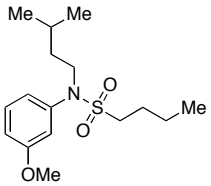


***N*-butyl-*N*-(4-*tert*-butylphenyl)benzenesulfonamide** (Table 2, Entry 7) Following general procedure D, a mixture of *N*-butylbenzenesulfonamide (463 mg, 2.5 mmol), 4-methylphenyl nonaflate[4] (390 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40

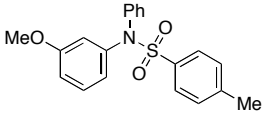
mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 2-40% EtOAc/hexanes) to provide the title compound as a tan solid (327 mg, 95%): mp 53 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.62–7.56 (m, 3H), 7.46 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 6.94 (d, J = 8.4 Hz, 2H), 3.50 (t, J = 7.2 Hz, 2H), 1.42–1.31(m, 4H), 1.30 (s, 9H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.8, 138.5, 136.2, 132.4, 128.6, 128.2, 127.6, 125.8, 50.4, 34.5, 31.3, 30.2, 19.5, 13.6; IR (thin film) 2961, 1507, 1349 cm^{-1}; Anal. Calcd. for $C_{20}H_{27}NO_2S$: C, 69.53; H, 7.88; N, 4.05. Found: C, 69.24; H, 7.86; N, 3.99.



***N*-hexyl-1-phenyl-*N*-*p*-tolylmethanesulfonamide** (Table 2, Entry 8) Following general procedure D, a mixture of *N*-hexyl-1-phenylmethanesulfonamide (637 mg, 2.5 mmol), 4-*t*-butylphenyl nonaflate[5] (432 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 2-20% EtOAc/hexanes) to provide the title compound as a tan solid (302 mg, 88%): mp 55 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44–7.41 (m, 2H), 7.39–7.37 (m, 3H), 7.18–7.13 (m, 4H), 4.23 (s, 2H), 3.40 (t, J = 6.8 Hz, 2H), 2.36 (s, 3H), 1.33–1.13 (m, 8H), 0.82 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.6, 136.2, 130.8, 129.9, 129.0, 128.7, 128.6, 56.7, 51.5, 31.3, 28.6, 25.9, 22.4, 21.0, 13.9; IR (thin film) 2971, 1539, 1495 cm^{-1}; Anal. Calcd. for $C_{20}H_{27}NO_2S$: C, 69.53; H, 7.88; N, 4.05. Found: C, 69.37; H, 7.93; N, 4.03.



***N*-isopentyl-*N*-(3-methoxyphenyl)butane-1-sulfonamide** (Table 2, Entry 9) Following general procedure D, a mixture of *N*-isopentylbutane-1-sulfonamide (517 mg, 2.5 mmol), 3-methoxyphenyl trifluoromethanesulfonate[7] (256 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 2-20% EtOAc/hexanes) to provide the title compound as an oil (286 mg, 91%): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.24 (t, J = 8.5 Hz, 1H), 6.93–6.86 (m, 2H), 6.84–6.79 (m, 1H), 3.75 (s, 3H), 3.70–3.61 (m, 2H), 2.97–2.90 (m, 2H), 1.82–1.69 (m, 2H), 1.60 (septet, J = 6.7 Hz, 1H), 1.44–1.26 (m, 4H), 0.87 (t, J = 7.35 Hz, 3H), 0.82 (d, J = 6.63 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 155.4, 142.4, 138.3, 128.7, 128.4, 127.7, 127.2, 126.7, 126.1, 69.3, 54.1, 22.0; IR (thin film) 2979, 1700.36, 1597, 1496, 1456, 1398, 1275, 1110, 1018, 697 cm^{-1}; Anal. Calcd. for $C_{13}H_{17}NO_3$: C, 61.31; H, 8.68. Found: C, 61.50; H, 8.81.

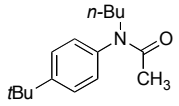


***N*-(3-methoxyphenyl)-4-methyl-*N*-phenylbenzenesulfonamide** (Table 2, Entry 10) Following general procedure D, a mixture of 4-methyl-*N*-phenylbenzenesulfonamide (618 mg, 2.5 mmol), 3-methoxyphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate[6] (406 mg, 1.0 mmol), K_3PO_4 (424 mg, 2.0 mmol, **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was

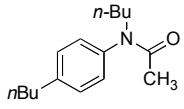
purified using a Biotage SP4 (silica-packed 50 g; 0-25% EtOAc/hexanes) to provide the title compound as a white solid (271 mg, 77%): mp = 74–76 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.61 (d, J = 8.1 Hz, 2H), 7.25 (m, 8H), 6.83 (m, 3H), 3.73 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 160.3, 144.0, 142.9, 141.7, 137.8, 130.1, 129.9, 129.5, 128.6, 128.0, 127.8, 120.5, 114.4, 113.2, 55.6, 21.9; IR (thin film) 2941, 2837, 1602, 1452, 1288, 1166, 1045, 814, 694, 608 cm^{-1}.

Experimental Procedures for Table 3

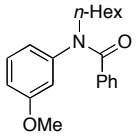
General procedure E: An oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with Cs_2CO_3 (648 mg, 2.0 mmol) and 3 Å mol sieves (200 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. The vessel was then charged with **L6** (40 mg, 5 mol%) and $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%); then the aryl chloride (1.0 mmol), amide (2.5 mmol), and toluene (4 mL) were added via syringe (aryl chlorides or amides that were solids were added with the ligand and [Pd]). The solution was heated to 130 °C for 17 h, cooled to room temperature, and diluted with ethyl acetate, filtered through celite, concentrated *in vacuo* and purified by column chromatography.



***N*-butyl-*N*-(4-*tert*-butylphenyl)acetamide** (Table 3, Entry 1) Following general procedure E, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), 1-*tert*-butyl-4-chlorobenzene (169 mg, 1.0 mmol), Cs_2CO_3 (648 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 5-60% EtOAc/hexanes) to provide the title compound as an oil (192 mg, 78%): Characterization matches Table 1, Entry 1.

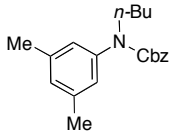


***N*-butyl-*N*-(4-butylphenyl)acetamide** (Table 3, Entry 2) Following general procedure E, a mixture of *N*-butyl acetamide (268 mg, 2.5 mmol), 1-*tert*-butyl-4-chlorobenzene (169 mg, 1.0 mmol), Cs_2CO_3 (648 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 5-60% EtOAc/hexanes) to provide the title compound as an oil (184 mg, 75%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.20 (d, J = 6.4 Hz, 2H), 7.04 (d, J = 8.0 Hz, 2H), 3.65 (t, J = 7.6 Hz, 2H), 2.63 (t, J = 7.6 Hz, 2H), 1.8 (s, 3H), 1.63–1.57 (m, 2H), 1.49–1.44 (m, 2H), 1.40–1.26 (m, 4H), 0.94 (t, J = 7.6 Hz, 3H), 0.87 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.2, 142.5, 140.6, 129.4, 127.7, 48.7, 35.1, 33.4, 29.8, 22.7, 22.3, 19.9, 13.8, 13.7; IR (thin film) 2931, 1653, 1509, 1395 cm^{-1}; Anal. Calcd. for $C_{16}H_{25}NO$: C, 77.68; H, 10.19. Found: C, 77.65; H, 10.25.

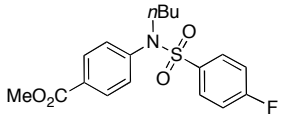


***N*-hexyl-*N*-(3-methoxyphenyl)benzamide** (Table 3, Entry 3) Following general procedure E, a mixture of *N*-hexylbenzamide (512 mg, 2.5 mmol), 1-chloro-3-methoxybenzene (123 μL, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol),

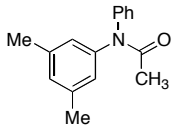
L6 (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 6-50% EtOAc/hexanes) to provide the title compound as an oil (167 mg, 54%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.30 (dd, J = 8.0, 1.6 Hz, 2H), 7.22–7.08 (m, 4H), 6.67 (ddd, J = 8.4, 2.4, 0.8 Hz, 1H), 6.60 (br d, J = 8.0 Hz, 1H), 6.55 (m, 1H), 3.89 (t, J = 7.6 Hz, 2H), 3.67 (s, 3H), 1.64–1.60 (m, 2H), 1.35–1.25 (m, 6H), 0.86 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.2, 159.8, 144.6, 136.4, 129.5, 129.4, 128.4, 127.6, 120.1, 113.6, 111.9, 55.2, 50.4, 31.5, 27.5, 26.5, 22.5, 14.0; IR (thin film) 2930, 1646, 1600, 1488 cm^{-1}; Anal. Calcd. for $C_{20}H_{25}NO$: C, 77.14; H, 8.09. Found: C, 77.16; H, 8.05.



benzyl butyl(3,5-dimethylphenyl)carbamate (Table 3, Entry 4) Following general procedure E, a mixture of benzyl butylcarbamate (518 mg, 2.5 mmol), 1-chloro-3,5-dimethylbenzene (141 μL, 1.0 mmol), Cs_2CO_3 (648 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 6-25% EtOAc/hexanes) to provide the title compound as an oil (285 mg, 92%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.32–7.26 (m, 5H), 6.89 (s, 1H), 6.80 (s, 2H), 5.14 (s, 2H), 3.63 (t, J = 7.6 Hz, 2H), 2.30 (s, 6H), 1.53–1.50 (m, 2H), 1.32–1.26 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 155.3, 141.5 (br s), 138.3, 136.8, 128.2, 127.6, 127.4 (br s), 124.9, 66.7, 50.1, 30.2 (br s), 21.1, 19.7, 13.7; IR (thin film) 2957, 1700, 1598, 1384 cm^{-1}; Anal. Calcd. for $C_{20}H_{25}NO_2$: C, 77.14; H, 8.09. Found: C, 77.01; H, 8.10.



methyl 4-(*N*-butyl-4-fluorophenylsulfonamido)benzoate (Table 3, Entry 5) Following general procedure E, a mixture of *N*-butyl-4-fluorobenzenesulfonamide (577 mg, 2.5 mmol), methyl 4-chlorobenzoate (171 mg, 1 mmol), Cs_2CO_3 (648 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 6-25% EtOAc/hexanes) to provide the title compound as a solid (321 mg, 88%): mp 97–98 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.92 (d, J = 8.53 Hz, 2H), 7.5 (dd, J = 8.8, 5.1 Hz, 2H), 7.12–7.02 (m, 4H), 3.83 (s, 3H), 3.51 (t, J = 6.62 Hz, 2H), 1.38–1.16 (m, 4H), 0.75 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.5, 165.9, 163.2, 142.9, 133.6, 133.5, 130.1, 130.0, 129.9, 129.1, 127.1, 116.1, 115.8, 52.0, 49.5, 29.8, 19.2, 13.2; IR (thin film) 2958, 1724, 1592, 1494, 1355, 1280, 1172, 1088, 839 cm^{-1}; Anal. Calcd. for $C_{18}H_{20}FNO_4S$: C, 59.16; H, 5.52. Found: C, 59.29; H, 5.43.



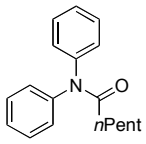
***N*-(3,5-dimethylphenyl)-*N*-phenylacetamide**[8] (Table 3, Entry 6) Following general procedure G, a mixture of *N*-phenylacetamide (336 mg, 2.5 mmol), 1-chloro-3,5-dimethylbenzene (135 μL, 1.0 mmol), K_3PO_4 (424 mg, 2.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 130 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 6-25% EtOAc/hexanes) to provide the title compound as a solid (162 mg, 68%): mp 91–93 °C (lit. 89–90 °C); ^{1}H NMR (400

[8] Klapars, A.; Antilla, J. C.; Huang, X., Buchwald. S. L. *J. Am. Chem. Soc.* **2001**, *123*, 7727.

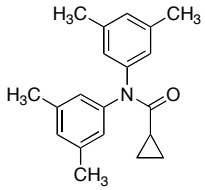
MHz, $CDCl_3$) δ: 7.34–7.26 (m, 5H), 6.95–6.86 (m, 3H), 2.30 (br s, 6H), 2.06 (s, 3H); IR (thin film) 3010, 2918, 1675, 1595, 1492 cm^{-1}; Anal. Calcd. for $C_{16}H_{17}NO$: C, 80.30; H, 7.16. Found: C, 80.12; H, 7.19.

Experimental Procedures for Table 4

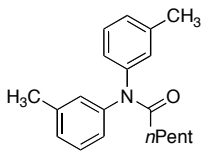
General procedure F: An oven-dried test tube fitted with a teflon septum and magnetic stir bar was charged with K_3PO_4 (636 mg, 3.0 mmol) and 3 Å mol sieves (200 mg). The powder was flame-dried under vacuum to activate the molecular sieves and remove trace water. The vessel was then charged with **L6** (40 mg, 5 mol%) and $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), then the aryl nonaflate/triflate (2.2 mmol), amide (1.0 mmol), and toluene (4 mL) were added via syringe (aryl nonaflates/triflates or amides that were solids were added with the ligand and [Pd]). The solution was heated to 110 °C for 17 h, cooled to room temperature, and diluted with ethyl acetate, filtered through celite, concentrated *in vacuo* and purified by column chromatography.



***N,N*-diphenylhexanamide** (Table 4, Entry 1) Following general procedure F, a mixture of hexanamide (115 mg, 1.0 mmol), phenyl trifluoromethanesulfonate (358 μL, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 3-30% EtOAc/hexanes) to provide the title compound as a white solid (223 mg, 84%): mp 50 °C; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.36–7.25 (m, 10H), 2.25 (t, J = 7.2 Hz, 2H), 1.68–1.61 (m, 2H), 1.27–1.22 (m, 4H), 0.85 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.3, 142.9, 128.8 (br s), 126.5 (br s), 35.2, 31.4, 25.2, 22.4, 13.9; IR (thin film) 2955, 1674, 1491 cm^{-1}.

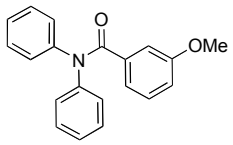


***N,N*-bis(3,5-dimethylphenyl)cyclopropanecarboxamide** (Table 4, Entry 2) Following general procedure F, a mixture of cyclopropanecarboxamide (85 mg, 1.0 mmol), 3,5-dimethylphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (888 mg, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (40 mg, 5 mol%), $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 3-30% EtOAc/hexanes) to provide the title compound as a white solid (205 mg, 70%): mp 122 °C; ^1H NMR (400 MHz, $CDCl_3$) δ: 6.90 (br s, 6H), 2.29 (br s, 12H), 1.56–1.52 (m, 1H), 1.11–1.08 (m, 2H), 0.72–0.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.8, 142.9, 138.6, 125.8, 124.3, 21.2, 13.6, 9.1; IR (thin film) 2918, 1667. 1594, 1394 cm^{-1}.

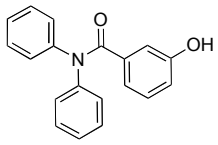


***N,N*-di-*m*-tolylhexanamide** (Table 4, Entry 3) Following general procedure F, a mixture of hexanamide (115 mg, 1.0 mmol), 1-chloro-3-methylbenzene (259 μL, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (80 mg, 10 mol%), $[Pd(allyl)Cl]_2$ (7.2 mg, 4 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified by

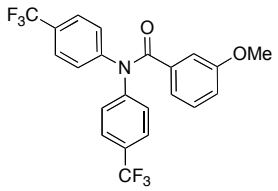
column chromatography (25:75 Et_2O/pentane) to provide the title compound as an oil (220 mg, 75%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26–6.99 (m, 8H), 2.33 (s, 6H), 2.24 (t, J = 7.2 Hz, 2H), 1.69–1.61 (m, 2H), 1.27–1.22 (m, 4H), 0.85 (t, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.2, 142.8, 128.7 (br s), 127.1 (br s), 125.5 (br s), 123.5 (br s), 35.0, 31.3, 25.1, 22.3, 21.2, 13.8; IR (thin film) 2935, 1674, 1604, 1488 cm^{-1}.



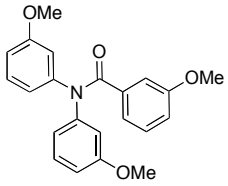
3-methoxy-*N*,*N*-diphenylbenzamide (Table 4, Entry 4) Following general procedure F, a mixture of 3-methoxybenzamide (151 mg, 1.0 mmol), trifluoromethanesulfonate (358 μL, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (60 mg, 7.5 mol%), $[Pd(allyl)Cl]_2$ (5.4 mg, 3 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 3-30% EtOAc/hexanes) to provide the title compound as a white solid (191 mg, 63%): mp 124–125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29–6.79 (m, 14H), 3.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.1, 158.7, 143.6, 137.0, 128.9, 128.7, 127.2, 126.1, 121.4, 116.3, 113.8, 55.0; IR (thin film) 3063, 1652, 1591 cm^{-1}; Anal. Calcd. for $C_{20}H_{17}NO_2$: C, 79.19; H, 5.65. Found: C, 78.91; H, 5.68.



3-hydroxy-*N*,*N*-diphenylbenzamide (Table 4) To a solution of 3-methoxy-*N*,*N*-diphenylbenzamide (100 mg, 0.33 mmol) in CH_2Cl_2 (3 mL, 1 M) cooled to -78 °C was added BBr_3 (1 M in CH_2Cl_2, 680 μL, 0.70 mmol) dropwise via syringe. The reaction was stirred 1 h at -78 °C then warmed to rt, stirred 10 min, then diluted with CH_2Cl_2 and brine. The organic layer was washed with sat. $Na_2S_2O_3$ and brine, then dried over Na_2SO_4, filtered and concentrated. The crude reaction mixture was purified by column chromatography (7-70% EtOAc/hexanes) to provide the title compound (78 mg, 82%): mp 147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (t, J = 7.6 Hz, 4H), 7.18–7.10 (m, 7H), 6.93 (t, J = 8.0 Hz, 1H), 7.75 (d, J = 7.6 Hz, 1H), 6.69 (dd, J = 8.4, 2.4 Hz, 1H), 6.49 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.2, 143.6, 136.8, 129.1, 128.8, 127.4, 126.6, 120.8, 117.8, 116.5; IR (thin film) 3305, 1634, 1581 cm^{-1}.



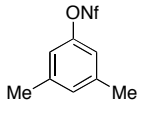
3-methoxy-*N*,*N*-bis(4-(trifluoromethyl)phenyl)benzamide (Table 4, Entry 5) Following general procedure F, a mixture of 3-methoxybenzamide (151 mg, 1.0 mmol), 4-(trifluoromethyl)phenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate[6] (977 mg, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (60 mg, 7.5 mol%), $[Pd(allyl)Cl]_2$ (5.4 mg, 3 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 2-20% EtOAc/hexanes) to provide the title compound as an oil (306 mg, 70%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55 (d, J = 8.8 Hz, 4H), 7.21 (d, J = 8.4 Hz, 4H), 7.10 (t, J = 8.0 Hz, 1H), 7.02–6.86 (m, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.3, 159.3, 146.4, 135.9, 129.2, 129.0, 128.6, 128.3, 128.0, 127.4, 126.4, 125.0, 122.3, 121.5, 117.2, 114.2, 55.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.7; IR (thin film) 1670, 1611, 1323 cm^{-1}; Anal. Calcd. for $C_{22}H_{15}F_6NO_2$: C, 60.14; H, 3.44. Found: C, 60.34; H, 3.47.



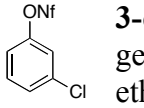
3-methoxy-*N*,*N*-bis(3-methoxyphenyl)benzamide (Table 4, Entry 6) Following general procedure F, a mixture of 3-methoxybenzamide (151 mg, 1.0 mmol), 3-methoxyphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate (893 mg, 2.2 mmol), K_3PO_4 (636 mg, 3.0 mmol), **L6** (60 mg, 7.5 mol%), $[Pd(allyl)Cl]_2$ (5.4 mg, 3 mol%), and toluene (4 mL) was heated to 110 °C for 17 h. The crude product was purified using a Biotage SP4 (silica-packed 25M; 4-40% EtOAc/hexanes) to provide the title compound as an oil (200 mg, 55%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.23–7.00 (m, 5H), 6.82–6.68 (m, 7H), 3.68 (s, 6H), 3.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.1, 159.9, 158.8, 144.7, 137.2, 129.6, 128.8, 121.3, 119.6, 116.5, 113.7, 113.1, 111.9, 55.1, 55.0; IR (thin film) 2940, 1652, 1599 cm^{-1}; Anal. Calcd. for $C_{22}H_{21}NO_4$: C, 72.71; H, 5.82. Found: C, 72.66; H, 5.77.

Synthesis of Aryl Nonaflates

General procedure G: Synthesis of Aryl Nonaflates To a solution of phenol (1 equiv), diisopropylethyl amine (1.2 equiv), and DMAP (0.05 equiv) in CH_2Cl_2 (1 M) was added perfluorobutanesulfonyl fluoride (1.1 equiv). The reaction was stirred 2 h at rt, then diluted with sat. NH_4Cl and CH_2Cl_2. The organic layer was washed with sat. $NaHCO_3$ and brine; dried over Na_2SO_4, filtered and concentrated *in vacuo*. The resulting oil was purified by column chromatography.

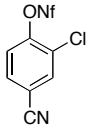


3,5-dimethylphenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate Following general procedure G, a mixture of 3,5-dimethylphenol (10.3 g, 84.3 mmol), diisopropyl ethylamine (18 mL, 101 mmol), DMAP (500 mg), and perfluorobutanesulfonyl fluoride (28 g, 92.7 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (5:95 EtOAc/hexanes) to provide the title compound as a clear oil (13.8 g, 41%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.02 (s, 1H), 6.91 (s, 2H), 2.36 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.8, 140.4, 130.0, 118.8, 116.0–109.9 (m, 4C) 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -81.1–(-81.2), -109.6–(-109.7), -121.3–(-121.4), -126.2–(-126.4); IR (thin film) 2928, 1625, 1426 cm^{-1}; Anal. Calcd. For $C_{12}H_9F_9O_3$: C, 35.65; H, 2.24. Found: C, 35.70; H, 2.26.



3-chlorophenyl 1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonate Following general procedure G, a mixture of 3-chlorophenol (1.2 g, 10 mmol), diisopropyl ethylamine (1.67 mL, 12 mmol), DMAP (61 mg), and perfluorobutanesulfonyl fluoride (3.3 g, 11 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (5:95 EtOAc/hexanes) to provide the title compound as a clear oil (3.3 g, 81%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44–7.37 (m, 2H), 7.32–7.31 (m, 1H), 7.23–7.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.8, 135.7, 130.9, 128.8, 122.1, 119.7 (4C not detected); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -80.88–(-80.9) (m), -109.0–

(-109.1), -121.1–(-121.2) (m), 126.1–(-126.2) (m); IR (thin film) 1582, 1470, 1241 cm^{-1}; Anal. Calcd. For $C_{10}H_4ClF_9O_3$: C, 29.25; H, 0.98. Found: C, 29.40; H, 0.97.



3-chloro-4-(perfluorobutoxy)benzonitrile Following general procedure G, a mixture of 3-chloro-4-hydroxybenzonitrile (5 g, 32.5 mmol), diisopropyl ethylamine (6.9 mL, 39 mmol), DMAP (200 mg), and perfluorobutanesulfonyl fluoride (10.9 g, 35.8 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (20% EtOAc/hexanes) to provide the title compound as a white solid (5.65 g, 40%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87 (d, J = 2.0 Hz, 1H), 7.68 (dd, J = 8.4, 2.0 Hz, 1H), 7.52 (d, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.7, 134.9, 134.5, 132.3, 129.0, 124.1, 116.0, 113.7 (4C not detected); ^{19}F NMR (376 MHz, $CDCl_3$) δ: -80.78–(-80.83) (m), -109.7–(-109.1), -120.9–(-120.9) (m), 126.0–(-126.1) (m); IR (thin film) 1426, 1202 cm^{-1}; Anal. Calcd. For $C_{11}H_3ClF_9O_3$: C, 30.33; H, 0.69. Found: C, 30.57; H, 0.54.

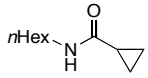
Synthesis of Secondary Amides and Related Nucleophiles

General procedure H: Synthesis of Secondary Amides To a solution of amine (1 equiv) and pyridine (1.2 equiv) in CH_2Cl_2 (1 M) cooled to 0 °C was added the acyl chloride (1.05 equiv). The reaction mixture was stirred for 1 h at rt, then diluted with sat. NH_4Cl and CH_2Cl_2. The organic layer was washed with sat. $NaHCO_3$ and brine, dried over Na_2SO_4, filtered and concentrated. The resulting oil was purified by column chromatography.

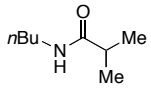
General procedure I: Synthesis of Ureas To a solution of secondary amine (1 equiv) and triethylamine (1.1 equiv) in CH_2Cl_2 (1 M) cooled to 0 °C was added the isocyanate (1.05 equiv). The reaction mixture was stirred for 2 h at rt, then diluted with EtOAc and sat NH_4Cl. The organic layer was washed with sat. $NaHCO_3$ and brine, dried over Na_2SO_4, filtered, and concentrated. The resulting solid was used directly.

General procedure J: Synthesis of Carbamates To a solution of amine (1 equiv) in THF/H_2O (50:50, 0.25 M) cooled to 0 °C was added $NaHCO_3$ (1.5 equiv) and the alkyl chloroformate (1.5 equiv). The reaction mixture was stirred for 2 h at rt, then diluted with EtOAc and sat NH_4Cl. The organic layer was washed with sat. $NaHCO_3$ and brine, dried over Na_2SO_4, filtered, and concentrated. The resulting oil was purified by column chromatography.

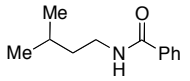
General procedure K: Synthesis of Sulfonamides To a solution of amine (1 equiv), triethylamine (1.2 equiv), and DMAP (0.05 equiv) in CH_2Cl_2 (1 M) cooled to 0 °C was added the sulfonyl chloride (1.1 equiv). The reaction mixture was stirred for 2 h at rt, then diluted with CH_2Cl_2 and sat. NH_4Cl. The organic layer was washed with sat. $NaHCO_3$ and brine, dried over Na_2SO_4, filtered, and concentrated. The resulting oil was purified by column chromatography.



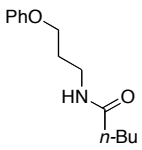
***N*-hexylcyclopropanecarboxamide** Following general procedure H, a mixture of *n*-hexylamine (6.7 mL, 50 mmol), pyridine (4.8 mL, 52.5 mmol), and cyclopropanecarbonyl chloride (4.77 mL, 52.5 mmol) was stirred for 1 h at rt. The crude product was purified by column chromatography (70:30 EtOAc/hexanes) to provide the title compound as a white solid (5.74 g, 68%): mp 49 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.73 (br s, 1H), 3.24 (q, *J* = 6.8, 2H), 1.52–1.45 (m, 1H), 1.34–1.23 (m, 6H), 0.96–0.92 (m, 2H), 0.87 (t, *J* = 6.8 Hz, 3H), 0.74–0.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.4, 39.7, 31.4, 29.6, 26.5, 22.5, 14.6, 14.0, 6.8; IR (thin film) 3302, 1636, 1549 cm^{-1}; Anal. Calcd. For $C_{10}H_{19}NO_3$: C, 70.96; H, 11.31. Found: C, 70.96; H, 11.62.



***N*-butylisobutyramide**[9] Following general procedure H, a mixture of *N*-butylamine (4.9 mL, 50 mmol), pyridine (4.8 mL, 60 mmol), and isobutyrylchloride (5.49 mL, 52.5 mmol) was stirred for 1 h at rt. The crude product was purified by column chromatography (50:50 EtOAc/hexanes) to provide the title compound as an oil (1.9 g, 27%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.46 (br s, 1H), 3.23 (q, 7.2 Hz, 2H), 2.32 (septet, *J* = 6.8 Hz, 1H), 1.49–1.45 (m, 2H), 1.37–1.31 (m, 2h), 1.14 (d, *J* = 7.2 Hz, 6H), 0.92 (t, *J* = 7.2 Hz, 3H).

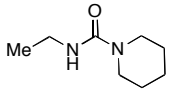


***N*-isopentylbenzamide**[10] Following general procedure H, a mixture of 3-methybutylamine (2.9 mL, 25 mmol), pyridine (2.4 mL, 30 mmol), and benzoyl chloride (3.0 mL, 26.3 mmol) was stirred for 1 h at rt. The crude product was purified by column chromatography (25:75 EtOAc/hexanes) to provide the title compound (3.62 g, 76%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75 (d, *J* = 6.8 Hz, 2H), 7.51–7.47 (m, 1H), 7.44–7.40 (m, 2H), 6.08 (br s, 1H), 3.50–3.45 (m, 2H), 1.68 (septet, *J* = 6.4 Hz, 1H), 1.51 (q, *J* = 7.6 Hz, 2H), 0.95 (d, *J* = 6.4 Hz, 6H).

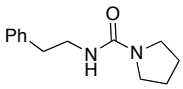


***N*-(3-phenoxypropyl)pentanamide** A mixture of 4-phenoxybutyric acid (3.6 g, 20 mmol), *N*-butylamine (2.0 mL, 20 mmol), HOBt (169 mg), and DCC (4.6 g, 22 mmol) was stirred for 1 h at rt. The reaction mixture was diluted with CH_2Cl_2 and sat. NH_4Cl. The organic layer was washed with brine, dried over Na_2SO_4, filtered, and concentrated. The crude product was purified by column chromatography (25:75 EtOAc/hexanes) to provide the title compound as a white solid (3.8 g, 85%): mp 65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.27–7.22 (m, 2H), 6.91 (t, *J* = 7.6 Hz, 1H), 6.87–6.83 (m, 2H), 5.53 (br s, 1H), 3.97 (t, *J* = 6.0 Hz, 2H), 3.21 (q, *J* = 6.8 Hz, 2H), 2.34 (t, *J* = 6.8 Hz, 2H), 2.12–2.06 (m, 2H), 1.45–1.37 (m, 2H), 1.32–1.29 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.2, 158.7, 129.4, 120.7, 114.3, 66.7, 39.2, 33.0, 31.6, 25.2, 20.0, 13.7; IR (thin film) 3323, 2963, 1541 cm^{-1}; Anal. Calcd. For $C_{14}H_{21}NO_2$: C, 71.46; H, 8.99. Found: C, 71.68; H, 8.92.

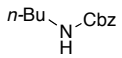
[9] Cashman, T. J.; Linton, B. R. *Org. Lett.* **2007**, *9*, 5457.
[10] Huang, P.-Q.; Zheng, X.; Deng, X.-M. *Tetrahedron Lett.* **2001**, *42*, 9039.



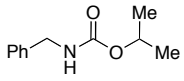
***N*-ethylpiperidine-1-carboxamide** Following general procedure I, a mixture of piperidine (4.94 mL, 50 mmol), triethylamine (7.6 mL, 55 mmol), and ethyl isocyanate (4.12 mL, 52.5 mmol) was stirred for 2 h at rt. After workup, the resulting solid was used directly (6.2 g, 79%): mp 83 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.40 (br s, 1H), 3.31–3.22 (m, 6H), 1.59–1.50 (m, 6H), 1.12 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.7, 44.7, 35.6, 25.5, 24.4, 15.5; IR (thin film) 3343, 2928, 1617, 1543 cm^{-1}.



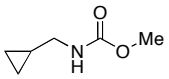
***N*-phenethylpyrrolidine-1-carboxamide**[11] Following general procedure I, a mixture of pyrrolidine (1.65 mL, 20 mmol), triethylamine (3.1 mL, 22 mmol), and phenylethyl isocyanate (3.1 mL, 21 mmol) was stirred for 2 h at rt. After workup, the resulting solid was used directly (4.01 g, 92%): mp 78–80 °C (lit 84–85 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77–7.75 (m, 2H), 7.49–7.44 (m, 1H), 7.43–7.37 (m, 2H), 6.34 (br s, 1H), 3.46–3.39 (m, 2H), 1.61–1.55 (m, 2H), 1.37–1.29 (m, 6H), 0.90–0.86 (m, 3H).



benzyl butylcarbamate[12] Following general procedure J, a mixture of *N*-butylamine (4.9 mL, 50 mmol), $NaHCO_3$ (6.3 g, 75 mmol), and benzyl chloroformate (10.7 mL, 75 mmol) was stirred for 2 h at rt. The crude reaction mixture was purified by column chromatography (8-80% EtOAc/hexanes) to provide the title compound as an oil (4.52 g, 44%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33–7.26 (m, 5H); 5.06 (s, 2H), 4.75 (br s, 1H), 3.16 (q, J = 6.8 Hz, 2H), 1.48–1.41 (m, 2H), 1.35–1.26 (m, 2H), 0.89 (t, J = 7.2 Hz, 3H).



isopropyl benzylcarbamate[13] Following general procedure J, a mixture of *N*-benzylamine (2.18 mL, 20 mmol), $NaHCO_3$ (2.52 g, 30 mmol), and isopropyl chloroformate (3 mL, 30 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (10-80% EtOAc/hexanes) to provide the title compound as an oil (3.4 g, 89%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36–7.26 (m, 5H), 4.96–4.88 (m, 2H), 4.37 (d, J = 5.6 Hz, 2H), 1.24 (d, J = 6.4 Hz, 6H).



methyl cyclopropylmethylcarbamate Following general procedure J, a mixture of cyclopropylmethanamine (1.97 mL, 20 mmol), $NaHCO_3$ (2.52 g, 30 mmol), and methyl chloroformate (2.31 mL, 30 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (10-80% EtOAc/hexanes) to provide the title compound as an oil (1.18 g, 60%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.79 (br s, 1H), 3.66 (s, 3H), 3.03 (t, J = 5.6 Hz, 2H), 0.98–0.91 (m, 1H), 0.51–0.46 (m, 2H), 0.19–0.15; ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.0, 51.9, 45.8, 11.0, 3.1; IR (thin film) 3335, 1704, 1537, 1256 cm^{-1}.

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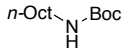
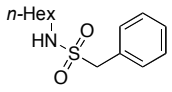
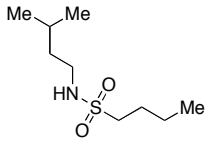
[11] Yamaguchi, J.; Murayama, Y.; Suyama, T.; *Bull. Chem. Soc. Jpn.* **2002**, *75*, 329.
[12] McGhee, W.; Riley, D.; Christ, K.; Pan, Y.; Parnas, B. *J. Org. Chem.* **1995**, *60*, 2820.
[13] Mormeneo, D.; Llebaria, A.; Delgado, A. *Tetrahedron Lett.* **2004**, *45*, 6831.



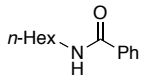
***tert*-butyl octylcarbamate**[14] Di-*tert*-butyl dicarbonate (5.7 mL, 25 mmol) was added to *N*-octylamine (4.1 mL, 25 mmol) and the reaction was stirred neat for 2 h. The resulting oil was purified by column chromatography (10:90 EtOAc/hexanes) to provide the title compound (4.6 g, 81%): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.46 (br s, 1H), 3.10 (q, J = 6.8 Hz, 2H), 1.43 (br s, 11H), 1.30–1.20 (m, 10H), 0.87 (t, J = 6.8 Hz, 3H).



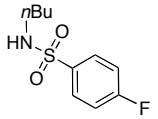
***N*-hexyl-1-phenylmethanesulfonamide** Following general procedure K, a mixture of *N*-hexylamine (3.3 mL, 25 mmol), triethylamine (4.21 mL, 30 mmol), DMAP (152 mg) and phenylmethanesulfonyl chloride (5.24 g, 27.5 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography to provide the title compound as a solid (1.6 g, 25%): mp 97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40–7.37 (m, 5H), 4.24 (s, 2H), 4.04 (br s, 1H), 2.97 (q, J = 6.4 Hz, 2H), 1.48–1.42 (m, 2H), 1.31–1.22 (m, 6H), 0.87 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 130.5, 129.4, 128.7, 128.6, 58.5, 43.7, 31.2, 30.2, 26.1, 22.4, 13.9; IR (thin film) 3240, 2923, 1305 cm^{-1}; Anal. Calcd. For $C_{13}H_{21}NO_2S$: C, 61.14; H, 8.29. Found: C, 61.19; H, 8.12.



***N*-isopentylbutane-1-sulfonamide** Following general procedure K, a mixture of isopentylamine (2.61 g, 30 mmol), triethylamine (5.05 mL, 36 mmol), DMAP (183 mg) and butanesulfonyl chloride (5.2 g, 33 mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography (10-80% EtOAc/hexanes) to provide the title compound as a solid (5.03 g, 81%): mp 62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.13 (br s, 1H), 3.12 (q, J = 7.2 Hz, 2H), 3.03–2.98 (m, 2H), 1.80–1.76 (m, 2H), 1.66 (septet, J = 6.4 Hz, 1H), 1.49–1.42 (m, 4H), 0.95 (t, J = 7.2 Hz, 3H), 0.91 (d, J = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 52.0, 41.4, 39.0, 25.5, 25.3, 22.2, 21.4, 13.5; IR (thin film) 3283, 2959, 1467, 1318 cm^{-1}; Anal. Calcd. For $C_9H_{21}NO_2S$: C, 52.14; H, 10.21. Found: C, 52.42; H, 10.14.



***N*-hexylbenzamide**[15] Following general procedure H, a mixture of *n*-hexylamine (3.3 mL, 25 mmol), pyridine (2.4 mL, 30 mmol), and benzoyl chloride (3.0 mL, 26.3 mmol) was stirred for 1 h at rt. The crude product was purified by column chromatography (5-50% EtOAc/hexanes) to provide the title compound (3.7 g, 73%): mp 46–47 °C (lit 42–44 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.78–7.75 (m, 2H), 7.49–7.44 (m, 1H), 7.44–7.37 (m, 2H), 6.34 (br s, 1H), 3.46–3.39 (m, 2H), 1.61–1.55 (m, 2H), 1.37–1.29 (m, 6H), 0.90–0.86 (m, 3H).



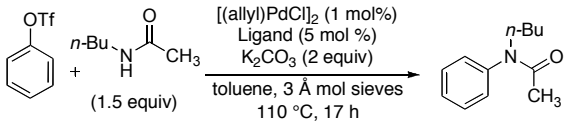
***N*-butyl-4-fluorobenzenesulfonamide** Following general procedure K, a mixture of *N*-butylamine (2.4 mL, 25 mmol), triethylamine (4.21 mL, 30 mmol), DMAP (152 mg) and phenylmethanesulfonyl chloride (5.35 g, 27.5

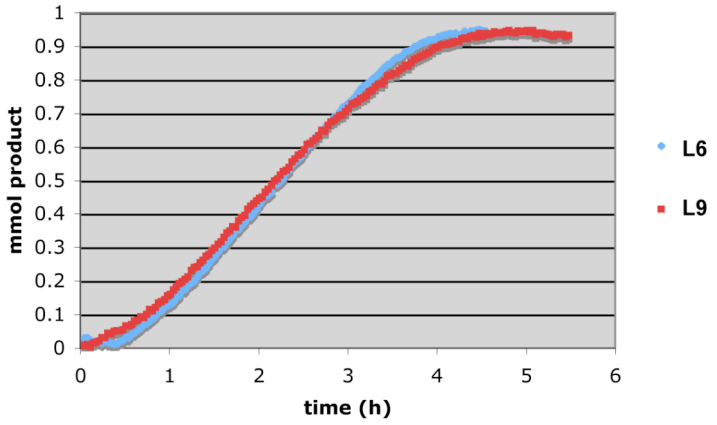
[14] Guin, J.; Frohlich, R.; Studer, A. *Angew. Chem., Int. Ed.* **2008**, *47*, 779.
[15] Erdik, E.; Daskapan, T.; *J. Chem. Soc., Perkin Trans. 1*, **1999**, 3139.

mmol) was stirred for 2 h at rt. The crude product was purified by column chromatography to provide the title compound as a white solid (1.24 g, 22%): mp 45 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91–7.86 (m, 2H), 7.22–7.16 (m, 2H), 2.95 (q, J = 6.8 Hz, 2H), 1.48–1.41 (m, 2H), 1.33–1.26 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.2, 163.7, 136.0, 136.7, 116.3, 116.1, 42.9, 31.4, 19.6, 13.4; IR (thin film) 3284, 2957, 1597, 1326 cm^{-1}.

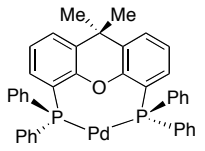
General procedure L: Representative Procedure for In Situ IR Spectroscopy: An oven-dried reaction tube fitted with a teflon septum, magnetic stir bar, and teflon screw valve was taken into the glove box and charged with K_2CO_3 (276 mg, 2.0 mmol, pre-dried under vacuum at 130 °C for 18 h), 3 Å mol sieves (200 mg, pre-dried under vacuum at 130 °C), **L6** (40 mg, 5 mol%), and $[Pd(allyl)Cl]_2$ (3.6 mg, 2 mol%). The tube was removed from the glove box and the React IR probe was secured in the reaction tube with a teflon adapter and evacuated and backfilled with Ar (this process was repeated a total of three times). Next, the aryl triflate/halide (1.0 mmol), amide (1.5 mmol), and toluene (4 mL) were added via syringe. The solution was placed in a 110 °C oil bath and the React IR scans started. The growing peak at 1670 cm^{-1} (height to single point baseline = 1722 cm^{-1}) was monitored over the course of the reaction. After completion of the reaction, the mixture was cooled to room temperature, diluted with ethyl acetate, and dodecane was added as an internal standard. An aliquot was analyzed by gas chromatography to obtain a GC yield. Full Characterization for *N*-butyl-*N*-phenylacetamide: ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.15 (d, *J* = 7.6 Hz, 2H), 3.68 (t, *J* = 7.6 Hz, 2H), 1.81 (s, 3H), 1.51–1.43 (m, 2H), 1.35–1.27 (m, 2H), 0.87 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.0, 143.2, 129.5, 128.1, 127.7, 48.7, 29.8, 22.8, 19.9, 13.7; IR (thin film) 2931, 1661, 1397 cm^{-1}.

In situ IR Comparison of L6 and L9





Cartesian Coordinates for all Calculated Complexes and Transition States:



Complex **1**
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P -2.147600 -0.658998 -0.321496
P 2.147552 -0.659073 -0.321410
O -0.000029 1.399872 0.394373
C -1.179288 2.011033 0.009806
C -2.279430 1.198022 -0.331888
C -3.458234 1.853243 -0.722641
H -4.325285 1.264086 -1.000791
C -3.531079 3.243598 -0.779437
H -4.452551 3.725168 -1.094622
C -2.425373 4.016366 -0.428758
H -2.498844 5.097665 -0.471500
C -1.233878 3.412463 -0.016845
C 0.000023 4.179994 0.470910
C 1.233922 3.412421 -0.016780
C 2.425456 4.016288 -0.428629
H 2.498959 5.097586 -0.471348
C 3.531150 3.243487 -0.779283
H 4.452655 3.725023 -1.094418
C 3.458241 1.853132 -0.722524
H 4.325263 1.263933 -1.000683
C 2.279394 1.197963 -0.331813
C 1.179280 2.010994 0.009859
C 0.000063 5.641429 -0.008071
H -0.876548 6.173577 0.373802
H 0.000114 5.714113 -1.100993
H 0.876655 6.173554 0.373881
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H -0.889809 4.688505 2.408486
H 0.889795 4.688442 2.408531
H -0.000058 3.153198 2.421126
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C -3.510048 -1.364256 -2.652900
H -2.533051 -1.215822 -3.107302
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H -4.458659 -1.906010 -4.507582
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H -6.679745 -2.308607 -3.458741
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H -5.051219 -1.268596 0.380400
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H -4.132464 0.065013 4.244246
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H -3.497965 -2.200358 5.050786
C -2.565346 -2.763637 3.187617
H -2.277901 -3.752297 3.535995
C -2.235907 -2.362600 1.893007
H -1.681031 -3.030767 1.239180
C 3.659830 -1.166349 -1.270385
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H 2.532636 -1.214823 -3.107423
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C 5.995581 -1.812028 -1.474734
H 6.960565 -1.995621 -1.008892
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C 2.599935 -1.090659 1.422013
C 2.235573 -2.362356 1.893331
H 1.680110 -3.030299 1.239772
C 2.565205 -2.763396 3.187899
H 2.277307 -3.751841 3.536511
C 3.250373 -1.892232 4.038375
H 3.498772 -2.200376 5.050669
C 3.606622 -0.621109 3.585305
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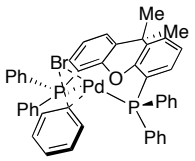

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O 0.000654 2.166876 -0.016852
C -0.001040 -3.160970 -0.487224
C -1.223144 -3.672956 -0.027308
H -2.156879 -3.340831 -0.465322
C -1.210601 -4.609104 1.011109
H -2.156060 -4.985467 1.394255
C -0.001962 -5.073415 1.538276
H -0.002323 -5.814167 2.333125
C 1.207135 -4.609840 1.011523

H 2.152235 -4.986785 1.394983
C 1.220599 -3.673701 -0.026896
H 2.154689 -3.342176 -0.464611
C -1.180521 2.643307 -0.554455
C -2.288769 1.776159 -0.552467
C -3.483873 2.260968 -1.104804
H -4.358863 1.621087 -1.124805
C -3.558858 3.544676 -1.641975
H -4.491109 3.896812 -2.074470
C -2.443562 4.380319 -1.617442
H -2.523046 5.380272 -2.029883
C -1.235160 3.949200 -1.060147
C 0.001353 4.838625 -0.894211
C 1.237352 3.948507 -1.060281
C 2.445934 4.378942 -1.617717
H 2.525930 5.378838 -2.030197
C 3.560763 3.542679 -1.642342
H 4.493163 3.894286 -2.074948
C 3.485133 2.259033 -1.105108
H 4.359776 1.618680 -1.125152
C 2.289820 1.774904 -0.552635
C 1.182043 2.642656 -0.554564
C 0.001635 6.018833 -1.881272
H -0.874285 6.655138 -1.724045
H 0.001488 5.679592 -2.922591
H 0.877930 6.654642 -1.724132
C 0.001593 5.407440 0.555001
H -0.888252 6.026011 0.720267
H 0.891818 6.025485 0.720180
H 0.001392 4.603340 1.297225
C -3.718276 -0.720003 -0.433603
C -3.748380 -1.358083 -1.685894
H -2.847335 -1.392181 -2.293585
C -4.918300 -1.964413 -2.146163
H -4.924000 -2.453318 -3.116695
C -6.070453 -1.955925 -1.356214
H -6.978769 -2.436385 -1.710337
C -6.047447 -1.335802 -0.105492
H -6.938728 -1.330366 0.516935
C -4.880613 -0.719792 0.353259
H -4.875901 -0.240257 1.327302
C -2.350920 0.266853 1.916924
C -2.874254 1.432719 2.495771
H -3.159457 2.269641 1.865386
C -3.031248 1.528684 3.880690
H -3.433347 2.440770 4.314536
C -2.675747 0.459108 4.703606
H -2.798657 0.534835 5.780872
C -2.154851 -0.706458 4.136613
H -1.869877 -1.541574 4.771232
C -1.984944 -0.799173 2.755321
H -1.562516 -1.701802 2.321908
C 3.718081 -0.721960 -0.433334
C 3.747920 -1.360484 -1.685403
H 2.846861 -1.394428 -2.293080
C 4.917592 -1.967447 -2.145473
H 4.923083 -2.456686 -3.115839
C 6.069754 -1.959152 -1.355541
H 6.977876 -2.440095 -1.709509
C 6.047005 -1.338598 -0.105027
H 6.938291 -1.333312 0.517395
C 4.880424 -0.721965 0.353524
H 4.875917 -0.242113 1.327413
C 2.350979 0.265898 1.916923
C 1.984281 -0.799778 2.755445
H 1.561339 -1.702211 2.322126
C 2.154113 -0.706959 4.136740
H 1.868569 -1.541804 4.771458
C 2.675660 0.458377 4.703607
H 2.798513 0.534192 5.780873
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H 3.434490 2.439525 4.314311
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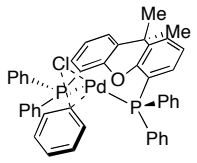

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C -0.000389 -3.151404 -0.831319
C -1.220935 -3.734399 -0.468372
H -2.154338 -3.331164 -0.842572
C -1.208640 -4.838990 0.388811
H -2.154631 -5.276426 0.698967
C -0.000800 -5.388963 0.827435
H -0.000962 -6.257052 1.480732
C 1.207250 -4.839197 0.389136
H 2.153083 -5.276798 0.699539
C 1.219960 -3.734610 -0.468048
H 2.153531 -3.331543 -0.842013
C -1.180566 2.585527 -0.385596
C -2.286992 1.722827 -0.494165
C -3.476817 2.266506 -1.001876
H -4.349396 1.631628 -1.107177
C -3.549422 3.603753 -1.387190
H -4.477432 4.001817 -1.787767
C -2.437576 4.433361 -1.251181
H -2.515199 5.474286 -1.545746
C -1.234447 3.941864 -0.734359
C 0.000568 4.804877 -0.456037
C 1.235371 3.941586 -0.734438
C 2.438581 4.432802 -1.251341
H 2.516423 5.473704 -1.545932
C 3.550233 3.602942 -1.387399

H 4.478307 4.000790 -1.788042
C 3.477357 2.265721 -1.002042
H 4.349791 1.630647 -1.107371
C 2.287440 1.722323 -0.494252
C 1.181208 2.585268 -0.385654
C 0.000683 6.100436 -1.284455
H -0.875440 6.711511 -1.047578
H 0.000574 5.896632 -2.360480
H 0.877007 6.711272 -1.047710
C 0.000659 5.184353 1.053872
H -0.889358 5.776705 1.296200
H 0.890686 5.776739 1.296083
H 0.000718 4.292549 1.687905
C -3.709655 -0.776491 -0.677325
C -3.704071 -1.298069 -1.982883
H -2.784381 -1.286488 -2.563107
C -4.862900 -1.851953 -2.529538
H -4.842211 -2.251534 -3.539880
C -6.037451 -1.906818 -1.775576
H -6.937007 -2.346853 -2.198060
C -6.049299 -1.403498 -0.473020
H -6.958569 -1.449373 0.121026
C -4.893995 -0.840272 0.073555
H -4.914276 -0.451635 1.087200
C -2.382719 -0.053236 1.792572
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C -2.206719 -1.266782 3.892550
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C -2.019840 -1.204474 2.511698
H -1.588262 -2.052979 1.987513
C 3.709592 -0.777312 -0.677152
C 3.703951 -1.299082 -1.982634
H 2.784276 -1.287439 -2.562880
C 4.862706 -1.853230 -2.529182
H 4.841975 -2.252955 -3.539466
C 6.037231 -1.908170 -1.775187
H 6.936727 -2.348407 -2.197588
C 6.049131 -1.404663 -0.472703
H 6.958380 -1.450599 0.121371
C 4.893905 -0.841172 0.073763
H 4.914224 -0.452397 1.087355
C 2.382631 -0.053584 1.792609
C 2.019227 -1.204595 2.511831
H 1.587352 -2.052984 1.987703
C 2.205949 -1.266820 3.892709
H 1.922482 -2.165815 4.433790
C 2.742724 -0.175093 4.579144
H 2.879318 -0.220596 5.656446
C 3.097426 0.976806 3.875709
H 3.512828 1.831911 4.402976
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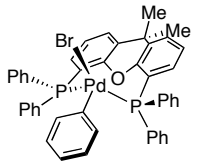

Complex **2a**
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C 0.011713 -2.872165 -0.064920
C -1.195922 -3.519276 0.202065
H -2.146435 -3.052250 -0.025901
C -1.178812 -4.807255 0.752611
H -2.123557 -5.303028 0.962618
C 0.029683 -5.452578 1.015109
H 0.036728 -6.453786 1.437386
C 1.228681 -4.808767 0.708725
H 2.179802 -5.305915 0.883765
C 1.227369 -3.521005 0.157584
H 2.169255 -3.054975 -0.105657
C -1.194970 2.540362 -0.469876
C -2.303386 1.675146 -0.455081
C -3.504886 2.156879 -0.995881
H -4.378417 1.514969 -1.008792
C -3.584488 3.441830 -1.528075
H -4.520100 3.795063 -1.951784
C -2.469097 4.278102 -1.510750
H -2.554114 5.278815 -1.919897
C -1.253505 3.848273 -0.968087
C -0.019537 4.742772 -0.809530
C 1.223002 3.859103 -0.962230
C 2.437197 4.299933 -1.499178
H 2.515237 5.301561 -1.907459
C 3.559952 3.473551 -1.511789
H 4.494397 3.835232 -1.930925
C 3.489009 2.187473 -0.981167
H 4.368075 1.553139 -0.991007
C 2.289335 1.694562 -0.446340
C 1.173656 2.550438 -0.464844
C -0.022292 5.912031 -1.810071
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H -0.018532 5.560412 -2.847119
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H 0.861741 5.949502 0.795385
H -0.024432 4.529914 1.384674
C -3.712530 -0.835490 -0.324292
C -3.737807 -1.445023 -1.591619

H -2.839914 -1.456377 -2.206840
C -4.905470 -2.053117 -2.055283
H -4.911090 -2.521091 -3.035800
C -6.052490 -2.073003 -1.258277
H -6.958013 -2.554603 -1.618008
C -6.030675 -1.480643 0.006323
H -6.918759 -1.498421 0.632886
C -4.868069 -0.863451 0.472534
H -4.860987 -0.404505 1.456544
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C -2.812914 1.354063 2.612939
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H -2.732184 0.449320 5.895626
C -2.150333 -0.811510 4.243596
H -1.889135 -1.657342 4.874020
C -1.999927 -0.909896 2.860545
H -1.618767 -1.830051 2.426027
C 3.717856 -0.804581 -0.323241
C 3.750163 -1.405746 -1.594402
H 2.853425 -1.420185 -2.211239
C 4.923219 -2.002038 -2.059844
H 4.934113 -2.463702 -3.043308
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H 6.978812 -2.490500 -1.622110
C 6.040341 -1.434000 0.007296
H 6.927472 -1.448818 0.635286
C 4.872194 -0.828765 0.475377
H 4.859972 -0.376053 1.462204
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C 2.009625 -0.910002 2.858010
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H 1.908755 -1.670464 4.867145
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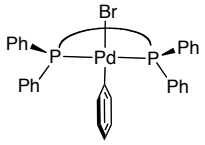

Complex **2b**
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C -0.002172 -2.443165 -0.234183
C -0.003690 -3.607271 0.549153
H -0.003917 -3.538935 1.635239
C -0.004956 -4.871031 -0.054317
H -0.006133 -5.763269 0.568470
C -0.004729 -4.985967 -1.446571
H -0.005738 -5.967101 -1.915156
C -0.003196 -3.830365 -2.229470
H -0.002969 -3.906526 -3.314539
C -0.001884 -2.567568 -1.627481
H -0.000553 -1.681197 -2.255831
C -1.183464 2.178413 -0.819876
C -2.300706 1.526851 -0.258622
C -3.472700 2.280282 -0.094105
H -4.343902 1.815784 0.354268
C -3.530869 3.619198 -0.468341
H -4.444793 4.185931 -0.316254
C -2.416508 4.229653 -1.039697
H -2.477513 5.270826 -1.336369
C -1.231462 3.516870 -1.238429
C 0.002315 4.085716 -1.945820
C 1.235743 3.515051 -1.239297
C 2.421989 4.226096 -1.041532
H 2.484311 5.267145 -1.338370
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H 4.450779 4.179404 -0.319605
C 3.475851 2.275367 -0.096168
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C 2.302578 1.523672 -0.259686
C 1.186014 2.176710 -0.820537
C 0.001418 3.580203 -3.418572
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H 0.000329 2.487089 -3.465013
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H -3.989892 -0.674251 -4.434680
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H -4.524402 -3.092597 -4.201756
C -3.853939 -3.192725 -2.152033
H -4.075813 -4.250700 -2.043207
C -3.306976 -2.490905 -1.080535
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C -4.953973 -0.611021 1.173012
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C -5.572803 -0.718093 3.509570
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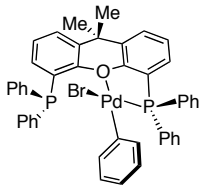
H 2.219808 -0.234594 3.167623
Br -0.000650 1.277040 2.608033



Complex **2c**
Pd 0.682851 -0.545008 -1.128300
P -2.233380 -0.649555 0.319256
P 2.040797 0.208175 0.611108
O -0.374875 1.599571 -0.422207
C 1.654303 -2.263711 -1.363681
C 1.194896 -3.361304 -0.628355
H 0.349487 -3.256178 0.046279
C 1.817959 -4.607083 -0.773745
H 1.453122 -5.457473 -0.201855
C 2.893084 -4.758982 -1.650739
H 3.374545 -5.726851 -1.764009
C 3.337255 -3.661673 -2.390574
H 4.163384 -3.773091 -3.089130
C 2.719811 -2.413366 -2.253126
H 3.058028 -1.577071 -2.854592
C -1.706387 2.010694 -0.519415
C -2.700157 1.056681 -0.253908
C -4.032665 1.465253 -0.409017
H -4.827611 0.746215 -0.239049
C -4.346517 2.775352 -0.763115
H -5.384966 3.075068 -0.872318
C -3.329501 3.705995 -0.971094
H -3.591527 4.724504 -1.235486
C -1.983902 3.339317 -0.862469
C -0.815499 4.284284 -1.160280
C 0.353525 3.887932 -0.251523
C 1.301501 4.779665 0.261354
H 1.171293 5.846108 0.113485
C 2.434995 4.324784 0.938330
H 3.159759 5.037951 1.319836
C 2.660655 2.957819 1.082814
H 3.573965 2.603853 1.550804
C 1.723435 2.028617 0.608705
C 0.564993 2.525467 -0.008867
C -0.374560 4.061545 -2.637787
H -1.192712 4.330999 -3.315109
H -0.113864 3.015842 -2.828005
H 0.494906 4.686113 -2.873912
C -1.205374 5.761731 -0.979404
H -2.011252 6.036161 -1.665786
H -0.361794 6.416384 -1.218503
H -1.533328 5.976775 0.043522
C -3.680022 -1.647753 -0.265384
C -3.609878 -2.160648 -1.573058
H -2.744761 -1.942957 -2.195299
C -4.648337 -2.943106 -2.079636
H -4.580977 -3.328634 -3.093500
C -5.760670 -3.238079 -1.287913
H -6.564242 -3.854907 -1.682232
C -5.833468 -2.741850 0.014815
H -6.694678 -2.968969 0.638509
C -4.801446 -1.949901 0.523933
H -4.869547 -1.572994 1.539920
C -2.544260 -0.529146 2.144564
C -3.028729 0.608667 2.807770
H -3.284193 1.498789 2.242044
C -3.198068 0.608277 4.195257
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H -2.165680 -2.560585 4.867278
C -2.224875 -1.663227 2.913591
H -1.830318 -2.550600 2.423940
C 3.863092 0.131958 0.361387
C 4.357466 0.414883 -0.922911
H 3.663600 0.640261 -1.728456
C 5.729052 0.406652 -1.168551
H 6.098484 0.628760 -2.165927
C 6.623861 0.100776 -0.139462
H 7.692872 0.085555 -0.333818
C 6.140259 -0.190553 1.136104
H 6.830575 -0.431969 1.939932
C 4.766109 -0.172662 1.389390
H 4.402650 -0.400235 2.386112

C 1.776707 -0.372600 2.332552
C 1.932032 -1.745199 2.597822
H 2.192467 -2.428707 1.794338
C 1.752795 -2.234601 3.890930
H 1.883935 -3.295508 4.086413
C 1.399982 -1.367399 4.928338
H 1.256083 -1.751693 5.934532
C 1.226679 -0.007979 4.667536
H 0.942046 0.669647 5.467633
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H 1.284270 1.550666 3.186623
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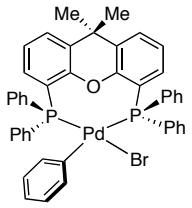

Complex **2d**
Pd 0.529538 -1.291506 -0.316895
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P 1.792527 0.692770 0.231959
O -0.705941 2.080621 -0.220930
C 2.239628 -2.173941 -0.947200
C 3.151147 -2.824983 -0.113397
H 2.987857 -2.860301 0.959219
C 4.271415 -3.457130 -0.661254
H 4.973258 -3.965795 -0.004077
C 4.485907 -3.448661 -2.041505
H 5.355486 -3.945941 -2.463984
C 3.567563 -2.809093 -2.875671
H 3.715420 -2.806558 -3.953642
C 2.444082 -2.174119 -2.330925
H 1.730777 -1.690914 -2.995098
C -1.948919 2.125615 -0.816460
C -2.719098 0.958737 -0.741587
C -4.002920 1.006003 -1.308439
H -4.636197 0.127198 -1.273559
C -4.462291 2.159947 -1.939796
H -5.455834 2.175345 -2.378577
C -3.649671 3.291505 -2.021924
H -4.022955 4.174661 -2.529347
C -2.372633 3.299467 -1.453915
C -1.441340 4.517776 -1.426355
C 0.000858 4.000206 -1.487933
C 1.069567 4.676092 -2.086690
H 0.893254 5.602138 -2.623635
C 2.371669 4.184942 -1.988697
H 3.190174 4.730172 -2.449728
C 2.635188 3.006579 -1.289604
H 3.654759 2.650072 -1.206471
C 1.590121 2.281310 -0.701346
C 0.296204 2.804641 -0.824923
C -1.747348 5.502416 -2.568230
H -2.769232 5.884895 -2.488127
H -1.628823 5.034509 -3.551248
H -1.086319 6.372834 -2.516871
C -1.635217 5.253116 -0.068310
H -2.667441 5.609602 0.025762
H -0.961311 6.115197 -0.002249
H -1.424583 4.589174 0.775797
C -3.114777 -1.838670 -0.791429
C -2.815325 -2.258897 -2.096555
H -1.913312 -1.902279 -2.585810
C -3.652198 -3.150837 -2.763587
H -3.402579 -3.472132 -3.771126
C -4.793889 -3.648397 -2.130104
H -5.440114 -4.353861 -2.645713
C -5.094522 -3.243951 -0.829682
H -5.976947 -3.631408 -0.327039
C -4.262265 -2.339912 -0.163508
H -4.507865 -2.034038 0.848340
C -2.543768 -0.542578 1.752131
C -3.187814 0.566074 2.318323
H -3.412270 1.435560 1.708780
C -3.551792 0.561189 3.667232
H -4.049568 1.429273 4.091749
C -3.286874 -0.553861 4.462513
H -3.578697 -0.559618 5.509595
C -2.646777 -1.664483 3.904922
H -2.439875 -2.539698 4.515505
C -2.267744 -1.659257 2.562538
H -1.763487 -2.522838 2.135700
C 3.633865 0.534643 0.314594
C 4.333123 0.658790 1.523804
H 3.799681 0.861296 2.445460
C 5.723208 0.521238 1.557049
H 6.247226 0.617553 2.504299
C 6.433582 0.264395 0.385277
H 7.514642 0.156952 0.413290
C 5.746186 0.136132 -0.823964
H 6.286172 -0.080842 -1.741200
C 4.358693 0.262152 -0.858750
H 3.839335 0.121862 -1.800408
C 1.343689 1.176887 1.956924
C 0.901901 0.186828 2.846083
H 0.781715 -0.835456 2.497681
C 0.602194 0.509341 4.171435
H 0.246838 -0.266064 4.843346
C 0.737506 1.823283 4.620470
H 0.498183 2.075009 5.650263
C 1.177839 2.815965 3.741465
H 1.286285 3.841252 4.085598
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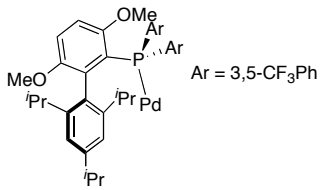
Br -0.279334 -3.740050 -0.020454



Complex **3**

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C -3.431124 -1.237961 0.266296
H -4.739983 -2.300819 -1.076671
H -4.276218 1.866331 -1.930109
C -1.868923 0.125524 1.712258
C -0.461436 0.132915 1.528647
C -2.390580 0.193928 3.027106
C 0.381442 0.168732 2.671823
C -1.542202 0.264933 4.129540
C -0.159605 0.245359 3.953590
H -1.939813 0.321779 5.135871
H 0.482638 0.274203 4.825681
P 0.266531 0.155830 -0.197872
C -3.121349 -2.507293 1.056612
H -2.403429 -2.250960 1.842107
C -5.464413 -0.418998 -2.897310
H -5.737150 -1.481432 -2.957075
C -4.749518 -0.051048 -4.211548
H -4.458148 1.006021 -4.224459
H -3.842764 -0.650649 -4.349135
H -5.408102 -0.224594 -5.071054
C -6.772056 0.383003 -2.739787
H -7.438988 0.206029 -3.592138
H -7.303799 0.098006 -1.825310
H -6.575004 1.460711 -2.690450
C -2.941835 2.587203 0.330683
H -2.065892 2.545123 0.987361
C -2.654098 3.636280 -0.758134
H -2.309434 4.570437 -0.299837
H -1.879211 3.288535 -1.452892
H -3.548608 3.873111 -1.346530
C -4.143000 3.037701 1.191163
H -3.943922 4.017331 1.642850
H -5.045535 3.128075 0.574316
H -4.350492 2.320077 1.989317
C -2.460372 -3.584639 0.173183
H -2.116771 -4.427042 0.784374
H -3.159826 -3.975323 -0.575264
H -1.593649 -3.181234 -0.360989
C -4.378568 -3.062198 1.754119
H -5.138168 -3.368159 1.024983
H -4.125924 -3.942227 2.358282
H -4.825483 -2.307995 2.409421
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O 1.724292 0.094443 2.441771
C -4.337820 0.241231 4.423530
H -4.067479 1.169362 4.944517
H -5.417336 0.218527 4.265620
H -4.043222 -0.618883 5.039248
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H 2.588799 -0.556477 4.228356
H 3.620159 0.341611 3.073980
H 2.419627 1.219031 4.057077
C 1.617908 1.428668 -0.100242
C 2.975859 1.137034 0.068558
C 1.238672 2.767664 -0.255742
C 3.923703 2.161869 0.102725
H 3.300429 0.110485 0.192291
C 2.187005 3.791101 -0.212081
H 0.194122 3.010213 -0.420896
C 3.538468 3.496065 -0.032343
H 4.276419 4.288116 -0.001317
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C 1.142337 -2.450027 0.637150
C 2.521052 -2.916633 -1.735386
H 1.908586 -0.943116 -2.308192
C 1.767458 -3.682924 0.414276
H 0.610844 -2.287582 1.567802
C 2.465311 -3.922812 -0.764266
H 2.956197 -4.874370 -0.930060
C 5.359998 1.803066 0.373533
C 1.737239 5.211766 -0.430224
C 3.222966 -3.197598 -3.038920
C 1.672504 -4.734346 1.488042
F 2.651642 6.105245 0.003960
F 1.519337 5.467666 -1.739704
F 0.576397 5.470314 0.215579
F 6.203442 2.819764 0.106440
F 5.543305 1.469625 1.680194
F 5.756452 0.736162 -0.351574
F 4.371494 -3.882808 -2.843307
F 3.529807 -2.064575 -3.703670
F 2.455044 -3.948437 -3.860793
F 2.244700 -4.315933 2.640908
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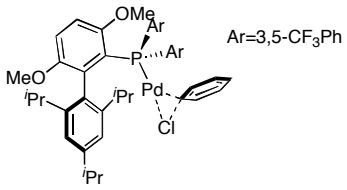
F 0.382456 -5.022005 1.782844
Pd -1.435842 0.618594 -1.617064



Transition State **3-TS**

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C 3.362082 -1.419736 0.595980
C 4.325332 -1.664603 -0.390279
C 4.906414 -0.642277 -1.142656
C 4.490727 0.667412 -0.887273
C 3.534271 0.971779 0.086410
C 2.056372 0.240985 2.004445
C 0.650762 0.380843 1.939798
C -0.071141 0.738814 3.110512
C 0.589980 0.921459 4.321793
C 1.974641 0.771866 4.389744
C 2.705176 0.447035 3.249409
H 4.637731 -2.689202 -0.577055
H 4.929608 1.482916 -1.456227
H 0.045198 1.196231 5.216990
H 2.469479 0.926126 5.341210
P -0.239040 0.073692 0.340427
Pd 0.941288 -0.773918 -1.451943
C -0.291276 -1.593428 -3.113108
C -1.040241 -0.612276 -3.782837
C -0.871720 -2.817929 -2.746362
C -2.406121 -0.824521 -3.978791
H -0.567290 0.303265 -4.120730
C -2.240377 -3.003150 -2.947159
H -0.268845 -3.599418 -2.297445
C -3.014348 -2.012111 -3.557540
H -2.993461 -0.046346 -4.458113
H -2.695262 -3.933412 -2.617930
Cl 1.650580 -1.684750 -3.617155
H -4.076174 -2.169885 -3.721869
C 3.184401 2.438263 0.335671
C 2.676014 3.148077 -0.934410
C 4.376415 3.198127 0.951774
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H 1.860792 2.585685 -1.402475
H 2.303697 4.149161 -0.687605
H 3.471801 3.261042 -1.679867
H 4.717091 2.712404 1.871982
H 5.224549 3.232393 0.257726
H 4.094783 4.231732 1.187127
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C 5.585979 -0.448156 -3.586842
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H 7.649588 -0.790817 -0.781739
H 8.118738 -0.677132 -2.490712
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C -3.336677 2.916311 -2.836385
C -0.819593 5.384972 0.757219
C -5.332116 -0.965791 1.716045
C -2.124752 -4.794580 1.006904
F -3.098935 -5.547909 1.556020
F -1.980470 -5.201781 -0.278852
F -0.967868 -5.098439 1.638562
F -6.264650 -1.935589 1.790899
F -5.312420 -0.338665 2.923048
F -5.757836 -0.052022 0.818890
F -4.305080 1.980329 -2.729977
F -2.635879 2.619769 -3.959234
F -3.937639 4.105271 -3.043400
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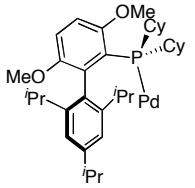
F -0.617702 5.229495 2.084494



Complex **4**
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C -2.356023 1.146343 -0.036155
C -1.572416 0.032392 0.416174
C -2.086588 -1.296049 0.190749
H -3.659756 -2.453117 -0.712720
H -4.137359 1.779032 -1.034474
C -0.454724 0.267218 1.427910
C 0.935766 0.310149 1.141354
C -0.886405 0.456307 2.768546
C 1.839022 0.557263 2.207686
C 0.025331 0.695179 3.791298
C 1.389683 0.748320 3.510910
H -0.305879 0.838511 4.812871
H 2.084019 0.933629 4.321591
P 1.538418 -0.064141 -0.612512
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H -0.529935 -2.252600 1.298100
C -5.349887 -0.585030 -1.738011
H -5.506832 -1.671080 -1.800316
C -5.278813 -0.048484 -3.181092
H -5.131150 1.038078 -3.193209
H -4.446438 -0.503634 -3.729705
H -6.206559 -0.265366 -3.725210
C -6.557759 0.010268 -0.989072
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H -6.633438 -0.397588 0.024985
H -6.476027 1.100557 -0.904414
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H -0.904976 2.586135 0.586628
C -1.948228 3.440052 -1.077761
H -1.507506 4.427378 -0.892154
H -1.385093 2.956352 -1.882502
H -2.969560 3.603218 -1.441297
C -2.811484 3.270371 1.286731
H -2.464859 4.293035 1.482675
H -3.855745 3.328798 0.956050
H -2.791045 2.709854 2.224630
C -1.281343 -3.717514 -0.064353
H -0.790186 -4.543029 0.465577
H -2.225385 -4.104841 -0.465452
H -0.649897 -3.422516 -0.910838
C -2.400924 -2.960218 2.072154
H -3.380478 -3.302898 1.716797
H -1.937025 -3.786741 2.625077
H -2.568731 -2.129198 2.762633
O -2.240336 0.379571 2.983874
O 3.172760 0.585718 1.886617
C -2.725430 0.549229 4.304687
H -2.482691 1.544598 4.700863
H -3.809681 0.443328 4.238074
H -2.327451 -0.216178 4.984665
C 4.121532 0.770268 2.922939
H 4.059610 -0.028309 3.674014
H 5.100361 0.737112 2.440580
H 3.997156 1.742031 3.419108
Pd -0.466932 -0.671424 -1.505995
C 2.491472 1.461495 -1.262560
C 1.731593 2.762936 -0.947304
C 3.990720 1.628598 -0.941610
H 2.408473 1.296753 -2.347112
C 2.330675 3.968597 -1.691398
H 1.767732 2.948805 0.135465
H 0.677340 2.653155 -1.216266
C 4.586350 2.825022 -1.707910
H 4.118086 1.784899 0.133781
H 4.550550 0.722660 -1.199362
C 3.830018 4.126121 -1.404517
H 1.789197 4.882538 -1.413753
H 2.181075 3.833430 -2.772862
H 5.649530 2.933429 -1.454724
H 4.542785 2.624278 -2.788863
H 4.246818 4.956850 -1.988768
H 3.970551 4.386358 -0.344569
C 2.890036 -1.369385 -0.406415
C 2.441632 -2.557422 0.463711
C 3.324223 -1.871412 -1.800715
H 3.747028 -0.897804 0.084852
C 3.545792 -3.623864 0.571417
H 1.544830 -3.010128 0.020982
H 2.161571 -2.212106 1.465389
C 4.430158 -2.936619 -1.699096
H 2.448262 -2.294499 -2.312298
H 3.671392 -1.037874 -2.424460
C 3.999188 -4.113014 -0.811587
H 3.188340 -4.468006 1.175861
H 4.408810 -3.199891 1.106646
H 4.695547 -3.292833 -2.703060
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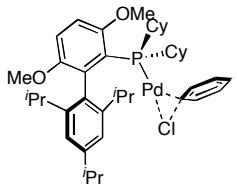
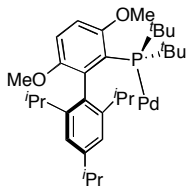
H 4.818007 -4.837510 -0.712199
H 3.166967 -4.643934 -1.296955



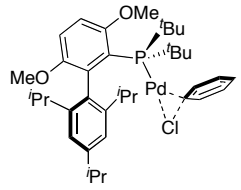
Transition State **4-TS**

C -2.078329 0.590547 -0.230994
C -2.377270 -0.224156 -1.352496
C -3.206616 -1.338279 -1.178843
C -3.767061 -1.671992 0.055081
C -3.466552 -0.850641 1.145038
C -2.644150 0.274040 1.030064
C -1.384661 1.918390 -0.439360
C 0.007271 2.164933 -0.335946
C 0.470977 3.484100 -0.607721
C -0.407940 4.504563 -0.957941
C -1.776262 4.258136 -1.042685
C -2.262086 2.982770 -0.785336
H -3.433671 -1.963205 -2.039544
H -3.900758 -1.080570 2.114335
H -0.044320 5.503820 -1.163438
H -2.441861 5.069612 -1.311546
P 1.166436 0.760021 0.162253
Pd 0.238726 -1.394780 0.023935
C 2.731621 0.982821 -0.867434
C 3.763947 -0.114205 -0.533897
C 2.394482 0.965656 -2.372443
H 3.167838 1.953634 -0.625619
C 5.027773 0.021711 -1.401279
H 3.319088 -1.102199 -0.692769
H 4.045447 -0.065631 0.524353
C 3.659446 1.097257 -3.237145
H 1.885939 0.022665 -2.615944
H 1.694198 1.773644 -2.614251
C 4.690763 0.011742 -2.898564
H 5.722027 -0.793821 -1.161784
H 5.546879 0.960040 -1.152526
H 3.388114 1.049560 -4.300098
H 4.109252 2.088457 -3.073949
H 5.600656 0.148283 -3.497684
H 4.280053 -0.972635 -3.166122
C 1.623498 1.207781 1.960525
C 1.979713 -0.062065 2.766843
C 2.693117 2.297131 2.184553
H 0.671528 1.588578 2.358511
C 2.170920 0.245947 4.261391
H 2.903558 -0.503951 2.369711
H 1.197717 -0.816791 2.624548
C 2.881620 2.599933 3.683323
H 3.652847 1.959341 1.768429
H 2.426728 3.212320 1.652581
C 3.225066 1.338631 4.486073
H 2.451383 -0.671918 4.794713
H 1.211863 0.573846 4.689049
H 3.664901 3.359437 3.809167
H 1.954551 3.039945 4.080626
H 3.310710 1.576116 5.554418
H 4.209462 0.963870 4.167876
C 1.429879 -3.310499 -0.108985
C 2.297996 -3.507745 0.979388
C 1.877724 -3.524909 -1.424532
C 3.636060 -3.809660 0.734777
H 1.924843 -3.413792 1.993107
C 3.222154 -3.828094 -1.644229
H 1.182171 -3.450572 -2.253212
C 4.109974 -3.966769 -0.573044
H 4.311841 -3.935024 1.577483
H 3.571261 -3.971263 -2.664151
Cl -0.454515 -3.750790 0.210587
H 5.150918 -4.219590 -0.752290
C -2.439748 1.158148 2.260120
C -1.952926 0.364778 3.487437
C -3.724975 1.940664 2.601233
H -1.666439 1.895460 2.019673
H -1.055810 -0.217659 3.255148
H -1.720119 1.047823 4.313899
H -2.717215 -0.333502 3.847949
H -4.067471 2.527239 1.743797
H -4.534918 1.257029 2.883336
H -3.551976 2.621348 3.444276
C -1.883808 0.108008 -2.760991
C -3.049652 0.554572 -3.667044
C -1.109999 -1.057101 -3.405496
H -1.190537 0.951476 -2.685744
H -3.593384 1.393680 -3.222343
H -2.675986 0.863789 -4.651249
H -3.764798 -0.262153 -3.823756
H -0.282875 -1.373065 -2.759341
H -1.754362 -1.927483 -3.577486
H -0.700006 -0.751751 -4.376425
C -4.718409 -2.855196 0.182698
C -6.172959 -2.376292 0.366367
C -4.318083 -3.830074 1.304531
H -4.671904 -3.408827 -0.765188
H -6.480921 -1.720240 -0.455435
H -6.862524 -3.228775 0.401274
H -6.286107 -1.814609 1.301658
H -3.292744 -4.189386 1.169871
H -4.378864 -3.355006 2.291000
H -4.988992 -4.697762 1.315564
O 1.820355 3.712131 -0.511866
O -3.595848 2.666444 -0.852933
C 2.330943 4.992748 -0.839370
H 3.413672 4.919401 -0.720267
H 2.097580 5.267039 -1.876461
H 1.945873 5.768903 -0.164764
C -4.514638 3.688945 -1.197528
H -5.499691 3.219134 -1.183340
H -4.495862 4.512941 -0.471354
H -4.318972 4.089483 -2.201516



Complex **5**

C 2.593203 -0.870185 -1.163429
C 3.443307 -0.831959 -0.033942
C 3.149703 0.079474 0.971465
C 1.984971 0.879771 0.959363
C 1.100577 0.789629 -0.134984
C 1.462444 -0.017262 -1.281885
H 2.912036 -1.445196 -2.028692
H 3.821872 0.159639 1.821054
C -0.222538 1.526593 -0.150776
C -1.498148 0.915752 0.063821
C -0.160789 2.923394 -0.398789
C -2.638536 1.763025 0.086764
C -1.300959 3.717862 -0.368991
C -2.539179 3.137119 -0.114091
H -1.246917 4.785518 -0.544414
H -3.418448 3.769015 -0.092001
P -1.670309 -0.980580 0.218894
C 0.906964 0.300009 -2.677994
H -0.101330 0.707301 -2.548366
C 4.667437 -1.736351 0.031036
H 4.678754 -2.331435 -0.892924
C 4.591048 -2.724486 1.210884
H 4.586070 -2.195041 2.171047
H 3.678333 -3.328497 1.158113
H 5.453212 -3.403102 1.206940
C 5.979283 -0.929059 0.074077
H 6.847989 -1.598759 0.056058
H 6.054101 -0.249084 -0.781786
H 6.044204 -0.324677 0.986596
C 1.769643 1.822935 2.146180
H 0.750074 2.219485 2.087360
C 1.924168 1.139150 3.520853
H 1.629166 1.832386 4.318424
H 1.311698 0.239356 3.607499
H 2.964912 0.853332 3.712417
C 2.743157 3.020580 2.077993
H 2.539461 3.729404 2.891073
H 3.780764 2.681404 2.185404
H 2.656271 3.545470 1.125204
C 0.802659 -0.910498 -3.620761
H 0.302491 -0.617100 -4.551954
H 1.790293 -1.299127 -3.896353
H 0.234477 -1.726816 -3.161463
C 1.771815 1.397303 -3.338496
H 2.786566 1.025231 -3.526707
H 1.340071 1.698518 -4.301459
H 1.848804 2.279361 -2.698116
O 1.083132 3.432144 -0.681854
O -3.852098 1.162816 0.301274
C 1.191115 4.807014 -1.009267
H 0.890498 5.450419 -0.171303
H 2.246301 4.977436 -1.230508
H 0.589869 5.060288 -1.892804
C -5.009334 1.972342 0.415935
H -5.221137 2.513659 -0.515646
H -5.833243 1.287591 0.626222
H -4.919380 2.692145 1.239954
Pd 0.429395 -1.764968 -0.395067
C -2.170954 -1.340027 2.048602
C -3.054397 -1.592481 -1.015437
C -4.498579 -1.712706 -0.493945
H -5.134329 -2.088781 -1.307936
H -4.584069 -2.428151 0.329455
H -4.901532 -0.756415 -0.167122
C -2.603386 -3.008090 -1.449799
H -1.595933 -2.993291 -1.877383
H -2.592748 -3.711698 -0.611151
H -3.303655 -3.395028 -2.203464
C -3.037903 -0.686116 -2.261470
H -2.028030 -0.573470 -2.667966
H -3.659331 -1.141612 -3.044626
H -3.440221 0.307650 -2.051624
C -3.441540 -0.680386 2.614238
H -4.344603 -0.959906 2.069549
H -3.568263 -1.002370 3.657740
H -3.365358 0.409273 2.610410
C -2.276703 -2.873019 2.193406
H -1.377308 -3.371505 1.815065
H -2.386311 -3.129008 3.255892
H -3.143493 -3.285331 1.667937
C -0.975257 -0.862597 2.892582
H -0.040123 -1.319832 2.553310
H -0.862875 0.224749 2.843882
H -1.135205 -1.136234 3.944570



Transition State **5-TS**

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C -3.566746 -1.334836 0.272995
C -3.079815 -0.976221 -0.986581
C -2.125549 0.028758 -1.167270
C -1.601852 0.707862 -0.029808
C -2.110590 0.375474 1.255054
H -3.442861 -0.893472 2.361441
H -3.472627 -1.480842 -1.864824
C -0.811636 1.994604 -0.204580
C 0.599295 2.173259 -0.159921

C -1.644834 3.135073 -0.392153
C 1.105601 3.497438 -0.279287
C -1.109088 4.405825 -0.558788
C 0.269321 4.587072 -0.498243
H -1.747270 5.266778 -0.717573
H 0.671514 5.586900 -0.605202
P 1.758438 0.693774 0.080130
Pd 0.459559 -1.256289 0.350647
C 1.302104 -3.370506 0.136291
C 1.397241 -3.717069 -1.224030
C 2.354845 -3.671928 1.018719
C 2.589740 -4.254979 -1.709237
H 0.549807 -3.563923 -1.883416
C 3.536034 -4.208999 0.510745
H 2.246313 -3.472045 2.078896
C 3.666920 -4.498927 -0.852677
H 2.668011 -4.496238 -2.766686
H 4.358682 -4.413034 1.192159
H 4.586665 -4.931102 -1.235845
C -1.720718 1.135847 2.521329
H -0.912069 1.825746 2.264984
C -1.747244 0.402971 -2.599934
H -0.871427 1.055806 -2.554755
C -1.376476 -0.822854 -3.457675
H -0.938673 -0.501976 -4.410573
H -0.655306 -1.466292 -2.945796
H -2.257714 -1.430504 -3.693873
C -2.875865 1.196050 -3.293010
H -2.571550 1.490921 -4.305229
H -3.782985 0.585508 -3.380383
H -3.133739 2.096313 -2.730304
C -1.203449 0.200184 3.631189
H -0.832315 0.784306 4.482604
H -1.996600 -0.456856 4.006309
H -0.392214 -0.437127 3.263169
C -2.894820 1.990757 3.042516
H -3.735290 1.359084 3.354389
H -2.582672 2.584153 3.911083
H -3.260266 2.673419 2.269427
C -4.660526 -2.380989 0.444390
H -4.748757 -2.579524 1.521496
C -4.332425 -3.717786 -0.244238
H -3.374535 -4.117880 0.102638
H -5.113739 -4.458167 -0.033439
H -4.272425 -3.605233 -1.333437
C -6.021302 -1.836495 -0.036483
H -6.284056 -0.909743 0.485752
H -5.998954 -1.618897 -1.111315
H -6.818883 -2.568433 0.141439
Cl -0.500161 -3.464205 0.884631
O -2.997554 2.902014 -0.390701
O 2.457963 3.656156 -0.136252
C -3.874930 4.003186 -0.551166
H -4.882832 3.587015 -0.504815
H -3.750171 4.741960 0.252098
H -3.732911 4.498414 -1.521453
C 3.026053 4.937719 -0.344737
H 2.817515 5.311958 -1.355469
H 2.665203 5.666596 0.392781
H 4.103541 4.810506 -0.223980
C 2.875076 0.556985 -1.502018
C 2.872737 1.054236 1.649131
C 4.249428 1.706819 1.416391
H 4.903842 1.099158 0.786568
H 4.165747 2.700379 0.980117
H 4.749632 1.807932 2.389621
C 2.083224 1.932884 2.637088
H 1.935775 2.946862 2.257606
H 1.107783 1.504519 2.877286
H 2.647943 2.005450 3.576696
C 3.116077 -0.318857 2.315664
H 2.173673 -0.806370 2.582396
H 3.665653 -1.003038 1.662588
H 3.708474 -0.174390 3.230225
C 3.825434 -0.637397 -1.267804
H 3.284829 -1.528759 -0.942778
H 4.331672 -0.876872 -2.212484
H 4.603603 -0.417747 -0.531698
C 1.929680 0.183543 -2.658682
H 1.359140 -0.719746 -2.431334
H 1.228871 0.993132 -2.885986
H 2.523972 -0.004198 -3.563430
C 3.699551 1.774860 -1.960816
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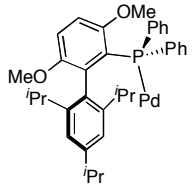
H 3.061028 2.605541 -2.270009
H 4.392986 2.138396 -1.202047



Complex **6**
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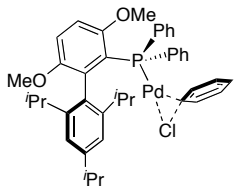
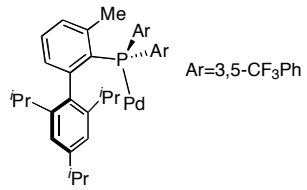
C -3.616406 -1.109353 0.194638
C -2.937721 -0.895623 -1.030564
C -1.925016 0.087785 -1.161184
C -1.508047 0.791191 0.030307
C -2.202735 0.608059 1.235036
H -3.798976 -0.462076 2.219385
H -3.303707 -1.389042 -1.926111
C -0.294430 1.684370 -0.031521
C 1.034840 1.187338 0.012361
C -0.506118 3.082271 -0.116425
C 2.110059 2.115808 0.008711
C 0.567460 3.967310 -0.164259
C 1.874108 3.484920 -0.096516
H 0.407111 5.036230 -0.241033
H 2.696871 4.190140 -0.109328

P 1.371694 -0.662338 -0.011555
C -1.836814 1.353228 2.516753
H -0.978962 1.997711 2.300659
C -4.736257 -2.135053 0.298716
H -5.080689 -2.127735 1.341995
C -4.246515 -3.562237 -0.014608
H -3.893199 -3.643162 -1.049490
H -3.418250 -3.846677 0.643863
H -5.057703 -4.288492 0.119207
C -5.942986 -1.761561 -0.585308
H -6.761822 -2.477886 -0.445563
H -6.317956 -0.761751 -0.339919
H -5.675652 -1.766808 -1.648878
C -1.547328 0.610122 -2.554992
H -0.572491 1.102997 -2.468948
C -1.418915 -0.476903 -3.634973
H -1.067189 -0.030984 -4.573475
H -0.708875 -1.255684 -3.331707
H -2.380695 -0.957861 -3.849518
C -2.570891 1.678645 -2.999764
H -2.269452 2.125131 -3.955790
H -3.562322 1.228897 -3.135817
H -2.660131 2.474753 -2.255760
C -1.409402 0.395128 3.646346
H -1.106399 0.963885 4.534527
H -2.229914 -0.268686 3.942829
H -0.565076 -0.230940 3.340528
C -2.987923 2.268205 2.980001
H -3.877997 1.687621 3.250833
H -2.688698 2.845778 3.863774
H -3.270478 2.968694 2.187874
O -1.817652 3.489013 -0.149636
O 3.364033 1.594647 0.145777
C -2.088138 4.878243 -0.225161
H -1.682045 5.321770 -1.144457
H -3.175733 4.969854 -0.232369
H -1.684835 5.416472 0.643213
C 4.488978 2.435117 -0.039289
H 4.567083 3.189650 0.755541
H 5.358152 1.776517 0.000162
H 4.458677 2.938422 -1.014279
C 2.818678 -0.836781 -1.158333
C 4.074175 -1.312858 -0.754422
C 2.609078 -0.568224 -2.520474
C 5.092802 -1.511684 -1.688908
H 4.262195 -1.521630 0.293723
C 3.633417 -0.747014 -3.450060
H 1.634706 -0.223312 -2.856946
C 4.879999 -1.224820 -3.038597
H 5.674742 -1.378692 -3.763889
C 2.059291 -1.056855 1.660364
C 2.179675 -2.418751 1.989474
C 2.403186 -0.102032 2.628462
C 2.662749 -2.814423 3.236343
H 1.880239 -3.170625 1.262914
C 2.865791 -0.499126 3.885614
H 2.308454 0.954319 2.405862
C 3.004887 -1.853509 4.191196
H 3.366985 -2.159219 5.169321
Pd -0.588782 -1.661387 -0.633906
H 3.452827 -0.525591 -4.499104
H 6.057969 -1.887527 -1.357529
H 2.755019 -3.872411 3.467853
H 3.120232 0.255030 4.626226



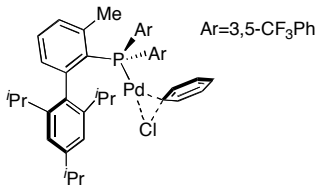
Transition State **6-TS**
C -2.032788 0.698432 -0.034347
C -2.496359 0.159326 -1.259582
C -3.347425 -0.952074 -1.230992
C -3.764299 -1.546760 -0.039804
C -3.295026 -0.997893 1.156866
C -2.445034 0.111946 1.188146
C -1.261515 1.996047 -0.028043
C 0.146110 2.109963 0.007617
C 0.737408 3.403412 0.003316
C -0.053322 4.547596 -0.055315
C -1.443533 4.434494 -0.083106
C -2.044855 3.179873 -0.057628
H -3.703807 -1.366559 -2.171264
H -3.608575 -1.440142 2.099208
H 0.395020 5.534079 -0.063702
H -2.040746 5.338063 -0.117382
P 1.228390 0.593963 0.046337
Pd 0.246503 -1.462035 -0.386753
C 1.497278 -3.316609 -0.376545
C 1.739669 -3.758821 0.935645
C 2.543635 -3.234348 -1.311963
C 3.053235 -4.011505 1.331993
H 0.913416 -3.889556 1.625715
C 3.847648 -3.484398 -0.888170
H 2.333821 -2.955628 -2.338590
C 4.113500 -3.870573 0.431115
H 3.243178 -4.330856 2.353917
H 4.661815 -3.383990 -1.601586
Cl -0.273904 -3.779111 -1.084929
H 5.131678 -4.082149 0.744682
C -2.030426 0.677570 2.545360
C -1.345735 -0.376852 3.435610
C -3.233063 1.316311 3.269257
H -1.299131 1.472740 2.371523
H -0.484003 -0.820884 2.926775
H -0.993529 0.082134 4.367238
H -2.033789 -1.186840 3.704757
H -3.706467 2.080218 2.643693
H -3.993938 0.564724 3.511837

H -2.914592 1.784505 4.209007
C -2.142752 0.776437 -2.612468
C -3.366357 1.473329 -3.242465
C -1.542845 -0.251481 -3.591374
H -1.382579 1.546026 -2.441320
H -3.788288 2.218246 -2.561244
H -3.086799 1.973900 -4.177983
H -4.154483 0.746969 -3.475105
H -0.683089 -0.765786 -3.147059
H -2.275019 -1.016548 -3.873978
H -1.217152 0.246562 -4.513447
C -4.718136 -2.734051 -0.054171
C -6.087340 -2.363725 0.549412
C -4.124055 -3.971430 0.644073
H -4.884589 -2.999854 -1.107209
H -6.533615 -1.510253 0.026785
H -6.783238 -3.208924 0.480872
H -5.993186 -2.094234 1.608380
H -3.164539 -4.252929 0.198153
H -3.954689 -3.784408 1.711282
H -4.807838 -4.825161 0.561712
O 2.097300 3.448401 0.086225
O -3.404836 2.999466 -0.059064
C 2.758515 4.695193 -0.031245
H 3.824855 4.464245 -0.018828
H 2.506741 5.197017 -0.974586
H 2.519301 5.361189 0.808941
C -4.235812 4.147532 -0.064487
H -5.260653 3.772430 -0.047809
H -4.064782 4.775116 0.820652
H -4.086813 4.752511 -0.969193
C 2.539584 0.957013 -1.216771
C 3.897882 1.112592 -0.908501
C 2.147575 0.999626 -2.563989
C 4.838511 1.307665 -1.922132
H 4.225314 1.089545 0.125445
C 3.085128 1.213948 -3.574648
H 1.103063 0.858566 -2.827115
C 4.437106 1.364218 -3.257885
H 5.888573 1.420958 -1.663386
H 2.759124 1.251519 -4.611083
H 5.170555 1.518402 -4.045037
C 2.092595 0.680938 1.678359
C 2.996427 -0.350844 1.988668
C 1.836023 1.660038 2.649204
C 3.644410 -0.383386 3.223491
H 3.190159 -1.138048 1.266527
C 2.471413 1.614538 3.892145
H 1.136333 2.461963 2.441594
C 3.382343 0.597974 4.182055
H 4.344211 -1.186738 3.438486
H 2.254393 2.380168 4.632874
H 3.878152 0.566262 5.148730



Complex **7**
C 4.502102 0.648635 -0.566884
C 4.616343 -0.422925 -1.443621
C 3.858756 -1.584717 -1.172121
C 3.014985 -1.682356 -0.042142
C 2.842512 -0.507337 0.777051
C 3.608843 0.645713 0.525039
H 5.096149 1.539951 -0.754078
H 4.019108 -2.471118 -1.778530
C 1.871372 -0.545535 1.929938
C 0.458489 -0.376865 1.803319
C 2.428397 -0.737648 3.203115
C -0.346500 -0.383990 2.976502
C 1.634390 -0.766824 4.343890
C 0.262101 -0.584825 4.223591
H 2.084108 -0.918571 5.321370
H -0.361625 -0.588854 5.113774
P -0.246008 -0.171439 0.075739
C 3.467844 1.923338 1.351166
H 2.666206 1.768261 2.079827
C 5.555604 -0.359993 -2.639800
H 6.006670 0.641592 -2.638933
C 4.803168 -0.525499 -3.974540
H 4.338263 -1.515926 -4.050001
H 4.011552 0.225154 -4.077453
H 5.490699 -0.415745 -4.821738
C 6.704170 -1.381776 -2.524892
H 7.402652 -1.273785 -3.363316
H 7.264954 -1.244010 -1.593871
H 6.326259 -2.411180 -2.539308
C 2.554818 -3.062222 0.447068
H 1.695305 -2.908103 1.108125
C 2.108328 -4.019317 -0.671130
H 1.668942 -4.924931 -0.237347
H 1.354870 -3.549966 -1.316099
H 2.946943 -4.335520 -1.302631
C 3.670128 -3.713136 1.293773
H 3.337573 -4.680683 1.688461
H 4.568454 -3.883900 0.688567
H 3.952099 -3.081244 2.142304
C 3.061918 3.128798 0.478772
H 2.799543 3.987191 1.107400
H 3.875883 3.437064 -0.187561
H 2.194314 2.889399 -0.145138
C 4.750318 2.232307 2.148290
H 5.605408 2.393940 1.481216
H 4.619900 3.140308 2.749254
H 5.007802 1.410309 2.825688

C -1.797569 -1.186831 0.073414
C -3.075688 -0.688914 -0.207252
C -1.647646 -2.571877 0.247816
C -4.169076 -1.553384 -0.314611
C -2.743960 -3.427390 0.159861
H -0.665307 -2.990317 0.441160
C -4.015336 -2.926089 -0.128930
C -0.826064 1.586302 0.014368
C -1.363598 2.059671 -1.193864
C -0.627890 2.500883 1.057618
C -1.729337 3.397889 -1.337286
H -1.487367 1.380974 -2.033169
C -0.969095 3.846830 0.898682
H -0.204814 2.170271 1.999193
C -1.529340 4.302941 -0.293211
H -1.808989 5.343171 -0.408366
Pd 1.349444 -0.831883 -1.390661
C -2.272226 3.874189 -2.660852
C -0.673289 4.822711 2.008475
F 0.579674 5.326916 1.901970
F -0.759392 4.240819 3.223939
F -1.521665 5.871730 1.994291
F -1.277584 4.088499 -3.550991
F -3.103569 2.963605 -3.211102
F -2.954242 5.032016 -2.537178
H -4.865328 -3.592615 -0.209840
H -3.237275 0.375923 -0.331957
C -5.517034 -0.987474 -0.682585
C -2.550627 -4.898711 0.422393
F -5.636164 -0.824694 -2.018827
F -6.526445 -1.791847 -0.287566
F -5.716195 0.225016 -0.119619
F -3.512789 -5.645288 -0.157714
F -2.579098 -5.171742 1.747225
F -1.357702 -5.335326 -0.041021
H 3.504490 -0.856373 3.286622
C -1.848327 -0.181833 2.985977
H -2.179254 0.587133 2.284788
H -2.382342 -1.103919 2.731428
H -2.175503 0.120580 3.985447



Transition State **7-TS**
C 2.965165 -0.319521 1.086216
C 3.338276 -1.659505 0.805058
C 4.327404 -1.897430 -0.157415
C 4.968090 -0.865794 -0.846463
C 4.586306 0.446659 -0.552002
C 3.604968 0.745208 0.398922
C 2.087841 -0.025697 2.282478
C 0.681428 0.188687 2.271453
C 0.002187 0.457482 3.493420
C 0.735955 0.506355 4.684796
C 2.111003 0.298574 4.698507
C 2.775379 0.037702 3.506485
H 4.613155 -2.923857 -0.374448
H 5.072267 1.268102 -1.071955
H 0.212594 0.715441 5.614115
H 2.662405 0.344366 5.633734
P -0.177700 0.104073 0.626305
Pd 1.030814 -0.700221 -1.164809
C -0.215784 -1.390627 -2.873833
C -0.913793 -0.349002 -3.506726
C -0.856460 -2.599715 -2.559664
C -2.288881 -0.483910 -3.707354
H -0.395610 0.554319 -3.809354
C -2.232241 -2.708955 -2.768292
H -0.293691 -3.427730 -2.142945
C -2.956823 -1.655335 -3.332963
H -2.835932 0.341522 -4.155541
H -2.732319 -3.629901 -2.480010
Cl 1.722598 -1.550683 -3.367461
H -4.026095 -1.750963 -3.496074
C 3.289002 2.209884 0.698323
C 2.900825 3.002281 -0.564690
C 4.455028 2.894633 1.439336
H 2.427469 2.235642 1.372203
H 2.100209 2.497384 -1.116727
H 2.551294 4.003131 -0.287174
H 3.751667 3.122169 -1.245017
H 4.688659 2.378680 2.377342
H 5.364256 2.902187 0.826683
H 4.200216 3.934369 1.677038
C 2.727200 -2.847689 1.548764
C 3.732426 -3.464023 2.542626
C 2.181158 -3.926770 0.593013
H 1.880767 -2.476110 2.136061
H 4.069371 -2.727118 3.279653
H 3.274810 -4.300686 3.084201
H 4.617879 -3.845341 2.020331
H 1.524428 -3.482989 -0.163975
H 2.986501 -4.449154 0.063931
H 1.609486 -4.677712 1.151144
C 6.055979 -1.168856 -1.867870
C 7.428286 -0.639532 -1.406989
C 5.701562 -0.636126 -3.269134
H 6.132393 -2.262291 -1.941176
H 7.704180 -1.048208 -0.428482
H 8.209440 -0.915641 -2.125319
H 7.424061 0.453956 -1.323811
H 4.736919 -1.027486 -3.608710
H 5.637703 0.458560 -3.275157
H 6.468956 -0.927805 -3.996218
C -1.693671 -0.932822 0.877763
C -3.009169 -0.457251 0.811413
C -1.488772 -2.312225 1.018944

C -4.088228 -1.340123 0.892224
H -3.207552 0.602622 0.703516
C -2.569055 -3.189503 1.107213
H -0.479924 -2.709721 1.042806
C -3.877457 -2.710723 1.042384
H -4.716872 -3.393070 1.110227
C -0.810632 1.811766 0.311067
C -1.553240 2.025922 -0.861308
C -0.444639 2.923711 1.079926
C -1.925217 3.314122 -1.244400
H -1.820335 1.185262 -1.493962
C -0.801841 4.213969 0.677966
H 0.127814 2.793400 1.991887
C -1.546342 4.420378 -0.482332
H -1.822476 5.421386 -0.789295
C -2.708895 3.478599 -2.521485
C -0.306436 5.384745 1.486082
C -5.496286 -0.819457 0.756394
C -2.307647 -4.671792 1.156024
F -3.332364 -5.349611 1.711803
F -2.126968 -5.174909 -0.089821
F -1.191725 -4.963253 1.860539
F -6.361394 -1.521690 1.519817
F -5.590253 0.477990 1.118694
F -5.933361 -0.909590 -0.519392
F -3.864991 2.779918 -2.485061
F -2.011402 3.013800 -3.586931
F -3.016385 4.766200 -2.771320
F -0.987989 6.516106 1.216985
F 1.001428 5.635816 1.233172
F -0.406269 5.149581 2.812718
C -1.489989 0.689265 3.599675
H -1.870181 1.364671 2.829380
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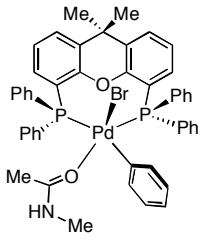
H -1.732547 1.128894 4.571670
H 3.849641 -0.119901 3.506700



Complex **8**
Pd 0.332869 -0.984930 -0.308090
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O -0.387742 2.284282 -0.533371
C 1.929693 -1.740083 -1.307510
C 2.455494 -2.978002 -0.918796
H 2.135095 -3.430673 0.016410
C 3.385233 -3.628017 -1.737773
H 3.791039 -4.588516 -1.426508
C 3.798419 -3.051035 -2.942521
H 4.528845 -3.555858 -3.570311
C 3.271469 -1.817763 -3.328441
H 3.582816 -1.358075 -4.264371
C 2.338340 -1.162075 -2.513535
H 1.935748 -0.205470 -2.833623
C -1.606435 2.354144 -1.170067
C -2.563742 1.398454 -0.798523
C -3.842875 1.533452 -1.361294
H -4.624375 0.833568 -1.088672
C -4.112285 2.533928 -2.293827
H -5.106693 2.617503 -2.723018
C -3.108131 3.417565 -2.692050
H -3.333476 4.171774 -3.438586
C -1.829695 3.349843 -2.130127
C -0.687522 4.325553 -2.448568
C 0.636628 3.564959 -2.292012
C 1.793960 3.793503 -3.046100
H 1.778391 4.510738 -3.859708
C 2.976926 3.106504 -2.768438
H 3.859442 3.286920 -3.375377
C 3.040993 2.195159 -1.712634
H 3.965316 1.665163 -1.514652
C 1.909455 1.945146 -0.924121
C 0.726980 2.616592 -1.269841
C -0.832483 4.936624 -3.853376
H -1.763748 5.504650 -3.937469
H -0.824902 4.167587 -4.633064
H -0.020571 5.642142 -4.054708
C -0.714953 5.473661 -1.398479
H -1.660220 6.024677 -1.463500
H 0.109705 6.173390 -1.577123
H -0.618519 5.082421 -0.380931
C -3.409403 -1.242138 -0.093630
C -3.601809 -1.640151 -1.429277
H -2.985627 -1.215948 -2.214408
C -4.576497 -2.580316 -1.760036
H -4.714651 -2.866838 -2.799588
C -5.366630 -3.157450 -0.761528
H -6.123340 -3.893901 -1.019132
C -5.175619 -2.780034 0.567081
H -5.782313 -3.220645 1.353774
C -4.208368 -1.826470 0.898962
H -4.081989 -1.542106 1.937363
C -2.523994 0.544339 1.995746
C -3.265602 1.710221 2.238009
H -3.559981 2.352148 1.413619
C -3.636105 2.051898 3.539736
H -4.206719 2.960457 3.714893
C -3.284884 1.226257 4.609586
H -3.583165 1.489442 5.621323
C -2.544286 0.066335 4.374811
H -2.257008 -0.578374 5.201301
C -2.149975 -0.270106 3.078212
H -1.542436 -1.159134 2.911363
C 3.515748 0.276232 0.915871

C 3.797111 -1.011595 1.391392
H 3.015404 -1.763070 1.418531
C 5.068119 -1.313612 1.886298
H 5.268812 -2.315138 2.256439
C 6.065989 -0.340013 1.913924
H 7.055508 -0.580862 2.293847
C 5.781797 0.955001 1.473682
H 6.544725 1.728022 1.516396
C 4.511087 1.266684 0.991929
H 4.296470 2.287844 0.693248
C 1.298974 1.656746 1.923376
C 1.358748 3.057505 1.972639
H 1.603009 3.629894 1.083325
C 1.116918 3.729330 3.171288
H 1.164280 4.815141 3.197571
C 0.822176 3.010197 4.331151
H 0.637549 3.534575 5.265194
C 0.768024 1.616788 4.285888
H 0.536440 1.049273 5.182556
C 1.001967 0.936581 3.089612
H 0.953486 -0.150725 3.064441
Br 0.530566 -2.814360 2.337647
O -0.758816 -2.471352 -1.632760
C -0.874849 -3.714418 -1.589574
C -1.375999 -4.446051 -0.374236
H -2.398864 -4.119949 -0.161734
H -1.366507 -5.533606 -0.500026
N -0.585214 -4.466456 -2.675160
H -0.678091 -5.467824 -2.583421
C -0.010348 -3.939535 -3.903381
H 1.050478 -4.200905 -3.984593
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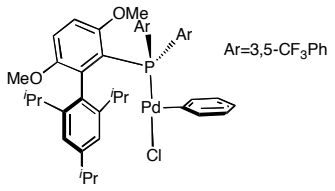

Complex **9a**
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C -4.601523 0.903222 -0.459584
C -3.486871 0.937819 0.380845
C -2.801607 -0.280201 0.671913
C -3.260581 -1.495294 0.082345
H -4.707545 -2.382248 -1.226863
H -5.114837 1.834294 -0.677184
C -1.896405 -0.352314 1.882765
C -0.491277 -0.249552 1.873386
C -2.547891 -0.566901 3.126497
C 0.242517 -0.344649 3.085050
C -1.813559 -0.653591 4.307435
C -0.422818 -0.542521 4.290703
H -2.310644 -0.815288 5.256450
H 0.124766 -0.623257 5.222039
P 0.367064 0.016937 0.267504
C -2.610416 -2.841985 0.392893
H -1.772770 -2.658633 1.073472
C -6.320306 -0.316458 -1.901853
H -6.297601 -1.266553 -2.452208
C -6.381208 0.815553 -2.941563
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H -7.237212 0.664674 -3.609998
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H -2.323229 3.064500 -0.894966
H -3.897821 3.706544 -0.437061
C -4.062855 2.701179 2.113528
H -3.726331 3.632346 2.585118
H -5.061067 2.878029 1.695746
H -4.156764 1.933772 2.887378
C -2.030738 -3.517268 -0.865094
H -1.465674 -4.414654 -0.586470
H -2.820735 -3.815642 -1.563513
H -1.359089 -2.837506 -1.400821
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H 2.354198 -1.174644 4.694599
H 3.400467 0.003358 3.845223
H 2.042028 0.583873 4.844027
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C 2.747923 1.474316 0.965378
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C 3.188088 -3.625292 -0.380727
H 3.825600 -4.483509 -0.557667
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C 0.953770 1.635202 -3.032638
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H 0.324926 -1.700869 -3.329756
C 2.469630 0.604983 -4.624564
H 2.466804 2.705473 -4.129677
H 2.204355 -1.516417 -4.922510
H 3.291273 0.686860 -5.330977
Cl -2.585011 0.368958 -3.340259
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F 4.131395 -2.852437 -3.260181
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H 3.225235 0.524209 1.166538
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F 5.281369 3.701705 2.262557
F 5.091253 1.538778 2.471936
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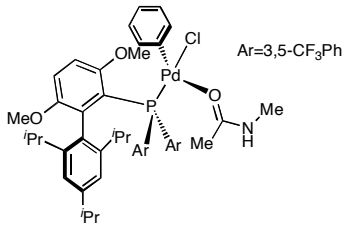

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C 2.410843 -1.125138 -1.266065
C 2.416646 -2.423347 -0.697527
H 3.498855 -3.784797 0.559643
H 5.367381 0.012398 -0.011327
C 1.363455 -0.724263 -2.277448
C 0.139836 -0.073928 -2.004235
C 1.700145 -0.967971 -3.638554
C -0.673935 0.367282 -3.088035
C 0.869223 -0.561869 -4.679327
C -0.315897 0.118938 -4.407258
H 1.139816 -0.749893 -5.711328
H -0.942711 0.455763 -5.224425
P -0.687384 0.286833 -0.374765
C 1.332431 -3.455202 -1.012560
H 0.419704 -2.917191 -1.288169
C 5.758626 -2.452173 1.185874
H 5.398068 -3.296510 1.790027
C 6.360788 -1.418356 2.151153
H 6.806020 -0.572960 1.613286
H 5.609926 -1.021190 2.838839
H 7.158465 -1.879749 2.745122
C 6.843247 -3.000303 0.234096
H 7.678126 -3.428947 0.802023
H 6.439592 -3.778283 -0.423112
H 7.241600 -2.199801 -0.401144
C 3.614578 1.130096 -1.686235
H 2.663180 1.353686 -2.178840
C 3.900249 2.280492 -0.701698
H 3.873681 3.239097 -1.230195
H 3.163599 2.333532 0.105497
H 4.887787 2.182493 -0.237301
C 4.700380 1.108429 -2.783581
H 4.731105 2.068857 -3.312551
H 5.691319 0.934701 -2.347056
H 4.511113 0.313660 -3.509662
C 0.979897 -4.374453 0.170501
H 0.088298 -4.958937 -0.076907
H 1.786784 -5.084791 0.388327
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H 2.619777 -4.930163 -1.981793
H 0.916990 -5.010943 -2.480052
H 1.973739 -3.721385 -3.098341
O 2.894992 -1.604207 -3.850425
O -1.789654 1.055441 -2.727030
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H 3.405083 -0.990527 -5.782143
H 4.238657 -2.416579 -5.104874
H 2.553227 -2.562710 -5.675109
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C 1.851272 -0.124552 2.883422

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H 0.476410 2.489881 -2.067790
C -0.071537 4.863013 0.296432
H 0.043309 5.929002 0.458717
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C -2.556471 -2.266045 -0.847220
C -2.309093 -2.593452 -2.186769
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C -5.435883 -0.602373 2.062527
H -4.679492 -1.326977 2.380034
H -4.977206 0.392081 2.080023
H -6.278520 -0.636575 2.759948
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H -8.753092 -1.348392 -0.910106
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F 0.492337 6.393376 -1.966422
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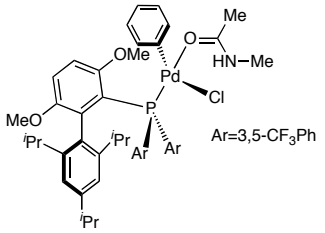

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C 0.599061 0.308036 -3.134878
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C 0.128663 0.332171 -4.442166
H -1.590740 0.215659 -5.708560
H 0.813680 0.440320 -5.274674
P 0.618189 0.353854 -0.414411
C -3.160433 2.264910 -0.974173
H -2.109504 2.342220 -1.272666
C -6.148821 -1.078001 1.340654
H -6.338483 -0.159803 1.913930
C -5.988059 -2.226108 2.350321
H -5.849687 -3.191438 1.849168
H -5.132928 -2.067160 3.012007
H -6.888254 -2.309243 2.970691
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H -7.533043 -0.478898 -0.251190
H -7.249183 -2.224429 -0.162991
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H -1.613072 -2.437726 -2.261152
C -1.954362 -3.887100 -0.727427
H -1.463514 -4.687385 -1.292104
H -1.218468 -3.493931 -0.019160
H -2.765256 -4.336324 -0.143730
C -3.454407 -3.430873 -2.704213
H -2.962482 -4.231946 -3.269579
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H -3.823525 -2.680553 -3.408531
C -3.373182 3.227147 0.208021
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H -4.437857 3.360745 0.435681
H -2.878322 2.887228 1.120483
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H -3.740691 3.776568 -2.431492

H -3.878807 2.115077 -3.048497
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O 1.923915 0.372048 -2.820454
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H -3.568214 -0.918283 -5.751658
H -5.063095 -0.268940 -5.022536
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C 1.457053 -2.287547 -1.180966
C 2.890058 -2.687444 1.171829
H 2.207780 -0.736525 1.741252
C 2.163055 -3.477083 -0.978283
H 0.916697 -2.146685 -2.109026
C 2.886463 -3.684230 0.195663
H 3.448588 -4.598940 0.341794
Pd 2.234120 2.108000 -0.364293
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C 0.369515 3.679032 -2.080023
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C 4.762192 1.570671 2.115909
H 4.603942 2.617641 1.837467
H 3.884883 1.232382 2.675332
H 5.645900 1.485434 2.755425
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H 6.014746 -0.017274 -1.486693
H 7.384345 -0.812796 -0.669172
H 5.758189 -1.540592 -0.610372
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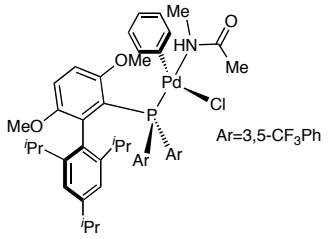

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C 0.298778 -0.144717 1.867247
C -0.836845 -1.220757 3.727304
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C 1.209569 -0.005482 4.140587
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H 1.961525 0.348888 4.835233
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H -6.615696 -1.018629 -0.849984
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H -5.161823 0.365048 3.309211
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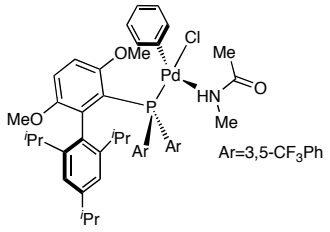
F -0.294032 4.491337 3.442472
F -0.609153 6.288654 2.248245
F -1.230383 5.092902 -3.052243
F 0.622633 6.080947 -2.506555
F 0.673832 4.165816 -3.547631
F -3.434544 1.715930 -3.580489
F -4.437368 -0.206285 -3.724447
F -4.365403 0.854316 -1.818650
F -0.467512 -2.533059 -5.395325
F 1.352527 -2.576892 -4.194830
F -0.286537 -3.929230 -3.741411
Cl 3.476088 2.255756 -1.210242



Complex **9e**
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C 4.271139 1.553612 -0.405573
C 3.104064 1.362731 -1.153807
C 2.619109 0.042907 -1.347270
C 3.322642 -1.055503 -0.796395
H 5.030220 -1.639665 0.366643
H 4.644396 2.565189 -0.272741
C 1.476048 -0.170620 -2.309208
C 0.098634 -0.206143 -1.991207
C 1.850167 -0.254292 -3.678981
C -0.857917 -0.255733 -3.046204
C 0.897015 -0.347967 -4.688971
C -0.459081 -0.335264 -4.375725

H 1.193488 -0.410375 -5.729008
H -1.191807 -0.385475 -5.171472
P -0.727997 -0.274753 -0.324263
C 2.900868 -2.505142 -1.046627
H 1.830354 -2.515103 -1.279808
C 6.320422 0.686486 0.853267
H 6.566802 -0.264521 1.345458
C 6.286396 1.772989 1.941299
H 6.079098 2.763074 1.518471
H 5.522546 1.566136 2.695046
H 7.257657 1.831248 2.446839
C 7.437423 0.975552 -0.171069
H 8.410833 1.054679 0.328134
H 7.501137 0.181623 -0.923232
H 7.250902 1.919853 -0.696983
C 2.449295 2.585244 -1.806263
H 1.477404 2.275809 -2.203436
C 2.190409 3.752113 -0.832772
H 1.600951 4.528803 -1.332227
H 1.636927 3.440586 0.058499
H 3.124276 4.211900 -0.490859
C 3.290237 3.088016 -2.999349
H 2.781138 3.916044 -3.507784
H 4.266567 3.453326 -2.658868
H 3.468235 2.288674 -3.723024
C 3.116701 -3.431729 0.163734
H 2.641854 -4.398394 -0.029725
H 4.181560 -3.620341 0.345968
H 2.688283 -3.027409 1.083801
C 3.640006 -3.097100 -2.266854
H 4.717486 -3.159660 -2.069156
H 3.271629 -4.108767 -2.473042
H 3.501216 -2.485816 -3.160658
O 3.195136 -0.212387 -3.933232
O -2.164302 -0.197470 -2.665160
C 3.637715 -0.334773 -5.276161
H 3.273258 0.491949 -5.900330
H 4.727323 -0.298517 -5.231267
H 3.324395 -1.289516 -5.718504
C -3.188447 -0.196266 -3.660648
H -3.188494 -1.138318 -4.221929
H -4.119787 -0.079417 -3.110217
H -3.056701 0.646759 -4.350054
C 0.446646 -0.376622 1.108232
C 1.171616 0.726069 1.583936
C 0.411535 -1.539761 1.884631
C 1.833457 0.662679 2.808936
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C 1.091261 -1.605341 3.104691
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H 2.305137 -0.544570 4.534032
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C -1.820590 1.831082 1.194889
C -1.455018 2.393032 -1.114335
C -2.390582 3.088259 1.412742
H -1.736528 1.143035 2.031791
C -1.999636 3.657272 -0.885326
H -1.106647 2.144028 -2.108250
C -2.482469 4.012103 0.374756
H -2.925727 4.985964 0.542301
Pd -2.461975 -1.930994 -0.055267
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C -0.994190 -3.514087 -2.092681
C -0.792529 -4.399883 0.144108
C -0.265264 -4.602530 -2.588111
H -1.369092 -2.771058 -2.787003
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H 0.766399 -6.436649 -2.106496
N -4.163447 -0.384983 0.779497
H -3.614938 0.471465 0.788946
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O -4.954011 0.590798 -1.119023
C -6.379562 -1.092028 -0.151751
H -6.993441 -0.902106 -1.033303
H -6.089916 -2.147804 -0.102109
H -6.961542 -0.860227 0.748411
C -4.560364 -0.805574 2.139574
H -4.948820 -1.823061 2.103247
H -3.667006 -0.811380 2.767999
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Cl -4.046452 -3.682080 0.327773
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C 2.494197 1.895178 3.370344
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F -2.992152 5.578698 -1.849047
F -0.841981 5.348051 -2.062150
F -2.181462 4.077905 -3.207613
F -1.971017 3.271581 3.729684
F -3.437438 4.636782 2.873379
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F -0.119241 -3.525270 3.768220
F 2.025108 -3.744865 3.492431
F 1.264407 -2.661180 5.215112
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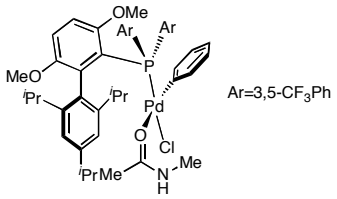
F 3.537284 1.579220 4.172613



Complex **9F**

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C -3.626574 -0.055020 1.155805
C -2.660789 -1.098541 1.117086
C -2.934452 -2.276139 0.376407
H -4.350059 -3.251266 -0.910457
H -5.551870 0.594869 0.475404
C -1.494129 -1.005322 2.077875
C -0.239589 -0.379508 1.852821
C -1.777025 -1.489110 3.386496
C 0.627390 -0.152525 2.964187
C -0.864135 -1.349755 4.427349
C 0.331069 -0.667839 4.221632
H -1.082422 -1.737751 5.415013
H 1.014628 -0.534846 5.051000
P 0.380438 0.143853 0.164982
C -1.995368 -3.486050 0.349465
H -0.974347 -3.117910 0.500134
C -6.405232 -1.499956 -1.082574
H -6.392329 -2.498842 -1.539193
C -6.510618 -0.474163 -2.227731
H -6.547529 0.551259 -1.839369
H -5.653604 -0.547100 -2.905598
H -7.423912 -0.641015 -2.811690
C -7.637681 -1.429323 -0.161334
H -8.556983 -1.600726 -0.734138
H -7.584255 -2.182891 0.632410
H -7.724098 -0.446013 0.316372
C -3.455614 1.214575 1.997640
H -2.387343 1.350838 2.198396
C -3.957845 2.486541 1.285648
H -3.598849 3.378589 1.808812
H -3.622535 2.542388 0.246520
H -5.053083 2.537031 1.279273
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H -4.017134 2.003694 3.953601
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C -2.017896 -4.240003 -0.994800
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H -2.957295 -4.789191 -1.129810
H -1.881975 -3.572639 -1.849621
C -2.316322 -4.485485 1.483228
H -3.336941 -4.872124 1.372933
H -1.629761 -5.340783 1.438942
H -2.239424 -4.031199 2.472079
O -3.002139 -2.073967 3.556103
O 1.747406 0.587768 2.726432
C -3.348238 -2.576763 4.836382
H -3.362077 -1.781270 5.593377
H -4.352695 -2.988890 4.728536
H -2.663062 -3.372269 5.158625
C 2.702119 0.786706 3.762515
H 3.204094 -0.153440 4.022692
H 3.427073 1.493907 3.357420
H 2.240048 1.224835 4.654839
C 0.641772 1.982940 0.324307
C 1.887944 2.531686 0.644481
C -0.442770 2.852649 0.130232
C 2.050001 3.910498 0.785957
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C 0.969096 4.769006 0.613143
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C 2.124796 -0.499657 0.087550
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C 2.636736 -1.474518 0.947214
C 4.244017 -0.512709 -1.107826
H 2.560764 0.694390 -1.661157
C 3.949485 -1.930650 0.805427
H 2.022049 -1.881666 1.740939
C 4.765470 -1.452859 -0.218765
H 5.785279 -1.802803 -0.322501
Pd -0.452624 -0.747188 -1.869578
C -1.323812 0.945817 -2.468109
C -2.698597 1.146645 -2.325323
C -0.547335 1.895560 -3.139650
C -3.289128 2.305942 -2.843274
H -3.313052 0.403007 -1.830863
C -1.145104 3.050899 -3.656957
H 0.518392 1.737520 -3.284170
C -2.516500 3.260215 -3.508280
H -4.361069 2.453385 -2.732110
H -0.533791 3.780685 -4.183199
H -2.980224 4.157233 -3.910031
O 0.765401 -2.686946 -1.379442
C 1.497456 -3.393315 -2.098795
N 1.949075 -4.594242 -1.664768
H 2.560490 -5.108101 -2.282196
C 1.960943 -2.975200 -3.473427
H 1.091598 -2.635241 -4.043717
H 2.653952 -2.132692 -3.381951
H 2.467543 -3.783482 -4.010244
C 1.658974 -5.170168 -0.361004
H 1.390835 -6.225558 -0.470900
H 2.516097 -5.085355 0.315066
H 0.817480 -4.631710 0.072542
Cl -1.237299 -1.678735 -3.927387
C 3.417669 4.434504 1.132331
C -1.449519 5.171169 0.155563

C 5.067895 -0.040008 -2.277112
C 4.496348 -2.880066 1.836582
F 3.891341 3.859223 2.269602
F 4.316403 4.156535 0.163423
F 3.424502 5.767226 1.326211
F -1.067104 6.377099 -0.319924
F -2.406516 4.693920 -0.658619
F -2.027062 5.396938 1.363633
F 4.830853 1.255302 -2.564743
F 4.782708 -0.750396 -3.397546
F 6.390255 -0.178790 -2.050193
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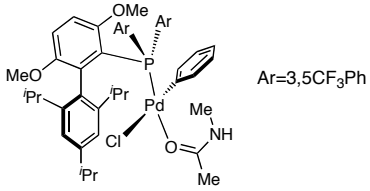

Complex **9g**
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C -2.551272 -0.604537 1.586481
C -3.030852 -1.857035 1.118994
H -4.646955 -2.838259 0.101725
H -5.210627 1.343349 0.710755
C -1.312832 -0.508800 2.449877
C 0.004095 -0.178744 2.037394
C -1.557809 -0.683627 3.841165
C 1.007507 0.030536 3.033134
C -0.541713 -0.552795 4.781977
C 0.738961 -0.188960 4.379528
H -0.735382 -0.709425 5.836248
H 1.515511 -0.070091 5.124809
P 0.569070 0.003892 0.262081
C -2.275555 -3.177988 1.319128
H -1.205270 -2.970315 1.220586
C -6.436478 -0.864148 -0.367424
H -6.553395 -1.906557 -0.694316
C -6.530967 0.025569 -1.621031
H -6.448807 1.088081 -1.362226
H -5.731355 -0.207344 -2.333189
H -7.493867 -0.118028 -2.126625
C -7.585221 -0.557494 0.613182
H -8.558695 -0.689889 0.125301
H -7.546923 -1.219230 1.485491
H -7.531668 0.476033 0.976070
C -2.977822 1.915414 2.051857
H -1.898518 1.915926 2.238996
C -3.288469 3.109721 1.128894
H -2.829192 4.019039 1.528989
H -2.920499 2.959914 0.110261
H -4.367088 3.295800 1.063327
C -3.677683 2.144915 3.409742
H -3.365398 3.104249 3.840555
H -4.766171 2.174618 3.277211
H -3.451733 1.350800 4.123397
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H -3.616454 -4.667865 0.423134
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C -2.520211 -3.797436 2.714135
H -3.592090 -3.958168 2.884326
H -2.020301 -4.771742 2.773904
H -2.141996 -3.175305 3.525658
O -2.849080 -0.974760 4.188195
O 2.227574 0.451720 2.596024
C -3.147108 -1.235257 5.549821
H -2.949341 -0.360229 6.183556
H -4.213195 -1.465923 5.578677
H -2.579746 -2.094947 5.930354
C 3.324824 0.525102 3.498418
H 3.605571 -0.472499 3.857940
H 4.144665 0.956250 2.922019
H 3.105187 1.183479 4.347166
C 1.240331 1.741756 0.216234
C 2.611677 2.015669 0.232705
C 0.345430 2.818632 0.179588
C 3.078616 3.330684 0.228765
H 3.329758 1.206653 0.267836
C 0.817748 4.134536 0.175440
H -0.721125 2.637462 0.137525
C 2.186529 4.399797 0.201843
H 2.549339 5.419994 0.195028
C 2.089141 -1.050415 0.130732
C 2.854678 -0.951744 -1.036423
C 2.445340 -2.005000 1.083934
C 3.970316 -1.766962 -1.228209
H 2.577774 -0.248480 -1.815304
C 3.572086 -2.806670 0.896906
H 1.845874 -2.142818 1.975556
C 4.343944 -2.695908 -0.257775
H 5.214901 -3.323164 -0.401827
Pd -0.679732 -0.683930 -1.557140
C -1.186310 1.162463 -2.196324
C -2.531231 1.551349 -2.193277
C -0.254742 1.948312 -2.888660
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C -0.661472 3.101627 -3.570676
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H -2.318780 4.385678 -4.083348
O -1.871772 -1.376739 -3.246942
C -1.428125 -1.873652 -4.302428

N -2.271513 -2.521527 -5.128277
H -1.901778 -2.919240 -5.978207
C 0.020134 -1.784794 -4.707371
H 0.327612 -0.734740 -4.683449
H 0.610257 -2.329201 -3.962180
H 0.211981 -2.194666 -5.703696
C -3.679033 -2.717020 -4.805438
H -4.129536 -3.344567 -5.576955
H -3.780219 -3.205797 -3.832255
H -4.205424 -1.757945 -4.766791
Cl 0.085468 -3.037874 -1.346124
C 4.565878 3.553491 0.286152
C -0.167224 5.275671 0.170220
C 4.722886 -1.670400 -2.528166
C 3.968638 -3.744026 2.004821
F 5.098362 3.006907 1.410740
F 5.197475 2.972487 -0.756245
F 4.891641 4.860919 0.284845
F 0.416698 6.444442 -0.172025
F -1.182497 5.059247 -0.688089
F -0.718603 5.456386 1.397076
F 4.881164 -0.383225 -2.914656
F 4.065235 -2.297530 -3.530145
F 5.950236 -2.225597 -2.448089
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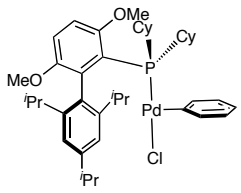

Complex **10a**

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C 1.828941 0.648852 -0.079196
C 2.331671 0.176800 -1.330721
H 3.813296 -1.034564 -2.297304
H 4.105957 -0.884737 1.956610
C 0.983333 1.909793 -0.055417
C -0.425719 1.994763 0.007354
C 1.742480 3.112566 -0.119029
C -1.037198 3.278814 0.002050
C 1.118942 4.354877 -0.109823
C -0.270775 4.438088 -0.049748
H 1.697720 5.269697 -0.154569
H -0.737587 5.415390 -0.050180
P -1.434069 0.424779 0.007417
C 1.754908 0.625358 -2.672116
H 0.839622 1.189324 -2.474923
C 5.357292 -1.920661 -0.256579
H 5.415960 -2.306258 -1.283214
C 5.305377 -3.134163 0.688413
H 5.329765 -2.826156 1.740829
H 4.391716 -3.713128 0.528288
H 6.173379 -3.782263 0.516990
C 6.623778 -1.075957 -0.005587
H 7.525576 -1.691161 -0.112110
H 6.694693 -0.240790 -0.711933
H 6.621842 -0.657444 1.008458
C 2.078970 0.754756 2.500617
H 1.111571 1.254012 2.394619
C 1.904854 -0.396562 3.511743
H 1.438295 -0.025551 4.432573
H 1.286185 -1.201560 3.103005
H 2.869203 -0.836134 3.790251
C 3.074274 1.796372 3.053081
H 2.736304 2.167878 4.028471
H 4.067918 1.353128 3.189323
H 3.180120 2.648844 2.376680
C 1.376077 -0.566709 -3.572092
H 0.866952 -0.211224 -4.476482
H 2.259420 -1.130900 -3.891863
H 0.715577 -1.263831 -3.046035
C 2.724120 1.571955 -3.410430
H 3.655901 1.055990 -3.670250
H 2.270762 1.932790 -4.341973
H 2.983289 2.437573 -2.793514
O 3.101175 2.963747 -0.194813
O -2.405436 3.315118 0.042208
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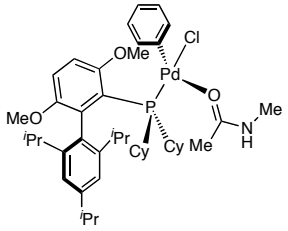
H 4.939308 3.766190 -0.317027
H 3.688255 4.720620 -1.161200
C -3.062104 4.572539 0.024508
H -2.838261 5.130988 -0.893603
H -4.129873 4.349817 0.061452
H -2.789059 5.182373 0.895396
Pd 0.080803 -1.372734 -0.082506
C -2.484932 0.318114 1.575139
C -1.609806 0.400774 2.840296
C -3.731304 1.213909 1.737737
H -2.836013 -0.720022 1.494946
C -2.404222 0.013752 4.099760
H -1.227334 1.425783 2.949129
H -0.739936 -0.254758 2.738775
C -4.538176 0.784341 2.976949
H -3.421275 2.256302 1.854288
H -4.369818 1.173158 0.848905
C -3.684123 0.848146 4.251135
H -1.766674 0.124979 4.986162
H -2.671960 -1.051052 4.039661
H -5.423229 1.425963 3.079221
H -4.910082 -0.241024 2.835725
H -4.262650 0.504593 5.118106

H -3.413019 1.895906 4.450124
C -2.688534 0.653762 -1.384363
C -2.007786 0.870698 -2.749548
C -3.708834 -0.501138 -1.469916
H -3.227799 1.571701 -1.131827
C -3.045170 1.124971 -3.857344
H -1.409743 -0.013996 -3.003002
H -1.316130 1.719666 -2.699222
C -4.751810 -0.225819 -2.567629
H -3.190302 -1.438794 -1.690036
H -4.217144 -0.650331 -0.510796
C -4.087355 0.000541 -3.932619
H -2.533112 1.239081 -4.821481
H -3.556100 2.079380 -3.659919
H -5.455723 -1.065888 -2.620115
H -5.343543 0.662608 -2.298888
H -4.843500 0.232357 -4.693647
H -3.594600 -0.929362 -4.252037
Cl 1.533846 -3.264355 -0.082858
C -1.377986 -2.759376 0.023370
C -1.772715 -3.445430 -1.130840
C -1.929237 -3.120190 1.256238
C -2.742049 -4.450854 -1.054363
H -1.317233 -3.214270 -2.089092
C -2.898518 -4.129181 1.328538
H -1.591642 -2.641412 2.170928
C -3.313856 -4.791767 0.173615
H -3.039957 -4.975790 -1.959434
H -3.316406 -4.401150 2.295495
H -4.063207 -5.577109 0.230622



Complex **10b**
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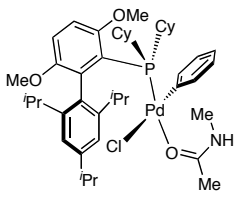
C -5.056570 -0.019721 -1.005187
C -4.499177 1.210230 -0.649005
C -3.377751 1.309600 0.181588
C -2.762884 0.125188 0.662739
C -3.333008 -1.135188 0.342762
H -4.892544 -2.134276 -0.744416
H -4.961390 2.123553 -1.013673
C -1.618982 0.202397 1.653011
C -0.227221 0.244859 1.369501
C -2.043781 0.216147 3.012021
C 0.675985 0.242656 2.476754
C -1.135725 0.188915 4.063339
C 0.228422 0.189529 3.792095
H -1.470168 0.176672 5.093599
H 0.935343 0.182721 4.612994
P 0.683583 0.426693 -0.283769
C -2.814117 -2.458461 0.917896
H -1.766713 -2.318113 1.204220
C -6.283174 -0.111451 -1.903552
H -6.511799 -1.178764 -2.027944
C -6.015801 0.468823 -3.305582
H -5.793558 1.541643 -3.256643
H -5.164156 -0.027285 -3.784349
H -6.892631 0.340115 -3.951681
C -7.515966 0.551758 -1.259576
H -8.400296 0.425319 -1.895814
H -7.734523 0.113602 -0.279568
H -7.359751 1.627725 -1.116904
C -2.901234 2.705356 0.586853
H -1.906904 2.606457 1.033510
C -2.781769 3.678123 -0.602363
H -2.311692 4.614373 -0.278405
H -2.180635 3.260105 -1.417192
H -3.762740 3.937797 -1.016166
C -3.827924 3.308023 1.664317
H -3.447296 4.280120 2.001860
H -4.837747 3.462390 1.264599
H -3.908458 2.643689 2.528375
C -2.864854 -3.636902 -0.075207
H -2.302661 -4.482313 0.333850
H -3.892921 -3.977950 -0.247403
H -2.426457 -3.388608 -1.044494
C -3.598718 -2.860481 2.186746
H -4.654990 -3.032894 1.944536
H -3.193195 -3.791195 2.602125
H -3.556409 -2.087803 2.955193
O -3.402374 0.262183 3.212351
O 2.004521 0.337454 2.181882
C -3.889862 0.293897 4.543124
H -3.524856 1.175152 5.087561
H -4.976786 0.346606 4.458483
H -3.614955 -0.612878 5.098656
C 2.980221 0.034355 3.172384
H 2.761385 -0.920164 3.664504
H 3.921783 -0.050841 2.629466
H 3.043154 0.832603 3.923975
Pd 2.734903 -0.876403 -0.260692
C 1.784699 -2.630053 -0.084067
C 1.170145 -3.013439 1.111355
C 1.878871 -3.563112 -1.126201
C 0.649281 -4.306650 1.260756
H 1.099368 -2.320834 1.943423
C 1.347562 -4.846832 -0.980077
H 2.388894 -3.300181 -2.047950
C 0.731429 -5.226446 0.215616
H 0.185846 -4.590254 2.203712
H 1.433395 -5.558003 -1.798962
H 0.331675 -6.230648 0.333294
C -0.535767 0.106631 -1.704797
C -0.224240 0.904807 -2.991680

C -0.601648 -1.392719 -2.048414
H -1.516356 0.432586 -1.350267
C -1.263836 0.613890 -4.090482
H 0.774434 0.635409 -3.364385
H -0.217993 1.981410 -2.799699
C -1.635951 -1.690340 -3.146216
H 0.387107 -1.718402 -2.390142
H -0.815104 -1.984228 -1.155968
C -1.352437 -0.881065 -4.417337
H -1.010530 1.191931 -4.988988
H -2.248314 0.970945 -3.754142
H -1.628759 -2.765271 -3.368726
H -2.642343 -1.449849 -2.776918
H -2.128052 -1.061541 -5.173010
H -0.400658 -1.213846 -4.857254
C 0.887566 2.333054 -0.365412
C 1.153209 3.054867 0.973824
C 1.955654 2.790907 -1.384856
H -0.097545 2.666326 -0.720421
C 1.122424 4.584266 0.791342
H 2.131470 2.747958 1.359849
H 0.411726 2.773303 1.727163
C 1.899989 4.313575 -1.597888
H 2.935372 2.513581 -0.991861
H 1.851018 2.278180 -2.343567
C 2.113992 5.064255 -0.276614
H 1.333270 5.069273 1.753666
H 0.106235 4.893500 0.504827
H 2.659949 4.610853 -2.332538
H 0.925873 4.595102 -2.025825
H 2.019524 6.147655 -0.426773
H 3.140304 4.883084 0.075303
Cl 4.772445 -2.168314 0.003570
O 4.197331 0.923006 -0.285814
C 5.245861 0.930135 -0.956876
N 6.379419 1.489179 -0.474720
C 5.324033 0.346002 -2.347078
H 5.337726 -0.744142 -2.243298
H 4.423218 0.623226 -2.901152
H 6.209566 0.675813 -2.900119
C 6.521825 1.951643 0.896623
H 7.046577 1.211882 1.512848
H 7.073176 2.896980 0.919072
H 5.522864 2.104756 1.304345
H 7.216542 1.395020 -1.031854



Complex **10g**
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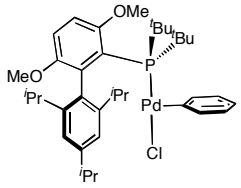
C 3.998278 1.353910 -0.169523
C 3.297658 2.000467 0.848970
C 1.923229 2.248785 0.766252
C 1.208840 1.830339 -0.392086
C 1.909810 1.214372 -1.459245
H 3.821501 0.483464 -2.107994
H 3.834041 2.328114 1.735912
C -0.212542 2.336796 -0.528683
C -1.419791 1.704150 -0.123945
C -0.259581 3.693307 -0.969113
C -2.589141 2.519607 -0.039942
C -1.437809 4.425897 -0.959115
C -2.598792 3.843214 -0.464249
H -1.463318 5.455317 -1.295228
H -3.505331 4.433150 -0.419238
P -1.678845 -0.157719 0.194956
C 1.249573 0.856802 -2.795249
H 0.228106 0.523714 -2.587439
C 5.493750 1.084118 -0.066552
H 5.783463 0.533330 -0.972191
C 5.840013 0.195713 1.143470
H 5.610222 0.703721 2.088030
H 5.271754 -0.740498 1.124229
H 6.909542 -0.048464 1.151058
C 6.309144 2.391230 -0.042385
H 7.385151 2.178392 -0.023256
H 6.097346 3.005422 -0.924602
H 6.071942 2.989732 0.845402
C 1.279800 3.036151 1.915243
H 0.194811 3.014255 1.780804
C 1.576273 2.439789 3.305498
H 1.008277 2.980791 4.072409
H 1.307174 1.382291 3.363132
H 2.637141 2.529356 3.567624
C 1.719528 4.515741 1.889658
H 1.203165 5.083078 2.674217
H 2.798033 4.603358 2.069508
H 1.505669 4.980273 0.924397
C 1.946906 -0.299482 -3.533806
H 1.312545 -0.635435 -4.358487
H 2.910226 0.014606 -3.957434
H 2.106708 -1.158787 -2.878185
C 1.170187 2.068802 -3.750132
H 2.171484 2.471718 -3.948480
H 0.736933 1.754365 -4.707450
H 0.557176 2.877699 -3.350099
O 0.935433 4.235129 -1.368192
O -3.715039 1.943394 0.486559
C 0.938904 5.540121 -1.919095
H 0.628471 6.294727 -1.183191
H 1.971713 5.732621 -2.214814
H 0.289937 5.608869 -2.802530
C -4.877474 2.735458 0.665907
H -5.282179 3.086780 -0.292062
H -5.609783 2.083534 1.145677
H -4.678072 3.597600 1.315075
Pd 0.021028 -1.716143 -0.357872

C 0.797687 -1.916399 1.493602
C 1.777113 -1.067932 2.014214
C 0.540503 -3.126618 2.159547
C 2.476205 -1.411907 3.179842
H 2.014132 -0.140672 1.509933
C 1.235506 -3.469579 3.324577
H -0.205003 -3.817793 1.772561
C 2.206019 -2.609298 3.842921
H 3.237248 -0.735437 3.563263
H 1.016504 -4.411504 3.823810
H 2.747241 -2.872970 4.748257
O 1.700571 -3.068474 -0.895357
C 1.688976 -4.236611 -1.324637
N 2.806088 -4.780913 -1.857574
H 2.753626 -5.734985 -2.182594
C 0.462985 -5.113198 -1.277308
H 0.117631 -5.181197 -0.241350
H -0.318816 -4.618265 -1.863189
H 0.641513 -6.121716 -1.663102
C 4.066070 -4.069063 -2.002398
H 4.837367 -4.499300 -1.352728
H 4.409487 -4.108323 -3.041482
H 3.899442 -3.030760 -1.716804
Cl -0.773493 -2.171194 -2.709219
C -2.406816 -0.259329 1.937199
C -2.584374 -1.707679 2.435417
C -1.630646 0.561548 2.983551
H -3.397844 0.189137 1.834674
C -3.341648 -1.725988 3.775197
H -1.601806 -2.159853 2.579592
H -3.108978 -2.325391 1.698101
C -2.356115 0.539228 4.341217
H -0.623906 0.143552 3.099603
H -1.513671 1.597686 2.647498
C -2.606738 -0.893032 4.835794
H -3.457476 -2.762098 4.118802
H -4.357806 -1.327360 3.632807
H -1.770674 1.100752 5.080798
H -3.319611 1.062103 4.242433
H -3.176950 -0.876950 5.773883
H -1.642461 -1.371301 5.060134
C -3.121004 -0.665260 -0.976024
C -4.534029 -0.865252 -0.386899
C -3.190848 0.187660 -2.261373
H -2.762156 -1.648164 -1.293016
C -5.446223 -1.540649 -1.430472
H -4.970679 0.095466 -0.102429
H -4.511341 -1.485508 0.513765
C -4.116582 -0.472261 -3.297988
H -3.566662 1.190915 -2.026920
H -2.193396 0.297543 -2.694630
C -5.519256 -0.729556 -2.731210
H -6.449830 -1.674434 -1.004267
H -5.061728 -2.546823 -1.651004
H -4.177504 0.164740 -4.190400
H -3.662623 -1.419521 -3.615648
H -6.141941 -1.250868 -3.470175
H -6.015011 0.232443 -2.527684



Complex **11a**
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C 3.725966 -1.006035 -0.257887
C 3.177017 -0.736582 1.000006
C 2.080107 0.102621 1.174470
C 1.464352 0.703518 0.028585
C 2.032953 0.453356 -1.256782
H 3.543856 -0.609648 -2.347628
H 3.628993 -1.190335 1.877183
C 0.618117 1.950147 0.210314
C -0.793185 2.062637 0.154049
C 1.399177 3.127240 0.400933
C -1.364780 3.364051 0.234940
C 0.802356 4.372233 0.552819
C -0.581402 4.490379 0.461501
H 1.397353 5.262721 0.716183
H -1.030243 5.472136 0.546809
P -1.866340 0.524323 -0.043382
C 1.560339 1.161732 -2.525024
H 0.690714 1.772513 -2.267560
C 4.956904 -1.886070 -0.418239
H 5.072230 -2.081373 -1.492708
C 4.813307 -3.247403 0.285364
H 4.770597 -3.133292 1.375486
H 3.901107 -3.757574 -0.036268
H 5.676939 -3.883503 0.056273
C 6.224202 -1.146694 0.058274
H 7.115131 -1.766642 -0.099458
H 6.364020 -0.203475 -0.482255
H 6.164134 -0.913270 1.128533
C 1.632982 0.408674 2.603078
H 0.698774 0.973544 2.547294
C 1.364227 -0.869638 3.420923
H 0.892001 -0.616546 4.377924
H 0.711612 -1.562016 2.882132
H 2.293589 -1.404306 3.646714
C 2.657248 1.294074 3.344282
H 2.297162 1.529573 4.353500
H 3.619484 0.778115 3.444460
H 2.835442 2.231289 2.811479
C 1.132060 0.166230 -3.620783
H 0.717579 0.703143 -4.483248
H 1.980365 -0.427936 -3.977448
H 0.381131 -0.538211 -3.248215
C 2.638358 2.125822 -3.063080
H 3.531020 1.580048 -3.389674

H 2.254291 2.683542 -3.926084
H 2.947448 2.843318 -2.296696
O 2.757538 2.953521 0.414816
O -2.714461 3.461801 0.040212
C 3.587662 4.092097 0.573308
H 3.417248 4.587680 1.538606
H 4.611778 3.717188 0.537857
H 3.437814 4.817816 -0.237218
C -3.346798 4.720344 0.207455
H -2.986129 5.454193 -0.524544
H -4.411308 4.544056 0.042305
H -3.198550 5.114012 1.221146
Pd -0.302342 -1.317461 -0.316670
Cl 1.168232 -3.083815 -0.934403
C -1.543373 -2.882694 0.018764
C -2.254800 -3.531706 -0.994226
C -1.577505 -3.408098 1.315947
C -3.048990 -4.644962 -0.696704
H -2.180359 -3.198497 -2.022374
C -2.370886 -4.523272 1.609134
H -0.981503 -2.967438 2.108746
C -3.120271 -5.139161 0.606378
H -3.599831 -5.133963 -1.497294
H -2.389983 -4.911688 2.625063
H -3.735168 -6.006301 0.833135
C -2.976543 0.390544 1.546796
C -2.974327 0.784565 -1.639024
C -3.966175 -0.780747 1.360343
H -4.456466 -0.971085 2.324091
H -4.754817 -0.550701 0.640355
H -3.473383 -1.702495 1.054005
C -2.017110 0.044543 2.701192
H -1.419468 -0.841996 2.486301
H -1.341470 0.876338 2.922583
H -2.605245 -0.153631 3.606976
C -3.775960 1.634102 1.983309
H -3.125636 2.472041 2.243908
H -4.494806 1.969403 1.235184
H -4.339334 1.361352 2.886338
C -2.220644 1.684703 -2.636393
H -1.233331 1.288469 -2.880126
H -2.794596 1.721770 -3.571912
H -2.110555 2.708541 -2.272935
C -4.382270 1.374238 -1.421575
H -4.869770 1.445307 -2.403289
H -5.016345 0.738026 -0.800874
H -4.353890 2.372755 -0.991355
C -3.145587 -0.601795 -2.287364
H -3.670500 -1.304491 -1.635335
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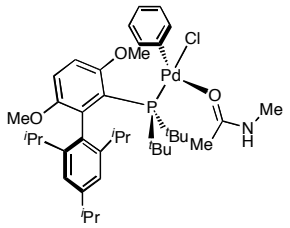

Complex **11b**
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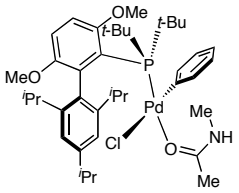
C 3.750228 -1.166037 -0.052308
C 2.880287 -0.090978 0.273696
C 3.187925 1.210649 -0.214539
H 4.495273 2.362383 -1.468631
H 5.457343 -1.780833 -1.192503
C 1.801439 -0.225303 1.337780
C 0.386260 -0.380630 1.190396
C 2.341057 -0.056270 2.648597
C -0.404260 -0.243802 2.380268
C 1.541018 -0.020299 3.782027
C 0.163080 -0.094905 3.641170
H 1.968263 0.092223 4.770818
H -0.463979 -0.030260 4.521342
P -0.760762 -0.838305 -0.292386
C 2.421051 2.469036 0.213989
H 1.409439 2.173490 0.507170
C 6.254720 0.534146 -2.432988
H 6.263721 1.603231 -2.686060
C 6.071006 -0.248937 -3.747015
H 6.064860 -1.330670 -3.567067
H 5.125725 0.013323 -4.234744
H 6.888047 -0.031454 -4.445627
C 7.610408 0.204892 -1.779162
H 8.435693 0.426988 -2.466497
H 7.760953 0.789119 -0.864666
H 7.676948 -0.856517 -1.512069
C 3.654278 -2.556561 0.581505
H 2.707598 -2.614208 1.122462
C 3.689258 -3.705947 -0.447691
H 3.462304 -4.658621 0.045383
H 2.971688 -3.565627 -1.260700
H 4.682323 -3.806998 -0.900793
C 4.784853 -2.779484 1.609855
H 4.673583 -3.759725 2.090325
H 5.766277 -2.756716 1.120851
H 4.774337 -2.007975 2.381257
C 2.281003 3.527931 -0.898500
H 1.556126 4.285573 -0.586296
H 3.230360 4.040945 -1.094763
H 1.927306 3.099968 -1.840532
C 3.083480 3.135787 1.440019
H 4.101493 3.464366 1.196374
H 2.506549 4.018121 1.742223

H 3.147180 2.458152 2.293025
O 3.705152 0.089743 2.721975
O -1.760371 -0.260683 2.231067
C 4.293764 0.344360 3.985990
H 4.139823 -0.489710 4.684056
H 5.362309 0.459954 3.795647
H 3.903725 1.267484 4.435199
C -2.612149 -0.086047 3.351654
H -2.407471 0.860774 3.866514
H -3.622212 -0.058082 2.941439
H -2.517344 -0.918517 4.061772
Pd -2.875018 0.399596 -0.321118
C -2.036188 2.213935 -0.219324
C -1.510881 2.741606 0.963871
C -2.144418 3.049526 -1.341433
C -1.102473 4.080463 1.026338
H -1.434110 2.125141 1.850827
C -1.728303 4.382547 -1.279073
H -2.581732 2.675337 -2.262400
C -1.209707 4.906774 -0.092649
H -0.708610 4.475067 1.960967
H -1.828658 5.015463 -2.158161
H -0.902375 5.948337 -0.039752
Cl -5.005366 1.556281 -0.179304
O -4.230778 -1.504599 -0.581079
C -5.338681 -1.421116 -1.146997
N -6.478645 -1.686320 -0.480068
C -5.473774 -1.038009 -2.602604
H -5.353454 0.048901 -2.664119
H -4.674365 -1.509057 -3.179823
H -6.442943 -1.315738 -3.029230
C -6.502202 -1.811722 0.972156
H -6.222114 -0.861043 1.439209
H -7.510239 -2.096188 1.282085
H -5.799453 -2.586352 1.287118
H -7.349015 -1.479896 -0.949420
C -1.066454 -2.749835 0.072235
C -0.012960 -0.670354 -2.075349
C -1.728000 -3.439968 -1.139897
H -1.963114 -4.473281 -0.851891
H -2.663484 -2.952416 -1.417675
H -1.071076 -3.496920 -2.009960
C 0.241312 -3.482401 0.407910
H 0.985277 -3.407683 -0.384277
H 0.681051 -3.108946 1.335795
H 0.020253 -4.548762 0.554032
C -2.017603 -2.943384 1.274327
H -1.555343 -2.640315 2.215370
H -2.960328 -2.412391 1.143925
H -2.235835 -4.017584 1.351276
C -1.208380 -0.795437 -3.054069
H -1.978864 -0.049610 -2.833602
H -0.830915 -0.609273 -4.068158
H -1.678060 -1.778732 -3.051929
C 0.541083 0.752377 -2.253221
H 1.475397 0.883752 -1.715862
H 0.750896 0.909772 -3.320165
H -0.167167 1.519281 -1.935277
C 1.082029 -1.672143 -2.477752
H 1.402097 -1.441222 -3.502868
H 1.962258 -1.588682 -1.839552
H 0.737758 -2.709219 -2.476103



Complex **11g**
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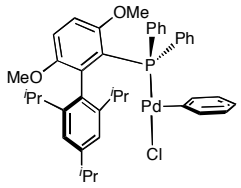
C 1.976332 3.382993 -0.052903
C 0.947445 3.473029 0.884606
C -0.244456 2.753043 0.752544
C -0.417598 1.889571 -0.369517
C 0.593567 1.823697 -1.358824
H 2.558998 2.494011 -1.900717
H 1.068629 4.126624 1.744788
C -1.827117 1.352378 -0.533141
C -2.396960 0.169951 0.035844
C -2.694085 2.346643 -1.075771
C -3.803500 0.207224 0.276466
C -4.075537 2.237532 -0.996920
C -4.624847 1.191184 -0.268332
H -4.728602 2.988425 -1.424576
H -5.697359 1.156532 -0.127996
P -1.513002 -1.543458 0.152366
C 0.437475 1.034241 -2.662094
H -0.110597 0.118599 -2.427903
C 3.271227 4.170057 0.100261
H 3.920102 3.886580 -0.739970
C 4.016828 3.812085 1.399721
H 3.441986 4.113932 2.283712
H 4.193002 2.733428 1.472180
H 4.985199 4.325619 1.444176
C 3.030638 5.689068 0.003874
H 3.978938 6.237451 0.063028
H 2.541223 5.952909 -0.940190
H 2.390265 6.041584 0.821464
C -1.331129 3.001310 1.809397
H -2.166406 2.324859 1.617849
C -0.859074 2.716362 3.248512
H -1.688248 2.869118 3.950415
H -0.503433 1.688508 3.360863
H -0.047045 3.387290 3.553381
C -1.877051 4.441402 1.708786
H -2.711165 4.585220 2.406910
H -1.102899 5.176518 1.959603
H -2.229047 4.663334 0.697368
C 1.776375 0.601963 -3.285945
H 1.586244 -0.124430 -4.080645

H 2.307686 1.454571 -3.730146
H 2.425144 0.117763 -2.552289
C -0.372489 1.805345 -3.727422
H 0.103930 2.767135 -3.955781
H -0.410997 1.218825 -4.653312
H -1.395879 2.006862 -3.408650
O -2.081113 3.445857 -1.620740
O -4.325264 -0.758328 1.090111
C -2.883427 4.428660 -2.250601
H -3.564069 4.916628 -1.539443
H -2.185985 5.169728 -2.644980
H -3.468764 4.006043 -3.078378
C -5.716469 -0.743143 1.366706
H -6.313124 -0.905825 0.459855
H -5.893463 -1.565839 2.061913
H -6.019365 0.199160 1.839794
Pd 0.941629 -1.643047 -0.216452
C 1.555349 -1.112076 1.646166
C 1.588735 0.200843 2.114191
C 2.260355 -2.089748 2.370247
C 2.281141 0.529182 3.288782
H 1.090735 0.983932 1.563016
C 2.949532 -1.765500 3.542818
H 2.289537 -3.120225 2.025192
C 2.959161 -0.450674 4.012398
H 2.287204 1.562303 3.628880
H 3.481225 -2.545329 4.084520
H 3.493252 -0.195013 4.924161
Cl 1.055297 -2.710377 -2.513647
O 3.134580 -1.458418 -0.561553
C 4.013512 -2.299357 -0.827059
N 5.237531 -1.879159 -1.213849
C 3.800846 -3.788290 -0.723707
H 3.514341 -4.037398 0.302356
H 2.966014 -4.048941 -1.382036
H 4.690708 -4.365113 -0.993990
C 5.559000 -0.471196 -1.402271
H 5.197622 0.104004 -0.546942
H 6.643682 -0.366237 -1.478616
H 5.090625 -0.072276 -2.309031
H 5.916592 -2.574292 -1.484420
C -2.457074 -2.479808 -1.294362
C -1.873321 -2.488393 1.838301
C -1.910709 -3.922570 -1.368281
H -2.301302 -4.389691 -2.281877
H -0.822505 -3.953722 -1.432012
H -2.251679 -4.530439 -0.524291
C -3.995471 -2.571926 -1.176758
H -4.346315 -3.046387 -0.262291
H -4.477398 -1.597993 -1.283431
H -4.336675 -3.187799 -2.019419
C -2.179073 -1.733755 -2.615756
H -2.563663 -0.709184 -2.585572
H -1.120571 -1.726833 -2.870218
H -2.708048 -2.260308 -3.421601
C -0.768960 -3.558078 1.993187
H 0.219710 -3.121447 2.054710
H -0.950572 -4.106320 2.927508
H -0.781107 -4.284992 1.175941
C -1.758817 -1.449821 2.970501
H -2.590361 -0.739701 2.943560
H -1.787715 -1.969337 3.937854
H -0.817283 -0.896639 2.923189
C -3.191015 -3.276483 1.997321
H -3.188193 -3.706808 3.007750
H -4.080077 -2.666967 1.900842
H -3.256157 -4.115034 1.299237



Complex **12a**
C 3.327635 -0.693686 -1.388976
C 4.001258 -1.108418 -0.238669
C 3.542534 -0.632242 0.991103
C 2.459497 0.241906 1.098261
C 1.800743 0.681581 -0.089424
C 2.254373 0.198501 -1.351867
H 3.661281 -1.073909 -2.351397
H 4.037741 -0.958327 1.900303
C 0.948354 1.931989 -0.040394
C -0.457599 1.976121 0.021555
C 1.663412 3.159676 -0.074605
C -1.127940 3.227133 0.070378
C 0.990861 4.377117 -0.015375
C -0.402158 4.414090 0.059992
H 1.537355 5.312697 -0.030914
H -0.902688 5.374094 0.100972
P -1.417559 0.398638 0.046219
C 1.650777 0.675827 -2.671732
H 0.830515 1.362210 -2.439407
C 5.221667 -2.011805 -0.348483
H 5.203926 -2.448308 -1.356186
C 5.213743 -3.176053 0.656937
H 5.328795 -2.819945 1.688041
H 4.277481 -3.737544 0.595979
H 6.050804 -3.854309 0.451977
C 6.517922 -1.183446 -0.225377
H 7.399486 -1.822510 -0.358027
H 6.557185 -0.386534 -0.976896
H 6.588750 -0.714449 0.763875
C 2.056936 0.744013 2.484657
H 1.119523 1.301173 2.379542
C 1.802426 -0.414847 3.469465
H 1.384427 -0.029796 4.408060
H 1.112823 -1.155017 3.050252
H 2.729286 -0.943915 3.717508

C 3.106466 1.715346 3.062618
H 2.772442 2.110437 4.029921
H 4.063805 1.205085 3.221902
H 3.286150 2.556588 2.387291
C 1.056708 -0.484819 -3.492132
H 0.582250 -0.102936 -4.404315
H 1.828651 -1.203059 -3.790302
H 0.303289 -1.029055 -2.912987
C 2.679609 1.470035 -3.501811
H 3.515329 0.833502 -3.814931
H 2.211366 1.873796 -4.407902
H 3.092926 2.303605 -2.924464
O 3.025224 3.059469 -0.170439
O -2.489431 3.181971 0.107910
C 3.792050 4.251686 -0.214344
H 3.666445 4.847528 0.699639
H 4.832016 3.931411 -0.295096
H 3.532869 4.867408 -1.086067
C -3.216019 4.395830 0.202085
H -3.056103 5.029380 -0.680101
H -4.267125 4.108194 0.255137
H -2.947107 4.955983 1.106822
C -2.508595 0.522675 1.533529
C -3.857575 0.899806 1.477462
C -1.941913 0.216739 2.780110
C -4.620170 0.970224 2.644105
H -4.312573 1.138958 0.523131
C -2.701187 0.303595 3.947998
H -0.907184 -0.106245 2.836957
C -4.044179 0.677851 3.882214
H -4.640560 0.734509 4.788942
C -2.533802 0.467015 -1.418036
C -3.589398 -0.454710 -1.526534
C -2.297478 1.352575 -2.480043
C -4.396591 -0.471840 -2.664827
H -3.782308 -1.162969 -0.728154
C -3.100985 1.324931 -3.620527
H -1.487332 2.071619 -2.418421
C -4.155072 0.414993 -3.715407
H -4.781370 0.394395 -4.603278
Pd 0.034583 -1.413582 0.086981
C -1.521751 -2.684304 0.018499
C -2.307159 -2.953725 1.141048
C -1.789853 -3.331875 -1.192177
C -3.377990 -3.852398 1.043848
H -2.102681 -2.470676 2.090718
C -2.859845 -4.227414 -1.281407
H -1.163928 -3.155764 -2.060958
C -3.660374 -4.487096 -0.166287
H -3.986475 -4.053820 1.922756
H -3.059225 -4.728388 -2.226124
H -4.490164 -5.185755 -0.238022
H -2.902636 2.018651 -4.433370
H -5.209537 -1.189696 -2.730272
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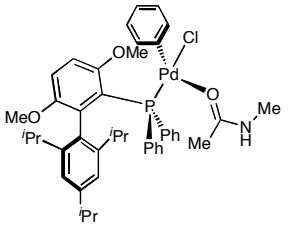
H -2.244996 0.064514 4.904799
Cl 1.416143 -3.344761 0.203532



Complex **12b**
C 4.155010 0.937469 -1.139847
C 4.856167 -0.266995 -1.212658
C 4.455202 -1.303497 -0.367039
C 3.387470 -1.166093 0.526952
C 2.675498 0.059318 0.563619
C 3.081370 1.134489 -0.263682
H 4.464792 1.755553 -1.784135
H 5.001035 -2.243692 -0.388370
C 1.593834 0.243628 1.599937
C 0.214218 -0.008440 1.418552
C 2.045045 0.650588 2.885637
C -0.656847 0.105187 2.541685
C 1.163803 0.805928 3.951495
C -0.189744 0.524066 3.782303
H 1.515967 1.126130 4.924639
H -0.866321 0.619528 4.623453
P -0.732010 -0.404435 -0.147018
C 2.430478 2.516167 -0.182267
H 1.409743 2.389857 0.192070
C 6.040124 -0.419697 -2.159616
H 6.121029 0.517923 -2.726420
C 5.831953 -1.554713 -3.179258
H 5.757539 -2.529766 -2.682667
H 4.913380 -1.400603 -3.755559
H 6.673075 -1.603463 -3.881479
C 7.362153 -0.606459 -1.389813
H 8.211240 -0.656465 -2.082530
H 7.535344 0.223197 -0.695668
H 7.353318 -1.534099 -0.804955
C 3.094683 -2.323818 1.486775
H 2.178044 -2.087565 2.036042
C 2.861547 -3.670725 0.776336
H 2.658686 -4.455150 1.515571
H 2.004266 -3.632923 0.097304
H 3.738526 -3.984853 0.198812
C 4.227577 -2.465932 2.525942
H 3.975009 -3.232842 3.268962
H 5.167147 -2.763912 2.044896
H 4.402921 -1.519977 3.045474
C 2.329083 3.243175 -1.535734
H 1.683482 4.121126 -1.429590
H 3.308465 3.594956 -1.883401
H 1.903944 2.601443 -2.311513

C 3.179764 3.420931 0.820480
H 4.199340 3.621406 0.467388
H 2.660497 4.381570 0.920974
H 3.255158 2.958336 1.806763
O 3.395320 0.863417 3.003415
O -1.953072 -0.254847 2.326875
C 3.905412 1.297754 4.252852
H 3.725875 0.557144 5.043935
H 4.980634 1.416500 4.108052
H 3.472452 2.260870 4.554525
C -2.958845 0.106420 3.266555
H -2.921086 1.177867 3.493562
H -3.904579 -0.125971 2.777299
H -2.860399 -0.474778 4.192876
C 0.286957 -0.353031 -1.687698
C 1.165144 -1.387507 -2.051132
C 0.017726 0.658838 -2.621191
C 1.766762 -1.400349 -3.307447
H 1.370118 -2.195009 -1.360347
C 0.622716 0.645283 -3.881017
H -0.668664 1.456275 -2.363610
C 1.497097 -0.383758 -4.227666
H 1.959633 -0.400972 -5.211164
C -1.067498 -2.224442 -0.015930
C -1.585745 -2.887714 -1.141009
C -0.869833 -2.957944 1.159975
C -1.890446 -4.246557 -1.092202
H -1.746493 -2.339995 -2.064867
C -1.180266 -4.320139 1.211455
H -0.466951 -2.473671 2.041882
C -1.690876 -4.969369 0.087569
H -1.925473 -6.029920 0.126399
Pd -2.788507 0.803422 -0.302626
C -1.918167 2.608736 -0.337991
C -1.315282 3.157110 0.799826
C -2.037097 3.407249 -1.485783
C -0.830757 4.471881 0.788332
H -1.226142 2.575522 1.711785
C -1.543190 4.715081 -1.499494
H -2.548443 3.024327 -2.364356
C -0.937308 5.254346 -0.361989
H -0.374096 4.881531 1.687026
H -1.652174 5.319106 -2.397754
H -0.566179 6.276226 -0.368627
H -1.012923 -4.872639 2.132475
H -2.283331 -4.741859 -1.976425
H 2.441304 -2.210655 -3.569266
H 0.399228 1.437969 -4.589985
O -3.963661 -1.133852 -0.147343
C -4.887559 -1.542710 -0.871371
N -5.683597 -2.546371 -0.439318
H -6.464535 -2.821977 -1.015205
C -5.171208 -0.981790 -2.242963
H -5.450949 0.070394 -2.123013
H -4.251426 -1.011009 -2.835545
H -5.959453 -1.524710 -2.774099
C -5.541697 -3.133359 0.885585
H -5.796075 -2.410098 1.668570
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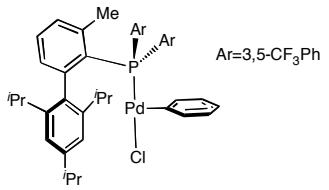
H -4.511073 -3.463276 1.040088
Cl -4.906556 1.951435 -0.350883



Complex **13a**
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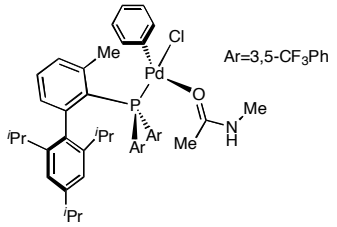
C 3.586922 0.825468 -0.701521
C 2.827363 -0.361562 -0.941698
C 3.251900 -1.589625 -0.349404
H 4.709186 -2.526182 0.914429
H 5.300030 1.655949 0.272512
C 1.916329 -0.408591 -2.152597
C 0.504730 -0.277863 -2.171336
C 2.592718 -0.621549 -3.366657
C -0.201030 -0.348775 -3.405257
C 1.906798 -0.697231 -4.572102
C 0.522085 -0.560704 -4.584080
H 2.447576 -0.865578 -5.499313
H -0.017883 -0.620607 -5.525262
P -0.314627 -0.023079 -0.533861
C 2.532959 -2.909567 -0.620166
H 1.652886 -2.689244 -1.231417
C 6.443005 -0.528477 1.491937
H 6.414994 -1.483754 2.032846
C 6.572076 0.590581 2.539667
H 6.704531 1.572134 2.068570
H 5.682748 0.637348 3.174241
H 7.450139 0.412212 3.171568
C 7.672089 -0.559312 0.559073
H 8.594585 -0.673613 1.140762
H 7.613466 -1.389070 -0.154604
H 7.750637 0.371928 -0.015474
C 3.215622 2.167580 -1.333661
H 2.233509 2.056869 -1.807347
C 3.101372 3.293438 -0.285665
H 2.668506 4.191836 -0.740361
H 2.475832 2.992307 0.561904
H 4.081111 3.567058 0.121502
C 4.208168 2.565864 -2.444843
H 3.915670 3.522844 -2.893033
H 5.222045 2.679075 -2.043768
H 4.242925 1.815260 -3.241514
C 2.030529 -3.582211 0.671532
H 1.410731 -4.452036 0.424928

H 2.860580 -3.925035 1.299477
H 1.432171 -2.886089 1.269219
C 3.412549 -3.875972 -1.438256
H 4.317255 -4.153799 -0.885652
H 2.859988 -4.796353 -1.661391
H 3.723983 -3.427683 -2.388376
C -1.374396 1.483917 -0.705248
C -2.759350 1.483603 -0.907215
C -0.715795 2.712442 -0.577143
C -3.462144 2.688265 -0.989301
C -1.419751 3.913325 -0.667506
H 0.350547 2.731261 -0.378275
C -2.798173 3.909725 -0.873036
C -1.471583 -1.443570 -0.311331
C -2.466611 -1.398314 0.679854
C -1.270831 -2.641243 -1.008360
C -3.241505 -2.526778 0.951122
H -2.636752 -0.494257 1.251249
C -2.038755 -3.771002 -0.717710
H -0.519572 -2.700859 -1.787731
C -3.029145 -3.721115 0.260550
H -3.633164 -4.594443 0.475885
Pd 1.253626 0.157125 1.164088
C -0.190832 0.540424 2.516908
C -0.624796 1.847073 2.752110
C -0.725316 -0.518431 3.256375
C -1.620283 2.085932 3.707439
H -0.195909 2.686099 2.213116
C -1.723409 -0.272075 4.206652
H -0.365687 -1.532036 3.107054
C -2.175968 1.029411 4.430839
H -1.953609 3.105605 3.886095
H -2.144598 -1.103369 4.765571
H -2.949564 1.219762 5.169905
Cl 2.748801 0.345055 2.986429
C -4.268045 -2.480368 2.056528
C -1.735270 -5.059085 -1.438941
F -0.636896 -5.661008 -0.923341
F -1.483101 -4.844820 -2.748784
F -2.750917 -5.940077 -1.353393
F -3.728386 -2.847326 3.240856
F -4.778348 -1.243639 2.214363
F -5.294191 -3.323708 1.812387
H -3.346637 4.841392 -0.937395
H -3.303482 0.551859 -1.008203
C -4.960403 2.651605 -1.160995
C -0.655182 5.201631 -0.499479
F -5.586923 2.434880 0.014331
F -5.435773 3.809219 -1.663809
F -5.333204 1.656329 -1.996763
F -1.454970 6.282996 -0.565402
F 0.294645 5.337278 -1.454369
F -0.016550 5.232269 0.691185
H 3.672407 -0.732107 -3.346359
C -1.700028 -0.193990 -3.537228
H -2.252464 -0.750466 -2.776650
H -2.003281 0.856117 -3.459629
H -2.030095 -0.557775 -4.514471



Complex **13b**
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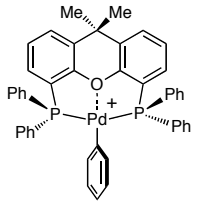
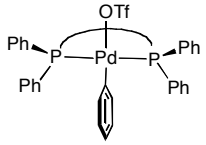
C -4.191534 -1.929049 -0.644878
C -3.023333 -1.705762 -1.382082
C -2.635150 -0.370699 -1.668251
C -3.454725 0.705900 -1.249392
H -5.245757 1.241730 -0.191193
H -4.483966 -2.952809 -0.428643
C -1.478579 -0.132130 -2.611226
C -0.114538 0.098017 -2.282698
C -1.838427 -0.211960 -3.969283
C 0.853477 0.191536 -3.331981
C -0.903823 -0.103326 -4.989174
C 0.433661 0.080479 -4.662586
H -1.212818 -0.174910 -6.028320
H 1.178725 0.147038 -5.450528
P 0.592128 0.341732 -0.576179
C -3.154907 2.154262 -1.640600
H -2.073980 2.252683 -1.787358
C -6.303737 -1.142276 0.551130
H -6.735065 -0.161629 0.794607
C -6.077811 -1.889477 1.877984
H -5.638364 -2.879545 1.711840
H -5.403375 -1.338216 2.539898
H -7.029592 -2.030282 2.404178
C -7.326051 -1.886020 -0.330998
H -8.279914 -2.001294 0.197584
H -7.515390 -1.342712 -1.263344
H -6.968469 -2.888569 -0.594797
C -2.257026 -2.917596 -1.921849
H -1.273258 -2.572754 -2.254393
C -2.026051 -4.029580 -0.879949
H -1.313794 -4.764331 -1.269716
H -1.628178 -3.643835 0.062833
H -2.953693 -4.563283 -0.644365
C -2.968225 -3.513084 -3.156063
H -2.408575 -4.373312 -3.542856
H -3.976395 -3.855641 -2.894353
H -3.061927 -2.779781 -3.962778
C -3.567230 3.187990 -0.577580
H -3.147697 4.164839 -0.837687
H -4.656766 3.303045 -0.524116

H -3.211347 2.926170 0.421336
C -3.832764 2.518467 -2.980179
H -4.922935 2.428364 -2.898090
H -3.596600 3.554561 -3.249877
H -3.500837 1.874544 -3.799225
C -0.652052 0.368010 0.801812
C -1.172790 -0.806836 1.361443
C -0.881489 1.584413 1.457682
C -1.904186 -0.763334 2.548961
H -0.989354 -1.763537 0.890123
C -1.613642 1.621561 2.647349
H -0.467783 2.499462 1.053075
C -2.125054 0.449896 3.200611
H -2.672506 0.477905 4.134955
C 1.422528 -1.280316 -0.208894
C 2.070307 -1.413341 1.026325
C 1.482156 -2.344662 -1.113568
C 2.769625 -2.575848 1.342571
H 2.041381 -0.602223 1.744176
C 2.169907 -3.517861 -0.785359
H 1.006662 -2.264804 -2.083802
C 2.822493 -3.639222 0.440210
H 3.367897 -4.542852 0.686683
Pd 2.160000 2.123215 -0.344273
C 0.856407 3.543579 -0.916134
C 0.426162 3.642983 -2.243388
C 0.483448 4.540119 -0.002989
C -0.368985 4.722202 -2.651620
H 0.709154 2.896835 -2.978801
C -0.321181 5.608313 -0.411436
H 0.841239 4.508281 1.021167
C -0.747322 5.706467 -1.738056
H -0.684535 4.789199 -3.690436
H -0.596088 6.374452 0.309629
H -1.358060 6.546873 -2.057809
O 3.863037 0.673666 0.125146
C 4.821782 0.836477 0.908266
N 6.060834 0.468820 0.536314
H 6.817696 0.595216 1.191439
C 4.659785 1.427414 2.286832
H 4.338129 2.466680 2.166053
H 3.879523 0.881544 2.825604
H 5.581269 1.395308 2.875573
C 6.356969 -0.040168 -0.795781
H 5.964510 0.643050 -1.553652
H 7.440146 -0.121160 -0.905535
H 5.906903 -1.027141 -0.947163
Cl 3.769636 3.877597 -0.102823
C -1.854896 2.942295 3.334676
C -2.365894 -2.050976 3.181190
C 3.554998 -2.623782 2.626165
C 2.167939 -4.681453 -1.743260
F 3.318955 -5.383539 -1.675395
F 2.004932 -4.280562 -3.020878
F 1.163944 -5.549202 -1.468675
F 3.796465 -3.885652 3.031042
F 2.919147 -1.979528 3.627726
F 4.760261 -2.015090 2.478088
F -1.355915 -2.666228 3.836555
F -2.825557 -2.928799 2.261741
F -3.354949 -1.844875 4.077823
F -2.081192 2.780295 4.656196
F -0.801841 3.774835 3.198862
F -2.934353 3.580303 2.826839
H -2.883127 -0.380965 -4.208953
C 2.338818 0.407594 -3.114817
H 2.558296 1.427347 -2.772600
H 2.776480 -0.265820 -2.373135
H 2.873622 0.252166 -4.056856



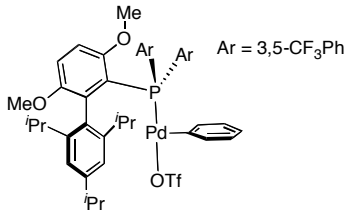
Complex **14**
Pd 0.001365 -0.509880 -0.140352
P -2.328068 -0.213165 -0.036344
P 2.320951 -0.199273 0.006150
O -0.004240 1.747159 0.000676
C 0.020838 -2.512601 -0.249434
C -0.313470 -3.270291 0.878192
H -0.592600 -2.787631 1.810375
C -0.293638 -4.669020 0.806768
H -0.553134 -5.251998 1.687043
C 0.052736 -5.311073 -0.383299
H 0.064528 -6.396010 -0.435812
C 0.386572 -4.550464 -1.505211
H 0.662459 -5.040639 -2.435400
C 0.376871 -3.151795 -1.441484
H 0.659769 -2.579008 -2.319854
C -1.227291 2.426824 -0.024242
C -2.395340 1.635635 -0.031749
C -3.634718 2.287192 -0.059607
H -4.545752 1.698092 -0.079697
C -3.708581 3.676757 -0.067572
H -4.673010 4.174174 -0.086119
C -2.535534 4.424014 -0.058932
H -2.604251 5.507007 -0.069964
C -1.268212 3.823570 -0.042573
C -0.008889 4.693542 -0.050868
C 1.252504 3.827548 -0.078022
C 2.517698 4.430186 -0.142292
H 2.583100 5.512997 -0.171880
C 3.691900 3.685630 -0.180925
H 4.653394 4.184953 -0.245135
C 3.622640 2.295829 -0.142269
H 4.532470 1.705105 -0.185931
C 2.385757 1.644056 -0.054932

C 1.215363 2.431566 -0.039996
C -0.030204 5.600949 -1.310550
H -0.913073 6.246952 -1.313903
H -0.042987 5.000767 -2.225927
H 0.848698 6.251654 -1.341023
C 0.010255 5.572465 1.228883
H -0.872663 6.217690 1.272996
H 0.892806 6.219558 1.244815
H 0.025463 4.952522 2.131116
C -3.402935 -0.750633 -1.414974
C -2.808755 -0.984702 -2.664913
H -1.731585 -0.895391 -2.774225
C -3.594050 -1.343761 -3.760230
H -3.126244 -1.525403 -4.723425
C -4.975900 -1.481953 -3.614084
H -5.586321 -1.768330 -4.465597
C -5.572660 -1.262407 -2.370336
H -6.646167 -1.378206 -2.252485
C -4.792695 -0.898294 -1.272534
H -5.264052 -0.747270 -0.306141
C -3.149511 -0.748123 1.509781
C -3.286333 0.112138 2.610557
H -2.973031 1.148759 2.539022
C -3.838757 -0.356815 3.803553
H -3.946582 0.319428 4.646686
C -4.256883 -1.684187 3.911061
H -4.690403 -2.044953 4.839243
C -4.116473 -2.547688 2.821964
H -4.439835 -3.581679 2.899629
C -3.560611 -2.088192 1.628270
H -3.453282 -2.770739 0.790676
C 3.460394 -0.752702 -1.314784
C 3.020824 -0.657781 -2.646083
H 2.023771 -0.281050 -2.862530
C 3.858803 -1.040559 -3.691449
H 3.512851 -0.961237 -4.718005
C 5.137978 -1.533283 -3.417492
H 5.788442 -1.837736 -4.232242
C 5.576720 -1.638299 -2.097025
H 6.569003 -2.023431 -1.880869
C 4.743784 -1.249419 -1.045246
H 5.092571 -1.340057 -0.021532
C 3.056611 -0.711825 1.602323
C 3.078399 -2.088263 1.895109
H 2.681245 -2.806447 1.183791
C 3.605103 -2.537742 3.104777
H 3.623650 -3.602372 3.318905
C 4.097546 -1.623846 4.040474
H 4.502481 -1.976830 4.984472
C 4.063116 -0.257253 3.761918
H 4.440651 0.457575 4.487399
C 3.546719 0.201142 2.547895
H 3.529361 1.266537 2.344723



Complex **15**
Pd -0.109445 0.625231 -0.812399
P -2.337809 0.204210 -0.062509
P 2.122764 0.909216 -0.000178
O 0.044572 -0.666657 1.702311
C -0.440699 2.582246 -1.081944
C -0.536988 2.958485 -2.430836
H -0.448765 2.213002 -3.218242
C -0.747040 4.297422 -2.777359
H -0.818842 4.574019 -3.826691
C -0.864301 5.271970 -1.782391
H -1.027987 6.312153 -2.052528
C -0.770127 4.898165 -0.441871
H -0.860213 5.646841 0.341991
C -0.558800 3.558867 -0.089973
H -0.489506 3.290100 0.959291
C -1.003276 -1.576250 1.738982
C -2.162590 -1.311360 0.981734
C -3.196221 -2.258051 1.021686
H -4.090502 -2.095712 0.430840
C -3.082256 -3.414395 1.787274
H -3.887791 -4.142572 1.792624
C -1.935994 -3.635259 2.547169
H -1.866586 -4.535144 3.147787
C -0.884265 -2.714508 2.548428
C 0.356363 -2.836273 3.438905
C 1.547731 -2.279871 2.652761
C 2.848573 -2.779587 2.758989
H 3.044692 -3.646334 3.379845
C 3.906638 -2.178202 2.081387
H 4.911710 -2.578831 2.174347
C 3.672552 -1.066143 1.279114
H 4.498246 -0.613871 0.741273
C 2.382160 -0.536764 1.128038
C 1.331653 -1.168553 1.824437
C 0.143081 -1.948077 4.699768
H -0.724285 -2.299737 5.270495
H -0.029339 -0.902455 4.425935
H 1.026044 -1.989588 5.348226
C 0.594350 -4.285150 3.898340
H -0.256039 -4.651415 4.480997
H 1.466677 -4.346852 4.555618
H 0.749738 -4.958539 3.048934
C -3.015013 1.464095 1.101900
C -2.988925 1.286729 2.492573
H -2.593055 0.370479 2.917503
C -3.485696 2.277025 3.343581
H -3.460965 2.121149 4.418852
C -4.019625 3.453351 2.816997

H -4.410817 4.220697 3.479688
C -4.048729 3.639702 1.432749
H -4.457481 4.554441 1.012357
C -3.543034 2.658521 0.581403
H -3.562612 2.822653 -0.491344
C -3.749001 -0.122309 -1.197459
C -5.085072 0.104352 -0.822023
H -5.317124 0.489963 0.165558
C -6.121533 -0.154255 -1.719210
H -7.150175 0.027342 -1.418920
C -5.837719 -0.642333 -2.997090
H -6.646685 -0.841220 -3.695135
C -4.514376 -0.875449 -3.373425
H -4.284821 -1.264663 -4.361152
C -3.472142 -0.614006 -2.482420
H -2.451299 -0.832591 -2.774800
C 2.464270 2.370462 1.065349
C 2.624829 3.630049 0.462387
H 2.563042 3.727547 -0.617104
C 2.863753 4.761614 1.240718
H 2.991921 5.726550 0.758058
C 2.925658 4.657580 2.632542
H 3.107910 5.541283 3.238201
C 2.749407 3.414496 3.241055
H 2.795085 3.324189 4.323108
C 2.522973 2.276451 2.463467
H 2.401949 1.313657 2.948961
C 3.538526 0.869970 -1.174075
C 4.772780 1.485438 -0.903549
H 4.923723 2.023482 0.027086
C 5.809920 1.417898 -1.834789
H 6.759405 1.900359 -1.617832
C 5.627632 0.735489 -3.040058
H 6.436703 0.686254 -3.764157
C 4.404207 0.121239 -3.312607
H 4.251511 -0.413911 -4.245460
C 3.359032 0.190400 -2.389673
H 2.415423 -0.296544 -2.618414
O 0.387401 -1.561920 -0.983785
S 0.220909 -2.376712 -2.252413
O 1.020985 -1.871739 -3.382389
O -1.171851 -2.757093 -2.534976
C 1.059668 -3.948674 -1.720339
F 1.006124 -4.853145 -2.705845
F 2.346378 -3.715688 -1.423914
F 0.460151 -4.461255 -0.635761



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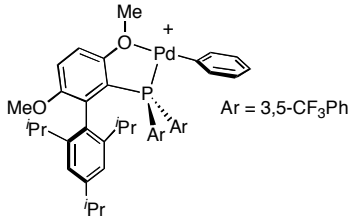
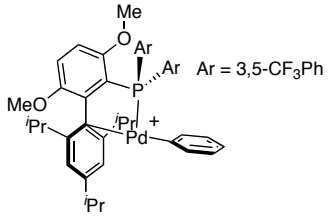
C 3.670466 -2.284109 0.394197
C 2.397810 -2.243872 0.964328
C 1.963283 -1.039293 1.599894
C 2.845920 0.079393 1.655965
H 4.773045 0.828471 1.090220
H 3.990819 -3.198644 -0.093735
C 0.764236 -1.079018 2.518756
C -0.550736 -0.725002 2.159730
C 1.008832 -1.500976 3.851599
C -1.600208 -0.799620 3.113105
C -0.032115 -1.572816 4.775353
C -1.332838 -1.224011 4.410939
H 0.154016 -1.895493 5.792780
H -2.121588 -1.278194 5.151536
P -0.898213 -0.177449 0.438658
C 2.495618 1.360696 2.413016
H 1.479159 1.249876 2.805652
C 5.950672 -1.269057 -0.150207
H 6.261305 -0.238391 -0.357520
C 6.018454 -2.041733 -1.477994
H 5.830361 -3.113208 -1.337546
H 5.290882 -1.653270 -2.195461
H 7.018282 -1.944031 -1.916101
C 6.933370 -1.857774 0.883721
H 7.954322 -1.865175 0.483692
H 6.935467 -1.275334 1.812029
H 6.663000 -2.890637 1.136492
C 1.545717 -3.513304 0.947155
H 0.524266 -3.242299 1.237379
C 1.473973 -4.164614 -0.448408
H 0.705323 -4.944971 -0.465453
H 1.240108 -3.429192 -1.226370
H 2.424207 -4.633943 -0.726067
C 2.053865 -4.539430 1.982104
H 1.402782 -5.421749 1.998142
H 3.067203 -4.873288 1.729573
H 2.085426 -4.111092 2.987614
C 2.509947 2.609314 1.511041
H 2.165144 3.483086 2.076422
H 3.514976 2.823954 1.132931
H 1.865464 2.490324 0.635037
C 3.423913 1.554534 3.630114
H 4.459976 1.722103 3.314287
H 3.108883 2.428889 4.211978

H 3.410109 0.677531 4.285117
O 2.303385 -1.819156 4.150417
O -2.837317 -0.422931 2.684033
C 2.616509 -2.222591 5.476180
H 2.086896 -3.143569 5.753074
H 3.691258 -2.409090 5.480955
H 2.380436 -1.433922 6.202251
C -3.958815 -0.627288 3.537766
H -3.930096 0.049535 4.400402
H -4.837831 -0.414392 2.928612
H -4.006676 -1.666097 3.885723
C -2.267873 -1.263214 -0.155069
C -3.622092 -0.925166 -0.066924
C -1.916263 -2.505179 -0.692589
C -4.601847 -1.823533 -0.493221
H -3.922494 0.032588 0.339570
C -2.899399 -3.399454 -1.119716
H -0.871375 -2.775119 -0.788374
C -4.249028 -3.065778 -1.020543
H -5.011763 -3.756947 -1.356891
C -1.609985 1.514527 0.590308
C -2.342632 2.075704 -0.464077
C -1.307543 2.310959 1.701528
C -2.753298 3.409291 -0.406550
H -2.585093 1.489077 -1.341987
C -1.720430 3.642484 1.751066
H -0.754528 1.897638 2.536967
C -2.442444 4.202181 0.696599
H -2.763296 5.235971 0.737732
C -6.046920 -1.431067 -0.326936
C -2.465361 -4.729406 -1.680306
C -3.477101 3.992350 -1.594543
C -1.323618 4.487055 2.935138
F -3.493130 -5.419812 -2.210001
F -1.530688 -4.574821 -2.643354
F -1.907650 -5.506622 -0.720062
F -6.887540 -2.322006 -0.884554
F -6.375226 -1.336963 0.989288
F -6.299040 -0.223680 -0.871648
F -4.102997 5.146369 -1.287622
F -4.403621 3.135870 -2.075141
F -2.619137 4.254646 -2.605844
F -1.373622 3.778578 4.086094
F -2.126489 5.560460 3.079830
F -0.057922 4.946224 2.812784
Pd 1.040552 -0.116576 -0.777857
C -0.039320 0.088603 -2.470235
C -0.271161 -1.054305 -3.238831
C -0.455253 1.342179 -2.919037
C -0.944857 -0.938567 -4.460153
H 0.070768 -2.032459 -2.915100
C -1.138554 1.444890 -4.137761
H -0.220020 2.240163 -2.359448
C -1.387757 0.307845 -4.906087
H -1.117629 -1.829713 -5.058630
H -1.463962 2.423982 -4.478812
H -1.912542 0.393157 -5.853781
O 2.852910 0.207274 -1.887921
S 3.008077 1.531419 -2.648319
O 2.876380 1.393076 -4.099369
O 2.324191 2.650229 -1.976935
C 4.820065 1.873720 -2.379597
F 5.575755 0.855687 -2.817851
F 5.093811 2.066005 -1.073812
F 5.168087 2.980154 -3.043347



Complex **17**
C -4.187955 0.361976 0.031500
C -4.285815 -0.201194 1.310099
C -3.426903 -1.257309 1.614084
C -2.492946 -1.757812 0.694882
C -2.394253 -1.147947 -0.577952
C -3.283376 -0.093208 -0.929774
H -4.867840 1.169402 -0.227497
H -3.495494 -1.729363 2.587887
C -1.487232 -1.701864 -1.647571
C -0.194266 -1.208369 -1.958437
C -2.020650 -2.741646 -2.456276
C 0.485360 -1.697752 -3.106629
C -1.310725 -3.236041 -3.550350
C -0.068539 -2.704574 -3.884941
H -1.723322 -4.023254 -4.168924
H 0.444699 -3.084222 -4.758757
P 0.767621 -0.038336 -0.893245
C -3.367407 0.480535 -2.348642
H -2.436932 0.238934 -2.875467
C -5.356782 0.305462 2.271761
H -5.360582 1.400796 2.188640
C -5.103151 -0.044457 3.745113
H -5.191410 -1.122392 3.926254
H -4.112007 0.279500 4.075582
H -5.848023 0.449723 4.377688
C -6.748730 -0.198494 1.831974
H -7.528510 0.216081 2.480710
H -6.977220 0.090172 0.800486
H -6.802154 -1.291944 1.894054
C -1.691760 -2.999134 1.091083
H -0.906354 -3.150548 0.341892
C -1.006592 -2.870147 2.465237
H -0.364871 -3.738728 2.643860
H -0.386296 -1.969892 2.536189
H -1.738127 -2.831905 3.279149
C -2.582847 -4.260330 1.075884

H -1.982492 -5.151629 1.292918
H -3.367681 -4.190831 1.837629
H -3.067472 -4.392878 0.105571
C -3.538958 2.009016 -2.405472
H -3.484317 2.348797 -3.445928
H -4.514192 2.324645 -2.019346
H -2.770497 2.537878 -1.838187
C -4.524501 -0.186768 -3.126501
H -5.487805 0.066832 -2.669126
H -4.541817 0.166618 -4.164212
H -4.436902 -1.275708 -3.128767
O -3.249000 -3.194338 -2.102577
O 1.714337 -1.134785 -3.441191
C -3.857280 -4.228179 -2.877012
H -3.255558 -5.144795 -2.860463
H -4.820327 -4.417505 -2.402869
H -4.017377 -3.906301 -3.913020
C 2.490312 -1.722952 -4.503547
H 1.977911 -1.602082 -5.462105
H 3.432841 -1.175046 -4.520260
H 2.680187 -2.779970 -4.296509
C -0.160501 1.354216 -0.156954
C -0.721837 1.296861 1.127874
C -0.188088 2.557634 -0.870834
C -1.280275 2.444722 1.686148
H -0.730757 0.374665 1.694252
C -0.758180 3.698323 -0.305849
H 0.256174 2.617693 -1.856991
C -1.296432 3.648906 0.978071
H -1.712822 4.542684 1.430738
C 1.519176 -1.019899 0.457826
C 2.068727 -0.372758 1.573592
C 1.724058 -2.396750 0.295416
C 2.808948 -1.097180 2.508956
H 1.946200 0.695261 1.713249
C 2.447370 -3.114257 1.247593
H 1.327127 -2.916557 -0.568890
C 2.998759 -2.470251 2.356222
H 3.574479 -3.028252 3.085279
Pd 2.506078 0.578092 -2.227698
C 3.271525 2.021997 -1.131119
C 3.154886 3.335514 -1.604538
C 4.148503 1.706166 -0.087453
C 3.982860 4.326964 -1.064704
H 2.441611 3.601929 -2.378725
C 4.961519 2.710537 0.449270
H 4.217963 0.697238 0.307503
C 4.878888 4.016316 -0.039529
H 3.909520 5.344115 -1.439311
H 5.647528 2.465715 1.255214
H 5.503378 4.795346 0.387796
C 3.484177 -0.343915 3.631214
C 2.581555 -4.610811 1.090708
C -1.870188 2.425118 3.077294
C -0.821220 4.980333 -1.102272
F 0.168212 5.037496 -2.023239
F -1.990370 5.080428 -1.766850
F -0.711762 6.058580 -0.307584
F -1.291269 3.357889 3.857138
F -3.191327 2.699439 3.043290
F -1.711740 1.227423 3.675505
F 3.660790 -5.084290 1.734466
F 1.496769 -5.247347 1.585704
F 2.683409 -4.955741 -0.211333
F 4.597537 0.276597 3.171200
F 3.854262 -1.157021 4.632652
F 2.677435 0.610548 4.133836



Complex **18**

C 4.041407 -1.389256 1.088342
C 4.525260 -0.161167 1.566505
C 4.173142 1.001232 0.862546
C 3.353924 0.973482 -0.282388
C 2.811689 -0.286897 -0.705225
C 3.209261 -1.488599 -0.031241
H 4.327968 -2.297453 1.610992
H 4.566584 1.956358 1.193828
C 1.954581 -0.373841 -1.946728
C 0.546280 -0.262979 -1.918334
C 2.592997 -0.601140 -3.186570
C -0.207635 -0.361202 -3.114347
C 1.837629 -0.686061 -4.359342
C 0.449334 -0.566300 -4.327319
H 2.321737 -0.853332 -5.313964
H -0.109230 -0.647161 -5.252158
P -0.319436 0.023774 -0.323068
C 2.756609 -2.869327 -0.497212
H 2.024409 -2.728163 -1.298229
C 5.429571 -0.105205 2.787658
H 5.533888 -1.133715 3.156514
C 4.814373 0.736054 3.923516
H 4.700680 1.786490 3.630765
H 3.828641 0.356306 4.215569
H 5.462299 0.707887 4.805940
C 6.838927 0.402060 2.419106
H 7.492196 0.367077 3.297441
H 7.292827 -0.211316 1.633540
H 6.812658 1.439649 2.066289
C 3.137572 2.263582 -1.075563
H 2.246722 2.125196 -1.697881
C 2.909127 3.505164 -0.191632
H 2.528494 4.332501 -0.798976
H 2.187479 3.317085 0.611731
H 3.837545 3.848849 0.277653

C 4.332544 2.507147 -2.023873
H 4.149127 3.395222 -2.638592
H 5.251113 2.678801 -1.450682
H 4.501491 1.652794 -2.683533
C 2.069644 -3.677535 0.621079
H 1.630917 -4.591916 0.209055
H 2.777741 -3.971644 1.403437
H 1.264916 -3.103734 1.094589
C 3.941829 -3.656448 -1.095546
H 4.705434 -3.861370 -0.336594
H 3.594299 -4.618669 -1.487373
H 4.414350 -3.099910 -1.910057
C -1.424148 1.474171 -0.515101
C -2.781630 1.359547 -0.833050
C -0.864130 2.744558 -0.357523
C -3.555970 2.507635 -1.005287
C -1.646997 3.887631 -0.517475
H 0.183257 2.847310 -0.096725
C -2.997508 3.777220 -0.846282
C -1.379180 -1.429463 0.017623
C -2.284353 -1.389136 1.088224
C -1.233759 -2.612841 -0.715096
C -3.032814 -2.520633 1.412117
H -2.409336 -0.485869 1.674804
C -1.981814 -3.741741 -0.377689
H -0.547159 -2.662325 -1.552128
C -2.883881 -3.702747 0.685017
H -3.469343 -4.578343 0.939661
Pd 1.373544 0.322826 1.141345
C 0.133430 0.619998 2.688395
C -0.257999 1.909615 3.064066
C -0.135484 -0.477600 3.515728
C -0.870550 2.102832 4.308478
H -0.093354 2.765804 2.416027
C -0.751500 -0.271511 4.755763
H 0.126976 -1.487462 3.210815
C -1.117438 1.016832 5.150898
H -1.160888 3.105646 4.610207
H -0.955243 -1.122156 5.400136
H -1.606159 1.172730 6.108197
C -3.951027 -2.470004 2.611646
C -1.750198 -5.024146 -1.140682
F -0.654606 -5.668998 -0.674949
F -1.535398 -4.780720 -2.451160
F -2.790705 -5.866484 -1.035458
F -3.250474 -2.643429 3.754371
F -4.571091 -1.276805 2.700755
F -4.890868 -3.429707 2.560174
H -3.607465 4.663944 -0.969479
H -3.238034 0.385032 -0.959487
C -5.003167 2.331211 -1.399534
C -0.985204 5.227284 -0.308231
F -5.650650 1.535414 -0.526331
F -5.657273 3.500762 -1.469298
F -5.093487 1.734466 -2.615072
F -1.854912 6.245048 -0.384131
F -0.014891 5.436820 -1.227186
F -0.386171 5.275369 0.905750
O -1.555751 -0.264338 -2.981667
O 3.949923 -0.729658 -3.143878
C -2.372397 -0.190462 -4.154187
H -3.374881 0.048021 -3.798366
H -2.026124 0.605633 -4.822544
H -2.382334 -1.148077 -4.686664
C 4.654044 -0.973864 -4.361919
H 5.705652 -1.044694 -4.083175
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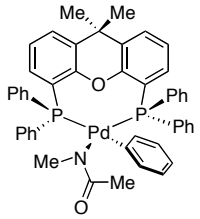
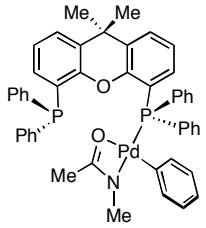
H 4.519788 -0.148759 -5.071563



Complex **19**
Pd 0.011557 -0.662742 0.797424
P -2.283214 -0.219505 0.237214
P 2.301384 -0.216319 0.255674
O 0.008250 1.346723 -1.193895
C 0.008584 -2.260831 -0.476703
C -0.008581 -3.521022 0.144564
H -0.021490 -3.594547 1.231176
C -0.009123 -4.699313 -0.611703
H -0.022445 -5.663618 -0.107052
C 0.007060 -4.637929 -2.006802
H 0.006567 -5.551397 -2.596685
C 0.023346 -3.391257 -2.635466
H 0.035739 -3.330162 -3.721726
C 0.023883 -2.216404 -1.876956
H 0.035956 -1.258435 -2.391118
C -1.174319 2.068571 -1.120142
C -2.287647 1.496970 -0.471652
C -3.453100 2.276251 -0.388062
H -4.324032 1.872563 0.116388
C -3.508100 3.559200 -0.923618
H -4.417902 4.145630 -0.834972
C -2.397425 4.086247 -1.580190
H -2.455758 5.082172 -2.004806
C -1.219187 3.345773 -1.701664
C 0.010211 3.814283 -2.485216
C 1.243663 3.337532 -1.713217
C 2.428922 4.068742 -1.606722
H 2.491001 5.062088 -2.036808
C 3.542264 3.535896 -0.959020
H 4.458293 4.114523 -0.884326
C 3.480304 2.258105 -0.412655
H 4.351811 1.849518 0.087132
C 2.306910 1.488325 -0.479374
C 1.193843 2.062116 -1.126748

C 0.001534 3.118346 -3.878335
H -0.889594 3.414148 -4.443862
H -0.001793 2.028642 -3.781277
H 0.889567 3.407830 -4.451974
C 0.014303 5.336226 -2.705126
H -0.864166 5.646019 -3.279014
H 0.888143 5.640225 -3.289117
H 0.021428 5.886540 -1.758220
C -3.055964 -1.220899 -1.108160
C -3.431235 -0.680845 -2.345257
H -3.280303 0.373839 -2.549195
C -4.008226 -1.491834 -3.326885
H -4.292469 -1.057381 -4.281827
C -4.221564 -2.847491 -3.082023
H -4.669919 -3.477053 -3.846032
C -3.850902 -3.394573 -1.850288
H -4.003544 -4.451993 -1.653423
C -3.268776 -2.590203 -0.873775
H -2.963641 -3.033283 0.069070
C -3.625089 -0.169468 1.512470
C -4.944864 -0.558867 1.223014
H -5.206843 -0.904970 0.229168
C -5.930024 -0.510028 2.210996
H -6.944680 -0.816891 1.970454
C -5.614660 -0.072493 3.498779
H -6.382787 -0.039524 4.267030
C -4.307814 0.318361 3.793957
H -4.042515 0.657679 4.791129
C -3.318300 0.270065 2.810949
H -2.311204 0.572262 3.065041
C 3.111791 -1.238773 -1.050358
C 3.281160 -2.612402 -0.805447
H 2.918248 -3.047311 0.120506
C 3.890691 -3.431755 -1.752745
H 4.008991 -4.492090 -1.548196
C 4.329576 -2.895930 -2.966719
H 4.797572 -3.537275 -3.708828
C 4.157764 -1.536410 -3.223166
H 4.493896 -1.110982 -4.165209
C 3.555492 -0.710424 -2.269951
H 3.436708 0.346588 -2.482240
C 3.607448 -0.112361 1.563535
C 4.899021 -0.635605 1.384815
H 5.168363 -1.123310 0.454599
C 5.848869 -0.535385 2.403863
H 6.843101 -0.947060 2.250512
C 5.525510 0.089221 3.609171
H 6.266245 0.163738 4.401041
C 4.244789 0.614584 3.793049
H 3.979239 1.098039 4.729154
C 3.290069 0.514361 2.781037
H 2.290358 0.905596 2.932497
N 0.021122 0.754243 2.445338
C -0.075143 0.270025 3.708001
C 0.140948 -1.233890 3.881180
H 0.821432 -1.654561 3.131117
H 0.539139 -1.421392 4.882605
H -0.820022 -1.758850 3.801123
C -0.184573 2.193671 2.339725
H -1.244950 2.482731 2.427432
H 0.346499 2.724245 3.140031
H 0.180068 2.554395 1.374347
O -0.345795 0.964276 4.704197



Complex **20**
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P 2.061793 0.440639 0.383734
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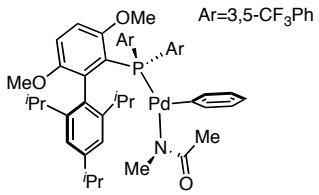
C 1.727299 -2.632022 -0.397496
C 0.723530 -3.471803 0.113360
H -0.310165 -3.137867 0.121698
C 1.038200 -4.740597 0.612383
H 0.244769 -5.374869 1.002771
C 2.359509 -5.194056 0.608427
H 2.603489 -6.180221 0.995778
C 3.362243 -4.367922 0.099231
H 4.395757 -4.708188 0.087556
C 3.050073 -3.096440 -0.398701
H 3.852075 -2.472861 -0.781885
C -1.825062 2.008686 -0.485785
C -2.690606 0.900319 -0.470011
C -3.927004 1.037582 -1.115343
H -4.610923 0.195540 -1.135917
C -4.286552 2.234091 -1.732634
H -5.244535 2.320208 -2.237942
C -3.428241 3.330035 -1.675922
H -3.739802 4.265039 -2.128477
C -2.186606 3.246205 -1.035436
C -1.280197 4.459180 -0.803252
C 0.170856 3.977101 -0.722896
C 1.262994 4.797069 -1.026334
H 1.094092 5.800563 -1.401038
C 2.571236 4.358046 -0.842480
H 3.404355 5.016140 -1.071527
C 2.811081 3.072406 -0.365153
H 3.832353 2.735748 -0.234486
C 1.750152 2.204779 -0.070326
C 0.437237 2.686236 -0.245483
C -1.463448 5.527987 -1.898250
H -2.496184 5.887027 -1.923004
H -1.207063 5.137224 -2.888303
H -0.840728 6.404822 -1.699111
C -1.659061 5.085847 0.570673

H -2.702405 5.422209 0.562729
H -1.015944 5.946740 0.788946
H -1.543144 4.359203 1.381388
C -3.361280 -1.885173 -0.294556
C -2.986877 -2.528706 -1.488244
H -2.043048 -2.270000 -1.963479
C -3.811626 -3.495946 -2.063801
H -3.508116 -3.982203 -2.987636
C -5.014964 -3.850286 -1.448858
H -5.652430 -4.610912 -1.892361
C -5.390415 -3.227517 -0.257511
H -6.323747 -3.499943 0.229240
C -4.571681 -2.250559 0.314927
H -4.876621 -1.772362 1.240655
C -2.841923 -0.371632 2.103116
C -3.745372 0.644994 2.450333
H -4.099732 1.335133 1.690956
C -4.198157 0.778311 3.765161
H -4.897404 1.572530 4.015370
C -3.761784 -0.106048 4.753144
H -4.117573 -0.002930 5.775114
C -2.860024 -1.119788 4.421760
H -2.508460 -1.808753 5.185576
C -2.397623 -1.243806 3.111518
H -1.676887 -2.020183 2.868183
C 3.906095 0.351408 0.434692
C 4.590517 0.106988 -0.767917
H 4.022535 -0.047894 -1.682461
C 5.984321 0.056483 -0.793202
H 6.499825 -0.132468 -1.730991
C 6.712435 0.235919 0.385759
H 7.797989 0.187619 0.368765
C 6.040702 0.472598 1.586003
H 6.601298 0.610378 2.506807
C 4.645388 0.534042 1.611820
H 4.134318 0.721756 2.550542
C 1.579045 0.287157 2.152936
C 1.559291 -0.987785 2.742352
H 1.767091 -1.866795 2.141585
C 1.268174 -1.128895 4.099346
H 1.261507 -2.120274 4.544635
C 0.980143 -0.006580 4.879234
H 0.747206 -0.120272 5.934630
C 0.988138 1.261495 4.297410
H 0.760096 2.139094 4.896419
C 1.290160 1.409747 2.942301
H 1.304384 2.401367 2.501404
O 0.297149 0.490231 -2.832499
C 0.070879 -0.533158 -3.571692
N 0.331269 -1.714791 -3.041384
C -0.459689 -0.339038 -4.976100
H -1.349664 -0.953462 -5.154631
H -0.712241 0.713027 -5.121250
H 0.294179 -0.630148 -5.718219
C 0.295122 -2.970576 -3.754995
H 0.276801 -3.790474 -3.031388
H -0.595993 -3.061521 -4.394472
H 1.180617 -3.114798 -4.394143



Complex **21**
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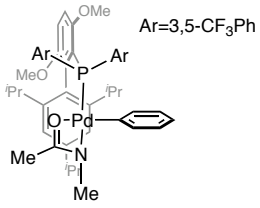
C -4.971125 0.195656 0.511111
C -4.456365 -0.943382 -0.115044
C -3.308901 -0.906907 -0.914536
C -2.643505 0.337549 -1.106909
C -3.153452 1.509279 -0.483907
H -4.677088 2.296471 0.805300
H -4.972117 -1.890815 0.009253
C -1.621887 0.477653 -2.211493
C -0.222656 0.393538 -2.054137
C -2.141781 0.741734 -3.506454
C 0.630660 0.568692 -3.177188
C -1.290384 0.897852 -4.597844
C 0.092246 0.812894 -4.436637
H -1.688069 1.095549 -5.586129
H 0.734013 0.952740 -5.298118
P 0.498037 0.037989 -0.391229
C -2.572789 2.897112 -0.761745
H -1.705919 2.771700 -1.418545
C -6.287231 0.174191 1.280200
H -6.327500 1.101372 1.867869
C -6.425646 -0.997677 2.266226
H -6.407388 -1.965708 1.749767
H -5.632273 -0.985246 3.019574
H -7.389306 -0.928646 2.785196
C -7.469678 0.206114 0.287455
H -8.422914 0.263653 0.826420
H -7.404990 1.067482 -0.387446
H -7.486232 -0.701172 -0.329244
C -2.865265 -2.180652 -1.636585
H -1.883236 -1.986334 -2.082596
C -2.708228 -3.388872 -0.693887
H -2.240763 -4.225513 -1.225663
H -2.090892 -3.144325 0.176843
H -3.675671 -3.737042 -0.314965
C -3.829445 -2.532907 -2.788698
H -3.464658 -3.408527 -3.339078
H -4.826390 -2.772394 -2.400237
H -3.935493 -1.699285 -3.488125
C -2.080029 3.616560 0.506870
H -1.608529 4.569668 0.241513
H -2.903570 3.827695 1.198295
H -1.341576 3.015127 1.046215
C -3.585811 3.776656 -1.524048
H -4.466113 3.992121 -0.907476

H -3.128667 4.734753 -1.799274
H -3.929468 3.279842 -2.436573
O -3.502978 0.835422 -3.598622
O 1.971354 0.502716 -2.938899
C -4.081006 1.102260 -4.868067
H -3.850800 0.308224 -5.590539
H -5.158391 1.135886 -4.699981
H -3.745137 2.067459 -5.269244
C 2.872266 0.499068 -4.040989
H 2.903222 1.478905 -4.533357
H 3.851845 0.264101 -3.623099
H 2.600224 -0.271346 -4.772495
C 1.649189 -1.381719 -0.681149
C 3.023772 -1.257173 -0.903679
C 1.085812 -2.661281 -0.662648
C 3.810305 -2.390332 -1.119598
H 3.488048 -0.278496 -0.917690
C 1.876049 -3.792688 -0.874045
H 0.025482 -2.780827 -0.466723
C 3.244192 -3.665672 -1.106761
H 3.859423 -4.542551 -1.265427
C 1.578074 1.487642 -0.018844
C 2.527754 1.409735 1.011247
C 1.380228 2.715616 -0.660257
C 3.261153 2.538762 1.380923
H 2.696903 0.477379 1.535835
C 2.110857 3.842524 -0.278837
H 0.661768 2.800449 -1.467194
C 3.055964 3.762061 0.742466
H 3.630789 4.634241 1.029815
C 5.275611 -2.194049 -1.407147
C 1.213375 -5.143890 -0.812666
C 4.232708 2.447200 2.531128
C 1.825913 5.160610 -0.951040
F 2.085583 -6.151992 -1.004962
F 0.617331 -5.339807 0.386164
F 0.243661 -5.259907 -1.750715
F 5.948740 -3.358499 -1.465345
F 5.457613 -1.565515 -2.599405
F 5.865547 -1.419959 -0.473349
F 5.208028 3.376011 2.434217
F 4.821639 1.236579 2.593033
F 3.609785 2.649594 3.715286
F 1.586356 5.002782 -2.271998
F 2.850574 6.027070 -0.820655
F 0.730082 5.757351 -0.424642
Pd -1.067671 -0.427431 1.304912
C 0.356343 -0.885037 2.656838
C 0.835866 -2.195283 2.759986
C 0.863426 0.101919 3.509773
C 1.829127 -2.508240 3.696109
H 0.449742 -2.985154 2.122287
C 1.860158 -0.215683 4.440613
H 0.492174 1.120768 3.459057
C 2.346454 -1.520593 4.535505
H 2.193610 -3.530616 3.765044
H 2.255069 0.565183 5.085171
H 3.118151 -1.766189 5.260051
N -2.428624 -0.913529 2.757297
C -2.978008 -0.055940 3.658551
C -2.504231 1.391053 3.645867
H -2.009927 1.604421 4.600531
H -1.813611 1.614971 2.828928
H -3.373470 2.052980 3.574189
O -3.845013 -0.393147 4.480161
C -2.759002 -2.323467 2.944825
H -3.077468 -2.503043 3.976230
H -3.573763 -2.640004 2.279053
H -1.884017 -2.944457 2.725051



Complex **22**
C -3.998169 -1.808825 -0.088467
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C -4.477691 0.532810 0.044357
C -3.466799 0.716080 0.993881
C -2.676753 -0.399024 1.367377
C -2.976283 -1.687096 0.860328
H -4.222402 -2.790653 -0.496519
H -5.079624 1.389762 -0.248009
C -1.582621 -0.237174 2.388842
C -0.215448 -0.072586 2.066984
C -1.961592 -0.271370 3.756285
C 0.740424 0.027758 3.120663
C -1.014293 -0.141093 4.767463
C 0.334833 0.004154 4.450929
H -1.306488 -0.163987 5.810494
H 1.060823 0.079480 5.251341
P 0.425727 0.036585 0.317334
C -2.307553 -2.951083 1.405115
H -1.355761 -2.657028 1.860289
C -5.837283 -0.896553 -1.574521
H -5.876049 -1.968151 -1.813651
C -5.498099 -0.148291 -2.878066
H -5.479286 0.936842 -2.718335
H -4.515022 -0.447698 -3.257474
H -6.247540 -0.356610 -3.651622
C -7.227325 -0.492429 -1.048091
H -7.998147 -0.689276 -1.803020
H -7.486115 -1.051210 -0.141853
H -7.267813 0.575961 -0.804527
C -3.317595 2.086561 1.661048
H -2.415166 2.063356 2.281973
C -3.157695 3.251941 0.669484
H -2.951314 4.182831 1.210551

H -2.344922 3.081502 -0.040135
H -4.070349 3.409418 0.082244
C -4.512692 2.363296 2.598958
H -4.364541 3.306152 3.140182
H -5.443881 2.450735 2.026138
H -4.639195 1.557828 3.326486
C -1.992690 -4.020946 0.344454
H -1.349580 -4.791153 0.786860
H -2.905450 -4.522674 -0.001175
H -1.484198 -3.599767 -0.526435
C -3.176649 -3.563725 2.526360
H -4.136150 -3.906633 2.119921
H -2.671613 -4.429966 2.971517
H -3.390031 -2.837228 3.315054
O -3.296629 -0.444472 4.002176
O 2.050745 0.116778 2.755518
C -3.733469 -0.512927 5.350795
H -3.523377 0.419357 5.891628
H -4.812665 -0.666812 5.304238
H -3.269778 -1.354435 5.882147
C 3.036171 0.404781 3.739376
H 3.180357 -0.443472 4.420268
H 3.957740 0.594936 3.187119
H 2.770995 1.298489 4.317377
C 1.514258 1.532670 0.411117
C 2.906002 1.486266 0.315329
C 0.887821 2.776910 0.559379
C 3.660579 2.659542 0.398826
H 3.416546 0.536379 0.205135
C 1.645053 3.945670 0.638674
H -0.192620 2.842157 0.615859
C 3.038109 3.895041 0.563019
H 3.625963 4.802280 0.635000
C 1.564028 -1.416012 0.154658
C 2.288442 -1.556231 -1.038244
C 1.616016 -2.449355 1.093453
C 3.066703 -2.689685 -1.269098
H 2.234405 -0.786972 -1.802049
C 2.376751 -3.595337 0.845931
H 1.063761 -2.375187 2.022646
C 3.110253 -3.721734 -0.331074
H 3.706144 -4.607129 -0.515320
Pd -0.675428 -0.168261 -1.782671
C -0.758509 1.764542 -2.301206
C -2.009749 2.351667 -2.537025
C 0.396515 2.480346 -2.645377
C -2.100705 3.638450 -3.081365
H -2.919084 1.808341 -2.296821
C 0.302793 3.765389 -3.192697
H 1.380862 2.045073 -2.495729
C -0.945489 4.350918 -3.408314
H -1.017296 5.350223 -3.829557
O -0.678819 -2.424263 -2.200712
C -1.050750 -2.138586 -3.394164
N -1.268952 -0.862416 -3.651647
C -1.202179 -3.239155 -4.420078
H -0.435963 -3.147371 -5.199588
H -1.090774 -4.206043 -3.925806
H -2.180077 -3.194143 -4.912871
C -1.564050 -0.311895 -4.955683
H -2.301336 -0.920176 -5.498706
H -1.977055 0.692407 -4.834696
H -0.664147 -0.227934 -5.583895
C 3.796050 -2.820386 -2.581158
C 2.351561 -4.705115 1.863621
F 4.808879 -3.709989 -2.507357
F 2.972109 -3.235523 -3.568542
F 4.317371 -1.637653 -2.976582
F 1.150694 -5.328427 1.887331
F 3.286315 -5.645389 1.618890
F 2.565279 -4.232139 3.114077
H 1.210766 4.305700 -3.450458
H -3.080140 4.081447 -3.248738
C 5.161083 2.544019 0.397365
C 0.954624 5.281869 0.736468
F 5.597533 1.724035 -0.581633
F 5.769287 3.735722 0.239767
F 5.609483 2.019197 1.569088
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F 1.702660 6.176987 1.421381
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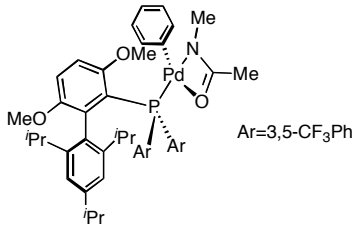

Complex **23**
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C 3.243079 1.056148 -0.951420
C 2.596917 -0.167514 -1.264630
C 3.081989 -1.381587 -0.719276
H 4.552340 -2.260876 0.575804
H 4.822495 1.980125 0.164462
C 1.498848 -0.174431 -2.299613
C 0.113243 -0.083105 -2.039066
C 1.924867 -0.226746 -3.655787
C -0.797220 -0.002219 -3.133080
C 1.013367 -0.180011 -4.706581
C -0.350642 -0.059250 -4.447425
H 1.349184 -0.220826 -5.735694
H -1.048348 -0.000877 -5.274099
P -0.801506 -0.143248 -0.419612
C 2.501155 -2.741265 -1.113877
H 1.454064 -2.595856 -1.400190

C 6.041149 -0.149269 1.400653
H 6.207484 -1.191608 1.705589
C 5.828340 0.677819 2.681294
H 5.636429 1.732128 2.452114
H 4.976612 0.308197 3.259783
H 6.718407 0.631405 3.320437
C 7.304525 0.315339 0.649475
H 8.187967 0.235589 1.294383
H 7.478859 -0.290924 -0.246265
H 7.217016 1.361688 0.333114
C 2.864682 2.387080 -1.610280
H 1.923816 2.243570 -2.151503
C 2.648645 3.542836 -0.615116
H 2.315414 4.438997 -1.149077
H 1.889239 3.311377 0.137208
H 3.570609 3.797211 -0.080842
C 3.927263 2.798270 -2.652827
H 3.614967 3.707997 -3.180207
H 4.888726 3.005933 -2.167908
H 4.086625 2.004089 -3.386332
C 2.522466 -3.787435 0.014933
H 1.922785 -4.654225 -0.280761
H 3.539325 -4.146741 0.215376
H 2.116982 -3.403097 0.953404
C 3.235721 -3.322376 -2.342520
H 4.284514 -3.530680 -2.096392
H 2.765428 -4.264176 -2.649379
H 3.224906 -2.633270 -3.189210
O 3.277972 -0.312779 -3.851062
O -2.108004 0.156792 -2.794565
C 3.768672 -0.403627 -5.179333
H 3.517940 0.490129 -5.766057
H 4.853225 -0.481705 -5.087987
H 3.382918 -1.294774 -5.691845
C -3.107170 0.171335 -3.805314
H -3.099534 -0.759758 -4.385130
H -4.054440 0.263838 -3.273471
H -2.975460 1.027377 -4.479069
C 0.280217 -0.317933 1.074117
C 0.963721 0.763285 1.644610
C 0.201602 -1.518280 1.791191
C 1.557274 0.642799 2.901436
H 1.015637 1.710877 1.124918
C 0.793743 -1.632779 3.051527
H -0.347267 -2.354429 1.375858
C 1.471187 -0.553396 3.614591
H 1.911156 -0.635175 4.601133
C -1.416275 1.590852 -0.185918
C -2.287299 1.842098 0.885301
C -1.067119 2.642252 -1.037117
C -2.778967 3.127929 1.103766
H -2.618724 1.032125 1.523638
C -1.571355 3.927726 -0.817342
H -0.416353 2.467689 -1.885725
C -2.424730 4.178130 0.254710
H -2.826204 5.172200 0.415748

Pd -2.649952 -1.589254 -0.280948
C -1.657752 -3.262160 -0.786347
C -1.223769 -3.497882 -2.098574
C -1.569923 -4.311082 0.144565
C -0.723910 -4.751074 -2.473779
H -1.277309 -2.709711 -2.844011
C -1.062418 -5.560849 -0.229348
H -1.905274 -4.164964 1.168624
C -0.640890 -5.787287 -1.541328
H -0.402096 -4.914683 -3.500138
H -1.002874 -6.357763 0.508623
H -0.254943 -6.760364 -1.834105
N -4.528836 -2.457841 0.055610
C -5.121995 -1.316904 0.336260
C -6.589470 -1.191375 0.676249
H -7.212945 -1.499368 -0.172173
H -6.852872 -1.834472 1.524316
H -6.814772 -0.153583 0.928904
O -4.380044 -0.265321 0.305023
C -5.182362 -3.745187 0.000737
H -5.806658 -3.932162 0.887284
H -5.821210 -3.850962 -0.890014
H -4.420551 -4.527625 -0.044468
C -1.146340 5.058263 -1.716958
C -3.669998 3.412049 2.286741
C 0.697608 -2.937907 3.799050
C 2.211084 1.848412 3.526238
F -0.498982 -3.534780 3.605902
F 1.644878 -3.817112 3.396689
F 0.859301 -2.767501 5.128270
F 1.294442 2.685690 4.059501
F 3.059051 1.502176 4.520222
F 2.914619 2.563793 2.620513
F -0.017719 5.657582 -1.265436
F -0.885500 4.630459 -2.972077
F -2.091500 6.017818 -1.799262
F -4.627272 4.315164 1.976806
F -2.960424 3.932909 3.315577
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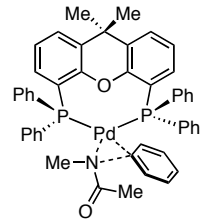

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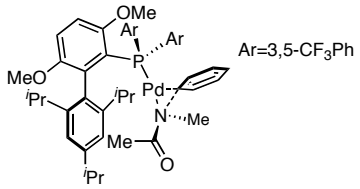
P -1.844342 -1.166540 0.097047
P 1.412712 1.253783 0.171378
O -1.555076 1.704547 -0.153035
C 2.425400 -2.044012 0.016773
C 1.926926 -3.323918 0.339182
H 1.072352 -3.723615 -0.198237

C 2.552753 -4.090641 1.328404
H 2.144550 -5.068124 1.577363
C 3.706491 -3.627359 1.964183
H 4.199342 -4.231156 2.721474
C 4.236565 -2.388905 1.589348
H 5.145689 -2.020800 2.060986
C 3.616684 -1.603576 0.613196
H 4.059089 -0.657225 0.330410
C -2.747311 1.329553 -0.744985
C -3.083022 -0.028351 -0.659917
C -4.286904 -0.433742 -1.252065
H -4.578255 -1.477656 -1.211573
C -5.099465 0.490764 -1.908396
H -6.026544 0.162565 -2.369951
C -4.729537 1.834682 -1.976662
H -5.376612 2.536141 -2.492424
C -3.543060 2.283651 -1.385988
C -3.081681 3.743419 -1.339109
C -1.549844 3.740685 -1.426804
C -0.797934 4.734156 -2.060379
H -1.298265 5.539983 -2.586364
C 0.594959 4.710052 -2.016019
H 1.166976 5.492349 -2.506790
C 1.259882 3.690202 -1.338102
H 2.342409 3.693252 -1.310666
C 0.550859 2.656372 -0.704562
C -0.850701 2.714427 -0.774534
C -3.723939 4.585695 -2.454363
H -4.813866 4.587549 -2.357344
H -3.465728 4.207909 -3.449372
H -3.404257 5.629973 -2.386619
C -3.492323 4.345019 0.036427
H -4.583019 4.332174 0.145961
H -3.146342 5.382123 0.116950
H -3.059161 3.775092 0.864089
C -2.607879 -2.828155 -0.191249
C -2.160007 -3.582771 -1.288686
H -1.356289 -3.201162 -1.912790
C -2.723734 -4.833363 -1.555400
H -2.368054 -5.410136 -2.405472
C -3.726778 -5.347512 -0.732268
H -4.157701 -6.323780 -0.939772
C -4.169822 -4.606209 0.365875
H -4.946529 -5.002526 1.015131
C -3.615078 -3.354350 0.635336
H -3.964311 -2.788299 1.493631
C -2.102125 -0.940214 1.914878
C -3.133590 -0.167785 2.467011
H -3.833169 0.348653 1.816667
C -3.275867 -0.059383 3.852854
H -4.079621 0.545874 4.264577
C -2.396295 -0.728546 4.704230
H -2.510483 -0.646621 5.781977
C -1.365508 -1.501267 4.163628
H -0.673256 -2.023552 4.818896
C -1.213330 -1.599405 2.781043
H -0.398171 -2.191218 2.371140
C 3.168664 1.648288 -0.264839
C 3.656197 1.172239 -1.494153
H 3.029604 0.531999 -2.109166
C 4.957671 1.469939 -1.899119
H 5.322908 1.093879 -2.851049
C 5.794274 2.230100 -1.077392
H 6.810812 2.453538 -1.390580
C 5.322721 2.691678 0.152571
H 5.970120 3.276430 0.801050
C 4.015746 2.406298 0.556446
H 3.658020 2.776197 1.512008
C 1.300772 1.754077 1.948809
C 1.629985 0.794946 2.920471
H 1.913098 -0.207506 2.612684
C 1.599869 1.121880 4.276203
H 1.861898 0.369967 5.015723
C 1.223183 2.403887 4.682219
H 1.191017 2.654616 5.739310
C 0.883120 3.360510 3.724492
H 0.585633 4.359737 4.032297
C 0.926130 3.040356 2.365812
H 0.668871 3.796199 1.630310
O 0.541820 -2.296580 -2.240410
C 1.682772 -2.470011 -2.805739
N 2.801446 -2.106265 -2.239126
C 1.657664 -3.147622 -4.172150
H 0.635601 -3.185893 -4.552725
H 2.293945 -2.619959 -4.891588
H 2.041711 -4.172709 -4.090037
C 4.094716 -2.441414 -2.788597
H 4.348586 -1.842704 -3.679963
H 4.854951 -2.228069 -2.027488
H 4.198997 -3.503241 -3.064927



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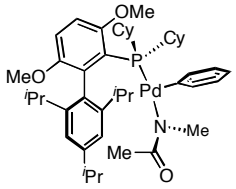
C -4.939174 -0.081367 0.560304
C -4.435580 -1.037381 -0.327913
C -3.358633 -0.773136 -1.181366
C -2.749878 0.508959 -1.144432
C -3.239171 1.491068 -0.249265
H -4.694280 1.923930 1.270137
H -4.906949 -2.015429 -0.373892
C -1.740448 0.895035 -2.199259
C -0.336226 0.826779 -2.053154
C -2.274891 1.385677 -3.419213

C 0.501282 1.256562 -3.117750
C -1.435522 1.778367 -4.458942
C -0.050494 1.716588 -4.309902
H -1.842946 2.148347 -5.392238
H 0.583061 2.046961 -5.124253
P 0.399000 0.167778 -0.484706
C -2.688566 2.916125 -0.219927
H -1.830262 2.958593 -0.897555
C -6.174638 -0.347028 1.412685
H -6.283444 0.508130 2.093920
C -6.062939 -1.613872 2.279369
H -5.949060 -2.513369 1.661579
H -5.215559 -1.564391 2.970106
H -6.974431 -1.742789 2.875396
C -7.439243 -0.394417 0.530214
H -8.336829 -0.516040 1.148351
H -7.549931 0.523703 -0.057741
H -7.398532 -1.237299 -0.170513
C -2.921456 -1.850721 -2.175114
H -1.998343 -1.509551 -2.656254
C -2.607169 -3.194806 -1.491568
H -2.147118 -3.891102 -2.202702
H -1.918249 -3.051678 -0.651660
H -3.511457 -3.672313 -1.096780
C -3.972571 -2.045658 -3.287014
H -3.619041 -2.773593 -4.027473
H -4.915471 -2.421490 -2.871989
H -4.184673 -1.102281 -3.798291
C -2.184852 3.333883 1.174421
H -1.696388 4.313617 1.122561
H -3.006237 3.405638 1.896630
H -1.458647 2.613260 1.565511
C -3.728735 3.922304 -0.753056
H -4.608572 3.965812 -0.100358
H -3.298810 4.930020 -0.802884
H -4.069110 3.639139 -1.754357
O -3.640286 1.447699 -3.492530
O 1.845441 1.215417 -2.890066
C -4.232948 1.955954 -4.677839
H -3.986539 1.337689 -5.551288
H -5.310070 1.923610 -4.506679
H -3.926614 2.992843 -4.869461
C 2.740368 1.463286 -3.967944
H 2.718770 2.518009 -4.269602
H 3.732728 1.205573 -3.595598
H 2.505935 0.830065 -4.832313
C 1.720196 -1.019959 -1.016193
C 3.074304 -0.693368 -1.139595
C 1.328189 -2.343617 -1.240460
C 4.007217 -1.665364 -1.505273
H 3.407936 0.321545 -0.959772
C 2.264470 -3.315740 -1.598549
H 0.286906 -2.623052 -1.119615
C 3.610966 -2.983384 -1.736858
H 4.338963 -3.736929 -2.010768
C 1.329696 1.593259 0.236826
C 2.080447 1.368438 1.400076
C 1.204295 2.904114 -0.237670
C 2.685281 2.432864 2.070930
H 2.177576 0.365051 1.802077
C 1.802782 3.965600 0.444625
H 0.637660 3.107491 -1.138417
C 2.546691 3.739258 1.602515
H 3.012086 4.563988 2.128294
C 5.438838 -1.244554 -1.703050
C 1.798094 -4.738511 -1.754115
C 3.432796 2.147626 3.348420
C 1.573771 5.372242 -0.042291
F 2.732533 -5.523636 -2.326273
F 1.491046 -5.289016 -0.553536
F 0.679129 -4.814930 -2.510390
F 6.274411 -2.295885 -1.807405
F 5.578993 -0.510774 -2.840575
F 5.875702 -0.466491 -0.691176
F 4.138001 3.215162 3.774562
F 4.292337 1.117545 3.203466
F 2.580844 1.806047 4.347164
F 1.512435 5.431127 -1.391176
F 2.547929 6.213452 0.360550
F 0.402590 5.871238 0.423558
Pd -0.970721 -0.848265 1.096529
C 0.143252 -1.871544 2.570812
C 0.673212 -3.104560 2.145307
C 0.856794 -1.126214 3.530104
C 1.904521 -3.550283 2.631531
H 0.156090 -3.709879 1.410630
C 2.085197 -1.588315 4.007704
H 0.483202 -0.176438 3.890350
C 2.620293 -2.801344 3.566169
H 2.301490 -4.490813 2.257044
H 2.627116 -0.976944 4.724381
H 3.574046 -3.155185 3.946402
N -1.787267 -1.891675 2.737351
C -2.370624 -1.200518 3.789096
C -2.039524 0.270958 3.975810
H -1.574581 0.415763 4.957358
H -1.397442 0.682499 3.193670
H -2.983360 0.825025 3.978235
O -3.182964 -1.743095 4.537201
C -2.253329 -3.275607 2.603229
H -1.830667 -3.921344 3.383117
H -3.341010 -3.297846 2.693396
H -1.974697 -3.663853 1.624142



Complex **24**

C -3.447451 0.299917 1.210542
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C -3.453664 0.147141 -1.172477
C -2.230094 0.818271 -1.248965
C -1.591561 1.243944 -0.046620
C -2.231693 0.992445 1.201067
H -3.940078 0.118566 2.162656
H -3.939335 -0.153652 -2.096683
C -0.490111 2.282614 -0.113435
C 0.899546 2.045243 -0.030703
C -0.950425 3.623288 -0.246677
C 1.787396 3.154699 -0.046379
C -0.057940 4.688312 -0.278553
C 1.312663 4.455093 -0.172231
H -0.409906 5.708090 -0.377791
H 1.991256 5.299023 -0.190328
P 1.562607 0.304912 0.102297
C -1.723799 1.582673 2.518277
H -0.718688 1.977936 2.346836
C -5.482829 -0.732586 0.112357
H -5.680851 -0.953366 1.170044
C -5.619805 -2.054166 -0.663058
H -5.435435 -1.911351 -1.735408
H -4.926479 -2.813835 -0.288847
H -6.641795 -2.439216 -0.558678
C -6.539042 0.294142 -0.348786
H -7.549607 -0.114779 -0.229582
H -6.474976 1.223716 0.228716
H -6.403876 0.548028 -1.407418
C -1.674315 1.170861 -2.629857
H -0.717253 1.681178 -2.482909
C -1.405574 -0.071254 -3.499262
H -0.949677 0.223958 -4.452616
H -0.733219 -0.772025 -2.993958
H -2.330914 -0.611139 -3.728284
C -2.602956 2.152215 -3.375095
H -2.143815 2.469546 -4.319495
H -3.564290 1.682888 -3.615058
H -2.805801 3.040494 -2.770499
C -1.626144 0.549907 3.655020
H -1.196727 1.016087 4.550209
H -2.609753 0.155444 3.933576
H -0.998600 -0.300730 3.375249
C -2.611127 2.766531 2.961100
H -3.625948 2.425539 3.197795
H -2.197642 3.239381 3.860582
H -2.688750 3.521819 2.174625
O -2.307812 3.787683 -0.331428
O 3.122909 2.871290 0.072734
C -2.824419 5.100478 -0.480227
H -2.461327 5.575054 -1.401541
H -3.908214 4.986673 -0.535721
H -2.570100 5.735365 0.379025
C 4.048154 3.945981 0.130251
H 3.841712 4.607553 0.981231
H 5.030078 3.487093 0.258710
H 4.043376 4.534416 -0.796393
Pd -0.202373 -1.301569 0.004244
C 0.998396 -2.889951 -0.321213
C 1.419197 -3.172533 -1.627853
C 1.363236 -3.767911 0.706136
C 2.221707 -4.289548 -1.895132
H 1.117260 -2.534715 -2.455078
C 2.164568 -4.882653 0.437595
H 1.017786 -3.599287 1.720619
C 2.602098 -5.145784 -0.862216
H 2.538340 -4.488761 -2.916663
H 2.435821 -5.552931 1.250327
H 3.221008 -6.015138 -1.068244
N -1.727596 -2.686212 -0.138482
C -2.320553 -3.311227 0.910292
C -1.796755 -3.006597 2.309378
H -1.528300 -3.952553 2.792740
H -0.930042 -2.338699 2.313930
H -2.597251 -2.554604 2.904913
O -3.271958 -4.103908 0.800256
C -2.121526 -3.156303 -1.462810
H -2.640680 -4.115524 -1.377145
H -2.794571 -2.446380 -1.959936
H -1.236553 -3.281070 -2.095981
C 2.760366 0.036320 -1.355711
C 2.333184 0.819668 -2.614246
C 4.275206 0.194363 -1.105922
H 2.590629 -1.025644 -1.564170
C 3.145204 0.380304 -3.845629
H 2.482491 1.893775 -2.445582
H 1.266035 0.675621 -2.812527
C 5.074632 -0.261529 -2.341222
H 4.510013 1.240092 -0.885786
H 4.591324 -0.397266 -0.240329
C 4.655748 0.503312 -3.604115
H 2.846003 0.978173 -4.716297
H 2.900891 -0.664766 -4.085254
H 6.148048 -0.129575 -2.152334
H 4.914780 -1.338131 -2.497899
H 5.212249 0.135481 -4.475603
H 4.919599 1.565548 -3.489461
C 2.659309 0.323475 1.645546
C 2.036176 1.069386 2.841378
C 3.059923 -1.101361 2.075814
H 3.561360 0.869228 1.352835
C 3.013220 1.113402 4.030157
H 1.116276 0.559412 3.152679

H 1.755909 2.089518 2.558902
C 4.047615 -1.064454 3.254762
H 2.158200 -1.647191 2.376030
H 3.490228 -1.666594 1.242190
C 3.469044 -0.291623 4.448613
H 2.540792 1.629459 4.876014
H 3.892632 1.712749 3.750496
H 4.304420 -2.089279 3.551189
H 4.985498 -0.588510 2.931107
H 4.207247 -0.227309 5.258226
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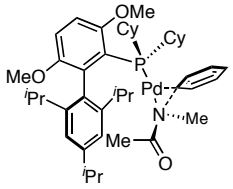

Transition State **10-TS**
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C -2.321265 0.830771 -1.214536
C -1.721161 1.305224 -0.017534
C -2.321592 0.984639 1.227888
H -3.943116 -0.036295 2.197649
H -3.930239 -0.302196 -2.063258
C -0.645468 2.370556 -0.080056
C 0.753884 2.164806 -0.022694
C -1.140995 3.699924 -0.191338
C 1.609698 3.298521 -0.053194
C -0.277470 4.788360 -0.230197
C 1.100487 4.588211 -0.156761
H -0.656583 5.799932 -0.312746
H 1.756984 5.449287 -0.183640
P 1.471252 0.439908 0.102309
C -1.824325 1.561696 2.553411
H -0.845952 2.017870 2.377762
C -5.403854 -1.038135 0.147644
H -5.601795 -1.237954 1.209816
C -5.376537 -2.395233 -0.576338
H -5.174105 -2.272764 -1.647749
H -4.617703 -3.063663 -0.158119
H -6.350745 -2.890944 -0.484342
C -6.557263 -0.157116 -0.375405
H -7.519620 -0.669839 -0.257630
H -6.607262 0.794997 0.164959
H -6.427293 0.069979 -1.440573
C -1.805978 1.227430 -2.597965
H -0.887629 1.806784 -2.461484
C -1.453967 0.006158 -3.467503
H -1.034544 0.327408 -4.429072
H -0.719042 -0.631325 -2.963779
H -2.337830 -0.606058 -3.680609
C -2.812836 2.139407 -3.329108
H -2.396311 2.484001 -4.283793
H -3.745931 1.606021 -3.546149
H -3.061603 3.014719 -2.721921
C -1.643450 0.490917 3.645071
H -1.199324 0.936928 4.543386
H -2.600417 0.046736 3.942388
H -0.991767 -0.319929 3.304537
C -2.766605 2.677809 3.052782
H -3.759373 2.275329 3.287999
H -2.367352 3.140254 3.964185
H -2.894059 3.455810 2.294677
O -2.505104 3.829865 -0.251213
O 2.955931 3.049121 0.025988
C -3.055549 5.130206 -0.379231
H -2.720145 5.622408 -1.302005
H -4.137329 4.991139 -0.417388
H -2.802314 5.764692 0.480854
C 3.853476 4.146808 0.061782
H 3.657830 4.798345 0.923276
H 4.850889 3.713493 0.155814
H 3.803990 4.741233 -0.859979
Pd -0.112322 -1.297975 0.017218
C 0.759002 -3.199941 -0.302384
C 1.300498 -3.360247 -1.597602
C 1.376798 -3.901094 0.757021
C 2.440036 -4.141721 -1.806626
H 0.851222 -2.856234 -2.445722
C 2.510703 -4.678592 0.530643
H 0.987727 -3.832249 1.764495
C 3.059472 -4.807681 -0.749196
H 2.840792 -4.223829 -2.814889
H 2.967044 -5.194118 1.373120
H 3.938763 -5.422575 -0.917350
N -1.125374 -3.144114 -0.261282
C -1.806653 -3.725974 0.797322
C -1.450665 -3.313808 2.216460
H -1.171984 -4.203357 2.792380
H -0.658793 -2.563517 2.272222
H -2.352975 -2.896884 2.675284
O -2.723492 -4.525990 0.609528
C -1.640832 -3.535229 -1.577919
H -1.352204 -4.562978 -1.832642
H -2.729701 -3.476277 -1.569422
H -1.259880 -2.854940 -2.337845
C 2.644632 0.200086 -1.390057
C 2.203651 1.008850 -2.626877
C 4.162764 0.357036 -1.162996
H 2.467239 -0.859775 -1.615159
C 2.992473 0.589284 -3.879876
H 2.365512 2.077763 -2.438804
H 1.132638 0.878180 -2.809590
C 4.946492 -0.074657 -2.416971
H 4.396113 1.400697 -0.928342
H 4.495136 -0.247238 -0.312529
C 4.507102 0.707745 -3.662091
H 2.679605 1.201517 -4.735920

H 2.742944 -0.451776 -4.132020
H 6.022423 0.057734 -2.242299
H 4.787596 -1.149327 -2.587748
H 5.049497 0.352748 -4.547912
H 4.772794 1.768306 -3.536434
C 2.615125 0.490693 1.610044
C 2.012066 1.236772 2.815120
C 3.008180 -0.941536 2.026528
H 3.515684 1.031069 1.303649
C 2.992656 1.257522 4.001236
H 1.084985 0.739072 3.125571
H 1.745581 2.262580 2.539178
C 3.992583 -0.930012 3.208428
H 2.099011 -1.487136 2.307702
H 3.438484 -1.498278 1.186567
C 3.425024 -0.158251 4.408384
H 2.532484 1.776027 4.852607
H 3.882046 1.842770 3.723048
H 4.234468 -1.960990 3.496826
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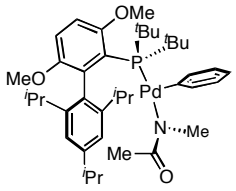
H 4.163228 -0.113272 5.219544
H 2.554608 -0.700245 4.806708



Complex **25**
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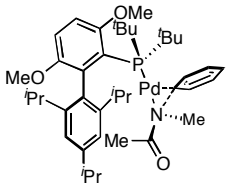
C 3.036679 -0.876302 -1.058783
C 1.688987 -1.209187 -1.212434
C 0.892103 -1.451447 -0.050433
C 1.514689 -1.384226 1.232943
H 3.331170 -0.967579 2.296450
H 3.636572 -0.722845 -1.951529
C -0.404688 -2.230684 -0.171505
C -1.728272 -1.735008 -0.047884
C -0.203287 -3.632240 -0.337805
C -2.793298 -2.680967 -0.020115
C -1.274341 -4.513936 -0.399483
C -2.570110 -4.037455 -0.228803
H -1.118503 -5.575572 -0.547479
H -3.392558 -4.741560 -0.237868
P -2.065018 0.121626 0.049279
C 0.831292 -1.884888 2.508564
H -0.226256 -2.044770 2.285734
C 5.149478 -0.540402 0.342665
H 5.337993 -0.363362 1.410087
C 5.670136 0.688779 -0.421620
H 5.516431 0.585372 -1.503273
H 5.176989 1.604933 -0.082792
H 6.749437 0.795491 -0.256425
C 5.923503 -1.814306 -0.058294
H 6.998294 -1.681512 0.114390
H 5.588463 -2.685420 0.516810
H 5.780686 -2.040984 -1.122149
C 1.157671 -1.417412 -2.633050
H 0.085711 -1.624730 -2.561372
C 1.337100 -0.177736 -3.529801
H 0.839847 -0.335692 -4.494621
H 0.920396 0.720648 -3.068860
H 2.395864 0.017542 -3.734513
C 1.815253 -2.636924 -3.314158
H 1.371470 -2.803083 -4.303607
H 2.890173 -2.474297 -3.455828
H 1.689744 -3.543178 -2.718508
C 0.914443 -0.902791 3.690396
H 0.373644 -1.309630 4.553585
H 1.949636 -0.731713 4.005384
H 0.480787 0.070018 3.444224
C 1.416059 -3.251613 2.930177
H 2.466938 -3.152072 3.226310
H 0.862479 -3.656004 3.786622
H 1.368707 -3.974677 2.112014
O 1.098709 -4.052879 -0.413087
O -4.043700 -2.203046 0.257952
C 1.359383 -5.441495 -0.540266
H 0.943318 -5.848923 -1.471407
H 2.446222 -5.536333 -0.560595
H 0.960816 -6.006937 0.312508
C -5.149430 -3.090111 0.205687
H -5.060707 -3.889688 0.951963
H -6.028902 -2.484884 0.433197
H -5.263840 -3.533372 -0.791811
Pd 0.112952 1.294403 0.025965
C -0.466731 3.230079 -0.207484
C -0.613168 3.757192 -1.497827
C -0.625001 4.094947 0.882531
C -0.947569 5.102995 -1.692898
H -0.473183 3.127810 -2.371711
C -0.958479 5.439842 0.688015
H -0.476393 3.737790 1.895099
C -1.126318 5.950344 -0.600041
H -1.062611 5.482825 -2.705787
H -1.073290 6.090097 1.552547
H -1.380696 6.996379 -0.749430
N 1.979908 2.177621 -0.010364
C 2.666637 2.610449 1.079113
C 2.025171 2.434128 2.448743
H 1.950692 3.417138 2.926639
H 1.033825 1.975218 2.409085
H 2.679446 1.817523 3.073767
O 3.796987 3.124971 1.025200
C 2.545484 2.549276 -1.302753
H 3.317550 3.311417 -1.163399
H 2.997057 1.686226 -1.805336
H 1.764610 2.950059 -1.956988
C -3.093924 0.546425 -1.548329

C -3.112566 0.447749 1.671423
C -3.594344 2.003666 -1.449332
H -2.812743 2.700670 -1.149088
H -3.950057 2.315154 -2.440495
H -4.436938 2.106363 -0.762109
C -4.295058 -0.348762 -1.902784
H -4.000092 -1.385334 -2.082446
H -5.076294 -0.332382 -1.142365
H -4.729456 0.035863 -2.835863
C -2.090827 0.444935 -2.713519
H -1.212153 1.071121 -2.549075
H -1.755478 -0.585633 -2.865017
H -2.579385 0.774819 -3.639956
C -4.647075 0.486185 1.525707
H -5.053454 -0.443332 1.134457
H -5.075508 0.646975 2.524448
H -4.988212 1.313820 0.900889
C -2.746452 -0.614355 2.725564
H -1.670101 -0.657715 2.904088
H -3.221816 -0.339898 3.676757
H -3.099069 -1.610504 2.451111
C -2.665803 1.819903 2.210638
H -1.597303 1.830873 2.439791
H -2.863412 2.631806 1.506609
H -3.215752 2.034518 3.137129



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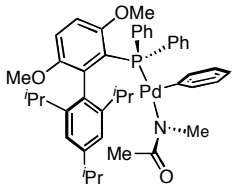
C 2.398251 2.791051 -0.266880
C 1.729551 2.727029 0.957544
C 0.413562 2.263909 1.076044
C -0.267893 1.803145 -0.085066
C 0.390857 1.878194 -1.343037
H 2.201177 2.414186 -2.363781
H 2.232175 3.086381 1.850051
C -1.768028 1.588642 -0.040597
C -2.470635 0.358457 0.079167
C -2.506582 2.801844 -0.155782
C -3.893741 0.411492 0.104706
C -3.893385 2.814848 -0.090168
C -4.586137 1.616387 0.045510
H -4.450464 3.741619 -0.155635
H -5.668113 1.638107 0.080324
P -1.549829 -1.301797 0.118543
C -0.328451 1.594811 -2.662940
H -1.310170 1.176439 -2.425084
C 3.777811 3.423309 -0.423400
H 4.237485 2.968615 -1.312369
C 4.731648 3.182910 0.757037
H 4.364591 3.653558 1.677700
H 4.883434 2.115068 0.940215
H 5.708853 3.629877 0.538218
C 3.630098 4.934337 -0.707281
H 4.609905 5.390649 -0.893907
H 2.994035 5.117938 -1.580542
H 3.176149 5.446938 0.149955
C -0.267153 2.390875 2.442229
H -1.217205 1.849173 2.397037
C 0.557677 1.794284 3.598513
H -0.027450 1.815203 4.525968
H 0.850019 0.760619 3.403285
H 1.471833 2.370837 3.781121
C -0.595069 3.864902 2.766897
H -1.136650 3.934435 3.718566
H 0.324721 4.454699 2.861834
H -1.203690 4.321254 1.983913
C 0.405814 0.571133 -3.547284
H -0.176650 0.362830 -4.453367
H 1.387155 0.940581 -3.866510
H 0.559172 -0.370952 -3.010133
C -0.569859 2.901925 -3.447262
H 0.378903 3.355456 -3.757725
H -1.158234 2.703932 -4.351879
H -1.105782 3.634018 -2.836690
O -1.768270 3.943548 -0.341017
O -4.559621 -0.781926 0.160471
C -2.452878 5.174575 -0.503761
H -3.032596 5.438906 0.391039
H -1.676641 5.924954 -0.662898
H -3.122072 5.153174 -1.374296
C -5.971245 -0.780600 0.290976
H -6.459213 -0.332443 -0.584286
H -6.265175 -1.829275 0.365765
H -6.291669 -0.250010 1.196786
Pd 0.839182 -0.980588 -0.098953
C 2.131504 -2.689117 -0.184327
C 2.321695 -3.456766 0.985640
C 2.229617 -3.354862 -1.424539
C 2.550370 -4.831110 0.908916
H 2.272606 -2.995752 1.963061
C 2.457632 -4.730306 -1.485491
H 2.105100 -2.809549 -2.352262
C 2.621019 -5.485349 -0.323154
H 2.675285 -5.391963 1.832786
H 2.506438 -5.210281 -2.460627
H 2.809067 -6.553764 -0.375409
N 2.947334 -0.972296 -0.241136
C 3.561496 -0.764711 -1.557303
C -1.893434 -2.108705 1.848650
C -2.300916 -2.411630 -1.310732
C -3.349024 -2.256655 2.327112
H -3.836756 -1.287494 2.451677
H -3.958480 -2.866028 1.659565
H -3.333385 -2.749868 3.309156

C -1.222353 -3.499146 1.847780
H -0.182075 -3.456794 1.517632
H -1.236070 -3.896849 2.871780
H -1.749505 -4.219214 1.216447
C -1.161883 -1.224438 2.875171
H -1.232136 -1.687733 3.868517
H -0.104238 -1.110983 2.623598
H -1.608047 -0.227620 2.941873
C -3.448761 -3.372800 -0.942236
H -4.328547 -2.849856 -0.575491
H -3.736214 -3.922601 -1.849132
H -3.149296 -4.119782 -0.202980
C -2.769430 -1.500857 -2.462311
H -3.025682 -2.130091 -3.325299
H -3.655294 -0.918464 -2.199680
H -1.983129 -0.812950 -2.784590
C -1.132521 -3.270951 -1.834085
H -0.326850 -2.652901 -2.234836
H -0.698275 -3.907948 -1.059512
H -1.500120 -3.921706 -2.639714
H 4.329873 -1.518920 -1.768947
H 2.793744 -0.799918 -2.328665
H 4.032953 0.219380 -1.576737
C 3.780745 -0.622792 0.808388
O 4.934602 -0.239233 0.606667
C 3.248834 -0.671244 2.228298
H 3.421805 0.309539 2.681108
H 2.184053 -0.899895 2.286830
H 3.822386 -1.405050 2.805644



Complex **26**
C -3.312992 0.142145 1.287593
C -3.964425 -0.324336 0.142556
C -3.393869 -0.017820 -1.095913
C -2.226838 0.743207 -1.215933
C -1.588968 1.222928 -0.036158
C -2.154605 0.924477 1.233692
H -3.751082 -0.079991 2.257955
H -3.883101 -0.363410 -2.001859
C -0.540056 2.305018 -0.146264
C 0.853600 2.104049 -0.103108
C -1.032775 3.629411 -0.295326
C 1.730548 3.217232 -0.215945
C -0.158204 4.704243 -0.426340
C 1.221928 4.500820 -0.389100
H -0.533701 5.713032 -0.550764
H 1.883868 5.353595 -0.482225
P 1.552981 0.399688 0.082425
C -1.616949 1.538154 2.527981
H -0.705098 2.092037 2.284550
C -5.306941 -1.037181 0.263914
H -5.394210 -1.376831 1.304907
C -5.450370 -2.276670 -0.634894
H -5.380008 -2.014709 -1.698237
H -4.690530 -3.030131 -0.405931
H -6.437345 -2.729986 -0.480715
C -6.452665 -0.033508 0.009644
H -7.426369 -0.513368 0.165438
H -6.385067 0.831451 0.679652
H -6.422936 0.339718 -1.021655
C -1.735253 1.122141 -2.614654
H -0.794831 1.672391 -2.501730
C -1.447383 -0.105037 -3.499399
H -1.032579 0.212482 -4.464452
H -0.735913 -0.785482 -3.020113
H -2.358567 -0.677105 -3.705325
C -2.732233 2.065796 -3.319214
H -2.331153 2.394697 -4.285841
H -3.685609 1.558978 -3.509214
H -2.939093 2.949320 -2.708900
C -1.235946 0.490252 3.588527
H -0.849447 0.987225 4.486520
H -2.096611 -0.117272 3.889685
H -0.460478 -0.186936 3.218302
C -2.623481 2.556371 3.103826
H -3.547607 2.061452 3.424673
H -2.196893 3.065181 3.977035
H -2.889668 3.310742 2.356888
O -2.395757 3.765962 -0.297136
O 3.062455 2.948338 -0.121550
C -2.945586 5.065205 -0.446916
H -2.659663 5.516810 -1.406252
H -4.028357 4.932978 -0.419212
H -2.640077 5.730548 0.371625
C 3.996405 3.993083 -0.337961
H 3.920955 4.768102 0.436201
H 4.979855 3.523648 -0.286740
H 3.862941 4.451305 -1.326190
C 2.837754 0.306407 -1.245116
C 4.209705 0.176977 -0.996553
C 2.388257 0.330706 -2.573852
C 5.112037 0.070431 -2.056640
H 4.579979 0.169382 0.022763
C 3.292724 0.240347 -3.632447
H 1.326324 0.416505 -2.785155
C 4.658537 0.104731 -3.376361
H 5.363528 0.022839 -4.199288
C 2.454463 0.420971 1.692961
C 3.192251 -0.713402 2.074477
C 2.363271 1.496897 2.588492
C 3.838705 -0.755953 3.310550
H 3.252366 -1.571722 1.414449
C 2.999843 1.444921 3.829680
H 1.793969 2.380080 2.321167

C 3.744017 0.321796 4.192953
H 4.241231 0.283855 5.158463
Pd -0.065775 -1.313458 -0.071031
C 1.304753 -2.784163 -0.197759
C 1.922978 -3.053343 -1.423441
C 1.612851 -3.578661 0.913448
C 2.851637 -4.095673 -1.532325
H 1.698791 -2.453384 -2.300099
C 2.543880 -4.617624 0.799723
H 1.131180 -3.401217 1.869756
C 3.166988 -4.879472 -0.422180
H 3.326449 -4.289290 -2.491602
H 2.769935 -5.229341 1.670477
H 3.885256 -5.690687 -0.508888
N -1.478252 -2.798224 -0.253220
C -2.108989 -3.434297 0.765995
C -1.717709 -3.055220 2.188997
H -1.303748 -3.940191 2.686016
H -0.989488 -2.241332 2.235428
H -2.616010 -2.764672 2.743856
O -2.987710 -4.298087 0.601287
C -1.747083 -3.324929 -1.588276
H -2.095996 -4.360345 -1.524392
H -2.520491 -2.739778 -2.105351
H -0.835051 -3.285350 -2.192967
H 2.927642 0.265420 -4.655823
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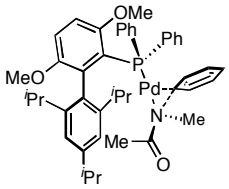
H 4.408571 -1.639617 3.584843
H 2.914411 2.287336 4.511110



Transition State **12-TS**
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C -3.914993 -0.746954 0.227841
C -3.426494 -0.364775 -1.024808
C -2.405052 0.579780 -1.174817
C -1.838144 1.172104 -0.016665
C -2.314054 0.796974 1.263239
H -3.703859 -0.441487 2.335920
H -3.867479 -0.799618 -1.917590
C -0.900692 2.347728 -0.154980
C 0.509047 2.278465 -0.127847
C -1.520643 3.616328 -0.308107
C 1.267634 3.474665 -0.253804
C -0.758010 4.771050 -0.455041
C 0.635119 4.702137 -0.428584
H -1.230731 5.737595 -0.583352
H 1.209840 5.614987 -0.530683
P 1.384393 0.647228 0.051442
C -1.818501 1.465327 2.545534
H -0.972014 2.108220 2.285733
C -5.100335 -1.694165 0.375961
H -5.164935 -1.963198 1.439511
C -4.953694 -3.002079 -0.421715
H -4.893613 -2.809416 -1.500115
H -4.064380 -3.567054 -0.125666
H -5.828890 -3.641937 -0.255870
C -6.412698 -0.971487 0.005831
H -7.276000 -1.626855 0.173536
H -6.550296 -0.063324 0.603511
H -6.413402 -0.679049 -1.051360
C -1.990683 0.992310 -2.587563
H -1.125316 1.658380 -2.503359
C -1.560016 -0.209450 -3.449320
H -1.192320 0.131867 -4.425197
H -0.764929 -0.779434 -2.955569
H -2.394300 -0.895870 -3.634501
C -3.112081 1.786475 -3.288700
H -2.775882 2.143468 -4.270126
H -3.998508 1.160323 -3.446884
H -3.415208 2.649657 -2.689069
C -1.310702 0.455637 3.590832
H -0.922525 0.984158 4.469756
H -2.109762 -0.211862 3.933326
H -0.503739 -0.161855 3.184167
C -2.911545 2.373939 3.145618
H -3.776650 1.786631 3.476094
H -2.525164 2.918431 4.016163
H -3.264484 3.101946 2.408246
O -2.892028 3.619562 -0.298034
O 2.621238 3.344340 -0.167809
C -3.564505 4.861515 -0.422378
H -3.346467 5.347130 -1.383227
H -4.629460 4.628476 -0.371136
H -3.303220 5.546631 0.395380
C 3.441461 4.480832 -0.375688
H 3.286007 5.239055 0.403550
H 4.468548 4.116065 -0.326168
H 3.263162 4.930832 -1.360843
C 2.688983 0.696347 -1.266767
C 4.063566 0.758004 -1.002671
C 2.262493 0.604297 -2.600358
C 4.988163 0.729523 -2.048429
H 4.416440 0.835566 0.020067
C 3.186285 0.596078 -3.646182
H 1.202087 0.534605 -2.824990
C 4.554348 0.653782 -3.373157
H 5.276057 0.634311 -4.185533
C 2.294645 0.771444 1.654808
C 3.104692 -0.313581 2.035361
C 2.148973 1.844444 2.546139
C 3.767768 -0.309771 3.262978
H 3.210766 -1.170671 1.377672
C 2.800385 1.837506 3.781403
H 1.524565 2.690971 2.282231
C 3.616231 0.764587 4.142291

H 4.125267 0.762524 5.102493
Pd 0.139283 -1.319367 -0.126386
C 1.334678 -3.063278 -0.179145
C 2.046581 -3.243334 -1.383216
C 1.910909 -3.546119 1.014547
C 3.303255 -3.851686 -1.380204
H 1.643656 -2.880466 -2.321459
C 3.164982 -4.157399 0.997362
H 1.397823 -3.434118 1.960414
C 3.874461 -4.318839 -0.195619
H 3.838068 -3.952537 -2.321903
H 3.585431 -4.514178 1.935319
H 4.846630 -4.803115 -0.201712
N -0.543765 -3.305277 -0.355208
C -1.243587 -3.941156 0.659610
C -1.129801 -3.412197 2.079602
H -0.724835 -4.198161 2.726978
H -0.528826 -2.504971 2.168829
H -2.142818 -3.191731 2.430353
O -1.991433 -4.889945 0.421808
C -0.837592 -3.832430 -1.692263
H -0.373923 -4.814334 -1.850604
H -1.918095 -3.942347 -1.803967
H -0.474901 -3.136064 -2.447628
H 2.670492 2.676748 4.460030
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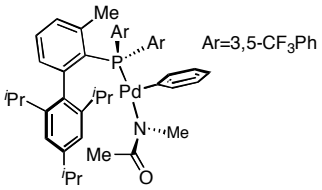
H 2.835858 0.532932 -4.673277



Complex **27**
C -4.313640 1.340206 0.021522
C -5.001523 0.148570 0.268194
C -4.488858 -1.025218 -0.294020
C -3.339765 -1.035412 -1.091513
C -2.665854 0.194626 -1.344469
C -3.172949 1.400750 -0.786315
H -4.707882 2.262926 0.440923
H -5.010188 -1.962466 -0.122668
C -1.667525 0.265942 -2.478452
C -0.253995 0.220793 -2.368467
C -2.244136 0.400750 -3.753383
C 0.553281 0.307257 -3.538608
C -1.459600 0.484619 -4.896457
C -0.073655 0.438591 -4.782729
H -1.924917 0.590518 -5.872569
H 0.543234 0.508642 -5.674584
P 0.459324 0.057651 -0.669147
C -2.587543 2.766167 -1.150224
H -1.667652 2.595225 -1.717328
C -6.319605 0.170886 1.034026
H -6.372646 1.140581 1.547177
C -6.442220 -0.922408 2.108796
H -6.409184 -1.927092 1.668604
H -5.649900 -0.842152 2.859177
H -7.407343 -0.827343 2.620863
C -7.501721 0.109203 0.042687
H -8.455169 0.198084 0.576683
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H -7.508806 -0.844294 -0.499871
C -2.900839 -2.343972 -1.753020
H -1.943794 -2.160017 -2.253567
C -2.674515 -3.486522 -0.745812
H -2.257745 -4.362353 -1.256947
H -1.979598 -3.186935 0.045393
H -3.607929 -3.795334 -0.262422
C -3.901838 -2.779970 -2.842907
H -3.558417 -3.699624 -3.331221
H -4.890764 -2.976945 -2.413021
H -4.018667 -2.010597 -3.613389
C -2.209791 3.622028 0.071787
H -1.714792 4.542712 -0.257122
H -3.089550 3.905469 0.660464
H -1.524043 3.087311 0.736168
C -3.545081 3.541119 -2.079510
H -4.494321 3.757796 -1.576255
H -3.097162 4.495981 -2.379231
H -3.770017 2.971220 -2.987677
C 1.705934 -1.301904 -0.801384
C 3.080677 -1.159662 -0.590002
C 1.190441 -2.582250 -1.039813
C 3.918255 -2.277858 -0.617019
H 3.515521 -0.185514 -0.399317
C 2.029302 -3.695416 -1.061746
H 0.125642 -2.721901 -1.194555
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C 1.399816 1.622959 -0.378714
C 2.177506 1.751192 0.781471
C 1.233371 2.745799 -1.201354
C 2.773602 2.971673 1.105491
H 2.299221 0.911432 1.455630
C 1.823085 3.965468 -0.864630
H 0.643019 2.677304 -2.107540
C 2.597430 4.087675 0.289508
H 3.057073 5.034515 0.546007
C 5.407085 -2.094684 -0.457670
C 1.414511 -5.063170 -1.212461
C 3.556818 3.066719 2.391709
C 1.551541 5.176219 -1.720766
F 2.309637 -5.978321 -1.632647
F 0.912859 -5.499262 -0.034524
F 0.389794 -5.052931 -2.094941
F 5.986876 -3.179710 0.094492
F 6.003514 -1.890833 -1.654816
F 5.698542 -1.029319 0.316400

F 4.250565 4.219074 2.477411
F 4.431855 2.047188 2.510623
F 2.735004 3.008394 3.465800
F 1.401085 4.844418 -3.020858
F 2.545036 6.083417 -1.638400
F 0.411121 5.799585 -1.338889
Pd -1.087997 -0.385802 1.057756
C 0.329598 -0.891663 2.401962
C 0.801157 -2.208015 2.450209
C 0.837351 0.053341 3.300801
C 1.791070 -2.566856 3.373337
H 0.410131 -2.966714 1.777967
C 1.835806 -0.308024 4.213930
H 0.468385 1.074321 3.299863
C 2.315280 -1.618315 4.252744
H 2.148561 -3.593641 3.399969
H 2.231538 0.443142 4.892768
H 3.085797 -1.898832 4.965746
N -2.436834 -0.805191 2.540003
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C -2.485240 1.541522 3.319153
H -2.048737 1.822926 4.283996
H -1.747597 1.706240 2.529021
H -3.344594 2.198333 3.148008
O -3.825906 -0.195320 4.251025
C -2.782295 -2.199581 2.805695
H -2.974331 -2.349300 3.872948
H -3.685000 -2.503292 2.258315
H -1.961056 -2.850429 2.491989
H -3.326054 0.442142 -3.832085
C 2.066680 0.255806 -3.537209
H 2.514745 0.859002 -2.743936
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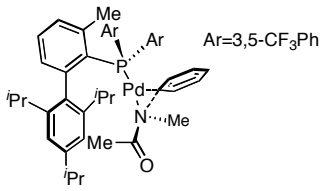

Transition State **13-TS**
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C -4.481774 -0.980839 -0.343376
C -3.395930 -0.909397 -1.223543
C -2.765677 0.345191 -1.438105
C -3.244568 1.495574 -0.763627
H -4.705670 2.245930 0.621198
H -4.968743 -1.940880 -0.194916
C -1.768074 0.492824 -2.563388
C -0.352824 0.422696 -2.451317
C -2.339901 0.723962 -3.825997
C 0.454158 0.581485 -3.613891
C -1.552502 0.877815 -4.960290
C -0.168034 0.806181 -4.847710
H -2.014500 1.057188 -5.927284
H 0.452175 0.930145 -5.731507
P 0.359663 0.132074 -0.762426
C -2.663271 2.886450 -1.017115
H -1.761712 2.766695 -1.625633
C -6.217413 0.070709 1.209914
H -6.299695 1.037350 1.725650
C -6.143591 -1.022734 2.290258
H -6.059915 -2.021730 1.844790
H -5.293030 -0.877335 2.963514
H -7.057424 -1.013649 2.896277
C -7.483053 -0.095563 0.342954
H -8.384024 -0.075606 0.967604
H -7.564999 0.704612 -0.401340
H -7.469297 -1.051725 -0.194323
C -2.968485 -2.167720 -1.980995
H -2.035956 -1.939473 -2.508051
C -2.682926 -3.361220 -1.050314
H -2.254856 -4.194469 -1.620130
H -1.973086 -3.082318 -0.263173
H -3.593304 -3.726216 -0.561569
C -4.007938 -2.554413 -3.052881
H -3.677697 -3.441552 -3.606413
H -4.978011 -2.784281 -2.596620
H -4.160755 -1.743267 -3.772839
C -2.240986 3.608742 0.275739
H -1.719374 4.540602 0.030043
H -3.104369 3.863140 0.901261
H -1.566123 2.987851 0.873850
C -3.640708 3.757939 -1.832056
H -4.577632 3.917820 -1.285667
H -3.198556 4.740125 -2.037641
H -3.888659 3.289649 -2.790924
C 1.638568 -1.190129 -0.984384
C 3.011429 -1.029794 -0.769982
C 1.149414 -2.473979 -1.259973
C 3.870674 -2.130511 -0.831218
H 3.426055 -0.053534 -0.546164
C 2.009299 -3.569363 -1.318566
H 0.086116 -2.627713 -1.410631
C 3.377810 -3.406539 -1.102306
H 4.045974 -4.258878 -1.134150
C 1.288541 1.680032 -0.355996
C 1.993685 1.730812 0.857145
C 1.178277 2.852992 -1.113733
C 2.573855 2.922799 1.292826
H 2.069176 0.847635 1.483362
C 1.748601 4.046466 -0.663098
H 0.642184 2.847263 -2.056211
C 2.450860 4.091059 0.540389
H 2.894239 5.016853 0.885551
C 5.354549 -1.923554 -0.661416
C 1.419680 -4.941874 -1.512546
C 3.277973 2.933687 2.626374
C 1.529988 5.304776 -1.462701

F 2.336827 -5.835685 -1.932173
F 0.897260 -5.414144 -0.356114
F 0.413795 -4.928846 -2.416789
F 5.959551 -3.022584 -0.165062
F 5.948177 -1.644242 -1.845026
F 5.623945 -0.893903 0.167716
F 3.948024 4.083756 2.838528
F 4.159367 1.917438 2.729411
F 2.394870 2.789133 3.645176
F 1.607004 5.069805 -2.790571
F 2.431210 6.260361 -1.160902
F 0.300959 5.826775 -1.229332
Pd -1.005119 -0.520847 1.004828
C 0.112261 -1.224324 2.657944
C 0.667382 -2.507811 2.489338
C 0.800477 -0.292718 3.460221
C 1.891095 -2.830049 3.081513
H 0.172910 -3.252951 1.877073
C 2.024340 -0.631381 4.041419
H 0.408721 0.703305 3.618898
C 2.579278 -1.900952 3.862896
H 2.304783 -3.822820 2.920120
H 2.544239 0.117963 4.632501
H 3.526553 -2.160462 4.326078
N -1.816834 -1.239209 2.811320
C -2.427489 -0.371874 3.705454
C -2.113307 1.112683 3.626510
H -1.664208 1.438058 4.571518
H -1.462533 1.383482 2.792284
H -3.062055 1.646867 3.515962
O -3.250334 -0.778966 4.524562
C -2.271048 -2.628702 2.932206
H -1.894543 -3.097300 3.849870
H -3.362408 -2.648183 2.960511
H -1.933930 -3.202437 2.070037
H -3.421342 0.783250 -3.902553
C 1.967001 0.511889 -3.616363
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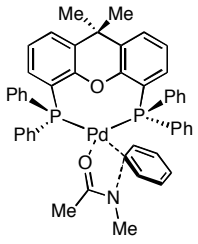
H 2.321221 -0.523302 -3.559963
H 2.359023 0.942709 -4.542370



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Pd 0.731396 -0.992934 -0.427612
P -1.844342 -1.166540 0.097047
P 1.412712 1.253783 0.171378
O -1.555076 1.704547 -0.153035
C 2.425400 -2.044012 0.016773
C 1.926926 -3.323918 0.339182
H 1.072352 -3.723615 -0.198237
C 2.552753 -4.090641 1.328404
H 2.144550 -5.068124 1.577363
C 3.706491 -3.627359 1.964183
H 4.199342 -4.231156 2.721474
C 4.236565 -2.388905 1.589348
H 5.145689 -2.020800 2.060986
C 3.616684 -1.603576 0.613196
H 4.059089 -0.657225 0.330410
C -2.747311 1.329553 -0.744985
C -3.083022 -0.028351 -0.659917
C -4.286904 -0.433742 -1.252065
H -4.578255 -1.477656 -1.211573
C -5.099465 0.490764 -1.908396
H -6.026544 0.162565 -2.369951
C -4.729537 1.834682 -1.976662
H -5.376612 2.536141 -2.492424
C -3.543060 2.283651 -1.385988
C -3.081681 3.743419 -1.339109
C -1.549844 3.740685 -1.426804
C -0.797934 4.734156 -2.060379
H -1.298265 5.539983 -2.586364
C 0.594959 4.710052 -2.016019
H 1.166976 5.492349 -2.506790
C 1.259882 3.690202 -1.338102
H 2.342409 3.693252 -1.310666
C 0.550859 2.656372 -0.704562
C -0.850701 2.714427 -0.774534
C -3.723939 4.585695 -2.454363
H -4.813866 4.587549 -2.357344
H -3.465728 4.207909 -3.449372
H -3.404257 5.629973 -2.386619
C -3.492323 4.345019 0.036427
H -4.583019 4.332174 0.145961
H -3.146342 5.382123 0.116950
H -3.059161 3.775092 0.864089
C -2.607879 -2.828155 -0.191249
C -2.160007 -3.582771 -1.288686
H -1.356289 -3.201162 -1.912790
C -2.723734 -4.833363 -1.555400
H -2.368054 -5.410136 -2.405472
C -3.726778 -5.347512 -0.732268
H -4.157701 -6.323780 -0.939772
C -4.169822 -4.606209 0.365875
H -4.946529 -5.002526 1.015131
C -3.615078 -3.354350 0.635336
H -3.964311 -2.788299 1.493631
C -2.102125 -0.940214 1.914878
C -3.133590 -0.167785 2.467011
H -3.833169 0.348653 1.816667
C -3.275867 -0.059383 3.852854
H -4.079621 0.545874 4.264577
C -2.396295 -0.728546 4.704230
H -2.510483 -0.646621 5.781977
C -1.365508 -1.501267 4.163628

H -0.673256 -2.023552 4.818896
C -1.213330 -1.599405 2.781043
H -0.398171 -2.191218 2.371140
C 3.168664 1.648288 -0.264839
C 3.656197 1.172239 -1.494153
H 3.029604 0.531999 -2.109166
C 4.957671 1.469939 -1.899119
H 5.322908 1.093879 -2.851049
C 5.794274 2.230100 -1.077392
H 6.810812 2.453538 -1.390580
C 5.322721 2.691678 0.152571
H 5.970120 3.276430 0.801050
C 4.015746 2.406298 0.556446
H 3.658020 2.776197 1.512008
C 1.300772 1.754077 1.948809
C 1.629985 0.794946 2.920471
H 1.913098 -0.207506 2.612684
C 1.599869 1.121880 4.276203
H 1.861898 0.369967 5.015723
C 1.223183 2.403887 4.682219
H 1.191017 2.654616 5.739310
C 0.883120 3.360510 3.724492
H 0.585633 4.359737 4.032297
C 0.926130 3.040356 2.365812
H 0.668871 3.796199 1.630310
O 0.541820 -2.296580 -2.240410
C 1.682772 -2.470011 -2.805739
N 2.801446 -2.106265 -2.239126
C 1.657664 -3.147622 -4.172150
H 0.635601 -3.185893 -4.552725
H 2.293945 -2.619959 -4.891588
H 2.041711 -4.172709 -4.090037
C 4.094716 -2.441414 -2.788597
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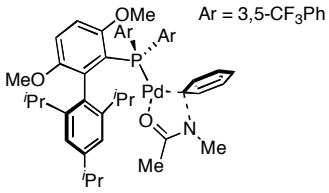

Transition State **15-TS**
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C -2.822379 0.263351 -0.928499
C -3.293797 1.430483 -0.270849
H -4.660728 2.203063 1.184000
H -4.840307 -2.024253 0.595001
C -1.897146 0.406590 -2.111475
C -0.488204 0.397628 -2.045120
C -2.517173 0.598663 -3.373832
C 0.276307 0.599360 -3.226711
C -1.751073 0.768085 -4.524413
C -0.357464 0.772264 -4.453343
H -2.223150 0.910309 -5.489228
H 0.215611 0.922128 -5.360440
P 0.373132 0.084910 -0.436577
C -2.770535 2.825546 -0.607212
H -1.951118 2.713722 -1.323868
C -6.001788 -0.035092 2.032434
H -6.132987 -1.104679 2.246838
C -7.333127 0.488906 1.458088
H -7.262200 1.556512 1.216337
H -7.608815 -0.043322 0.540589
H -8.145727 0.363040 2.184082
C -5.654940 0.662530 3.360279
H -6.417667 0.443180 4.117588
H -4.679149 0.328948 3.724968
H -5.617607 1.752539 3.243144
C -2.999633 -2.276624 -1.355675
H -2.144042 -2.037670 -1.997711
C -2.565879 -3.407602 -0.402466
H -2.162669 -4.253177 -0.972533
H -1.798736 -3.068044 0.303099
H -3.411823 -3.779705 0.187321
C -4.134906 -2.756526 -2.283455
H -3.812893 -3.629132 -2.864817
H -5.017748 -3.049379 -1.702852
H -4.436598 -1.966520 -2.977768
C -2.200704 3.554880 0.624980
H -1.712301 4.487595 0.320480
H -2.988463 3.807541 1.344355
H -1.462836 2.935704 1.146223
C -3.855668 3.676799 -1.297312
H -4.700185 3.862281 -0.623198
H -3.447772 4.649532 -1.597817
H -4.243680 3.172049 -2.188187
O -3.885659 0.609704 -3.372884
O 1.630929 0.635925 -3.072115
C -4.561300 0.816860 -4.603652
H -4.335378 0.022849 -5.327791
H -5.625548 0.793912 -4.364085
H -4.309092 1.790894 -5.043455
C 2.453360 0.809707 -4.216900
H 2.268155 1.777927 -4.699247
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H 2.302028 0.003013 -4.945184
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C 2.999394 -1.074002 -0.719598
C 1.120410 -2.415428 -1.398835
C 3.854563 -2.139999 -1.005480
H 3.420127 -0.145157 -0.353830
C 1.981781 -3.471960 -1.703011
H 0.052393 -2.548137 -1.538033
C 3.354956 -3.344592 -1.502543
H 4.022970 -4.166717 -1.728353
C 1.328113 1.634804 -0.106599

C 2.189299 1.707972 1.000651
C 1.114133 2.791642 -0.867866
C 2.844389 2.906251 1.304668
H 2.353332 0.840457 1.631346
C 1.745842 3.989819 -0.537038
H 0.452184 2.766763 -1.724302
C 2.622603 4.053747 0.545061
H 3.129204 4.979502 0.788353
Pd -0.988811 -0.550679 1.349924
C 0.479132 -1.051046 2.720747
C 1.611378 -1.796850 2.347993
C 0.594886 -0.104911 3.760909
C 2.846848 -1.553356 2.958013
H 1.527067 -2.561241 1.582751
C 1.831948 0.117111 4.366875
H -0.281778 0.446189 4.087094
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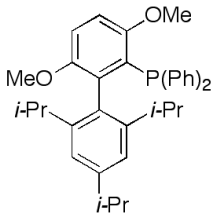
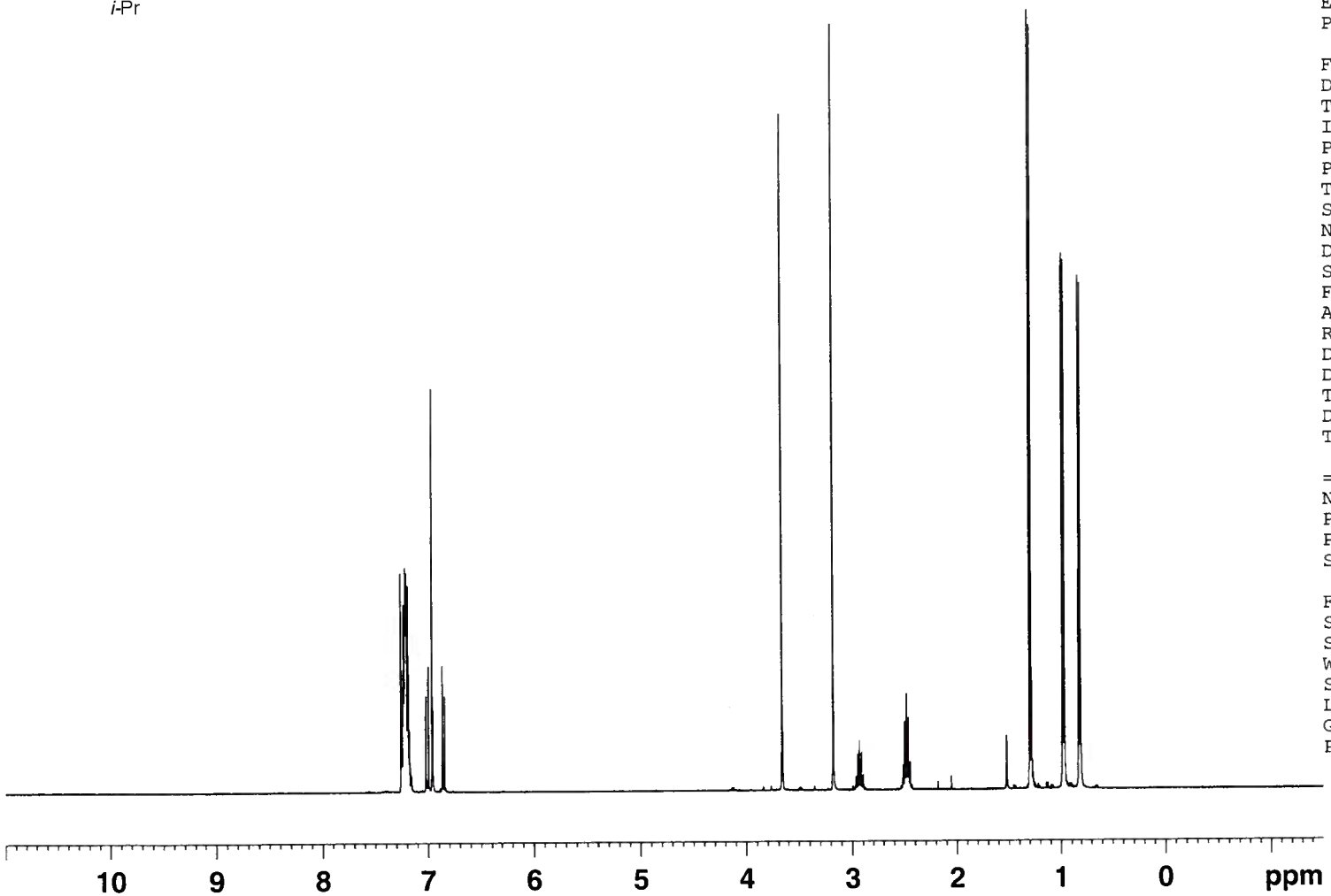
O -2.458566 -0.828898 2.974061
C -2.114027 -1.903809 3.568017
N -0.968773 -2.482778 3.282435
C -0.460620 -3.627730 4.005684
H 0.593901 -3.755710 3.737650
H -0.511069 -3.516355 5.099733
H -0.986053 -4.554921 3.731953
C -3.052928 -2.472561 4.619486
H -2.628475 -2.320312 5.620105
H -4.019891 -1.970151 4.569115
H -3.195430 -3.550545 4.487598
C 3.766624 2.965414 2.497615
C 1.426645 5.231291 -1.326593
C 5.324742 -2.009678 -0.704908
C 1.392477 -4.742149 -2.258641
F 2.418147 6.143766 -1.260059
F 0.302884 5.834899 -0.868420
F 1.212919 4.953600 -2.632681
F 4.572846 1.885316 2.556693
F 4.558757 4.060596 2.462917
F 3.076886 3.013820 3.658362
F 6.073204 -2.805145 -1.499207
F 5.760440 -0.742199 -0.869006
F 5.599426 -2.359696 0.574136
F 2.313663 -5.717114 -2.393951
F 0.838936 -4.535834 -3.475975
F 0.408216 -5.219660 -1.462351

Reference 32: Gaussian 03, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al- Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.





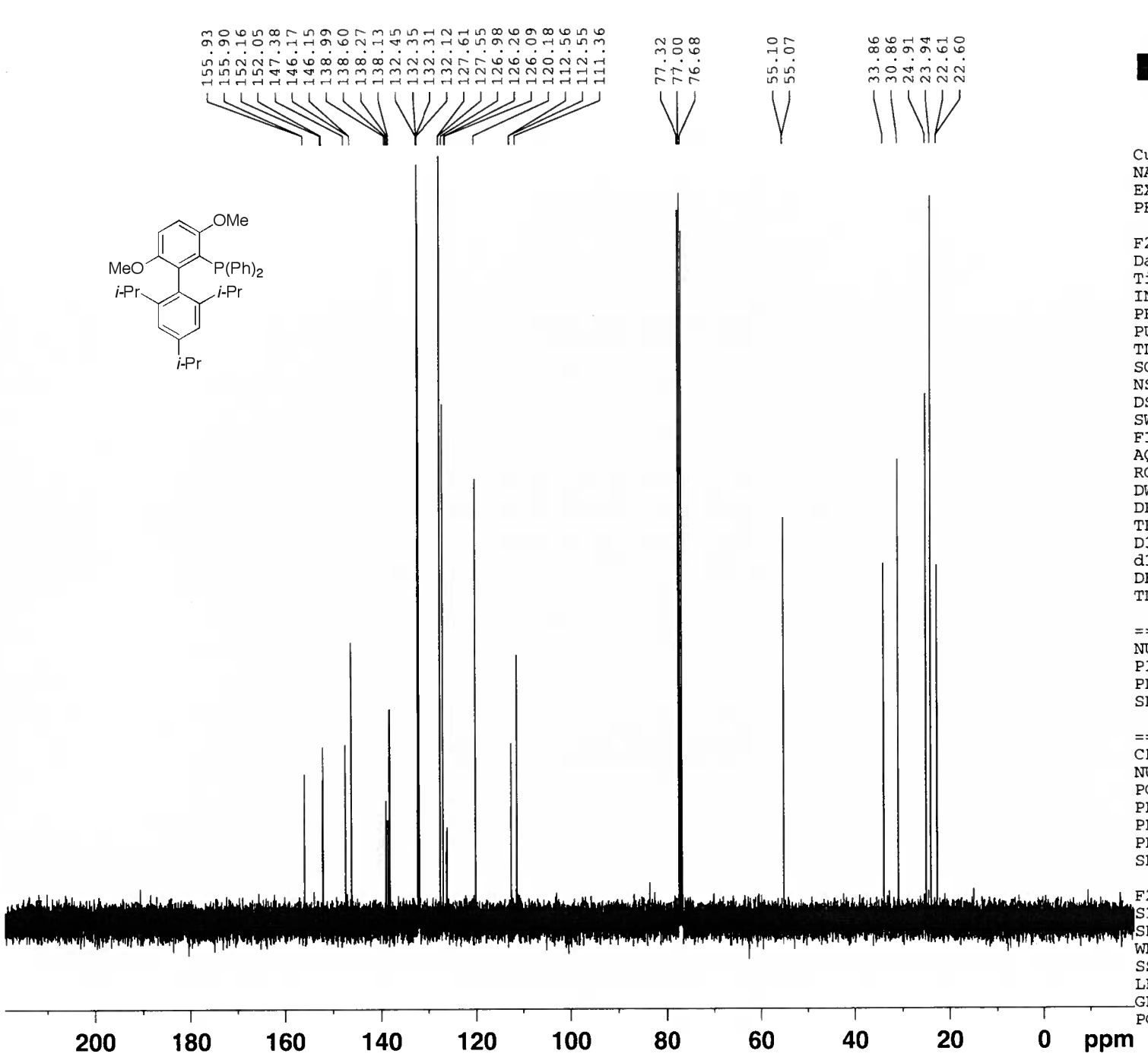
BRUKER

```
Current Data Parameters
NAME                  jdh-2-282
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080930
Time                      20.01
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          256
DW                       60.400 usec
DE                        6.00 usec
TE                       291.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.88 usec
PL1                       0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300094 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```



BRUKER

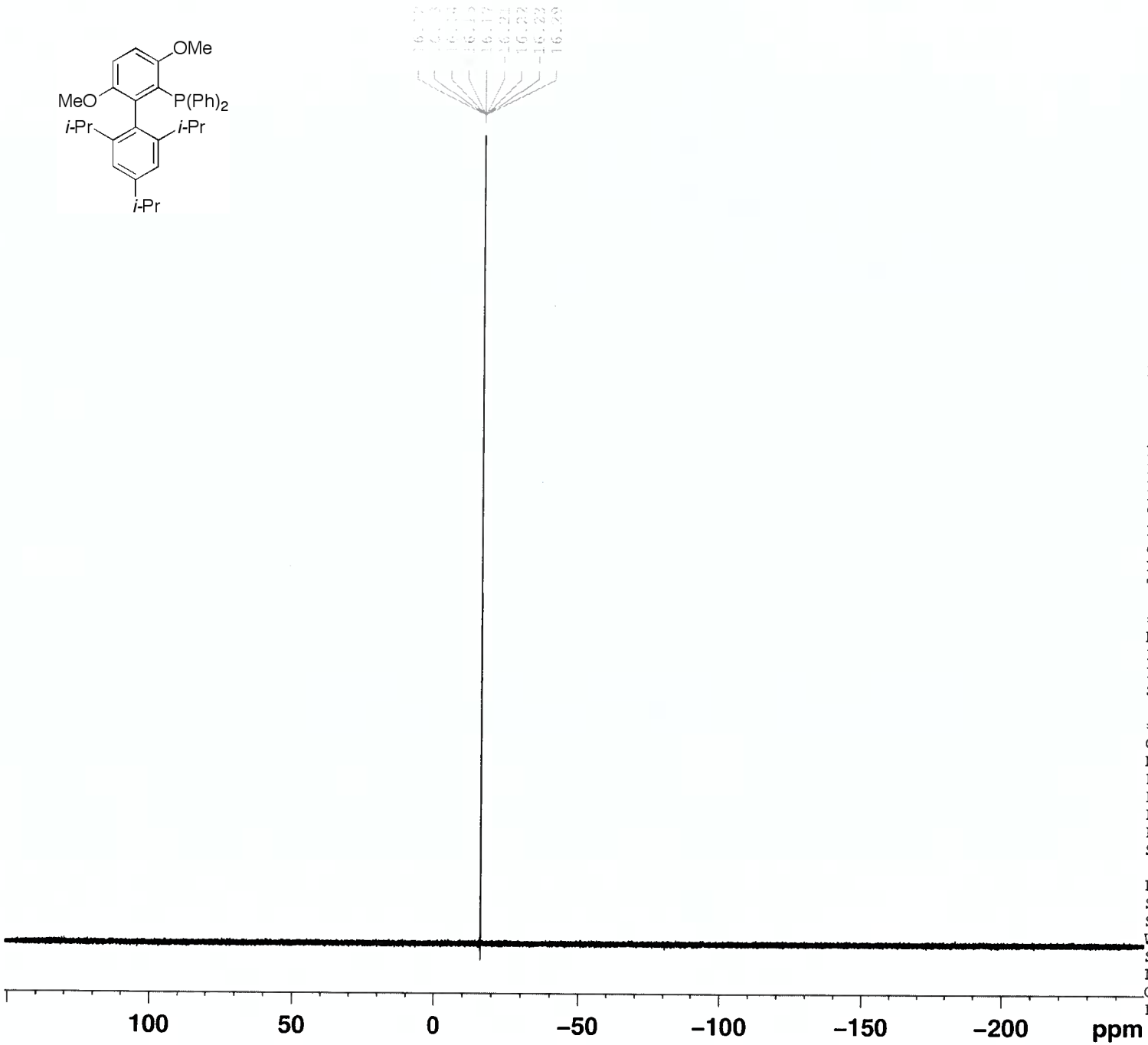
Current Data Parameters
NAME jdh-2-282-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080929
Time 16.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5160.6
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127768 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



BRUKER

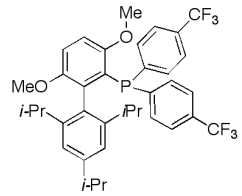
```
Current Data Parameters
NAME       jdh-2-282-p31
EXPNO                  1
PROCNO                 1

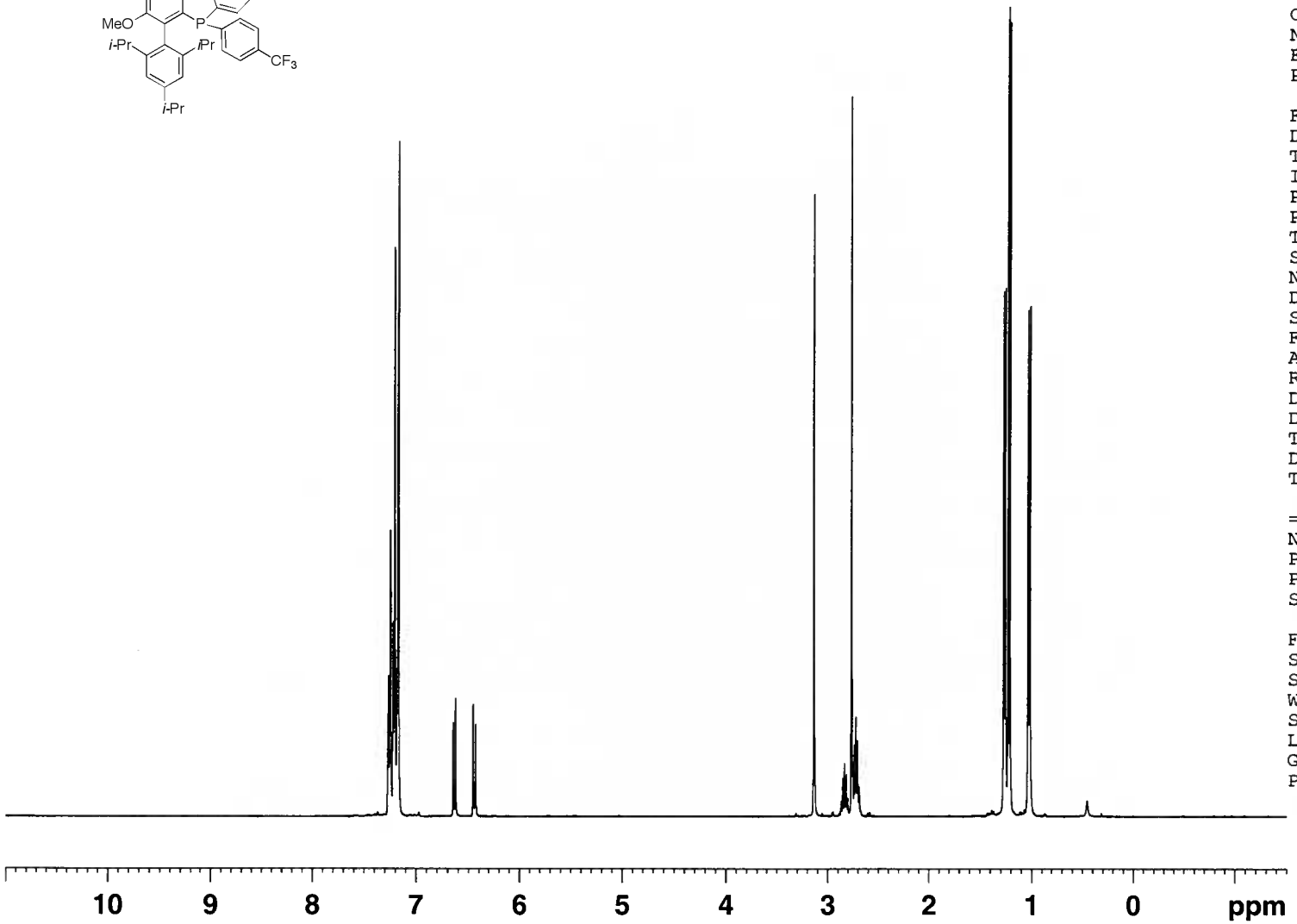
F2 - Acquisition Parameters
Date_           20080930
Time               20.03
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    4
SWH           64935.066 Hz
FIDRES         0.990830 Hz
AQ             0.5046772 sec
RG                 6502
DW                7.700 usec
DE                6.00 usec
TE                291.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                  9.25 usec
PL1                 3.00 dB
SFO1        161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2        400.1316000 MHz

F2 - Processing parameters
SI                 65536
SF          161.9755024 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.40
```





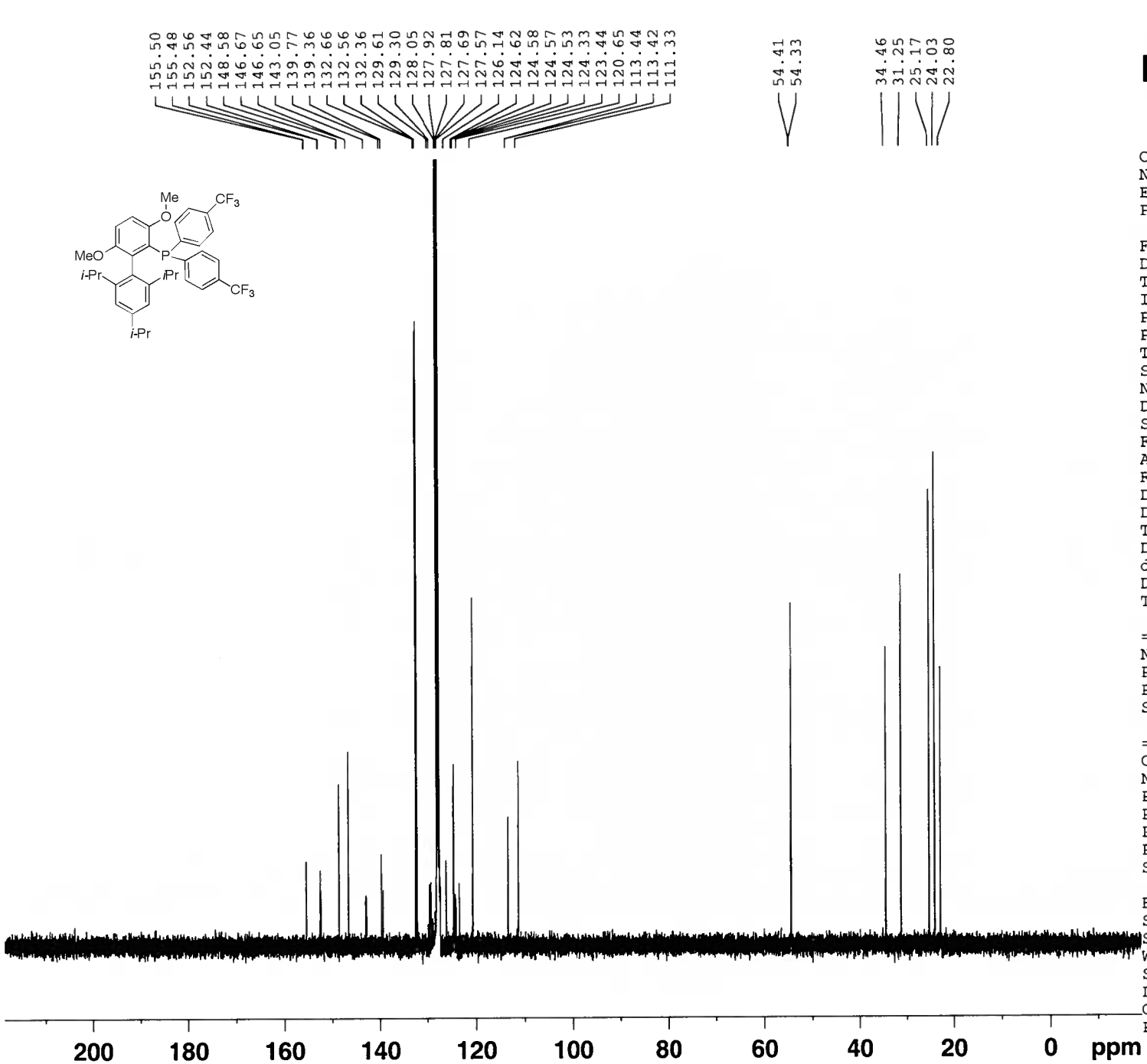
BRUKER

```
Current Data Parameters
NAME                  jdh-1-183
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080909
Time                      19.41
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          181
DW                        60.400 usec
DE                         6.00 usec
TE                        291.2 K
D1                   1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        13.88 usec
PL1                        0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                  400.1300220 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         1.00
```



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Current Data Parameters
NAME jdh-2-183-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080909	
Time	22.05	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	C6D6	
NS	1024	
DS	4	
SWH	23980.814	Hz
FIDRES	0.365918	Hz
AQ	1.3664756	sec
RG	1625.5	
DW	20.850	usec
DE	6.00	usec
TE	293.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	

======== CHANNEL f1 ========

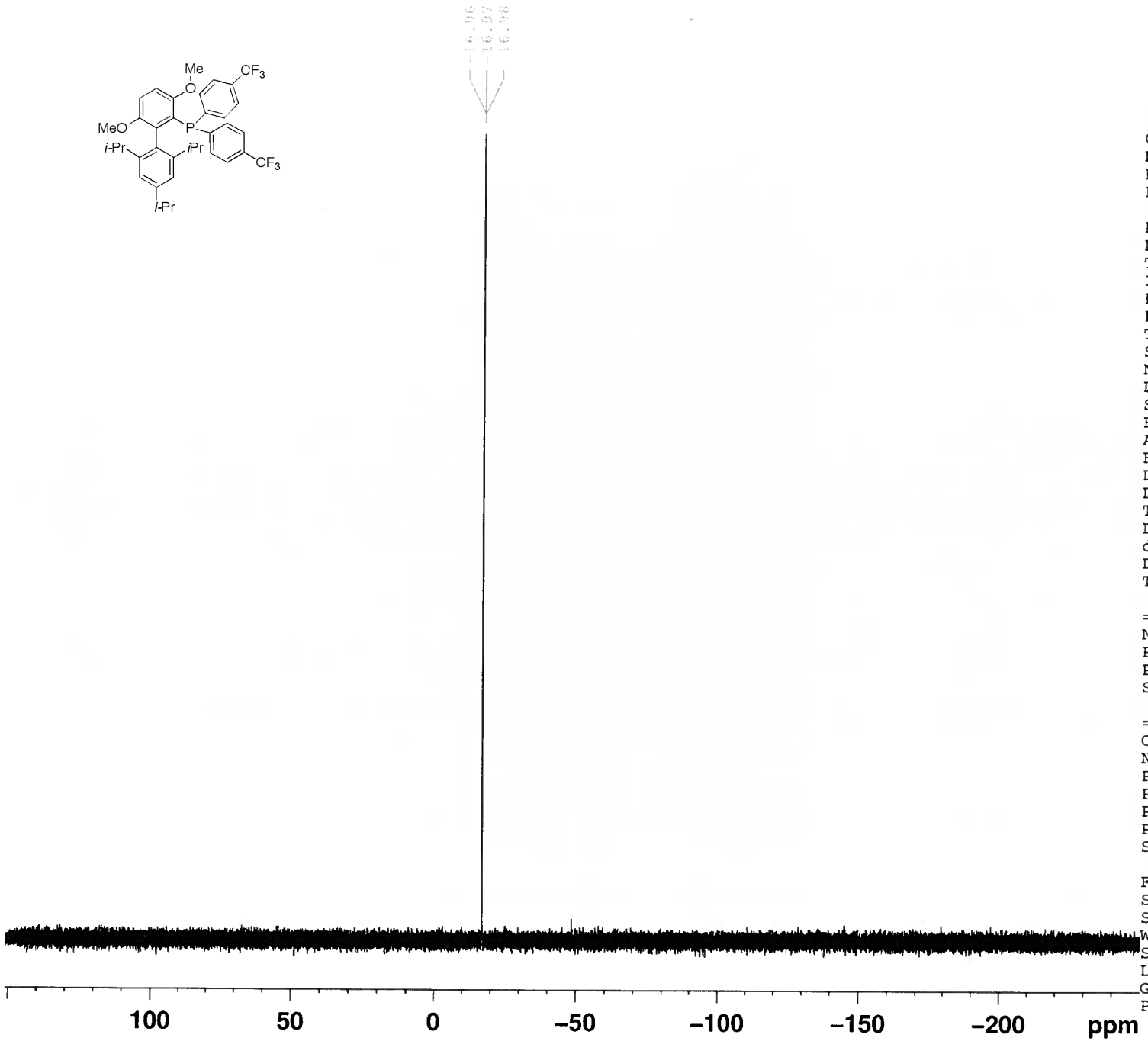
NUC1	13C	
P1	9.38	usec
PL1	0.00	dB
SFO1	100.6228298	MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	0.00	dB
PL12	16.10	dB
PL13	19.00	dB
SFO2	400.1316005	MHz

F2 - Processing parameters

SI	32768	
SF	100.6127690	MHz
WDW	no	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	



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Current Data Parameters
NAME jdh-1-183-p31
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080909
Time	19.43
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	16
DS	4
SWH	64935.066 Hz
FIDRES	0.990830 Hz
AQ	0.5046772 sec
RG	3649.1
DW	7.700 usec
DE	6.00 usec
TE	291.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

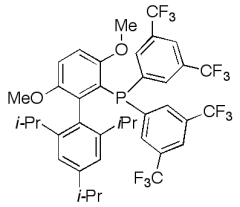
NUC1	31P
P1	9.25 usec
PL1	3.00 dB
SFO1	161.9674940 MHz

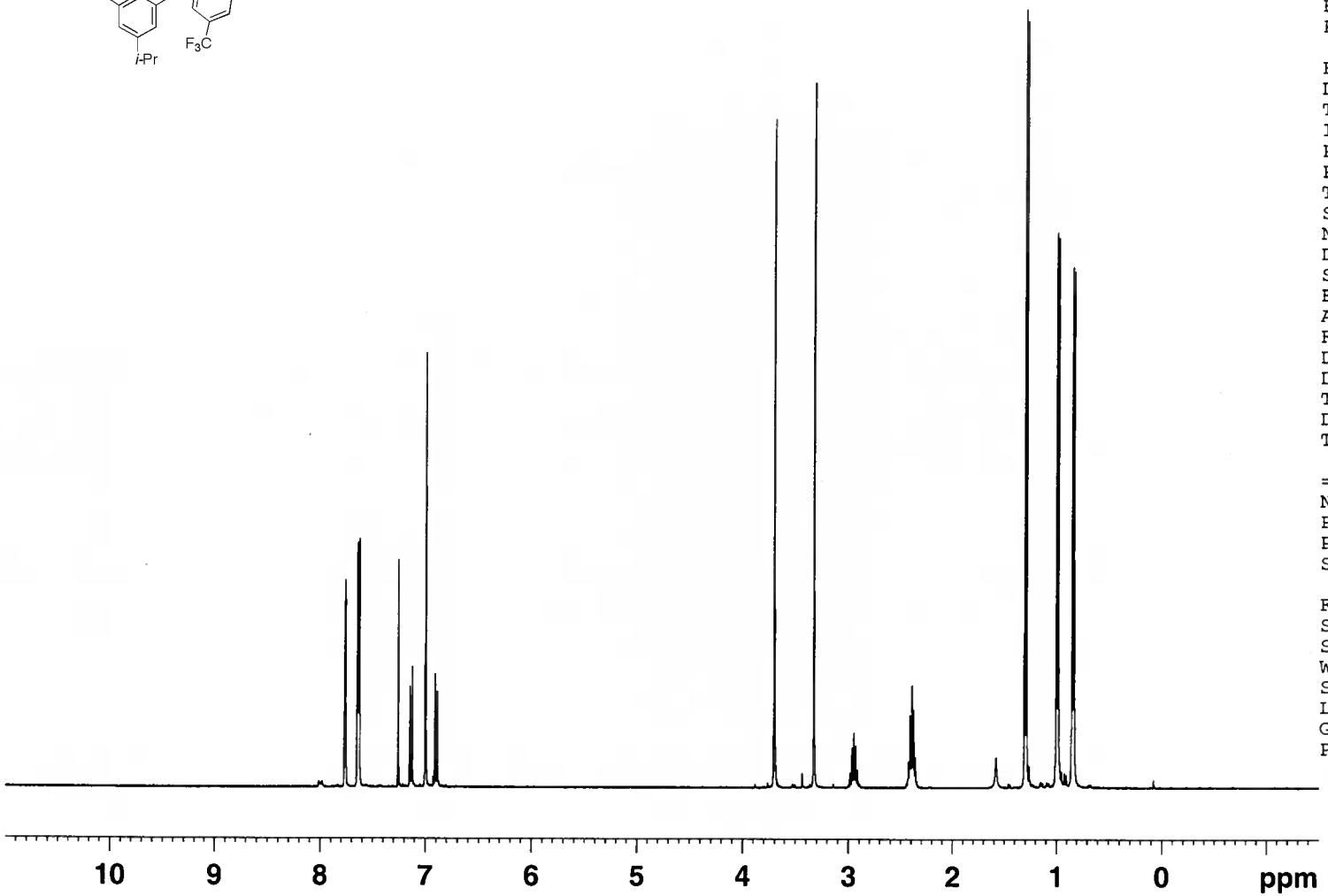
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316000 MHz

F2 - Processing parameters

SI	65536
SF	161.9755024 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40





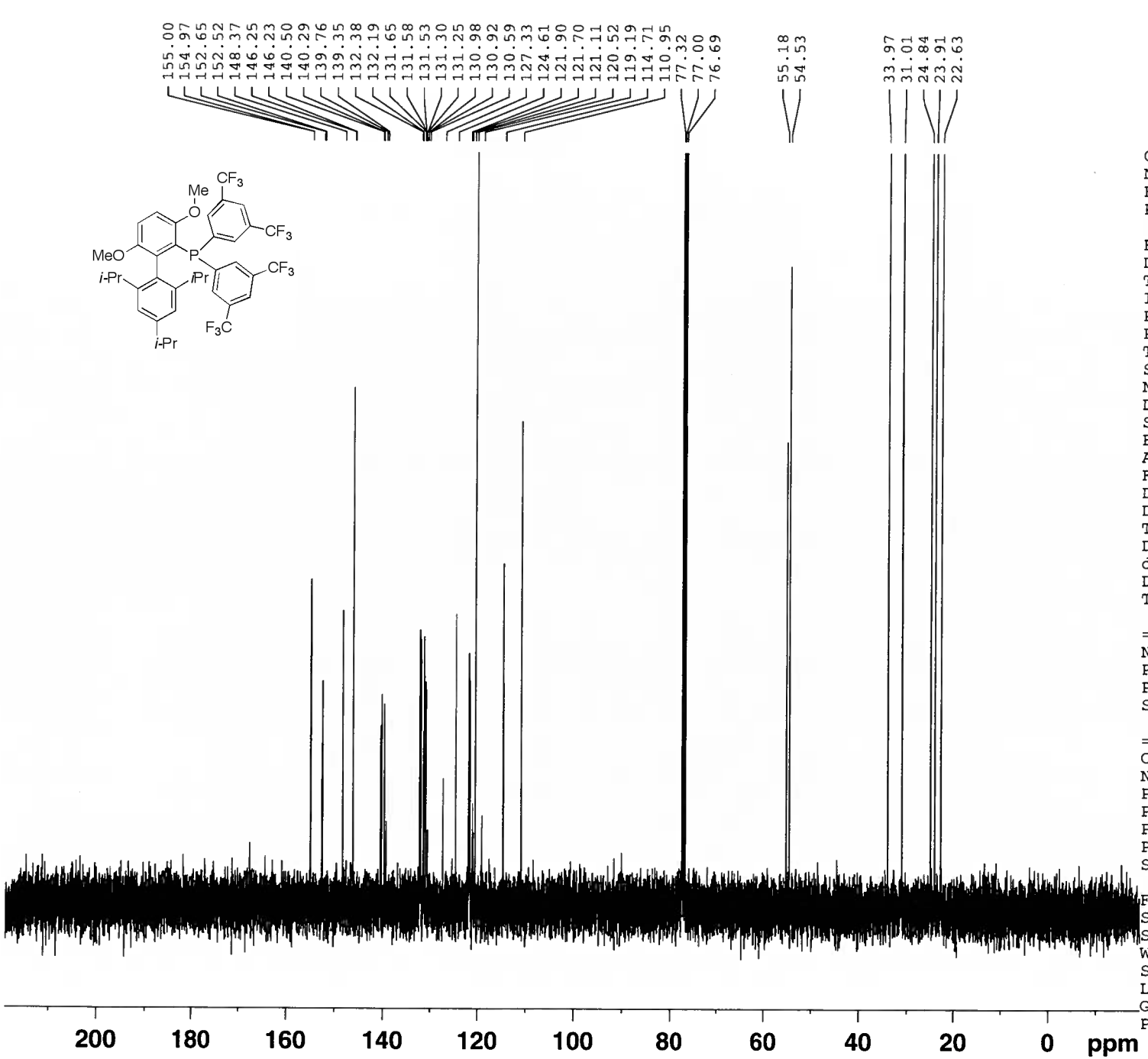
BRUKER

```
Current Data Parameters
NAME        jdh-2-233-H1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080906
Time               17.02
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                 287.4
DW                60.400 usec
DE                 6.00 usec
TE                292.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.88 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300095 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```



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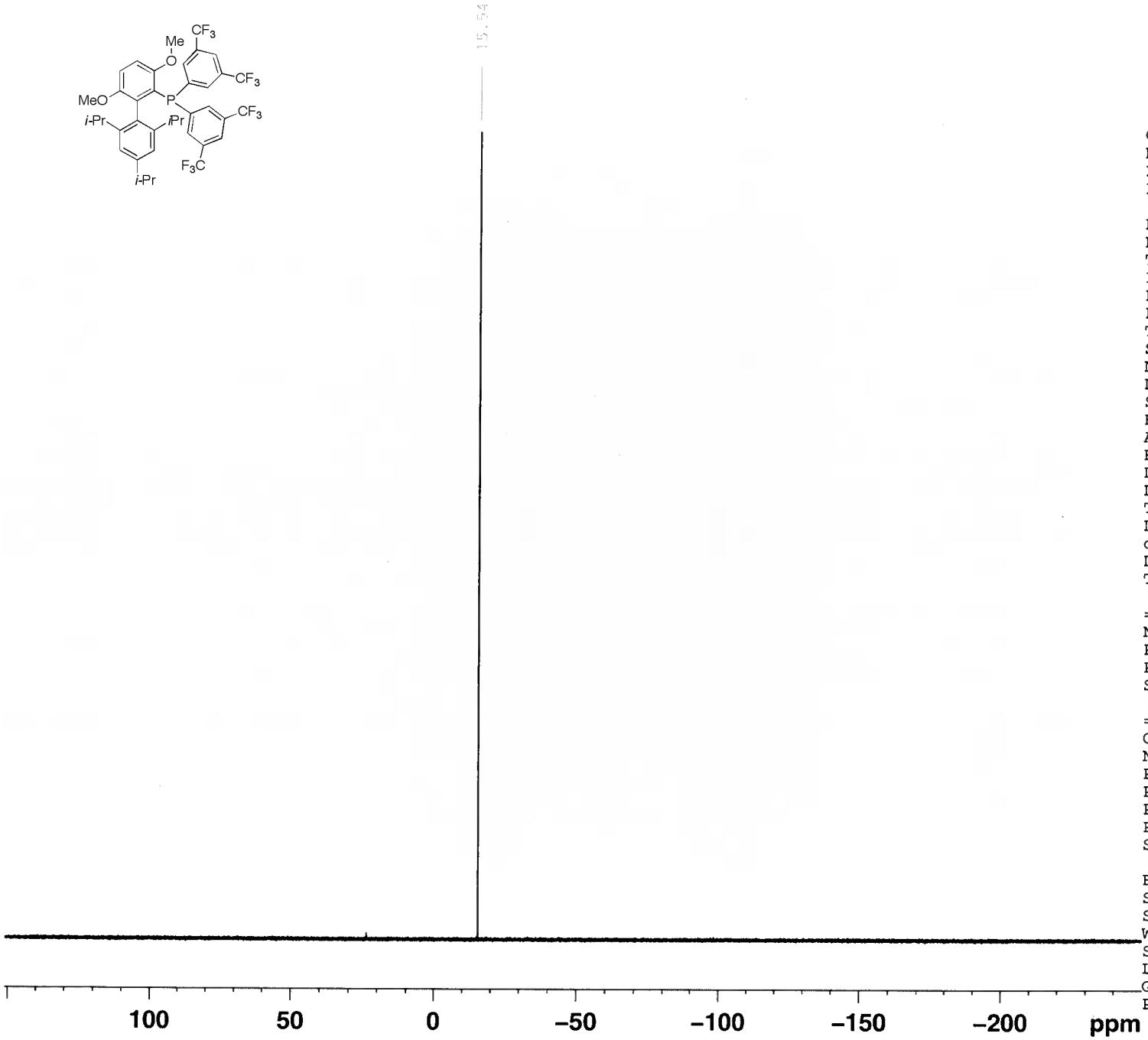
Current Data Parameters
NAME jdh-2-233-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080906
Time 14.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127701 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME jdh-2-233-p31
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080906
Time	14.07
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	16
DS	4
SWH	64935.066 Hz
FIDRES	0.990830 Hz
AQ	0.5046772 sec
RG	3251
DW	7.700 usec
DE	6.00 usec
TE	292.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

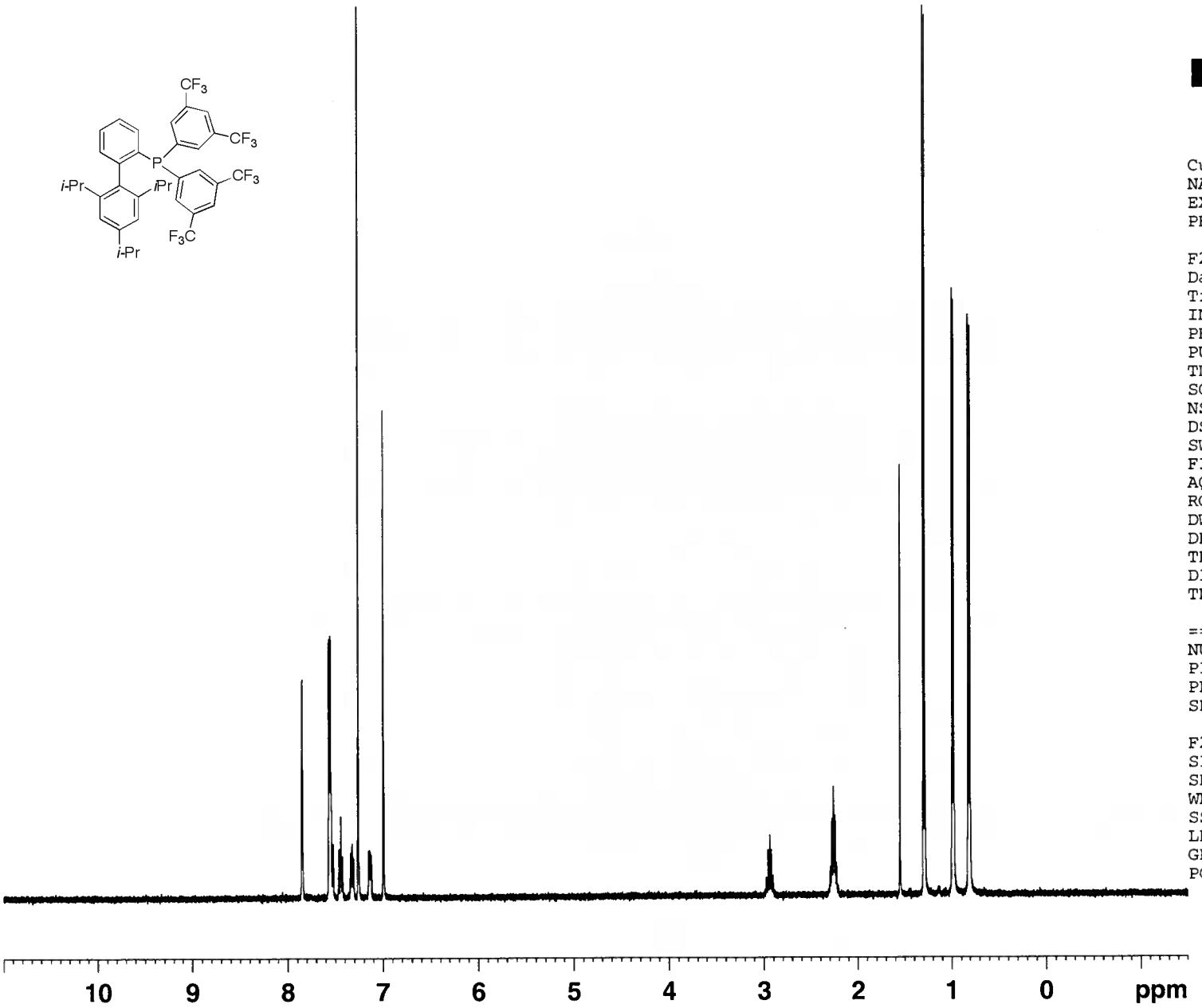
NUC1	31P
P1	9.25 usec
PL1	3.00 dB
SFO1	161.9674940 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316000 MHz

F2 - Processing parameters

SI	65536
SF	161.9755024 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



BRUKER

Current Data Parameters

NAME	jdh-1-253
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

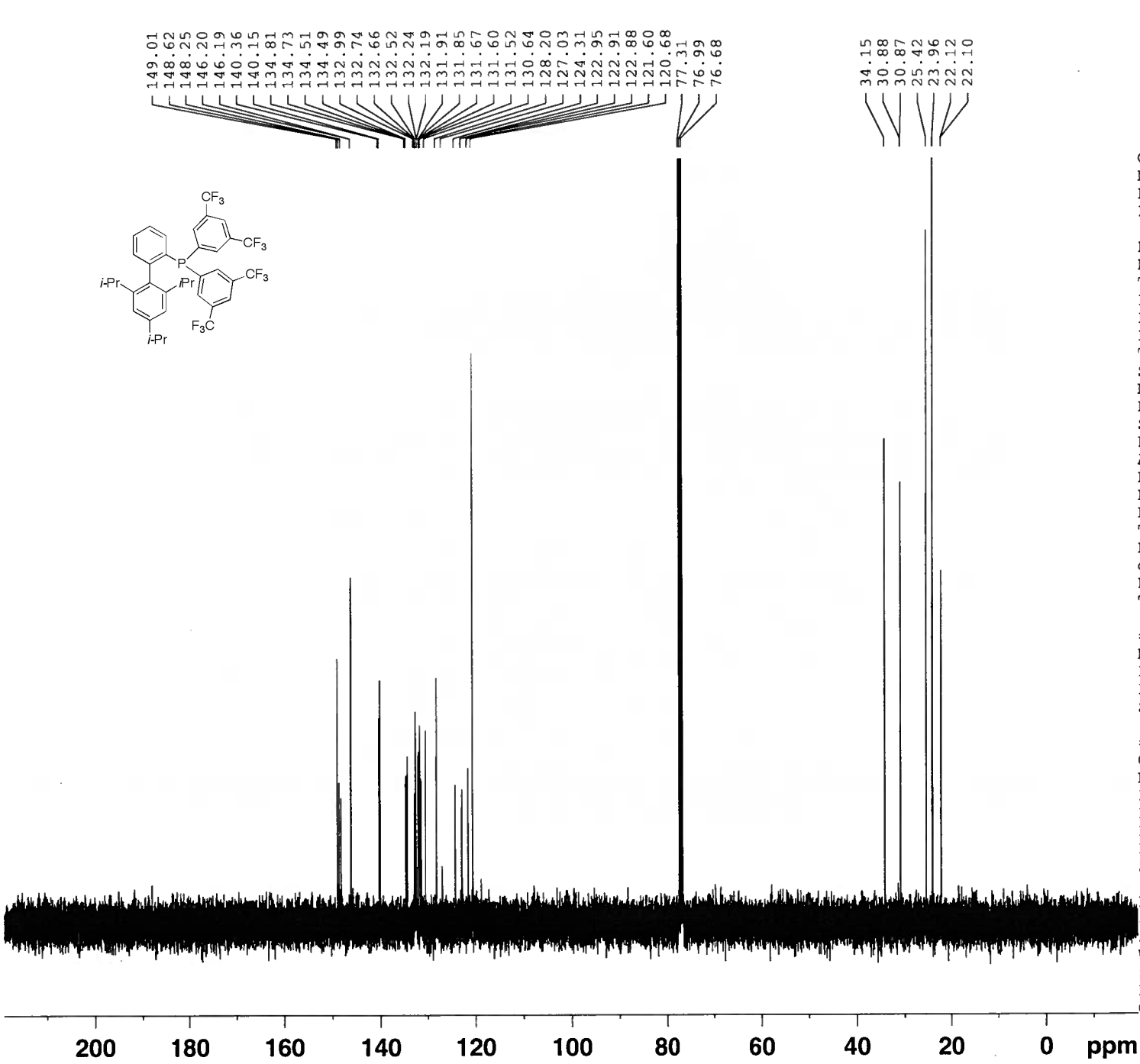
Date_	20080923
Time	12.19
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	287.4
DW	60.400 usec
DE	6.00 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	13.88 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	65536
SF	400.1300093 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



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Current Data Parameters

NAME	jdh-2-253
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080923
Time	17.21
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

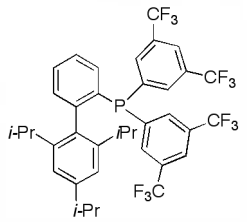
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

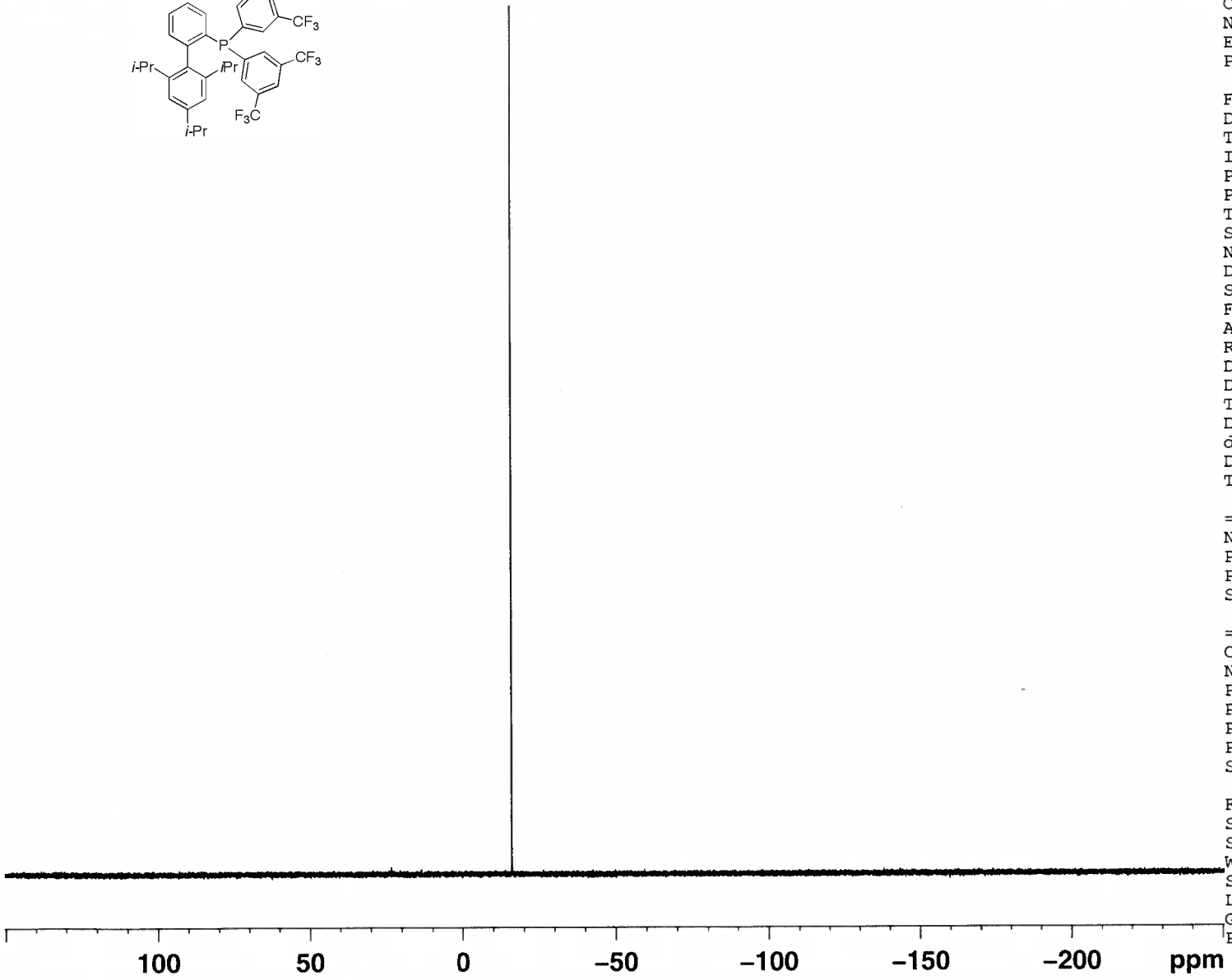
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127719 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40





BRUKER

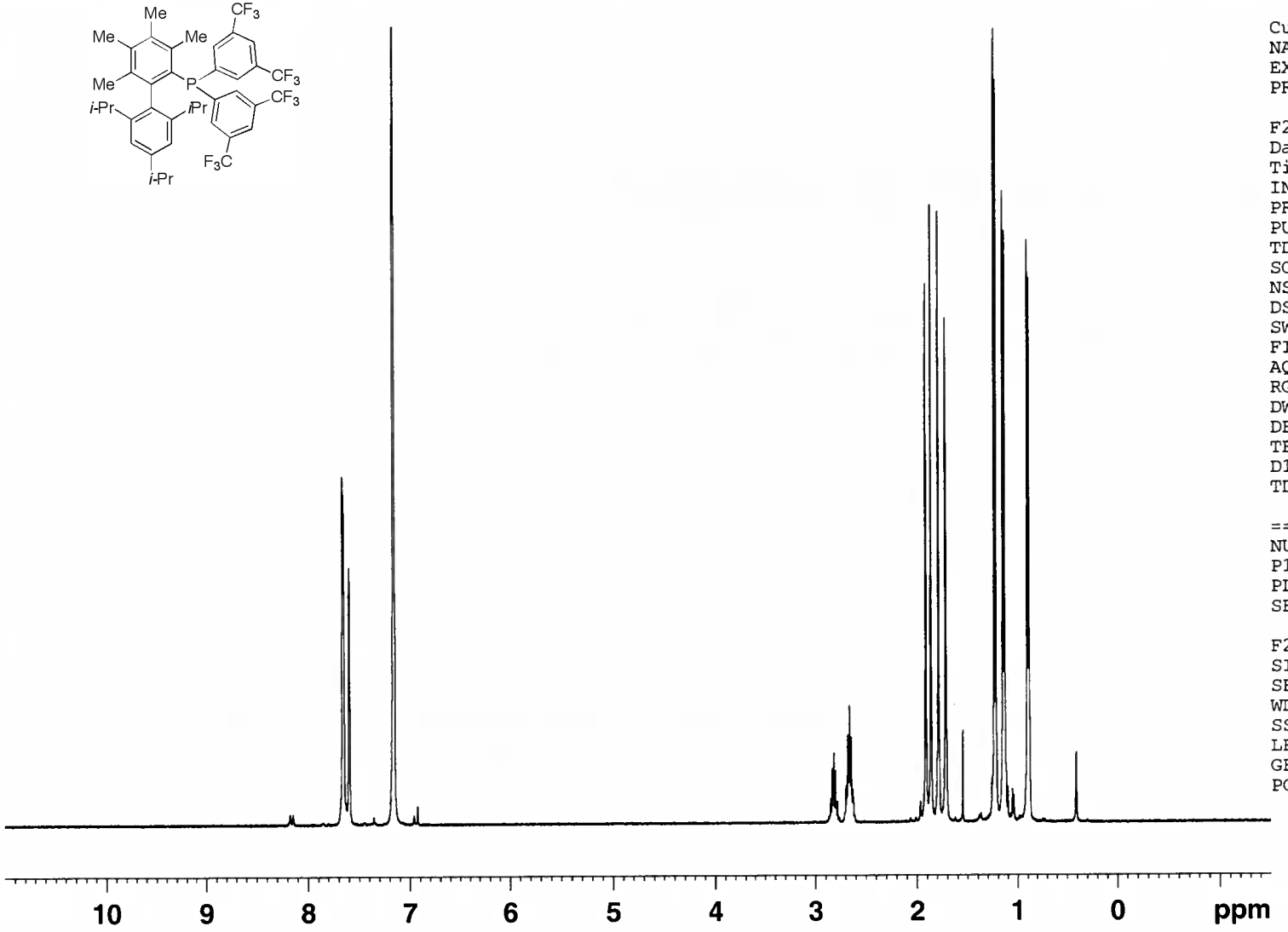
```
Current Data Parameters
NAME       jdh-2-253-p31
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080923
Time               17.26
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    4
SWH           64935.066 Hz
FIDRES        0.990830 Hz
AQ            0.5046772 sec
RG                22800
DW                7.700 usec
DE                6.00 usec
TE                293.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                10.00 usec
PL1                0.00 dB
SFO1        161.9674942 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -1.00 dB
PL12              14.52 dB
PL13              18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          161.9755930 MHz
WDW                  no
SSB                   0
LB                0.00 Hz
GB                    0
PC                1.40
```



BRUKER

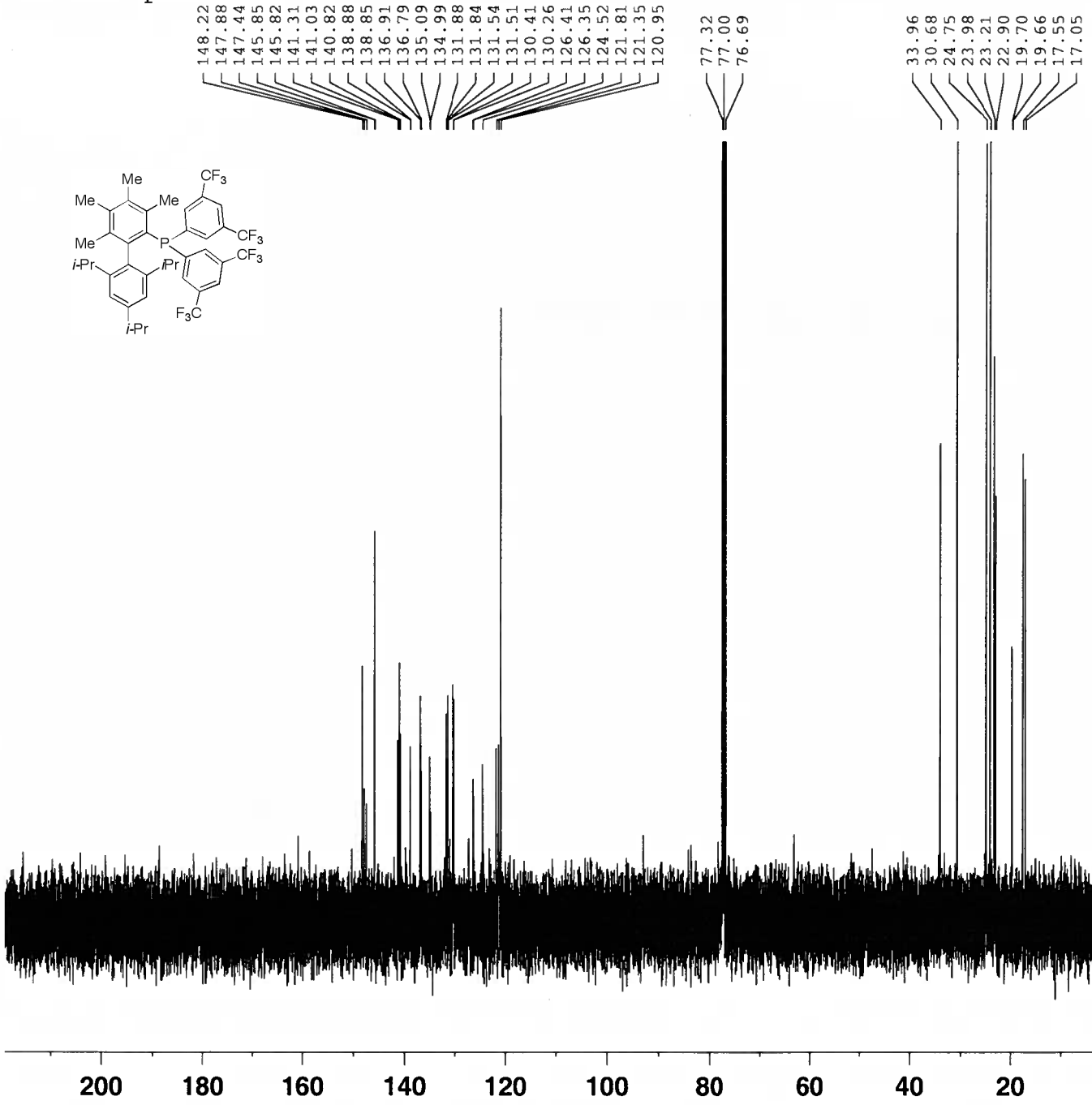
```
Current Data Parameters
NAME         jdh-2-286-6
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20081008
Time               13.09
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   256
DW                60.400 usec
DE                 6.00 usec
TE                292.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.88 usec
PL1                 0.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300282 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

13C-dcif parameter set



Current Data Parameters

NAME	jdh-2-286-c13
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20081006
Time	21.03
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

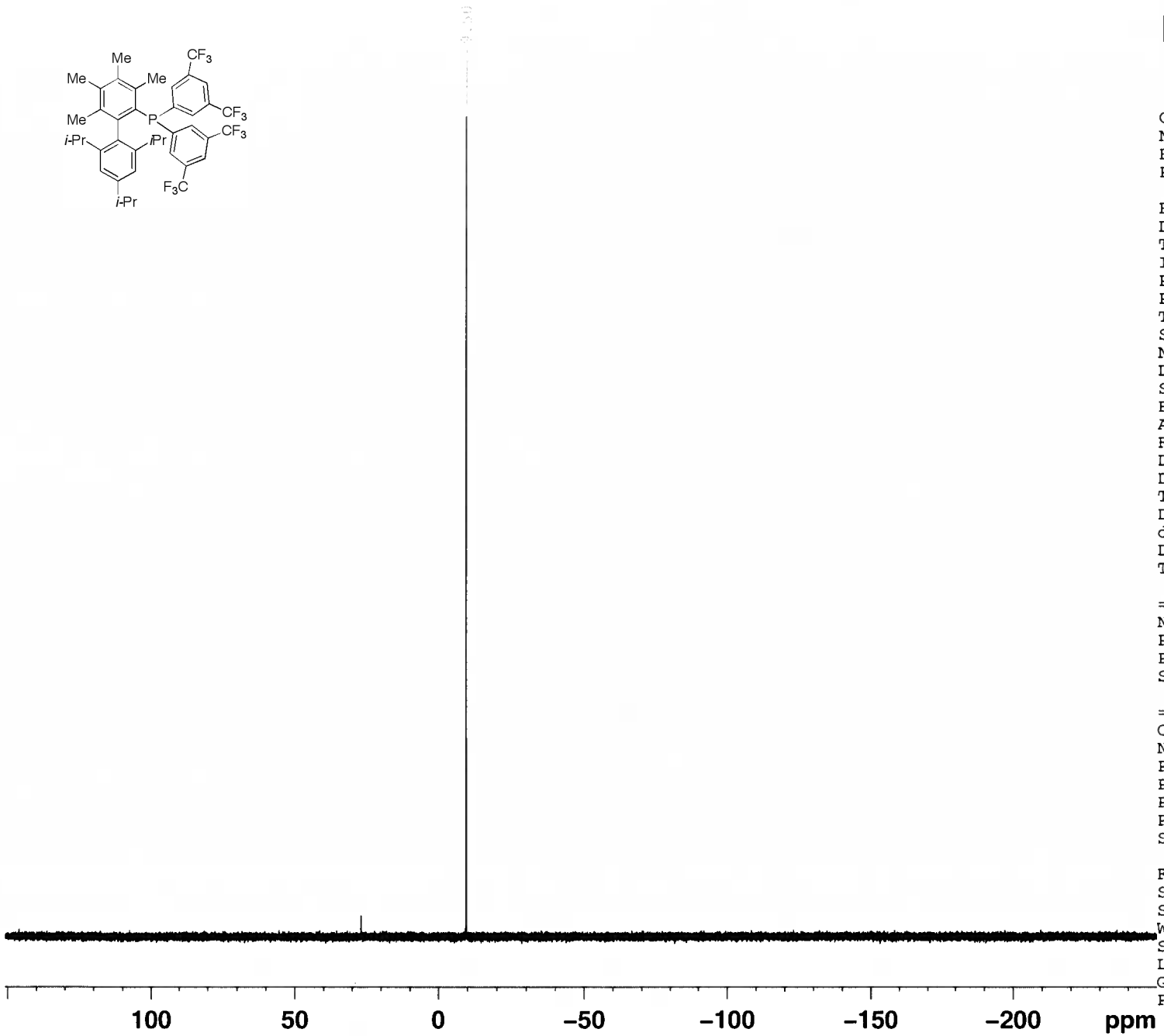
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127681 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



BRUKER

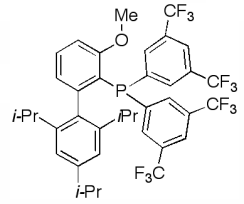
```
Current Data Parameters
NAME      jdh-2-286-4-p31
EXPNO                   1
PROCNO                  1

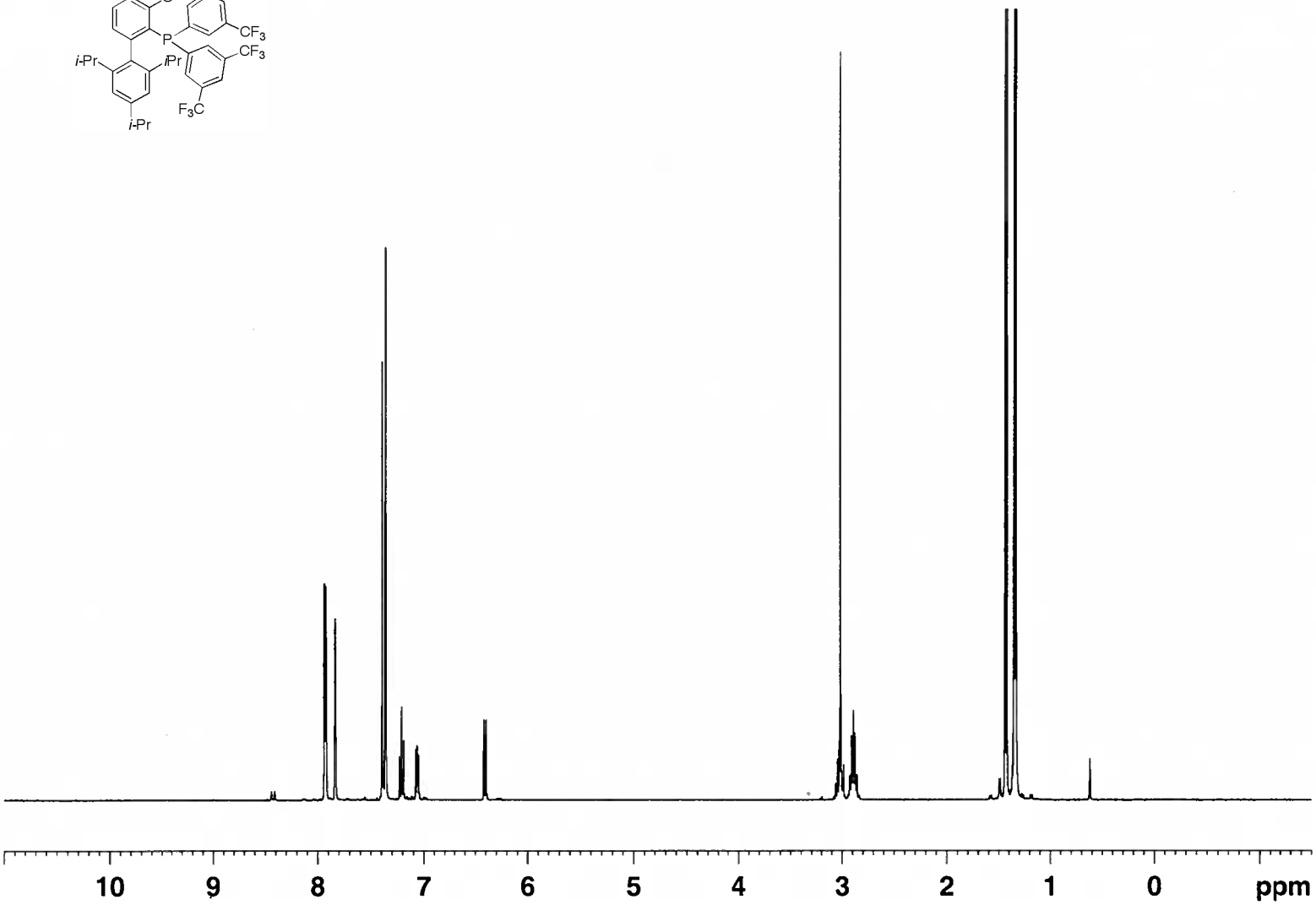
F2 - Acquisition Parameters
Date_           20081006
Time               14.10
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    4
SWH           64935.066 Hz
FIDRES         0.990830 Hz
AQ             0.5046772 sec
RG                7298.2
DW                7.700 usec
DE                6.00 usec
TE                291.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                9.25 usec
PL1               3.00 dB
SFO1        161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL2               0.00 dB
PL12             16.10 dB
PL13             19.00 dB
SFO2        400.1316000 MHz

F2 - Processing parameters
SI                65536
SF          161.9755024 MHz
WDW                  no
SSB                   0
LB                0.00 Hz
GB                    0
PC                1.40
```





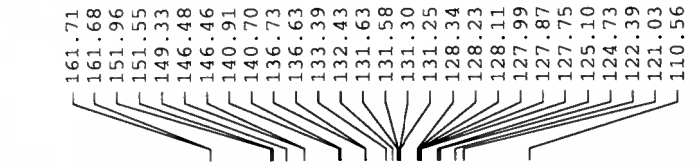

```
Current Data Parameters
NAME                  jdh-2-216
EXPNO                         1
PROCNO                        1

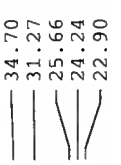
F2 - Acquisition Paramet
Date_                  20080924
Time                      17.06
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                    C6D6
NS                           16
DS                            2
SWH                    8278.146
FIDRES                 0.126314
AQ                     3.9584243
RG                          128
DW                       60.400
DE                        6.00
TE                       293.2
D1                    1.00000000
TD0                           1

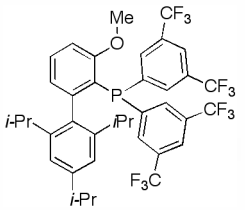
======== CHANNEL f1 ====
NUC1                         1H
P1                        15.07
PL1                        0.00
SFO1               400.1324710

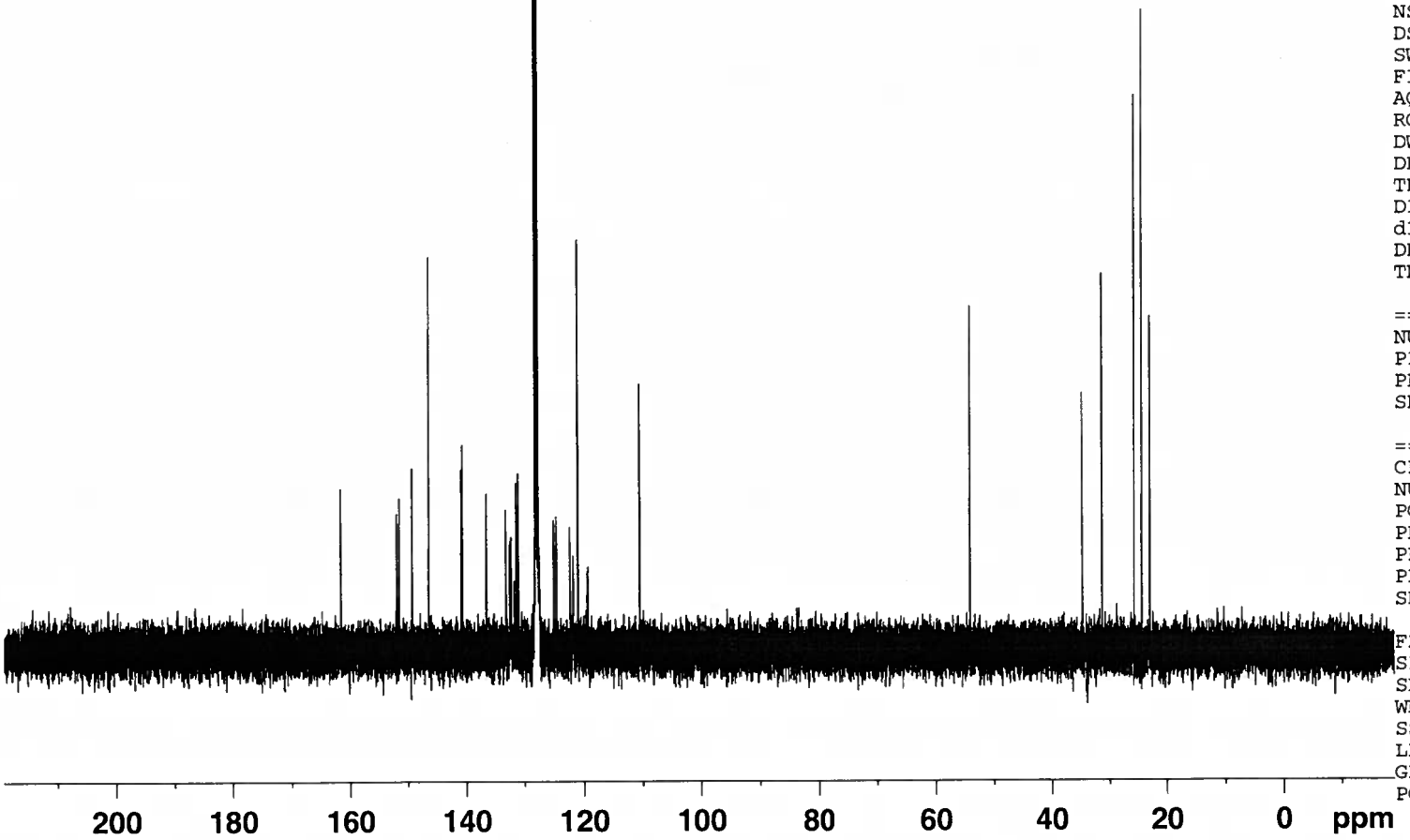
F2 - Processing paramete
SI                        65536
SF                 400.1299644
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.00
```

SI-100









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Current Data Parameters

NAME	jdh-2-216-c13
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080924	
Time	17.23	
INSTRUM	spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	256	
DS	2	
SWH	23980.814	Hz
FIDRES	0.365918	Hz
AQ	1.3664756	sec
RG	8192	
DW	20.850	usec
DE	6.00	usec
TE	293.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	

======== CHANNEL f1 ========

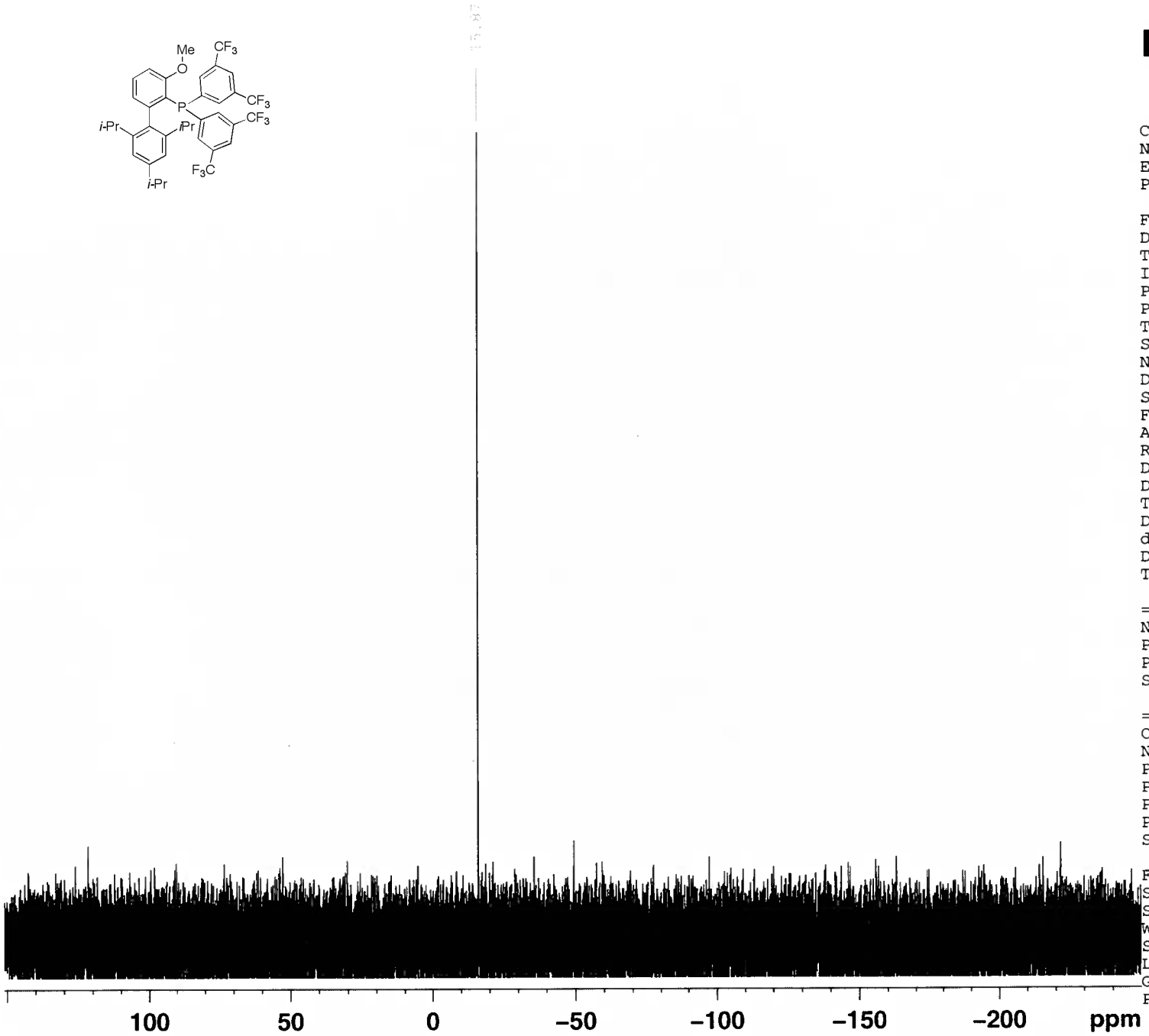
NUC1	13C	
P1	8.75	usec
PL1	-3.00	dB
SFO1	100.6228298	MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-1.00	dB
PL12	14.52	dB
PL13	18.00	dB
SFO2	400.1316005	MHz

F2 - Processing parameters

SI	65536	
SF	100.6127513	MHz
WDW	no	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	



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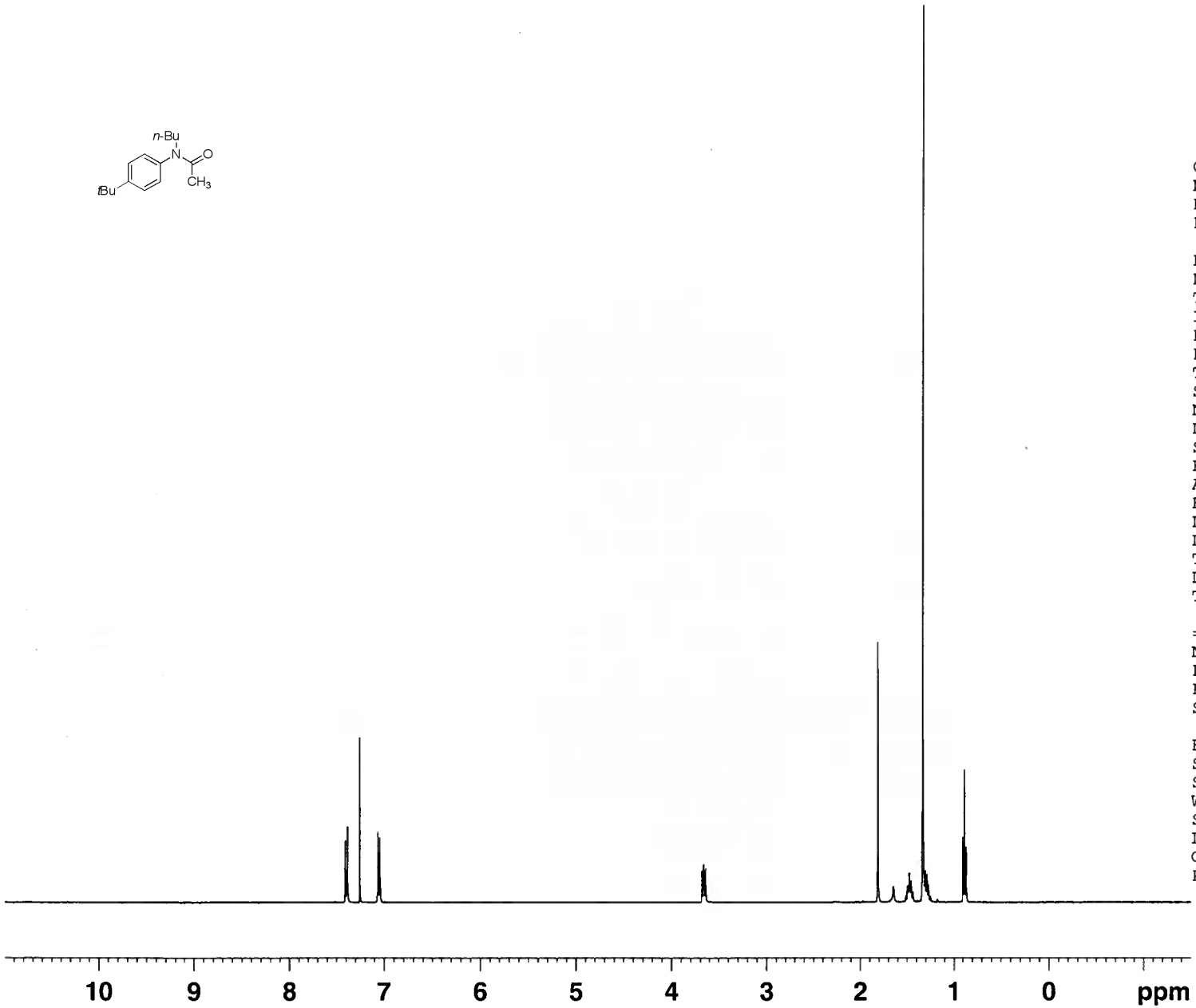
```
Current Data Parameters
NAME       jdh-2-216-p31
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20080901
Time              14.29
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    4
SWH           64935.066 Hz
FIDRES         0.990830 Hz
AQ             0.5046772 sec
RG                 6502
DW                7.700 usec
DE                6.00 usec
TE                291.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                  9.25 usec
PL1                 3.00 dB
SFO1        161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2        400.1316000 MHz

F2 - Processing parameters
SI                65536
SF          161.9755024 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
```



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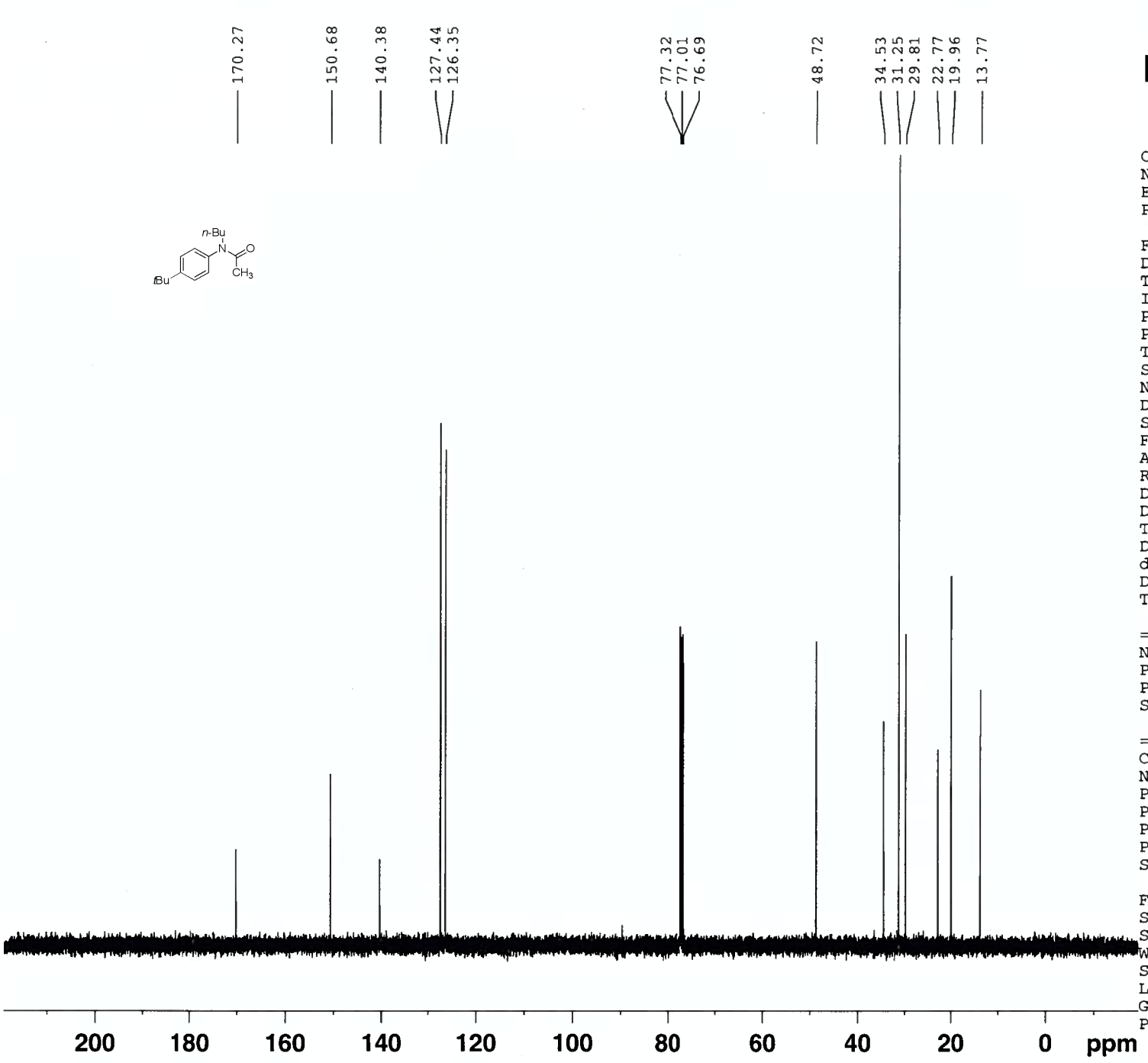
```
Current Data Parameters
NAME                  jdh-2-229
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080905
Time                      11.10
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          256
DW                       60.400 usec
DE                        6.00 usec
TE                       292.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.88 usec
PL1                       0.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF              400.1300098 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```



Current Data Parameters
NAME jdh-2-229-Carbon
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080905
Time	15.08
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1625.5
DW	20.850 usec
DE	6.00 usec
TE	292.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

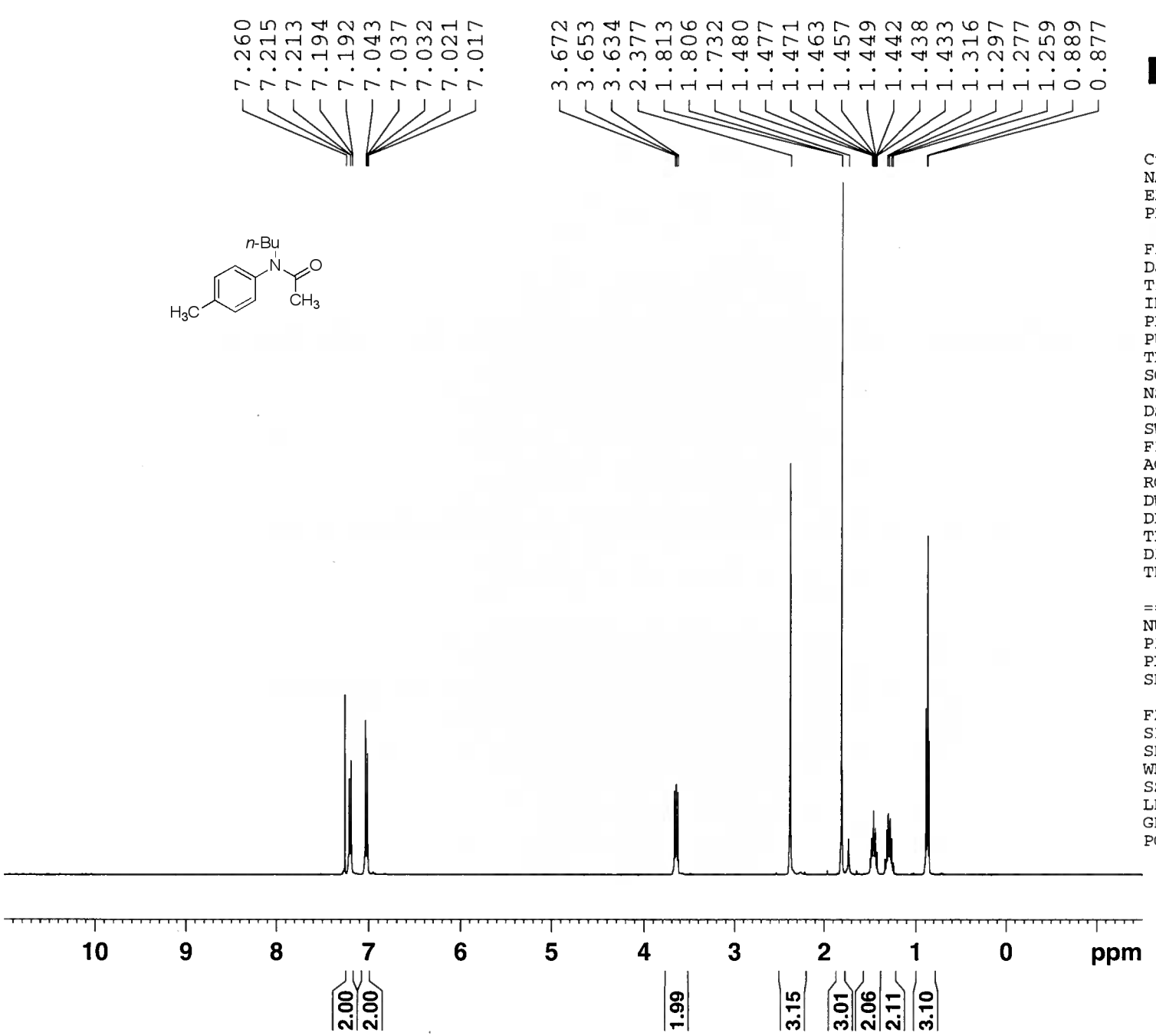
NUC1	13C
P1	9.38 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127776 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



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Current Data Parameters
NAME jdh-2-237
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

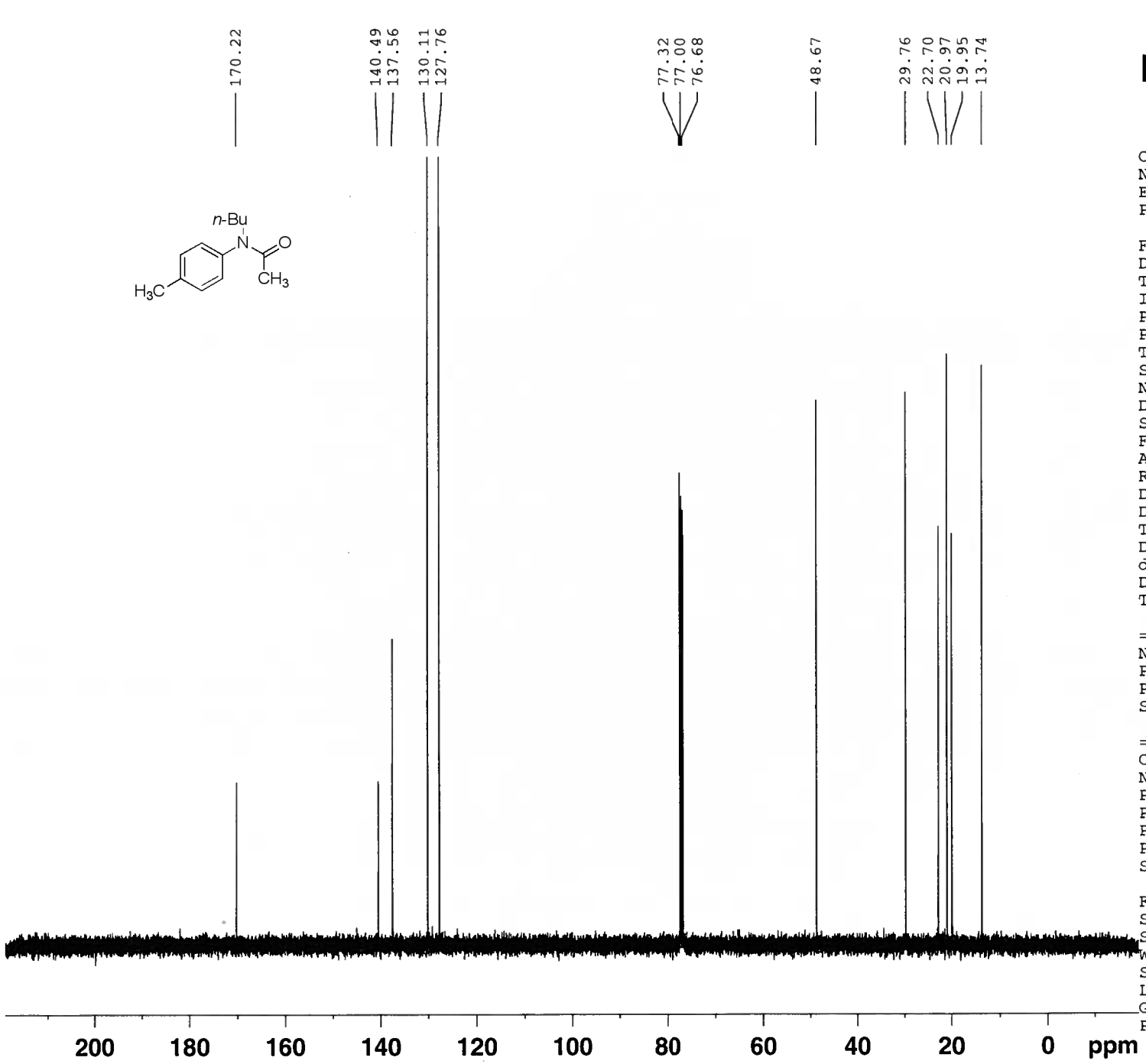
Date_	20080908	
Time	18.34	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8278.146	Hz
FIDRES	0.126314	Hz
AQ	3.9584243	sec
RG	406.4	
DW	60.400	usec
DE	6.00	usec
TE	291.2	K
D1	1.00000000	sec
TD0	1	

======== CHANNEL f1 ========

NUC1	1H	
P1	13.88	usec
PL1	0.00	dB
SFO1	400.1324710	MHz

F2 - Processing parameters

SI	65536	
SF	400.1300096	MHz
WDW	no	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



Current Data Parameters
NAME jdh-2-237-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080908
Time	19.01
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	2896.3
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

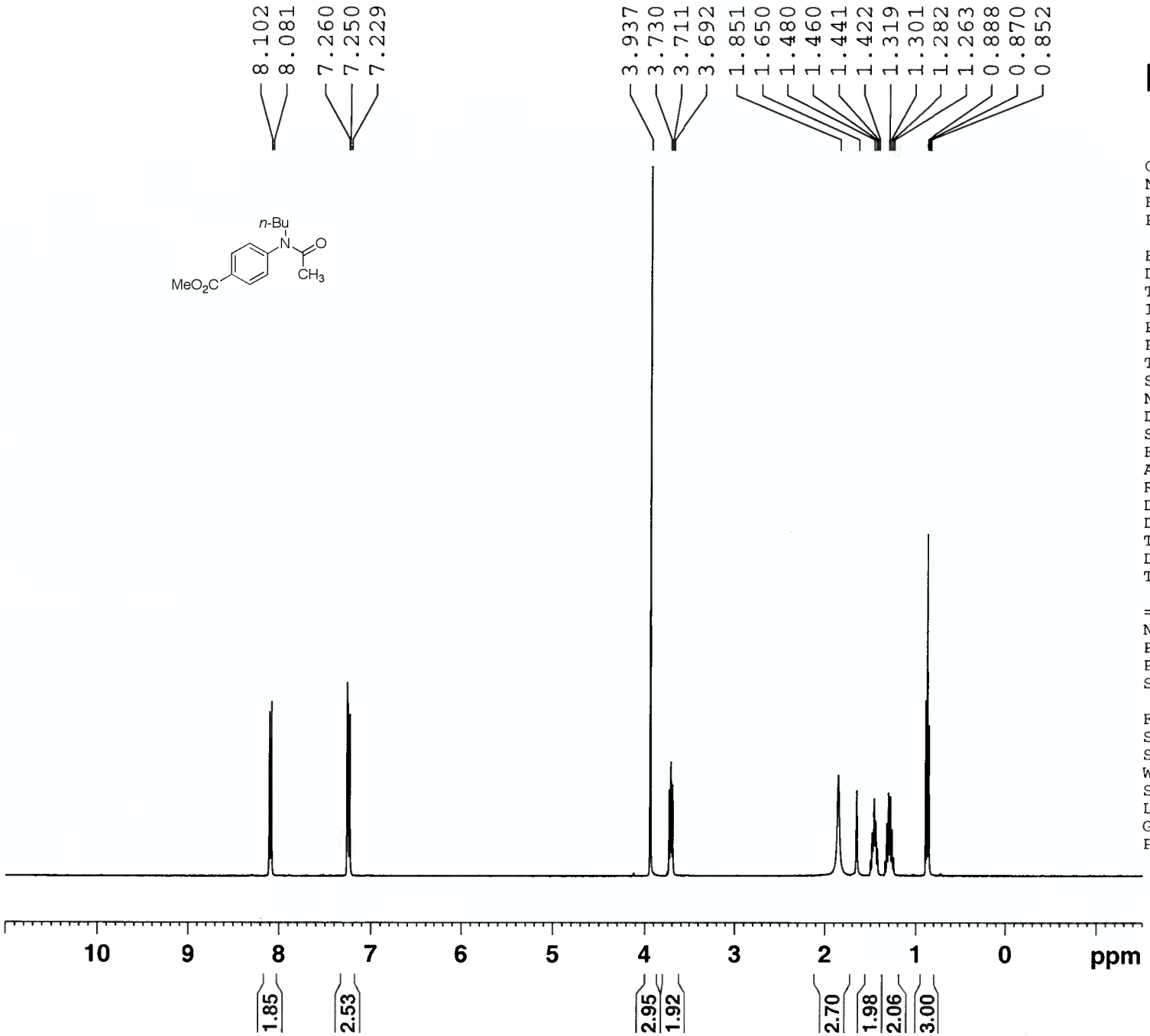
NUC1	13C
P1	9.38 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127782 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



Current Data Parameters

NAME	jdh-2-241
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

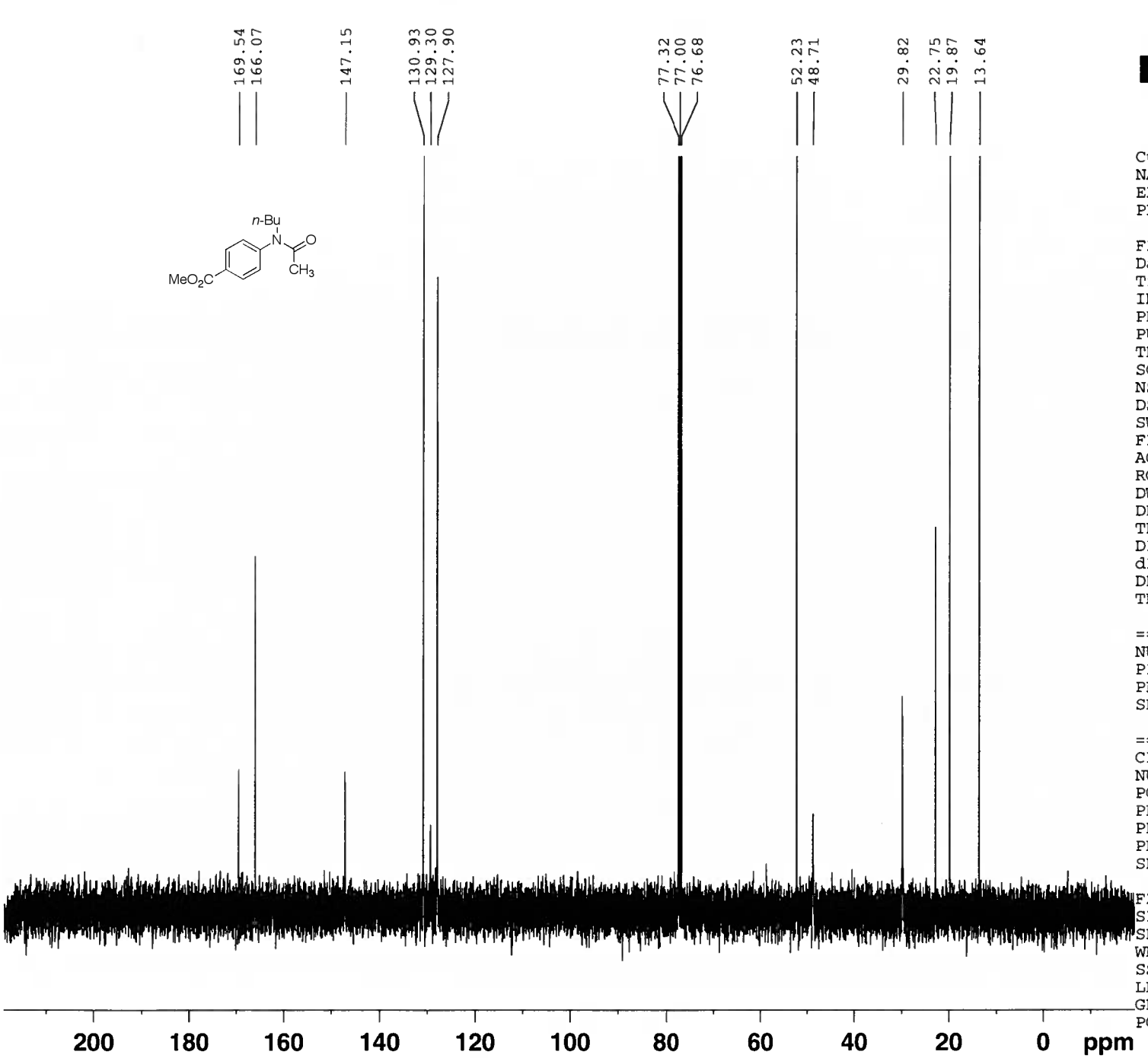
Date_	20080909
Time	12.25
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	406.4
DW	60.400 usec
DE	6.00 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	13.88 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	65536
SF	400.1300096 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



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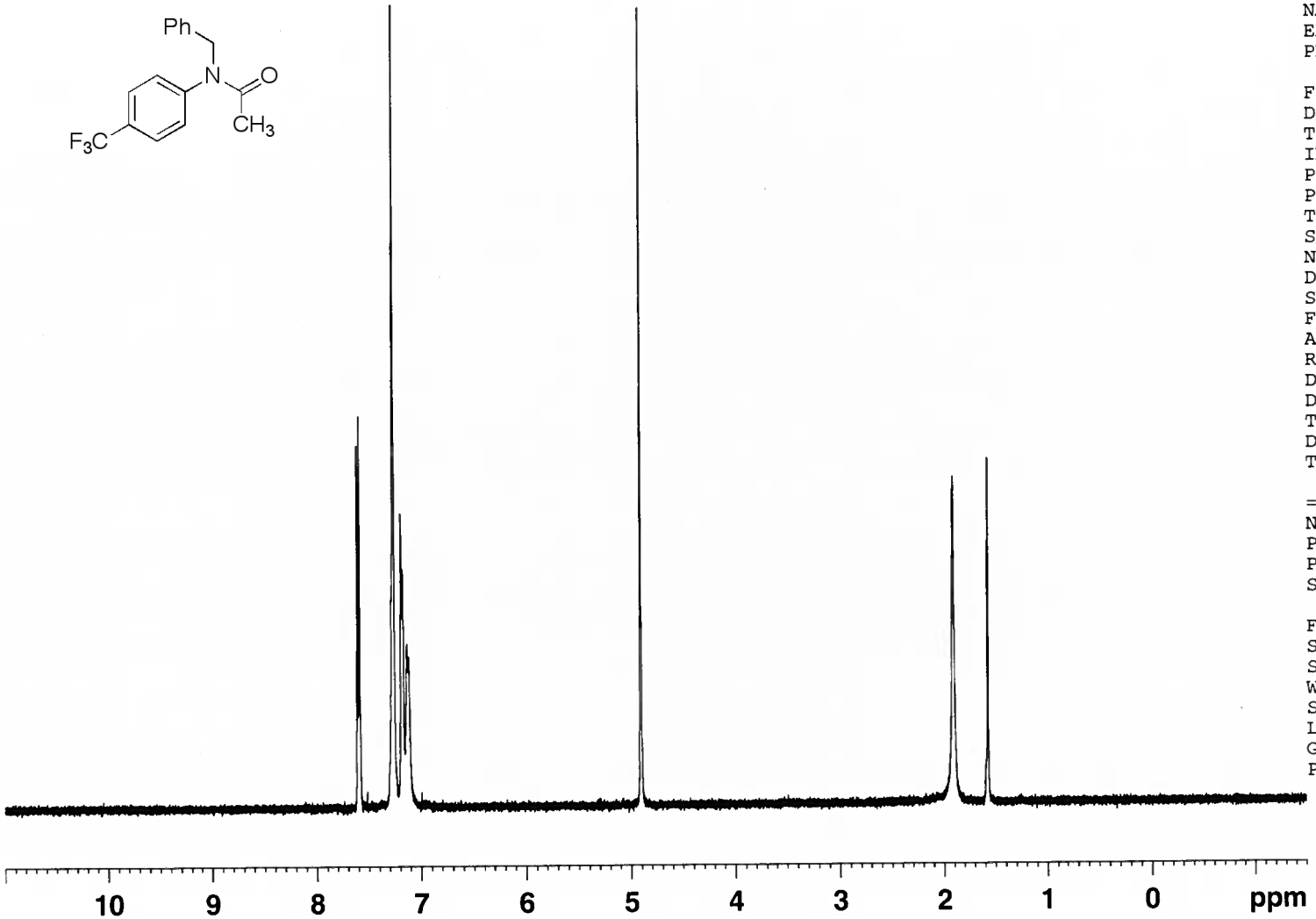
Current Data Parameters
NAME jdh-2-241-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080909
Time 14.24
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 292.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127797 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



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Current Data Parameters

NAME	jdh-2-232
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

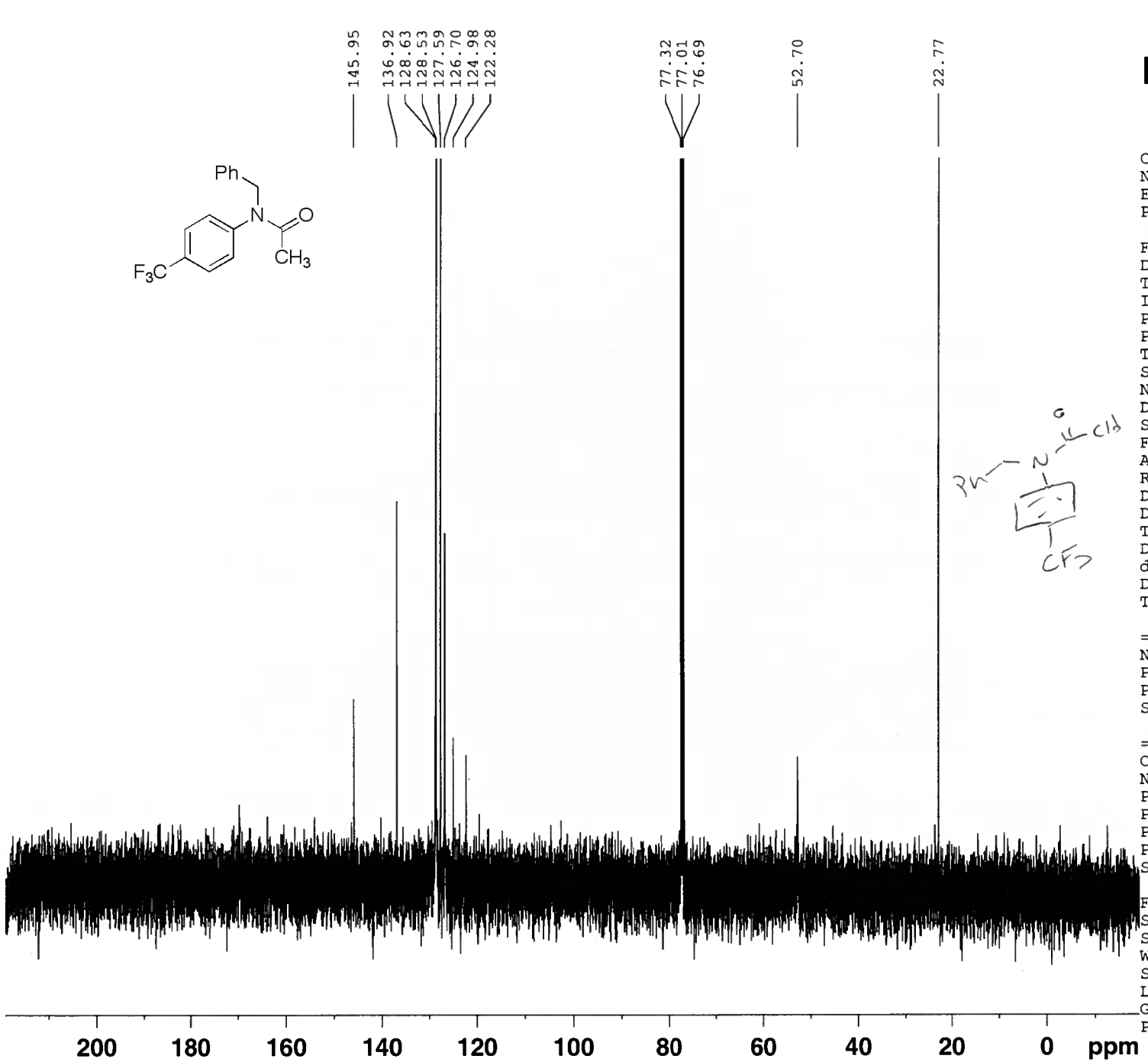
Date_	20080906
Time	11.51
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	322.5
DW	60.400 usec
DE	6.00 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	13.88 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	65536
SF	400.1300100 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



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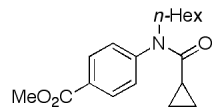
```
Current Data Parameters
NAME       jdh-2-232-c13
EXPNO                 1
PROCNO                1

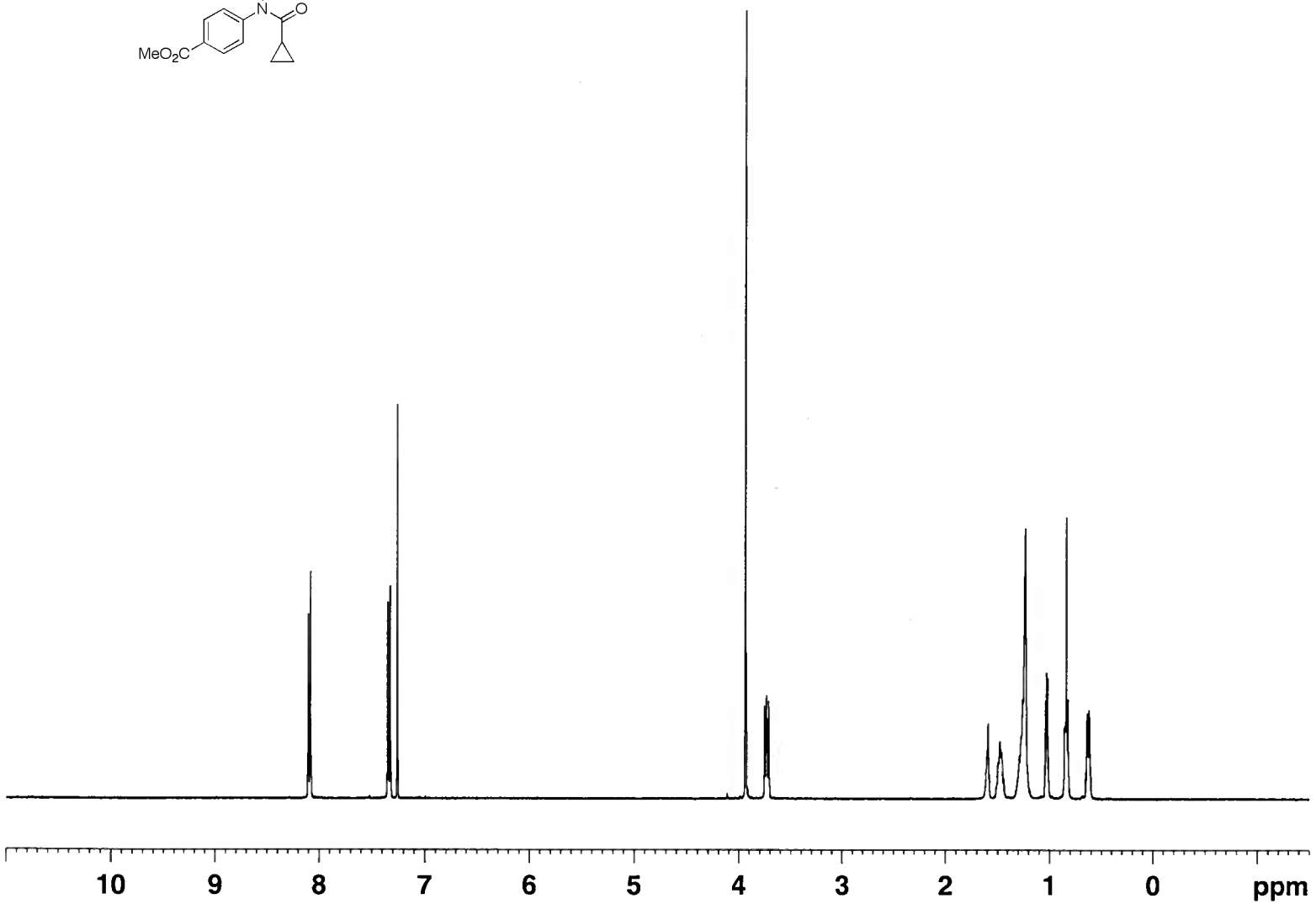
F2 - Acquisition Parameters
Date_          20080906
Time              13.11
INSTRUM           spect
PROBHD   5 mm QNP 1H/13
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                2298.8
DW               20.850 usec
DE                6.00 usec
TE               293.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.38 usec
PL1               0.00 dB
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2               0.00 dB
PL12             16.10 dB
PL13             19.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127740 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
```





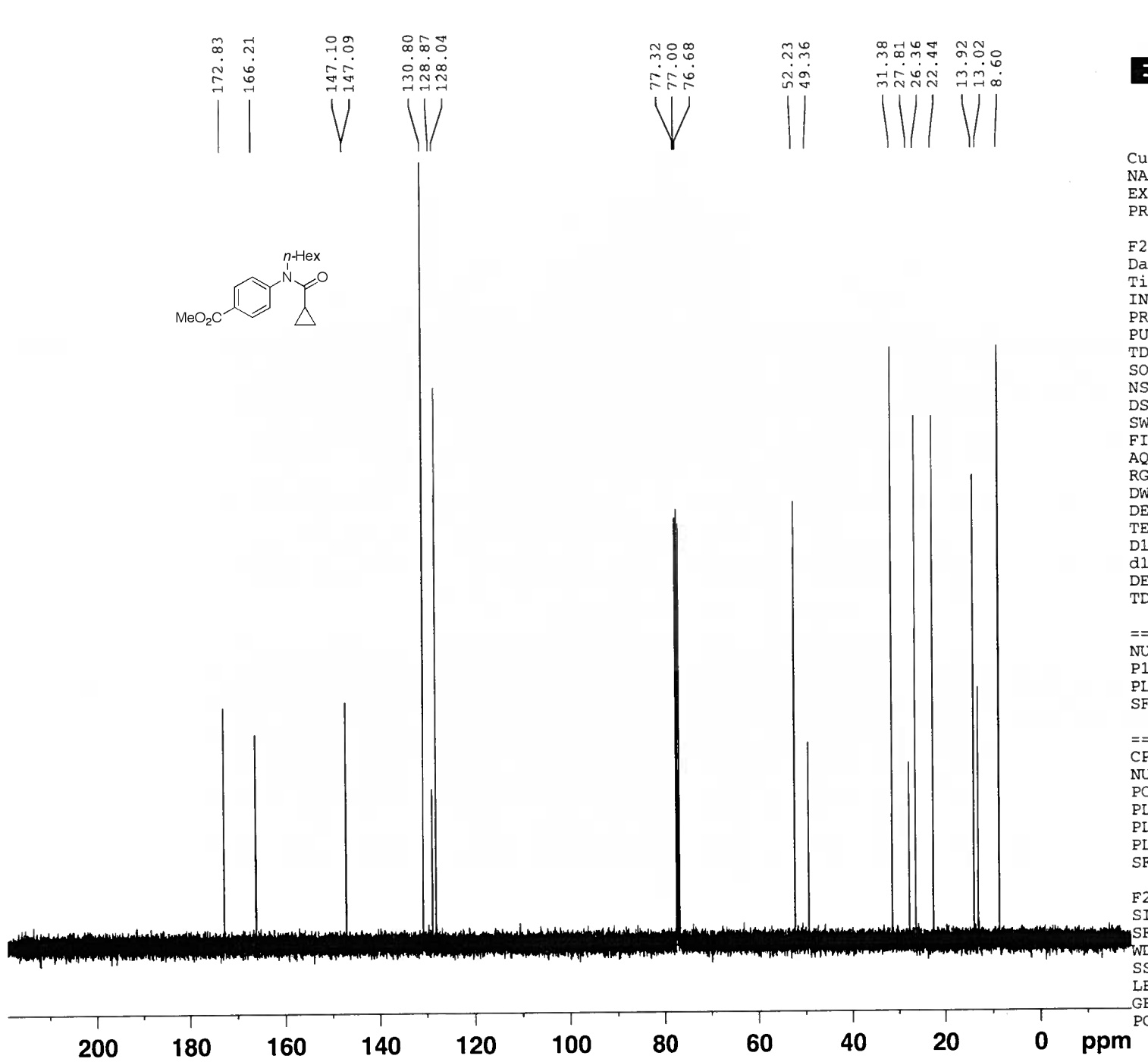

```
Current Data Parameters
NAME                  jdh-2-243
EXPNO                         1
PROCNO                        1

F2 - Acquisition Paramet
Date_                  20080911
Time                      17.31
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146
FIDRES                 0.126314
AQ                     3.9584243
RG                          181
DW                       60.400
DE                         6.00
TE                        293.2
D1                     1.0000000
TD0                           1

======== CHANNEL f1 ====
NUC1                         1H
P1                        15.07
PL1                        0.00
SFO1               400.1324710

F2 - Processing paramete
SI                        65536
SF                 400.1300102
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.00
```

SI-1 (1)



Current Data Parameters

NAME	jdh-2-243-C13
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080911
Time	17.48
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	129
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

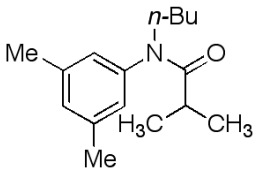
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

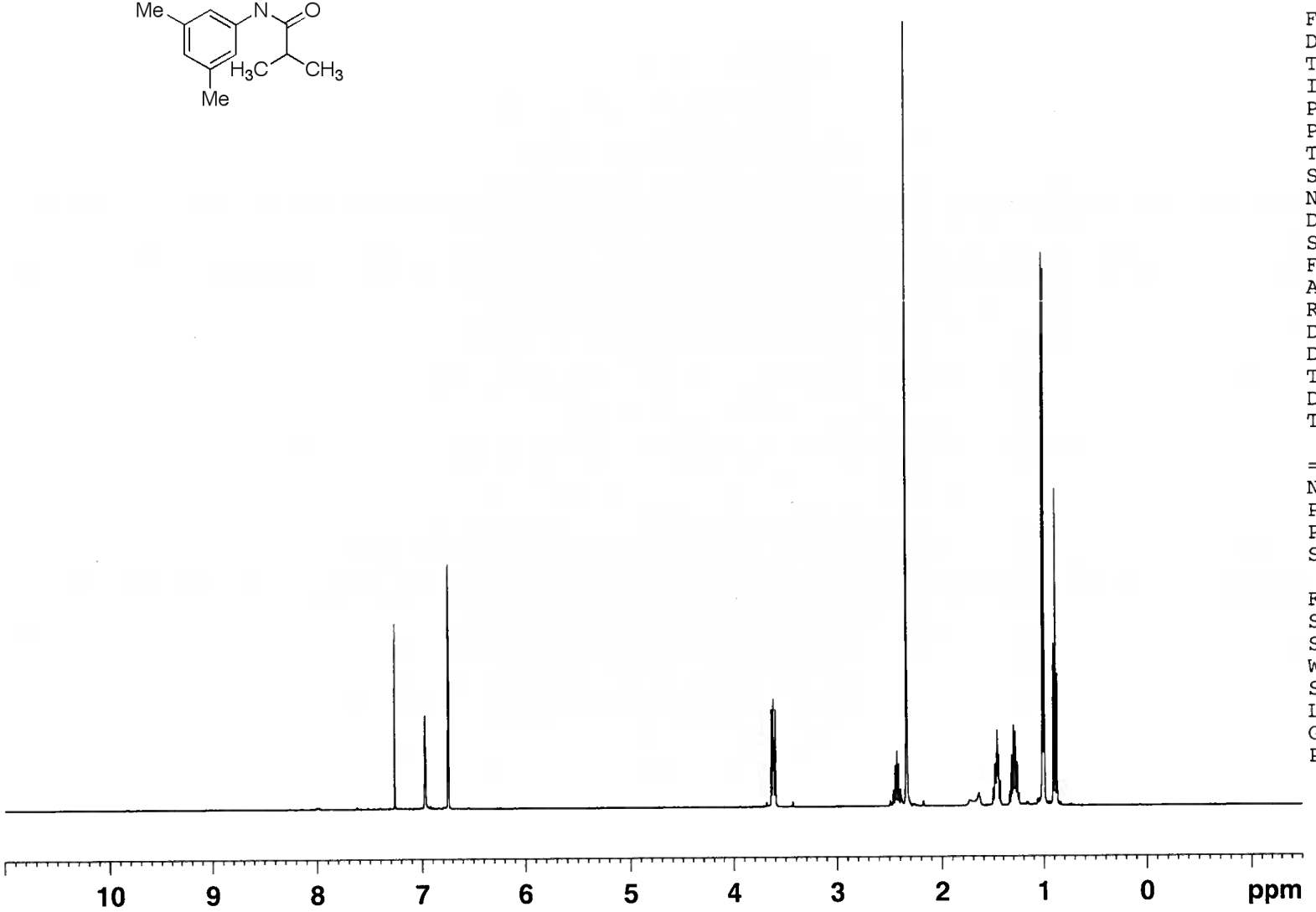
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127773 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



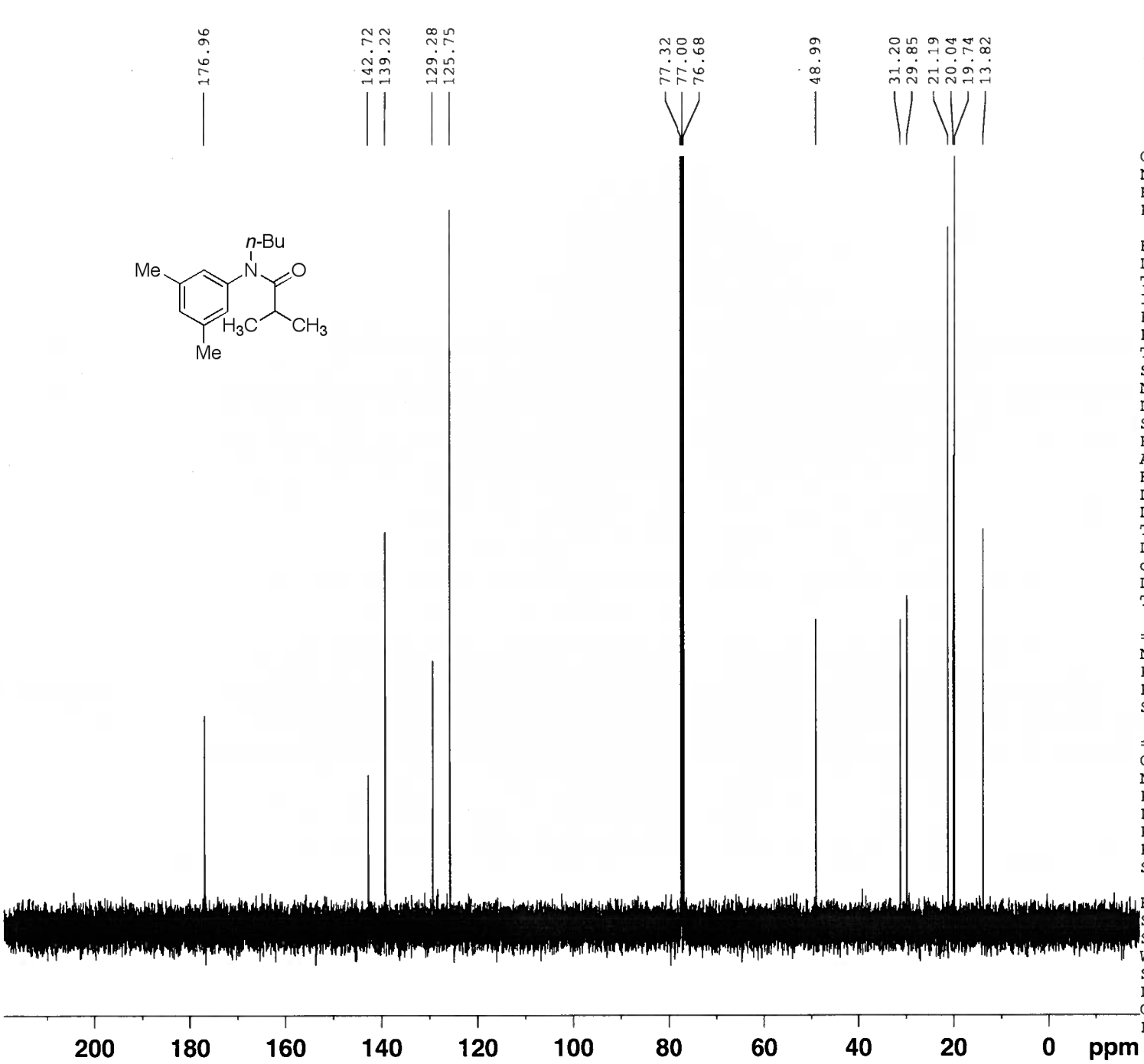



```
Current Data Parameters
NAME                  jdh-2-244
EXPNO                         1
PROCNO                        1

F2 - Acquisition Paramet
Date_                  20080911
Time                      17.35
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146
FIDRES                 0.126314
AQ                     3.9584243
RG                          128
DW                       60.400
DE                        6.00
TE                       293.2
D1                    1.00000000
TD0                           1

======== CHANNEL f1 ====
NUC1                         1H
P1                        15.07
PL1                        0.00
SFO1               400.1324710

F2 - Processing paramete
SI                        65536
SF                 400.1300096
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.00
```



Current Data Parameters
NAME jdh-2-244-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080911
Time	17.59
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	129
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

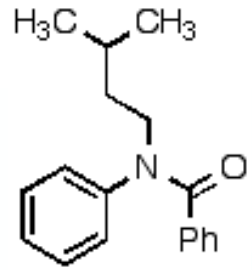
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

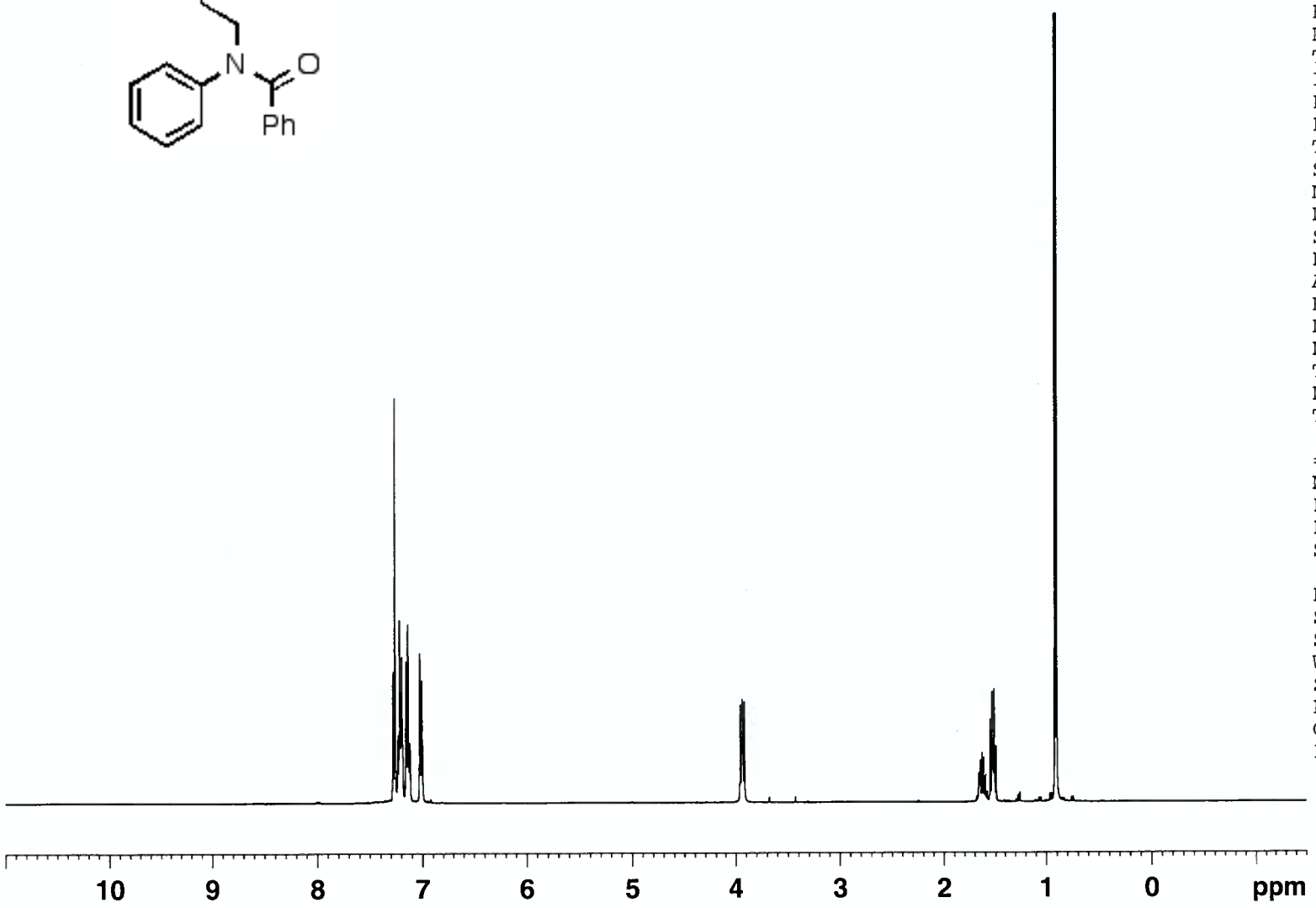
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127743 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40






```
Current Data Parameters
NAME                  jdh-2-248-2
EXPNO                           1
PROCNO                          1

F2 - Acquisition Paramet
Date_                    20080917
Time                        12.01
INSTRUM                     spect
PROBHD    5 mm BBO BB-1H
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                      8278.146
FIDRES                   0.126314
AQ                       3.9584243
RG                            128
DW                         60.400
DE                          6.00
TE                         293.2
D1                     1.00000000
TD0                             1

======== CHANNEL f1 ====
NUC1                           1H
P1                          15.07
PL1                          0.00
SFO1                400.1324710

F2 - Processing paramete
SI                          65536
SF                400.1300098
WDW                            no
SSB                             0
LB                           0.00
GB                              0
PC                           1.00
```

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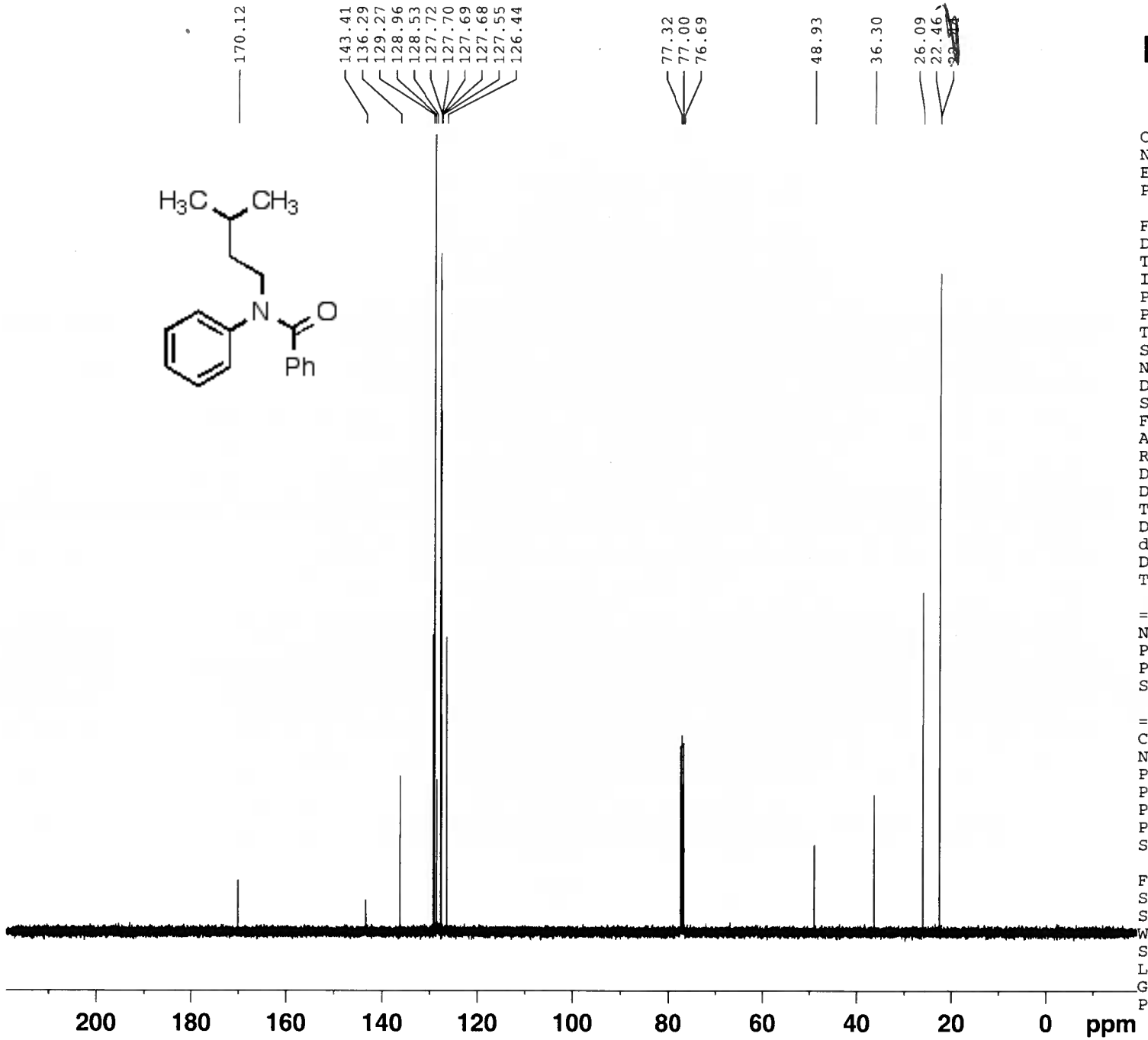


BRUKER

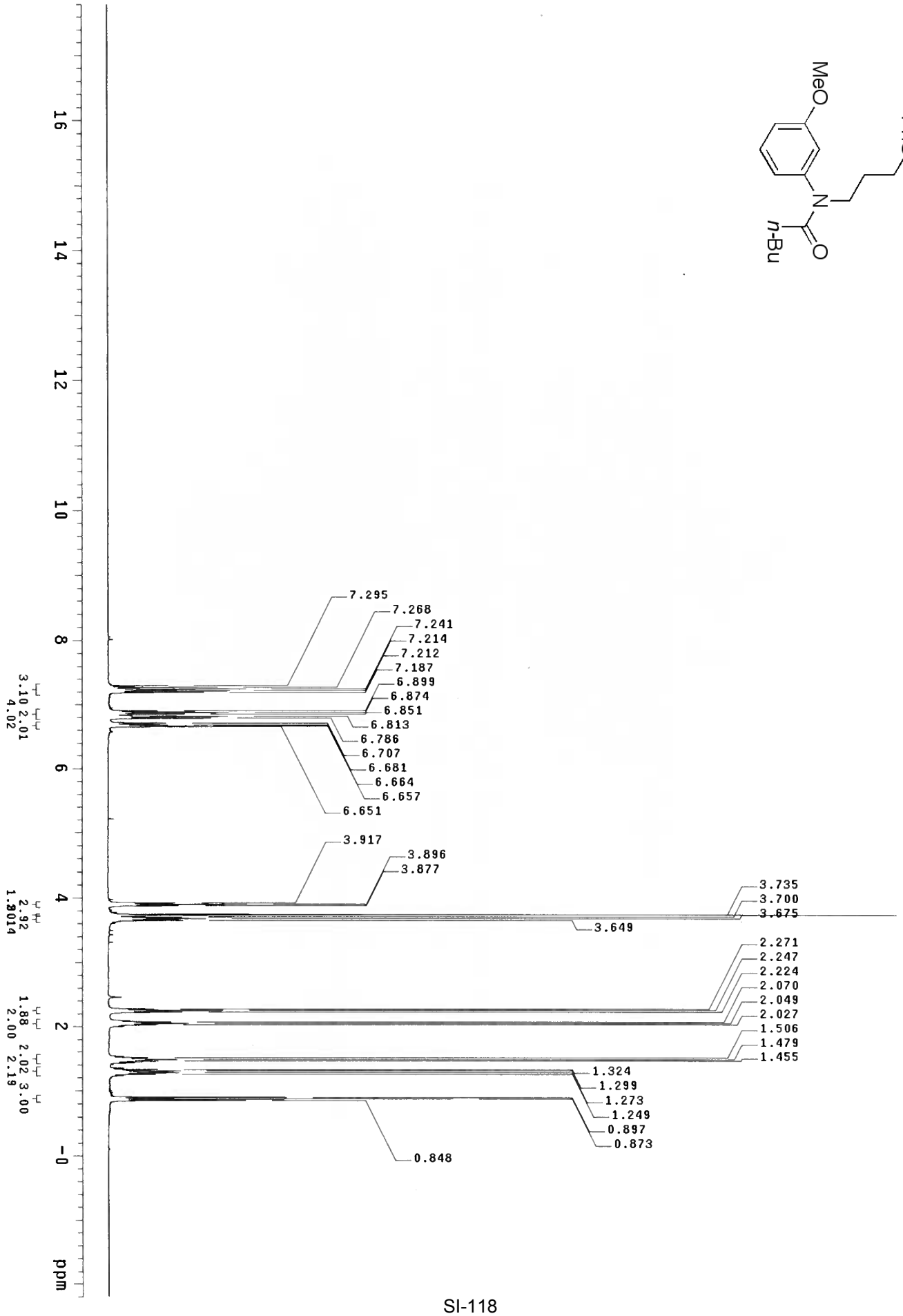
Current Data Parameters
NAME jdh-2-248-c13
EXPNO 1
PROCNO 1

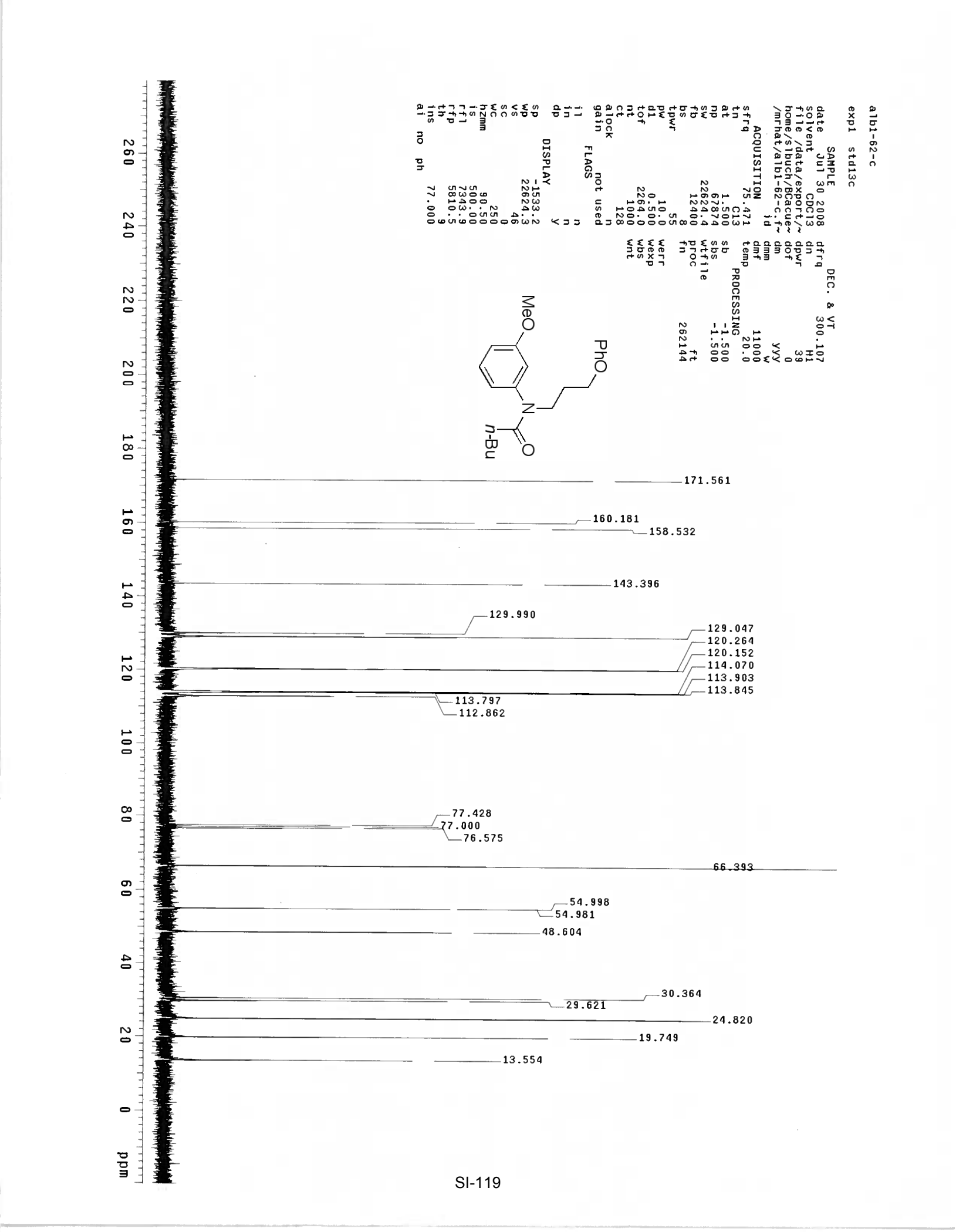
F2 - Acquisition Parameters
Date_ 20080917
Time 12.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

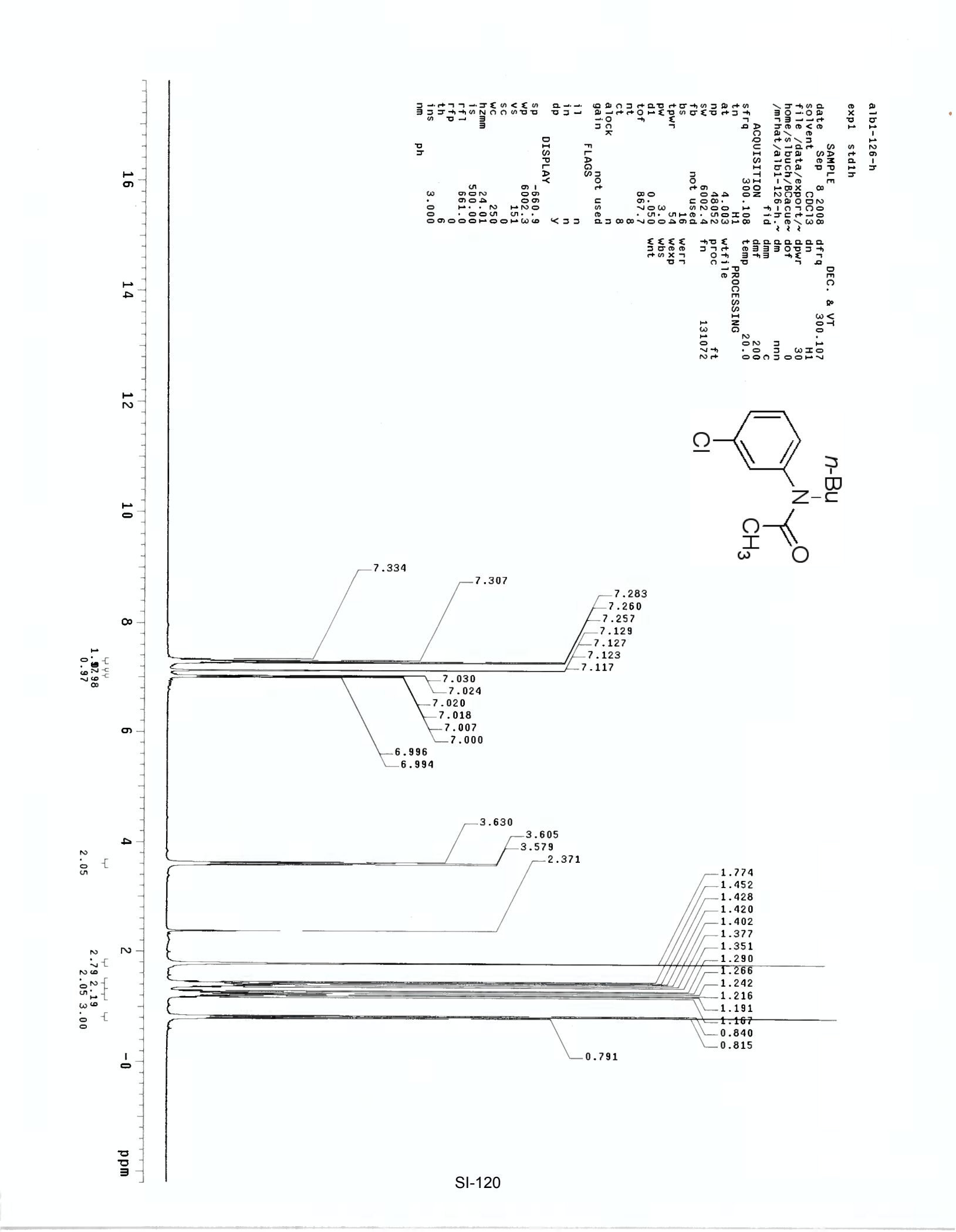
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

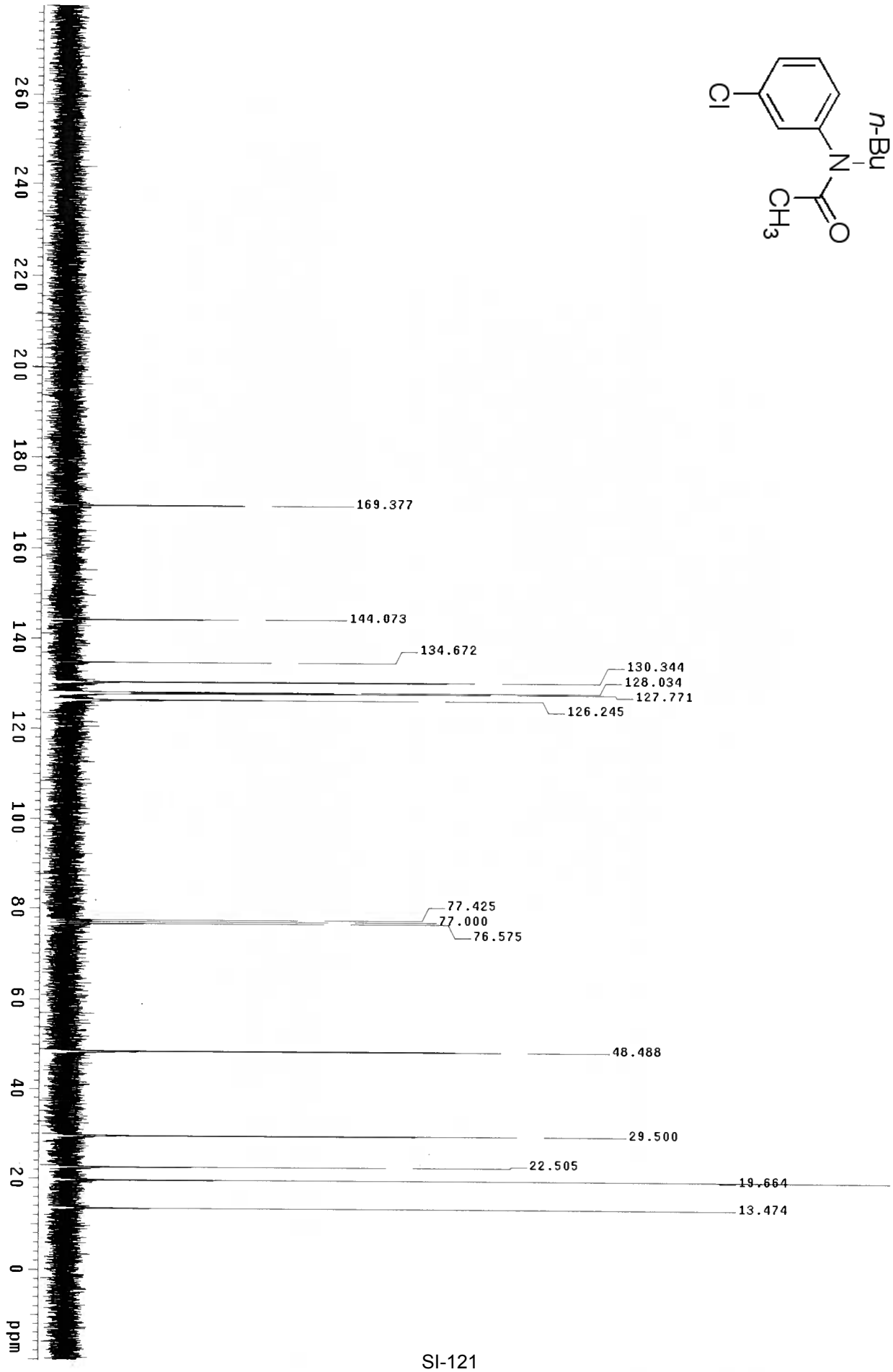
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

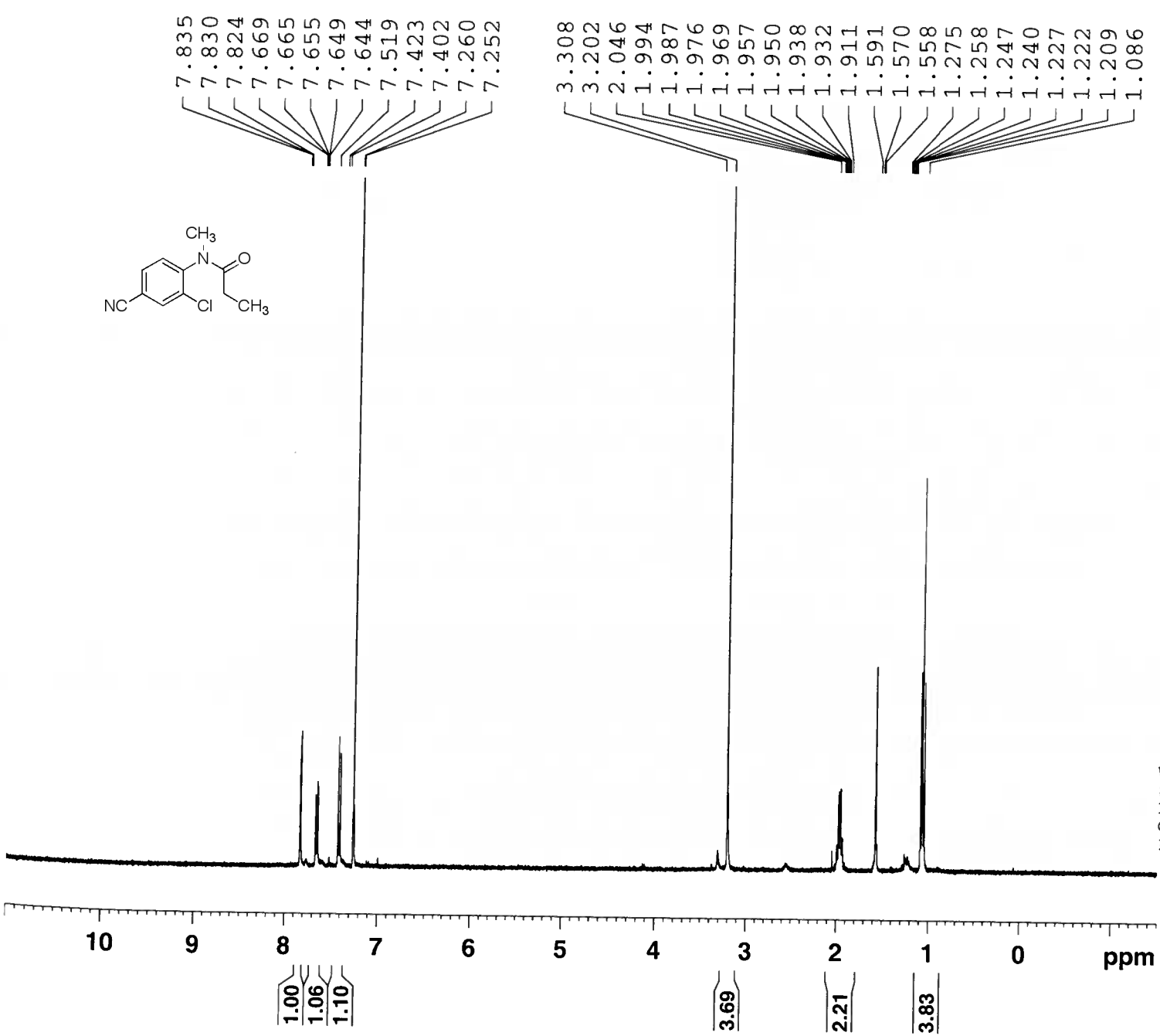
F2 - Processing parameters
SI 65536
SF 100.6127811 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40


MeO
PhO
N
O
n-Bu
7.295
7.268
7.241
7.214
7.212
7.187
6.899
6.874
6.851
6.813
6.786
6.707
6.681
6.664
6.657
6.651
3.917
3.896
3.877
3.735
3.700
3.675
3.649
2.271
2.247
2.224
2.070
2.049
2.027
1.506
1.479
1.455
1.324
1.299
1.273
1.249
0.897
0.873
0.848
3.10 2.01
4.02
2.92
1.8014
1.88 2.02 3.00
2.00 2.19
16
14
12
10
8
6
4
2
-0
ppm


alb1-62-c
exp1 std13c
SAMPLE
date Jul 30 2008
solvent CDCl3
file /data/export/~
home/slbuch/BGacue~
/mrhat/alb1-62-c.f~
id
ACQUISITION
sfrq 75.471
tn C13
at 1.500
np 67874
sw 22624.4
fb 12400
bs 8
tpwr 55
pw 10.0
d1 0.500
tof 2264.0
nt 1000
ct 128
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1533.2
wp 22624.3
vs 46
sc 0
wc 250
hzmm 90.50
is 500.00
rfl 7343.9
rfp 5810.5
th 9
ins 77.000
ai no ph
DEC. & VT
dfrq 300.107
dn H1
dpwr 39
dof 0
dm yyy
dmm w
dmf 11000
temp 20.0
PROCESSING
sb -1.500
sbs -1.500
wtfile
proc
fn ft
262144
wnt
wbs
wexp
werr
MeO
PhO
N
O
n-Bu
171.561
160.181
158.532
143.396
129.990
129.047
120.264
120.152
114.070
113.903
113.845
113.797
112.862
77.428
77.000
76.575
66.393
54.998
54.981
48.604
30.364
29.621
24.820
19.749
13.554
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm


alb1-126-h
expl stdih
SAMPLE
date Sep 8 2008
solvent CDCl3
file /data/export/~
home/slbuch/BCacue~
/mrhat/alb1-126-h.~
fid
ACQUISITION
sfrq 300.108
tn H1
at 4.003
np 48052
sw 6002.4
fb not used
bs 16
tpwr 54
pw 3.0
d1 0.050
tof 867.7
nt 8
ct 8
alock n
gain n
FLAGS
not used
il n
in n
dp y
DISPLAY
sp -660.9
wp 6002.3
vs 151
sc 0
wc 250
hzmm 24.01
is 500.00
rfl 661.0
rfp 0
th 6
ins 3.000
nm
ph
DEC. & VT
dfrq 300.107
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
temp 20.0
PROCESSING
wtfile
proc ft
fn 131072
n-Bu
N
CH3
O
Cl
7.334
7.307
7.283
7.260
7.257
7.129
7.127
7.123
7.117
7.030
7.024
7.020
7.018
7.007
7.000
6.996
6.994
3.630
3.605
3.579
2.371
1.774
1.452
1.428
1.420
1.402
1.377
1.351
1.290
1.266
1.242
1.216
1.191
1.167
0.840
0.815
0.791
1.98
0.97
2.05
2.79
2.19
2.05
3.00
16
14
12
10
8
6
4
2
-0
ppm


Cl
n-Bu
N
CH3
O
169.377
144.073
134.672
130.344
128.034
127.771
126.245
77.425
77.000
76.575
48.488
29.500
22.505
19.664
13.474
ppm



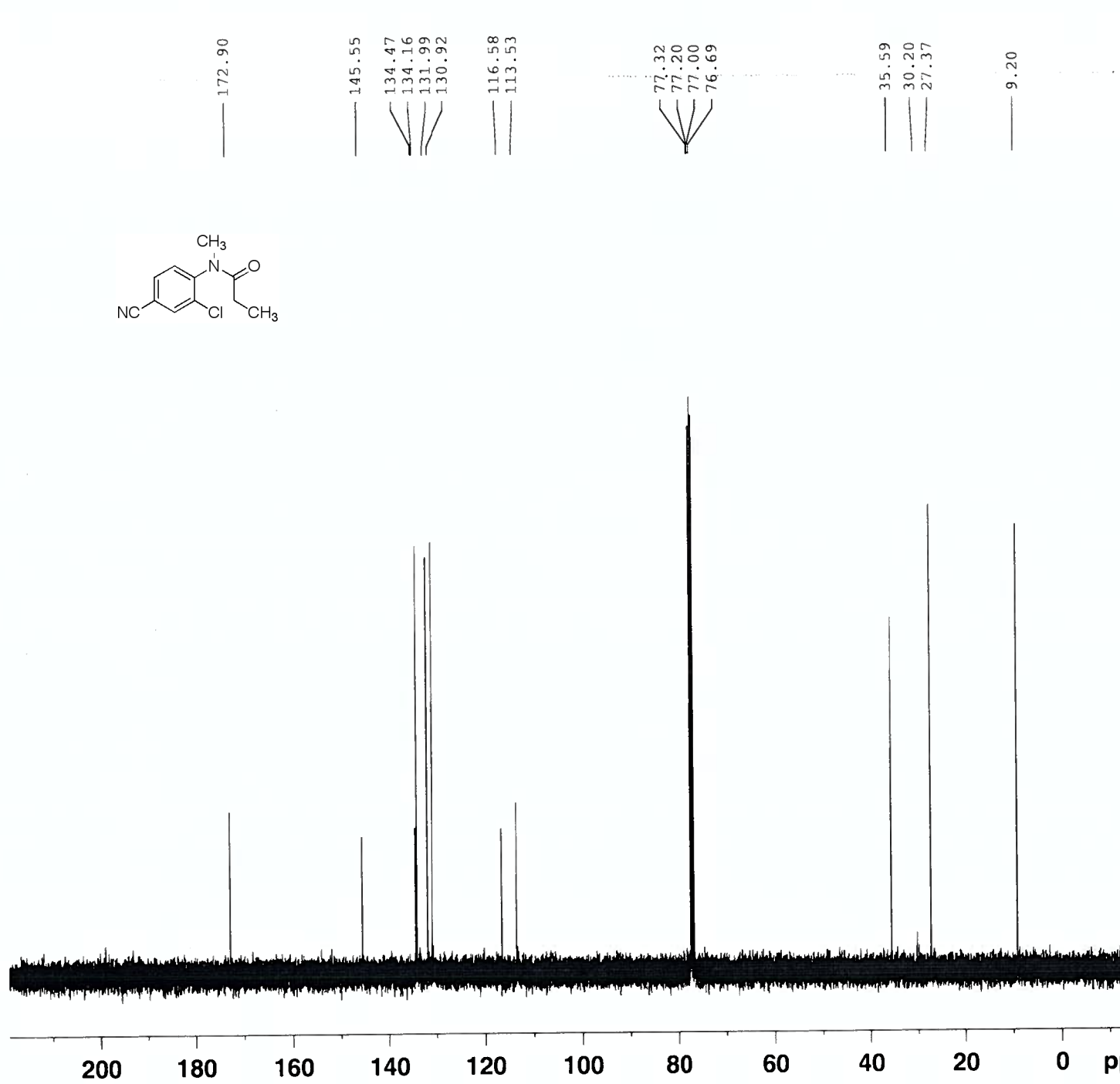
BRUKER

Current Data Parameters
NAME jdh-3-38
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081031
Time 18.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300096 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



BRUKER

Current Data Parameters
NAME jdh-3-257-2-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090416
Time	18.43
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	16384
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

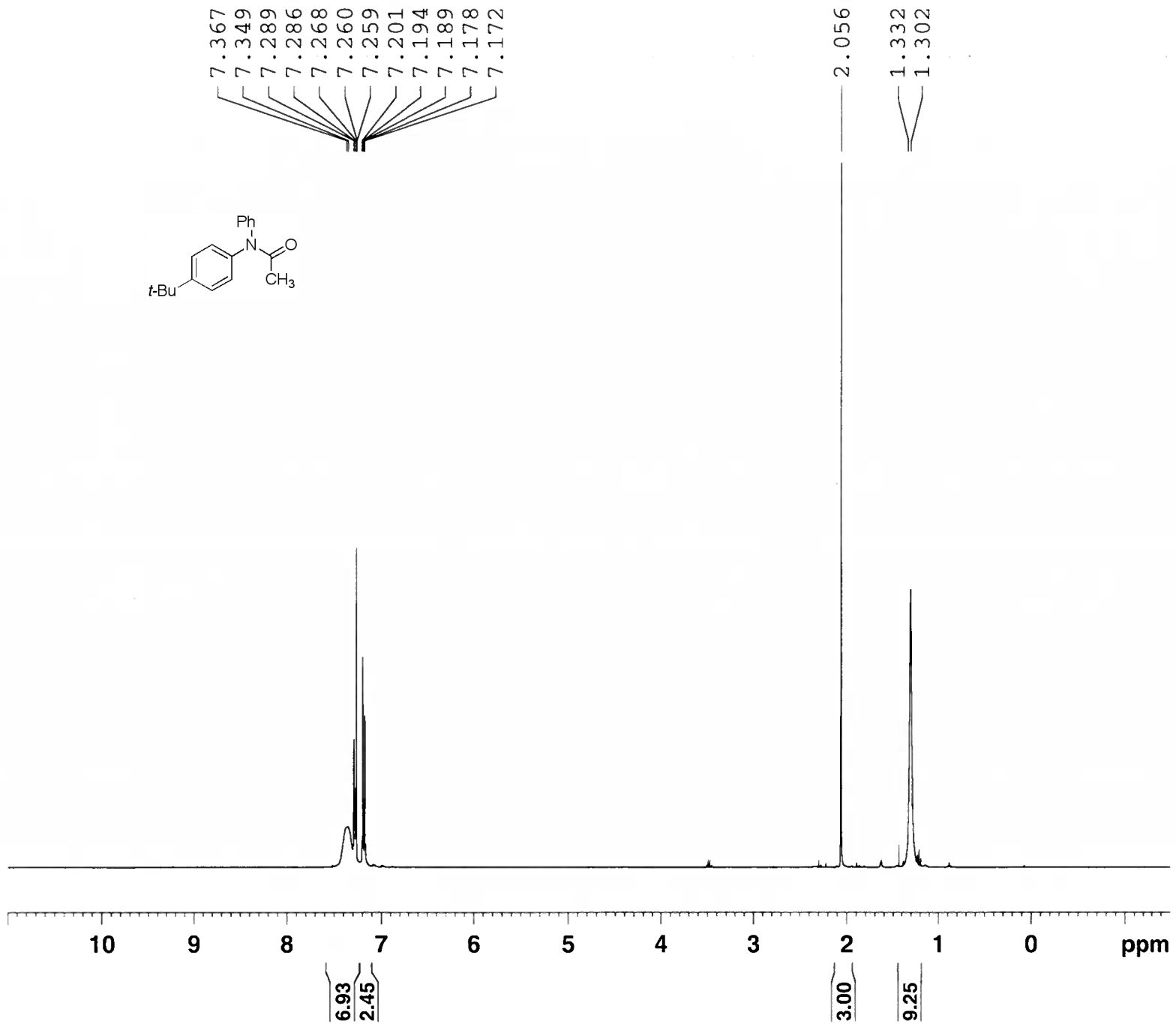
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127792 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



Current Data Parameters
NAME jdh-3-260-2
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090416
Time 11.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

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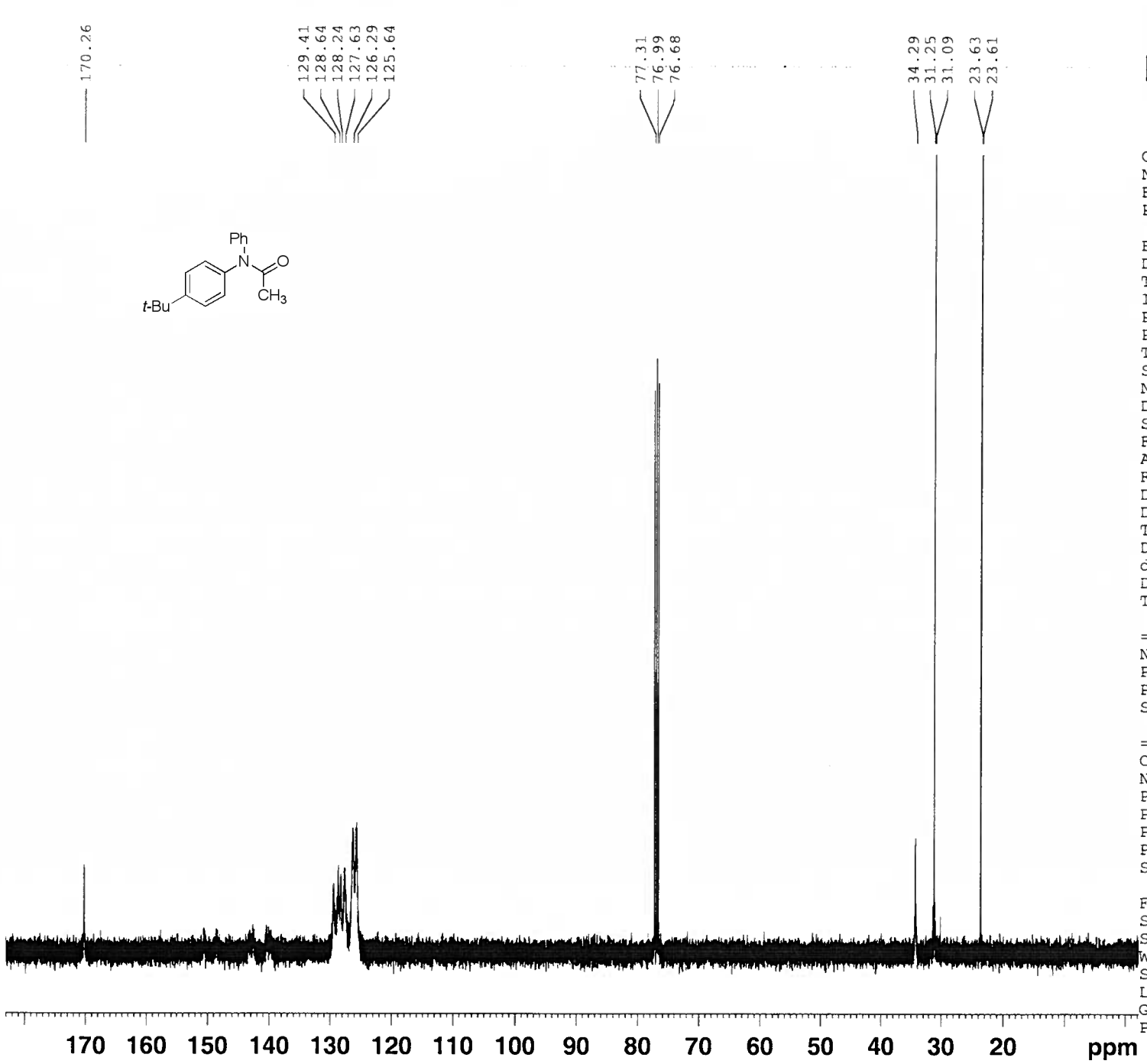
======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300096
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

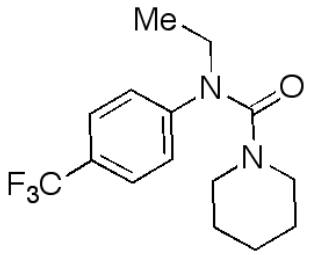
Current Data Parameters
NAME jdh-3-260-c13-2
EXPNO 1
PROCNO 1

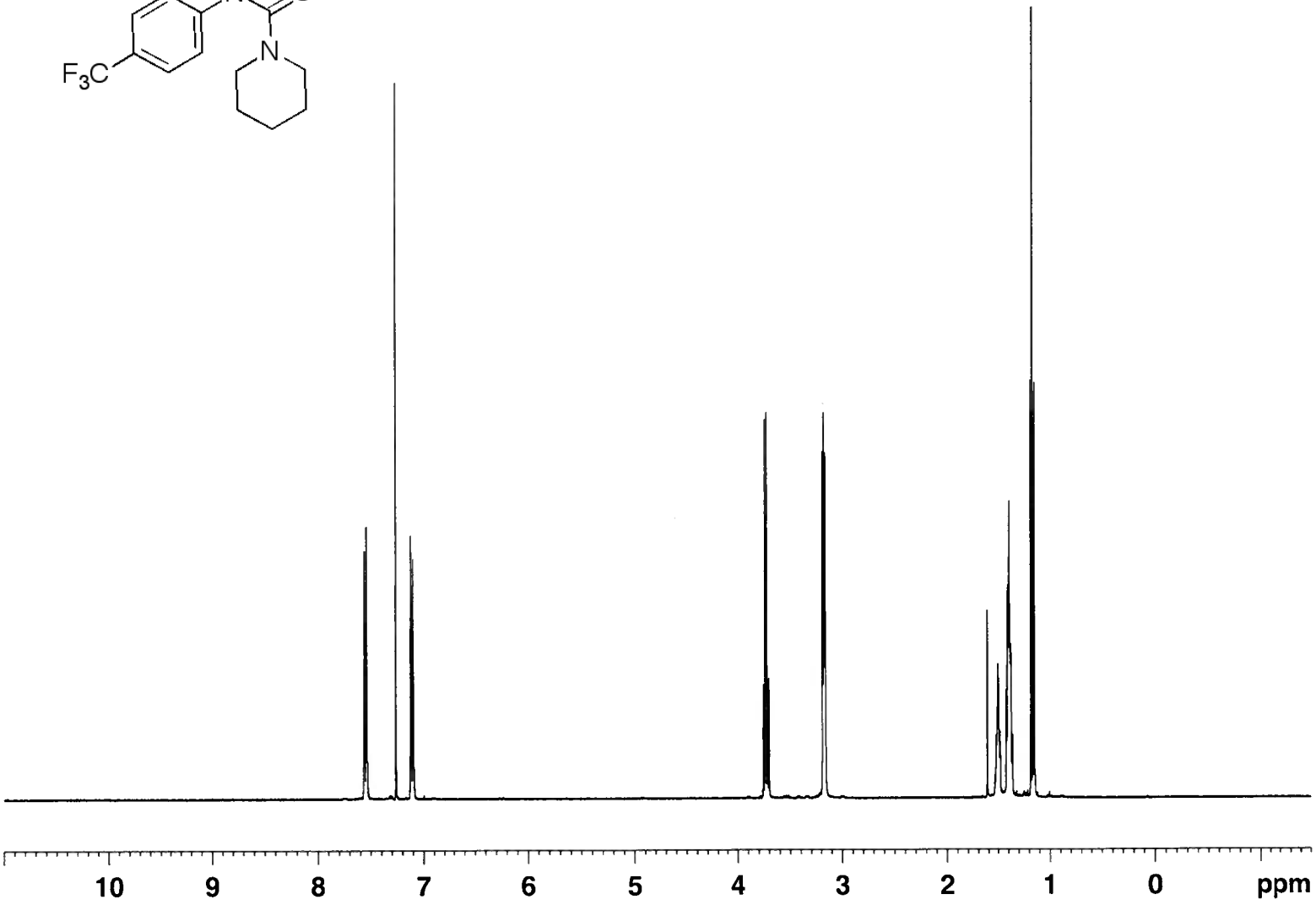
F2 - Acquisition Parameters
Date_ 20090416
Time 11.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 257
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127980 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME                  jdh-2-249-2
EXPNO                           1
PROCNO                          1

F2 - Acquisition Paramet
Date_                    20080917
Time                        12.05
INSTRUM                     spect
PROBHD    5 mm BBO BB-1H
PULPROG                      zg30
TD                          65536
SOLVENT                     CDCl3
NS                             16
DS                              2
SWH                      8278.146
FIDRES                   0.126314
AQ                       3.9584243
RG                            181
DW                         60.400
DE                          6.00
TE                         293.2
D1                    1.00000000
TD0                             1

======== CHANNEL f1 ====
NUC1                           1H
P1                          15.07
PL1                          0.00
SFO1                400.1324710

F2 - Processing paramete
SI                          65536
SF                400.1300097
WDW                            no
SSB                             0
LB                           0.00
GB                              0
PC                           1.00
```

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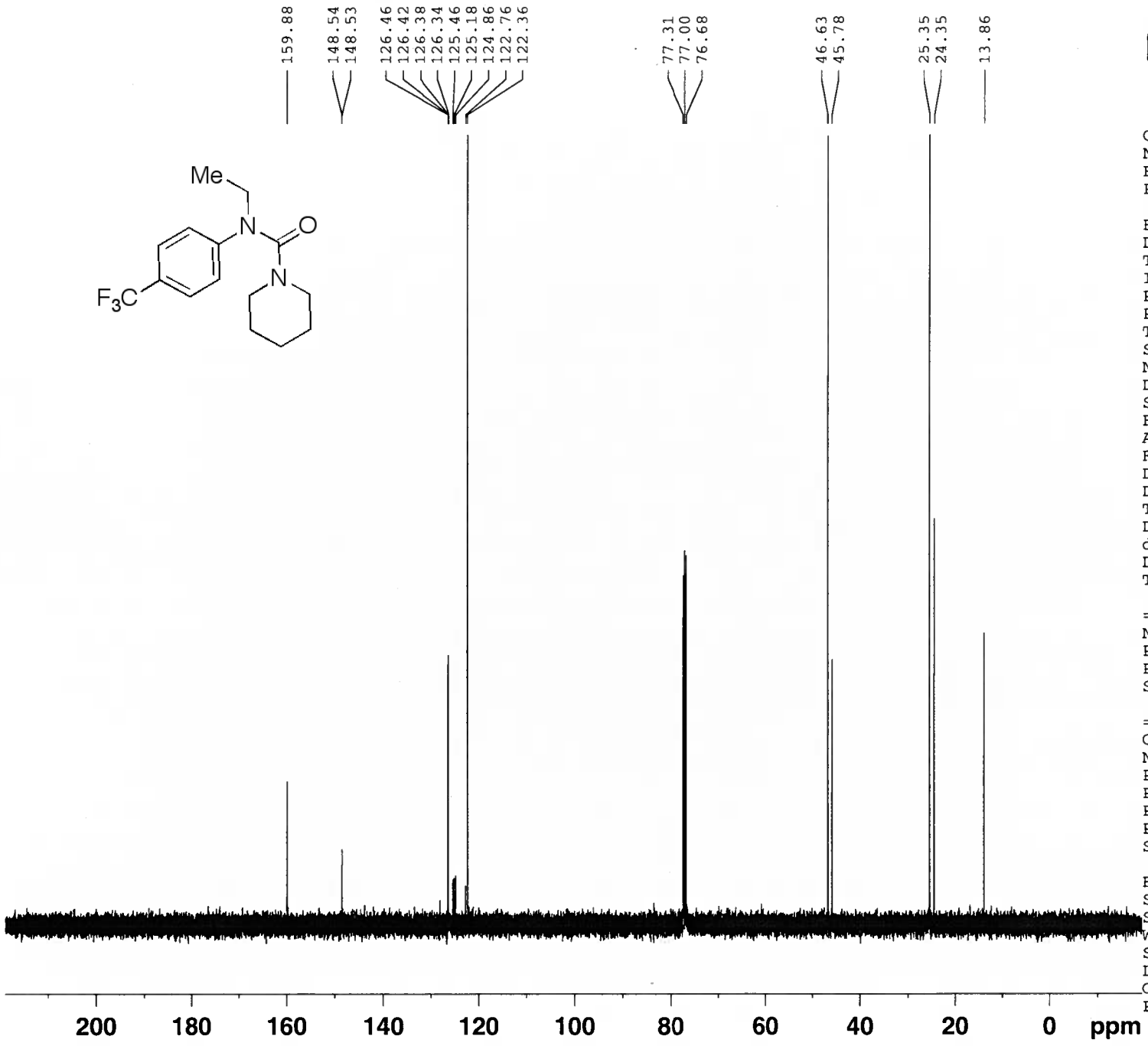


BRUKER

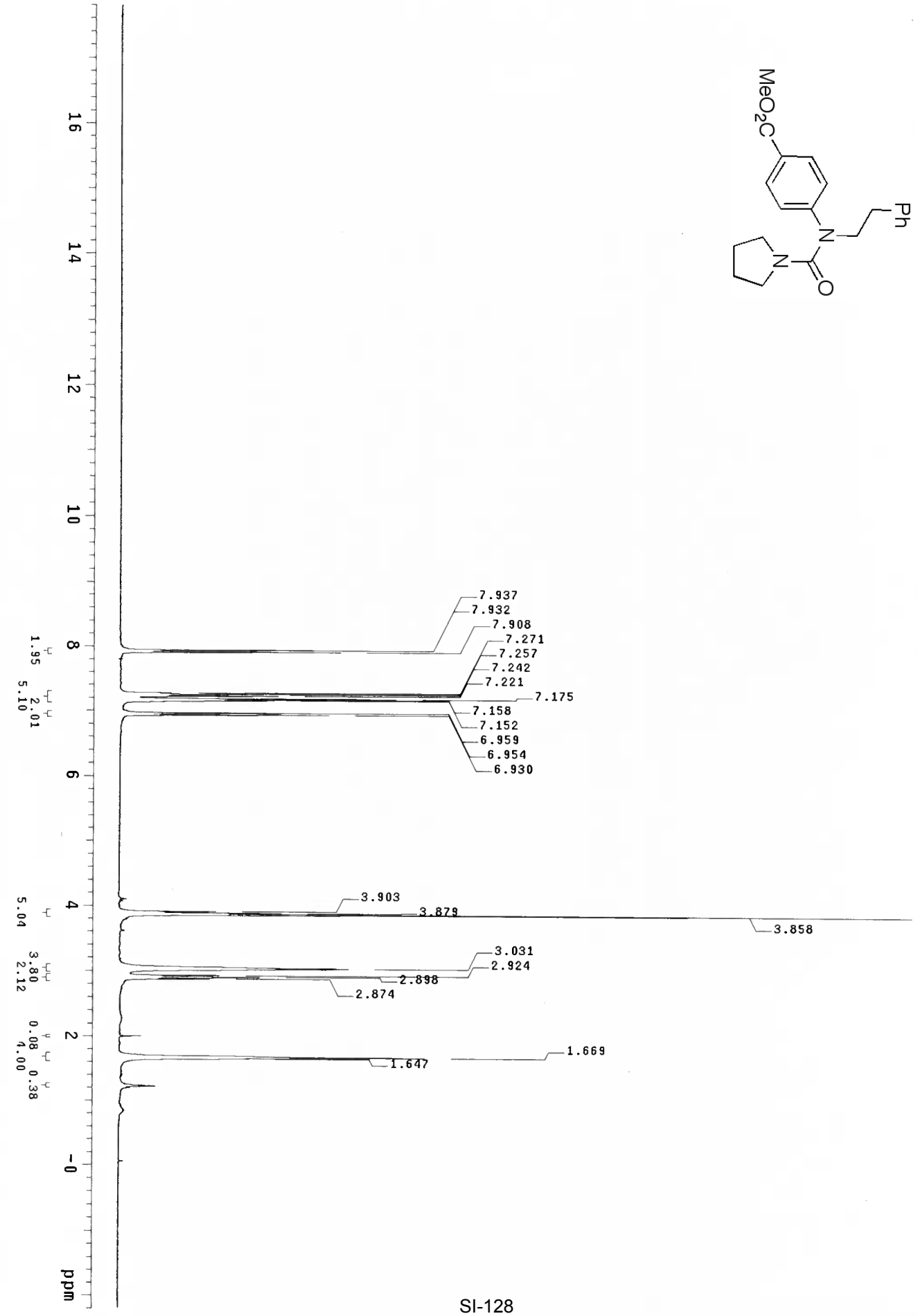
Current Data Parameters
NAME jdh-2-249-c13
EXPNO 1
PROCNO 1

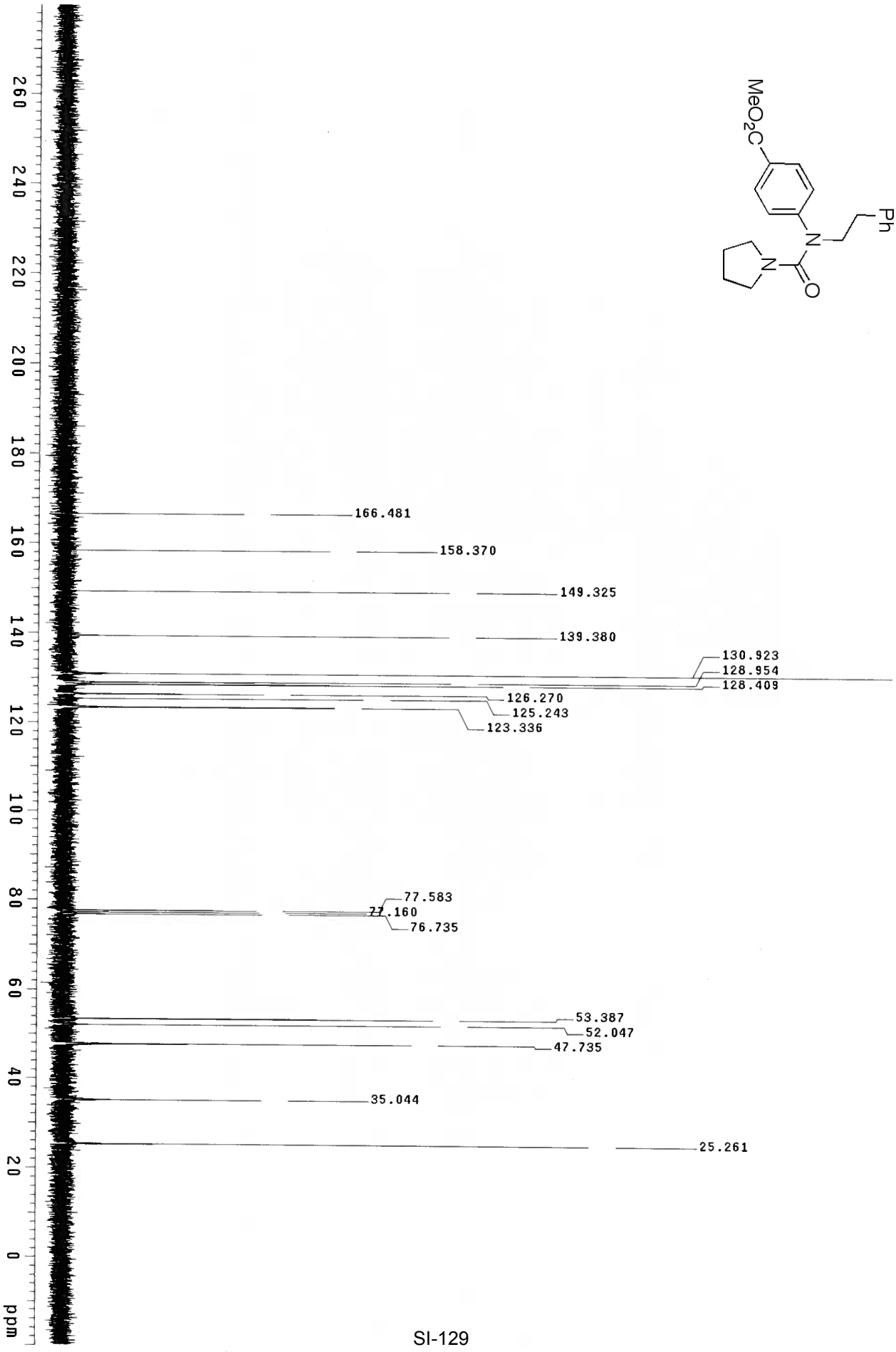
F2 - Acquisition Parameters
Date_ 20080917
Time 12.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

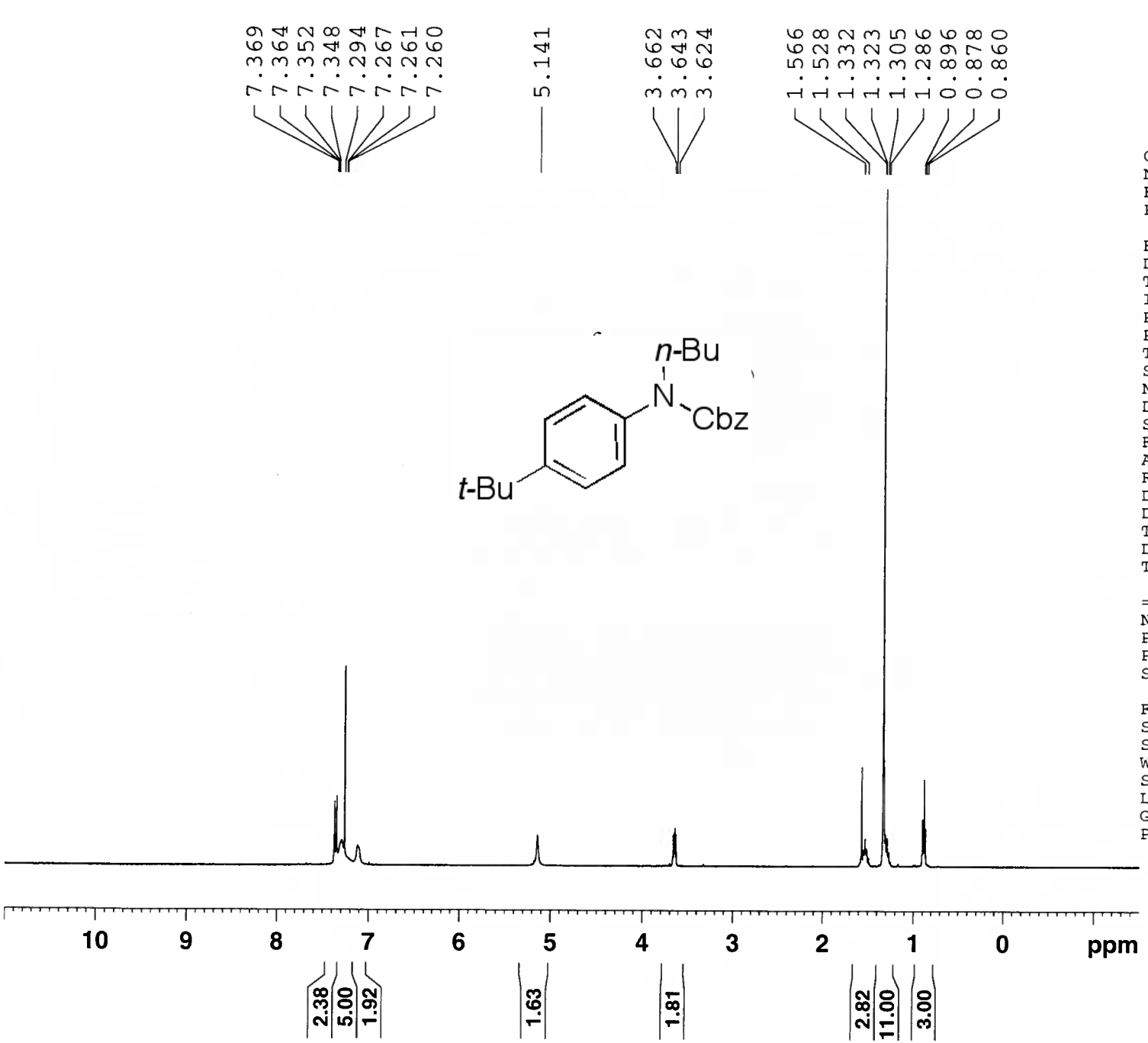
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127741 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40


MeO2C
Ph
N
N
O
7.937
7.932
7.908
7.271
7.257
7.242
7.221
7.175
7.158
7.152
6.959
6.954
6.930
3.903
3.879
3.858
3.031
2.924
2.898
2.874
1.669
1.647
1.95
2.01
5.10
5.04
3.80
2.12
0.08
1.00
0.38
16
14
12
10
8
6
4
2
-0
ppm


MeO2C
Ph
N
N
O
166.481
158.370
149.325
139.380
130.923
128.954
128.409
126.270
125.243
123.336
77.583
77.160
76.735
53.387
52.047
47.735
35.044
25.261
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm



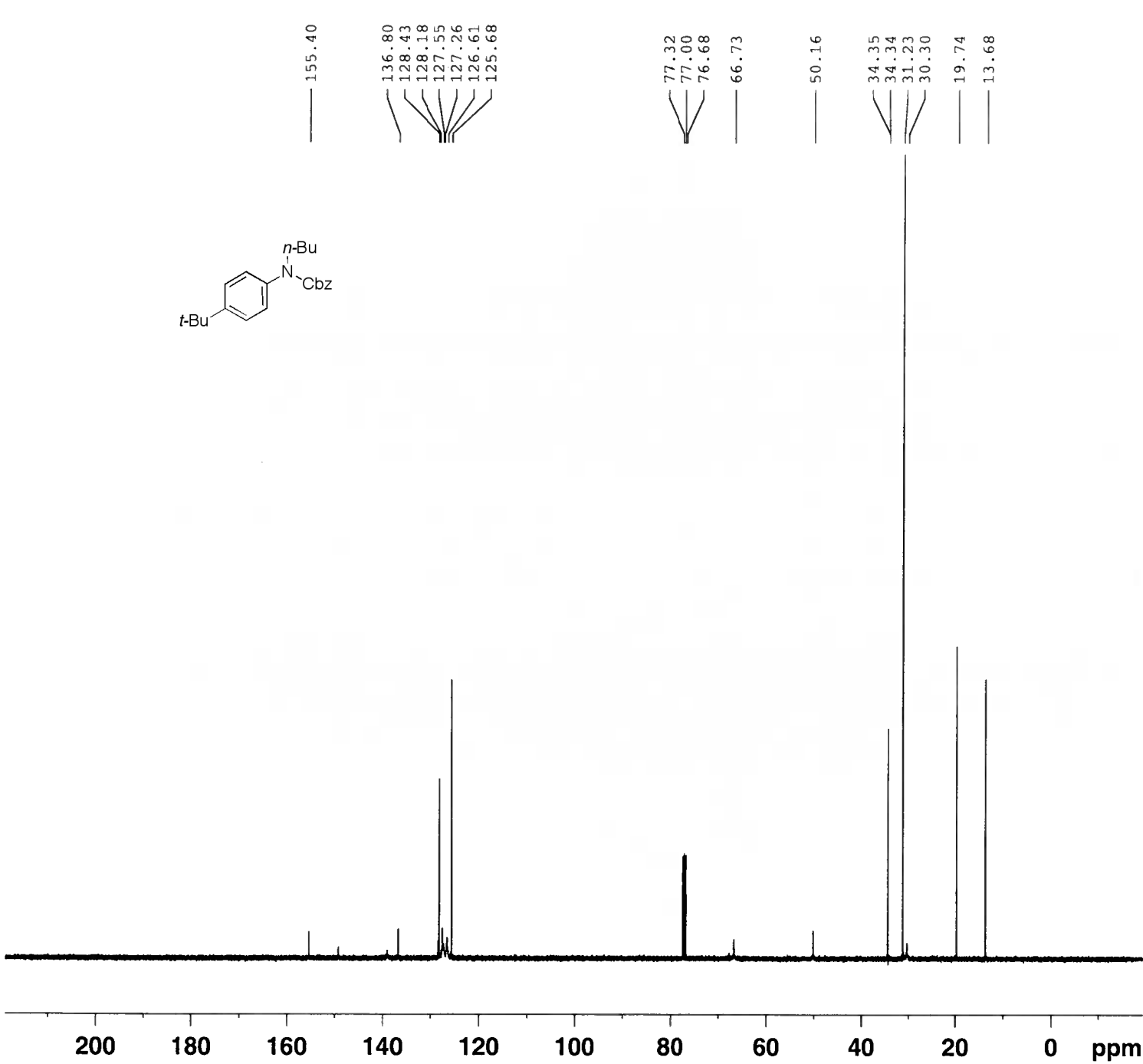
BRUKER

Current Data Parameters
NAME jdh-2-278
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080927
Time 17.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



BRUKER

Current Data Parameters

NAME	jdh-2-278-2-c13
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080929
Time	16.48
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	184
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	5792.6
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

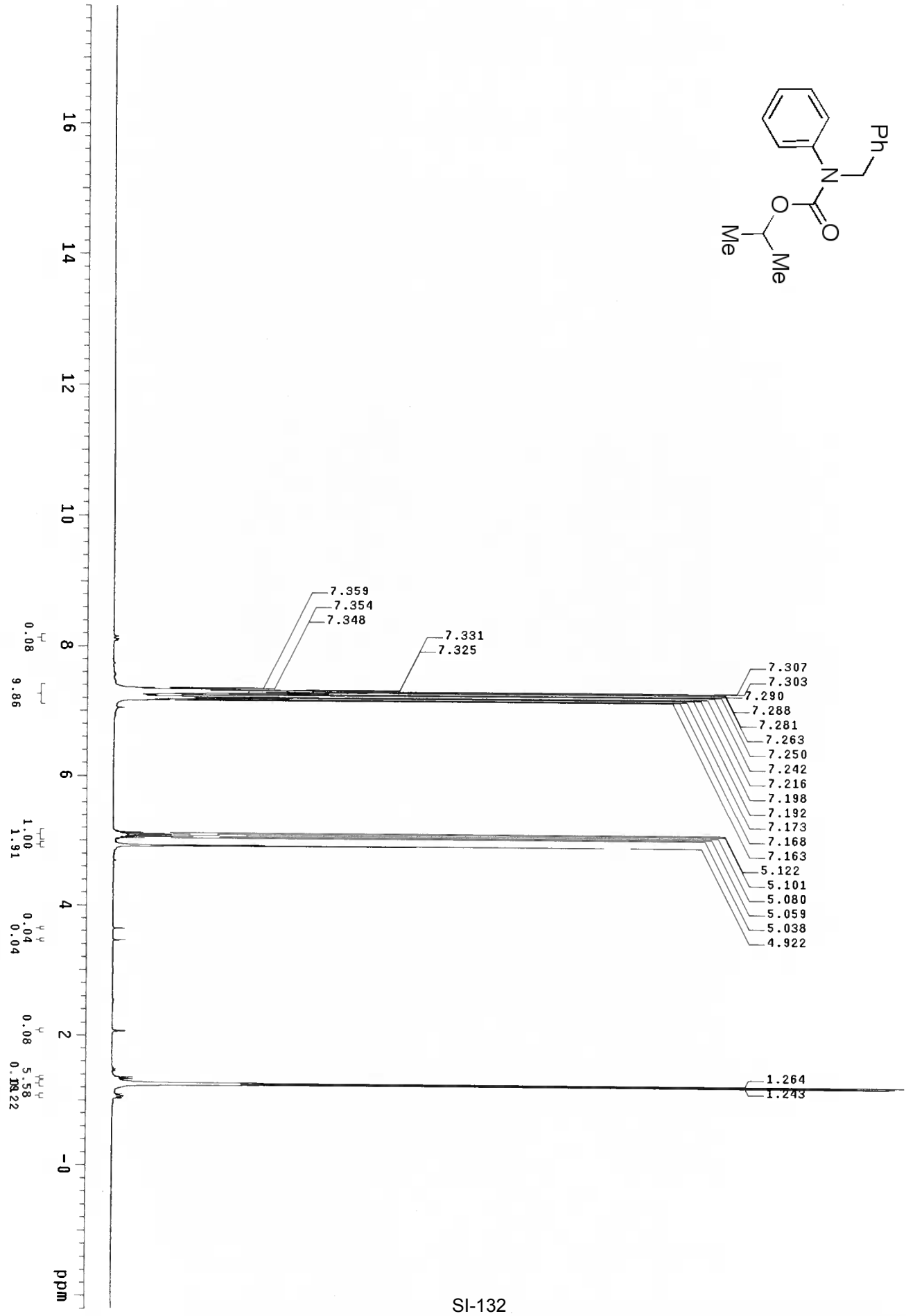
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

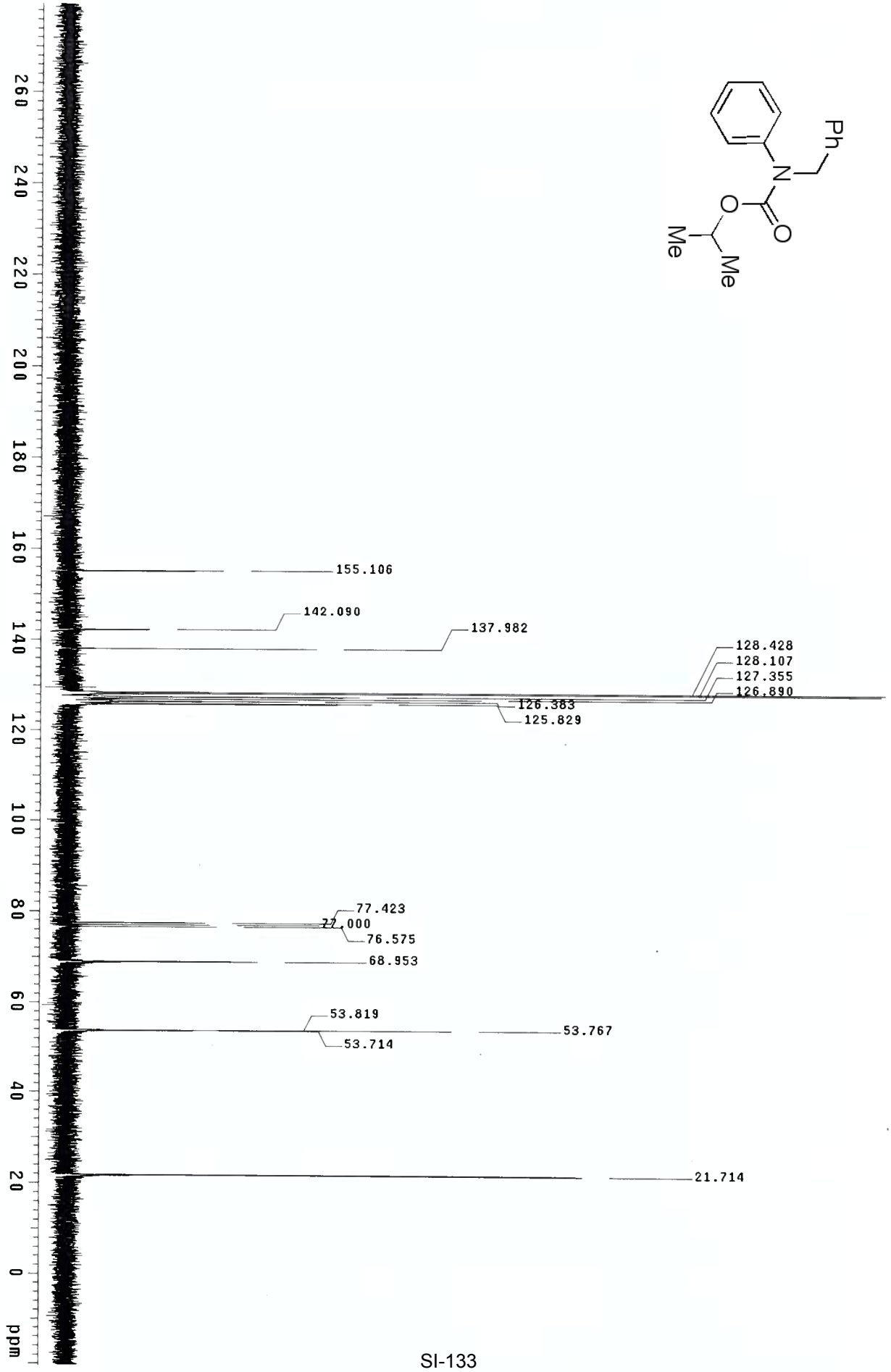
======== CHANNEL f2 ========

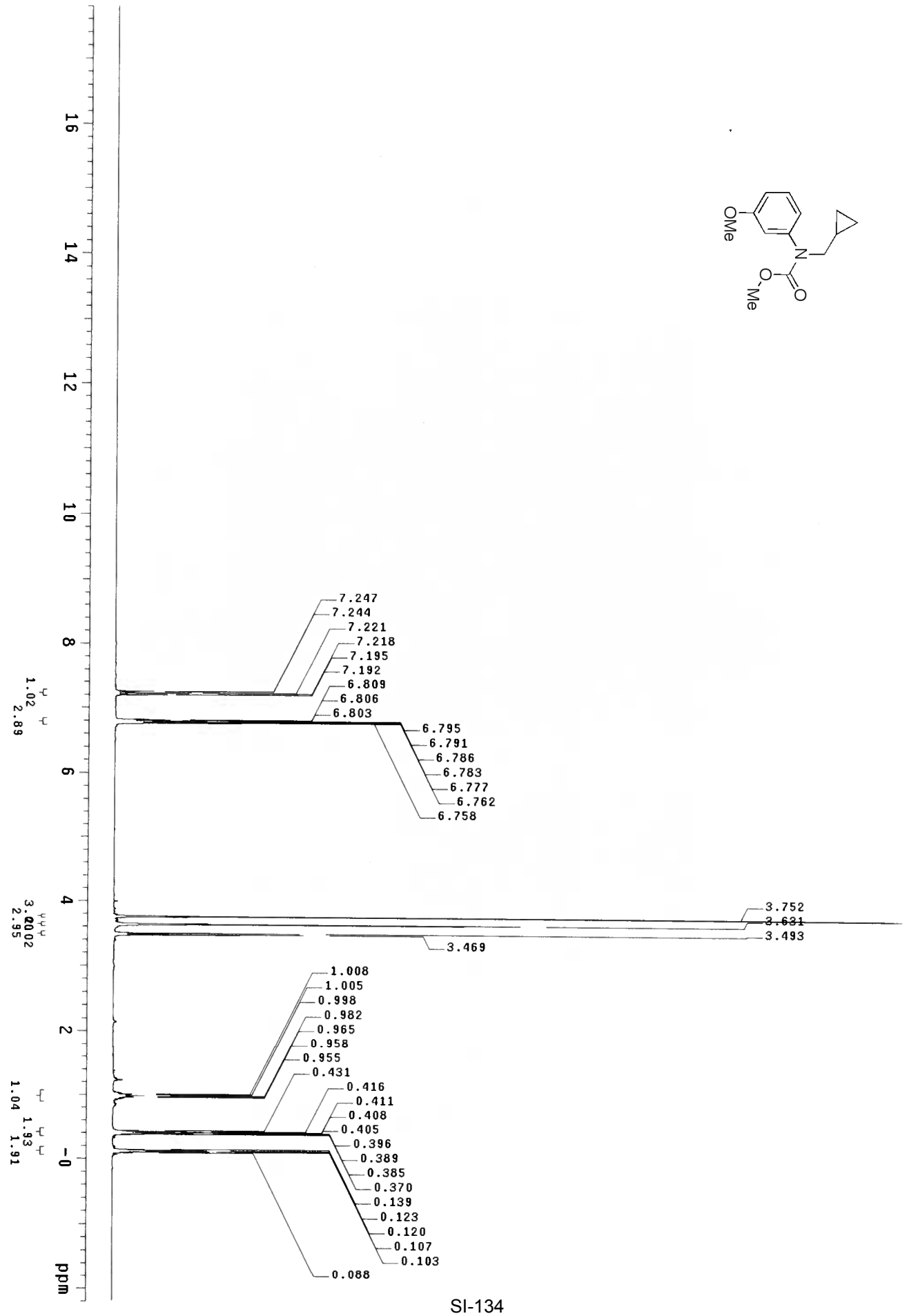
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

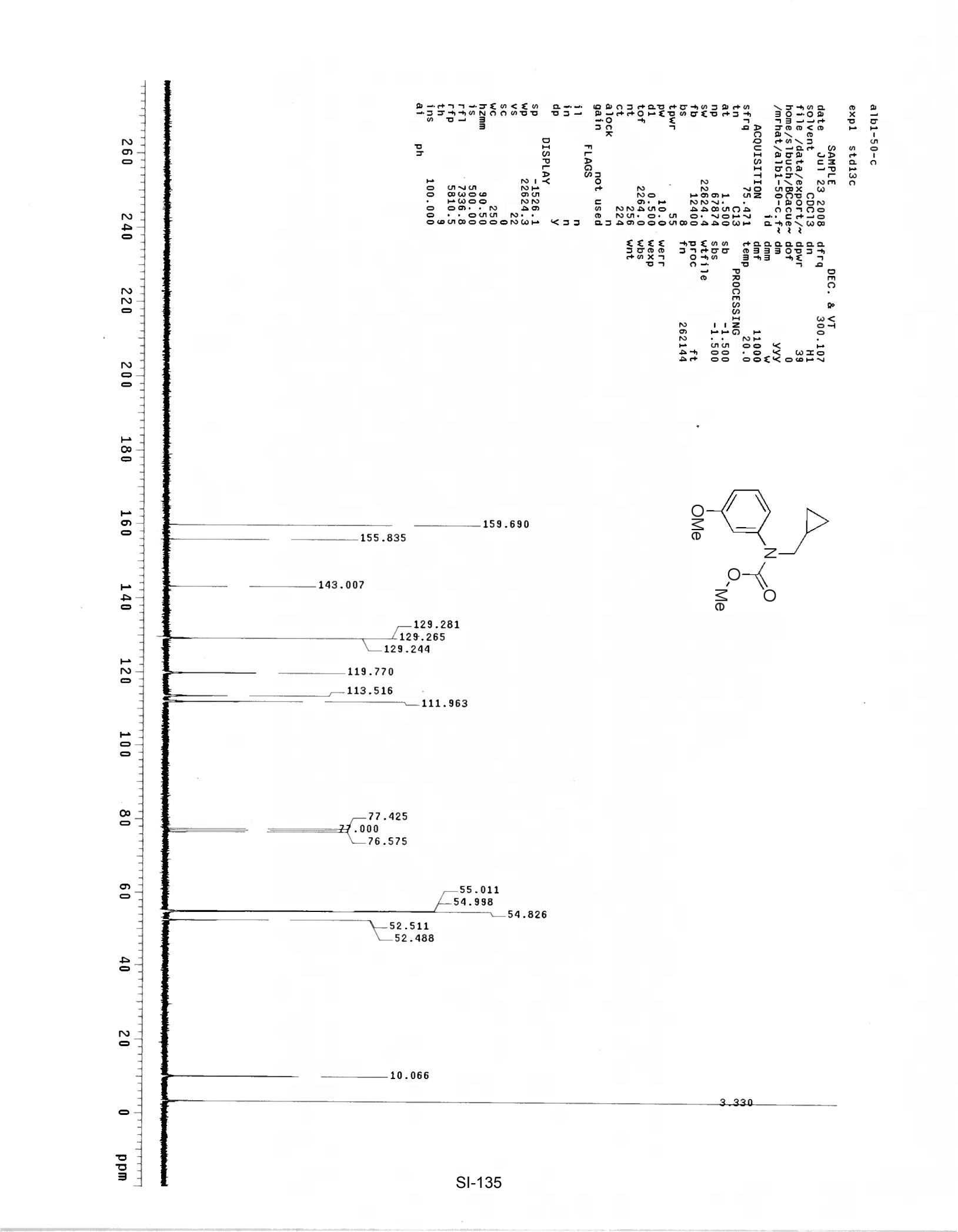
F2 - Processing parameters

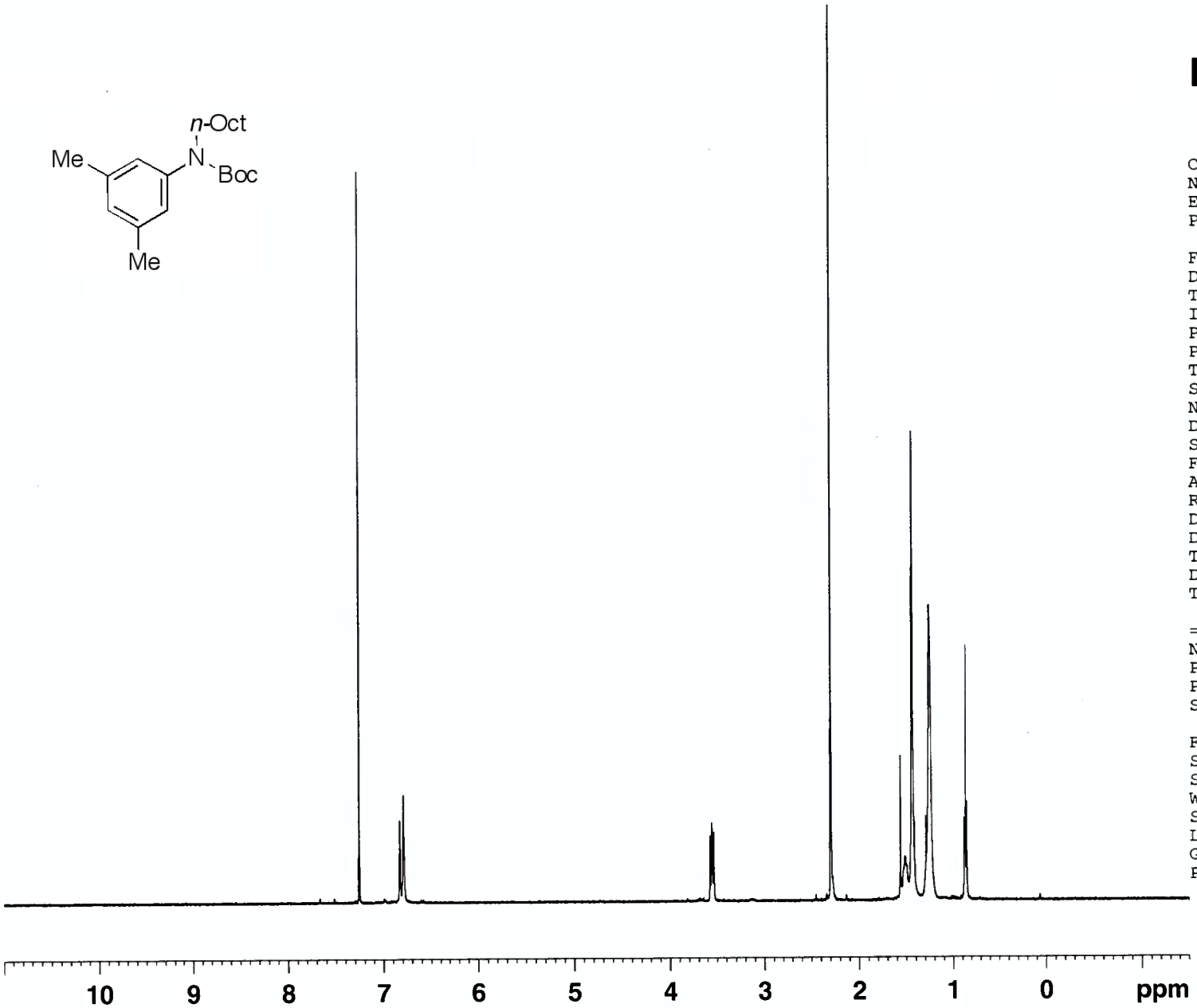
SI	65536
SF	100.6127905 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40


Ph
N
O
O
Me
Me
7.359
7.354
7.348
7.331
7.325
7.307
7.303
7.290
7.288
7.281
7.263
7.250
7.242
7.216
7.198
7.192
7.173
7.168
7.163
5.122
5.101
5.080
5.059
5.038
4.922
1.264
1.243
16
14
12
10
8
6
4
2
-0
ppm


Ph
N
O
O
Me
Me
155.106
142.090
137.982
128.428
128.107
127.355
126.890
126.383
125.829
77.423
77.000
76.575
68.953
53.819
53.767
53.714
21.714
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm


OMe
N
O
O
Me
7.247
7.244
7.221
7.218
7.195
7.192
6.809
6.806
6.803
6.795
6.791
6.786
6.783
6.777
6.762
6.758
3.752
3.631
3.493
3.469
1.008
1.005
0.998
0.982
0.965
0.958
0.955
0.431
0.416
0.411
0.408
0.405
0.396
0.389
0.385
0.370
0.139
0.123
0.120
0.107
0.103
0.088
1.02
2.89
3.00
2.95
1.04
1.93
1.91
ppm


alb1-50-c
exp1 std13c
SAMPLE
date Jul 23 2008
solvent CDCl3
file /data/export/~
home/slbuch/BCacue~
/mrhat/alb1-50-c.f~
id
ACQUISITION
sfrq 75.471
tn C13
at 1.500
np 67874
sw 22624.4
fb 12400
bs 8
tpwr 55
pw 10.0
d1 0.500
tof 2264.0
nt 256
ct 224
alock n
gain n
FLAGS
not used
il n
in n
dp y
DISPLAY
sp -1526.1
wp 22624.3
vs 22
sc 0
wc 250
hzmm 90.50
is 500.00
rfl 7336.8
rfp 5810.5
th 9
ins 100.000
ph
af
DEC. & VT
dfrq 300.107
dn H1
dpwr 39
dof 0
dm yyy
dmm w
dmf 11000
temp 20.0
PROCESSING
sb -1.500
sbs -1.500
wtfile
proc ft
fn 262144
werr
wexp
wbs
wnt
OMe
N
O
O
Me
159.690
155.835
143.007
129.281
129.265
129.244
119.770
113.516
111.963
77.425
77.000
76.575
55.011
54.998
54.826
52.511
52.488
10.066
3.330
ppm



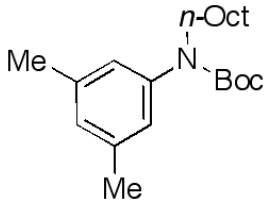
BRUKER

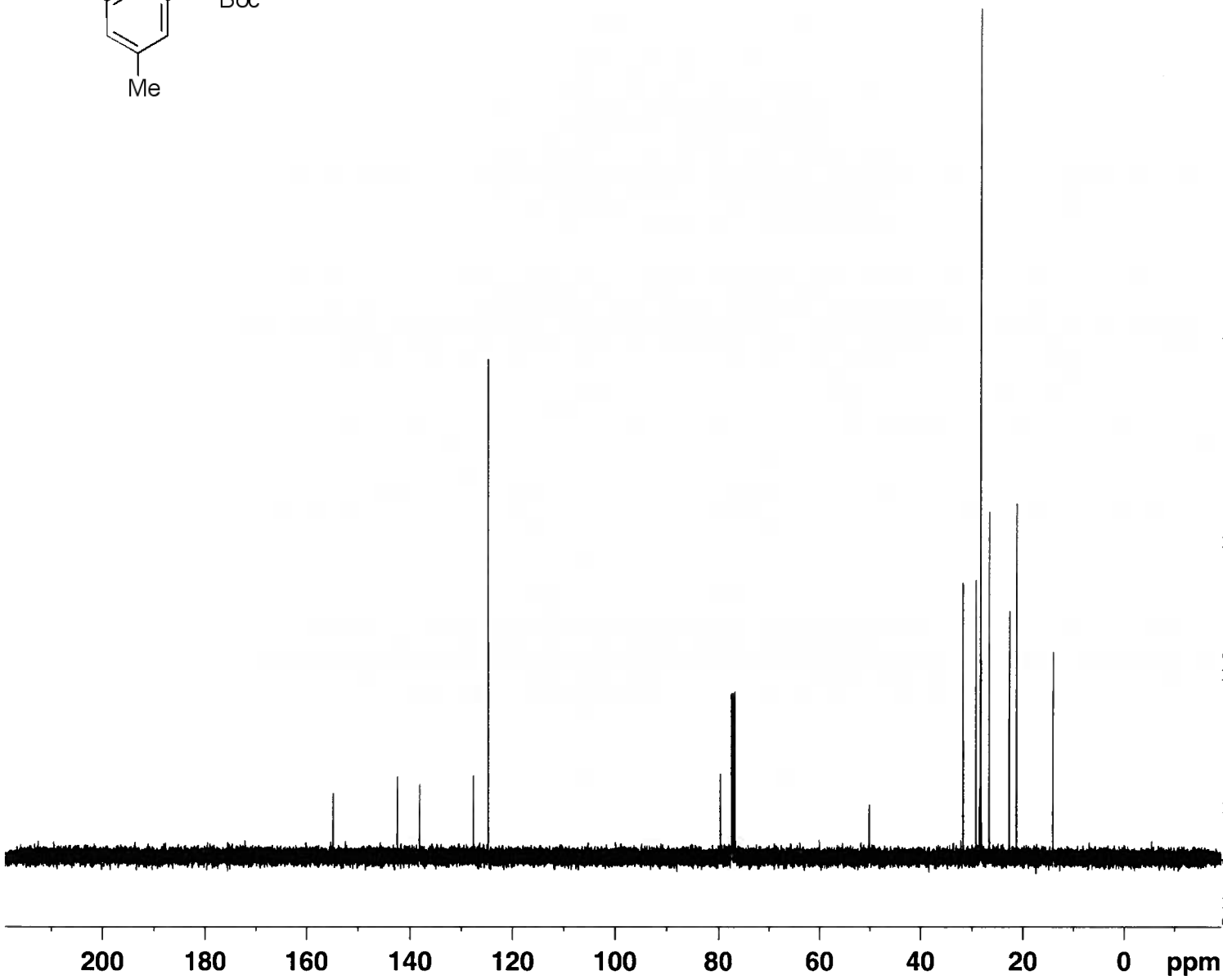
```
Current Data Parameters
NAME                  jdh-2-221
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080902
Time                      11.06
INSTRUM                   spect
PROBHD   5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                        406.4
DW                       60.400 usec
DE                        6.00 usec
TE                       291.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.88 usec
PL1                       0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300097 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```





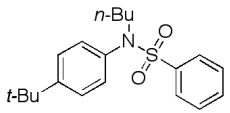

```
Current Data Parameters
NAME      jdh-2-267-c13
EXPNO                1
PROCNO               1

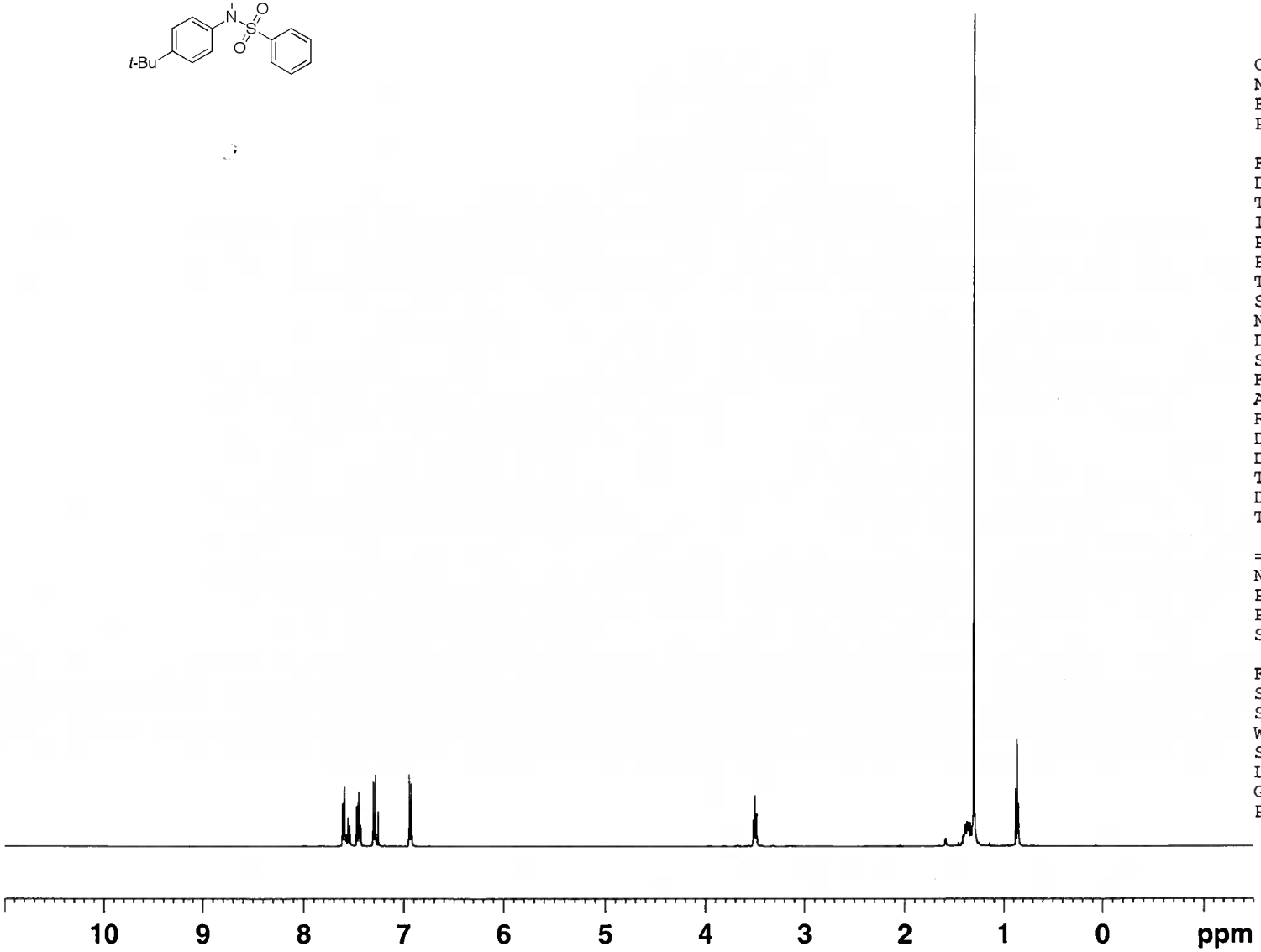
F2 - Acquisition Parameters
Date_           20080923
Time               12.15
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    2
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                2896.3
DW                20.850 usec
DE                 6.00 usec
TE                292.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                 0.00 dB
PL12               16.10 dB
PL13               19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                65536
SF          100.6127751 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
```





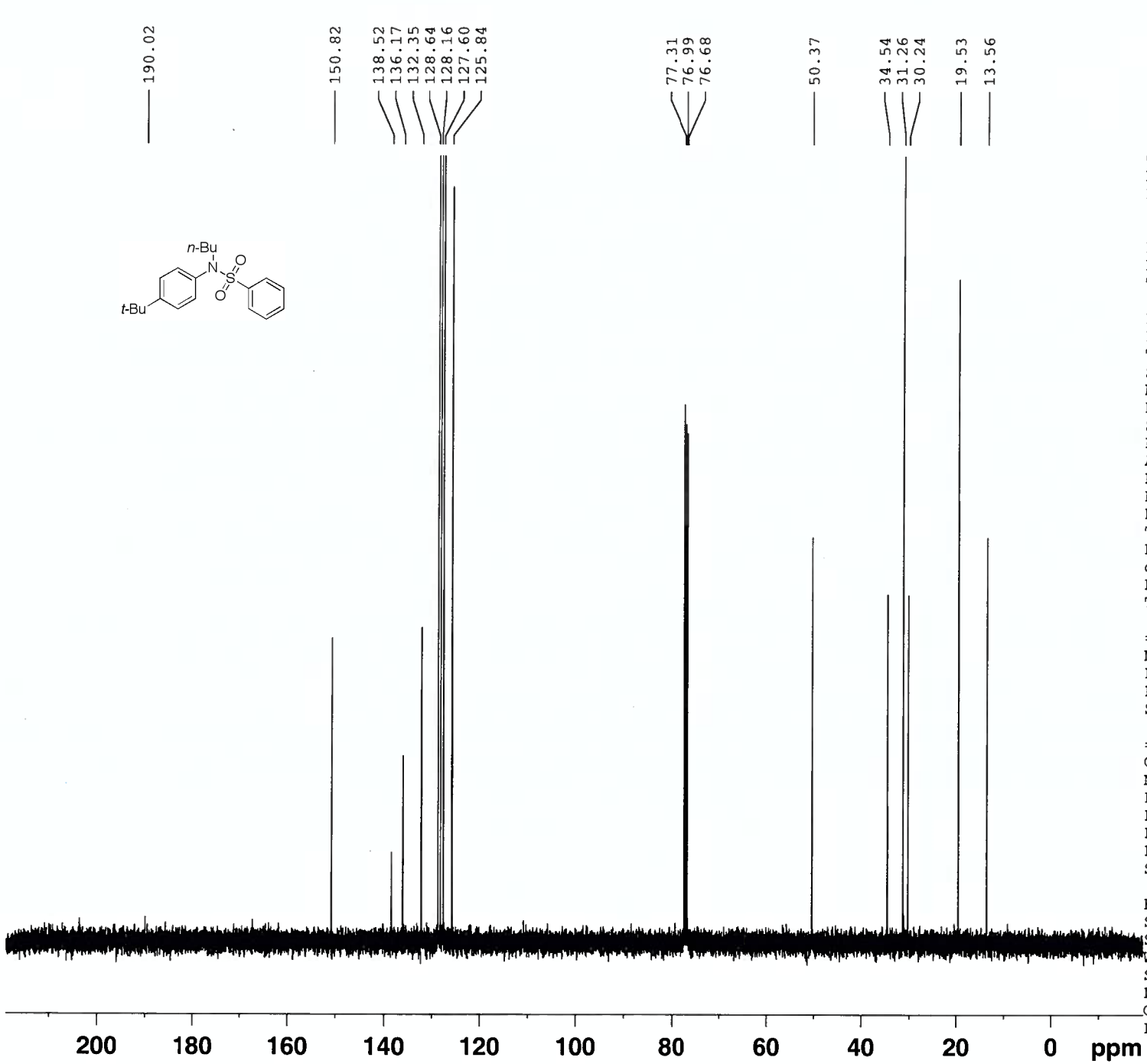
BRUKER

```
Current Data Parameters
NAME                  jdh-2-238
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080908
Time                      20.19
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                         256
DW                      60.400 usec
DE                       6.00 usec
TE                      291.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.88 usec
PL1                       0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                  400.1300094 MHz
WDW                         no
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.00
```



BRUKER

Current Data Parameters
NAME jdh-2-238-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080908
Time	20.37
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	2580.3
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

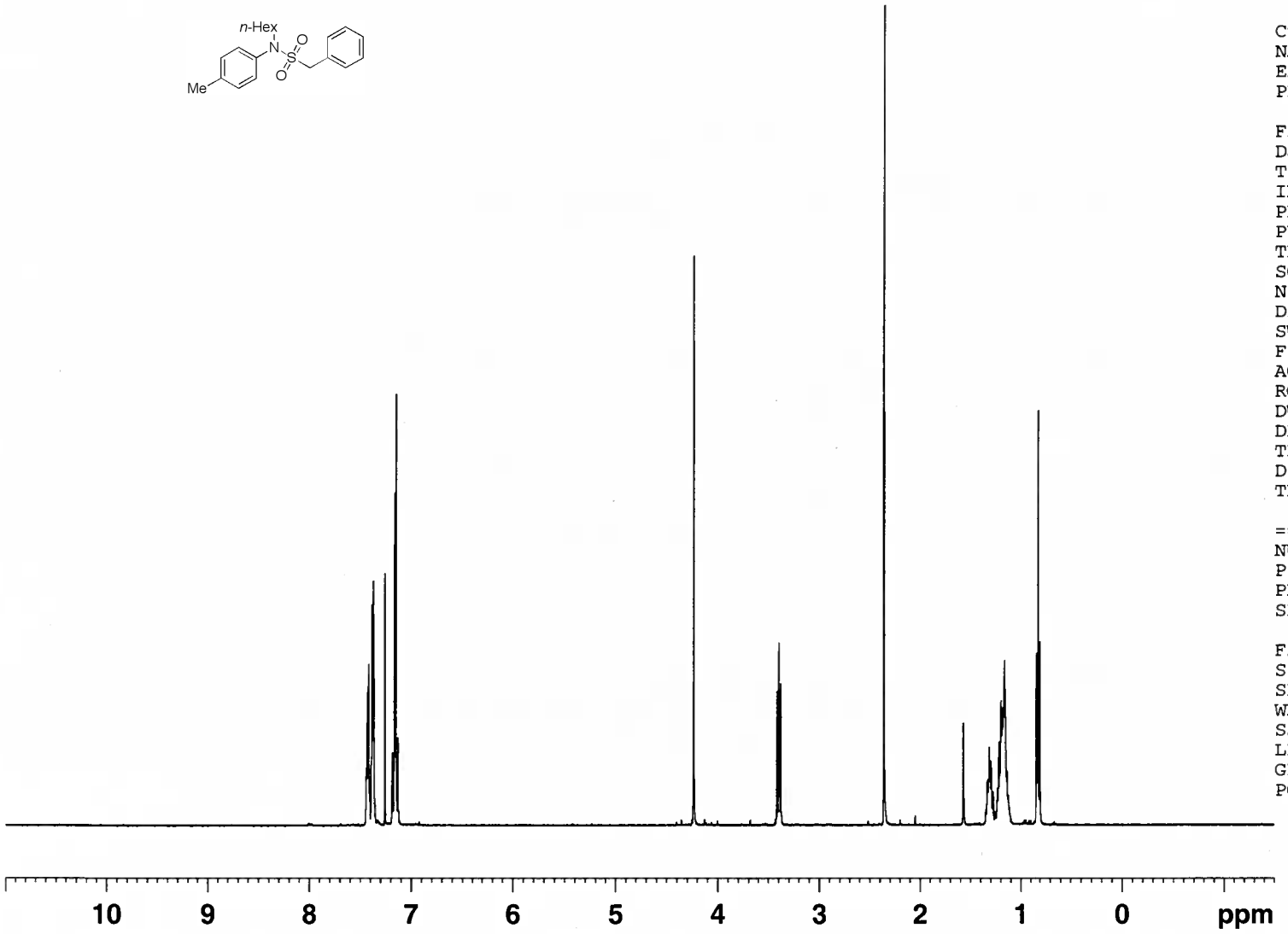
NUC1	13C
P1	9.38 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	16.10 dB
PL13	19.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127760 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



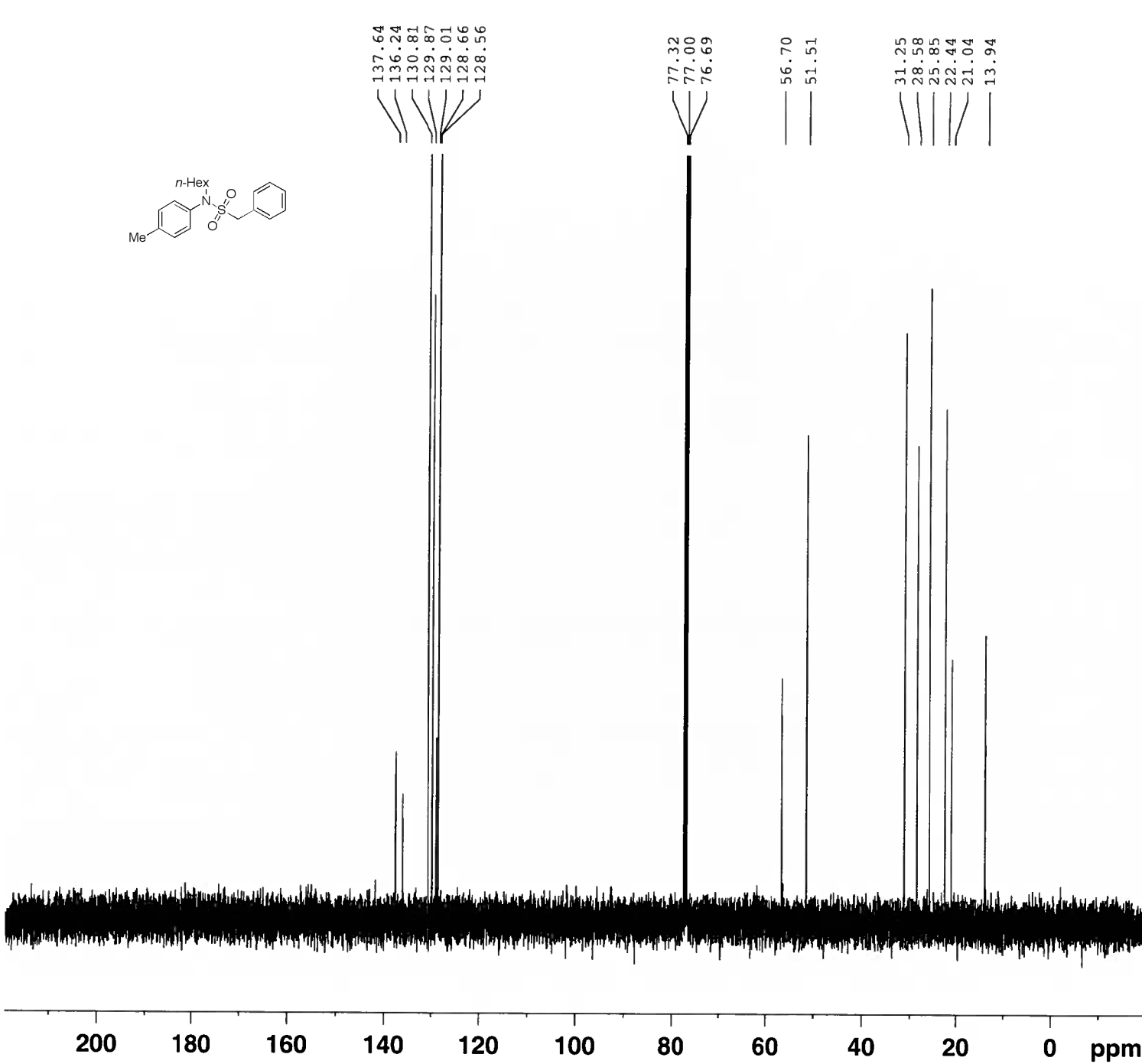
BRUKER

Current Data Parameters
NAME jdh-2-240
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080909
Time 12.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 287.4
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



BRUKER

```
Current Data Parameters
NAME       jdh-2-240-c13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080909
Time               12.21
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664756 sec
RG                1625.5
DW               20.850 usec
DE                6.00 usec
TE                292.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.38 usec
PL1                0.00 dB
SFO1        100.6228298 MHz

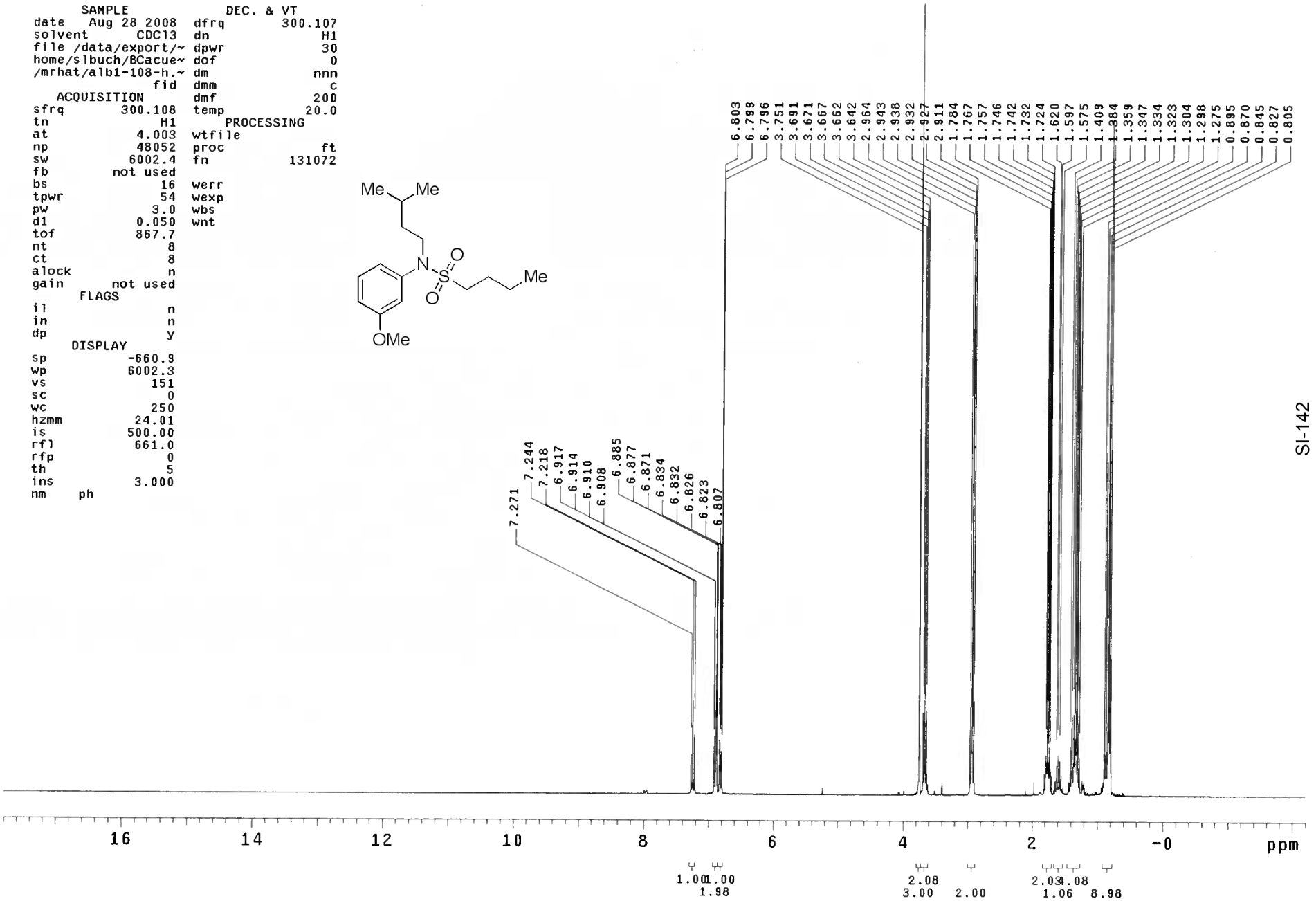
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              16.10 dB
PL13              19.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127756 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.40
```

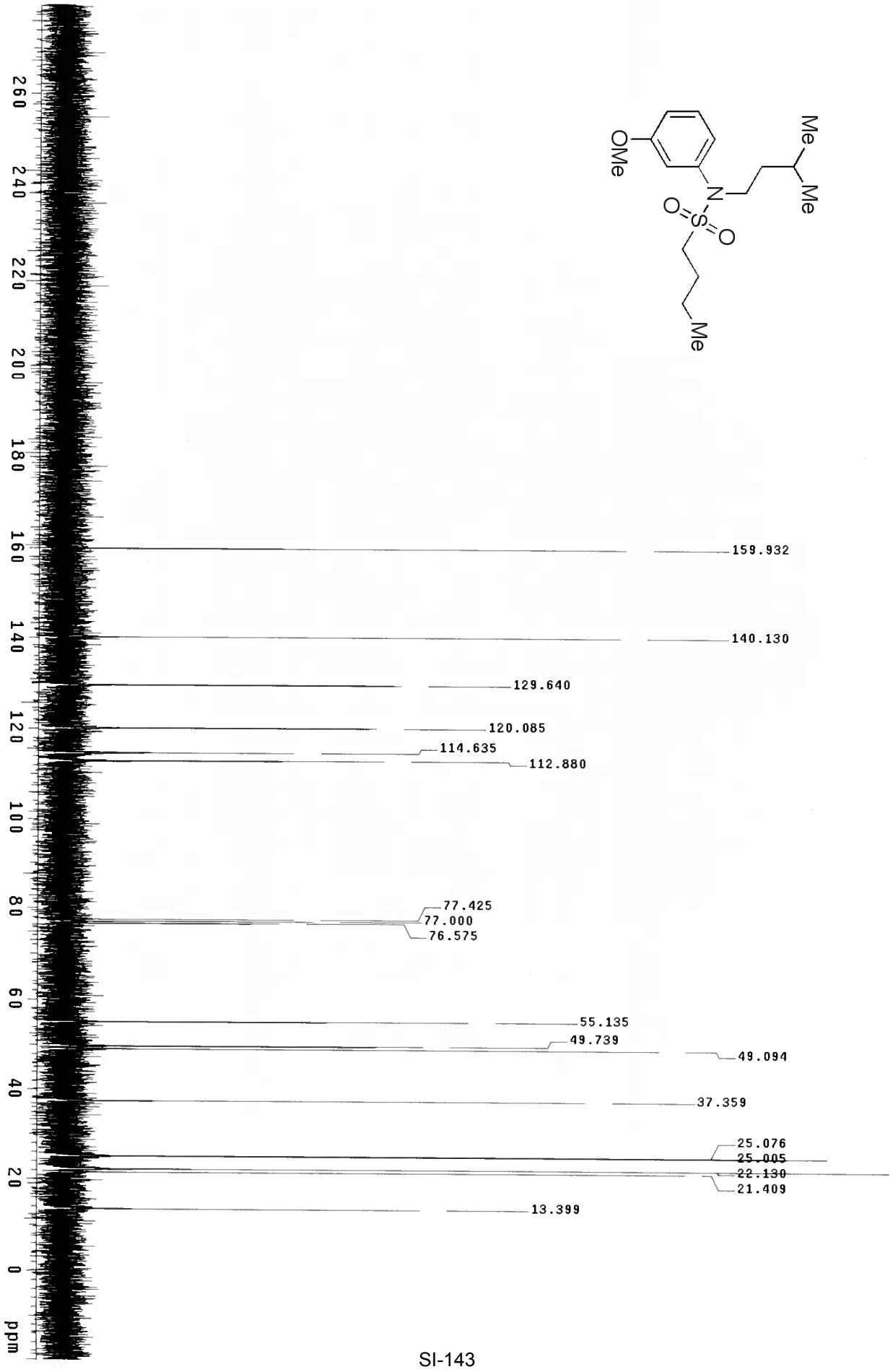
alb1-108-h

exp1 std1h

SAMPLE		DEC. & VT	
date	Aug 28 2008	dfrq	300.107
solvent	CDCl3	dn	H1
file	/data/export/~	dpwr	30
	home/slbuch/BCacue~	dof	0
	/mrhat/alb1-108-h.~	dm	nnn
	fid	dmm	c
ACQUISITION		dmf	200
sfrq	300.108	temp	20.0
tn	H1	PROCESSING	
at	4.003	wtfile	
np	48052	proc	ft
sw	6002.4	fn	131072
fb	not used		
bs	16	werr	
tpwr	54	wexp	
pw	3.0	wbs	
d1	0.050	wnt	
tof	867.7		
nt	8		
ct	8		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-660.9		
wp	6002.3		
vs	151		
sc	0		
wc	250		
hzmm	24.01		
is	500.00		
rfl	661.0		
rfp	0		
th	5		
ins	3.000		
nm	ph		

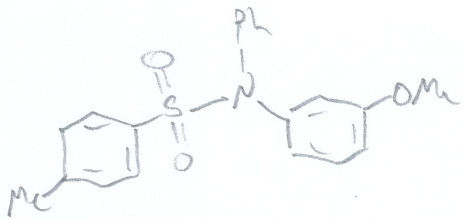


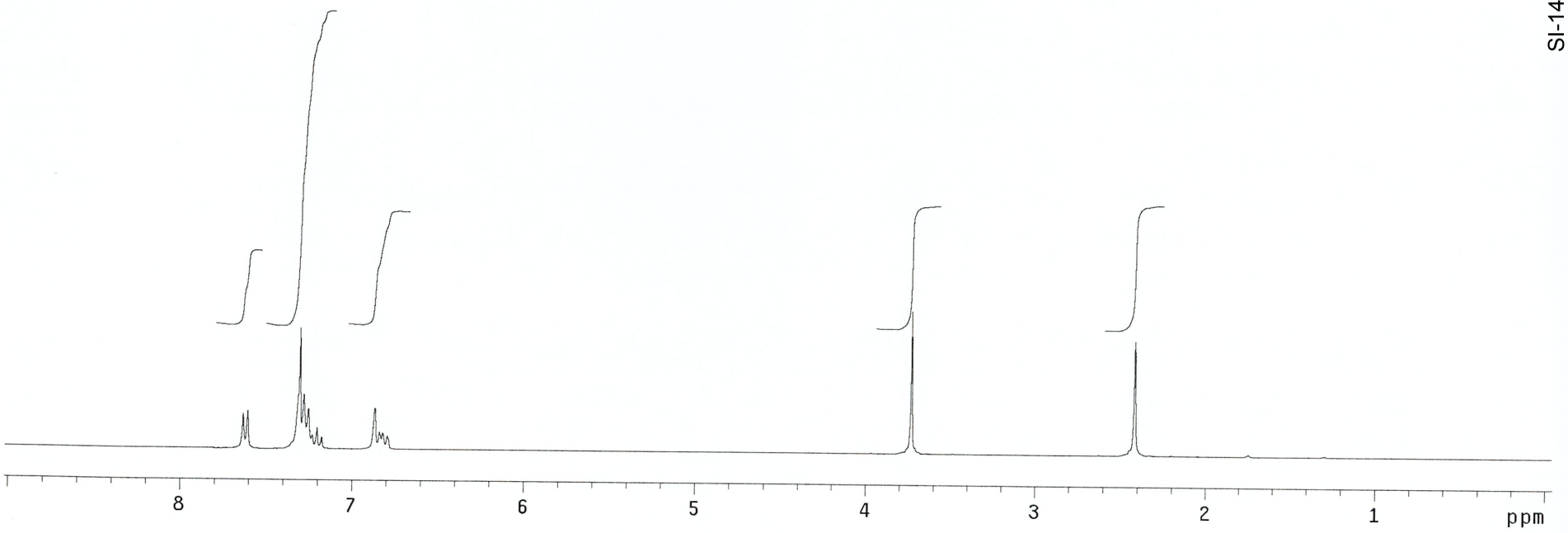
SI-142


OMe
N
O=S=O
Me
Me
Me
159.932
140.130
129.640
120.085
114.635
112.880
77.425
77.000
76.575
55.135
49.739
49.094
37.359
25.076
25.005
22.130
21.409
13.399
ppm

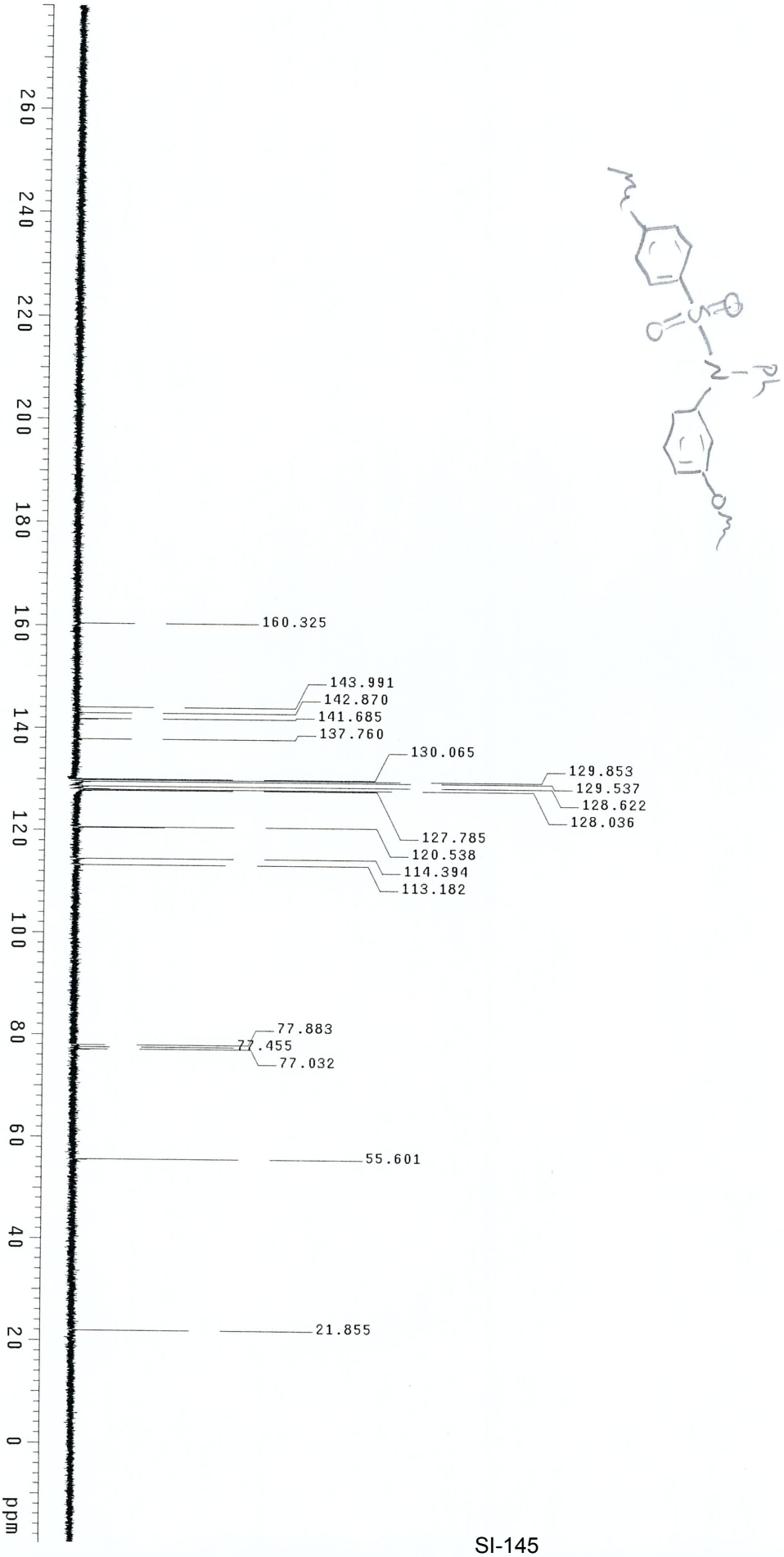
BF-VII-JACKIEPAPER

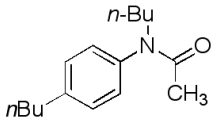
Pulse Sequence: s2pul

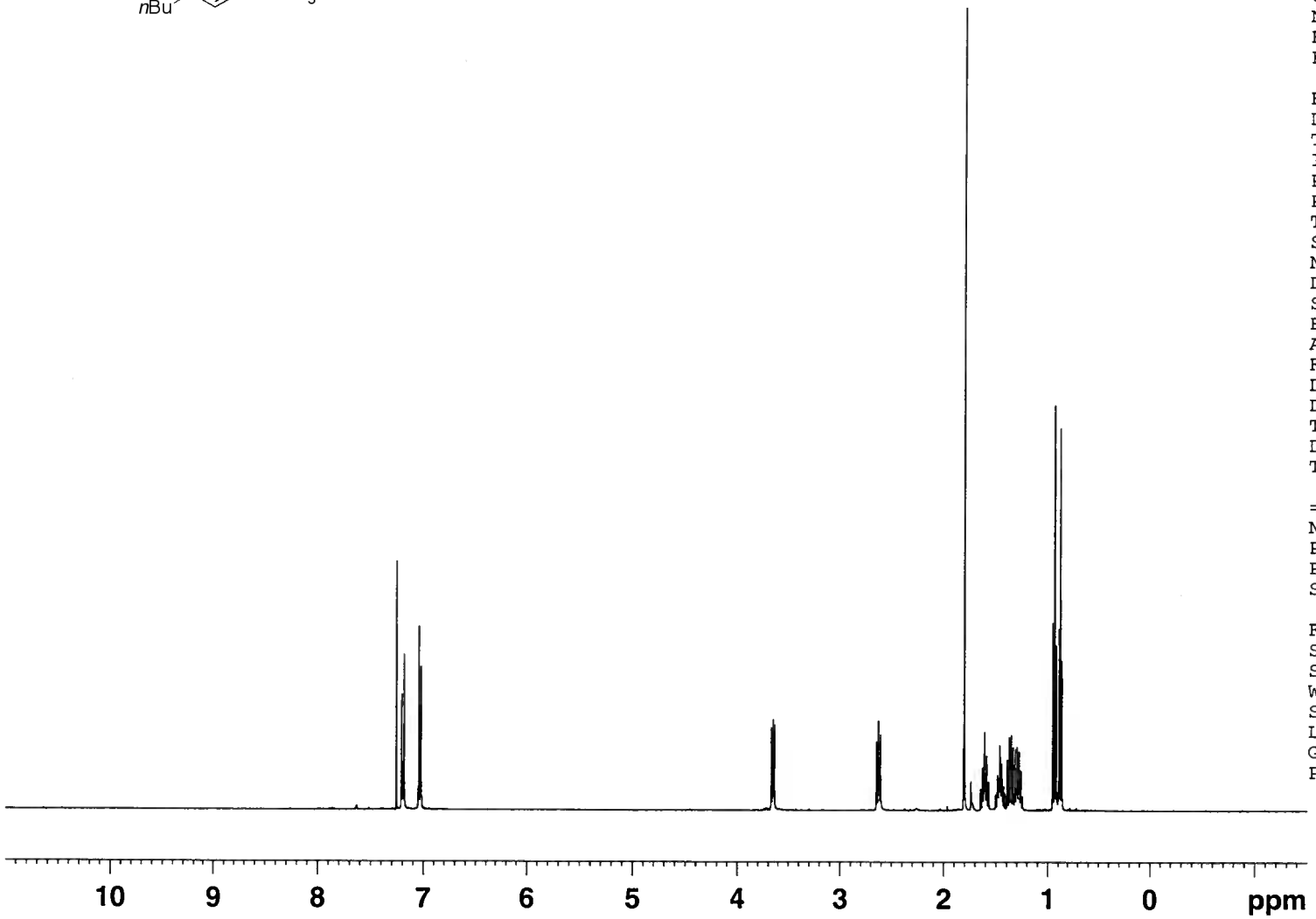




BF-VII-JACKIEPAPER-13C
Pulse Sequence: s2pul







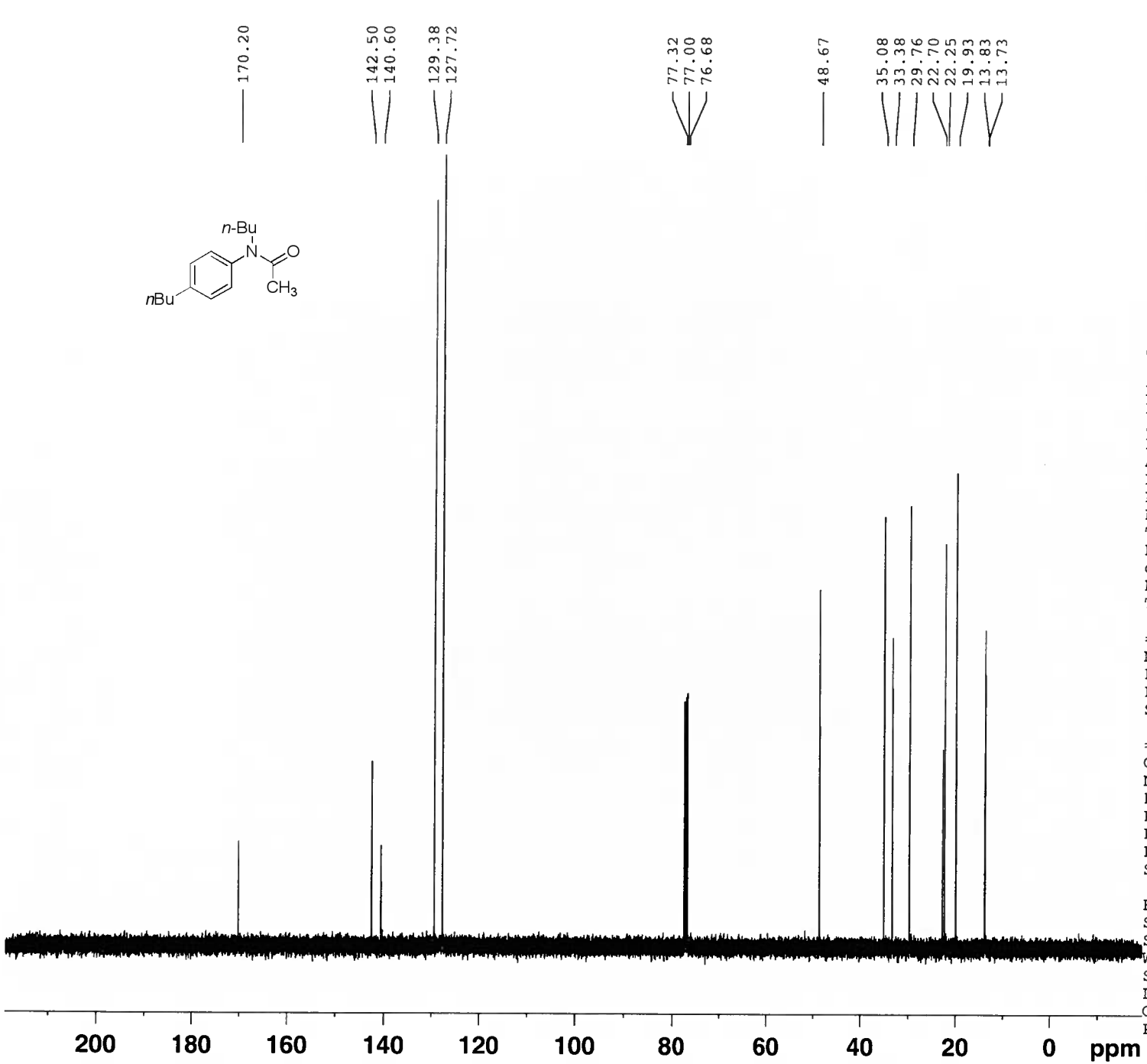
BRUKER

```
Current Data Parameters
NAME                  jdh-2-264
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20080922
Time                      12.29
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                        287.4
DW                       60.400 usec
DE                        6.00 usec
TE                       291.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.88 usec
PL1                       0.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                 400.1300098 MHz
WDW                          no
SSB                           0
LB                        0.00 Hz
GB                            0
PC                         1.00
```



BRUKER

Current Data Parameters
NAME jdh-2-264-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080922	
Time	12.40	
INSTRUM	spect	
PROBHD	5 mm QNP 1H/13	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	129	
DS	2	
SWH	23980.814	Hz
FIDRES	0.365918	Hz
AQ	1.3664756	sec
RG	1149.4	
DW	20.850	usec
DE	6.00	usec
TE	292.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	

======== CHANNEL f1 ========

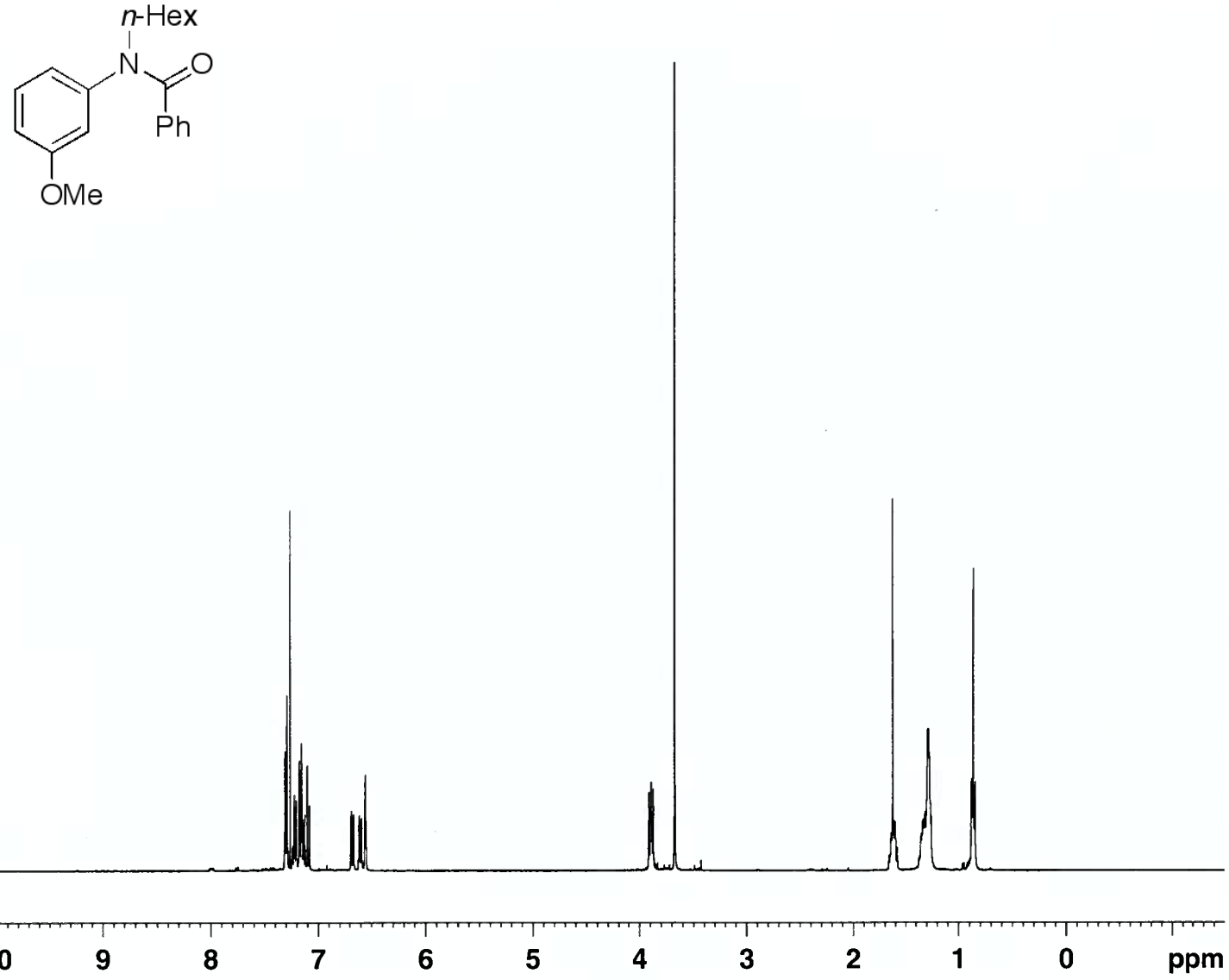
NUC1	13C	
P1	9.38	usec
PL1	0.00	dB
SFO1	100.6228298	MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	0.00	dB
PL12	16.10	dB
PL13	19.00	dB
SFO2	400.1316005	MHz

F2 - Processing parameters

SI	65536	
SF	100.6127798	MHz
WDW	no	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	



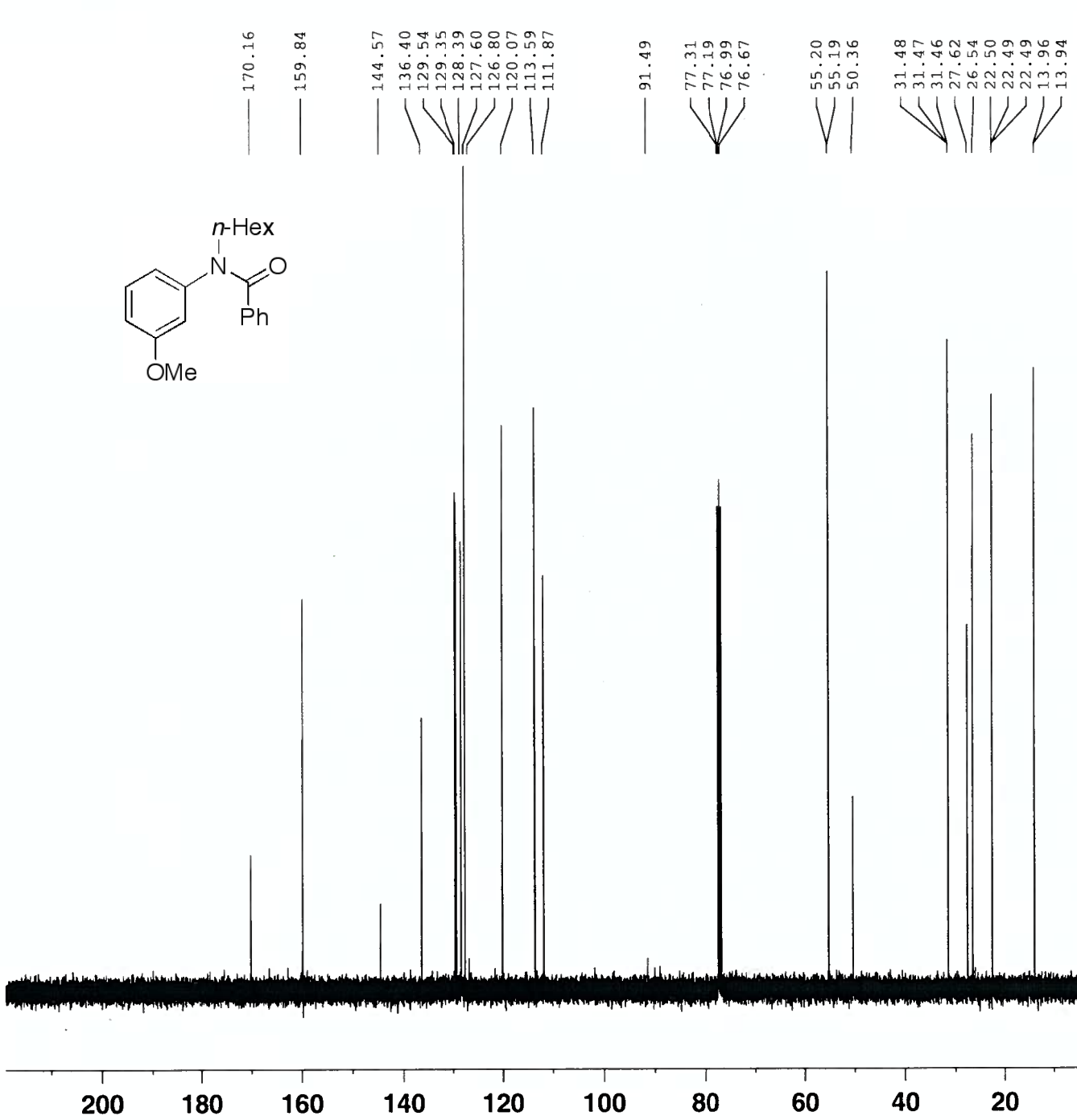

```
Current Data Parameters
NAME                  jdh-2-273
EXPNO                         1
PROCNO                        1

F2 - Acquisition Paramet
Date_                  20080924
Time                      17.52
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146
FIDRES                 0.126314
AQ                     3.9584243
RG                          181
DW                       60.400
DE                         6.00
TE                        293.2
D1                  1.00000000
TD0                           1

======== CHANNEL f1 ====
NUC1                         1H
P1                        15.07
PL1                        0.00
SFO1               400.1324710

F2 - Processing paramete
SI                        65536
SF                 400.1300095
WDW                          no
SSB                           0
LB                         0.00
GB                            0
PC                         1.00
```

SI-148



BRUKER

Current Data Parameters
NAME jdh-2-273-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20080924
Time	18.02
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	13004
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

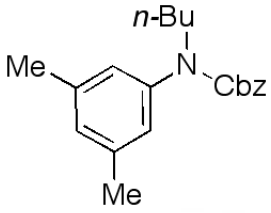
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

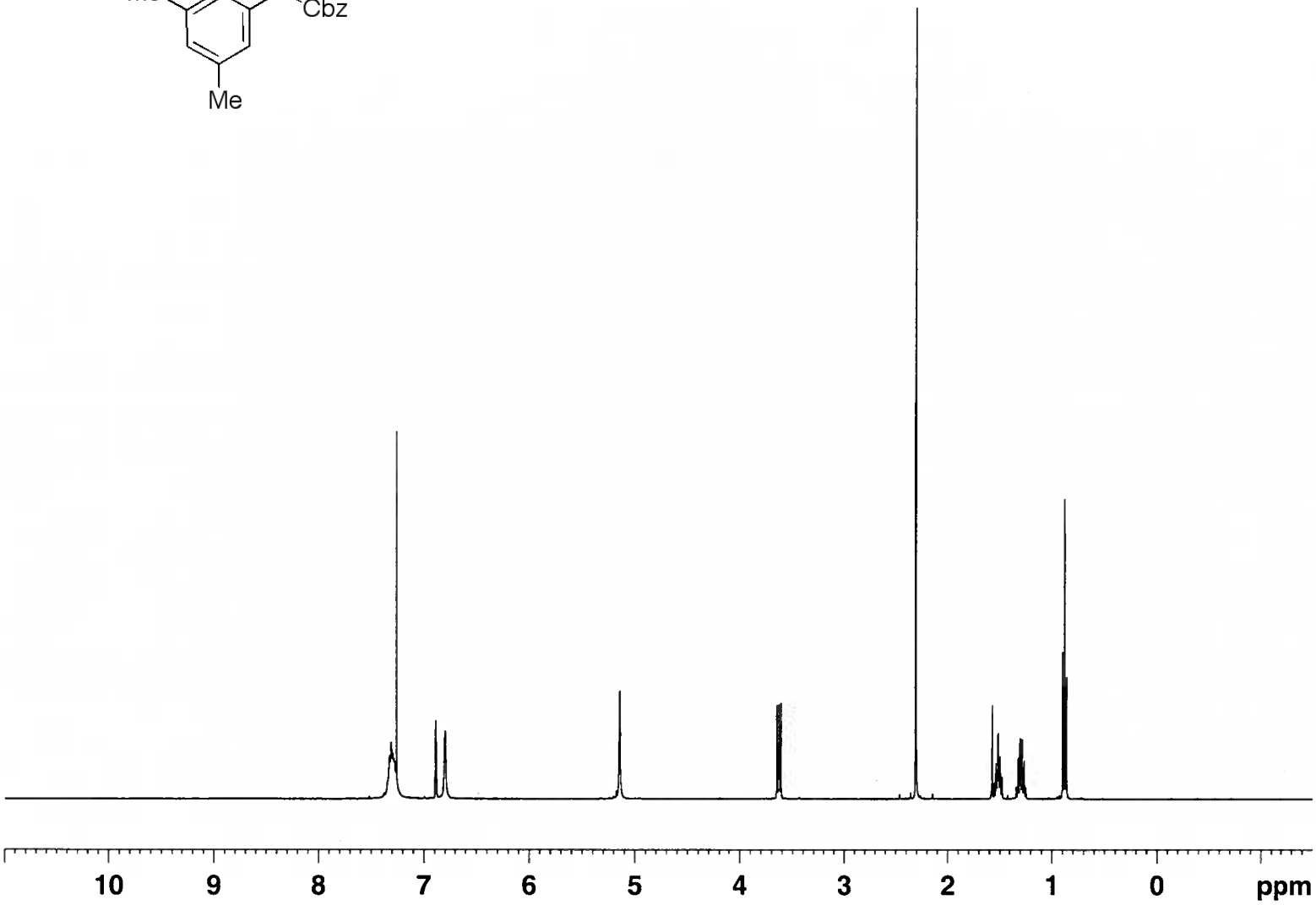
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127792 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40






```
Current Data Parameters
NAME          jdh-2-281-2
EXPNO                   1
PROCNO                  1

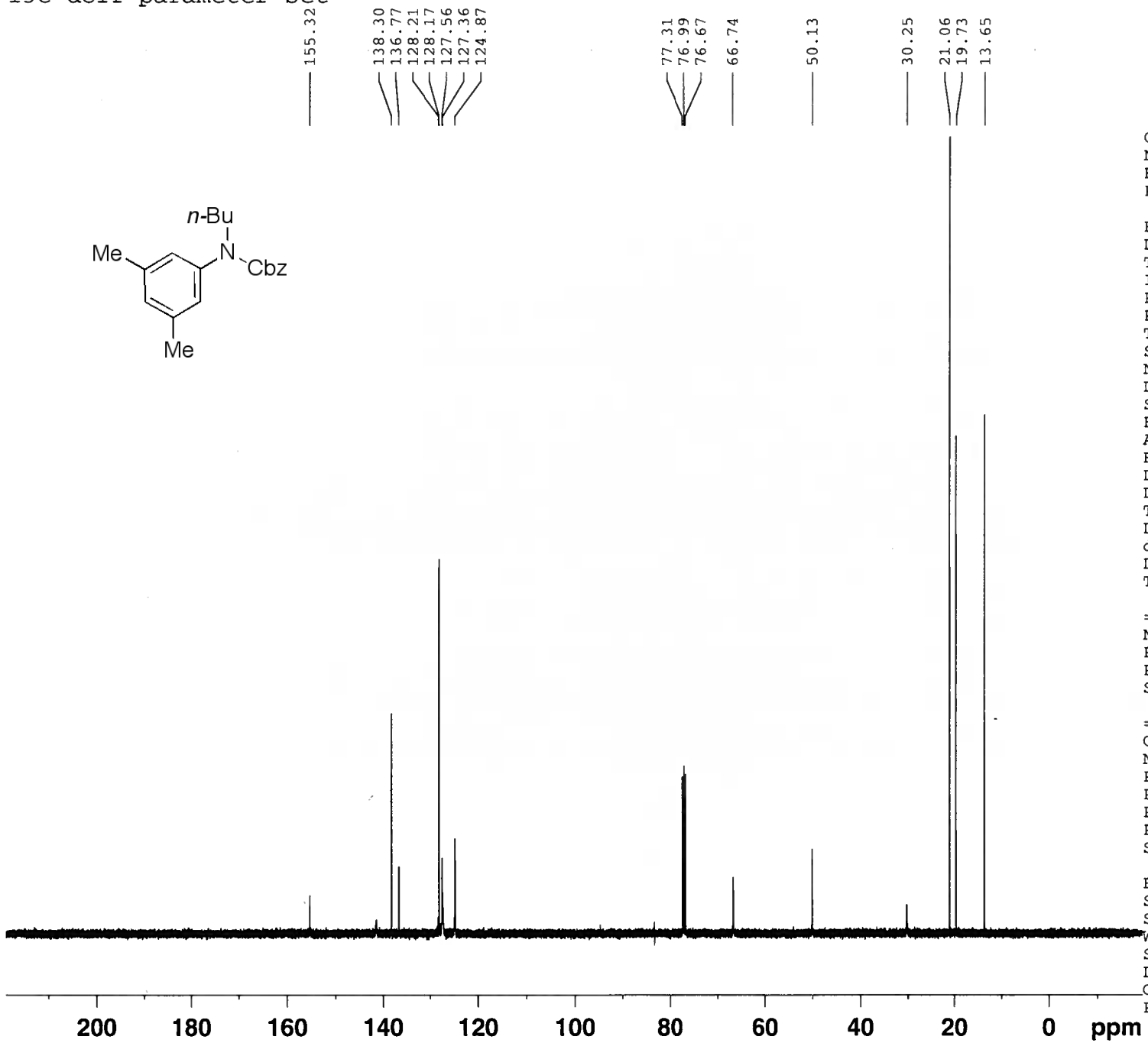
F2 - Acquisition Paramet
Date_            20081001
Time                15.02
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146
FIDRES           0.126314
AQ               3.9584243
RG                    128
DW                 60.400
DE                   6.00
TE                  293.2
D1             1.00000000
TD0                     1

======== CHANNEL f1 ====
NUC1                   1H
P1                  15.07
PL1                  0.00
SFO1         400.1324710

F2 - Processing paramete
SI                  65536
SF           400.1300101
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.00
```

SI-150

13C-dcif parameter set



BRUKER

Current Data Parameters
NAME jdh-2-281-C13-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20081002
Time	15.41
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	14596.5
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

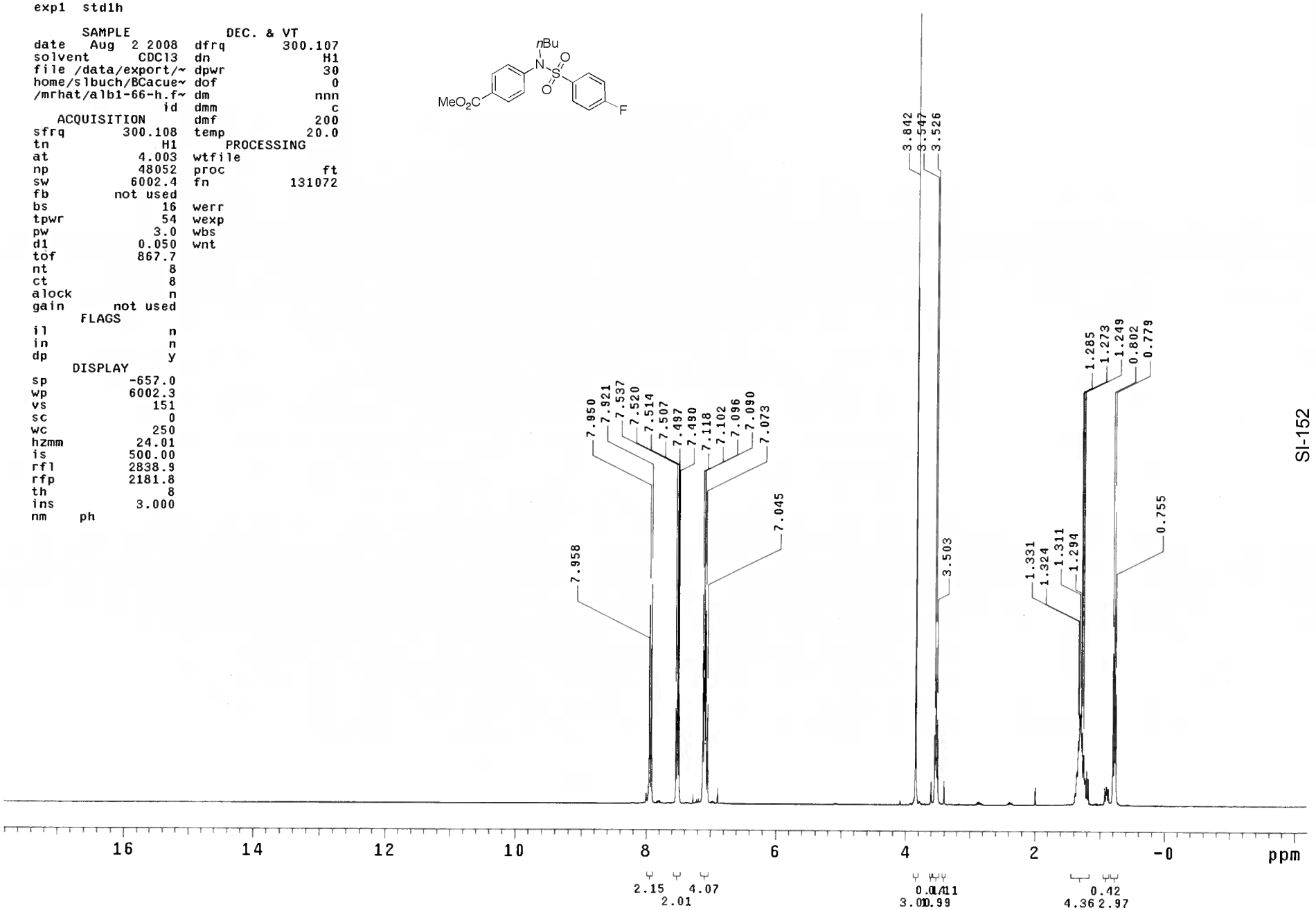
F2 - Processing parameters

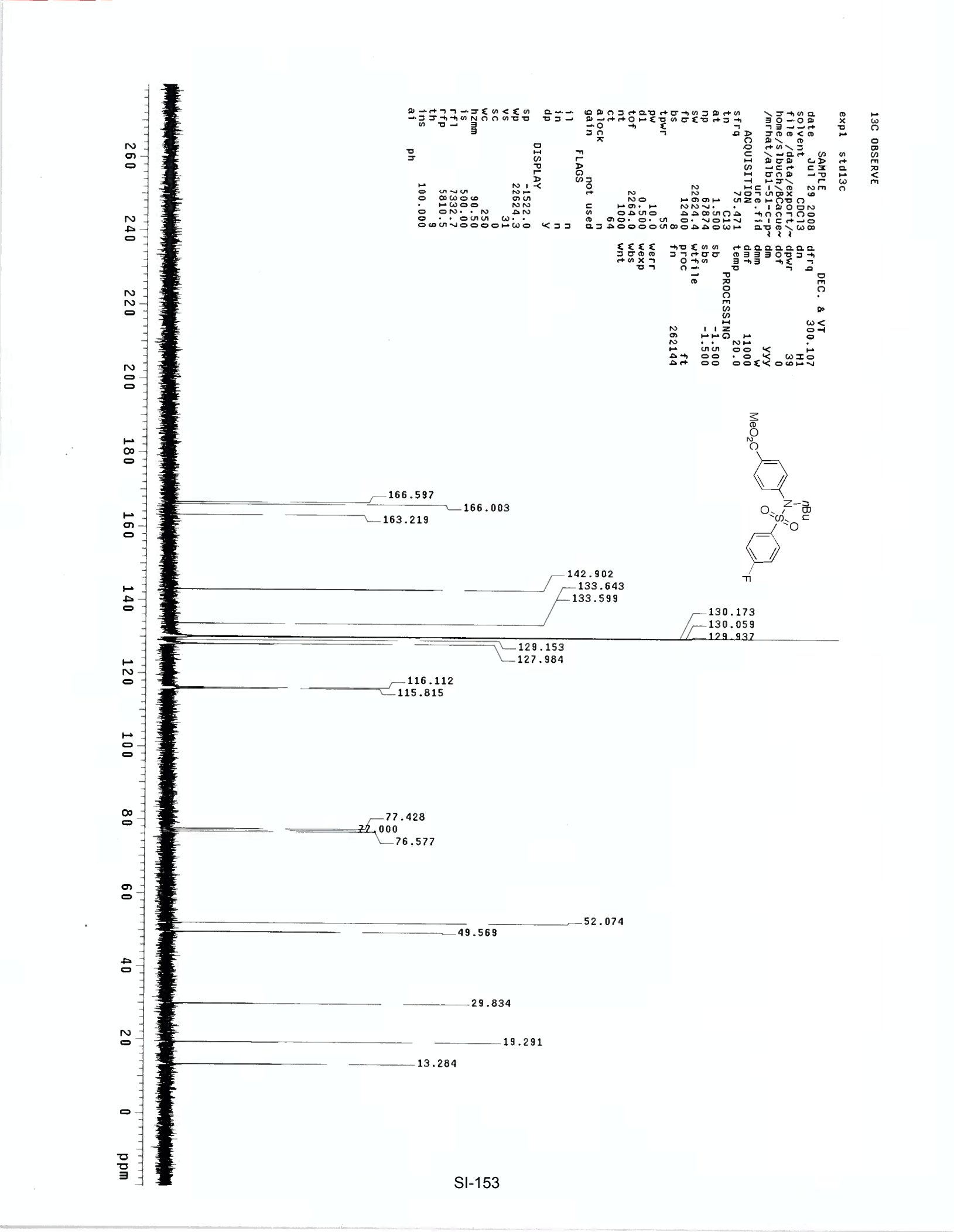
SI	65536
SF	100.6127939 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

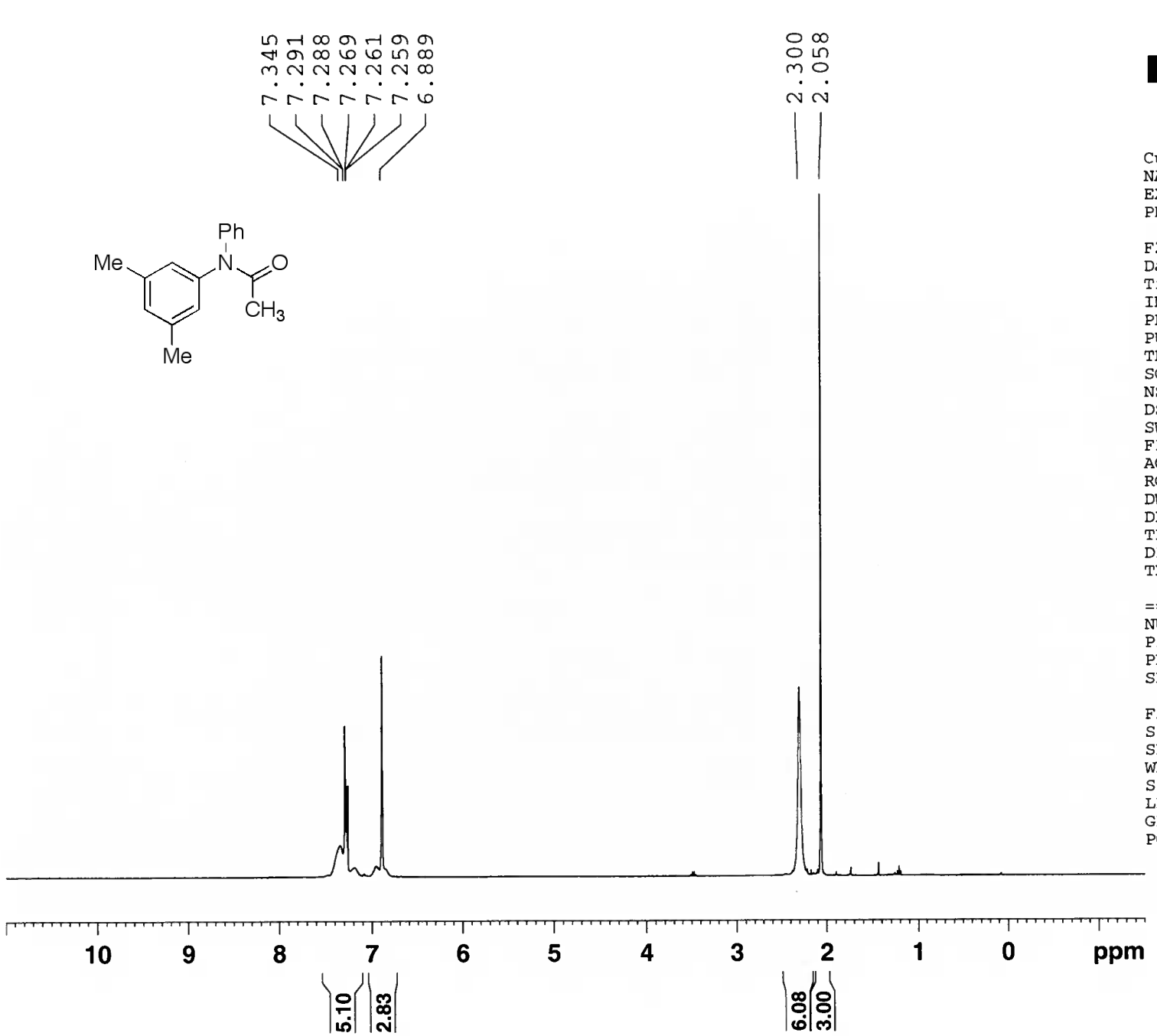
STANDARD 1H OBSERVE

exp1 std1h

SAMPLE		DEC. & VT	
date	Aug 2 2008	dfrq	300.107
solvent	CDCl3	dn	H1
file	/data/export/~	dpwr	30
home/slbuch/BCacue~		dof	0
/mrhat/alb1-66-h.f~		dm	nnn
	id	dmm	c
ACQUISITION		dmf	200
sfrq	300.108	temp	20.0
tn	H1	PROCESSING	
at	4.003	wtfile	
np	48052	proc	ft
sw	6002.4	fn	131072
fb	not used		
bs	16	werr	
tpwr	54	wexp	
pw	3.0	wbs	
d1	0.050	wnt	
tof	867.7		
nt	8		
ct	8		
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-657.0		
wp	6002.3		
vs	151		
sc	0		
wc	250		
hzmm	24.01		
is	500.00		
rfl	2838.9		
rfp	2181.8		
th	8		
ins	3.000		
nm	ph		




13C OBSERVE
expl std13c
SAMPLE
date Jul 29 2008
solvent CDCl3
file /data/export/~
home/slbuch/BCacue~
/mrhat/alb1-51-c-pr~
ure.fid
ACQUISITION
sfrq 75.471
tn C13
at 1.500
np 67874
sw 22624.4
fb 12400
bs 8
tpwr 55
pw 10.0
d1 0.500
tof 2264.0
nt 1000
ct 64
alock n
gain n
FLAGS
il n
in n
dp y
DISPLAY
sp -1522.0
wp 22624.3
vs 31
sc 0
wc 250
hzmm 90.50
is 500.00
rfl 7332.7
rfp 5810.5
th 9
ins 100.000
ai ph
DEC. & VT
dfrq 300.107
dn H1
dpwr 39
dof 0
dm yyy
dmm w
dmf 11000
temp 20.0
PROCESSING
sb -1.500
sbs -1.500
wtfile
proc ft
fn 262144
MeO2C
nBu
F
166.597
166.003
163.219
142.902
133.643
133.599
130.173
130.059
129.937
129.153
127.984
116.112
115.815
77.428
77.000
76.577
52.074
49.569
29.834
19.291
13.284
260
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm



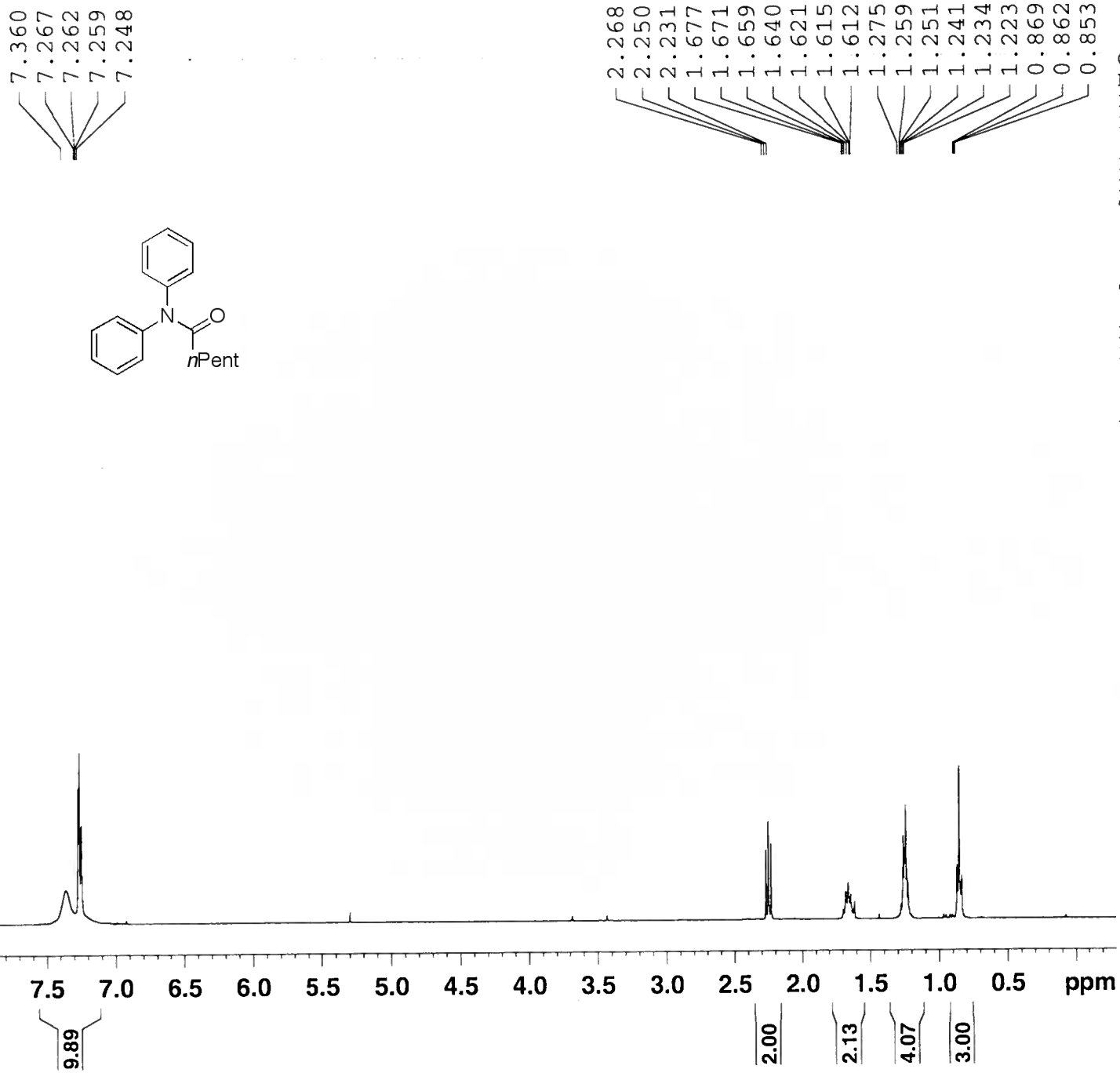
BRUKER

Current Data Parameters
NAME jdh-3-258
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090414
Time 18.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



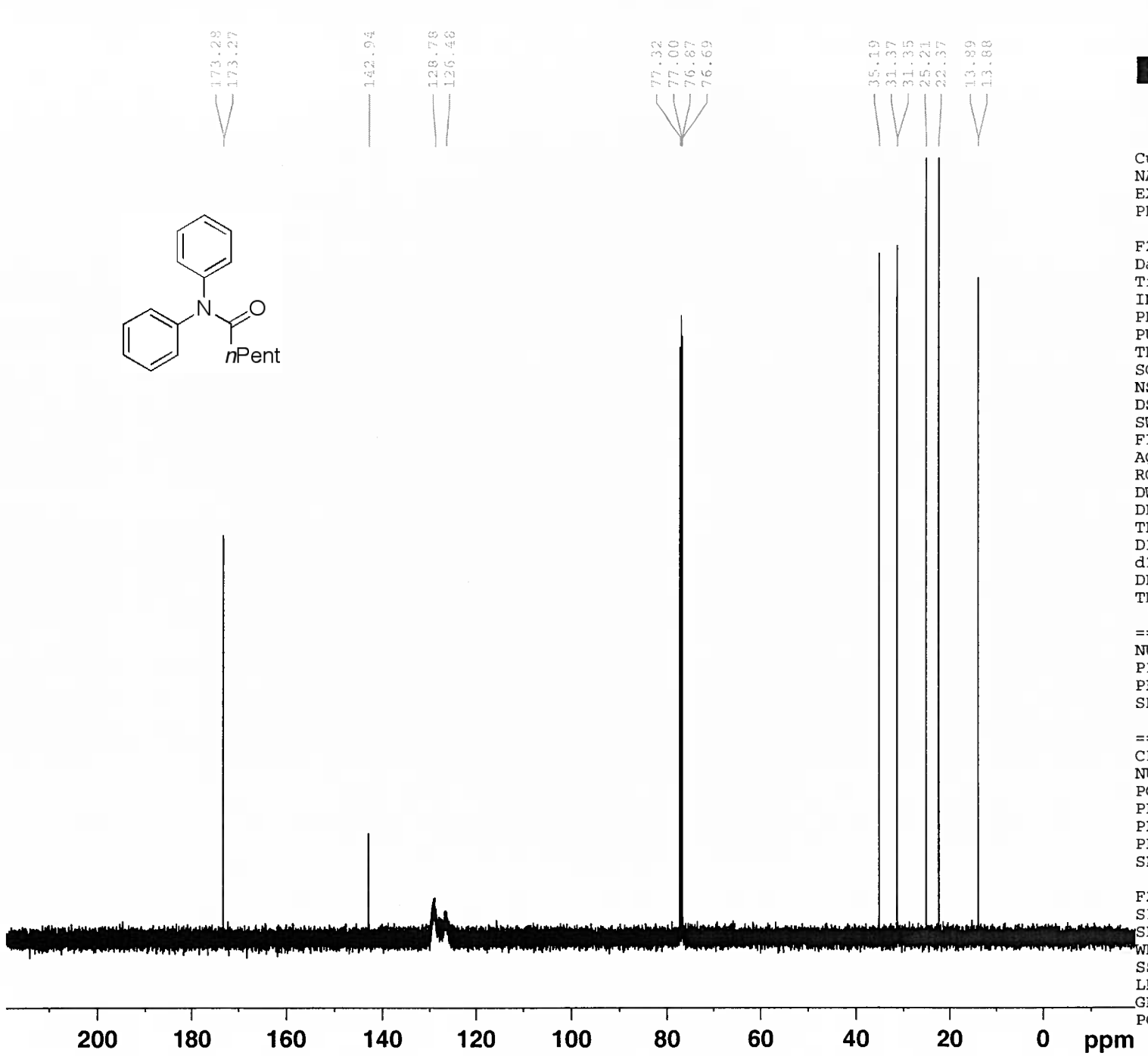
Current Data Parameters
NAME jdh-3-261-2
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090416
Time 11.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-156

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300094
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

Current Data Parameters
NAME jdh-3-261-c13-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090415
Time	21.58
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

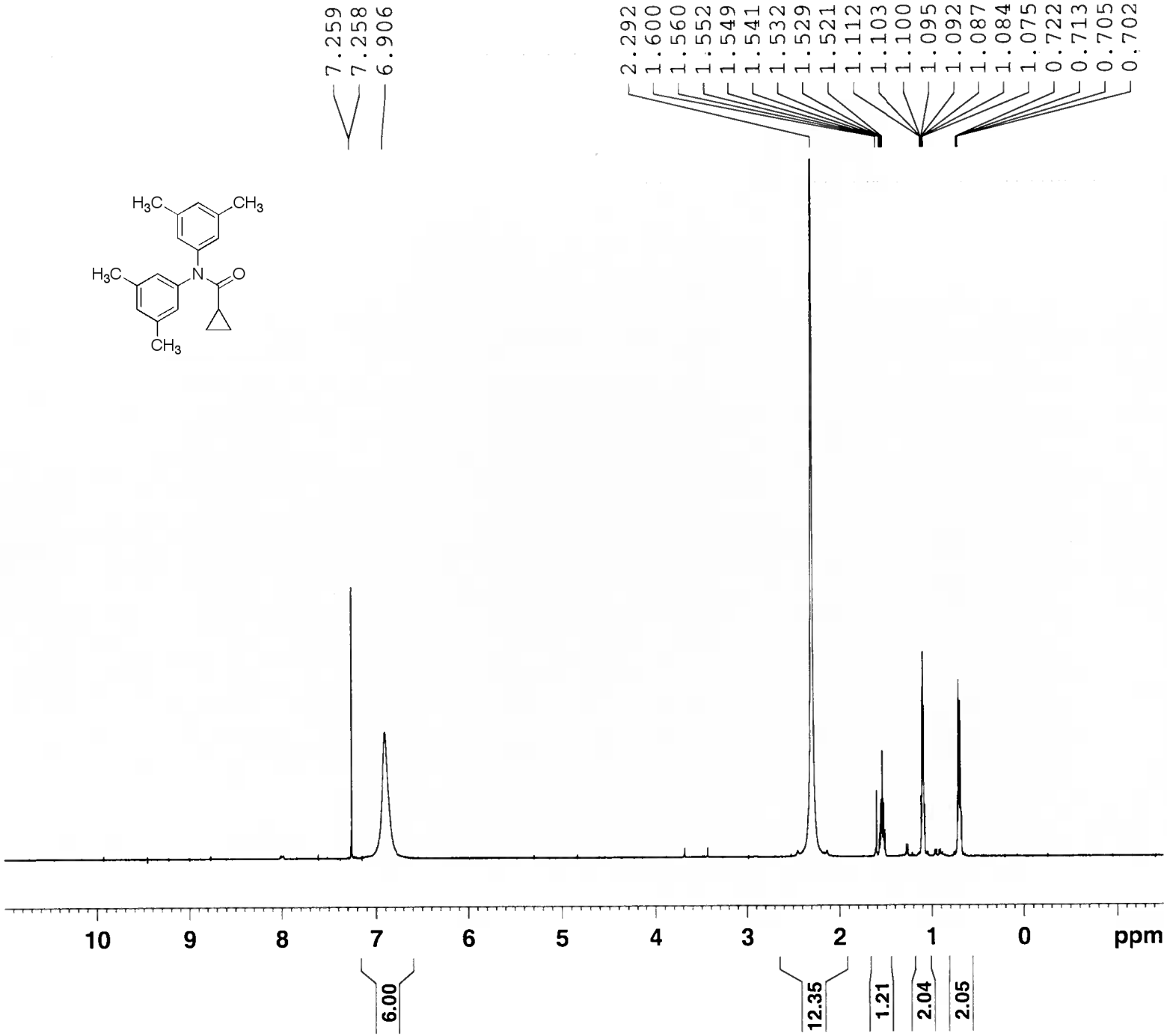
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127771 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



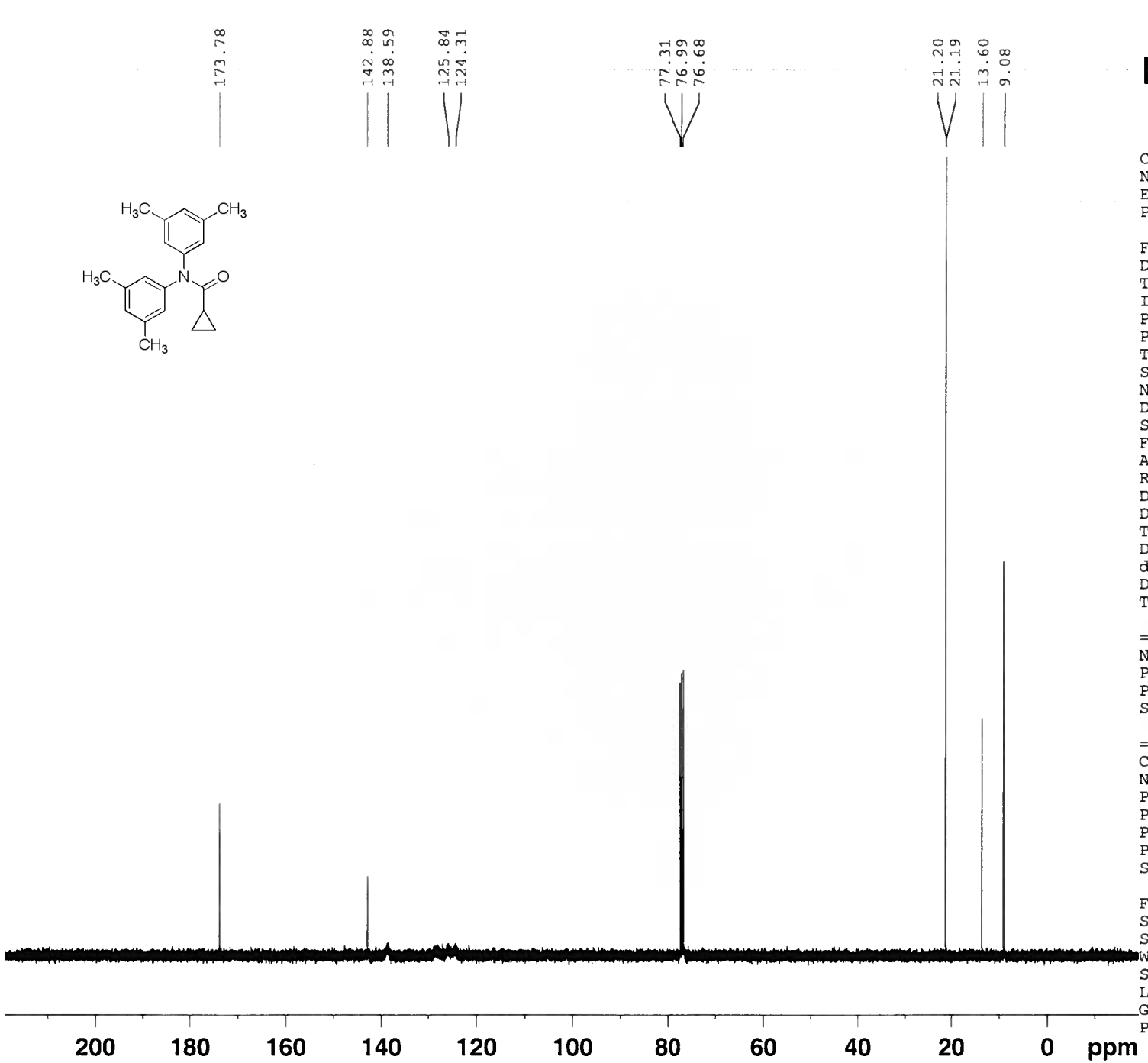
Current Data Parameters
NAME jdh-3-262-h1-2
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090428
Time 12.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-152

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300100
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

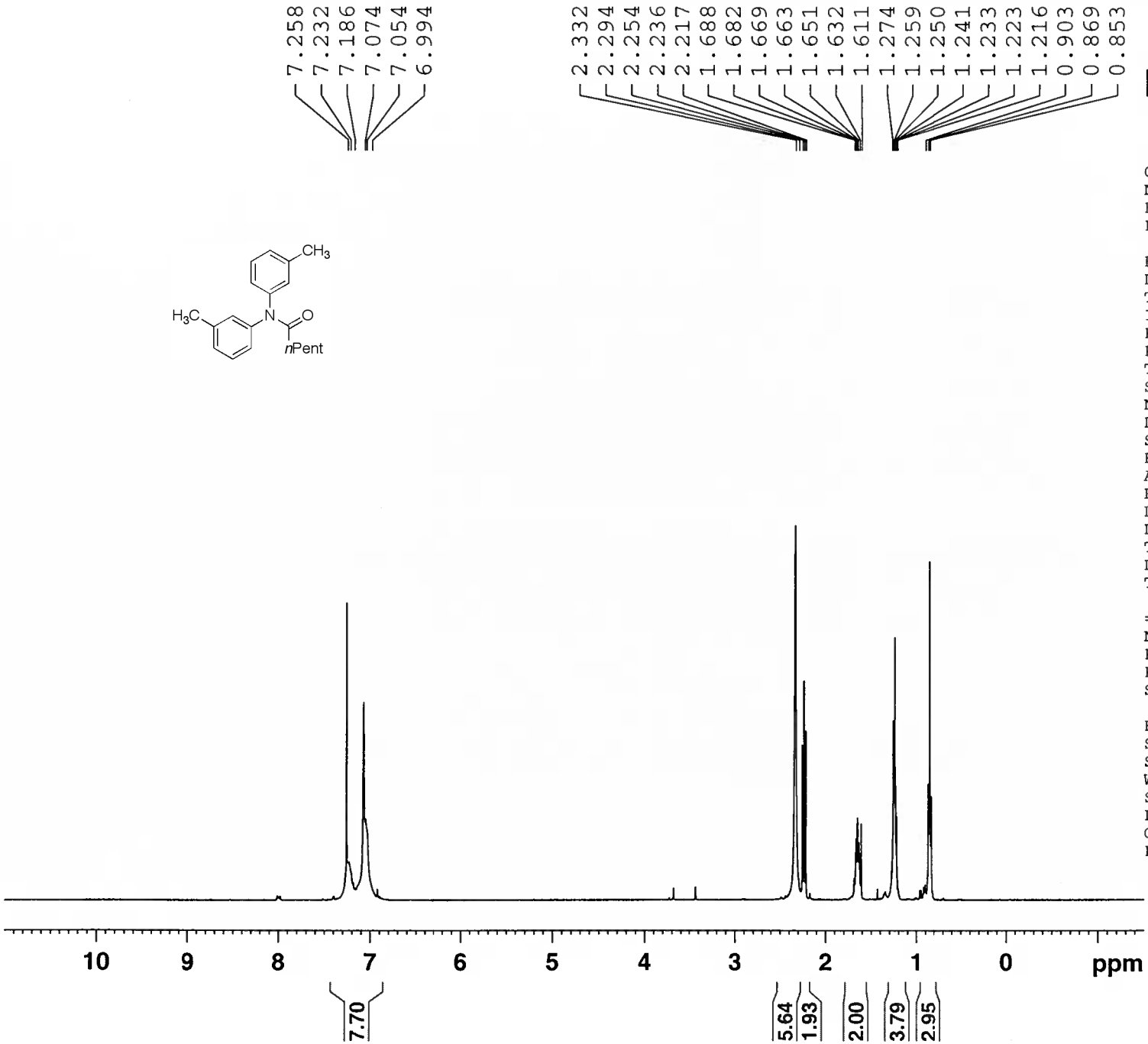
```
Current Data Parameters
NAME      jdh-3-262-C13-2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20090428
Time                 12.36
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     385
DS                       2
SWH              23980.814 Hz
FIDRES           0.365918 Hz
AQ               1.3664756 sec
RG                    8192
DW                 20.850 usec
DE                  6.00 usec
TE                 293.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  8.75 usec
PL1                -3.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -1.00 dB
PL12               14.52 dB
PL13               18.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   65536
SF           100.6127775 MHz
WDW                     no
SSB                      0
LB                  0.00 Hz
GB                       0
PC                   1.40
```



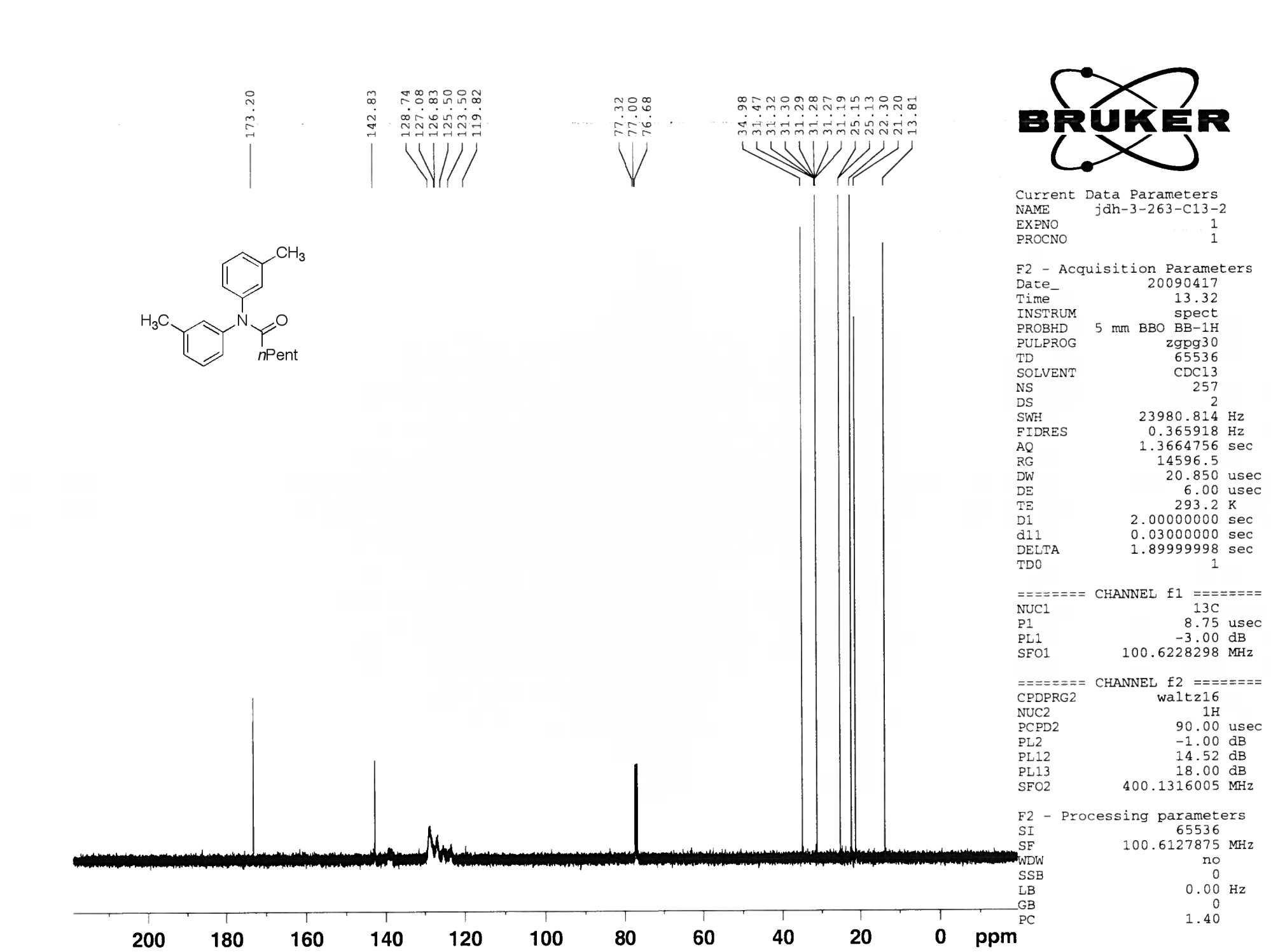
BRUKER

Current Data Parameters
NAME jdh-3-263
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090416
Time 15.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 228.1
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



BRUKER

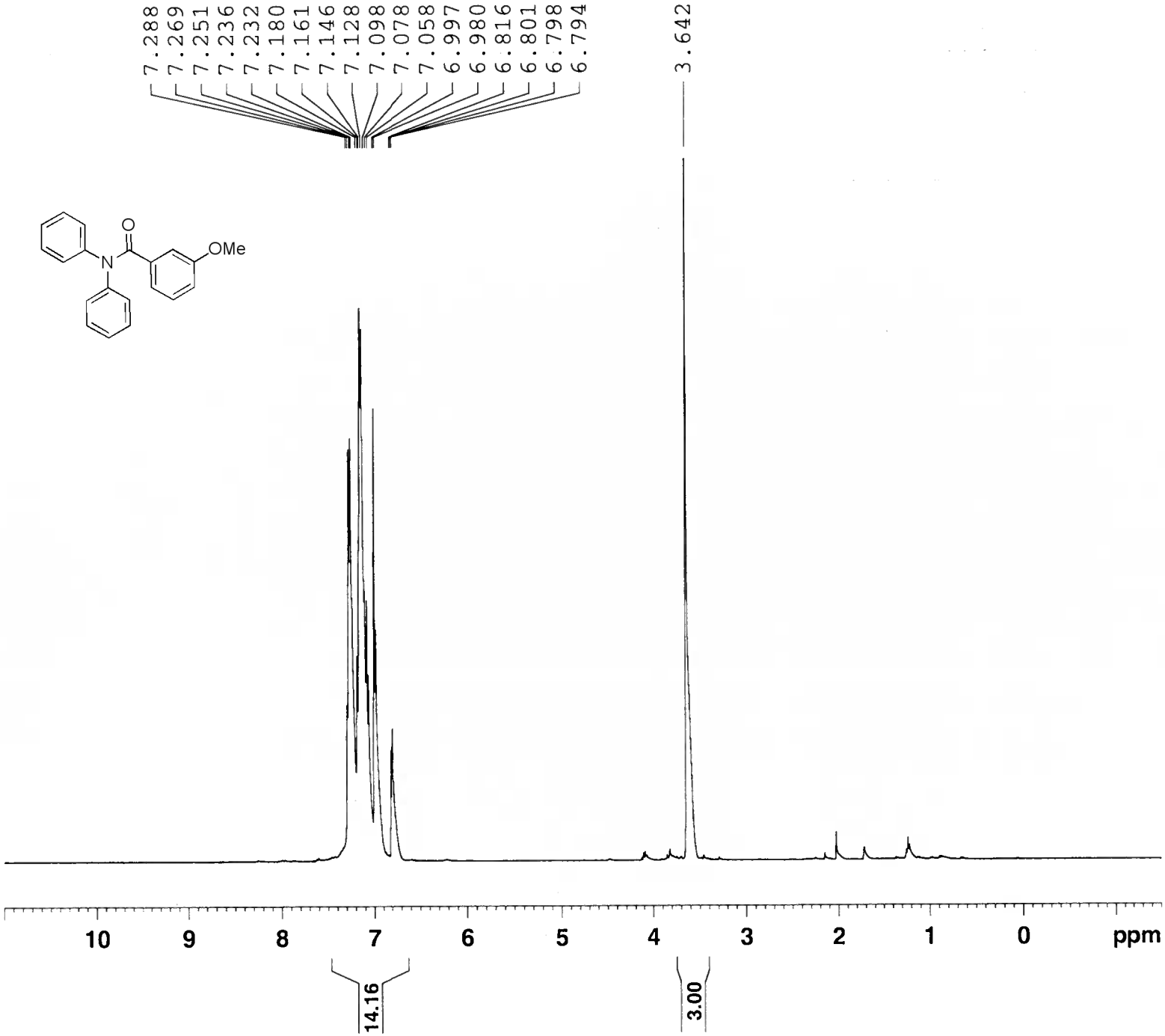
Current Data Parameters
NAME jdh-3-263-C13-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090417
Time 13.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 257
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127875 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



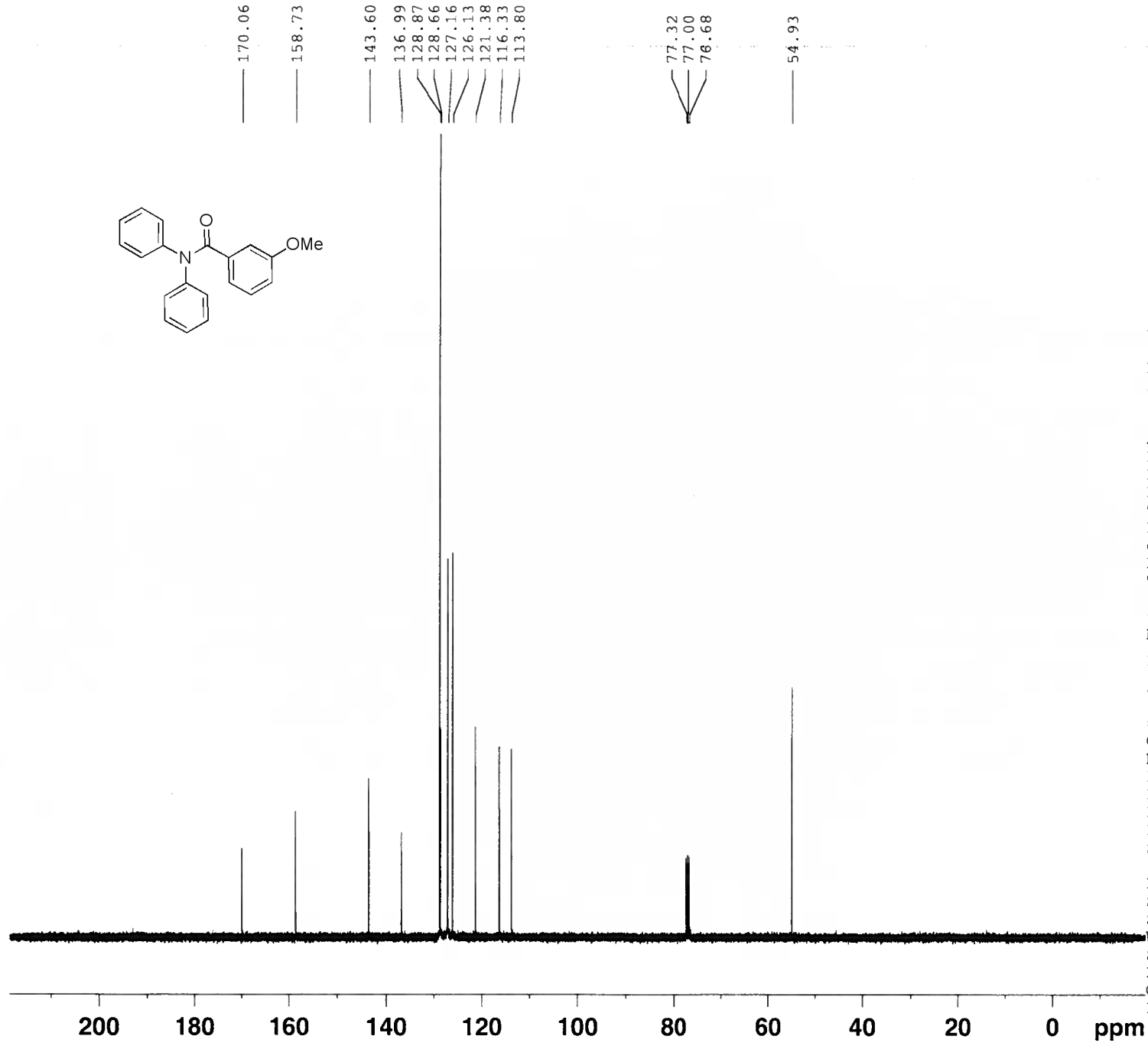
Current Data Parameters
NAME jdh-3-265a
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090420
Time 11.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 64
DW 60.400
DE 6.00
TE 285.2
D1 1.00000000
TD0 1

SI-164

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300212
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

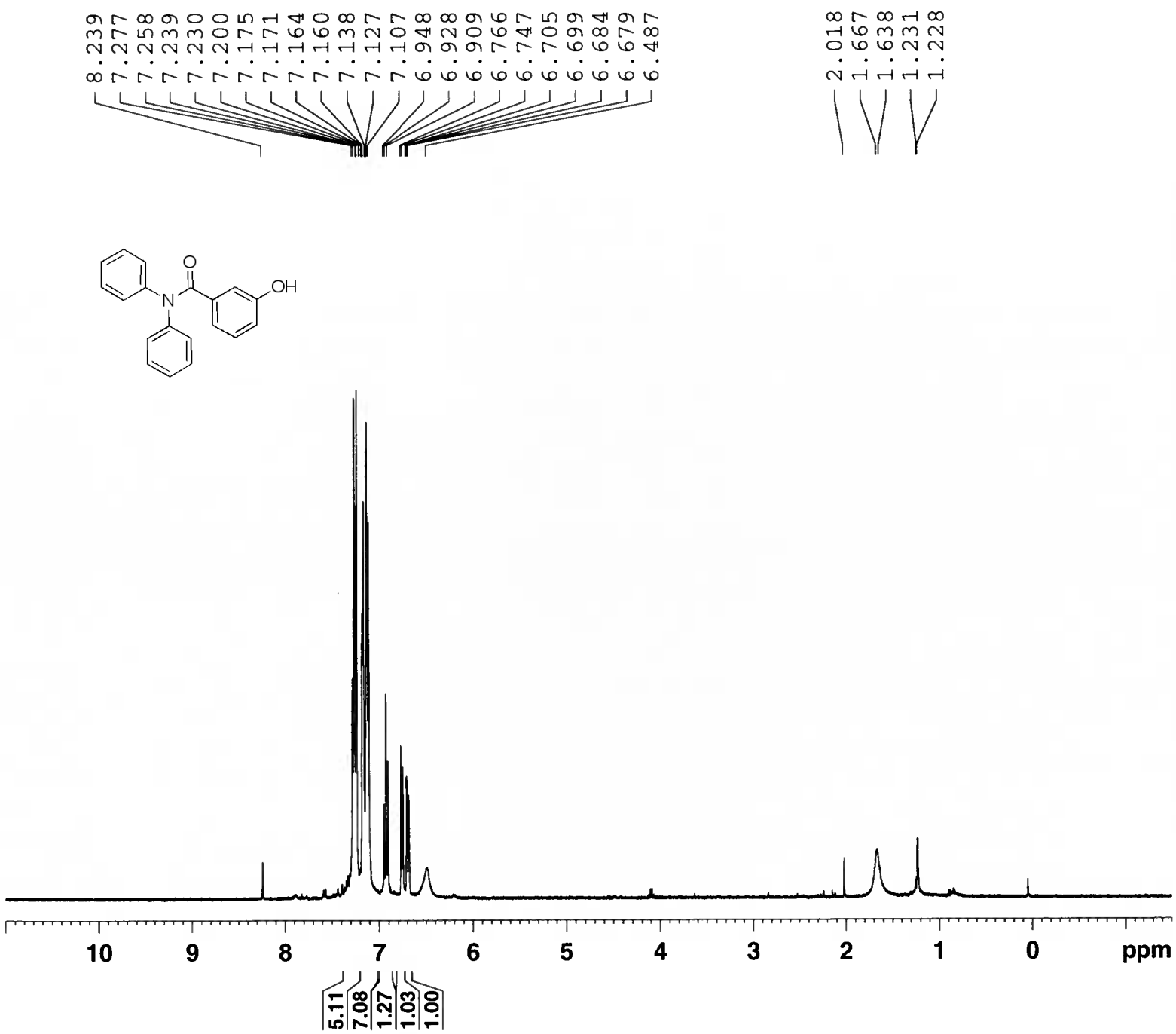
Current Data Parameters
NAME jdh-3-265a-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090420
Time 11.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 usec
DE 6.00 usec
TE 288.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6128031 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



Current Data Parameters

NAME	jdh-3-288
EXPNO	1
PROCNO	1

F2 - Acquisition Paramet

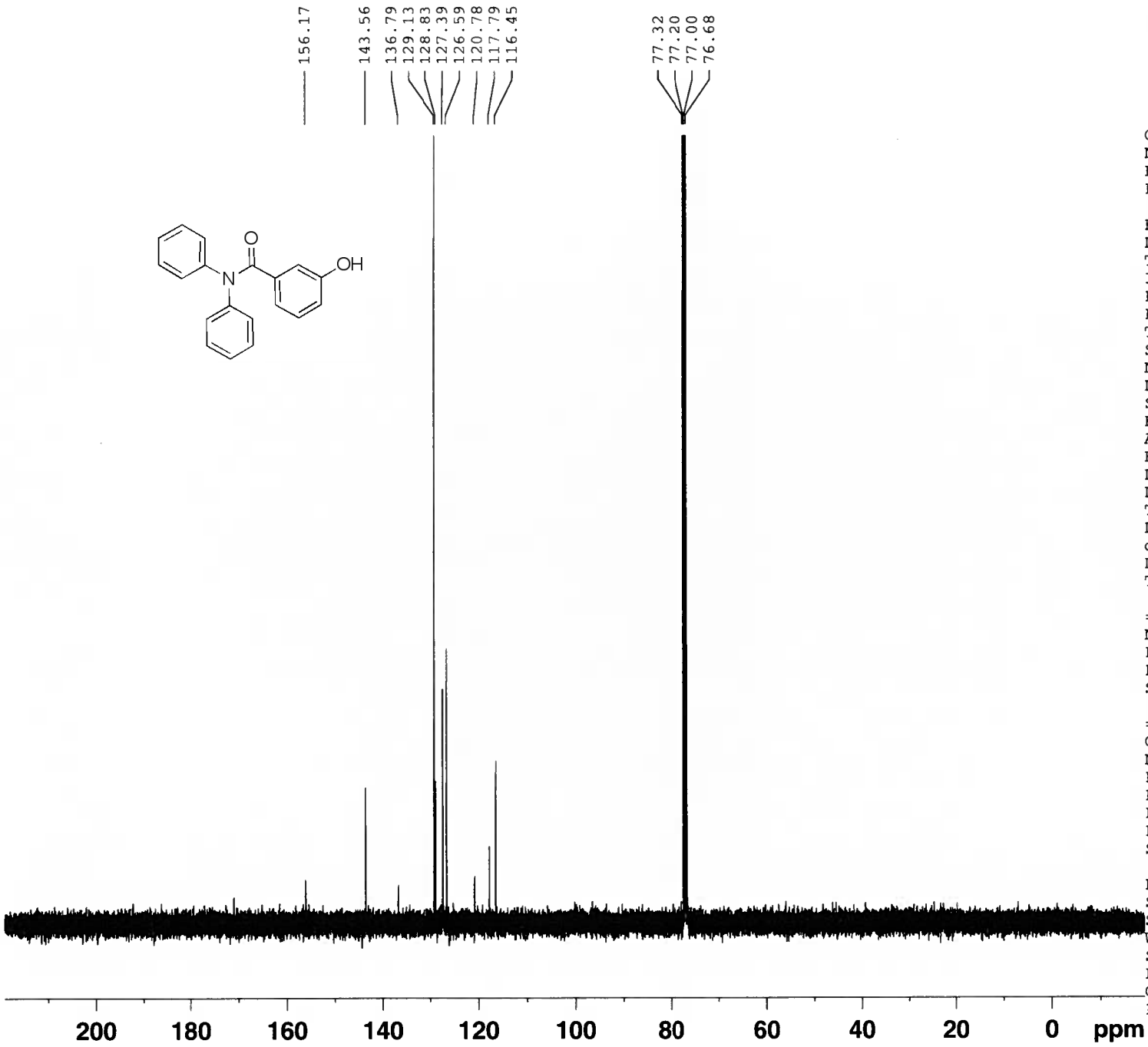
Date_	20090520
Time	13.15
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146
FIDRES	0.126314
AQ	3.9584243
RG	228.1
DW	60.400
DE	6.00
TE	298.2
D1	1.00000000
TD0	1

======== CHANNEL f1 ====

NUC1	1H
P1	15.07
PL1	0.00
SFO1	400.1324710

F2 - Processing paramete

SI	65536
SF	400.1300212
WDW	no
SSB	0
LB	0.00
GB	0
PC	1.00



Current Data Parameters
NAME jdh-3-288-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090520
Time	13.52
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	601
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	18390.4
DW	20.850 usec
DE	6.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

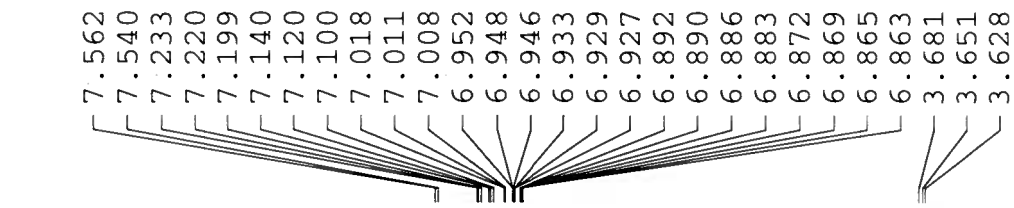
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

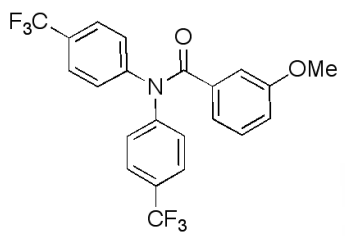
======== CHANNEL f2 ========

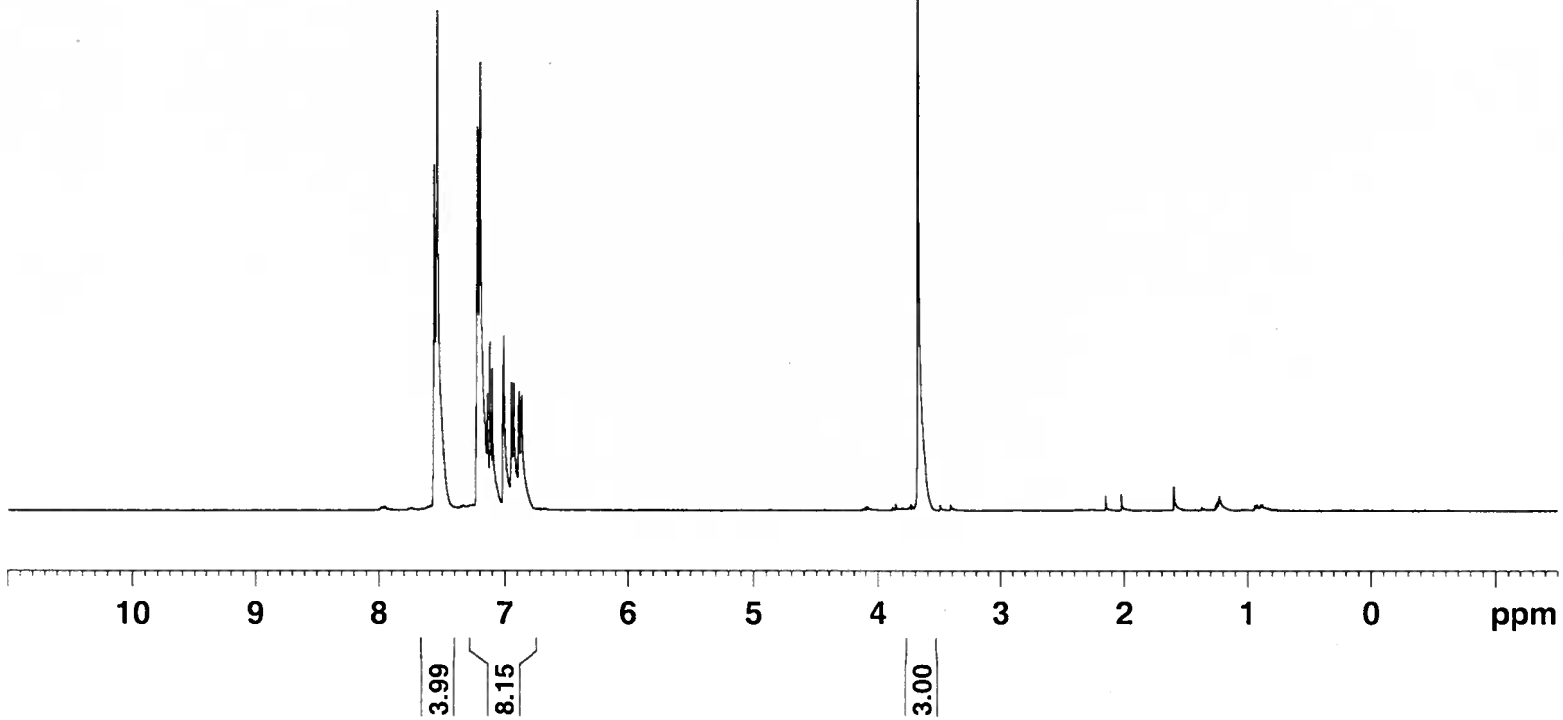
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127725 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40







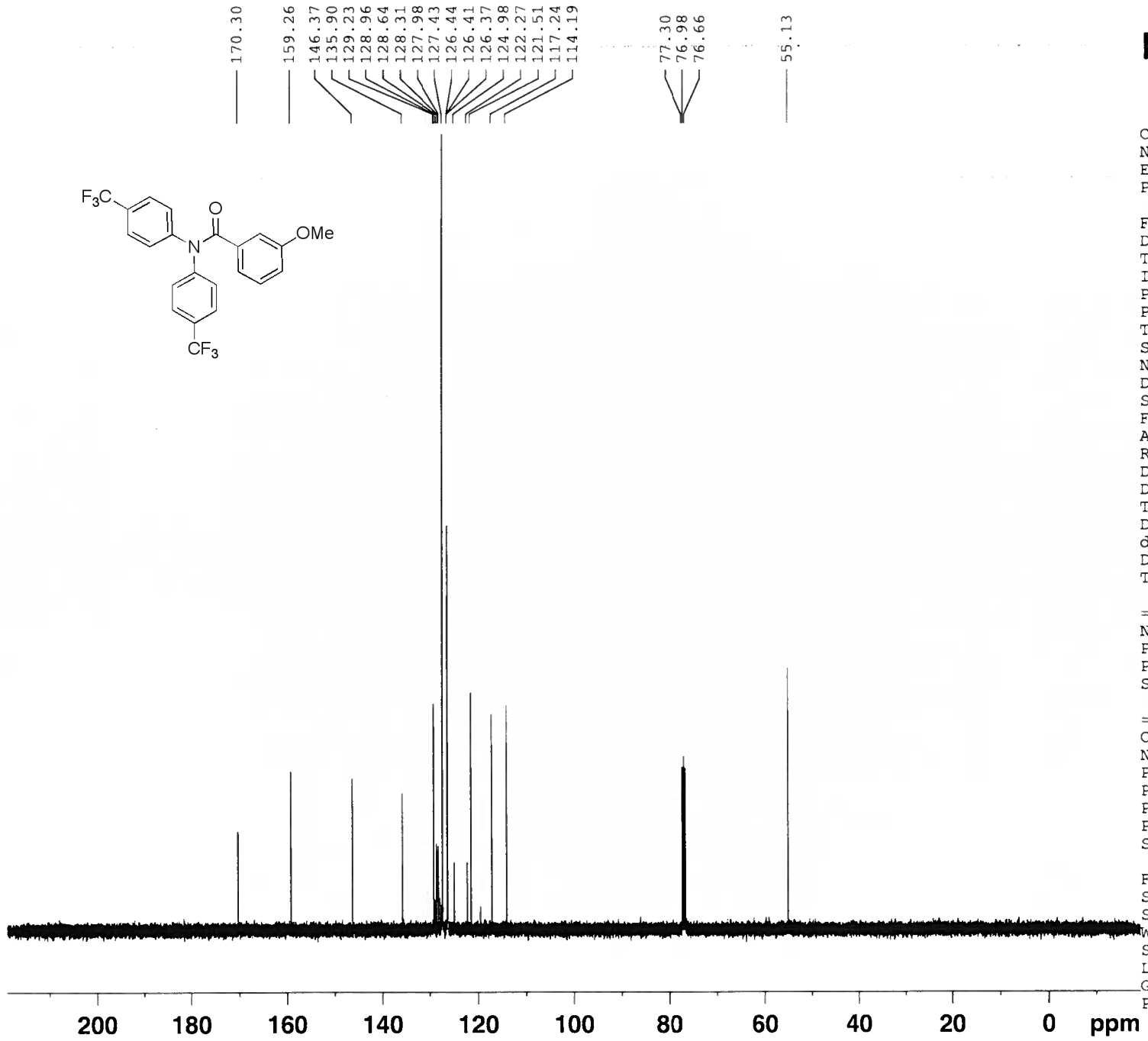
Current Data Parameters
NAME jdh-3-265b
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090420
Time 11.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 286.2
D1 1.00000000
TD0 1

SI-165

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300212
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

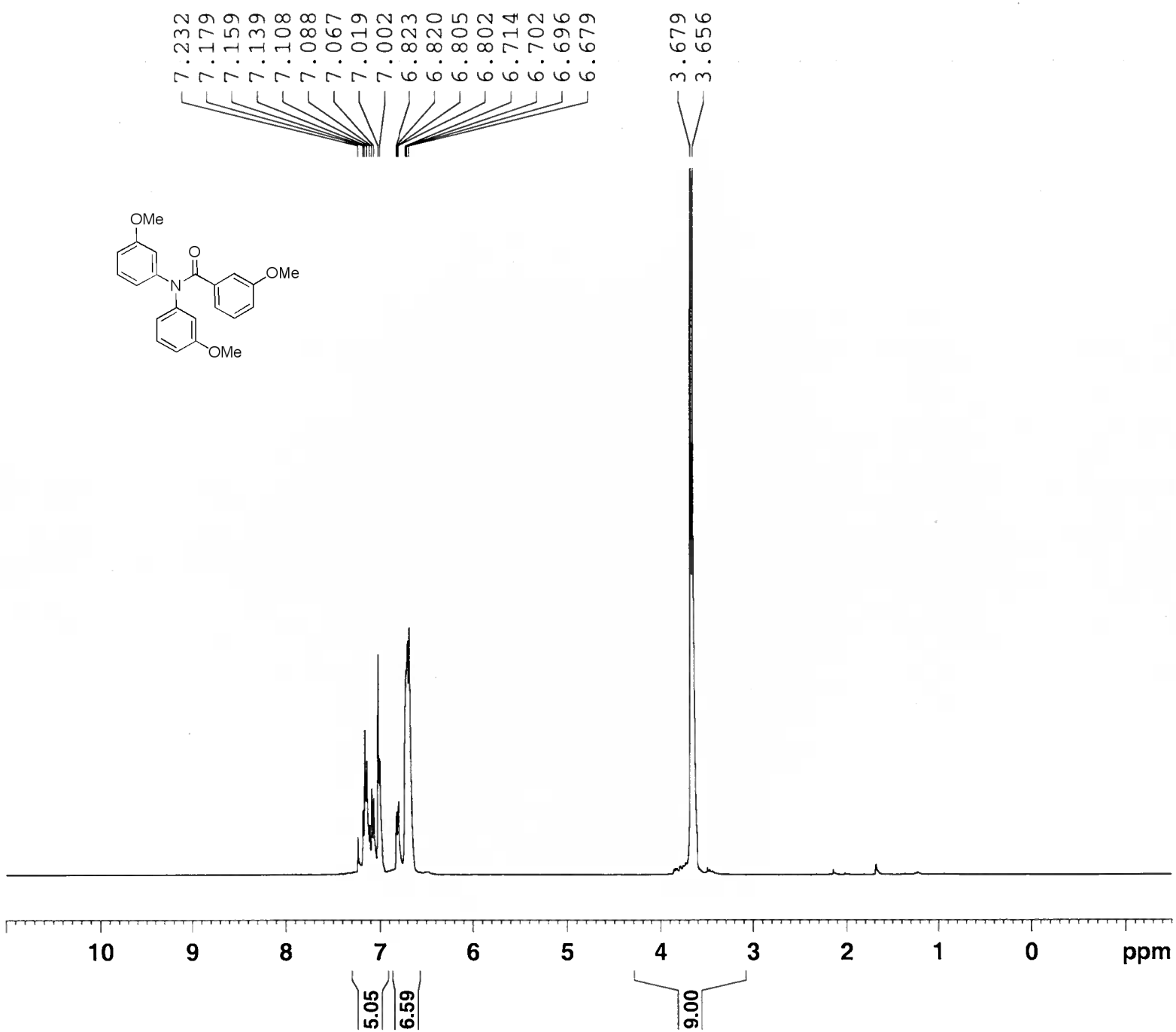
Current Data Parameters
NAME jdh-3-265b-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090420
Time 11.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 290.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127816 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



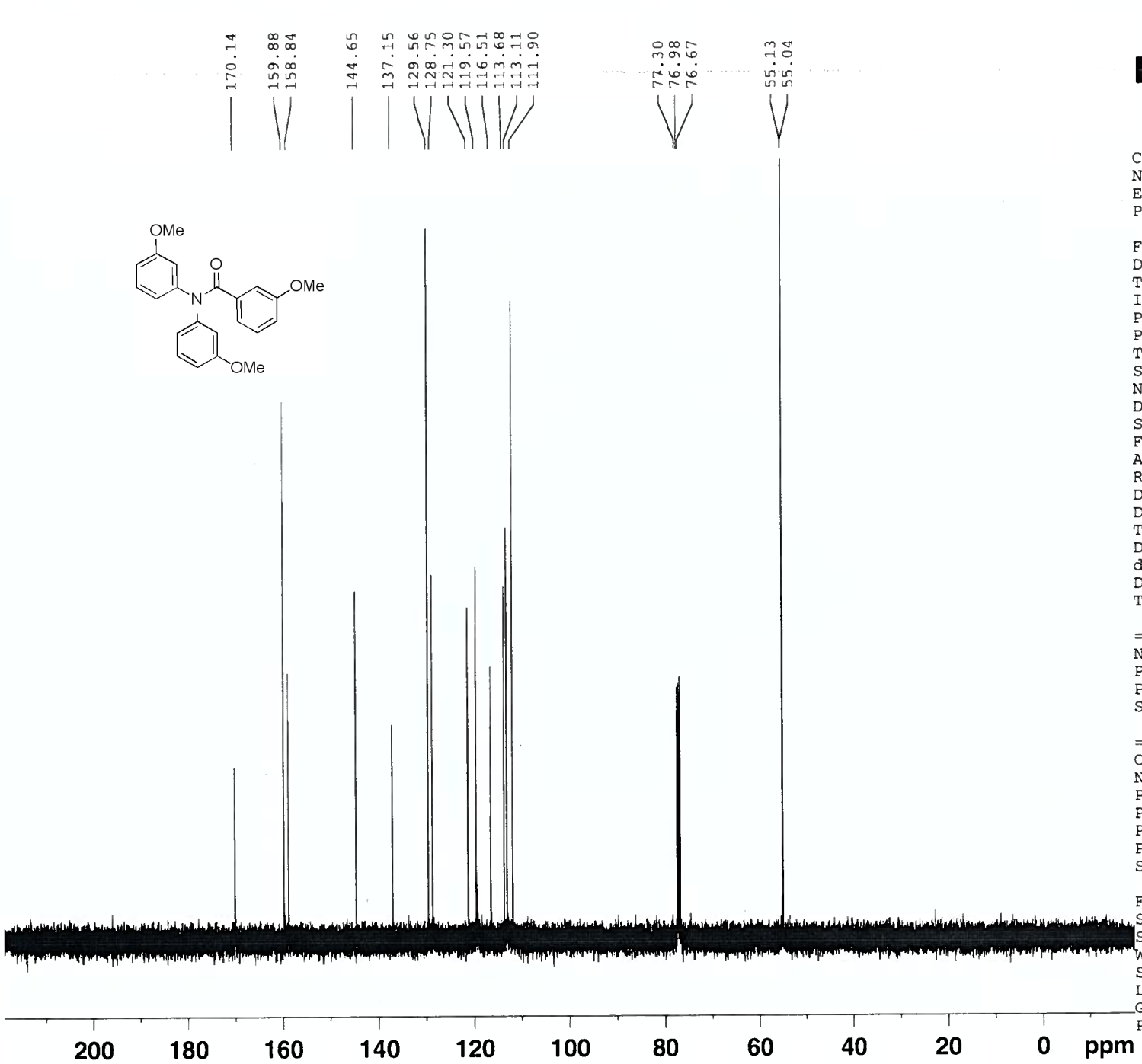
Current Data Parameters
NAME jdh-3-265c
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090420
Time 11.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 64
DW 60.400
DE 6.00
TE 287.2
D1 1.00000000
TD0 1

SI-163

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300212
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

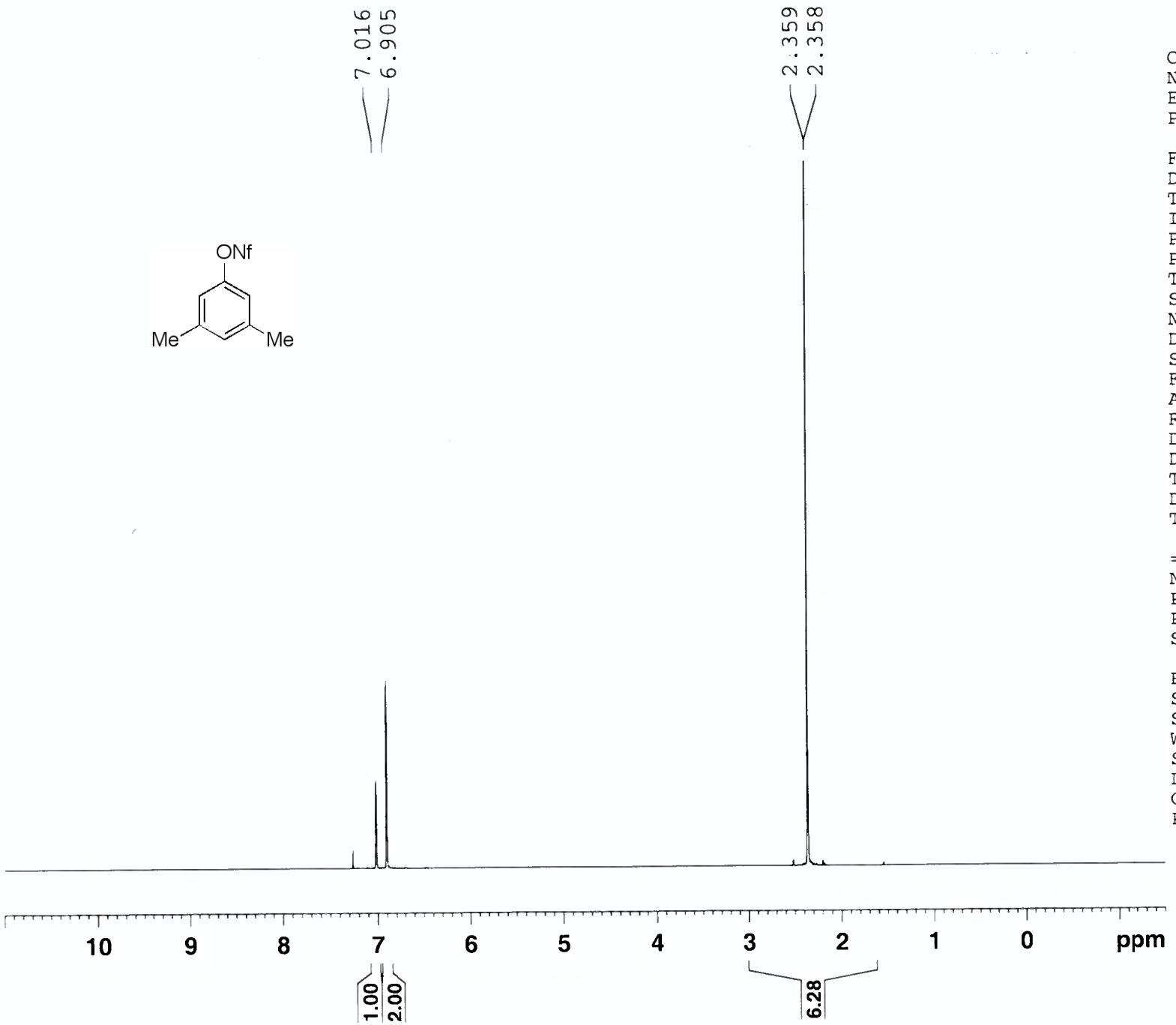
```
Current Data Parameters
NAME      jdh-3-265c-c13
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20090420
Time              11.52
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 115
DS                   2
SWH          23980.814 Hz
FIDRES        0.365918 Hz
AQ           1.3664756 sec
RG               13004
DW              20.850 usec
DE               6.00 usec
TE              291.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               8.75 usec
PL1             -3.00 dB
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2                1H
PCPD2           90.00 usec
PL2             -1.00 dB
PL12            14.52 dB
PL13            18.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                65536
SF         100.6127919 MHz
WDW                  no
SSB                   0
LB             0.00 Hz
GB                    0
PC                 1.40
```



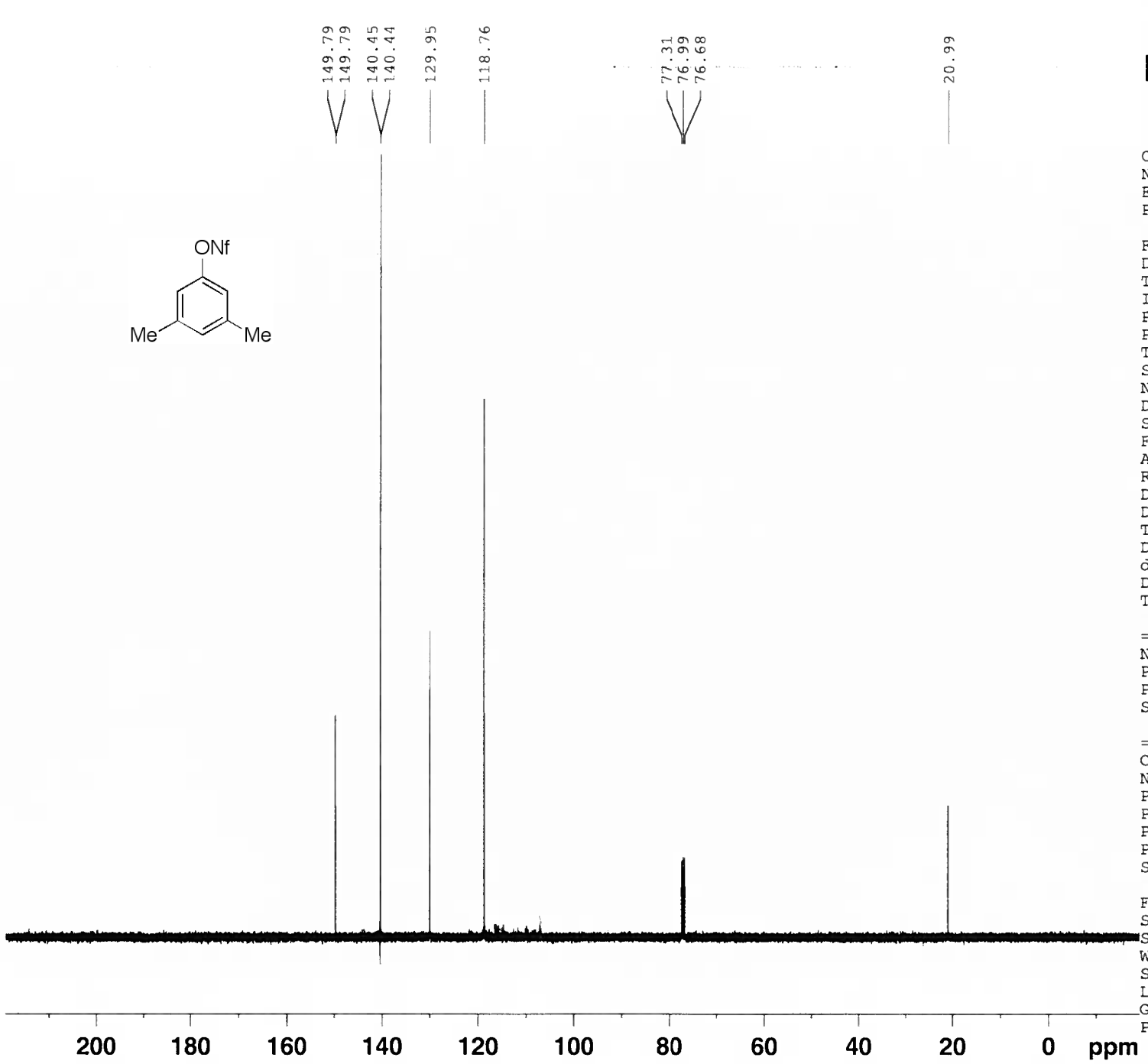
Current Data Parameters
NAME jdh-1-282
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090408
Time 19.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 64
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-169

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300096
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



Current Data Parameters
NAME jdh-1-282-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090408
Time	19.09
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

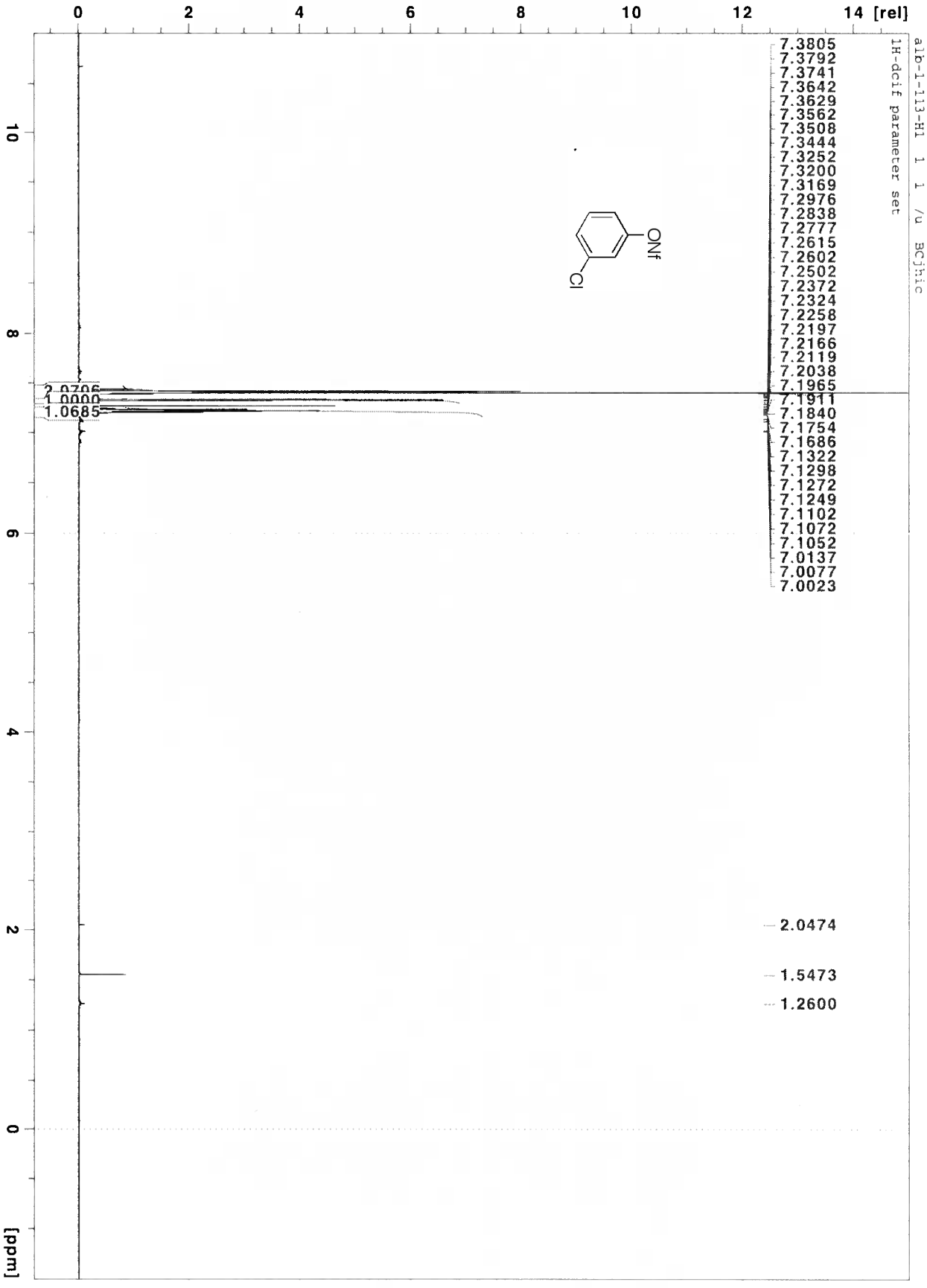
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127655 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40


0
2
4
6
8
10
12
14 [rel]
10
8
6
4
2
0 [ppm]
alb-1-113-H1 1 1 /u BCjhic
1H-dcif parameter set
ONf
Cl
7.3805
7.3792
7.3741
7.3642
7.3629
7.3562
7.3508
7.3444
7.3252
7.3200
7.3169
7.2976
7.2838
7.2777
7.2615
7.2602
7.2502
7.2372
7.2324
7.2258
7.2197
7.2166
7.2119
7.2038
7.1965
7.1911
7.1840
7.1754
7.1686
7.1322
7.1298
7.1272
7.1249
7.1102
7.1072
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7.0023
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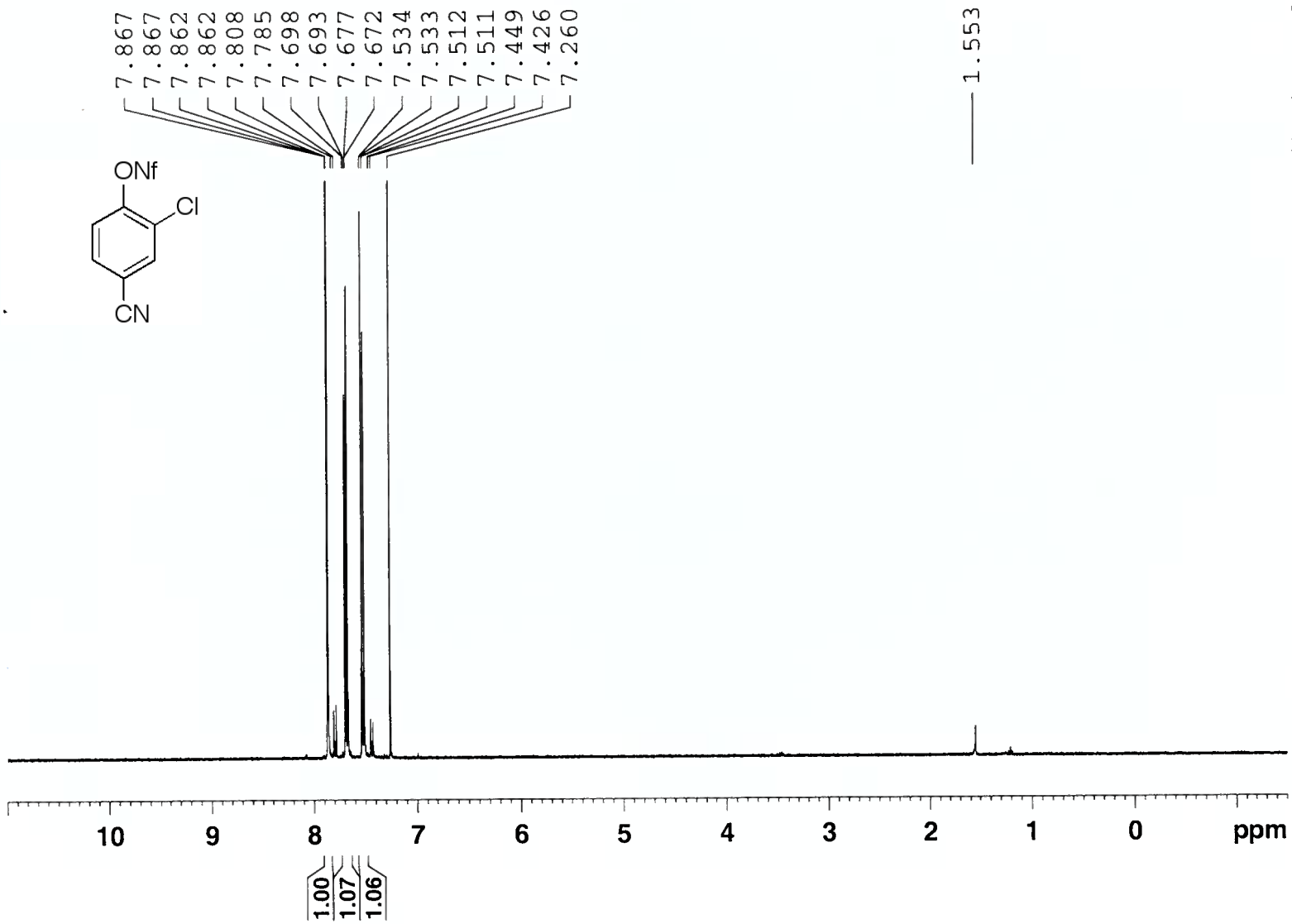
1.0685
2.0474
1.5473
1.2600



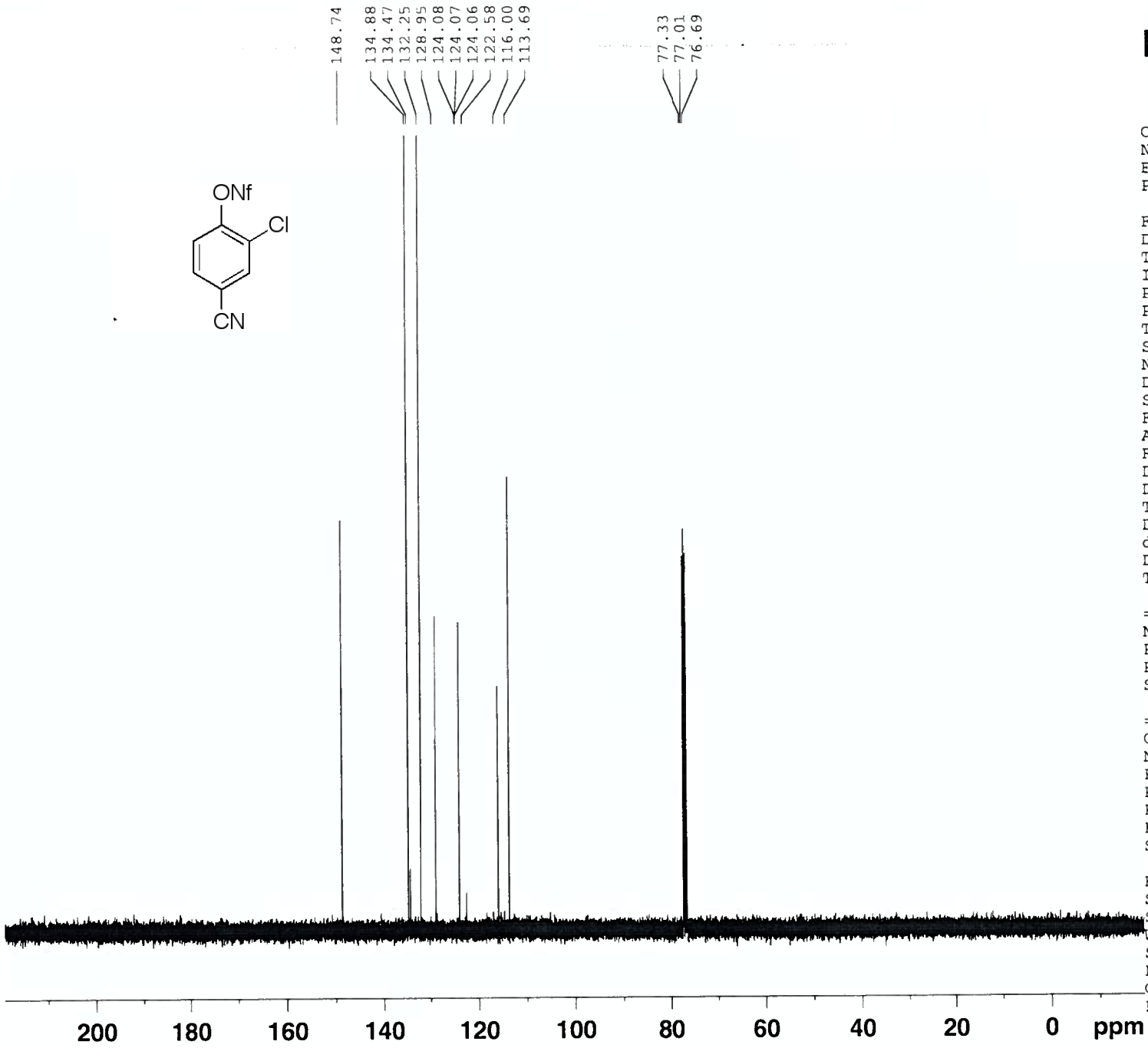
Current Data Parameters
NAME jdh-3-45-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090408
Time 18.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 362
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-172

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300096
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



Current Data Parameters
NAME jdh-3-48-C13-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090408
Time	18.45
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	10321.3
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

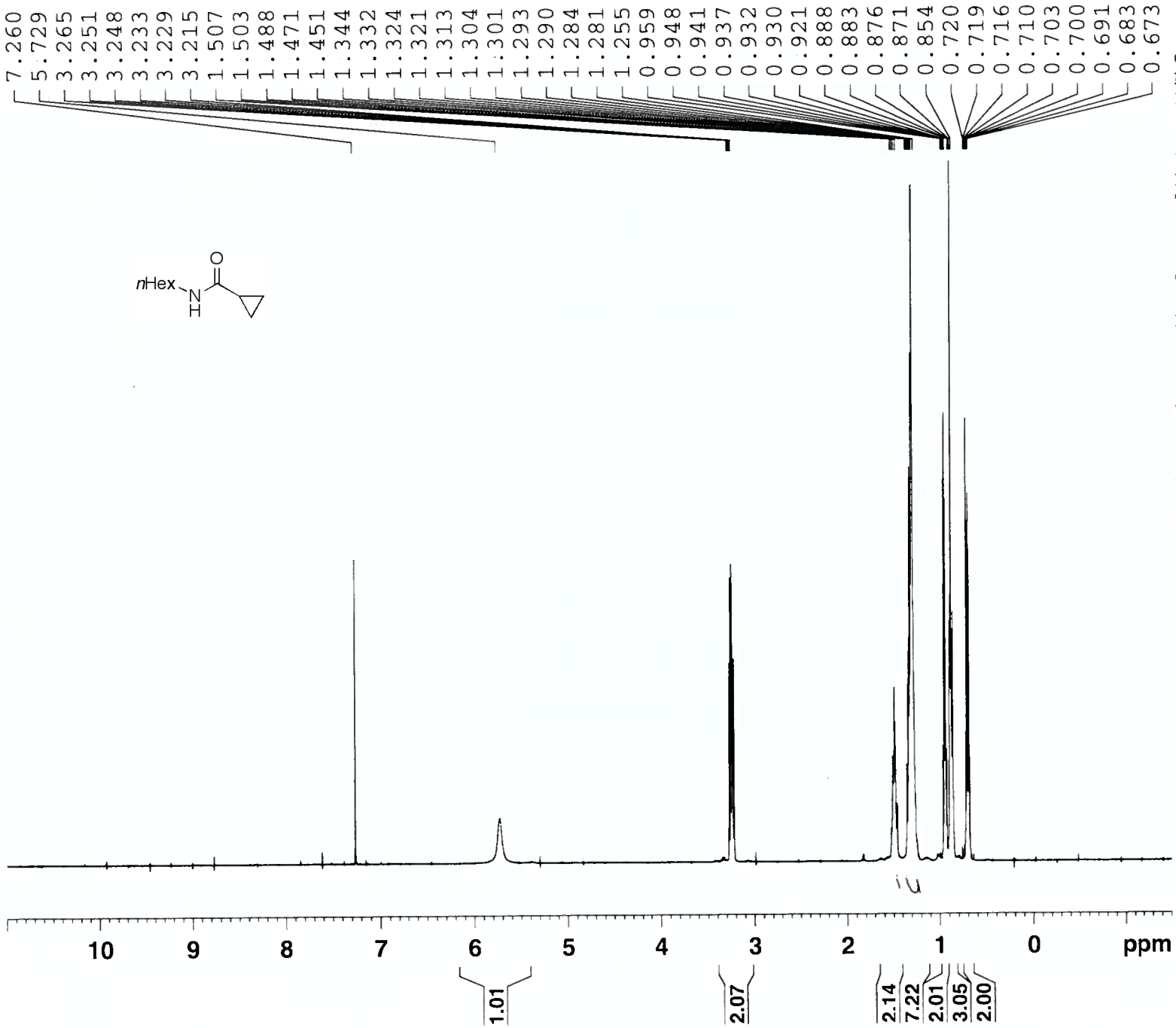
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127711 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



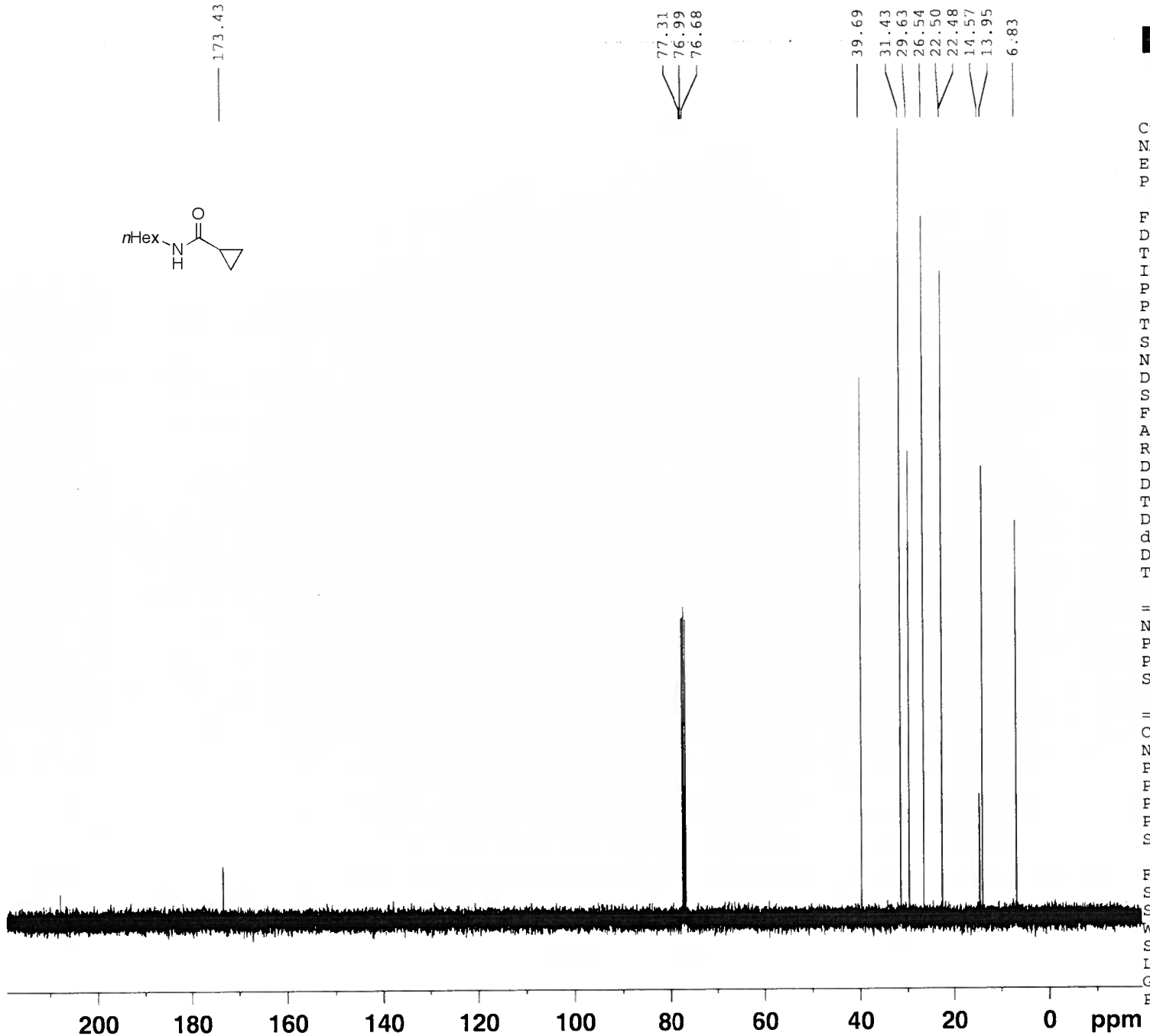
Current Data Parameters
NAME jdh-1-291
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090408
Time 14.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-174

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300093
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



Current Data Parameters
NAME jdh-1-291-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090408
Time	15.11
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	2
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	8192
DW	20.850 usec
DE	6.00 usec
TE	293.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

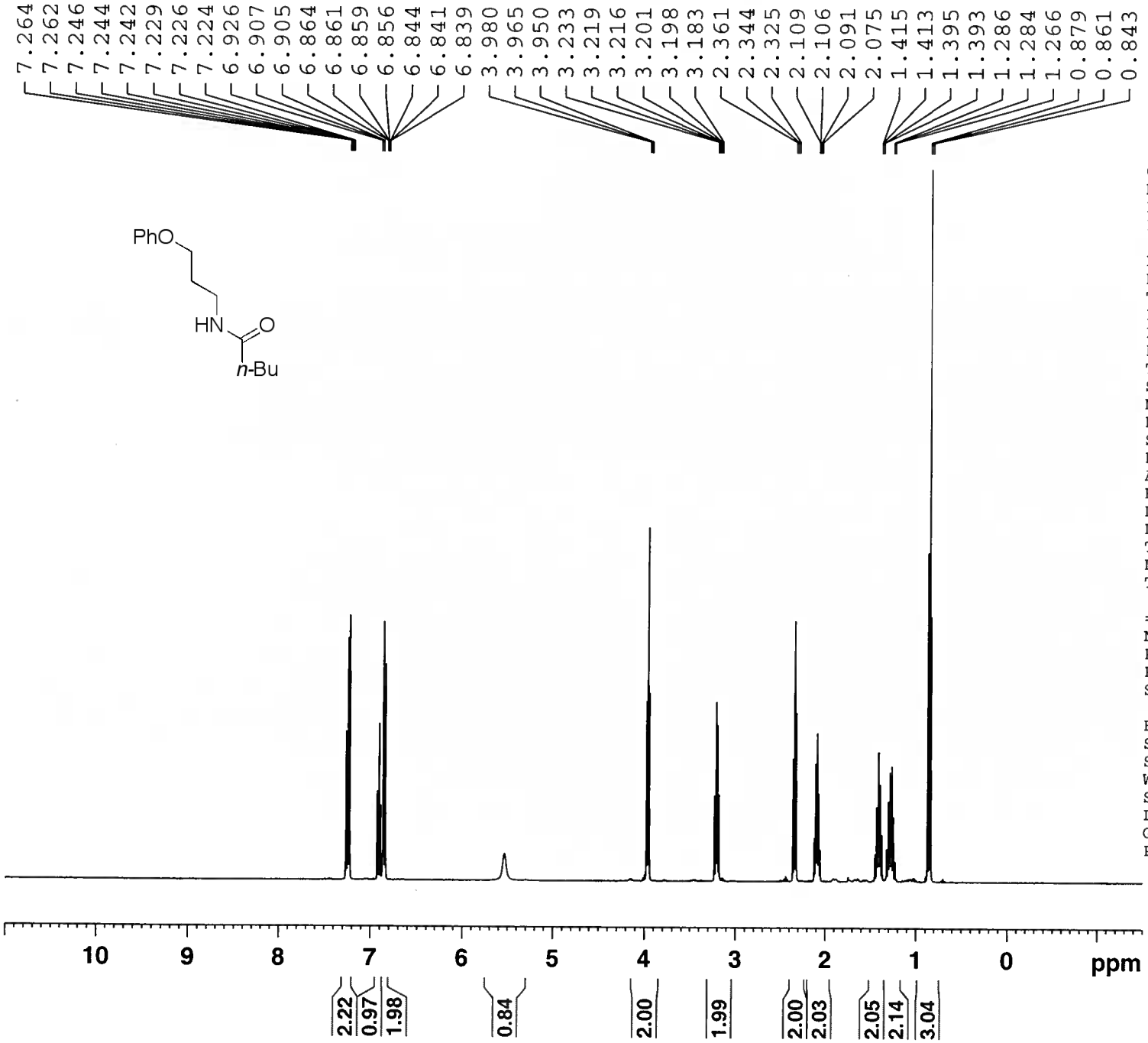
NUC1	13C
P1	8.75 usec
PL1	-3.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.00 dB
PL12	14.52 dB
PL13	18.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	65536
SF	100.6127773 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40



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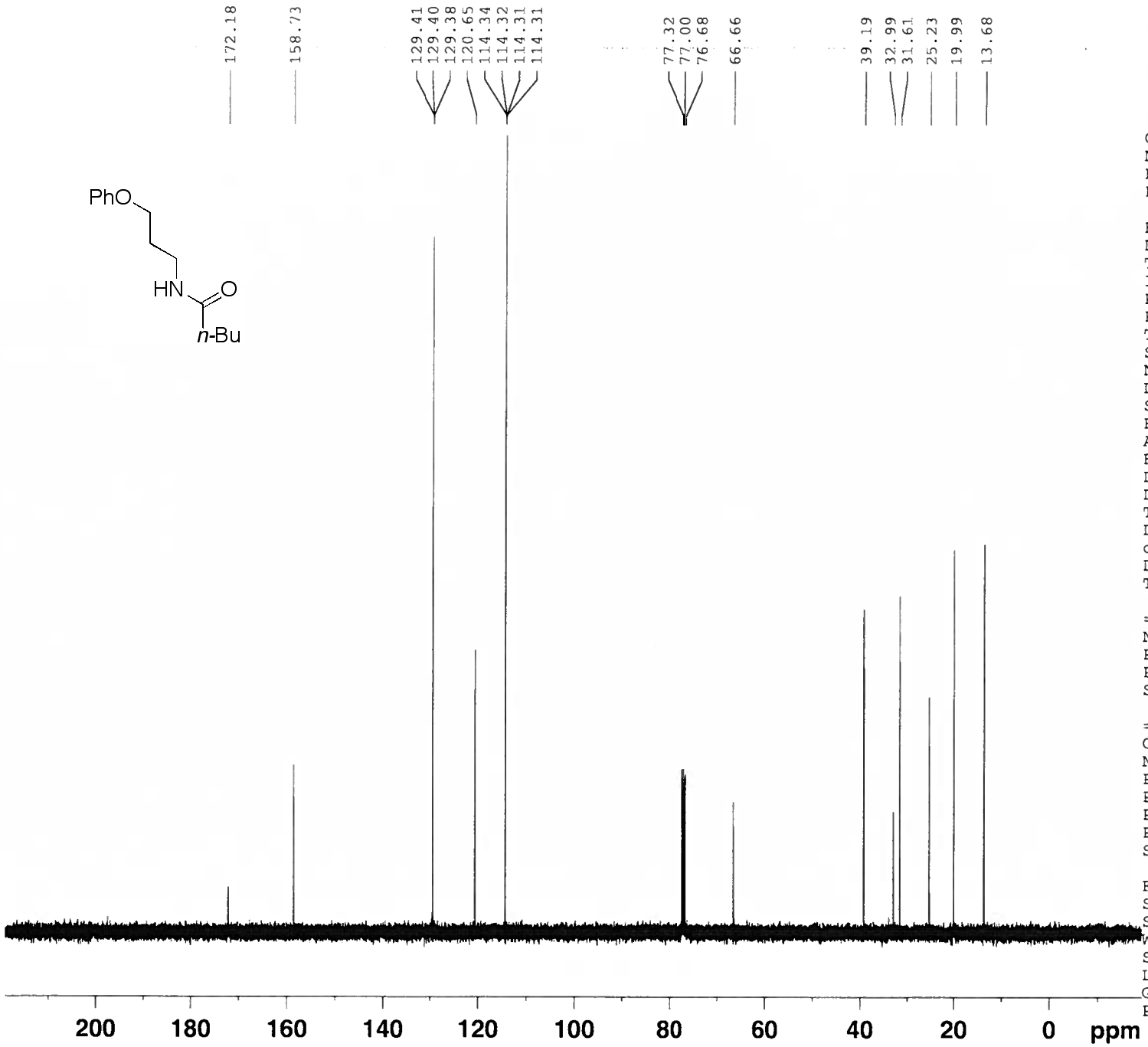
Current Data Parameters
NAME alb-1-48
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090408
Time 14.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 203.2
DW 60.400 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.88 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300220 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



BRUKER

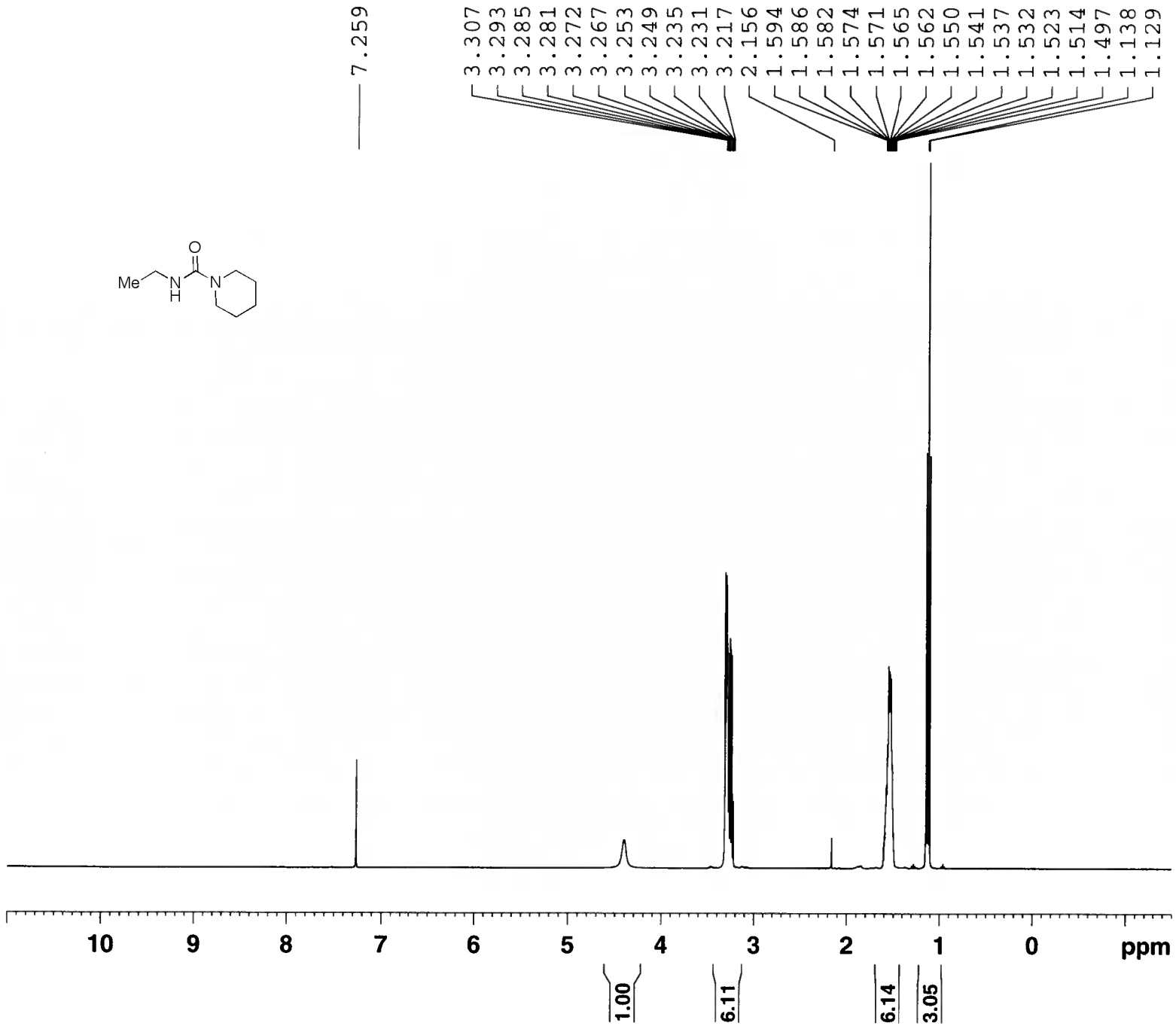
Current Data Parameters
NAME alb-1-48-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090408
Time 15.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127785 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



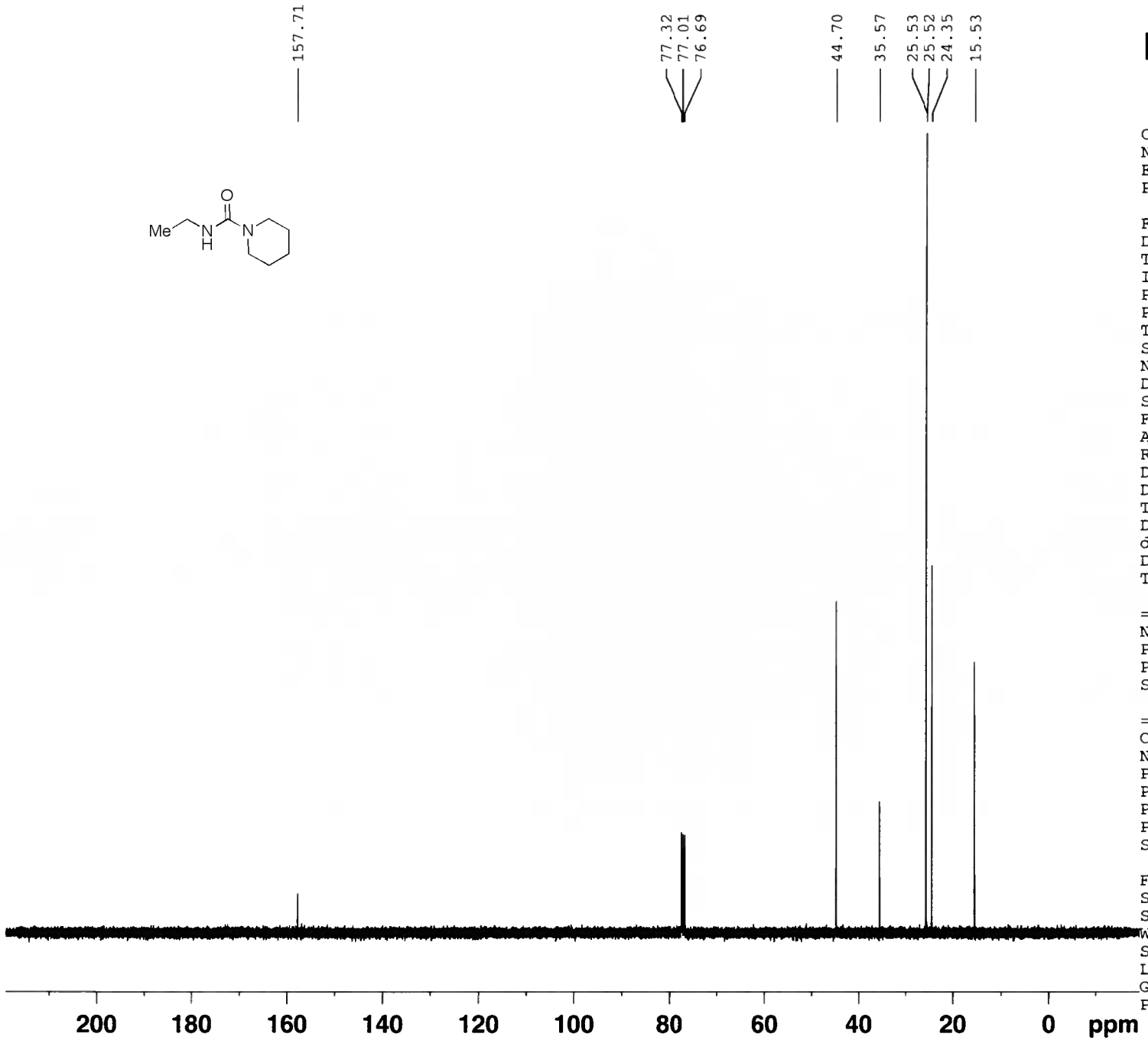
Current Data Parameters
NAME jdh-2-31-h1
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090514
Time 20.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 298.2
D1 1.00000000
TD0 1

SI-178

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300092
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



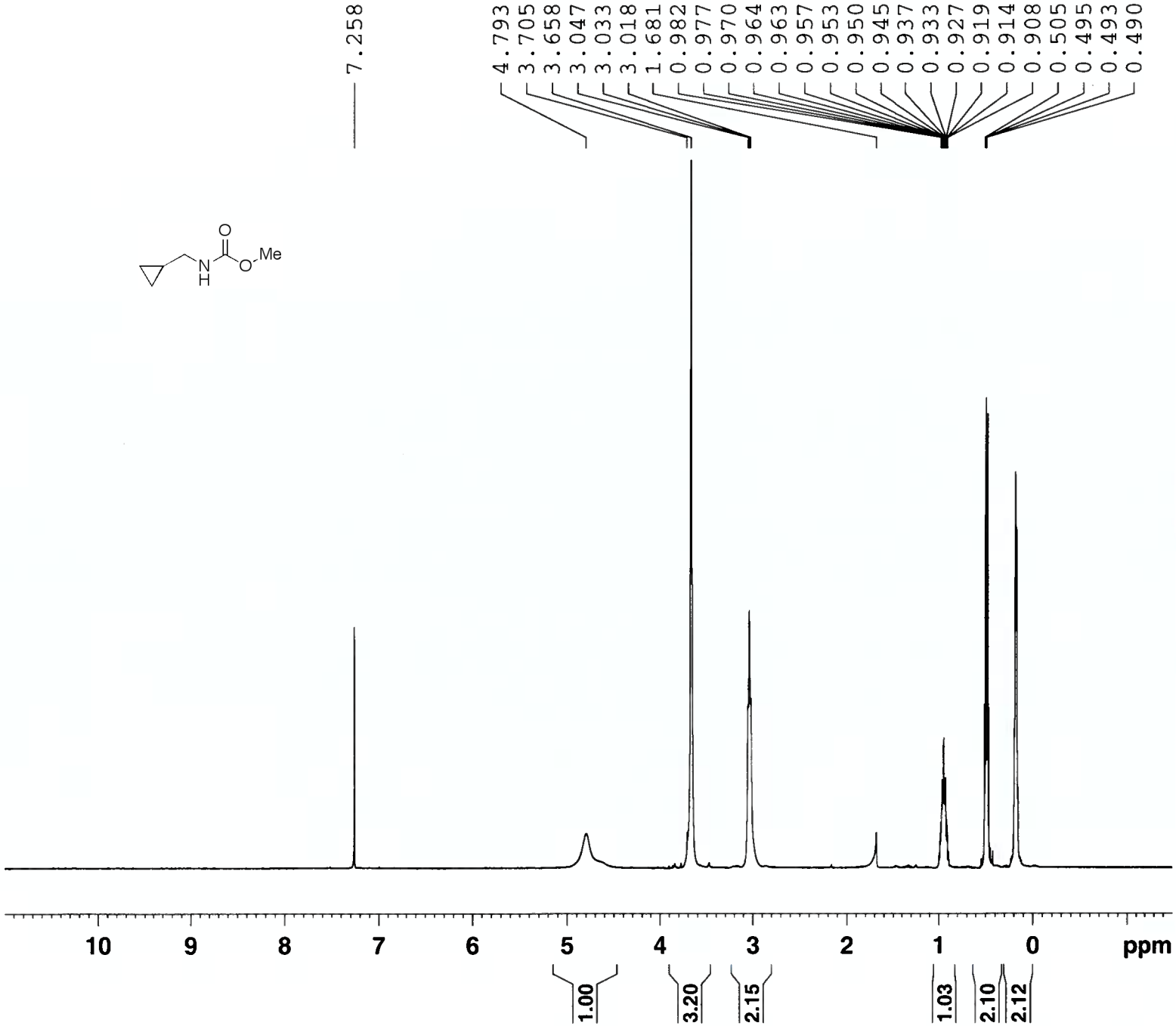
Current Data Parameters
NAME jdh-2-31-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090514
Time 20.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127766 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



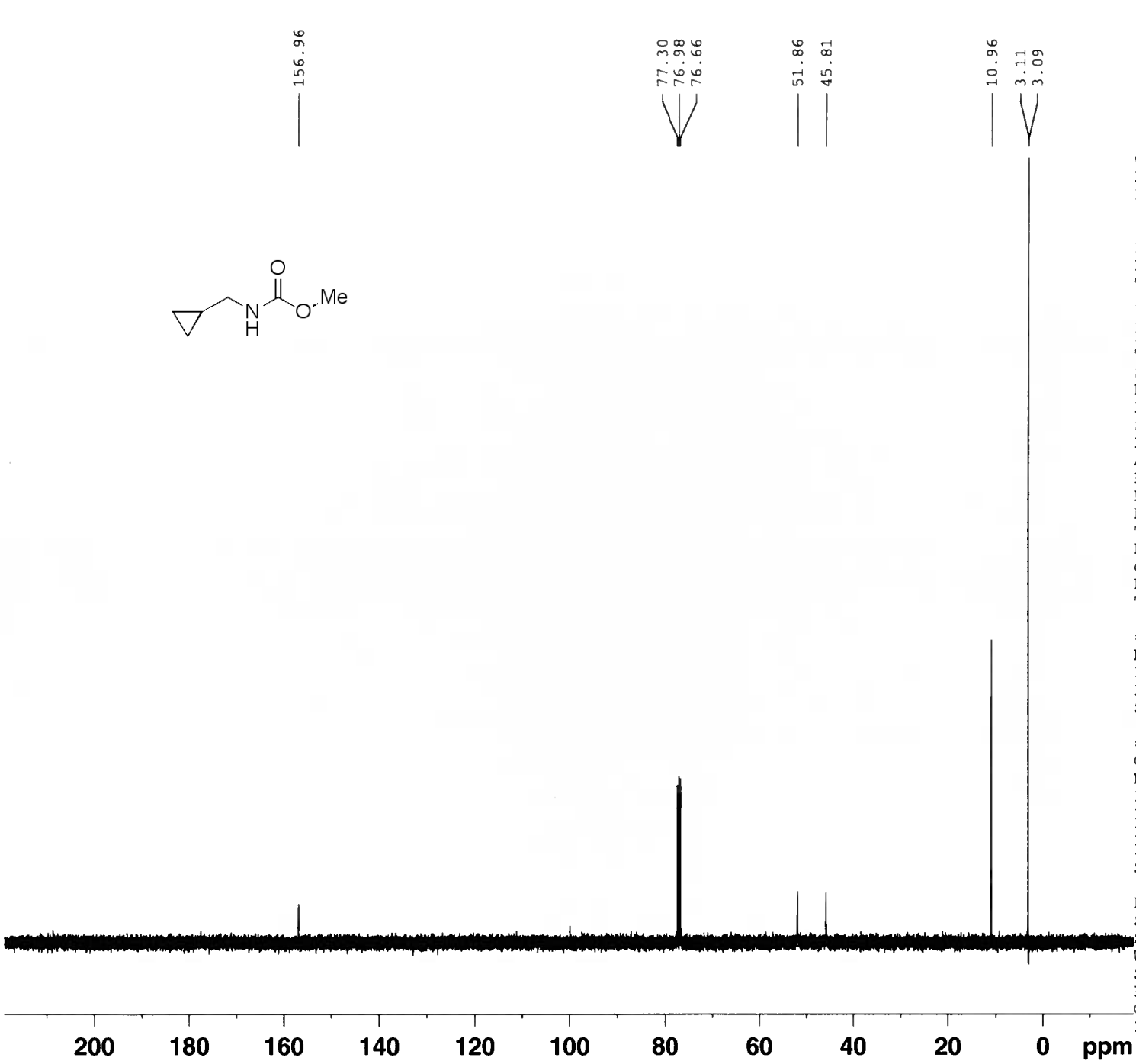
Current Data Parameters
NAME alb-1-38-h1
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090514
Time 20.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 128
DW 60.400
DE 6.00
TE 298.2
D1 1.00000000
TD0 1

SI-189

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300098
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



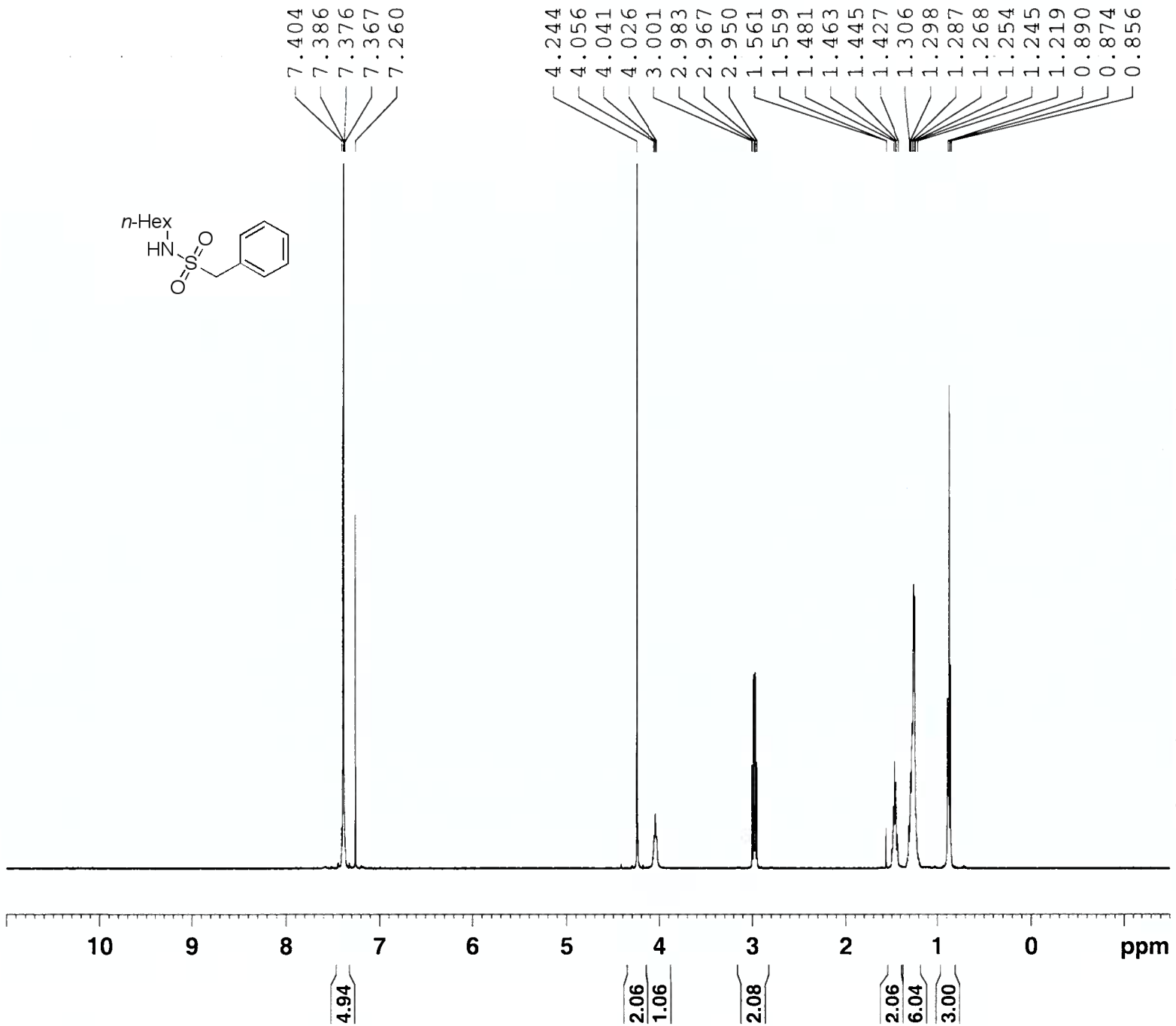
Current Data Parameters
NAME alb-1-38-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090514
Time 20.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 7298.2
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127768 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



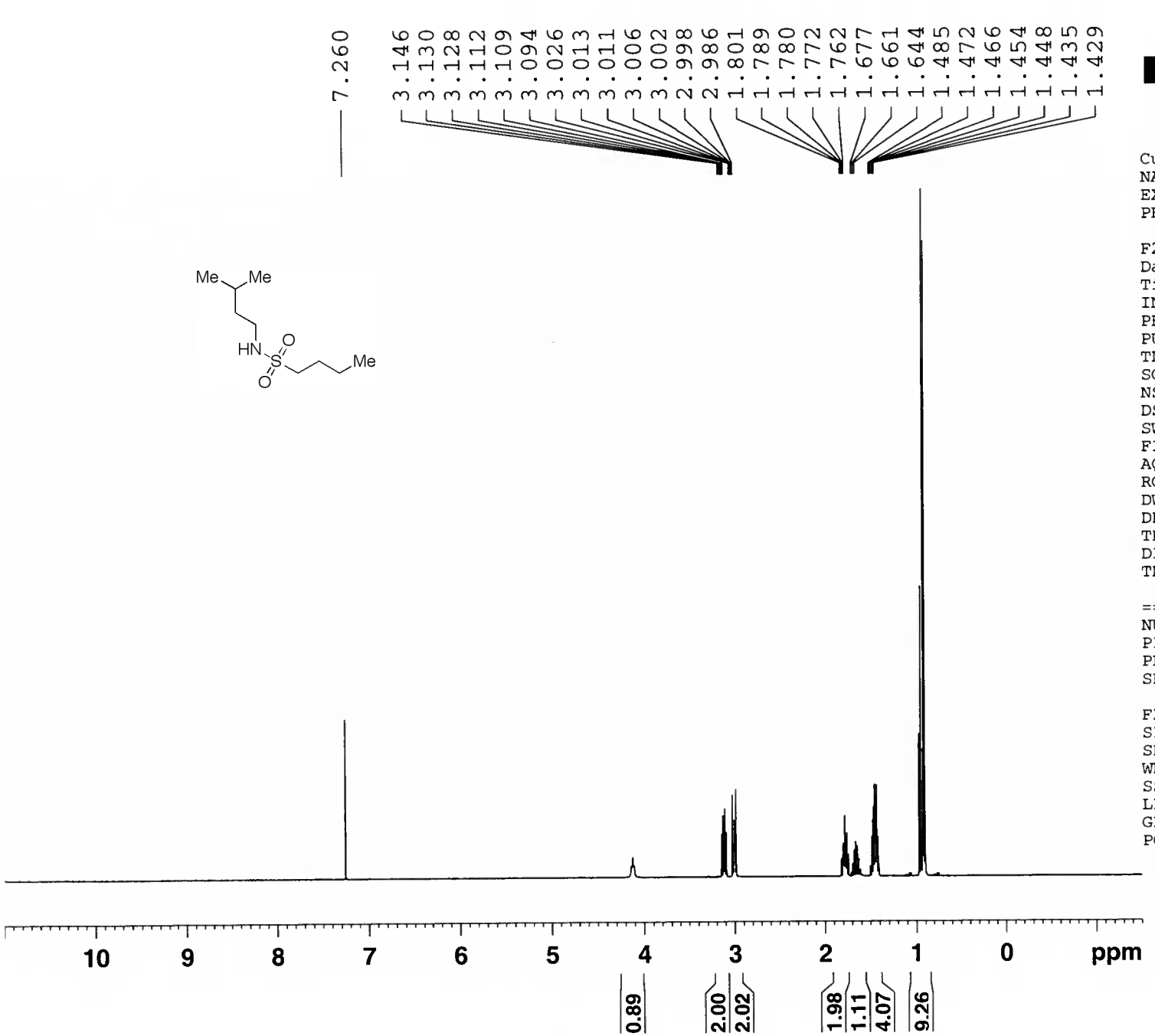
Current Data Parameters
NAME jdh-1-299
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090408
Time 14.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 203.2
DW 60.400
DE 6.00
TE 293.2
D1 1.00000000
TD0 1

SI-182

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300097
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

Current Data Parameters

NAME	alb-1-102
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

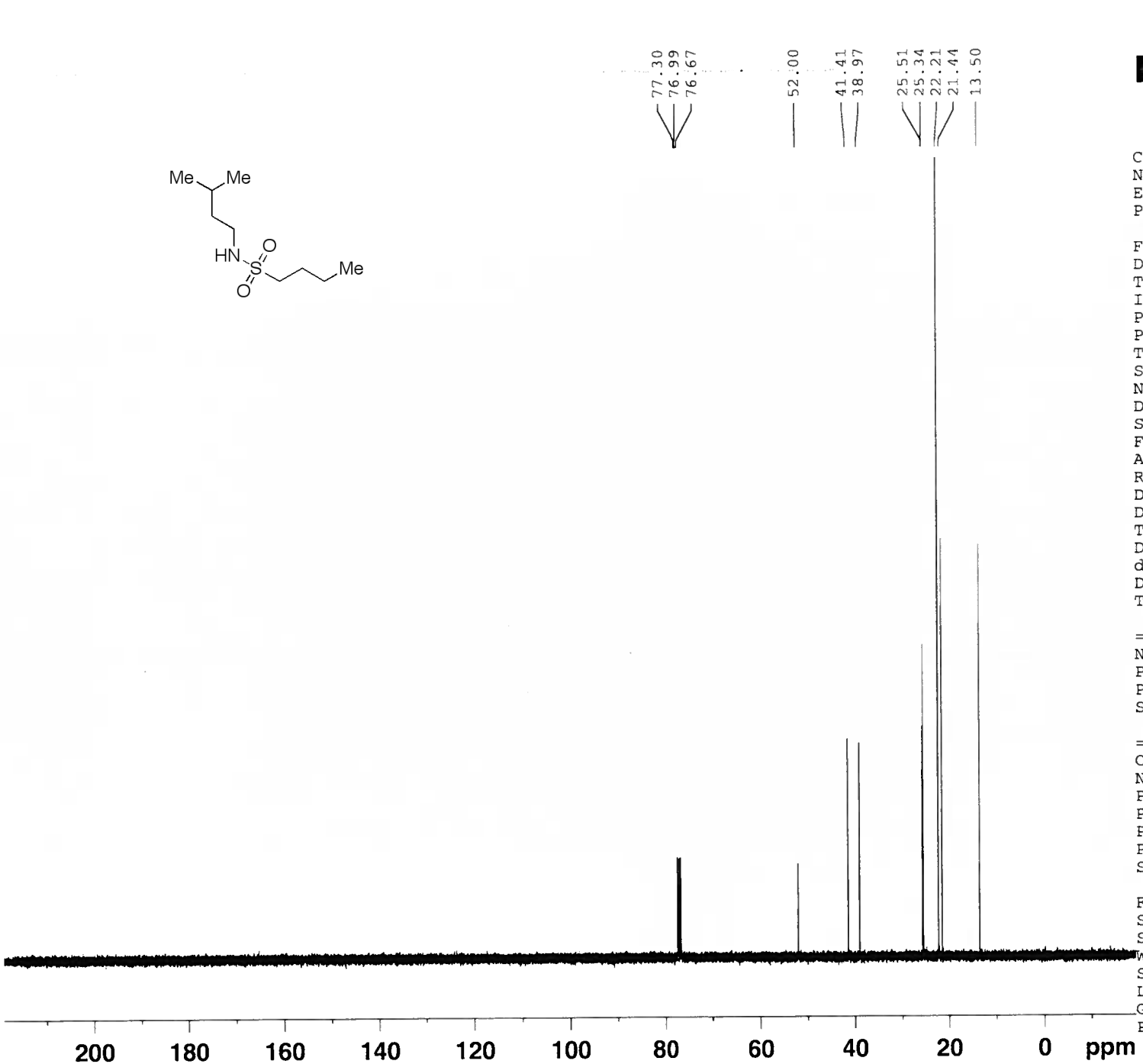
Date_	20090408
Time	14.29
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	287.4
DW	60.400 usec
DE	6.00 usec
TE	291.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	13.88 usec
PL1	0.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	65536
SF	400.1300094 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



BRUKER

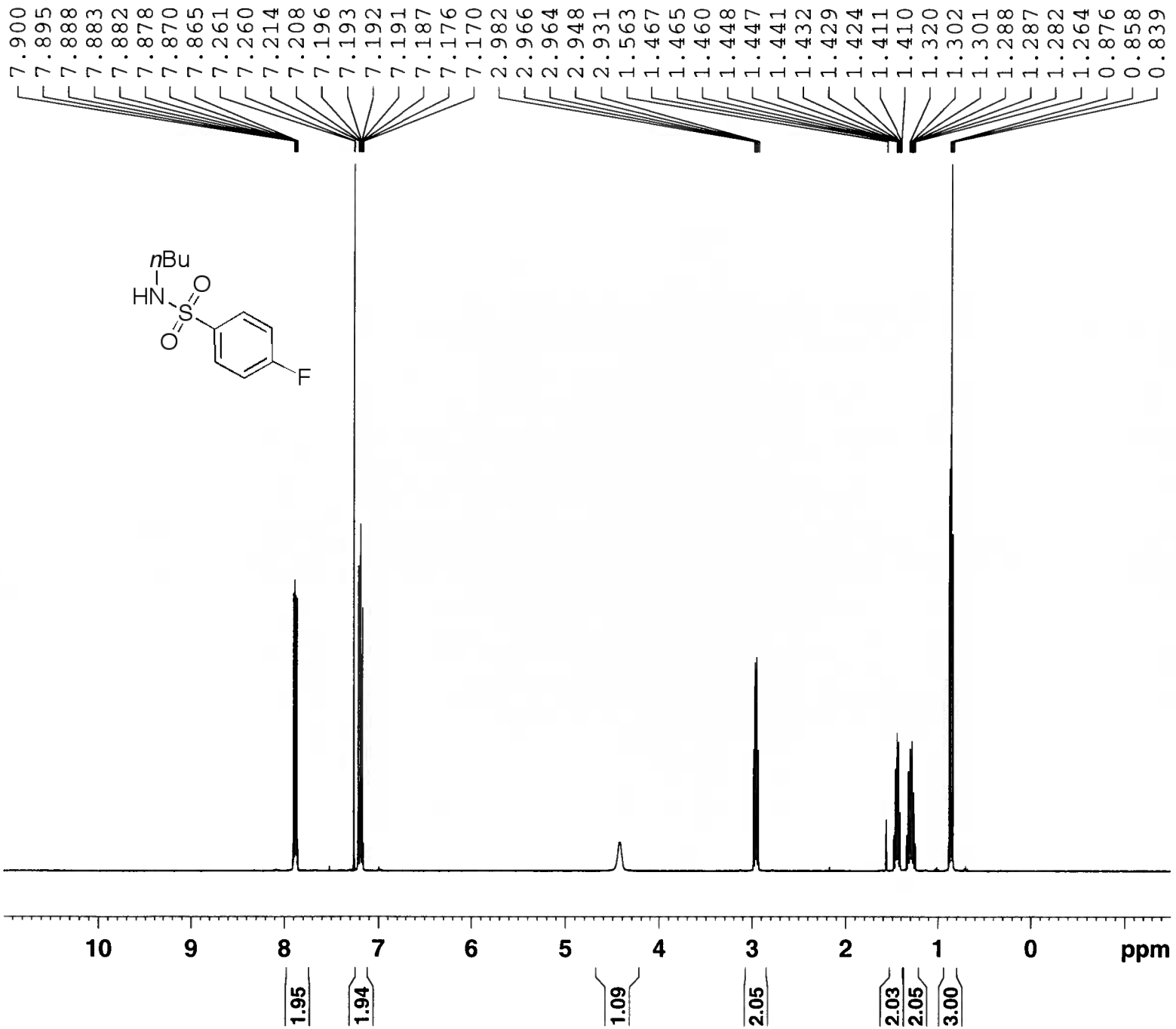
Current Data Parameters
NAME alb-1-102-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090408
Time 15.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127801 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40



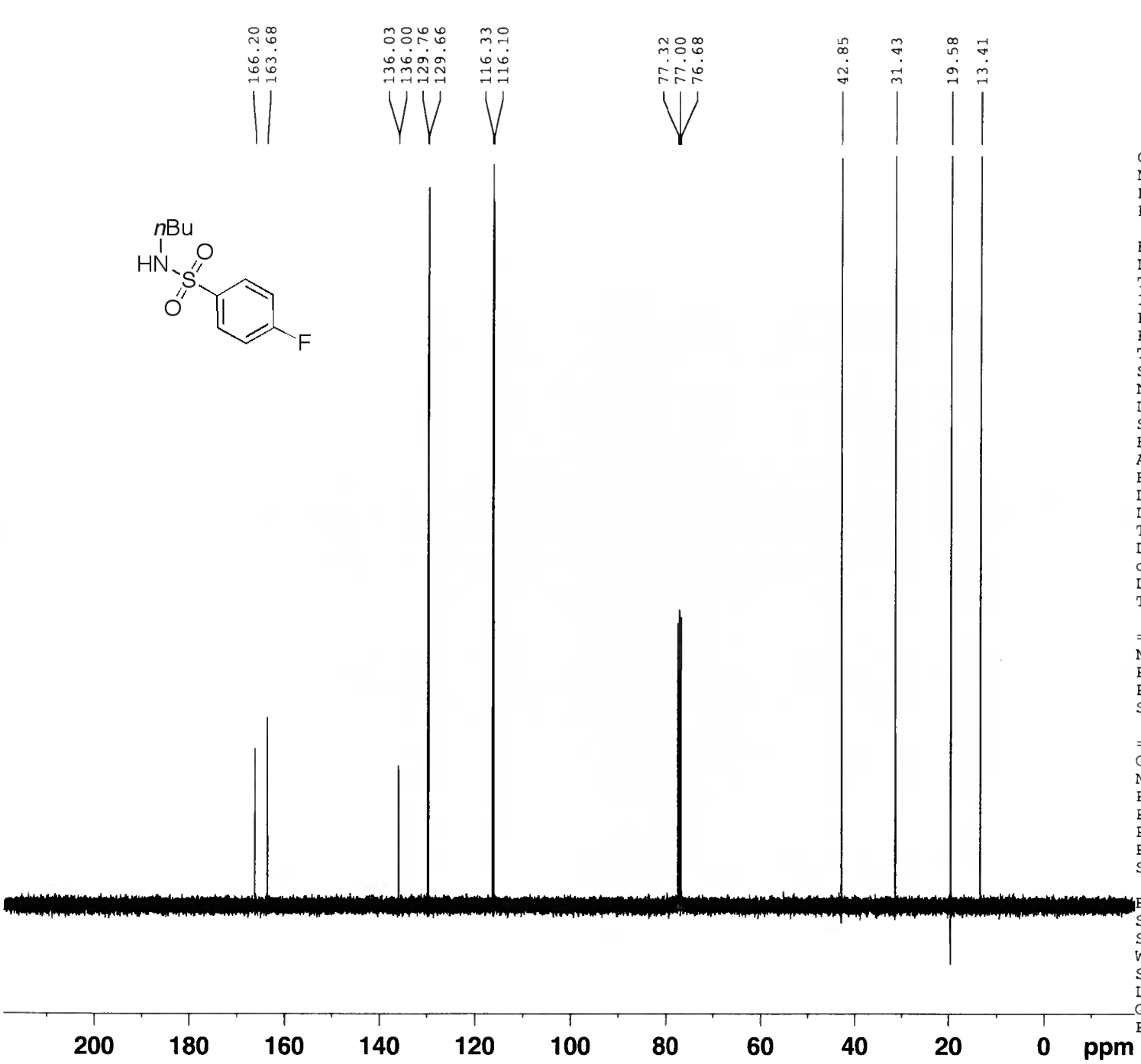
Current Data Parameters
NAME alb-1-29-h1
EXPNO 1
PROCNO 1

F2 - Acquisition Paramet
Date_ 20090514
Time 20.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146
FIDRES 0.126314
AQ 3.9584243
RG 203.2
DW 60.400
DE 6.00
TE 298.2
D1 1.00000000
TD0 1

SI-185

======== CHANNEL f1 ====
NUC1 1H
P1 15.07
PL1 0.00
SFO1 400.1324710

F2 - Processing paramete
SI 65536
SF 400.1300095
WDW no
SSB 0
LB 0.00
GB 0
PC 1.00



BRUKER

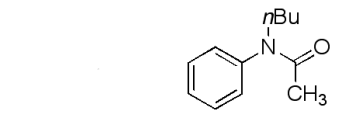
Current Data Parameters
NAME alb-1-29-C13
EXPNO 1
PROCNO 1

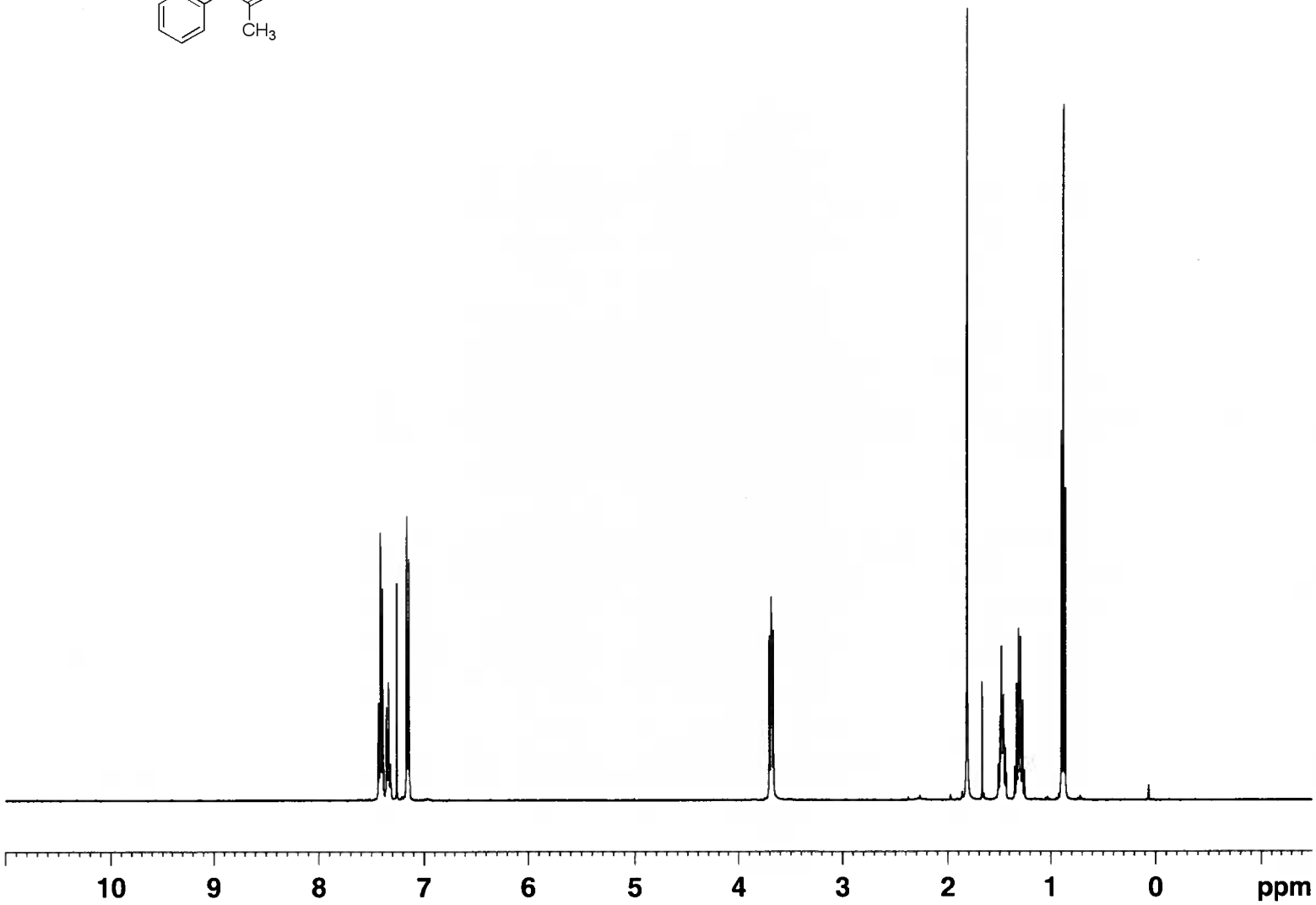
F2 - Acquisition Parameters
Date_ 20090514
Time 20.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 129
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127757 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME        jdh-4-151-H1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20090526
Time               17.06
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146
FIDRES          0.126314
AQ              3.9584243
RG                 203.2
DW                60.400
DE                 6.00
TE                298.2
D1           1.00000000
TD0                    1

======== CHANNEL f1 ====
NUC1                  1H
P1                 15.07
PL1                 0.00
SFO1        400.1324710

F2 - Processing paramete
SI                 65536
SF          400.1300102
WDW                   no
SSB                    0
LB                  0.00
GB                     0
PC                  1.00
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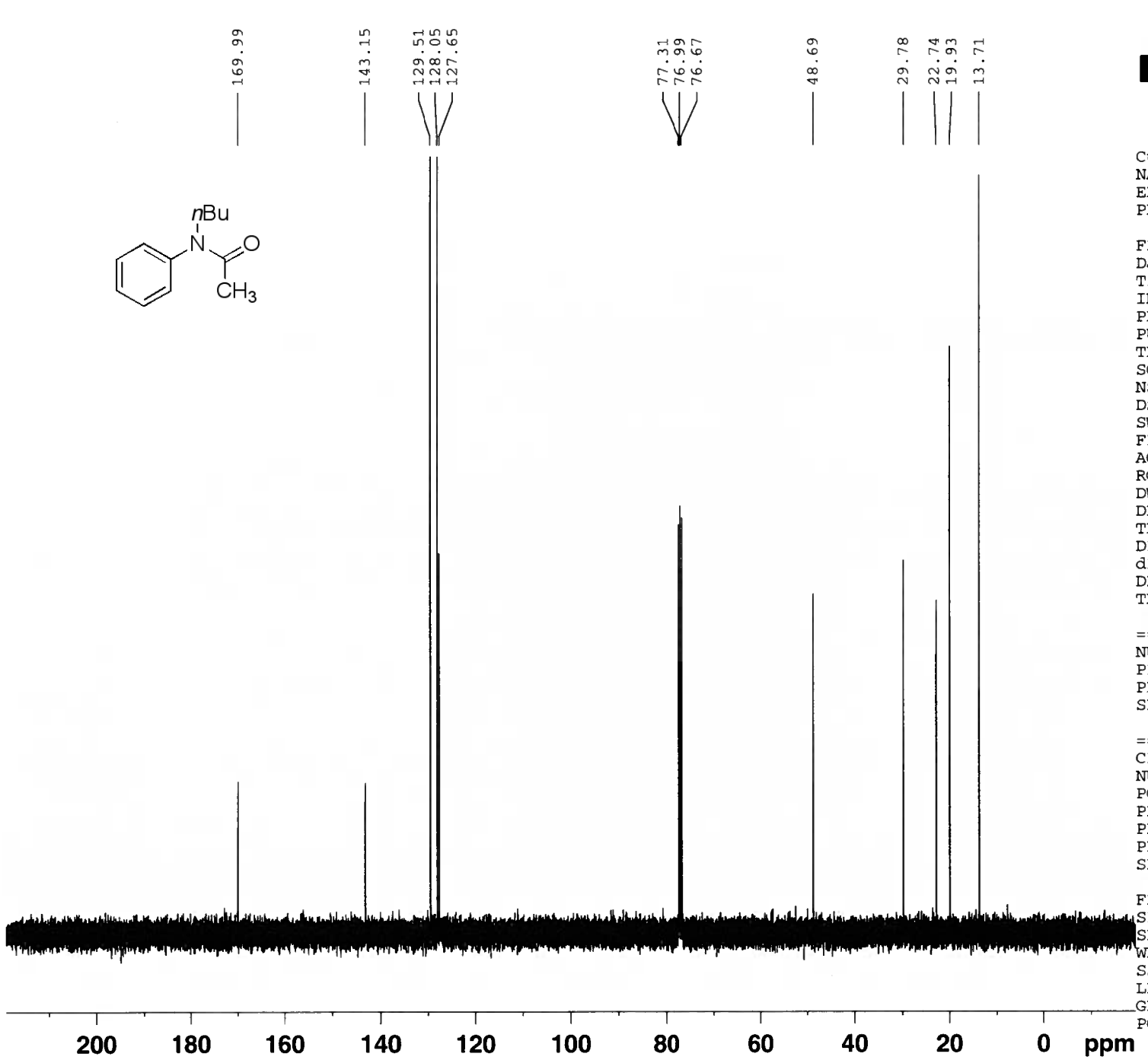
SI-187



BRUKER

Current Data Parameters
NAME jdh-4-151-c13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_	20090526	
Time	17.16	
INSTRUM	spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	128	
DS	2	
SWH	23980.814	Hz
FIDRES	0.365918	Hz
AQ	1.3664756	sec
RG	8192	
DW	20.850	usec
DE	6.00	usec
TE	298.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	

======== CHANNEL f1 ========

NUC1	13C	
P1	8.75	usec
PL1	-3.00	dB
SFO1	100.6228298	MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-1.00	dB
PL12	14.52	dB
PL13	18.00	dB
SFO2	400.1316005	MHz

F2 - Processing parameters

SI	65536	
SF	100.6127783	MHz
WDW	no	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	