Supporting Information

General Reagent Information

All reactions were carried out under an argon atmosphere. THF 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 under argon pressure through two packed columns of neutral alumina and copper (II) oxide. Aryl halides were purchased from Aldrich Chemical Co., Alfa Aesar, Acros Organics, TCI America, Frontier Scientific or Combi Blocks and were used as received without further purification. Vinyl triflates and nonaflates were prepared using literature procedures.[1] Ligands **L1-L4** were purchased from Strem Chemicals. Ligand **L5** was synthesized according to literature procedure[2] and is commercially available from Sigma-Aldrich. Precatalysts **5** were synthesized using literature procedures.[3] Pd-PEPPSI-IPent (**6**) was purchased from Sigma-Aldrich. Flash chromatography was performed using a Biotage Isolera instrument with prepacked silica cartridges.

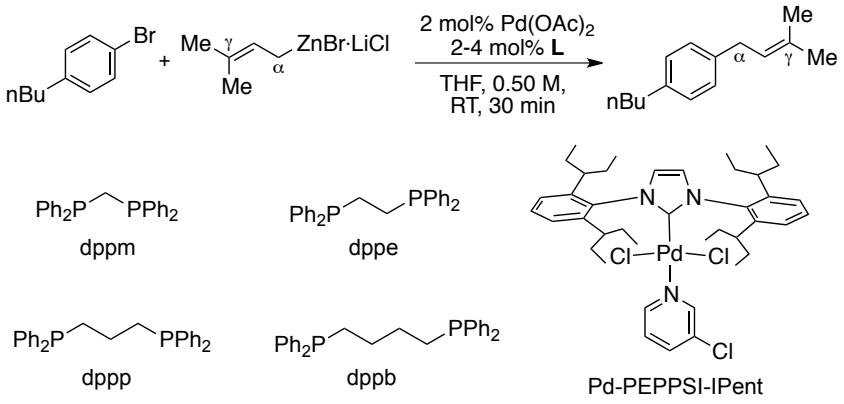
General Analytical Information

All compounds were characterized by ^{1}H NMR, ^{13}C NMR and ^{19}F NMR (where applicable). New compounds were characterized by IR spectroscopy, melting point (where applicable) and elemental analysis or high-resolution mass spectroscopy. Copies of the ^{1}H and ^{13}C spectra can be found at the end of the Supporting Information. Nuclear Magnetic Resonance spectra were recorded on a Bruker 400 MHz instrument. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvent. All ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (77.16 ppm) and all were obtained with ^{1}H decoupling. All ^{19}F NMR spectra are reported in ppm relative to

[1] E. J. Cho, S. L. Buchwald, *Org. Lett.* **2011**, *13*, 6552-6555.
[2] C. Han, S. L. Buchwald, *J. Am. Chem. Soc.* **2009**, *131*, 7532–7533.
[3] N. C. Bruno, M. T. Tudge, S. L. Buchwald, *Chem. Sci.* **2013**, *4*, 916-920.

$CFCl_3$ (0.00 ppm). All IR spectra were taken on a Thermo Scientific Nicolet iS5 spectrometer (iD5 ATR, diamond). All GC analyses were performed on a Agilent 6890 gas chromatograph with an FID detector using a J & W DB-1 column (10 m, 0.1 mm I.D.). Elemental analyses were performed by Atlantic Microlabs Inc., Norcross, GA. ESI-MS spectra were recorded on a Bruker Daltonics APEXIV 4.7 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS).

Table S1. Ligand Evaluation: Some Representative Unsuccessful Catalysts[a]



entry	ligand	conv.	yield of Ar-(prenyl)	yield of Ar-H	conv. to Ar-Ar
1	PPh_3	0	0	0	0
2	PPh_3[b]	100	6	3	80
3	dppm	0	0	0	0
4	dppm[b]	32	0	25	7
5	dppe	0	0	0	0
6	dppe[b]	100	10	5	80
7	dppp	0	0	0	0
8	dppp[b]	100	14	10	56
9	dppb	0	0	0	0
10	dppb[b]	100	8	15	75
11	Pd-PEPPSI-IPent[c]	1	0	0	0

a. 1-Bromo-4-butylbenzene (0.5 mmol), prenylzinc bromide (0.65 mmol), $Pd(OAc)_2$ (2 mol%) were used. Yields were determined by GC analysis of the crude reaction mixture using dodecane as an internal standard. *b*. Reaction was run at 70 °C for 24 h. *c*. No $Pd(OAc)_2$ was used.

Preparation of Allylzinc Reagents Using Knochel's Protocol[4]

[4] A. Krasovskiy, V. Malakhov, A. Gavryushin, P. Knochel, *Angew. Chem., Int. Ed.* **2006**, *45*, 6040-6044.

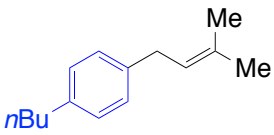
Representative Procedure (Prepration of Prenylzinc Bromide): An oven-dried round-bottom flask equipped with a magnetic stir bar and a rubber septum was charged with LiCl (4.2 g, 100 mmol). The vessel was heated with a heat gun for 10 min under high vacuum and backfilled with argon after cooling to room temperature. Zinc dust (4.88 g, 75 mmol) was added. The vessel was evacuated and backfilled with argon. THF (40 mL) and 1,2-dibromoethane (215 μL, 2.5 mmol) were added via syringe and the reaction mixture was heated at 40 °C until bubbling occurred (10 min). Trimethylsilyl chloride (63 μL, 0.5 mmol) and a solution of iodine (64 mg, 0.25 mmol) in THF (1 mL) were added via syringe. The reaction mixture was then cooled to 0 °C in an ice bath. 3,3-Dimethylallyl bromide (5.8 mL, 50 mmol) was added dropwise over 1 h using a syringe pump. The reaction mixture was allowed to warm to room temperature and stir for an additional 2 h. After the completion of the reaction, the reaction mixture was allowed to stand at room temperature for 1 h and the supernatant solution was carefully transferred to a dry vessel via cannula. The concentration of the organozinc solution was determined by iodometric titration using Knochel's procedure[5] (0.81 M, ca. 75% yield).

Experimental Procedures for Examples Described in Scheme 3-5

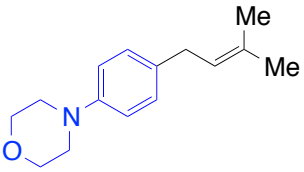
General Procedure: An oven-dried screw-cap test tube, which was equipped with a magnetic stir bar and fitted with a teflon septum, was charged with CPhos Precat (16.2 mg, 0.02 mmol) and CPhos (8.7 mg, 0.02 mmol). If the (hetero)aryl halide (1.0 mmol) was a solid, it was also added at this time. The test tube was evacuated and backfilled with argon (this process was repeated a total of 3 times) and THF (0.4 mL) were added via syringe. If the (hetero)aryl halide was a liquid, it was added to the test tube via syringe at this time. A THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) was added dropwise via syringe. The reaction mixture was allowed to stir at room temperature for 2-12 h, and then quenched by water (5 mL) and extracted with ethyl acetate (3×10 mL). The combined organic phases were dried over $MgSO_4$ and concentrated in vacuo, and purified by a Biotage SP4 instrument.

[5] A. Krasovskiy, P. Knochel, *Synthesis* **2006**, 890-891.

1-Butyl-4-(3-methylbut-2-en-1-yl)benzene (4)



Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.87 mL, 0.81 M) and 1-bromo-4-butylbenzene (213 mg, 176 µL, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-2% EtOAc/hexanes) to provide the title compound as a colorless liquid (192 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.24-7.22 (m, 4H), 5.47 (t, J = 7.2 Hz, 2H), 3.45 (d, J = 7.2 Hz, 2H), 2.71 (t, J = 7.8 Hz, 2H), 1.87 (s, 3H), 1.86 (s, 3H), 1.73 (m, 2H), 1.50 (m, 2H), 1.07 (t, J = 7.2 Hz, 3H), ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.3, 139.0, 132.3, 128.5, 128.3, 123.6, 35.4, 34.1, 34.0, 25.9, 22.6, 17.9, 14.1 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

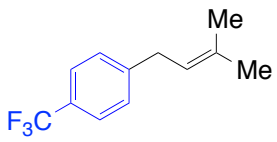


4-(4-(3-Methylbut-2-en-1-yl)phenyl)morpholine (7a)

Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.87 mL, 0.81 M) and (4-bromophenyl)morphorline (242 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-30% EtOAc/hexanes) to provide the title compound as a pale yellow oil (208 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.15 (d, J = 8.4 Hz, 1H), 6.90 (d, J = 8.4 Hz, 1H), 5.38 (t, J = 7.2 Hz, 1H), 3.90 (t, J = 4.8 Hz, 4H), 3.33 (d, J = 7.2 Hz, 2H), 3.15 (t, J = 4.8 Hz, 4H), 1.80 (s, 3H), 1.78 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.5, 133.5, 132.1, 129.0, 123.7, 116.0, 67.0, 49.8, 33.5, 25.8, 17.8 ppm. IR (neat, cm^{-1}): 2854, 1513, 1230, 1121, 926, 813. Anal. Calcd. for $C_{15}H_{21}NO$: C, 77.88; H, 9.15. Found: C, 77.76; H, 9.17. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

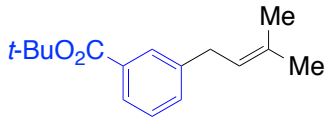
1-(3-Methylbut-2-en-1-yl)-4-(trifluoromethyl)benzene (7b)

[6] Y, Yang, S. L. Buchwald, *J. Am. Chem. Soc.* **2013**, *135*, 10642–10645.



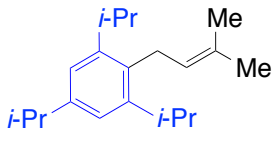
Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and 4-chlorobenzotrifluoride (180 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h.The coupling product was found to be highly volatile and the yield (89%) was determined by ^{1}H NMR spectroscopy of the crude reaction mixture using 1,3,5-trimethoxybenzene as internal standard. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.53 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 5.32 (t, J = 7.2 Hz, 1H), 3.39 (d, J = 7.6 Hz, 2H), 1.77 (s, 3H), 1.76 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.1, 133.8, 128.7, 128.0, 127.1 (q, J = 270 Hz), 125.3 (q, J = 3.6 Hz), 122.1, 34.3, 25.8, 18.0 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.3 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

***Tert*-butyl 3-(3-methylbut-2-en-1-yl)benzoate (7c)**



Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and *tert*-butyl 3-bromobenzoate (257 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-8% EtOAc/hexanes) to provide the title compound as a colorless oil (235 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81-7.78 (m, 2H), 7.34-7.29 (m, 2H), 5.32 (t, J = 7.2 Hz, 1H), 3.28 (d, J = 7.2 Hz, 2H), 1.75 (s, 3H), 1.73 (s, 3H), 1.59 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.9, 141.9, 132.9, 132.5, 132.1, 129.3, 128.2, 126.9, 122.7, 80.7, 34.2, 28.2, 25.7, 17.8 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

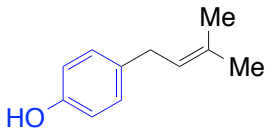
1,3,5-Triisopropyl-2-(3-methylbut-2-en-1-yl)benzene (7d)



Following general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and bromo-2,4,6-triisopropylbenzene (227 mg, 253 µL, 1.0 mmol) were used. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 100%

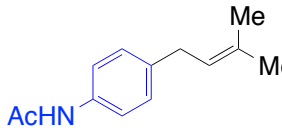
hexanes) to provide the title compound as a colorless oil (253 mg, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.19 (s, 2H), 5.25 (t, *J* = 6.0 Hz, 1H), 3.58 (d, *J* = 6.0 Hz, 2H), 3.36 (septet, *J* = 6.8 Hz, 2H), 3.06 (septet, *J* = 6.8 Hz, 1H), 1.95 (s, 3H), 1.87 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 6H), 1.42 (d, *J* = 6.8 Hz, 12H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.8, 146.4, 133.4, 130.7, 124.9, 121.0, 34.3, 29.4, 26.8, 25.8, 24.4, 24.3, 18.1 ppm. IR (neat, cm^{-1}): 2958, 2868, 1458, 1362, 1097, 875. Anal. Calcd. for $C_{18}H_{28}N_4O_2$: C, 67.22; H, 6.94. Found: C, 67.02; H, 6.99. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

4-(3-Methylbut-2-en-1-yl)phenol (7e)



Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.85 mL, 0.81 M) and 4-bromophenol (173 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-15% EtOAc/hexanes) to provide the title compound as a colorless oil (154 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.09 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 5.93 (s, 1H), 5.37 (t, *J* = 7.2 Hz, 1H), 3.33 (d, *J* = 7.2 Hz, 2H), 1.81 (s, 3H), 1.77 (s, 3H), 1.45 (d, *J* = 6.8 Hz, 6H), 1.42 (d, *J* = 6.8 Hz, 12H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.3, 134.2, 132.3, 129.5, 123.7, 115.4, 33.5, 25.8, 17.8 ppm. IR (neat, cm^{-1}): 3331, 2912, 1511, 1440, 1222, 818. Spectral data were in accordance with those in literature.[7] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

***N*-(4-(3-methylbut-2-en-1-yl)phenyl)acetamide (7f)**

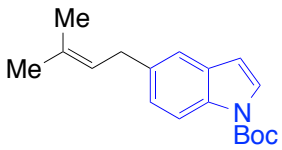


Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.85 mL, 0.81 M) and N-(4-bromophenyl)acetamide (214 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-15% EtOAc/hexanes) to provide the title compound as a slightly yellow solid (183 mg, 90%). ^{1}H NMR (400 MHz,

[7] T. Ollevier, Mwene-Mbeja, T, M. *Synthesis* **2006**, *23*, 3963-3966.

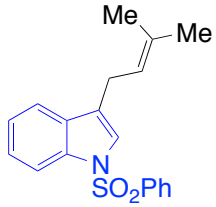
$CDCl_3$) δ: 8.58 (s, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 5.29 (t, *J* = 7.2 Hz, 1H), 3.30 (d, *J* = 7.2 Hz, 2H), 2.12 (s, 3H), 1.76 (s, 3H), 1.72 (s, *3*H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.2, 137.7, 135.9, 132.5, 128.6, 123.1, 120.5, 33.7, 25.7, 24.2, 17.8 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

***Tert*-butyl 5-(3-methylbut-2-en-1-yl)-1H-indole-1-carboxylate (7g)**



Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and *N*-Boc-5-bromoindole (296 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-10% EtOAc/hexanes) to provide the title compound as a colorless oil (284 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 3.2 Hz, 1H), 7.34 (d, *J* = 1.2 Hz, 1H), 7.13 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.51 (d, *J* = 3.2 Hz, 1H), 5.38 (t, *J* = 4.4 Hz, 1H), 3.43 (d, *J* = 7.2 Hz, 2H), 1.758 (s, 3H), 1.755 (s, 3H), 1.67 (s, 9H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.9, 136.3, 133.7, 132.2, 130.9, 126.0, 125.0, 124.0, 120.2, 115.0, 107.3, 83.5, 34.3, 28.3, 25.9, 17.9 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

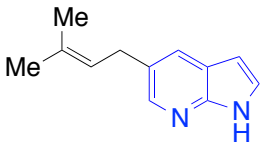
3-(3-Methylbut-2-en-1-yl)-1-(phenylsulfonyl)-1H-indole (7h)



Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and 1-phenylsulfonyl-3-bromoindole (336 mg, 1.0 mmol were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 50 g SNAP cartridge; 0-10% EtOAc/hexanes) to provide the title compound as a colorless solid (172 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.05 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.2 Hz, 2H), 7.52-7.49 (m, 2H), 7.38-7.34 (m, 2H), 7.27 (dd, *J* = 7.2, 7.2 Hz, 1H), 5.41 (t, *J* = 7.2 Hz, 1H), 3.39 (d, *J* = 7.2 Hz, 2H), 1.82 (s, 3H), 1.77 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.3, 135.6, 133.8, 133.7, 131.1, 129.2, 126.7, 124.8, 123.15, 123.09, 122.7, 120.8, 119.7, 113.8, 25.8, 23.9,

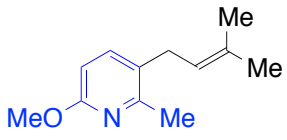
17.9 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

5-(3-Methylbut-2-en-1-yl)-1H-pyrrolo[2,3-b]pyridine (7i)



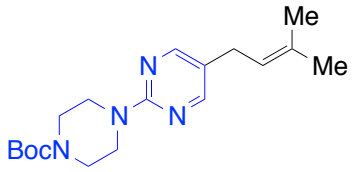
Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.87 mL, 0.81 M) and *tert*-butyl 3-bromobenzoate (257 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-100% EtOAc/hexanes) to provide the title compound as a yellowish solid (173 mg, 95%). m.p. = 157-158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, J = 1.2 Hz, 1H), 7.92 (d, J = 1.2 Hz, 1H), 7.37 (dd, J = 3.2, 2.0 Hz, 1H), 6.51 (dd, J = 3.2, 2.0 Hz, 1H), 5.32 (t, J = 7.2 Hz, 1H), 3.36 (d, J = 7.2 Hz, 2H), 1.70 (s, 3H), 1.65 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.4, 141.2, 133.9, 132.4, 129.7, 126.7, 123.2, 121.9, 101.2, 31.1, 25.6, 17.9 ppm. IR (neat, cm^{-1}): 3363, 2930, 1591, 1325, 889, 726. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{14}N_2$, 187.1230; found, 187.1222. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

6-Methoxy-2-methyl-3-(3-methylbut-2-en-1-yl)pyridine (7j)



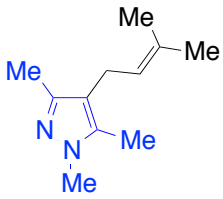
Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.62 mL, 0.81 M) and 3-bromo-6-methoxy-3-methylpyridine (201 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-5% EtOAc/hexanes) to provide the title compound as a yellowish liquid (140 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.30 (d, J = 8.4 Hz, 1H), 6.49 (d, J = 8.4 Hz, 1H), 5.19 (t, J = 7.2 Hz, 1H), 3.89 (s, 3H), 3.21 (d, J = 7.2 Hz, 1H), 2.41 (s, 3H), 1.73 (s, 3H), 1.71 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.9, 153.8, 139.4, 132.8, 127.1, 122.3, 107.2, 55.3, 30.6, 25.8, 22.0, 17.9 ppm. IR (neat, cm^{-1}): 2913, 1473, 1423, 1304, 1040, 818. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{12}H_{17}NO$, 192.1383; found, 192.1378. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

***Tert*-butyl 4-(5-(3-methylbut-2-en-1-yl)pyrimidin-2-yl)piperazine-1-carboxylate (7k)**



Following the general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.62 mL, 0.81 M) and tert-butyl 4-(5-bromopyrimidin-2-yl)piperazine-1-carboxylate (343 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-20% EtOAc/hexanes) to provide the title compound as a yellowish liquid (259 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06 (s, 2H), 5.13 (t, J = 7.2 Hz, 1H), 3.69 (t, J = 4.8 Hz, 4H), 3.41 (t, J = 4.8 Hz, 4H), 3.05 (d, J = 7.2 Hz, 1H), 1.65 (s, 3H), 1.62 (s, 3H), 1.41 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.7, 157.4, 154.8, 133.4, 122.7, 121.9, 79.8, 43.8, 28.4, 28.0, 25.6, 17.8 ppm. Spectral data were in accordance with those in literature.[6] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

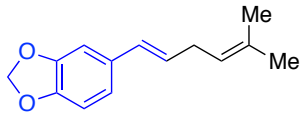
1,3,5-Trimethyl-4-(3-methylbut-2-en-1-yl)-1*H*-pyrazole (7l)



Following the general procedure, a THF solution of prenylzinc bromide (2.30 mmol, 2.87 mL, 0.81 M) and 4-bromo-1,3,5-trimethylpyrazole (189 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h and then quenched with water (10 mL) and extracted with ethyl acetate (3 × 20 mL). The combined organic phases were dried over $MgSO_4$ and concentrated in vacuo. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-100% EtOAc/hexanes) to provide the title compound as a yellow oil (178 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 4.96 (t, J = 7.2 Hz, 1H), 3.75 (s, 3H), 2.96 (d, J = 7.2 Hz, 2H), 2.10 (s, 3H), 2.09 (s, 3H), 1.66 (s, 3H), 1.63 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.4, 135.8, 130.7, 123.1, 115.5, 35.7, 25.5, 22.4, 17.6, 11.7, 9.5 ppm. Spectral data were in accordance with those in literature.[8] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

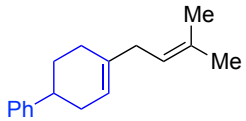
[8] Farmer, J. L.; Hunter, H. N.; Organ, M. G. *J. Am. Chem. Soc.* **2012**, *134*, 17470-17473.

(*E*)-5-(5-Methylhexa-1,4-dien-1-yl)benzo[*d*][1,3]dioxole (8a)



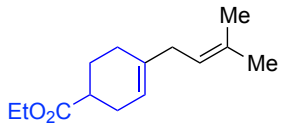
Following general procedure, a THF solution of prenylzinc bromide (1.30 mmol, 1.60 mL, 0.81 M) and (*E*)-5-(2-bromovinyl)benzo[*d*][1,3]dioxole (227 mg, 1.0 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-8% EtOAc/hexanes) to provide the title compound as a colorless oil (190 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.93 (d, *J* = 1.2 Hz, 1H), 6.79-6.75 (m, 2H), 6.31 (d, *J* = 15.6 Hz, 1H), 6.07-6.03 (m, 1H), 5.94 (s, 2H), 5.25 (t, *J* = 7.2 Hz, 1H), 2.90 (dd, *J* = 7.2, 7.2 Hz, 2H), 1.78 (s, 3H), 1.70 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.0, 146.6, 132.9, 132.4, 129.2, 127.8, 121.8, 120.4, 108.2, 105.5, 101.0, 31.7, 25.8, 17.8 ppm. IR (neat, cm^{-1}): 2882, 1489, 1247, 1038, 961, 934. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{14}H_{16}O_2$, 217.1223; found, 217.1250. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

4-(3-Methylbut-2-en-1-yl)-1,2,3,6-tetrahydro-1,1'-biphenyl (8b)



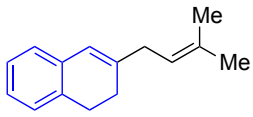
Following general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and cyclohex-1-en-1-yl nonaflate (115 mg, 0.50 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h.The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (104 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.34 (m, 2H), 7.28-7.23 (m, 3H), 5.57-5.56 (m, 1H), 5.28-5.25 (m, 1H), 2.82-2.78 (m, 1H), 2.75 (d, *J* = 6.8 Hz, 2H), 2.38-2.24 (m, 1H), 2.24-2.21 (m, 2H), 2.18-2.09 (m, 1H), 2.04-2.00 (m, 1H), 1.88-1.78 (m, 4H), 1.72 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.5, 137.4, 132.7, 128.4, 127.0, 126.0, 122.4, 120.5, 40.4, 36.4, 33.8, 30.3, 29.4, 25.9, 17.8 ppm. IR (neat, cm^{-1}): 2965, 2912, 1543, 1375, 754, 698. Anal. Calcd. for $C_{17}H_{22}$: C, 90.20; H, 9.80. Found: C, 90.26; H, 9.93. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

Ethyl 4-(3-methylbut-2-en-1-yl)cyclohex-3-enecarboxylate (8c)



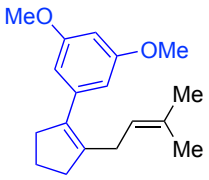
Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and ethyl 4-(((trifluoromethyl)sulfonyl)oxy)cyclohex-3-enecarboxylate (151 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (100 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.78-5.70 (m, 1H), 5.13-5.08 (m, 1H), 4.12 (q, J = 6.8 Hz, 2H), 2.60 (d, J = 7.2 Hz, 2H), 2.49-2.43 (m, 1H), 2.23-2.20 (m, 2H), 2.02-1,96 (m, 3H), 1.72-1.64 (m, 4H), 1.60 (s, 3H), 1.24 (t, J = 6.8 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 176.1, 137.1, 132.8, 122.1, 118.9, 60.3, 39.6, 36.2, 27.9, 27.8, 25.9, 25.7, 17.8, 14.4 ppm. IR (neat, cm^{-1}): 2925, 1733, 1376, 1222, 1164, 1032. Anal. Calcd. for $C_{14}H_{22}O_2$: C, 75.63; H, 9.97. Found: C, 75.92; H, 9.95. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

3-(3-Methylbut-2-en-1-yl)-1,2-dihydronaphthalene (8d)



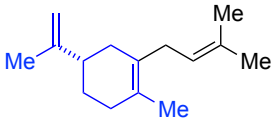
Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and 3,4-dihydronaphthalen-2-yl trifluoromethanesulfonate (139 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (94 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.17-7.15 (m, 1H), 7.14-7.09 (m, 2H), 7.01 (d, J = 7.2 Hz, 1H), 6.24 (s, 1H), 5.30-5.27 (m, 1H), 2.91 (d, J = 7.2 Hz, 2H), 2.84 (t, J = 8.0 Hz, 2H), 2.71 (t, J = 8.0 Hz, 2H), 1.80 (d, J = 0.8 Hz, 3H), 1.71 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.6, 135.2, 134.5, 133.6, 127.2, 126.5, 126.1, 125.5, 122.1, 121.3, 36.1, 28.3, 27.6, 26.0, 17.9 ppm. IR (neat, cm^{-1}): 2925, 2882, 1485, 1451, 839, 753, 745. Anal. Calcd. for $C_{15}H_{18}$: C, 90.85; H, 9.15. Found: C, 91.02; H, 9.24. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

1,3-Dimethoxy-5-(2-(3-methylbut-2-en-1-yl)cyclopent-1-en-1-yl)benzene (8e)



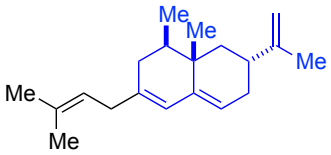
Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and 2-(3,5-dimethoxyphenyl)cyclopent-1-en-1-yl trifluoromethanesulfonate (176 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (125 mg, 92%). ^{1}H NMR (600 MHz, $CDCl_3$) δ: 6.452 (s, 2H), 6.448 (s, 2H), 5.20-5.17 (m, 1H), 3.80(s, 6H), 2.95 (d, J = 7.2 Hz, 2H), 2.73 (t, J = 7.2 Hz, 2H), 2.50 (t, J = 7.2 Hz, 2H), 1.92-1.87 (m, 1H), 1.73 (d, J = 0.6 Hz, 3H), 1.64 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.5, 140.9, 139.2, 135.2, 132.5, 122.0, 105.9, 98.5, 55.3, 37.7, 37.3, 28.7, 25.9, 22.0, 18.0 ppm. IR (neat, cm^{-1}): 2837, 1419, 1203, 1151, 1065, 829. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{18}H_{24}O_2$, 273.1849; found, 273.1853. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

(*S*)-1-Methyl-2-(3-methylbut-2-en-1-yl)-4-(prop-1-en-2-yl)cyclohex-1-ene (8f)



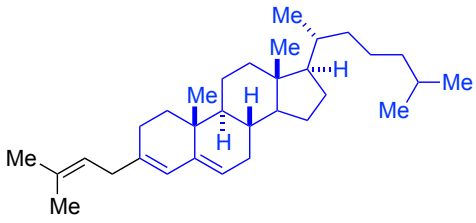
Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and (*S*)-2-methyl-5-(prop-1-en-2-yl)cyclohex-1-en-1-yl trifluoromethanesulfonate (142 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (92 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.83-5.76 (m, 1H), 4.71 (m, 2H), 2.72-2.68 (m, 2H), 2.16-1.90 (m, 6H), 1.74 (s, 3H), 1.71 (s, 3H), 1.67 (s, 3H), 1.65 (s, 3H), 1.47-1.37 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.5, 131.5, 129.2, 125.6, 122.9, 108.4, 42.1, 35.1, 32.5, 32.4, 28.3, 25.9, 21.0, 18.8, 17.9 ppm. IR (neat, cm^{-1}): 2967, 2917, 2831, 1644, 1436, 885. Anal. Calcd. for $C_{15}H_{24}$: C, 88.16; H, 11.84. Found: C, 88.33; H, 11.88. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

(2*R*,8*R*,8a*S*)-8,8a-Dimethyl-6-(3-methylbut-2-en-1-yl)-2-(prop-1-en-2-yl)-1,2,3,7,8,8a-hexahydronaphthalene (8g)



Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and (4*R*,4a*S*,6*R*)-4,4a-dimethyl-6-(prop-1-en-2-yl)-3,4,4a,5,6,7-hexahydronaphthalen-2-yl trifluoromethanesulfonate (175 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (128 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.75 (s, 1H), 5.38-5.36 (m, 1H), 5.19-5.15 (m, 1H), 4.76-4.75 (m, 2H), 2.46 (d, *J* = 7.2 Hz, 2H), 2.46-2.40 (m, 1H), 2.22 (ddd, *J* = 18.4, 5.2, 5.2 Hz, 1H), 2.01-1.96 (m, 1H), 1.92-1.89 (m, 2H), 1.77 (s, 3H), 1.74 (s, 3H), 1.741-1.740 (m, 1H), 1.64 (s, 3H), 1.56-1.51 (m, 1H), 1.18 (t, *J* = 12.4 Hz, 1H), 0.91-0.90 (m, 6H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.5, 142.6, 137.3, 132.8, 123.5, 122.0, 121.0, 108.7, 40.4, 39.3, 36.1, 36.0, 35.9, 35.8, 31.3, 25.9, 20.8, 17.9, 17.6, 14.9 ppm. IR (neat, cm^{-1}): 2966, 2909, 2827, 1441, 1373, 885. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{20}H_{30}$, 271.2420; found, 271.2432. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

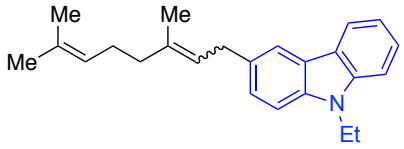
(8*S*,9*S*,10*R*,13*R*,17*R*)-10,13-dimethyl-3-(3-methylbut-2-en-1-yl)-17-((*R*)-6-methylheptan-2-yl)-2,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene (8h)



Following the general procedure, a THF solution of prenylzinc bromide (0.65 mmol, 0.80 mL, 0.81 M) and (8*S*,9*S*,10*R*,13*R*,17*R*)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl trifluoromethanesulfonate (258 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 2 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; hexanes) to provide the title compound as a colorless oil (187 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 5.71 (s, 1H), 5.33-5.32 (m, 1H), 5.19-5.15 (m, 1H), 2.70 (d, *J* = 7.2 Hz, 2H), 2.13-2.08 (m, 2H), 2.01-1.83 (m, 2H),

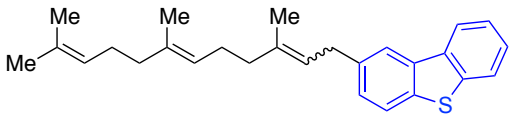
1.88-1.75 (m, 1H), 1.72 (d, J = 0.8 Hz, 3H), 1.63-1.02 (m, 24H), 0.94-0.92 (m, 6H), 0.88 (d, J = 1.6 Hz, 3H), 0.87 (d, J = 2.0 Hz, 3H), 0.71 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 142.1, 136.5, 132.8, 123.9, 122.1, 121.5, 57.2, 56.3, 48.6, 42.6, 40.0, 39.7, 36.4, 36.1, 36.0, 35.1, 34.4, 32.02, 31.96, 28.4, 28.2, 26.5, 25.9, 24.4, 24.0, 23.0, 22.7, 21.3, 19.1, 18.9, 17.9, 12.1 ppm. IR (neat, cm^{-1}): 2931, 2868, 1467, 1443, 1375, 892. HRMS-ESI (*m/z*) $[M + H]^+$ calcd for $C_{32}H_{53}$, 437.4142; found, 437.4160. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture.

3-(3,7-Dimethylocta-2,6-dien-1-yl)-9-ethyl-9H-carbazole (9a)



Following the general procedure, a THF solution of geranylzinc bromide (0.65 mmol, 1.20 mL, 0.56 M) and 3-bromo-9-ethyl-9*H*-carbazole (137 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-3% EtOAc/hexanes) to provide the title compound as a colorless oil (154 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) of the major stereoisomer δ: 8.17 (d, J = 7.6 Hz, 1H), 8.00 (s, 1H), 7.53 (ddd, J = 7.6, 7.2, 1.2 Hz, 1H), 7.44 (d, J = 8.4 Hz, 1H), 7.39-7.38 (m, 2H), 7.29 (ddd, J = 7.6, 7.2, 5.59-5.54 (m, 1H), 5.31-5.29 (m, 1H), 4.38 (q, J = 7.2 Hz, 2H), 3.65 (d, J = 7.2 Hz, 2H), 2.37-2.30 (m, 2H), 2.27-2.18 (m, 2H), 1.89 (s, 3H), 1.80 (d, J = 0.8 Hz, 3H), 1.76 (s, 3H), 1.48 (t, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.3, 138.6, 135.7, 135.6, 132.3, 131.8, 126.4, 125.5, 124.5, 124.4, 123.2, 123.0, 120.5, 119.9, 118.6, 108.5, 39.9, 37.6, 34.4, 32.2, 26.9, 25.9, 16.4, 13.9 ppm. IR (neat, cm^{-1}): 2913, 1484, 1470, 1324, 1230, 744. Anal. Calcd. for $C_{24}H_{29}N$: C, 86.96; H, 8.82. Found: C, 86.69; H, 8.92. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture. The *E*/*Z* ratio was determined to be 75:25 by ^{1}H NMR and GC analysis of the crude reaction mixture.

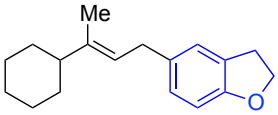
2-((6*E*)-3,7,11-Trimethyldodeca-2,6,10-trien-1-yl)dibenzo[b,d]thiophene (9b)



Following the general procedure, a THF solution of farnesylzinc bromide (0.65 mmol, 1.50 mL, 0.43 M) and 2-

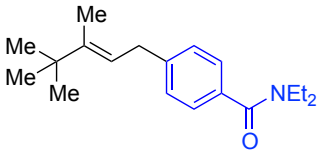
bromodibenzo[b,d]thiophene (131 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-3% EtOAc/hexanes) to provide the title compound as a colorless oil (173 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) of the major stereoisomer δ: 8.22-8.19 (m, 1H), 8.15 (d, *J* = 1.6 Hz, 1H), 7.88-7.86 (m, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.50-7.44 (m, 3H), 6.18 (dd, *J* = 17.2, 10.4 Hz, 1H), 5.23 (m, 4H), 2.10-2.06 (m, 2H), 2.02-1.95 (m, 2H), 1.91-1.87 (m, 2H), 1.72 (s, 3H), 1.64 (s, 3H), 1.56 (s, 3H), 1.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.1, 144.1, 140.0, 137.0, 135.9, 135.6, 135.1, 131.4, 126.2, 126.5, 124.6, 124.5, 124.3, 123.0, 122.5, 121.6, 119.5, 112.2, 44.6, 41.4, 39.8, 26.8, 25.9, 25.5, 23.4, 17.8, 16.1. Spectral data were in accordance with those in literature.[2] The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture. The *E*/*Z* ratio was determined to be 75:25 by GC analysis of the crude reaction mixture.

(*E*)-5-(3-Cyclohexylbut-2-en-1-yl)-2,3-dihydrobenzofuran (9c)



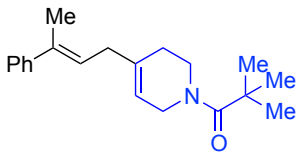
Following the general procedure, a THF solution of 3-methyl-3-cyclohexylallylzinc bromide (0.65 mmol, 2.50 mL, 0.26 M) and 5-bromo-2,3-dihydrobenzofuran (100 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-5% EtOAc/hexanes) to provide the title compound as a yellowish oil (118 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) of the major stereoisomer δ: 7.03 (s, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.35-5.33 (m, 1H), 4.56 (t, *J* = 8.4 Hz, 2H), 3.31 (d, *J* = 7.2 Hz, 2H), 3.20 (t, *J* = 8.4 Hz, 2H), 1.91-1.81 (m, 1H), 1.77-1.69 (m, 8H), 1.45-1.18 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.3, 141.3, 134.0, 127.8, 127.0, 124.9, 123.4, 121.8, 71.2, 47.5, 33.5, 32.1, 30.0, 26.9, 26.5, 14.6. IR (neat, cm^{-1}): 2921, 2850, 1490, 1242, 985, 812. Anal. Calcd. for $C_{18}H_{24}O$: C, 84.32; H, 9.44. Found: C, 84.03; H, 9.71. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture. The *E*/*Z* ratio was determined to be 84:16 by ^{1}H NMR and GC analysis of the crude reaction mixture.

(*E*)-*N*,*N*-diethyl-4-(3,4,4-trimethylpent-2-en-1-yl)benzamide (9d)



Following the general procedure, a THF solution of 3-methyl-3-*tert*-butylallylzinc bromide (0.65 mmol, 2.50 mL, 0.26 M) and 4-bromo-N,N-diethylbenzamide (143 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-30% EtOAc/hexanes) to provide the title compound as a colorless oil (118 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 8.4 Hz, 2H), 5.37-5.34 (m, 1H), 3.50 (broad, 2H), 3.33 (d, J = 7.2 Hz, 2H), 3.26 (broad, 2H), 1.67 (s, 3H), 1.23-1.10 (broad, 6H), 1.03 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.5, 144.8, 143.2, 134.7, 128.3, 126.4, 119.1, 43.3 (broad), 39.2 (broad), 36.2, 24.2, 29.1, 14.2 (broad), 13.0. IR (neat, cm^{-1}): 2964, 1630, 1422, 1284, 1093, 832. Anal. Calcd. for $C_{19}H_{29}NO$: C, 79.39; H, 10.17. Found: C, 79.16; H, 10.17. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture. The *E*/*Z* ratio was determined to be >99:1 by ^{1}H NMR and GC analysis of the crude reaction mixture.

(*E*)-2,2-Dimethyl-1-(4-(3-phenylbut-2-en-1-yl)-5,6-dihydropyridin-1(2H)-yl)propan-1-one (9e)

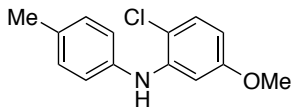


Following the general procedure, a THF solution of 3-methyl-3-phenylallylzinc phosphate (0.65 mmol, 2.00 mL, 0.33 M) and1-pivaloyl-1,2,3,6-tetrahydropyridin-4-yl trifluoromethanesulfonate (158 mg, 0.5 mmol) were used. The reaction mixture was allowed to stir at room temperature for 12 h. The crude product was purified via Biotage SP4 (silica-packed 25 g SNAP cartridge; 0-30% EtOAc/hexanes) to provide the title compound as a colorless oil (111 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31-7.29 (m, 2H), 7.26-7.23 (m, 2H), 7.23-7.21 (m, 1H), 5.78 (td, J = 7.2, 1.6 Hz, 1H), 5.46-5.45 (m, 1H), 4.05 (d, J = 2.8 Hz, 2H), 3.69 (t, J = 6.0 Hz, 2H), 2.89 (d, J = 7.2 Hz, 2H), 2.13 (s, 2H), 2.04 (d, J = 0.4 Hz, 3H), 1.29 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 176.6, 143.6, 136.8, 135.7, 128.3, 126.9, 125.7, 124.7, 118.6, 44.8, 42.7, 38.8, 36.1, 29.0, 28.3, 15.9. IR (neat, cm^{-1}): 2972, 1625, 1416, 1175, 758, 697. HRMS-ESI (*m/z*) $[M + H]^+$ calcd

for $C_{20}H_{27}NO$, 298.2165; found, 298.2171. The α/γ ratio was determined to be >99:1 by ^{1}H NMR spectroscopy of the crude reaction mixture. The *E*/*Z* ratio was determined to be >99:1 by ^{1}H NMR and GC analysis of the crude reaction mixture.

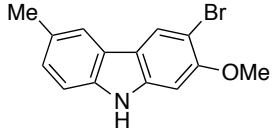
Synthesis of Siamenol

2-Chloro-5-methoxy-*N*-(p-tolyl)aniline (12)



An oven-dried screw-cap test tube, which was equipped with a magnetic stir bar and fitted with a teflon septum, was charged with BrettPhos Precat (45 mg, 0.05 mmol, 1 mol%) and BrettPhos (27 mg, 0.05 mmol, 1 mol%), 4-bromotoluene (855 mg, 5 mmol, 1 equiv), 2-chloro-4-methoxyaniline (830 mg, 5.25 mmol, 1.05 equiv) and sodium *tert*-butoxide (576 mg, 6 mmol, 1,2 equiv). The test tube was evacuated and backfilled with argon (this process was repeated a total of three times). Dioxane (5 mL, 1.0 M) was added and the reaction mixture was heated at 80 °C for 1 h and then cooled to room temperature. The reaction mixture was allowed to pass through a silica plug eluting with EtOAc (30-50 mL), concentrated in vacuo, and purified via Biotage Isolera (0-10% EtOAc/hexanes, 50 g SNAP cartridge) to afford the title compound as a colorless oil (1.11 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (s, 1H), 7.25 (d, *J* = 5.6 Hz, 1H), 7.18 (d, *J* = 5.2 Hz, 2H), 7.12 (d, *J* = 5.2 Hz, 2H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.35 (dd, *J* = 5.6, 2.0 Hz, 1H), 6.05 (s, 1H), 3.74 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.8, 143.9, 137.3, 131.1, 130.24, 130.22, 128.2, 122.6, 117.6, 111/4, 107.2, 104.6, 55.4, 20.5. IR (neat, cm^{-1}): 3401, 1594, 1490, 1156, 1048, 687. Anal. Calcd. for $C_{14}H_{14}ClNO$: C, 67.88; H, 5.70. Found: C, 67.91; H, 5.69.

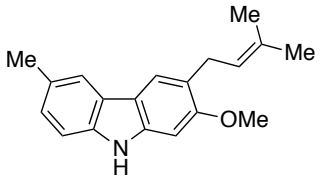
3-Bromo-2-methoxy-6-methyl-9*H*-carbazole (13)



An oven-dried screw-cap test tube, which was equipped with a magnetic stir bar and fitted with a teflon septum, was charged with 2-chloro-5-methoxy-*N*-(p-tolyl)aniline (99 mg, 0.40 mmol), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol), XPhos (19 mg, 0.04 mmol), pivalic acid (40 mg, 0.40 mmol) and K_3PO_4 (170 mg, 0.8 mmol). The test tube was evacuated and backfilled with

argon (this process was repeated a total of three times). DMA (2 mL, 0.2 M) was added and the reaction mixture was heated at 180 °C for 12 h and then cooled to room temperature. The reaction mixture was washed with water and the combined aqueous layers were extracted with EtOAc. The Combined organic phases were dried over $MgSO_4$, concentrated in vacuo and purified via Biotage Isolera (0-30% EtOAc/hexanes, 50 g SNAP cartridge) to afford the carbazole as a pale brown solid (70 mg, 83%). To the carbazole (40 mg, 0.19 mmol) was added NBS (35 mg, 0.20 mmol, 1.05 equiv) and carbon tetrachloride (2.5 mL). The reaction mixture was heated at 70 °C until the reaction went to completion as indicated by TLC (ca. 30 min). The reaction mixture was washed by water, and the aqueous phase was extracted with EtOAc. Combined organic phases were dried over $MgSO_4$, concentrated in vacuo and purified via Biotage Isolera (0-30% EtOAc/hexanes, 25 g SNAP cartridge) to afforded the brominated carbazole as an off-white solid (55 mg, 99%). ^{1}H NMR (400 MHz, acetone) δ: 10.17 (s, 1H), 8.23 (s, 1H), 7.83 (d, J = 0.8 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.17-7.15 (m, 2H), 3.93 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, acetone) δ: 155.7, 142.0, 139.8, 129.6, 127.5, 125.4, 123.9, 120.7, 118.9, 111.8, 103.6, 95.9, 57.1, 21.9. Spectral data were in accordance with those in literature.[9]

2-Methoxy-6-methyl-3-(3-methylbut-2-en-1-yl)-9*H*-carbazole (15)

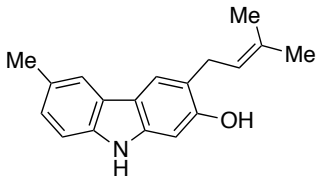


An oven-dried screw-cap test tube, which was equipped with a magnetic stir bar and fitted with a teflon septum, was charged with CPhos Precat (3.1 mg, 0.0038 mmol) and CPhos (1.7 mg, 0.0038 mmol) and 3-bromo-2-methoxy-6-methyl-9*H*-carbazole (55 mg, 0.19 mmol). The test tube was evacuated and backfilled with argon (this process was repeated a total of three times). THF (0.2 mL) was added. A THF solution of prenylzinc bromide (0.56 mL, 0.78 M, 0.44 mmol) was then added dropwise, and the reaction mixture was allowed to stir at room temperature for 2 h and then quenched by water and extracted with EtOAc. The combined organic phases were dried over $MgSO_4$, concentrated in vacuo, and purified via Biotage Isolera (0-25% EtOAc/hexanes, 25 g SNAP cartridge) to afford the title compound as a white solid (51

[9] W. Kong, C. Fu, S. Ma, *Chem. Eur. J.* **2011**, *17*, 13134-13137.

mg, 96%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80-7.77 (m, 2H), 7.46 (s, 1H), 7.15-7.13 (m, 2H), 6.60 (s, 1H), 5.47-5.43 (m, 1H), 3.82 (s, 3H), 2.54 (s, 3H), 3.48 (d, *J* = 7.2 Hz, 2H), 1.809 (s, 3H), 1.807 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 157.0, 139.6, 137.7, 132.2, 128.6, 125.5, 123.8, 123.5, 122.7, 120.4, 119.5, 116.2, 110.1, 92.8, 55.6, 29.0, 26.0, 21.6, 17.9. Spectral data were in accordance with those in literature.[9]

6-Methyl-3-(3-methylbut-2-enyl)-9*H*-carbazol-2-ol (16)



To an oven-dried test tube was added 2-methoxy-6-methyl-3-(3-methylbut-2-en-1-yl)-9*H*-carbazole (10 mg, 0.036 mmol). The test tube was evacuated and backfilled with argon (this process was repeated a total of three times). MeMgI (0.073 mL, 3 M in Et_2O, 0.22 mmol, 6.0 equiv) was added, and the solvent was removed under vacuum. The reaction mixture was heated at 180 °C for 10 min, during which time white smoke evaporated and vanished. The reaction mixture was then cooled to 0 °C, carefully diluted with Et_2O and quenched with water. The aqueous layer was extracted with Et_2O for 3 times and combined organic layers were dried over $MgSO_4$, concentrated in vacuo, and purified by column chromatography (2:1 hexanes/EtOAc) to afford the title compound as a white solid (6.1 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75 (s, 1H), 7.72 (s, 1H), 7.70 (broad, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.14 (dd, *J* = 8.0, 1.2 Hz, 1H, ArH), 6.81 (s, 1H), 5.43-5.39 (m, 1H, CH), 5.29 (s, 1H), 3.51 (d, *J* = 7.2 Hz, 2H), 2.51 (s, 3H), 1.85 (s, 3H), 1.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.6, 140.0, 137.9, 134.9, 128.7, 125.8, 123.8, 122.8, 120.9, 119.6, 117.9, 110.1, 97.4, 30.6, 26.0, 21.6, 18.1. Spectral data were in accordance with those in literature.[9]

Computed Reaction Coordinate

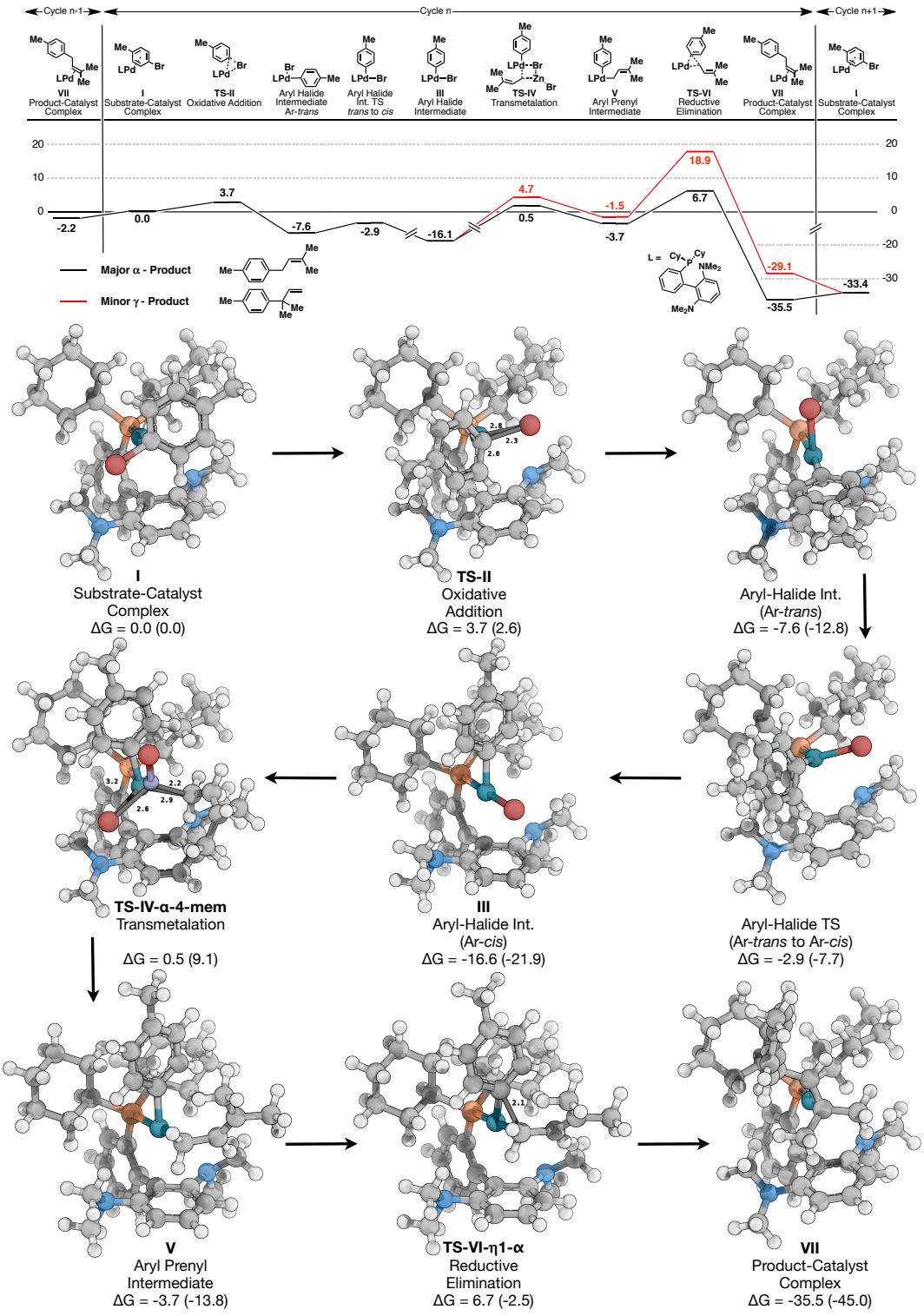
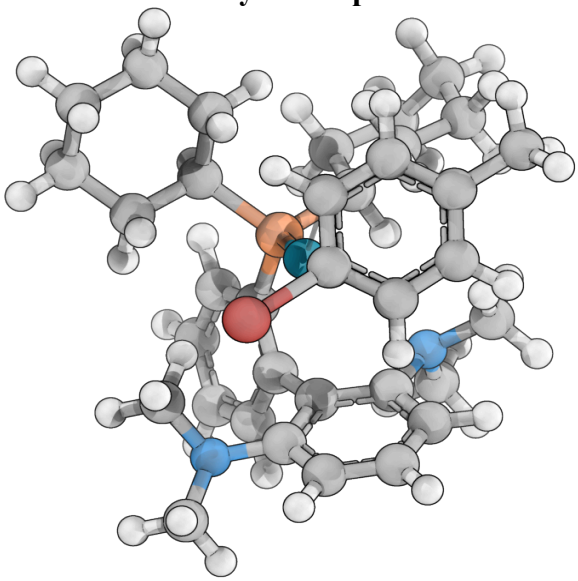


Figure S1. Reaction coordinate of Pd(0)-catalyzed cross-coupling of prenylZnBr with p-bromotoluene (above) and all structures (below).[10] All energies are displayed in kcal/mol,

[10] (a) The B3LYP hybrid functional with the 6-31G* (for H, C, N, and P) and LANL2DZ+ECP (for Zn, Br and Pd) basis sets were used. (b) M. J. Frisch,; et al. Gaussian, Inc.: Pittsburgh, PA, 2004. (c) The B3LYP hybrid functional and PCM solvation model with tetrahydrofuran with the 6-31++G(d,p) (for H, C, N, and

solvation energies in parentheses and distances in Å. Computed structures are rendered in Pymol.[11]

I Substrate-Catalyst Complex:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

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freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

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Pointgroup= C1 Stoichiometry= C35H48BrN2PPd C1[X(C35H48BrN2PPd)]
#Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.40661501 Predicted Change= -3.929247D-08

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Optimization completed on the basis of negligible forces. {Found 2 times}

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Displ	0.02082	0.00180	[NO]	0.02082	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.886710	4.287479	-0.122124

P) and LANL2DZ+ECP (for Zn, Br and Pd) basis sets were used. (d) M. J. Frisch,; et al. Gaussian, Inc.: Wallingford, CT, 2010.

[11] *The PyMOL Molecular Graphics System, version 1.3*; Schrödinger, LLC.

H	3.226395	5.315168	-0.220653
C	3.681545	3.331744	0.508026
H	4.655657	3.596789	0.910798
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H	3.838730	1.308253	1.142633
C	1.958247	1.620879	0.125078
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Pd	-0.875674	-0.678074	0.332087
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C	2.142344	-0.555551	2.089547
H	3.230222	-0.407380	2.056081
C	1.157052	2.594077	-0.526883
C	-0.196995	2.377091	-1.147885
C	1.644637	3.913174	-0.623094
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C	-3.217759	-1.295558	-1.026242
H	-3.659298	-0.371464	-1.380893
C	-3.005228	-2.366006	-1.889232
H	-3.266662	-2.252137	-2.939325

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

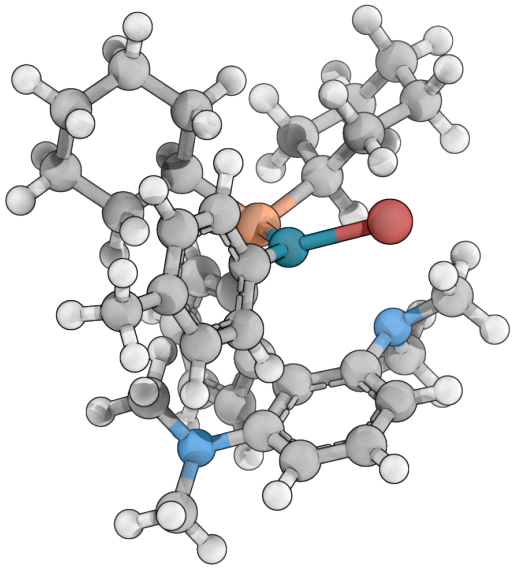
SCF Energy= -1953.40661501 Predicted Change= -3.929247D-08

Zero-point correction (ZPE)= -1952.6449 0.76168
Internal Energy (U)= -1952.6017 0.80486
Enthalpy (H)= -1952.6008 0.80580
Gibbs Free Energy (G)= -1952.7257 0.68081

Frequencies -- 7.0878 18.4940 26.8622

$\Delta G_{Solvation}$ = -0.00751849000016591

TS-II Oxidative Addition:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd C1[X(C35H48BrN2PPd)]
#Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.40310422 Predicted Change= -7.374393D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00891	0.00180	[NO]	0.00891	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.789941	3.643699	2.346027

H	3.124070	4.583172	2.778322
C	3.386627	2.438614	2.712662
H	4.195694	2.416581	3.438031
C	2.931809	1.253025	2.142739
H	3.398303	0.327489	2.459712
C	1.887650	1.216382	1.195114
P	1.351996	-0.440614	0.517472
Pd	-0.831836	-0.743594	-0.401288
C	1.551877	-1.588615	2.008900
H	2.594874	-1.554295	2.351247
C	2.783146	-0.867471	-0.656953
H	2.891612	0.079418	-1.202053
C	1.279947	2.444572	0.826707
C	0.146944	2.637007	-0.144711
C	1.750948	3.632599	1.422574
H	1.273764	4.566492	1.142993
C	-1.089479	3.153113	0.337033
N	-1.272975	3.358873	1.734898
C	-1.406944	2.152443	2.548859
H	-2.399101	1.680721	2.432545
H	-1.266734	2.410664	3.605187
H	-0.651285	1.419622	2.271107
C	-2.233501	4.377298	2.128216
H	-2.080281	5.286817	1.540396
H	-2.071669	4.618784	3.185225
H	-3.289333	4.065588	2.020297
C	-2.105555	3.492295	-0.568903
H	-3.051896	3.871995	-0.200127
C	-1.916807	3.327185	-1.937287
H	-2.710144	3.594340	-2.631109
C	-0.713271	2.830269	-2.421894
H	-0.573561	2.726305	-3.491132
C	0.331163	2.497522	-1.543282
N	1.592550	2.057505	-2.060401
C	1.543946	1.406760	-3.366785
H	1.386074	2.108849	-4.205415
H	0.750015	0.656066	-3.380914
H	2.502131	0.904808	-3.540944
C	2.648219	3.074099	-2.026663
H	2.464257	3.889427	-2.749564
H	3.605606	2.603856	-2.279183
H	2.735708	3.506532	-1.029435
C	0.644978	-1.142963	3.176737
H	-0.397749	-1.126341	2.827685
H	0.892230	-0.120789	3.483536
C	0.758581	-2.086692	4.386006

H	0.079997	-1.749774	5.180406
H	1.776509	-2.026723	4.799771
C	0.452650	-3.540235	4.000903
H	-0.602824	-3.620655	3.701834
H	0.585299	-4.202351	4.866228
C	1.343776	-3.996005	2.838068
H	1.080886	-5.016571	2.530943
H	2.390262	-4.032726	3.176414
C	1.235318	-3.051846	1.627600
H	0.218192	-3.098081	1.212315
H	1.909837	-3.400621	0.838520
C	4.137980	-1.208052	-0.006169
H	4.048709	-2.130335	0.585443
H	4.446168	-0.413942	0.681750
C	5.234276	-1.408510	-1.068973
H	6.180100	-1.675202	-0.579235
H	5.408922	-0.453988	-1.587201
C	4.841496	-2.478354	-2.097290
H	4.777140	-3.455816	-1.595971
H	5.619526	-2.572535	-2.865920
C	3.487235	-2.150417	-2.741848
H	3.190786	-2.946071	-3.437269
H	3.586569	-1.233695	-3.341773
C	2.386161	-1.949277	-1.686316
H	2.210129	-2.906327	-1.177604
H	1.439462	-1.680669	-2.166831
C	-3.538071	-0.027833	-0.755461
H	-3.283600	0.862682	-1.319032
C	-2.764592	-1.193794	-0.882961
C	-3.124790	-2.377481	-0.214971
H	-2.566640	-3.292229	-0.383010
C	-4.219650	-2.353102	0.651871
H	-4.489502	-3.261471	1.186933
C	-4.987928	-1.193303	0.830107
C	-6.204711	-1.199565	1.726342
H	-7.117248	-1.434942	1.161544
H	-6.360599	-0.223052	2.198204
H	-6.113819	-1.947757	2.521118
C	-4.623747	-0.037566	0.121810
H	-5.206882	0.872731	0.247699
Br	-1.786749	-1.512311	-2.906652

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

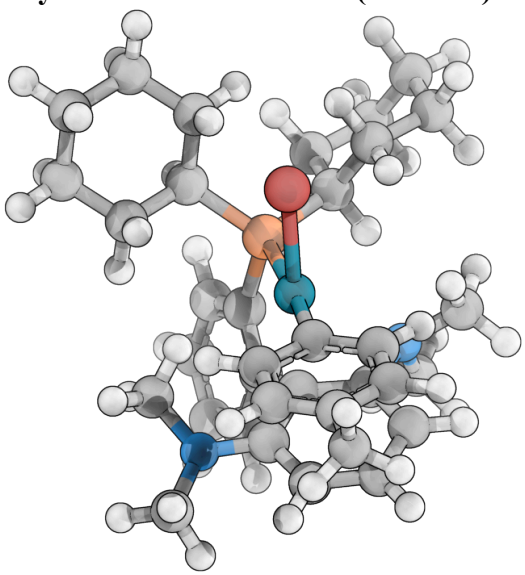
==========

SCF Energy= -1953.40310422 Predicted Change= -7.374393D-09

Zero-point correction (ZPE)= -1952.6410 0.76202
Internal Energy (U)= -1952.5987 0.80433
Enthalpy (H)= -1952.5978 0.80528
Gibbs Free Energy (G)= -1952.7199 0.68314

Frequencies -- -94.7250 8.1236 19.9197
$\Delta G_{Solvation}$ = -0.00927111999999397

Aryl Halide Intermediate (Ar-*trans*):



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd C1[X(C35H48BrN2PPd)]
#Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.42433037 Predicted Change= -5.019004D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.02019	0.00180	[NO]	0.02019	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.350420	4.305700	1.959891
H	1.244931	5.300398	2.384825

C	2.572394	3.635655	2.020078
H	3.433040	4.096696	2.497062
C	2.679226	2.361160	1.467593
H	3.629833	1.842973	1.539727
C	1.586927	1.727935	0.848309
P	1.685032	0.012614	0.160658
Pd	-0.696419	-0.550017	-0.194593
C	2.810167	0.175077	-1.350065
H	2.372838	1.052463	-1.842350
C	2.688996	-0.900662	1.474587
H	3.601676	-0.310393	1.644194
C	0.347517	2.402591	0.792194
C	-0.921893	1.887204	0.133523
C	0.258345	3.692169	1.351290
H	-0.691783	4.216582	1.306715
C	-1.047157	2.031381	-1.301322
N	0.140932	2.156029	-2.100193
C	0.063377	1.501865	-3.406163
H	1.069037	1.466214	-3.838876
H	-0.297618	0.477755	-3.283066
H	-0.585623	2.025099	-4.129939
C	0.601982	3.542543	-2.240441
H	-0.086582	4.152209	-2.852242
H	0.704356	4.011821	-1.260992
H	1.584603	3.542988	-2.725725
C	-2.300867	2.155664	-1.899558
H	-2.380464	2.251275	-2.976150
C	-3.450221	2.207251	-1.113733
H	-4.421290	2.315872	-1.588693
C	-3.381884	2.097637	0.264400
H	-4.300795	2.086478	0.835076
C	-2.145557	1.923434	0.917978
N	-2.112665	1.846759	2.299040
C	-1.119821	1.043547	3.003834
H	-1.617335	0.473001	3.796483
H	-0.664303	0.325554	2.316566
H	-0.328119	1.653244	3.456490
C	-3.299648	2.175350	3.076112
H	-3.762645	3.093011	2.702727
H	-4.052611	1.371893	3.067481
H	-2.998198	2.352577	4.112255
C	2.647360	-1.025245	-2.311960
H	3.003376	-1.945658	-1.834241
H	1.587281	-1.193553	-2.526515
C	3.433919	-0.807544	-3.615995
H	3.331620	-1.691270	-4.258335

H	2.994928	0.034557	-4.172221
C	4.915321	-0.510086	-3.344471
H	5.386329	-1.395739	-2.892917
H	5.447025	-0.319105	-4.285487
C	5.071652	0.684927	-2.394216
H	6.131962	0.865083	-2.173911
H	4.696640	1.593444	-2.888653
C	4.298647	0.473844	-1.078396
H	4.757847	-0.358760	-0.528754
H	4.403685	1.366893	-0.452651
C	3.118925	-2.319703	1.039801
H	2.227782	-2.908227	0.792854
H	3.728027	-2.275174	0.131214
C	3.922550	-3.024881	2.146950
H	4.185403	-4.037327	1.815304
H	4.872445	-2.491686	2.307412
C	3.146420	-3.081134	3.469282
H	2.254197	-3.709784	3.338650
H	3.755245	-3.554172	4.250576
C	2.715200	-1.675165	3.906614
H	2.116819	-1.724704	4.825632
H	3.608234	-1.078383	4.146831
C	1.909688	-0.964194	2.806261
H	0.969210	-1.506593	2.638941
H	1.647450	0.046579	3.139256
C	-3.412028	-1.324021	0.780203
H	-2.939002	-1.336077	1.759443
C	-2.662493	-1.034914	-0.364879
C	-3.297451	-1.080204	-1.608474
H	-2.735261	-0.903453	-2.521690
C	-4.665886	-1.359093	-1.698145
H	-5.140818	-1.387317	-2.678098
C	-5.430938	-1.621416	-0.555802
C	-6.899601	-1.967450	-0.660130
H	-7.457098	-1.630677	0.221633
H	-7.359216	-1.509808	-1.543541
H	-7.052277	-3.052411	-0.742371
C	-4.779833	-1.598337	0.684847
H	-5.346925	-1.810545	1.590570
Br	-0.340242	-3.062202	-0.476314

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

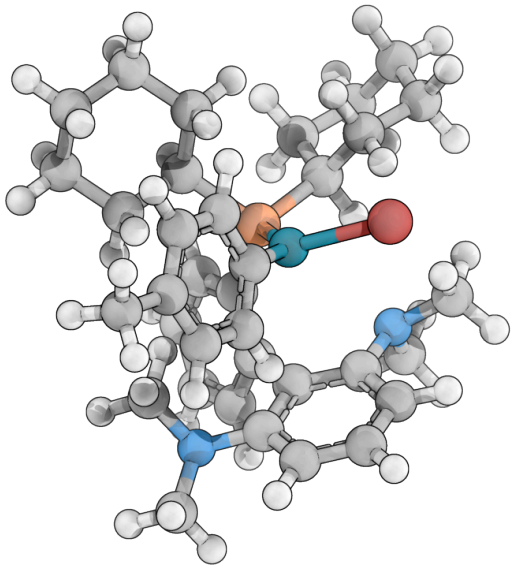
==========

SCF Energy= -1953.42433037 Predicted Change= -5.019004D-07
Zero-point correction (ZPE)= -1952.6610 0.76330

Internal Energy (U)= -1952.6182 0.80603
Enthalpy (H)= -1952.6173 0.80698
Gibbs Free Energy (G)= -1952.7379 0.68641

Frequencies -- 18.1927 27.7029 33.3282
$\Delta G_{Solvation}$ = -0.0157666000000063

Ar-*trans* to Ar-*cis* TS:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd C1[X(C35H48BrN2PPd)]
#Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.41397203 Predicted Change= -1.743349D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00363	0.00180	[NO]	0.00363	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.852907	3.465340	2.607518

H	3.208610	4.376642	3.080801
C	3.306954	2.218441	3.034848
H	4.021748	2.136205	3.849280
C	2.830623	1.070044	2.409278
H	3.182449	0.110686	2.771219
C	1.904950	1.116183	1.346425
P	1.325960	-0.491259	0.601483
Pd	-0.892323	-0.675418	-0.702558
C	2.844526	-1.093070	-0.368020
H	3.134943	-0.171829	-0.889012
C	1.171643	-1.628459	2.104819
H	2.142902	-1.673200	2.615709
C	1.438342	2.386181	0.917417
C	0.438718	2.648290	-0.174721
C	1.929270	3.535049	1.570678
H	1.562682	4.502556	1.243909
C	0.751703	2.430983	-1.541367
N	2.015292	1.862993	-1.903270
C	2.059910	1.200336	-3.205698
H	2.982870	0.613133	-3.264183
H	1.208889	0.523889	-3.314759
H	2.067320	1.905584	-4.055783
C	3.154557	2.775267	-1.753624
H	3.138590	3.583257	-2.506584
H	3.163560	3.225745	-0.760882
H	4.084871	2.209730	-1.880201
C	-0.170253	2.797253	-2.535161
H	0.061919	2.626748	-3.578921
C	-1.376201	3.397352	-2.196275
H	-2.077456	3.678295	-2.977543
C	-1.686312	3.644186	-0.863111
H	-2.632587	4.109675	-0.610880
C	-0.793733	3.279198	0.156628
N	-1.100760	3.570133	1.518375
C	-1.414651	2.420253	2.364002
H	-2.409745	1.996057	2.141423
H	-0.671564	1.635594	2.229446
H	-1.397006	2.729371	3.415633
C	-2.015014	4.675816	1.760955
H	-1.729769	5.539251	1.153428
H	-3.074697	4.437558	1.553122
H	-1.945305	4.959133	2.817565
C	2.467626	-2.136440	-1.444146
H	2.107726	-3.056933	-0.966138
H	1.639035	-1.769900	-2.058762
C	3.674460	-2.482884	-2.332979

H	3.382922	-3.247421	-3.063808
H	3.965700	-1.593936	-2.912073
C	4.875656	-2.959629	-1.505246
H	4.626340	-3.914832	-1.019433
H	5.736757	-3.156364	-2.156675
C	5.246488	-1.926948	-0.431906
H	6.074896	-2.294861	0.187460
H	5.605364	-1.009124	-0.920704
C	4.045705	-1.577807	0.467710
H	3.765118	-2.469857	1.045132
H	4.349120	-0.811248	1.188219
C	0.797995	-3.067433	1.682183
H	-0.129305	-3.042467	1.091992
H	1.568209	-3.488898	1.028244
C	0.605077	-3.990368	2.898741
H	0.308664	-4.989332	2.554484
H	1.567583	-4.112335	3.418018
C	-0.431831	-3.430730	3.880817
H	-1.419854	-3.416822	3.397801
H	-0.519557	-4.085511	4.757107
C	-0.059694	-2.006407	4.312554
H	-0.829947	-1.592294	4.975626
H	0.872565	-2.034891	4.896409
C	0.128190	-1.077287	3.101142
H	-0.836718	-0.964760	2.584602
H	0.422370	-0.079951	3.445389
C	-3.355245	-2.102041	-0.046275
H	-2.773075	-3.014210	-0.131515
C	-2.826675	-0.874434	-0.445615
C	-3.603530	0.283565	-0.441650
H	-3.208921	1.221017	-0.821876
C	-4.902421	0.219674	0.075520
H	-5.506814	1.124613	0.098174
C	-5.445872	-0.984938	0.541284
C	-6.845651	-1.039045	1.110049
H	-6.838829	-0.936152	2.203939
H	-7.471198	-0.232888	0.712080
H	-7.336185	-1.991013	0.878691
C	-4.655705	-2.140444	0.466099
H	-5.066382	-3.093657	0.793774
Br	-1.399376	-1.396117	-3.068185

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

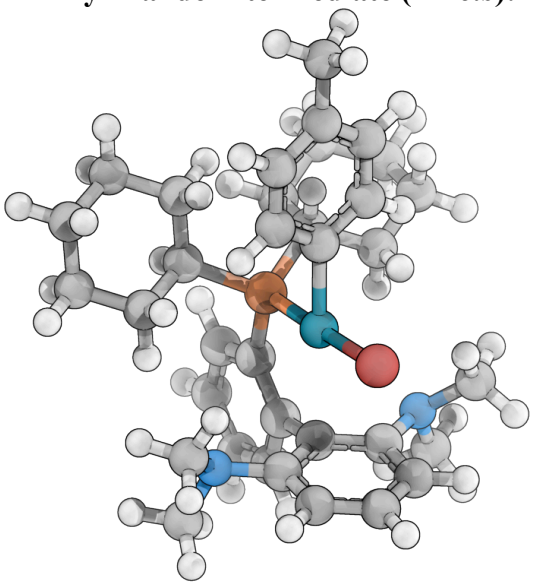
==========

SCF Energy= -1953.41397203 Predicted Change= -1.743349D-09

Zero-point correction (ZPE)= -1952.6513 0.76258
Internal Energy (U)= -1952.6090 0.80487
Enthalpy (H)= -1952.6081 0.80581
Gibbs Free Energy (G)= -1952.7304 0.68349

Frequencies -- -64.1653 9.7209 22.6338
$\Delta G_{Solvation}$ = -0.0151901799999905

III Aryl Halide Intermediate (Ar-*cis*):



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C35H48BrN2PPd C1[X(C35H48BrN2PPd)]
#Atoms= 88
Charge = 0 Multiplicity = 1

SCF Energy= -1953.43608789 Predicted Change= -1.389398D-04

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00023	0.00045	[YES]	0.00004	0.00030	[YES]
Displ	0.31456	0.00180	[NO]	0.31456	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.813666	3.314628	0.586672
H	-4.778338	3.807123	0.674528

C	-2.631303	4.039353	0.720968
H	-2.653768	5.107497	0.918400
C	-1.411863	3.377953	0.605051
H	-0.502952	3.955218	0.727217
C	-1.332709	1.995536	0.346717
P	0.329222	1.195264	0.191228
Pd	0.111848	-1.119842	-0.082515
C	1.221817	1.827943	1.722891
H	0.974329	2.896766	1.791298
C	1.192964	2.021279	-1.263541
H	2.170318	1.517529	-1.259553
C	-2.527808	1.255068	0.230177
C	-2.651798	-0.234801	0.026344
C	-3.750928	1.943812	0.351557
H	-4.673600	1.376024	0.266733
C	-2.828343	-1.077587	1.162036
N	-2.557204	-0.563039	2.479864
C	-3.739596	-0.034235	3.163001
H	-4.214240	0.741847	2.560130
H	-3.429899	0.415655	4.113091
H	-4.489802	-0.816223	3.382430
C	-1.833161	-1.495831	3.346696
H	-0.999701	-1.939226	2.796477
H	-2.461320	-2.312287	3.745273
H	-1.434719	-0.939557	4.202942
C	-3.259234	-2.397620	0.987606
H	-3.380127	-3.039739	1.853346
C	-3.512992	-2.900689	-0.282553
H	-3.838168	-3.929515	-0.403811
C	-3.331097	-2.094478	-1.401034
H	-3.507436	-2.505175	-2.389128
C	-2.902672	-0.768934	-1.270950
N	-2.691861	0.049931	-2.434251
C	-2.090666	-0.659491	-3.565181
H	-1.706972	0.080330	-4.277317
H	-2.799547	-1.306951	-4.111559
H	-1.259246	-1.276494	-3.215320
C	-3.872196	0.799803	-2.869127
H	-4.255654	1.418655	-2.057047
H	-4.686462	0.141805	-3.224880
H	-3.586631	1.462491	-3.694008
C	0.675944	1.136075	2.989181
H	0.906611	0.063943	2.930683
H	-0.415976	1.214179	3.029035
C	1.311335	1.724636	4.259831
H	0.929470	1.195593	5.142560

H	1.002553	2.775144	4.368497
C	2.844231	1.646003	4.211739
H	3.152023	0.590423	4.233193
H	3.279281	2.117731	5.102054
C	3.394197	2.304436	2.937998
H	4.484347	2.188873	2.889284
H	3.196000	3.386509	2.974159
C	2.759562	1.711102	1.666333
H	3.048443	0.658958	1.572628
H	3.162126	2.225111	0.786311
C	0.497004	1.665124	-2.593369
H	-0.502944	2.117393	-2.614310
H	0.341609	0.583617	-2.655832
C	1.320085	2.152324	-3.798264
H	0.785341	1.920596	-4.728452
H	2.267154	1.594225	-3.835702
C	1.622911	3.655691	-3.717956
H	0.684322	4.220769	-3.817453
H	2.262800	3.961326	-4.555391
C	2.286305	4.016877	-2.381127
H	2.443685	5.101027	-2.312643
H	3.281174	3.551323	-2.326627
C	1.435353	3.542752	-1.188342
H	0.472402	4.067221	-1.221664
H	1.924405	3.826185	-0.248872
C	2.848013	-1.807505	0.816734
H	2.372064	-2.008520	1.771270
C	2.093742	-1.362454	-0.273185
C	2.726958	-1.154129	-1.500072
H	2.160168	-0.846079	-2.372993
C	4.105405	-1.365668	-1.624038
H	4.580638	-1.198129	-2.589163
C	4.877990	-1.797117	-0.540493
C	6.359057	-2.061008	-0.691429
H	6.898373	-1.876840	0.244479
H	6.803412	-1.426854	-1.466684
H	6.552136	-3.104282	-0.975995
C	4.224010	-2.013909	0.679451
H	4.794766	-2.360695	1.539232
Br	-0.072384	-3.647103	-0.392994

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

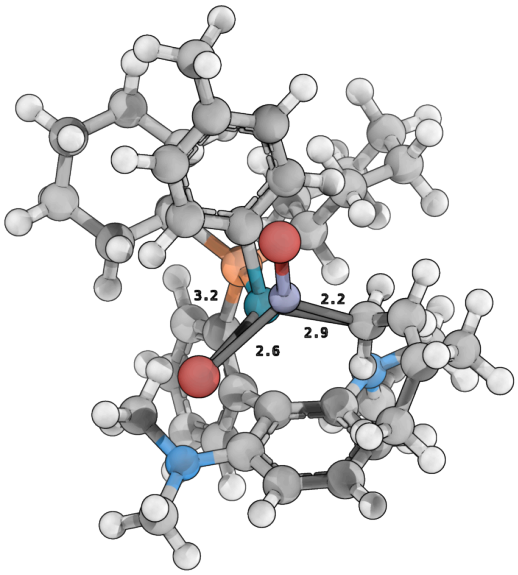
==========

SCF Energy= -1953.43608789 Predicted Change= -1.389398D-04
Zero-point correction (ZPE)= -1952.6725 0.76353

Internal Energy (U)= -1952.6298 0.80623
Enthalpy (H)= -1952.6289 0.80718
Gibbs Free Energy (G)= -1952.7513 0.68471

Frequencies -- 11.8890 18.5342 23.4070
$\Delta G_{Solvation}$ = -0.0167777399999522

TS-IV-α-4-mem Transmetalation:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

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# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn C1[X(C40H57Br2N2PPdZn)]
#Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00311	0.00180	[NO]	0.00311	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.004554	-2.651548	-1.665480

H	5.643498	-3.418568	-2.094586
C	5.464856	-1.343193	-1.522539
H	6.467381	-1.069806	-1.839555
C	4.621010	-0.378701	-0.978227
H	4.992821	0.636124	-0.897370
C	3.311318	-0.686255	-0.561371
P	2.203857	0.644041	0.112177
Pd	-0.012339	-0.172776	-0.058016
C	2.876710	0.894170	1.866718
H	2.980571	-0.148702	2.191381
C	2.715941	2.162949	-0.883413
H	3.807934	2.222240	-0.777272
C	2.847028	-2.012796	-0.694003
C	1.492355	-2.535099	-0.278807
C	3.714721	-2.971753	-1.253164
H	3.353439	-3.989322	-1.366254
C	1.272997	-2.892095	1.096041
N	2.161988	-2.398831	2.112864
C	1.545653	-2.203537	3.425976
H	2.224921	-1.606426	4.044446
H	0.600586	-1.665355	3.323277
H	1.354978	-3.145207	3.969231
C	3.395782	-3.184146	2.255192
H	3.199914	-4.190103	2.666186
H	3.899003	-3.293182	1.294660
H	4.073563	-2.660644	2.939207
C	0.238889	-3.760644	1.445479
H	0.073171	-4.021941	2.483431
C	-0.564884	-4.327281	0.454762
H	-1.367274	-5.003586	0.736822
C	-0.368429	-4.029176	-0.880658
H	-1.037602	-4.446680	-1.620195
C	0.665926	-3.154985	-1.287988
N	0.914178	-2.987244	-2.639288
C	1.319579	-1.708669	-3.217864
H	0.613814	-1.434390	-4.009740
H	1.273336	-0.919252	-2.470173
H	2.333388	-1.752923	-3.637690
C	0.290244	-3.883253	-3.605084
H	0.352440	-4.920609	-3.264630
H	-0.761451	-3.626489	-3.798398
H	0.842574	-3.807444	-4.546954
C	1.874103	1.579148	2.817892
H	1.641543	2.591820	2.466020
H	0.931434	1.022062	2.810972
C	2.417604	1.660174	4.255693

H	1.699353	2.198578	4.886798
H	2.497056	0.645358	4.671454
C	3.795265	2.332840	4.313810
H	3.702061	3.385863	4.009545
H	4.173749	2.337496	5.343585
C	4.786402	1.621347	3.384203
H	5.761370	2.124830	3.401487
H	4.956405	0.597260	3.747639
C	4.265985	1.565007	1.935794
H	4.213488	2.589203	1.543764
H	4.985309	1.019607	1.316093
C	2.148679	3.498815	-0.353906
H	1.057136	3.485578	-0.398375
H	2.422690	3.645037	0.696189
C	2.674569	4.682338	-1.186335
H	2.239547	5.614248	-0.804346
H	3.764208	4.768750	-1.056513
C	2.351658	4.512031	-2.676829
H	1.261264	4.533815	-2.812749
H	2.759708	5.351075	-3.254284
C	2.903140	3.182070	-3.208538
H	2.623682	3.043186	-4.260407
H	4.002928	3.205954	-3.177988
C	2.398490	1.985002	-2.383810
H	1.314215	1.886664	-2.510094
H	2.850626	1.061220	-2.761835
C	-1.090620	2.423140	1.096022
H	-0.865766	2.007538	2.071330
C	-0.841791	1.687289	-0.072504
C	-1.169581	2.263101	-1.311207
H	-1.023143	1.708091	-2.230935
C	-1.741393	3.537991	-1.367538
H	-2.010628	3.949817	-2.337713
C	-2.002247	4.274886	-0.206648
C	-2.685689	5.619156	-0.272831
H	-2.405910	6.256854	0.572749
H	-2.441218	6.151204	-1.198587
H	-3.775776	5.494136	-0.244507
C	-1.664248	3.694948	1.022757
H	-1.869629	4.234658	1.944913
Br	-2.119411	-1.081046	-2.219722
C	-2.141770	-1.047271	1.713501
H	-1.435636	-0.488781	2.330762
H	-1.713519	-1.995667	1.392084
C	-3.466033	-1.159009	2.364070
H	-3.721739	-0.331591	3.027147

C	-4.414584	-2.113481	2.200995
C	-4.277025	-3.285837	1.265040
H	-5.087924	-3.281419	0.522369
H	-4.362103	-4.239213	1.808461
H	-3.332492	-3.288165	0.715609
C	-5.722264	-2.034039	2.945336
H	-6.565629	-1.931399	2.246983
H	-5.751226	-1.179966	3.629221
H	-5.908301	-2.947890	3.529380
Br	-4.970761	1.386250	-0.070632
Zn	-2.894431	0.048737	-0.002394

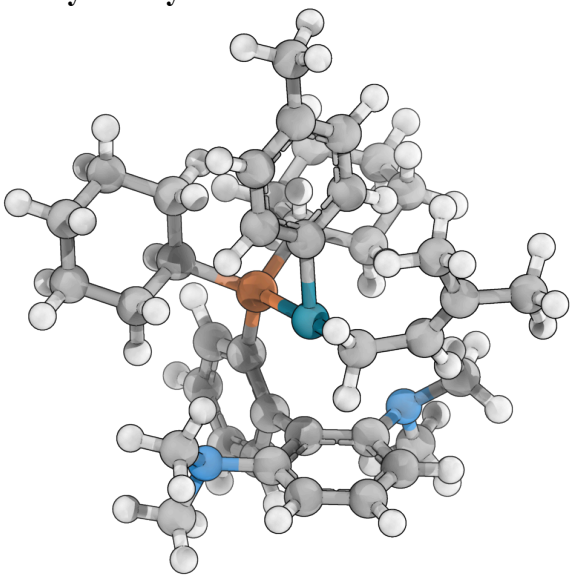
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09
Zero-point correction (ZPE)= -2227.2867 0.89270
Internal Energy (U)= -2227.2328 0.94656
Enthalpy (H)= -2227.2319 0.94750
Gibbs Free Energy (G)= -2227.3781 0.80131

Frequencies -- -68.2928 17.3940 18.2056
$\Delta G_{Solvation}$ = -0.0281542599996101

V Aryl Prenyl Intermediate:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)] #Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.14026159 Predicted Change= -1.724614D-05

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00032	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.13319	0.00180	[NO]	0.13319	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.167027	-1.217492	0.668217
H	-6.251647	-1.212013	0.736225
C	-4.437351	-2.349445	1.023268
H	-4.940064	-3.247060	1.373192
C	-3.048787	-2.323834	0.919639
H	-2.500003	-3.219344	1.186814
C	-2.346624	-1.186716	0.476197
P	-0.491932	-1.238203	0.348126
Pd	0.585477	0.763429	-0.577697
C	0.154299	-1.564509	2.091609
H	1.227440	-1.708478	1.896679
C	-0.220537	-2.875241	-0.552207
H	-0.896626	-3.616626	-0.103844
C	-3.088326	-0.042875	0.103395
C	-2.533131	1.246517	-0.448596
C	-4.491763	-0.088447	0.211738
H	-5.062475	0.789662	-0.079256
C	-2.280638	2.358128	0.402709
N	-2.308340	2.189177	1.829102
C	-3.631366	2.353904	2.434929
H	-3.573646	2.077194	3.493689
H	-3.998645	3.395027	2.371878
H	-4.358173	1.698483	1.954770
C	-1.310132	2.969081	2.558497
H	-0.334710	2.870424	2.075916
H	-1.556401	4.043343	2.641865
H	-1.234339	2.571635	3.576845
C	-2.002047	3.612203	-0.161598
H	-1.816928	4.460687	0.488498
C	-1.970850	3.786465	-1.542034
H	-1.765402	4.767980	-1.960695

C	-2.202008	2.702606	-2.383059
H	-2.167450	2.837602	-3.459417
C	-2.474931	1.433356	-1.855707
N	-2.694877	0.310214	-2.729460
C	-4.072444	0.199109	-3.210918
H	-4.359275	1.027788	-3.885018
H	-4.182382	-0.741569	-3.762318
H	-4.767613	0.180841	-2.369598
C	-1.742092	0.216545	-3.835079
H	-0.725043	0.329830	-3.450172
H	-1.832850	-0.775583	-4.291450
H	-1.904626	0.964227	-4.632801
C	-0.363884	-2.801190	2.850713
H	-1.433673	-2.677298	3.061852
H	-0.259603	-3.709978	2.244931
C	0.380633	-2.981234	4.186579
H	-0.012720	-3.860016	4.714101
H	1.442682	-3.185032	3.986008
C	0.258351	-1.729663	5.067122
H	-0.794123	-1.596796	5.359163
H	0.827067	-1.860185	5.996768
C	0.738214	-0.478091	4.317867
H	0.589099	0.416781	4.936354
H	1.820991	-0.557224	4.140355
C	0.020209	-0.303557	2.968520
H	-1.042961	-0.084515	3.134174
H	0.432154	0.558739	2.432602
C	1.220441	-3.412190	-0.420920
H	1.926823	-2.669179	-0.808676
H	1.481841	-3.574609	0.630839
C	1.391672	-4.734837	-1.190373
H	2.431704	-5.074762	-1.105097
H	0.769208	-5.512103	-0.721195
C	0.995354	-4.594022	-2.666499
H	1.694693	-3.905471	-3.162833
H	1.087236	-5.559931	-3.179969
C	-0.432771	-4.047400	-2.803730
H	-0.685463	-3.899424	-3.862004
H	-1.145987	-4.789500	-2.414236
C	-0.604475	-2.724405	-2.038879
H	0.040664	-1.957544	-2.488644
H	-1.632884	-2.356984	-2.130859
C	3.231954	0.166220	0.654345
H	2.796100	0.606250	1.547599
C	2.500596	0.129302	-0.540544
C	3.126790	-0.407921	-1.675312

H	2.601664	-0.440031	-2.626787
C	4.429237	-0.915044	-1.605665
H	4.886869	-1.330163	-2.502953
C	5.156898	-0.894998	-0.408969
C	6.576736	-1.411862	-0.346737
H	6.732692	-2.245031	-1.041618
H	7.303153	-0.631073	-0.611937
H	6.832939	-1.761762	0.659678
C	4.532905	-0.345991	0.718085
H	5.073029	-0.310872	1.663559
C	1.427128	2.526881	-1.362217
C	1.821678	3.482583	-0.308813
H	0.987066	3.905246	0.255144
C	3.055879	3.897784	0.054986
C	4.335033	3.450900	-0.606064
H	4.976535	2.909735	0.103797
H	4.164400	2.787170	-1.456210
H	4.916320	4.317194	-0.956883
C	3.238837	4.882764	1.184539
H	3.860506	4.462670	1.990080
H	3.756180	5.793063	0.844774
H	2.281269	5.184881	1.623475
H	2.212398	2.309848	-2.087573
H	0.522577	2.863117	-1.889086

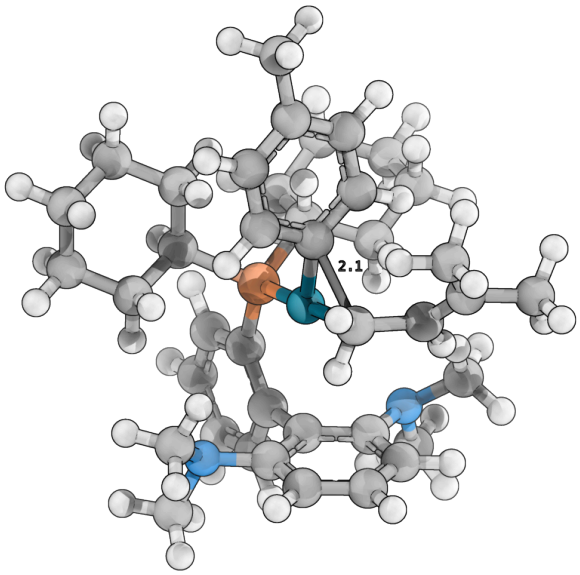
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.14026159 Predicted Change= -1.724614D-05
Zero-point correction (ZPE)= -2135.2517 0.88846
Internal Energy (U)= -2135.2034 0.93680
Enthalpy (H)= -2135.2025 0.93775
Gibbs Free Energy (G)= -2135.3385 0.80171

Frequencies -- 8.3086 18.6557 21.1872
$\Delta G_{Solvation}$ = -0.00806345000000874

TS-VI-η^1-α Reductive Elimination:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00246	0.00180	[NO]	0.00246	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.394518	0.744090	0.160557
H	6.476648	0.659059	0.105930
C	4.793472	1.915501	0.612632
H	5.395440	2.767327	0.917868
C	3.403416	1.990837	0.665757
H	2.960196	2.918580	1.007247
C	2.569888	0.920613	0.286226
P	0.715854	1.139926	0.386585
Pd	-0.799548	-0.468409	-0.478624

C	0.497302	2.850464	-0.382306
H	1.211558	3.535884	0.094483
C	0.334107	1.430498	2.218313
H	-0.728818	1.711161	2.175527
C	3.183584	-0.264581	-0.188366
C	2.463824	-1.483551	-0.703454
C	4.589506	-0.320421	-0.236438
H	5.057280	-1.228212	-0.608812
C	2.163219	-1.584045	-2.084920
N	2.429860	-0.468722	-2.952764
C	1.405376	-0.218714	-3.963424
H	1.563522	0.782150	-4.381162
H	0.416621	-0.246935	-3.498045
H	1.421961	-0.934134	-4.806616
C	3.762558	-0.485415	-3.555713
H	4.529158	-0.575188	-2.784861
H	3.926086	0.458764	-4.087831
H	3.893032	-1.313409	-4.277544
C	1.574758	-2.751915	-2.590293
H	1.343781	-2.821533	-3.648282
C	1.277888	-3.817782	-1.747267
H	0.824163	-4.720542	-2.148023
C	1.580396	-3.734846	-0.391517
H	1.357463	-4.575391	0.256784
C	2.172674	-2.582003	0.146147
N	2.447521	-2.496244	1.552938
C	3.822633	-2.829685	1.929382
H	3.966218	-2.602024	2.991757
H	4.533662	-2.232848	1.358883
H	4.054908	-3.899563	1.772993
C	1.501525	-3.200066	2.414165
H	0.477995	-2.969170	2.109798
H	1.641744	-2.852385	3.443910
H	1.630422	-4.298112	2.417310
C	0.818814	2.804017	-1.890187
H	0.133429	2.093557	-2.371553
H	1.830762	2.416697	-2.053341
C	0.661114	4.186931	-2.542645
H	0.870777	4.116080	-3.618211
H	1.410470	4.875832	-2.124280
C	-0.743442	4.761739	-2.308999
H	-1.481270	4.133908	-2.829904
H	-0.823701	5.766954	-2.743014
C	-1.082311	4.798270	-0.811897
H	-2.108565	5.157186	-0.661398
H	-0.421535	5.521458	-0.310030

C	-0.919846	3.416835	-0.152390
H	-1.663068	2.722105	-0.563659
H	-1.132015	3.503812	0.919549
C	0.417477	0.112236	3.012066
H	1.457474	-0.239819	3.026790
H	-0.164728	-0.657881	2.493261
C	-0.100009	0.284703	4.450468
H	0.013178	-0.658317	5.001709
H	-1.178404	0.500373	4.420267
C	0.620088	1.422661	5.188097
H	1.676485	1.151019	5.332389
H	0.192593	1.560682	6.189707
C	0.542873	2.731696	4.389665
H	1.102375	3.525628	4.901695
H	-0.503464	3.067765	4.340301
C	1.087227	2.550984	2.960676
H	2.152913	2.297005	3.022254
H	1.014155	3.501960	2.418044
C	-3.354007	0.616407	-1.595613
H	-2.849022	0.637631	-2.558579
C	-2.851032	-0.193620	-0.557769
C	-3.566813	-0.229144	0.648178
H	-3.244555	-0.890811	1.447019
C	-4.702220	0.566815	0.831212
H	-5.224850	0.533090	1.786278
C	-5.187414	1.396754	-0.185966
C	-6.437826	2.225244	0.001236
H	-6.319616	3.234992	-0.410488
H	-6.695340	2.324759	1.061340
H	-7.303716	1.774191	-0.503232
C	-4.490432	1.401943	-1.404517
H	-4.846695	2.027956	-2.221750
C	-2.183288	-2.055871	-1.188354
C	-2.422451	-3.075157	-0.145330
H	-1.529377	-3.395855	0.390894
C	-3.592678	-3.641636	0.216221
C	-4.926719	-3.320853	-0.409302
H	-5.627082	-2.938719	0.346369
H	-5.386215	-4.226907	-0.830985
H	-4.861183	-2.570521	-1.199854
C	-3.639033	-4.687405	1.304100
H	-4.301243	-4.378967	2.126446
H	-2.647355	-4.884563	1.725001
H	-4.042099	-5.638615	0.926109
H	-1.227487	-2.249184	-1.712841
H	-2.957634	-1.990442	-1.947485

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

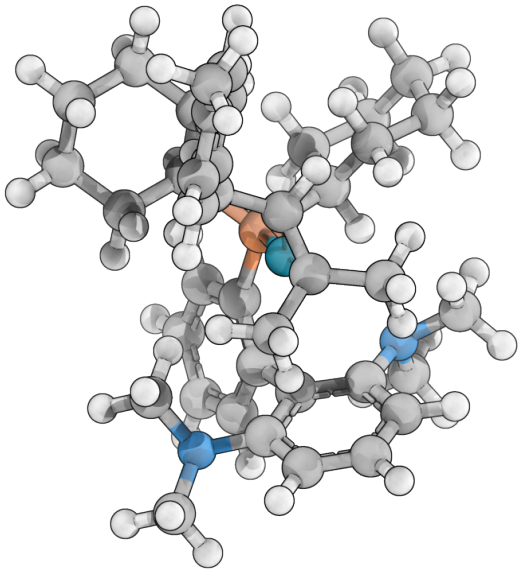
==========

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10
Zero-point correction (ZPE)= -2135.2360 0.88782
Internal Energy (U)= -2135.1882 0.93563
Enthalpy (H)= -2135.1872 0.93657
Gibbs Free Energy (G)= -2135.3218 0.80200

Frequencies -- -320.7174 9.9835 15.8974

$\Delta G_{Solvation}$ = -0.00681763000011415

VII Product-Catalyst Complex:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis) iop(1/8=18)
freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)]
#Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.19510844 Predicted Change= -6.272816D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.05684	0.00180	[NO]	0.05684	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-5.053959	-0.757535	2.338863
H	-5.924155	-1.183032	2.831773
C	-4.708723	0.578943	2.530895
H	-5.303879	1.219288	3.176804
C	-3.583198	1.090961	1.890974
H	-3.325149	2.127380	2.074711
C	-2.771954	0.312445	1.040399
P	-1.254329	1.086069	0.259561
Pd	0.496482	-0.302998	-0.454501
C	-2.036899	2.176375	-1.087267
H	-2.753169	1.473438	-1.532905
C	-0.673888	2.283199	1.607077
H	-1.502508	2.951364	1.878545
C	-3.130379	-1.046251	0.843158
C	-2.411597	-2.049265	-0.018407
C	-4.266109	-1.548682	1.510111
H	-4.523654	-2.593106	1.364116
C	-2.497346	-2.007707	-1.432484
N	-3.189704	-0.930348	-2.076995
C	-2.758025	-0.630153	-3.437862
H	-3.180512	0.336926	-3.732066
H	-1.668187	-0.557017	-3.474446
H	-3.090515	-1.372999	-4.185807
C	-4.651015	-1.024545	-2.008178
H	-5.044858	-1.852719	-2.624918
H	-4.978799	-1.170953	-0.978710
H	-5.087139	-0.088004	-2.374358
C	-1.949319	-3.049685	-2.199288
H	-2.026561	-3.022870	-3.279999
C	-1.347477	-4.140547	-1.584271
H	-0.938246	-4.946278	-2.188696
C	-1.279144	-4.211127	-0.196741
H	-0.804445	-5.065486	0.272588
C	-1.806390	-3.181941	0.598563
N	-1.790997	-3.292325	2.016825
C	-0.916975	-2.369081	2.736241
H	0.141761	-2.681938	2.688422
H	-0.988632	-1.368054	2.316111
H	-1.218189	-2.328999	3.789892

C	-1.726221	-4.633697	2.573758
H	-2.436930	-5.289364	2.062587
H	-0.722552	-5.095476	2.518590
H	-2.004161	-4.583709	3.633010
C	-1.020269	2.556480	-2.187631
H	-0.238798	3.206514	-1.771784
H	-0.507691	1.654614	-2.540759
C	-1.699781	3.287789	-3.358575
H	-0.945650	3.577517	-4.102121
H	-2.388641	2.597126	-3.867177
C	-2.484553	4.519502	-2.885568
H	-1.781968	5.265469	-2.484568
H	-2.996302	4.996144	-3.731781
C	-3.495408	4.140326	-1.794723
H	-4.020345	5.033473	-1.430877
H	-4.263343	3.480247	-2.224999
C	-2.817158	3.419362	-0.614480
H	-2.136952	4.125279	-0.117776
H	-3.578911	3.139153	0.120596
C	0.486521	3.169216	1.104230
H	1.297672	2.521566	0.745222
H	0.166378	3.770636	0.246534
C	1.012961	4.103512	2.207996
H	1.854197	4.692951	1.820475
H	0.226651	4.823949	2.479617
C	1.436510	3.324825	3.460415
H	2.299381	2.687676	3.216541
H	1.768582	4.015460	4.246330
C	0.287046	2.445191	3.970182
H	0.613175	1.851316	4.834059
H	-0.532023	3.088379	4.325780
C	-0.241539	1.508917	2.870300
H	0.544004	0.794095	2.586951
H	-1.079679	0.920295	3.260027
C	5.759404	-1.147256	0.449478
H	5.266253	-2.035283	0.838276
C	5.007096	0.011871	0.217040
C	3.505980	0.045295	0.468471
C	2.713006	-0.268992	-0.793190
H	2.823206	0.484820	-1.574143
C	2.253692	-1.518100	-1.196472
C	2.397062	-2.775093	-0.362067
H	3.276775	-3.352979	-0.688397
H	1.521489	-3.422009	-0.485299
H	2.509450	-2.567837	0.705349
C	1.987731	-1.786996	-2.667595

H	2.817695	-2.367633	-3.102430
H	1.893568	-0.857677	-3.238702
H	1.073266	-2.374129	-2.812368
H	3.226741	1.044099	0.824751
H	3.252227	-0.653702	1.270989
C	5.678707	1.135634	-0.281466
H	5.121300	2.051637	-0.468764
C	7.049249	1.101784	-0.539766
H	7.543591	1.990823	-0.926448
C	7.801819	-0.055743	-0.304035
C	9.293562	-0.082791	-0.547436
H	9.629253	-1.073369	-0.874211
H	9.588300	0.642662	-1.313478
H	9.853445	0.163159	0.365335
C	7.129923	-1.180232	0.193223
H	7.688165	-2.094508	0.385617

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.19510844 Predicted Change= -6.272816D-08
Zero-point correction (ZPE)= -2135.3035 0.89160
Internal Energy (U)= -2135.2558 0.93923
Enthalpy (H)= -2135.2549 0.94018
Gibbs Free Energy (G)= -2135.3892 0.80588

Frequencies -- 9.6702 13.4988 15.3959

$\Delta G_{Solvation}$ = -0.00707439999996495

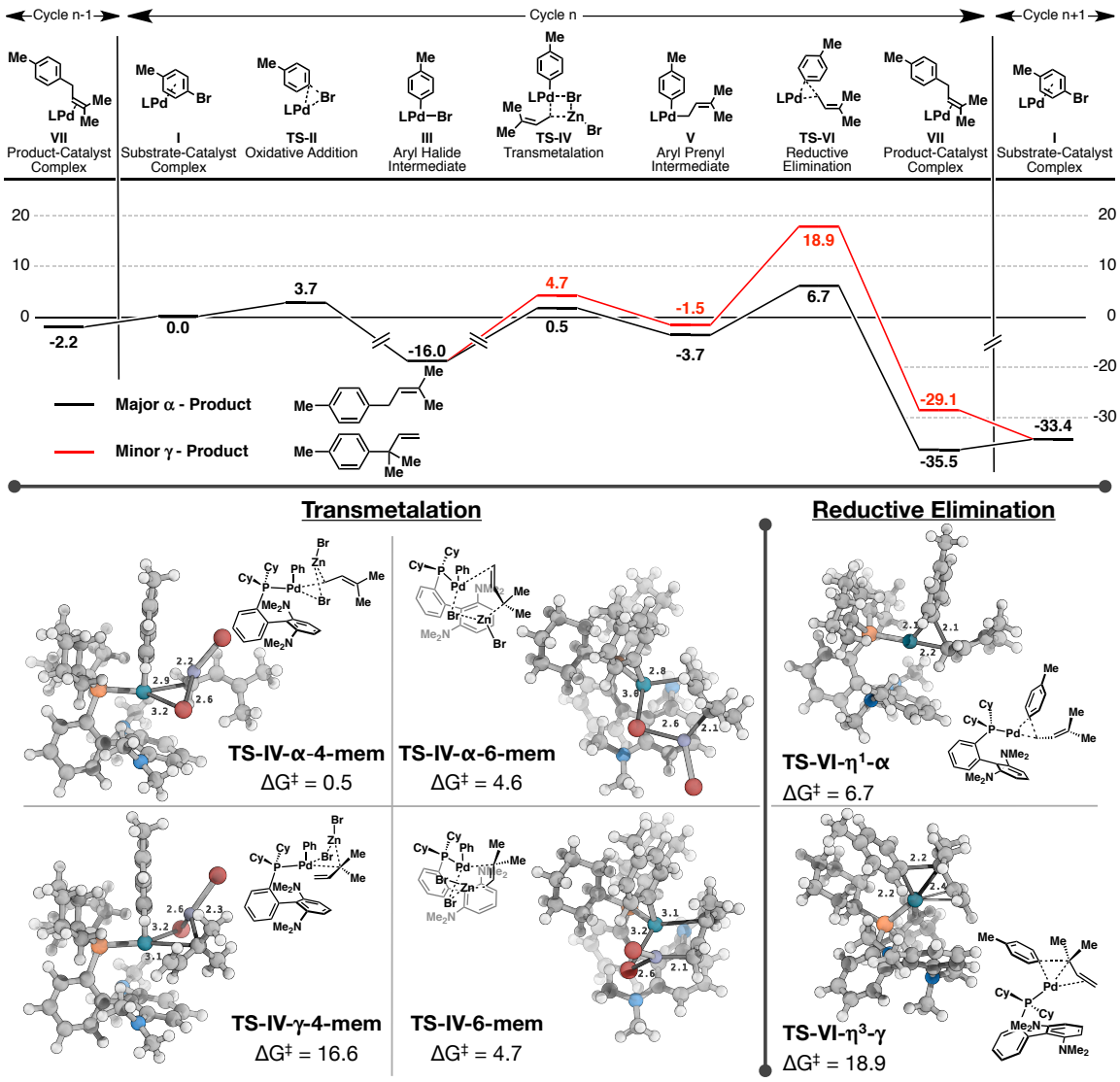
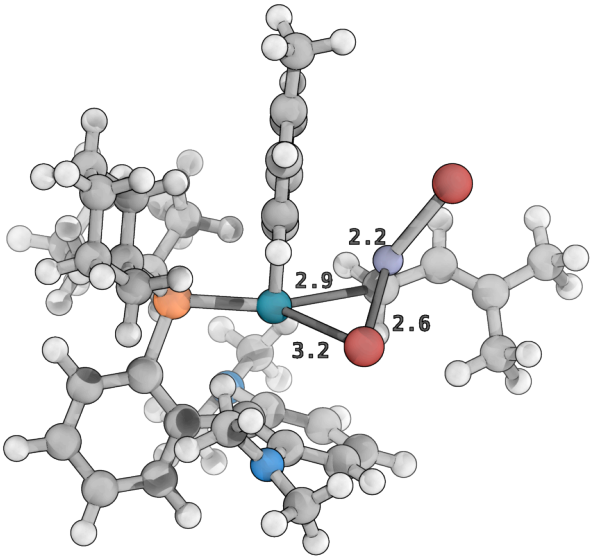


Figure X. Reaction coordinate of Pd(0)-catalyzed cross-coupling of prenylZnBr with p-bromotoluene (above) and transmetalation and reductive elimination transition (below).[10] Energies are displayed in kcal/mol and distances in Å. Computed structures are rendered in Pymol.[11]

TS-IV-α-4-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn C1[X(C40H57Br2N2PPdZn)]
#Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00311	0.00180	[NO]	0.00311	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.004554	-2.651548	-1.665480
H	5.643498	-3.418568	-2.094586
C	5.464856	-1.343193	-1.522539
H	6.467381	-1.069806	-1.839555
C	4.621010	-0.378701	-0.978227
H	4.992821	0.636124	-0.897370
C	3.311318	-0.686255	-0.561371
P	2.203857	0.644041	0.112177

Pd	-0.012339	-0.172776	-0.058016
C	2.876710	0.894170	1.866718
H	2.980571	-0.148702	2.191381
C	2.715941	2.162949	-0.883413
H	3.807934	2.222240	-0.777272
C	2.847028	-2.012796	-0.694003
C	1.492355	-2.535099	-0.278807
C	3.714721	-2.971753	-1.253164
H	3.353439	-3.989322	-1.366254
C	1.272997	-2.892095	1.096041
N	2.161988	-2.398831	2.112864
C	1.545653	-2.203537	3.425976
H	2.224921	-1.606426	4.044446
H	0.600586	-1.665355	3.323277
H	1.354978	-3.145207	3.969231
C	3.395782	-3.184146	2.255192
H	3.199914	-4.190103	2.666186
H	3.899003	-3.293182	1.294660
H	4.073563	-2.660644	2.939207
C	0.238889	-3.760644	1.445479
H	0.073171	-4.021941	2.483431
C	-0.564884	-4.327281	0.454762
H	-1.367274	-5.003586	0.736822
C	-0.368429	-4.029176	-0.880658
H	-1.037602	-4.446680	-1.620195
C	0.665926	-3.154985	-1.287988
N	0.914178	-2.987244	-2.639288
C	1.319579	-1.708669	-3.217864
H	0.613814	-1.434390	-4.009740
H	1.273336	-0.919252	-2.470173
H	2.333388	-1.752923	-3.637690
C	0.290244	-3.883253	-3.605084
H	0.352440	-4.920609	-3.264630
H	-0.761451	-3.626489	-3.798398
H	0.842574	-3.807444	-4.546954
C	1.874103	1.579148	2.817892
H	1.641543	2.591820	2.466020
H	0.931434	1.022062	2.810972
C	2.417604	1.660174	4.255693
H	1.699353	2.198578	4.886798
H	2.497056	0.645358	4.671454
C	3.795265	2.332840	4.313810
H	3.702061	3.385863	4.009545
H	4.173749	2.337496	5.343585
C	4.786402	1.621347	3.384203
H	5.761370	2.124830	3.401487

H	4.956405	0.597260	3.747639
C	4.265985	1.565007	1.935794
H	4.213488	2.589203	1.543764
H	4.985309	1.019607	1.316093
C	2.148679	3.498815	-0.353906
H	1.057136	3.485578	-0.398375
H	2.422690	3.645037	0.696189
C	2.674569	4.682338	-1.186335
H	2.239547	5.614248	-0.804346
H	3.764208	4.768750	-1.056513
C	2.351658	4.512031	-2.676829
H	1.261264	4.533815	-2.812749
H	2.759708	5.351075	-3.254284
C	2.903140	3.182070	-3.208538
H	2.623682	3.043186	-4.260407
H	4.002928	3.205954	-3.177988
C	2.398490	1.985002	-2.383810
H	1.314215	1.886664	-2.510094
H	2.850626	1.061220	-2.761835
C	-1.090620	2.423140	1.096022
H	-0.865766	2.007538	2.071330
C	-0.841791	1.687289	-0.072504
C	-1.169581	2.263101	-1.311207
H	-1.023143	1.708091	-2.230935
C	-1.741393	3.537991	-1.367538
H	-2.010628	3.949817	-2.337713
C	-2.002247	4.274886	-0.206648
C	-2.685689	5.619156	-0.272831
H	-2.405910	6.256854	0.572749
H	-2.441218	6.151204	-1.198587
H	-3.775776	5.494136	-0.244507
C	-1.664248	3.694948	1.022757
H	-1.869629	4.234658	1.944913
Br	-2.119411	-1.081046	-2.219722
C	-2.141770	-1.047271	1.713501
H	-1.435636	-0.488781	2.330762
H	-1.713519	-1.995667	1.392084
C	-3.466033	-1.159009	2.364070
H	-3.721739	-0.331591	3.027147
C	-4.414584	-2.113481	2.200995
C	-4.277025	-3.285837	1.265040
H	-5.087924	-3.281419	0.522369
H	-4.362103	-4.239213	1.808461
H	-3.332492	-3.288165	0.715609
C	-5.722264	-2.034039	2.945336
H	-6.565629	-1.931399	2.246983

H	-5.751226	-1.179966	3.629221
H	-5.908301	-2.947890	3.529380
Br	-4.970761	1.386250	-0.070632
Zn	-2.894431	0.048737	-0.002394

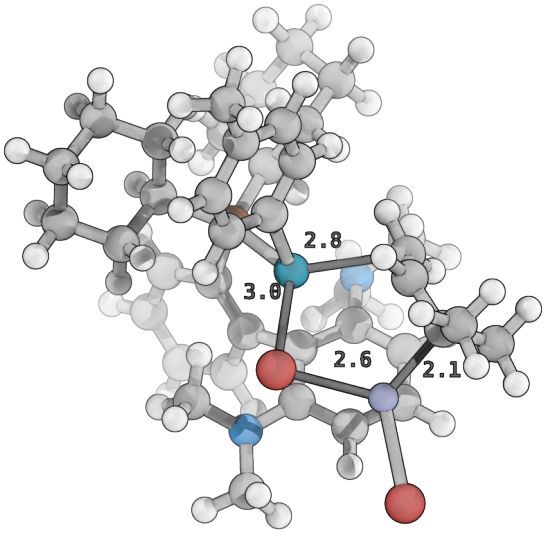
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17945412 Predicted Change= -7.865138D-09
Zero-point correction (ZPE)= -2227.2867 0.89270
Internal Energy (U)= -2227.2328 0.94656
Enthalpy (H)= -2227.2319 0.94750
Gibbs Free Energy (G)= -2227.3781 0.80131

Frequencies -- -68.2928 17.3940 18.2056

TS-IV-α-6-mem



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn C1[X(C40H57Br2N2PPdZn)]
#Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17505355 Predicted Change= -1.703331D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00065	0.00180	[YES]	0.00065	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.095916	-4.666571	-2.110210
H	2.011641	-5.645006	-2.575155
C	3.282631	-3.940352	-2.193171
H	4.141432	-4.338224	-2.726479
C	3.358265	-2.685449	-1.594493
H	4.284905	-2.133008	-1.693337
C	2.269793	-2.122008	-0.900109
P	2.423539	-0.426888	-0.150778
Pd	0.230319	0.380124	0.220706
C	3.464113	-0.769181	1.399503
H	2.949194	-1.654203	1.793302
C	3.560046	0.463380	-1.367988
H	4.430521	-0.196491	-1.480134
C	1.068581	-2.859945	-0.809127
C	-0.195376	-2.435610	-0.103824
C	1.012474	-4.126111	-1.424918
H	0.083876	-4.685478	-1.365289
C	-0.297165	-2.611605	1.316632
N	0.890100	-2.877973	2.084965
C	0.860622	-2.384532	3.461405
H	1.873480	-2.447052	3.874689
H	0.542772	-1.340264	3.478504
H	0.201756	-2.966296	4.128923
C	1.288410	-4.292721	2.072508
H	0.570423	-4.928972	2.618952
H	1.371864	-4.661775	1.050422
H	2.268832	-4.390822	2.552483
C	-1.545176	-2.613858	1.944379
H	-1.616380	-2.753124	3.016550
C	-2.708448	-2.498679	1.183301
H	-3.680011	-2.519945	1.669898
C	-2.652278	-2.365005	-0.193859
H	-3.577913	-2.264651	-0.745506
C	-1.411941	-2.353201	-0.877020
N	-1.407780	-2.345374	-2.259876
C	-0.408460	-1.636928	-3.055606
H	-0.920982	-0.967676	-3.754616
H	0.214589	-1.010508	-2.420544
H	0.229325	-2.328782	-3.622048

C	-2.646255	-2.608328	-2.986804
H	-3.182881	-3.450260	-2.541718
H	-3.312058	-1.734293	-3.017326
H	-2.385818	-2.882577	-4.013754
C	3.364137	0.340832	2.465814
H	3.758725	1.285898	2.072651
H	2.310753	0.516712	2.706086
C	4.129347	-0.029058	3.748777
H	4.076509	0.806555	4.458147
H	3.631852	-0.880859	4.234509
C	5.589944	-0.400108	3.462069
H	6.124843	0.483430	3.083111
H	6.096172	-0.698590	4.388539
C	5.669499	-1.525795	2.423373
H	6.715500	-1.765994	2.194116
H	5.223176	-2.439994	2.841427
C	4.935342	-1.150809	1.122884
H	5.464687	-0.310539	0.654818
H	4.988021	-1.993203	0.425603
C	4.105817	1.820923	-0.872475
H	3.282005	2.518877	-0.707505
H	4.619163	1.702672	0.087553
C	5.081221	2.420899	-1.901683
H	5.439677	3.391741	-1.537273
H	5.966771	1.773382	-1.990796
C	4.423928	2.575793	-3.279886
H	5.144204	2.978738	-4.003018
H	3.605173	3.305545	-3.207686
C	3.866667	1.234282	-3.775240
H	3.351320	1.362799	-4.735289
H	4.700527	0.540226	-3.959069
C	2.899376	0.605779	-2.756421
H	2.005360	1.233065	-2.666751
H	2.567571	-0.372383	-3.121861
C	1.330299	2.984311	1.267809
H	1.507779	2.475897	2.207364
C	0.827265	2.305913	0.155002
C	0.642758	3.011337	-1.040328
H	0.239911	2.519373	-1.916460
C	0.941445	4.375327	-1.104427
H	0.775154	4.903968	-2.041272
C	1.435607	5.072823	0.006129
C	1.724680	6.554414	-0.067605
H	2.423042	6.866691	0.716066
H	2.156301	6.832339	-1.035796
H	0.807457	7.145182	0.057588

C	1.624350	4.351756	1.188877
H	2.009813	4.857700	2.072155
Br	-2.126366	1.065738	-1.555697
C	-3.577268	1.554079	2.116529
C	-4.093958	0.544700	3.150416
H	-3.920238	0.912011	4.175893
H	-3.606975	-0.432465	3.069004
H	-5.171540	0.379900	3.037160
C	-4.358333	2.878875	2.203986
H	-5.429087	2.731775	2.018860
H	-3.994517	3.619633	1.480750
H	-4.265986	3.328571	3.206999
C	-2.128788	1.766395	2.122202
H	-1.798446	2.718205	1.701305
C	-1.145915	0.933310	2.568524
H	-1.374632	-0.023062	3.026763
H	-0.129180	1.289059	2.672035
Br	-6.046356	-0.374405	-0.568967
Zn	-3.972573	0.756844	0.200458

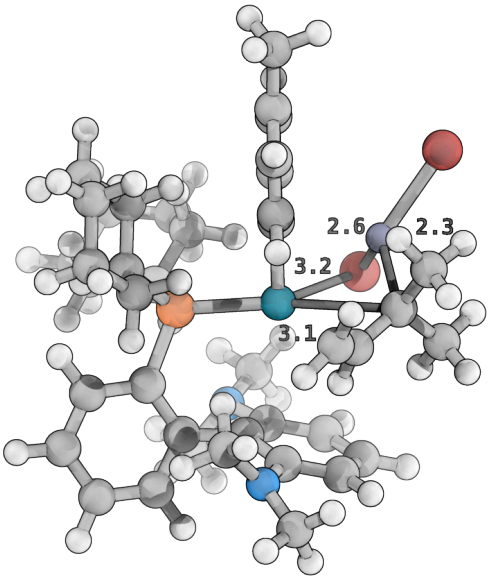
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17505355 Predicted Change= -1.703331D-10
Zero-point correction (ZPE)= -2227.2816 0.89338
Internal Energy (U)= -2227.2282 0.94678
Enthalpy (H)= -2227.2273 0.94772
Gibbs Free Energy (G)= -2227.3716 0.80337

Frequencies -- -69.5245 15.5364 23.4922

TS-IV-γ-4-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn C1[X(C40H57Br2N2PPdZn)]
#Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.15420473 Predicted Change= -1.109863D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00122	0.00180	[YES]	0.00122	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.825076	-0.360261	-1.338158
H	6.798581	-0.720296	-1.659532
C	5.554469	1.004496	-1.273419
H	6.311329	1.736147	-1.542122
C	4.294192	1.432871	-0.865911
H	4.120500	2.500504	-0.839617
C	3.265416	0.535822	-0.508404
P	1.604635	1.240944	0.010978

Pd	-0.226958	-0.303103	-0.269311
C	1.934635	1.697252	1.818648
H	2.395605	0.767339	2.177045
C	1.531266	2.853692	-0.974081
H	2.490572	3.351690	-0.788138
C	3.549646	-0.850371	-0.555544
C	2.613929	-1.975987	-0.213406
C	4.829977	-1.262045	-0.979553
H	5.030762	-2.327887	-1.027374
C	2.371374	-2.336830	1.146151
N	2.904873	-1.534306	2.206482
C	2.214108	-1.642513	3.493981
H	2.564976	-0.829813	4.139656
H	1.136438	-1.542721	3.356893
H	2.423239	-2.590253	4.020064
C	4.350878	-1.694659	2.413536
H	4.598167	-2.690772	2.820760
H	4.901901	-1.551763	1.485306
H	4.690051	-0.939269	3.131017
C	1.670870	-3.516016	1.440752
H	1.452242	-3.776831	2.467574
C	1.282190	-4.373742	0.419706
H	0.747924	-5.288692	0.661339
C	1.574191	-4.082313	-0.907133
H	1.255950	-4.766724	-1.684392
C	2.252800	-2.897275	-1.251566
N	2.628836	-2.687009	-2.585370
C	2.480507	-1.398980	-3.255783
H	1.932278	-1.539082	-4.196085
H	1.903226	-0.706312	-2.643302
H	3.448859	-0.937609	-3.491647
C	2.685812	-3.818751	-3.495577
H	3.109079	-4.692377	-2.992729
H	1.702889	-4.095858	-3.913696
H	3.343991	-3.561353	-4.332733
C	0.650710	1.931958	2.641210
H	0.098526	2.793801	2.245784
H	-0.003913	1.059003	2.557239
C	0.972235	2.185778	4.125066
H	0.041234	2.398562	4.664675
H	1.381488	1.266624	4.566893
C	1.978401	3.328155	4.312958
H	1.527119	4.274312	3.978512
H	2.218638	3.455429	5.376043
C	3.256605	3.065055	3.506361
H	3.961167	3.900002	3.613083

H	3.763237	2.174540	3.906271
C	2.949294	2.844670	2.013104
H	2.548910	3.780197	1.599740
H	3.881265	2.628917	1.480053
C	0.447632	3.857894	-0.524604
H	-0.547044	3.427295	-0.652202
H	0.557945	4.092167	0.539061
C	0.544825	5.157235	-1.345054
H	-0.243180	5.848373	-1.021108
H	1.503702	5.655069	-1.134560
C	0.432291	4.886725	-2.851442
H	0.532709	5.822392	-3.415821
H	-0.568725	4.489509	-3.071376
C	1.491600	3.874225	-3.308019
H	1.367070	3.641546	-4.373235
H	2.491477	4.321403	-3.201968
C	1.428367	2.572986	-2.488928
H	0.480890	2.059460	-2.690521
H	2.231951	1.899197	-2.808191
C	-2.239080	1.788054	0.565590
H	-1.959336	1.550810	1.585227
C	-1.651659	1.118759	-0.518270
C	-2.050316	1.443533	-1.820896
H	-1.619762	0.921319	-2.671730
C	-3.030018	2.417111	-2.029966
H	-3.336174	2.648670	-3.048524
C	-3.633892	3.091186	-0.957333
C	-4.726958	4.107241	-1.189836
H	-5.714895	3.632378	-1.132084
H	-4.704369	4.901517	-0.436076
H	-4.642281	4.571537	-2.178121
C	-3.222860	2.757830	0.337012
H	-3.684259	3.246024	1.192042
Br	-1.466645	-1.572178	2.433153
C	-2.359474	-2.193371	-1.541082
C	-3.687331	-1.924558	-2.249786
H	-4.549215	-2.161328	-1.621687
H	-3.743466	-2.551843	-3.155976
H	-3.790156	-0.881946	-2.570022
C	-2.325912	-3.560574	-0.843569
H	-1.405279	-3.710513	-0.272177
H	-2.390117	-4.362672	-1.598424
H	-3.172974	-3.702691	-0.161376
C	-1.185000	-1.974475	-2.400846
H	-0.244947	-2.374348	-2.017313
C	-1.178763	-1.431721	-3.638463

H	-0.259179	-1.336720	-4.206106
H	-2.082507	-1.080290	-4.125945
Br	-5.266825	-0.665938	0.823972
Zn	-2.861009	-1.027748	0.351448

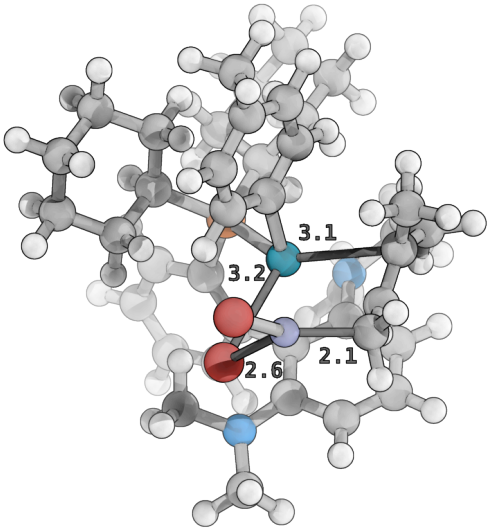
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.15420473 Predicted Change= -1.109863D-09
Zero-point correction (ZPE)= -2227.2620 0.89220
Internal Energy (U)= -2227.2082 0.94599
Enthalpy (H)= -2227.2072 0.94693
Gibbs Free Energy (G)= -2227.3525 0.80162

Frequencies -- -60.7485 17.7116 22.9111

TS-IV-γ-6-mem:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest,gdiis) iop(1/8=18) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57Br2N2PPdZn C1[X(C40H57Br2N2PPdZn)]
#Atoms= 104
Charge = 0 Multiplicity = 1

SCF Energy= -2228.17166772 Predicted Change= -1.718430D-08

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.01050	0.00180	[NO]	0.01050	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-4.699844	-2.198171	2.666420
H	-5.365216	-2.905328	3.154121
C	-4.626790	-0.875759	3.095984
H	-5.229895	-0.526584	3.929381
C	-3.762245	0.005928	2.451365
H	-3.723032	1.022629	2.820217
C	-2.948716	-0.386910	1.369424
P	-1.865391	0.909074	0.554013
Pd	0.027169	-0.064446	-0.560712
C	-3.156216	1.789456	-0.527439
H	-3.664375	0.923292	-0.970799
C	-1.446474	2.069726	1.984668
H	-2.403705	2.308999	2.465237
C	-3.016357	-1.735227	0.941428
C	-2.201511	-2.366388	-0.152325
C	-3.899184	-2.609185	1.605899
H	-3.930253	-3.645023	1.280943
C	-2.602519	-2.203479	-1.512370
N	-3.698546	-1.321790	-1.821376
C	-3.668472	-0.730383	-3.157810
H	-4.425290	0.060305	-3.203801
H	-2.690880	-0.285352	-3.351413
H	-3.898080	-1.446092	-3.966464
C	-5.018471	-1.922441	-1.582008
H	-5.232498	-2.742844	-2.289224
H	-5.089714	-2.310229	-0.566583
H	-5.787456	-1.151737	-1.706789
C	-1.996255	-2.949730	-2.529164
H	-2.313356	-2.833555	-3.558499
C	-1.005891	-3.876390	-2.208347
H	-0.518192	-4.441071	-2.999107
C	-0.640935	-4.100603	-0.891845
H	0.139740	-4.818534	-0.679062
C	-1.263615	-3.408390	0.177930
N	-1.014633	-3.836598	1.474054
C	-0.958204	-2.978971	2.658475
H	0.010307	-3.111151	3.149837
H	-1.033012	-1.930526	2.391187
H	-1.759453	-3.227807	3.367210

C	-0.337728	-5.109898	1.683402
H	-0.729435	-5.875024	1.007284
H	0.752342	-5.033443	1.553674
H	-0.535409	-5.436345	2.709185
C	-2.547663	2.615466	-1.676801
H	-1.931512	3.429321	-1.275587
H	-1.882847	1.976516	-2.267055
C	-3.630802	3.214700	-2.591741
H	-3.154234	3.836231	-3.360539
H	-4.147159	2.403250	-3.124198
C	-4.661232	4.031380	-1.802657
H	-4.171925	4.913710	-1.364102
H	-5.443785	4.408435	-2.472928
C	-5.278865	3.185400	-0.682220
H	-5.992359	3.780382	-0.098024
H	-5.850354	2.355740	-1.123781
C	-4.200828	2.613614	0.257535
H	-3.713329	3.448568	0.777918
H	-4.681005	1.994097	1.020914
C	-0.836785	3.422852	1.557460
H	0.103368	3.261810	1.027035
H	-1.506811	3.945190	0.865684
C	-0.576417	4.312768	2.786433
H	-0.124430	5.257143	2.458258
H	-1.533579	4.572836	3.263912
C	0.328618	3.610864	3.807841
H	0.485015	4.252976	4.683702
H	1.316787	3.442371	3.357448
C	-0.270020	2.264166	4.235710
H	0.406847	1.744357	4.924557
H	-1.204816	2.442020	4.788938
C	-0.557874	1.355980	3.027251
H	0.385463	1.053775	2.559135
H	-1.041867	0.434311	3.369654
C	2.165380	1.706943	0.322032
H	2.310134	0.949203	1.083546
C	1.108104	1.618009	-0.592413
C	0.928386	2.631883	-1.532563
H	0.127169	2.590643	-2.258863
C	1.813854	3.716928	-1.566801
H	1.664143	4.492465	-2.315813
C	2.887216	3.817336	-0.675351
C	3.848177	4.982900	-0.723052
H	4.875275	4.642268	-0.901089
H	3.584893	5.686004	-1.519829
H	3.854310	5.536945	0.223867

C	3.048562	2.790943	0.264810
H	3.880373	2.817646	0.965036
Br	1.921003	-1.772179	1.326512
C	3.272871	-1.754313	-2.168098
H	3.391104	-2.842622	-2.113868
H	4.010376	-1.353810	-2.869584
C	1.889344	-1.406608	-2.531908
H	1.124723	-2.151022	-2.306265
C	1.501997	-0.305335	-3.247452
C	2.519027	0.719142	-3.687833
H	2.044110	1.664739	-3.966857
H	3.068304	0.358012	-4.571450
H	3.259381	0.930461	-2.910086
C	0.156563	-0.215907	-3.922906
H	0.279942	-0.327767	-5.012339
H	-0.325081	0.760405	-3.772155
H	-0.522541	-1.001962	-3.584147
Br	5.920409	-0.229087	0.719113
Zn	3.860252	-1.162386	-0.266214

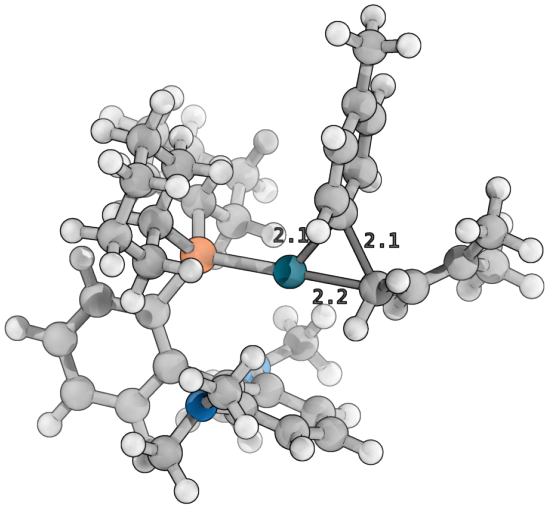
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2228.17166772 Predicted Change= -1.718430D-08
Zero-point correction (ZPE)= -2227.2787 0.89292
Internal Energy (U)= -2227.2250 0.94664
Enthalpy (H)= -2227.2240 0.94758
Gibbs Free Energy (G)= -2227.3715 0.80015

Frequencies -- -54.0448 12.8572 17.7196

TS-VI-η^1-α:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)] #Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00246	0.00180	[NO]	0.00246	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	5.394518	0.744090	0.160557
H	6.476648	0.659059	0.105930
C	4.793472	1.915501	0.612632
H	5.395440	2.767327	0.917868
C	3.403416	1.990837	0.665757
H	2.960196	2.918580	1.007247
C	2.569888	0.920613	0.286226
P	0.715854	1.139926	0.386585
Pd	-0.799548	-0.468409	-0.478624
C	0.497302	2.850464	-0.382306
H	1.211558	3.535884	0.094483
C	0.334107	1.430498	2.218313
H	-0.728818	1.711161	2.175527
C	3.183584	-0.264581	-0.188366
C	2.463824	-1.483551	-0.703454
C	4.589506	-0.320421	-0.236438
H	5.057280	-1.228212	-0.608812
C	2.163219	-1.584045	-2.084920
N	2.429860	-0.468722	-2.952764
C	1.405376	-0.218714	-3.963424
H	1.563522	0.782150	-4.381162
H	0.416621	-0.246935	-3.498045
H	1.421961	-0.934134	-4.806616
C	3.762558	-0.485415	-3.555713
H	4.529158	-0.575188	-2.784861

H	3.926086	0.458764	-4.087831
H	3.893032	-1.313409	-4.277544
C	1.574758	-2.751915	-2.590293
H	1.343781	-2.821533	-3.648282
C	1.277888	-3.817782	-1.747267
H	0.824163	-4.720542	-2.148023
C	1.580396	-3.734846	-0.391517
H	1.357463	-4.575391	0.256784
C	2.172674	-2.582003	0.146147
N	2.447521	-2.496244	1.552938
C	3.822633	-2.829685	1.929382
H	3.966218	-2.602024	2.991757
H	4.533662	-2.232848	1.358883
H	4.054908	-3.899563	1.772993
C	1.501525	-3.200066	2.414165
H	0.477995	-2.969170	2.109798
H	1.641744	-2.852385	3.443910
H	1.630422	-4.298112	2.417310
C	0.818814	2.804017	-1.890187
H	0.133429	2.093557	-2.371553
H	1.830762	2.416697	-2.053341
C	0.661114	4.186931	-2.542645
H	0.870777	4.116080	-3.618211
H	1.410470	4.875832	-2.124280
C	-0.743442	4.761739	-2.308999
H	-1.481270	4.133908	-2.829904
H	-0.823701	5.766954	-2.743014
C	-1.082311	4.798270	-0.811897
H	-2.108565	5.157186	-0.661398
H	-0.421535	5.521458	-0.310030
C	-0.919846	3.416835	-0.152390
H	-1.663068	2.722105	-0.563659
H	-1.132015	3.503812	0.919549
C	0.417477	0.112236	3.012066
H	1.457474	-0.239819	3.026790
H	-0.164728	-0.657881	2.493261
C	-0.100009	0.284703	4.450468
H	0.013178	-0.658317	5.001709
H	-1.178404	0.500373	4.420267
C	0.620088	1.422661	5.188097
H	1.676485	1.151019	5.332389
H	0.192593	1.560682	6.189707
C	0.542873	2.731696	4.389665
H	1.102375	3.525628	4.901695
H	-0.503464	3.067765	4.340301
C	1.087227	2.550984	2.960676

H	2.152913	2.297005	3.022254
H	1.014155	3.501960	2.418044
C	-3.354007	0.616407	-1.595613
H	-2.849022	0.637631	-2.558579
C	-2.851032	-0.193620	-0.557769
C	-3.566813	-0.229144	0.648178
H	-3.244555	-0.890811	1.447019
C	-4.702220	0.566815	0.831212
H	-5.224850	0.533090	1.786278
C	-5.187414	1.396754	-0.185966
C	-6.437826	2.225244	0.001236
H	-6.319616	3.234992	-0.410488
H	-6.695340	2.324759	1.061340
H	-7.303716	1.774191	-0.503232
C	-4.490432	1.401943	-1.404517
H	-4.846695	2.027956	-2.221750
C	-2.183288	-2.055871	-1.188354
C	-2.422451	-3.075157	-0.145330
H	-1.529377	-3.395855	0.390894
C	-3.592678	-3.641636	0.216221
C	-4.926719	-3.320853	-0.409302
H	-5.627082	-2.938719	0.346369
H	-5.386215	-4.226907	-0.830985
H	-4.861183	-2.570521	-1.199854
C	-3.639033	-4.687405	1.304100
H	-4.301243	-4.378967	2.126446
H	-2.647355	-4.884563	1.725001
H	-4.042099	-5.638615	0.926109
H	-1.227487	-2.249184	-1.712841
H	-2.957634	-1.990442	-1.947485

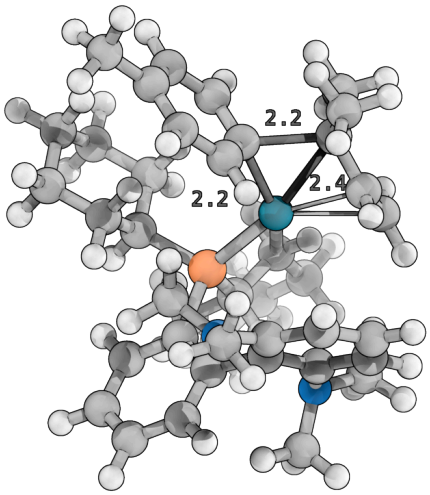
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2136.12385141 Predicted Change= -9.024289D-10
Zero-point correction (ZPE)= -2135.2360 0.88782
Internal Energy (U)= -2135.1882 0.93563
Enthalpy (H)= -2135.1872 0.93657
Gibbs Free Energy (G)= -2135.3218 0.80200

Frequencies -- -320.7174 9.9835 15.8974

TS-VI- η^3-γ:



Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C40H57N2PPd C1[X(C40H57N2PPd)] #Atoms= 101
Charge = 0 Multiplicity = 1

SCF Energy= -2136.11180380 Predicted Change= -5.083163D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00213	0.00180	[NO]	0.00213	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.736981	-0.915160	4.078125
H	-3.192691	-1.365575	4.956044
C	-2.440612	0.445148	4.045108
H	-2.660588	1.083768	4.896617
C	-1.845017	0.986877	2.908644
H	-1.608005	2.042982	2.925389
C	-1.528916	0.219287	1.768768
P	-0.673109	1.074747	0.322638
Pd	0.577895	-0.196488	-1.247086
C	-2.151356	1.975696	-0.474188
H	-2.886512	1.161643	-0.522376

C	0.302525	2.438242	1.207427
H	-0.395754	3.030843	1.813060
C	-1.853073	-1.162132	1.801106
C	-1.615877	-2.162207	0.705613
C	-2.440405	-1.695547	2.965949
H	-2.660162	-2.758809	2.983087
C	-2.458891	-2.208157	-0.430391
N	-3.518883	-1.247965	-0.565958
C	-3.944509	-0.961908	-1.931566
H	-4.515410	-1.782160	-2.404075
H	-4.597912	-0.082269	-1.914708
H	-3.074281	-0.732040	-2.549411
C	-4.683304	-1.521370	0.282245
H	-4.380755	-1.656892	1.320554
H	-5.366988	-0.665889	0.236335
H	-5.235114	-2.421575	-0.044521
C	-2.298731	-3.224694	-1.385512
H	-2.951375	-3.266943	-2.249932
C	-1.328608	-4.204892	-1.210168
H	-1.209895	-4.989132	-1.954141
C	-0.524599	-4.204675	-0.075386
H	0.221024	-4.981921	0.049772
C	-0.666509	-3.208136	0.908173
N	0.053608	-3.312705	2.117106
C	0.558349	-4.615003	2.509288
H	0.769412	-4.596698	3.585216
H	-0.191728	-5.388571	2.322105
H	1.494428	-4.903277	1.995714
C	0.897692	-2.222611	2.598107
H	1.962301	-2.450417	2.436320
H	0.681359	-1.299419	2.067333
H	0.741121	-2.057522	3.672438
C	-1.856714	2.422391	-1.922610
H	-1.075382	3.194067	-1.928903
H	-1.459024	1.574759	-2.490946
C	-3.111866	2.988579	-2.609064
H	-2.857936	3.331574	-3.620825
H	-3.853645	2.185350	-2.729427
C	-3.736616	4.132915	-1.798448
H	-3.039693	4.984160	-1.777058
H	-4.653625	4.491631	-2.283760
C	-4.032197	3.687619	-0.359917
H	-4.437494	4.524017	0.224789
H	-4.810432	2.910054	-0.373078
C	-2.775371	3.130621	0.335117
H	-2.048599	3.947069	0.450515

H	-3.041330	2.793918	1.342649
C	0.953395	3.413089	0.203242
H	1.619318	2.853752	-0.463880
H	0.190392	3.879860	-0.428417
C	1.749415	4.515439	0.925626
H	2.225983	5.170429	0.184313
H	1.053436	5.147929	1.497602
C	2.801556	3.931481	1.878003
H	3.563264	3.398566	1.292725
H	3.318733	4.738151	2.414172
C	2.161733	2.952458	2.871955
H	2.931852	2.498632	3.508966
H	1.486293	3.505283	3.542806
C	1.371733	1.846030	2.150937
H	2.062104	1.224985	1.568189
H	0.901325	1.191076	2.892861
C	3.537973	0.877285	-0.948693
H	3.284776	1.698406	-1.613264
C	2.728492	-0.269378	-0.906115
C	3.125759	-1.293424	-0.026688
H	2.548822	-2.213624	0.023033
C	4.248161	-1.160581	0.792370
H	4.511433	-1.969589	1.472983
C	5.051784	-0.012464	0.746987
C	6.298436	0.106219	1.593224
H	6.176181	-0.392930	2.561431
H	7.166577	-0.354631	1.101440
H	6.554980	1.153974	1.785237
C	4.674185	1.001276	-0.142389
H	5.277321	1.905993	-0.208195
C	2.181860	-0.965079	-2.891774
C	2.509479	0.217896	-3.789883
H	2.450146	-0.102320	-4.840653
H	1.820639	1.057083	-3.657855
H	3.525644	0.578253	-3.609280
C	3.264278	-2.036513	-2.938107
H	3.044305	-2.871265	-2.266667
H	3.313624	-2.438467	-3.962376
H	4.248405	-1.636896	-2.679135
C	0.832632	-1.526618	-3.019953
H	0.707850	-2.544154	-2.648212
C	-0.288085	-0.900182	-3.518536
H	-1.220830	-1.448950	-3.571388
H	-0.244700	0.048762	-4.042625

Statistical Thermodynamic Analysis

Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -2136.11180380 Predicted Change= -5.083163D-09
Zero-point correction (ZPE)= -2135.2223 0.88941
Internal Energy (U)= -2135.1754 0.93638
Enthalpy (H)= -2135.1744 0.93733
Gibbs Free Energy (G)= -2135.3024 0.80939

Frequencies -- -287.5205 13.7402 24.9558

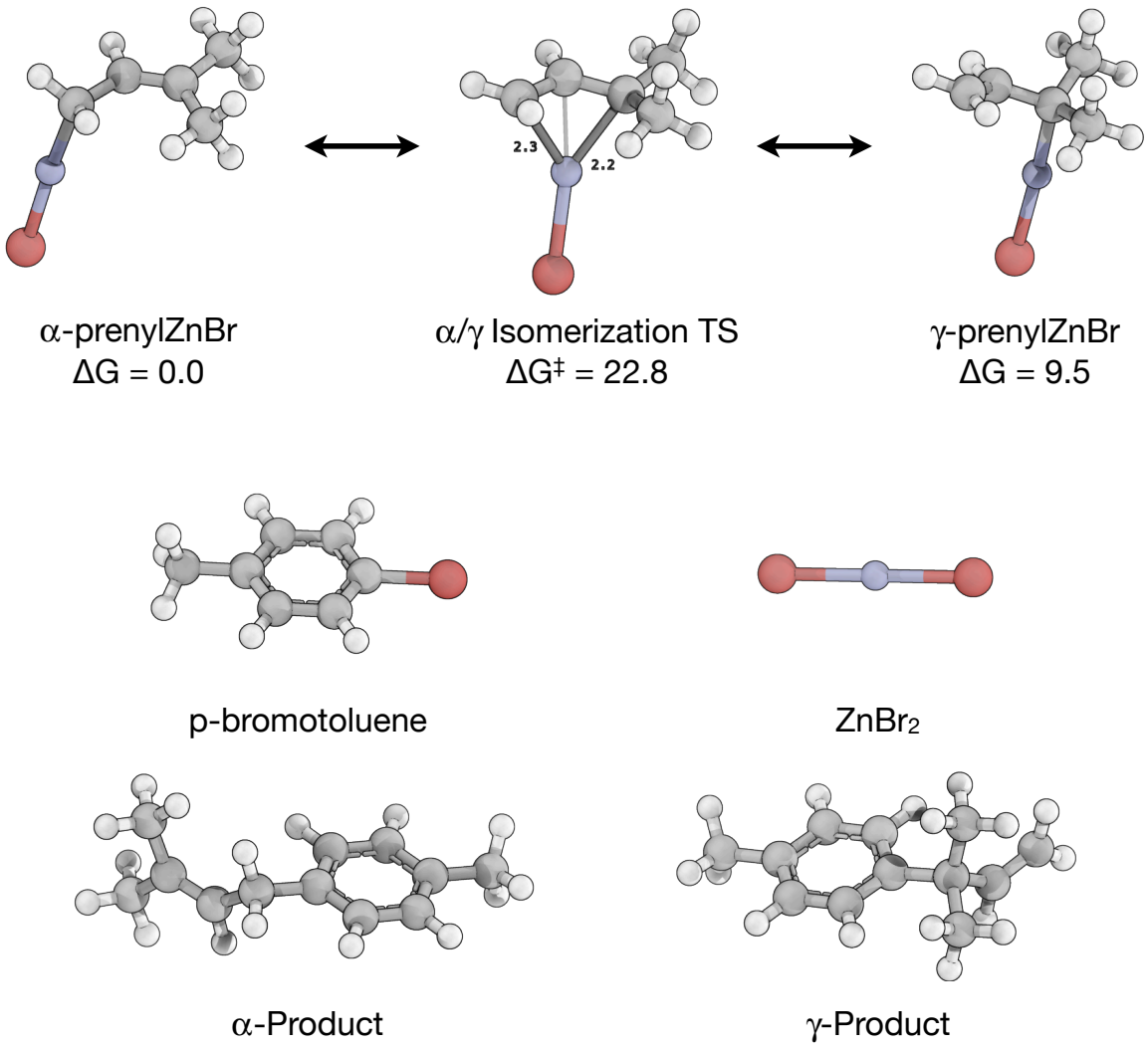


Figure X. Structures for all relevant minor intermediates, starting materials, and products; including the interconversion of prenylZnBr.[10] Energies are displayed in kcal/mol and distances in Å. Computed structures are rendered in Pymol.[11]

α-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.741185418 Predicted Change= -4.179115D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.02094	0.00180	[NO]	0.02094	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.270521	1.511996	-0.037352
H	1.511769	1.792602	0.991438
H	1.171115	2.430130	-0.624438
C	2.247675	0.567028	-0.653786
H	2.265395	0.581095	-1.744980
C	3.080623	-0.296948	-0.041655
C	4.003082	-1.182749	-0.843001
H	3.893022	-1.020053	-1.920040
H	3.811053	-2.246371	-0.639658
H	5.055165	-1.003238	-0.579211
C	3.169857	-0.471564	1.453816
H	2.898708	-1.497276	1.743669
H	2.523243	0.213116	2.009323
H	4.199195	-0.315174	1.805332
Zn	-0.564866	0.642611	-0.000526
Br	-2.657521	-0.542278	-0.008394

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -274.741185418 Predicted Change= -4.179115D-07
Zero-point correction (ZPE)= -274.6140 0.12715
Internal Energy (U)= -274.6038 0.13735
Enthalpy (H)= -274.6028 0.13829
Gibbs Free Energy (G)= -274.6531 0.08802

Frequencies -- 25.6209 41.5671 81.0463
$\Delta G_{Solvation}$ = -0.0342800329999591

α/γ-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,calcfc,ts,noeigentest) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.706185584 Predicted Change= -1.259105D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.412138	2.042563	0.112499
H	1.429291	2.148402	1.195352
H	1.301640	2.960498	-0.452652
C	1.979163	0.917340	-0.515565
H	2.158515	1.009877	-1.591490
C	2.083705	-0.419332	-0.000677
C	2.807395	-1.456878	-0.836251
H	3.888154	-1.470557	-0.619343
H	2.692988	-1.266227	-1.910055
H	2.432104	-2.467367	-0.638489
C	2.205932	-0.613696	1.508628
H	3.215361	-0.348924	1.863236
H	2.024357	-1.657827	1.783638
H	1.508270	0.000346	2.097135
Zn	-0.033637	0.231208	-0.142269
Br	-2.359187	-0.247555	0.026541

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -274.706185584 Predicted Change= -1.259105D-09
Zero-point correction (ZPE)= -274.5804 0.12574
Internal Energy (U)= -274.5709 0.13523
Enthalpy (H)= -274.5700 0.13618
Gibbs Free Energy (G)= -274.6168 0.08929

Frequencies -- -223.1991 54.6105 76.0052
$\Delta G_{Solvation}$ = -0.0264277869999887

γ-prenylZnBr:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C5H9BrZn C1[X(C5H9BrZn)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -274.727231796 Predicted Change= -1.076481D-07

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00864	0.00180	[NO]	0.00864	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.869635	1.977353	-0.090616
H	3.051944	2.044971	0.978143
H	3.145044	2.845575	-0.681958
C	2.330649	0.893173	-0.668302
H	2.194840	0.910581	-1.752702
C	1.890703	-0.376113	-0.005726
C	2.302865	-1.603594	-0.838198
H	3.400252	-1.698878	-0.846755
H	1.976256	-1.526897	-1.882278
H	1.897087	-2.534507	-0.425979
C	2.366088	-0.516086	1.445721
H	3.467049	-0.510452	1.482224
H	2.025815	-1.459194	1.887916
H	2.018049	0.299075	2.090560
Zn	-0.158090	-0.193226	-0.007030
Br	-2.542665	0.147946	0.008699

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -274.727231796 Predicted Change= -1.076481D-07
Zero-point correction (ZPE)= -274.6001 0.12706
Internal Energy (U)= -274.5901 0.13712
Enthalpy (H)= -274.5891 0.13806
Gibbs Free Energy (G)= -274.6379 0.08924

Frequencies -- 35.1449 44.4986 104.6673
$\Delta G_{Solvation}$ = -0.0345173110000019

p-bromotoluene:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C7H7Br C1[X(C7H7Br)] #Atoms= 15
Charge = 0 Multiplicity = 1

SCF Energy= -284.120087119 Predicted Change= -1.537413D-07

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00009	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00064	0.00180	[YES]	0.00064	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.312390	0.000006	-0.000567
C	0.366574	1.214021	-0.004396
C	0.366566	-1.214020	-0.004399
C	1.762788	-1.201156	-0.010221
C	1.762795	1.201172	-0.010223
C	2.484003	0.000004	-0.010181
H	2.297508	-2.148246	-0.016771
C	3.994889	-0.000010	0.015526
H	-0.177564	2.152182	-0.006892
H	2.297524	2.148256	-0.016765
H	-0.177559	-2.152182	-0.006886
H	4.374545	-0.000391	1.046110
H	4.404203	0.886293	-0.480638
H	4.404203	-0.885961	-0.481274
Br	-2.284978	-0.000002	0.003140

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -284.120087119 Predicted Change= -1.537413D-07
Zero-point correction (ZPE)= -284.0020 0.11803
Internal Energy (U)= -283.9943 0.12572
Enthalpy (H)= -283.9934 0.12666
Gibbs Free Energy (G)= -284.0363 0.08373

Frequencies -- 29.5690 104.8033 206.9485
$\Delta G_{Solvation}$ = -0.00293244800002412

$ZnBr^2$:

Using Gaussian 09: AM64L-G09RevC.01 23-Sep-2011

==========

# b3lyp/gen pseudo=read gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= Br2Zn C1[X(Br2Zn)] #Atoms= 3
Charge = 0 Multiplicity = 1

SCF Energy= -92.0235652765 Predicted Change= -2.393722D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Br	1.727500	-0.163127	-1.583811
Br	-1.727508	0.162957	1.583836
Zn	0.000009	0.000199	-0.000029

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -92.0235652765 Predicted Change= -2.393722D-09
Zero-point correction (ZPE)= -92.0222 0.00136
Internal Energy (U)= -92.0176 0.00594
Enthalpy (H)= -92.0166 0.00689
Gibbs Free Energy (G)= -92.0463 -0.02280

Frequencies -- 63.5376 187.9715 347.2022
$\Delta G_{Solvation}$ = -0.0497805409999899

α-Product:

Using Gaussian 03: EM64L-G03RevE.01 11-Sep-2007

==========

# b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman

#N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C12H16 C1[X(C12H16)] #Atoms= 28
Charge = 0 Multiplicity = 1

SCF Energy= -466.901455254 Predicted Change= -3.719157D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.01570	0.00180	[NO]	0.01570	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.418386	0.663281	0.141582
C	-1.496130	1.493665	-0.181332
C	-0.684904	-0.692577	0.381346
C	-1.982791	-1.192838	0.307898
C	-2.797304	0.991098	-0.255955
C	-3.065096	-0.360521	-0.014758
H	-2.160866	-2.248596	0.503500
C	-4.467473	-0.915020	-0.119429
H	-1.319144	2.550214	-0.372774
H	-3.616264	1.661822	-0.507621
C	0.996633	1.214692	0.252969
H	0.137698	-1.360841	0.624392
H	-4.610395	-1.469918	-1.056492
H	-5.216440	-0.116532	-0.095046
H	-4.687946	-1.608487	0.700576
C	2.005418	0.440906	-0.560044
H	1.292092	1.246422	1.308722
H	0.986865	2.260482	-0.086970
C	3.131954	-0.159748	-0.144143
C	3.633802	-0.176596	1.279905
C	4.023183	-0.885129	-1.125955
H	4.141506	-1.941982	-0.847443
H	5.034017	-0.452967	-1.137296
H	3.626211	-0.845345	-2.145210
H	3.790641	-1.208917	1.622461
H	2.957153	0.310774	1.985830
H	4.609542	0.324284	1.352113
H	1.761888	0.372312	-1.621252

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

```
=====================================================================
 SCF Energy=     -466.901455254  Predicted Change= -3.719157D-08
 Zero-point correction (ZPE)=          -466.6551  0.24630
 Internal Energy (U)=                  -466.6422  0.25924
 Enthalpy (H)=                         -466.6412  0.26019
 Gibbs Free Energy (G)=                -466.6963  0.20510
---------------------------------------------------------------------------------------------------
 Frequencies --    21.3677              36.1636              48.3462
```
$\Delta G_{Solvation}$ = -0.00262043399999357

γ-Product:

```
---------------------------------------------------------------------------------------------------
 Using  Gaussian 03:  EM64L-G03RevE.01 11-Sep-2007
=====================================================================
 # b3lyp/gen gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman
 #N Geom=AllCheck Guess=Read SCRF=Check GenChk RB3LYP/ChkBas Freq
---------------------------------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C12H16   C1[X(C12H16)]  #Atoms= 28
 Charge = 0 Multiplicity = 1
---------------------------------------------------------------------------------------------------
 SCF Energy= -466.888865594   Predicted Change= -4.168447D-10
=====================================================================
 Optimization completed. {Found  2 times}
 Item      Max Val.   Criteria   Pass?      RMS Val.   Criteria   Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00156 ||  0.00180   [ YES ]      0.00156 ||  0.00180   [ YES ]
---------------------------------------------------------------------------------------------------
     Atomic      Coordinates (Angstroms)
      Type    X                Y                Z
---------------------------------------------------------------------------------------------------
      C       -0.125222        0.213696         0.013463
      C        0.449791       -1.058129         0.176842
      C        0.746934        1.293058        -0.167978
      C        2.132914        1.109974        -0.181668
      C        1.829773       -1.238675         0.164609
      C        2.702147       -0.155532        -0.017607
      H        2.780325        1.972802        -0.324337
      C        4.199117       -0.359275        -0.055190
      H       -0.198463       -1.920601         0.307251
      H        2.238005       -2.239111         0.295220
      C       -1.659255        0.368179         0.080653
      H        0.357960        2.297261        -0.299838
      H        4.536871       -1.008915         0.760996
      H        4.734632        0.592072         0.028851
      H        4.515627       -0.832983        -0.994084
```

C	-2.287568	-0.670488	-0.838331
C	-2.129412	1.754040	-0.420411
C	-2.110782	0.200701	1.548219
C	-3.161203	-1.624834	-0.512673
H	-1.973252	-0.584044	-1.879872
H	-1.798905	1.946903	-1.447345
H	-1.753379	2.561925	0.217304
H	-3.223358	1.798273	-0.403519
H	-3.517700	-1.773807	0.502726
H	-3.557558	-2.301604	-1.265176
H	-1.828854	-0.778868	1.947285
H	-3.197815	0.310056	1.640385
H	-1.637541	0.964357	2.174582

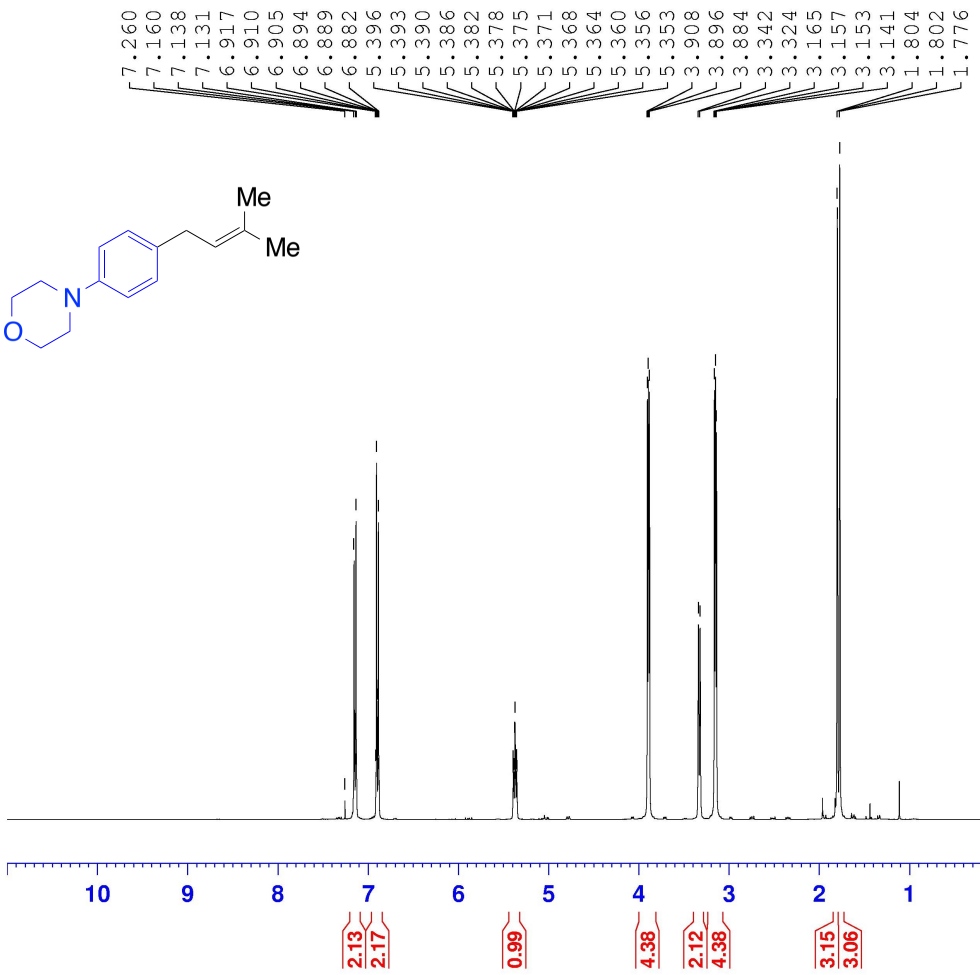
Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -466.888865594 Predicted Change= -4.168447D-10
Zero-point correction (ZPE)= -466.6424 0.24643
Internal Energy (U)= -466.6299 0.25893
Enthalpy (H)= -466.6289 0.25988
Gibbs Free Energy (G)= -466.6814 0.20742

Frequencies -- 35.7079 41.2865 87.3352

$\Delta G_{Solvation}$ = -0.00246640799997522



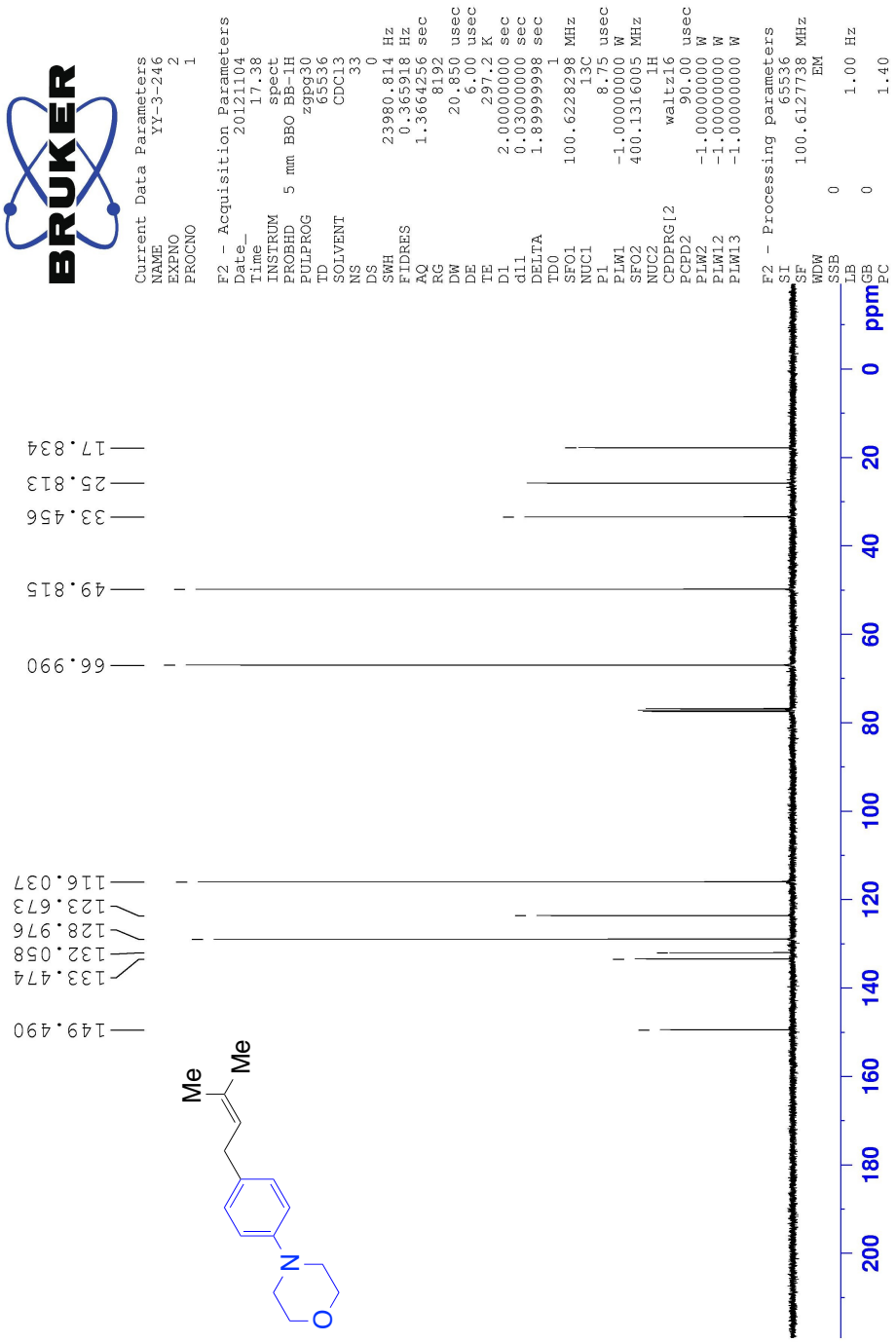
BRUKER

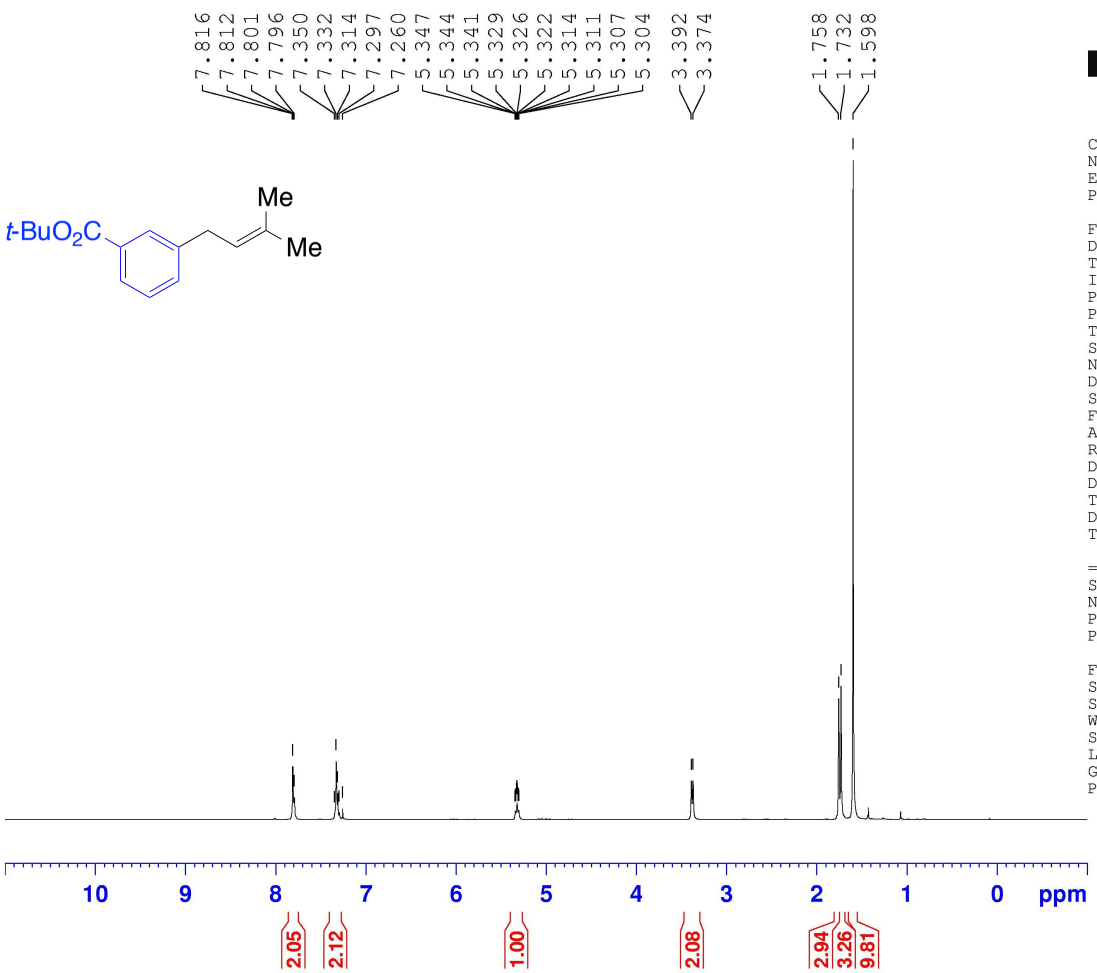
```
Current Data Parameters
NAME                  YY-3-246
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20121104
Time                   17.34
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9583745 sec
RG                      20.2
DW                    60.400 usec
DE                     6.00 usec
TE                    297.2 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.07 usec
PL1       0 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                     65536
SF              400.1300091 MHz
WDW                       EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```


Current Data Parameters
NAME YY-3-246
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121104
Time_ 17.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.36644256 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127738 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.834
25.813
33.456
49.815
66.990
116.037
123.673
128.976
132.058
133.474
149.490
Me
Me
N
O
ppm
0
20
40
60
80
100
120
140
160
180
200



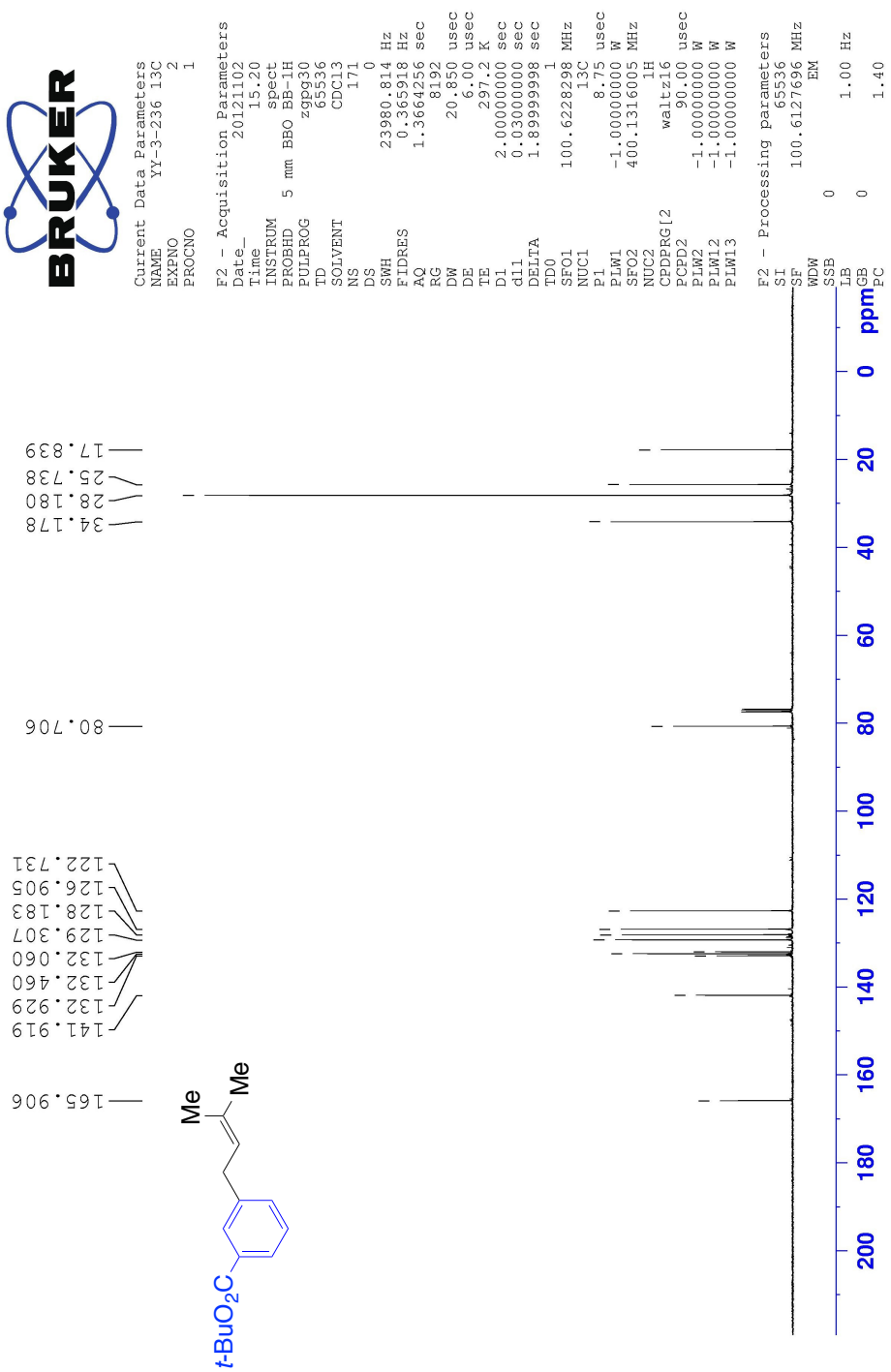
BRUKER

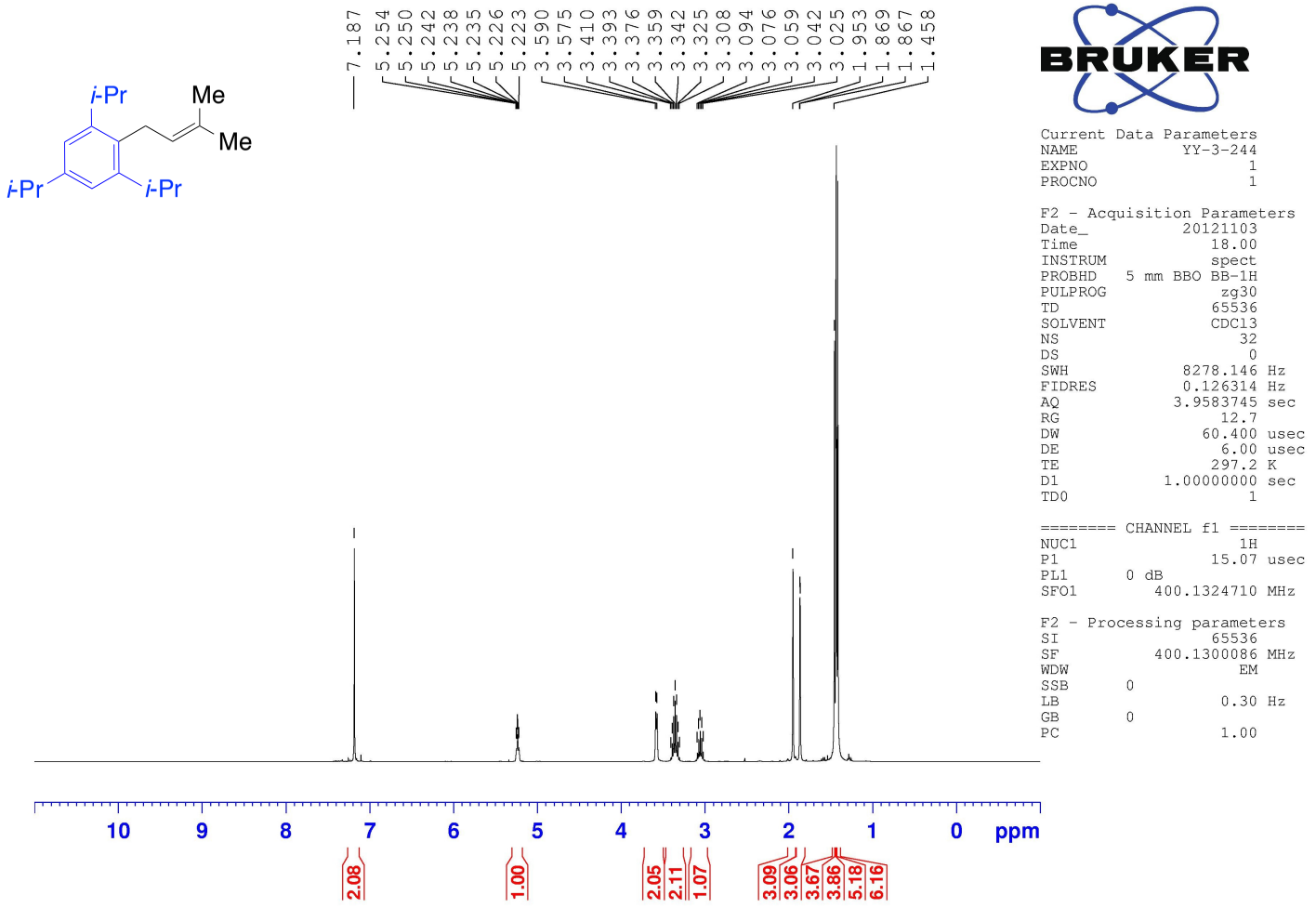
```
Current Data Parameters
NAME                  YY-4-40
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121130
Time                   17.04
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                8012.820 Hz
FIDRES                0.122266 Hz
AQ                 4.0894465 sec
RG                        57
DW                    62.400 usec
DE                     6.50 usec
TE                     298.1 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                     14.50 usec
PLW1            10.00000000 W

F2 - Processing parameters
SI                     65536
SF               400.1300094 MHz
WDW                        EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```


Current Data Parameters
NAME YY-3-236 13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121102
Time_ 15.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 171
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127696 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.839
25.738
28.180
34.178
80.706
122.731
126.905
128.183
129.307
132.060
132.460
132.929
141.919
165.906
Me
Me
t-BuO2C
ppm
0
20
40
60
80
100
120
140
160
180
200



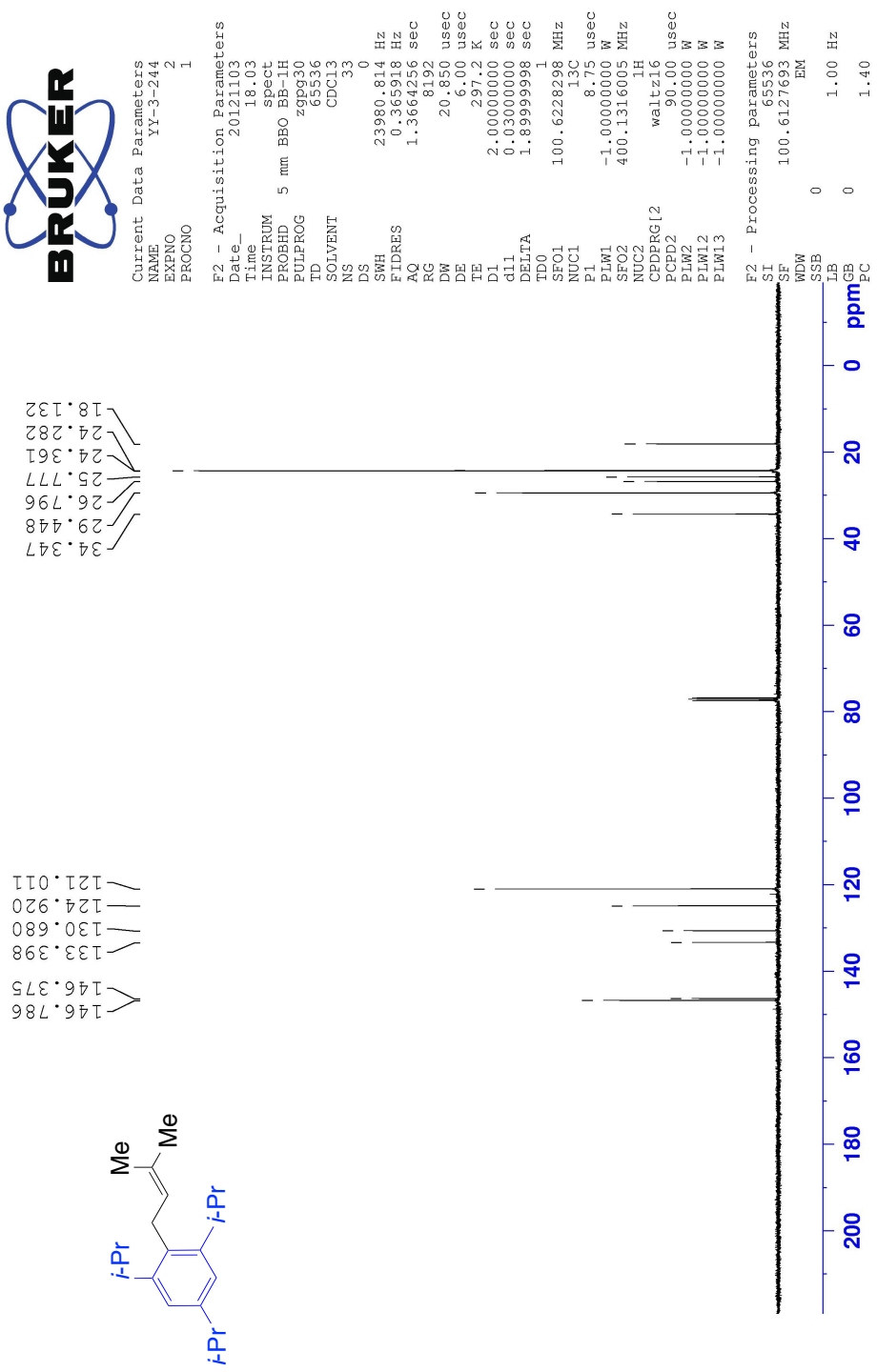
BRUKER

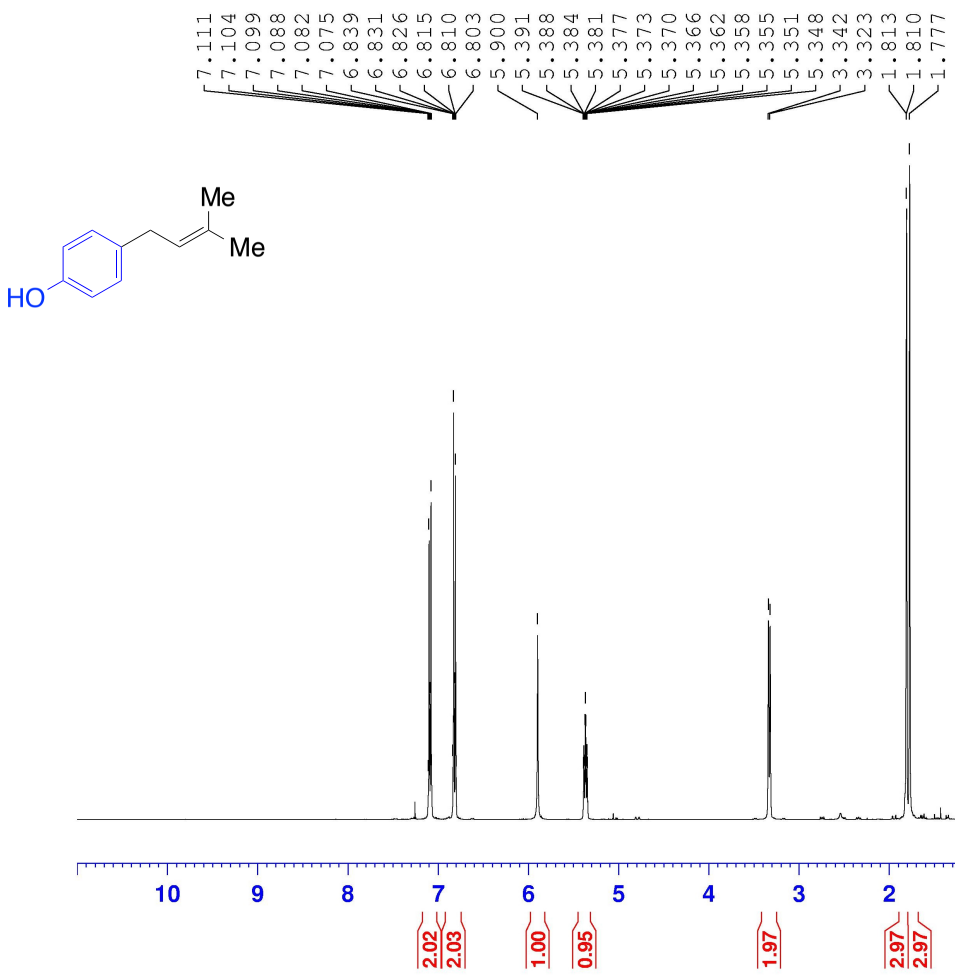
```
Current Data Parameters
NAME                  YY-3-244
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20121103
Time                     18.00
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          32
DS                           0
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9583745 sec
RG                        12.7
DW                      60.400 usec
DE                       6.00 usec
TE                       297.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1       0 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                400.1300086 MHz
WDW                         EM
SSB       0
LB                       0.30 Hz
GB        0
PC                       1.00
```


Current Data Parameters
NAME YY-3-244
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121103
Time 18.03
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
18.132
24.282
24.361
25.777
26.796
29.448
34.347
121.011
124.920
130.680
133.398
146.375
146.786
Me
Me
i-Pr
i-Pr
i-Pr
ppm



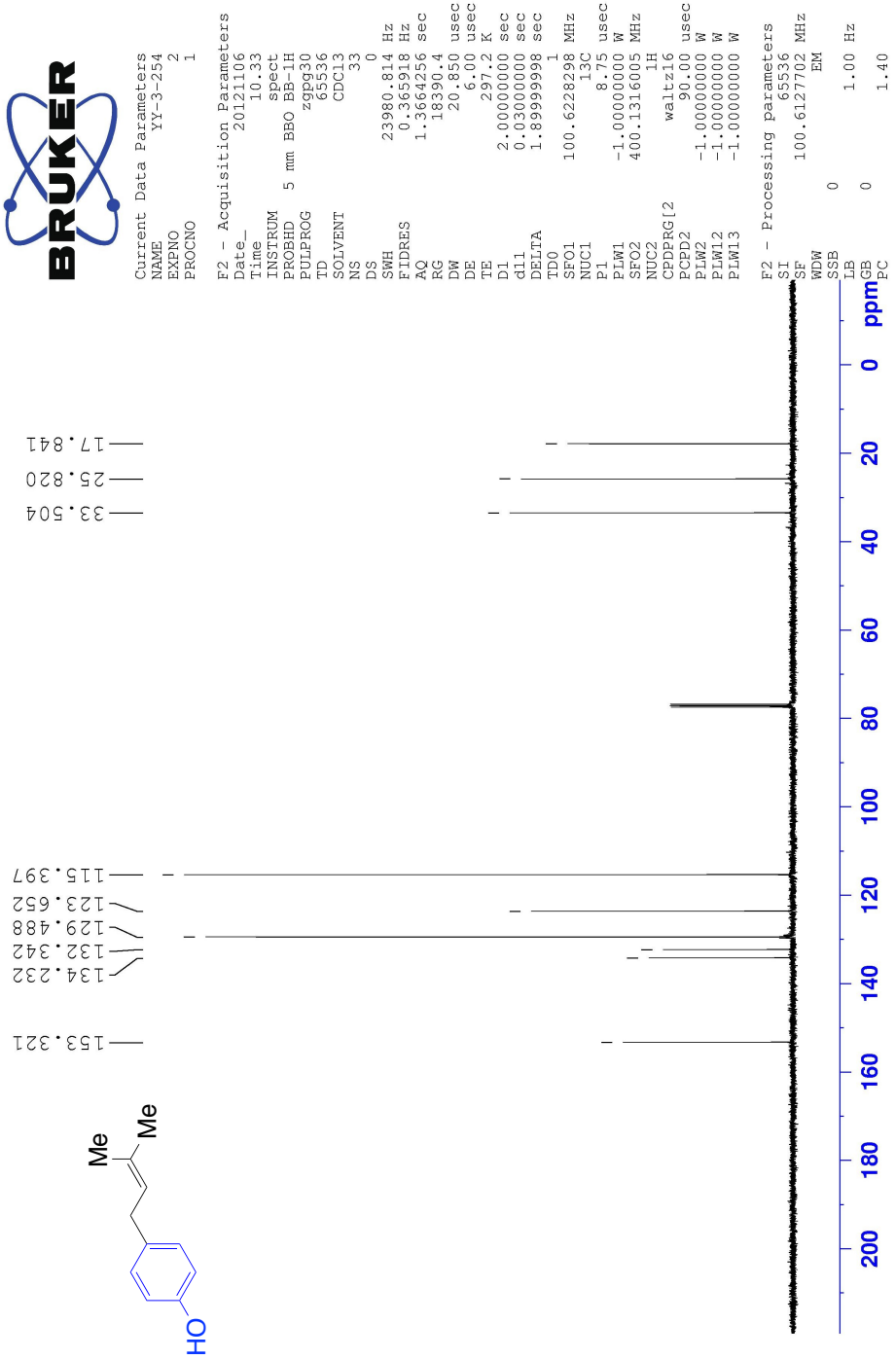
BRUKER

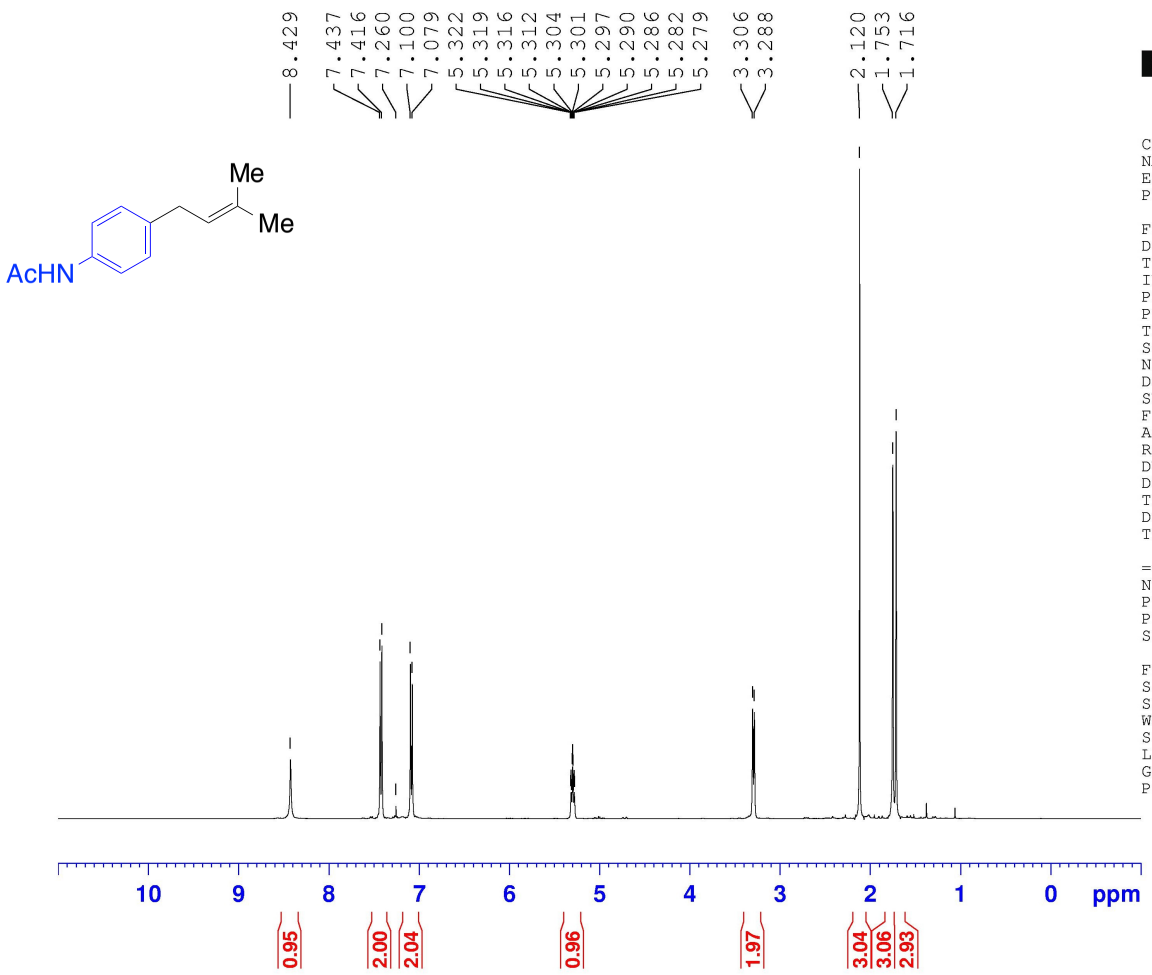
```
Current Data Parameters
NAME                  YY-3-293
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20121126
Time                     7.48
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9583745 sec
RG                       22.6
DW                     60.400 usec
DE                      6.00 usec
TE                     297.2 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1       0 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF                400.1300091 MHz
WDW                        EM
SSB       0
LB                      0.30 Hz
GB        0
PC                      1.00
```


Current Data Parameters
NAME YY-3-254
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121106
Time_ 10.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127702 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.841
25.820
33.504
115.397
123.652
129.488
132.342
134.232
153.321
Me
Me
HO
ppm
200
180
160
140
120
100
80
60
40
20
0



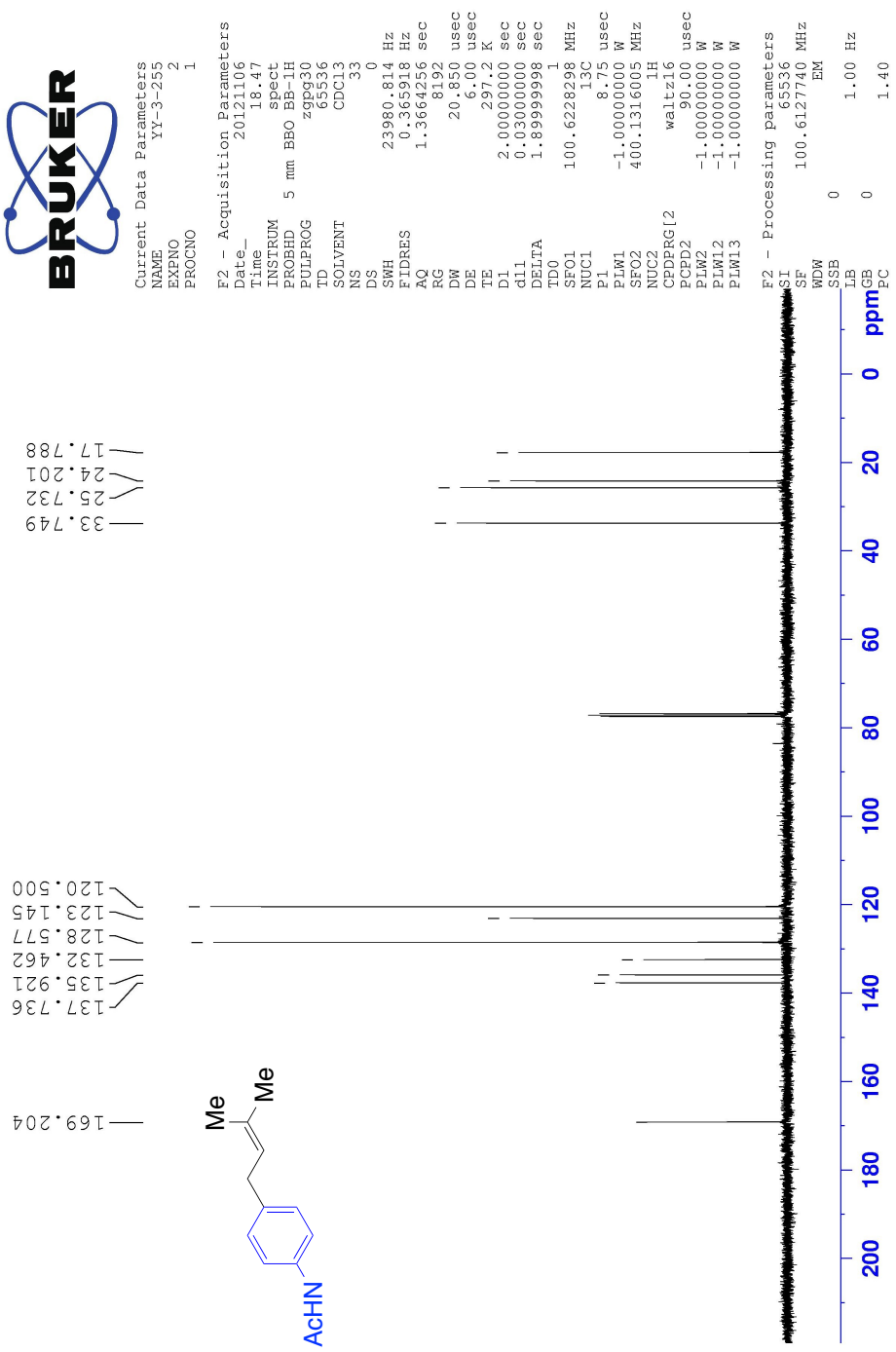
BRUKER

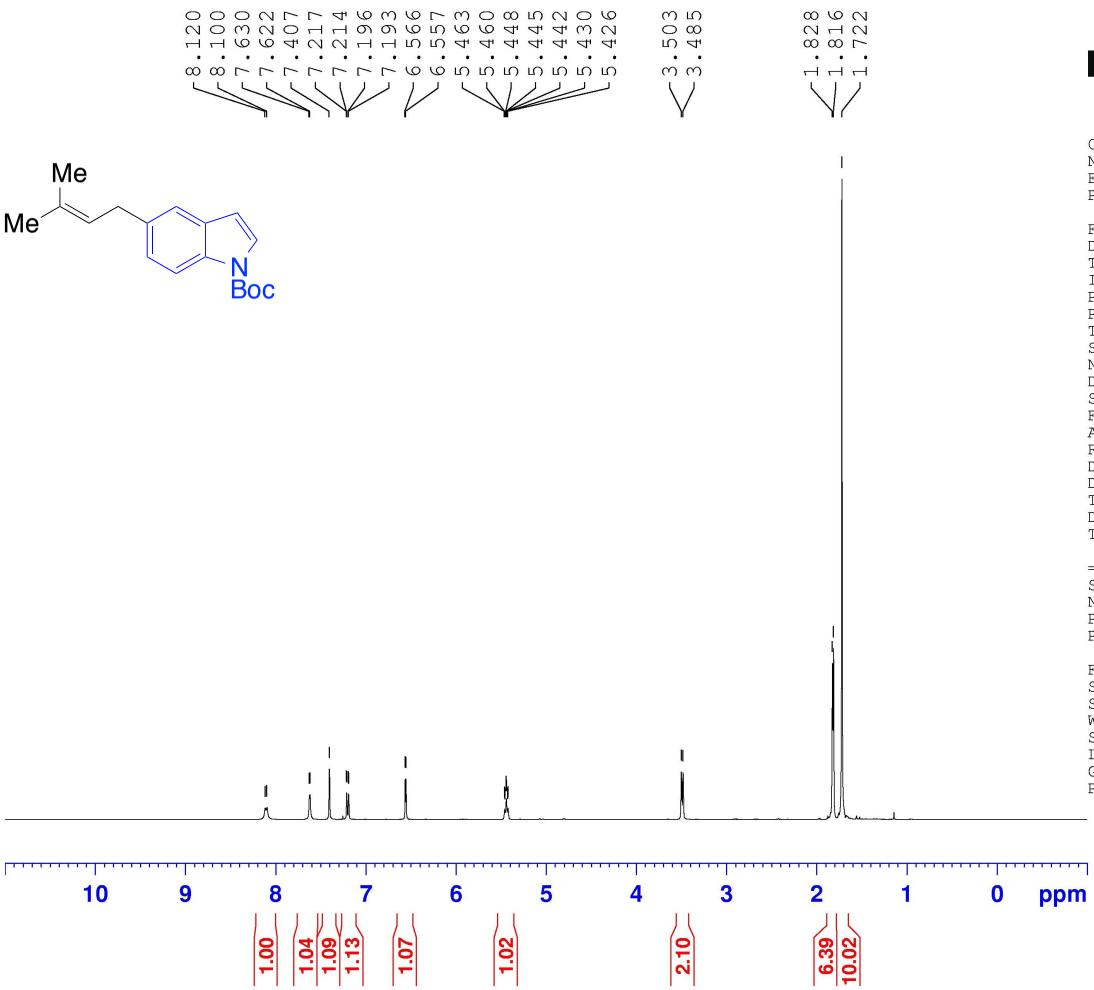
```
Current Data Parameters
NAME                  YY-3-288
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20121117
Time                     9.24
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9583745 sec
RG                       28.5
DW                     60.400 usec
DE                      6.00 usec
TE                     297.2 K
D1                 2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.07 usec
PL1       0 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                          65536
SF                400.1300092 MHz
WDW                           EM
SSB       0
LB                       0.30 Hz
GB        0
PC                       1.00
```


Current Data Parameters
NAME YY-3-255
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121106
Time 18.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 33
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.36664256 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
169.204
137.736
135.921
132.462
128.577
123.145
120.500
33.749
25.732
24.201
17.788
Me
Me
AcHN
ppm
200
180
160
140
120
100
80
60
40
20
0



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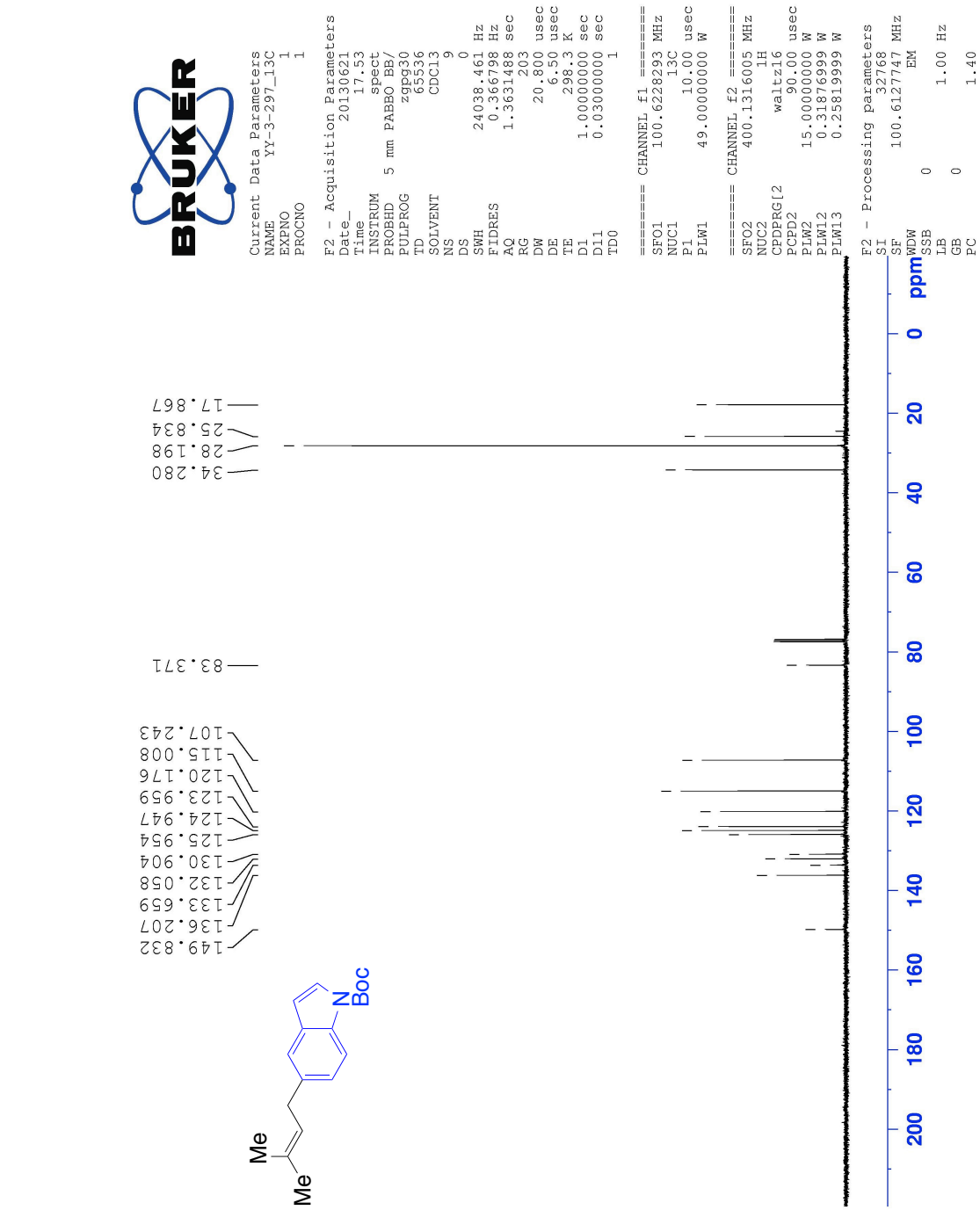
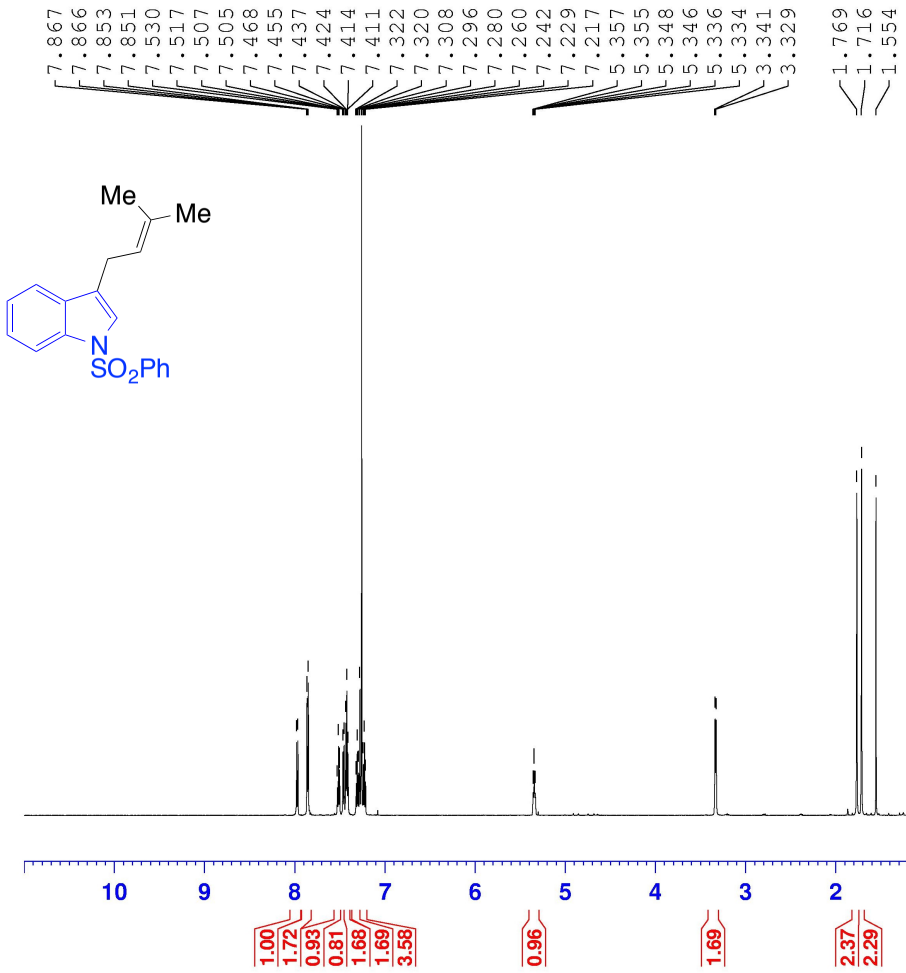
```
Current Data Parameters
NAME                  YY-3-297
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20121126
Time                     20.43
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                       12.25
DW                       62.400 usec
DE                        6.50 usec
TE                       298.1 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       14.50 usec
PLW1                10.00000000 W

F2 - Processing parameters
SI                       65536
SF                  400.1300092 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
```


Current Data Parameters
NAME YY-3-297_13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130621
Time 17.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.867
25.834
28.198
34.280
83.371
107.243
115.008
120.176
123.959
124.947
125.954
130.904
132.058
133.659
136.207
149.832
ppm
Me
Me
N
Boc



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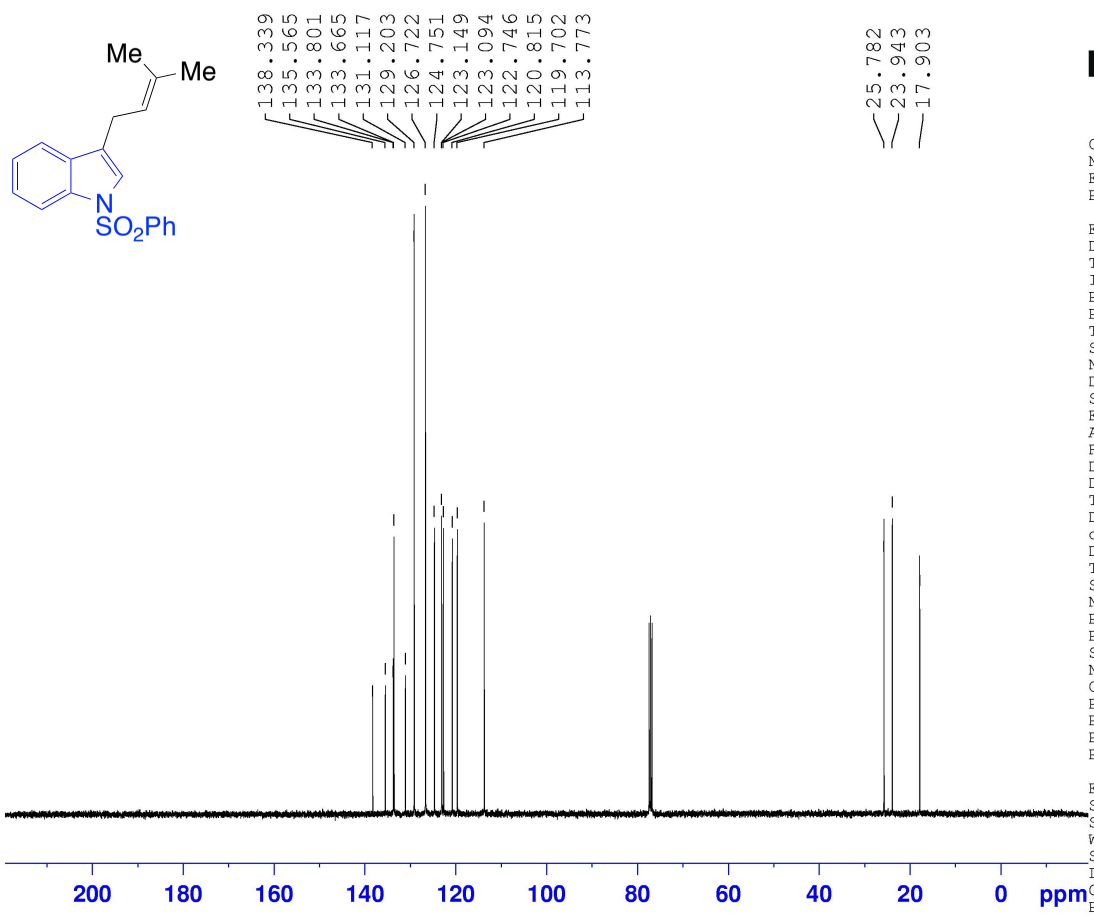
```
Current Data Parameters
NAME                  YY-4-33
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20121129
Time                   14.42
INSTRUM                spect
PROBHD    5 mm CPTXI 1H-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         0
SWH               12376.237 Hz
FIDRES             0.188846 Hz
AQ                 2.6476543 sec
RG                      50.8
DW                    40.400 usec
DE                     6.00 usec
TE                     293.0 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                     4.00 dB
SFO1             600.1337060 MHz

F2 - Processing parameters
SI                         65536
SF               600.1300181 MHz
WDW                           EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



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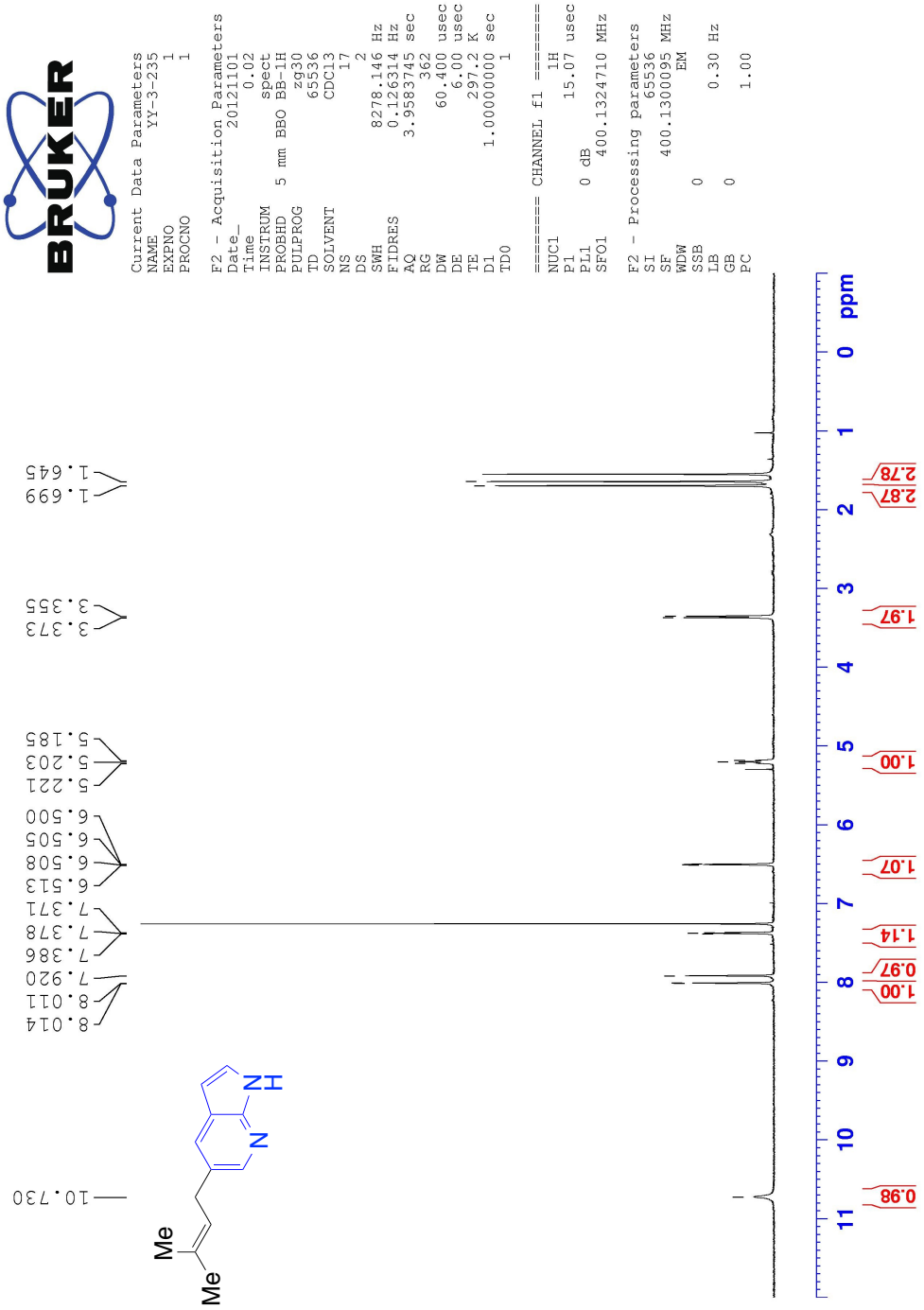
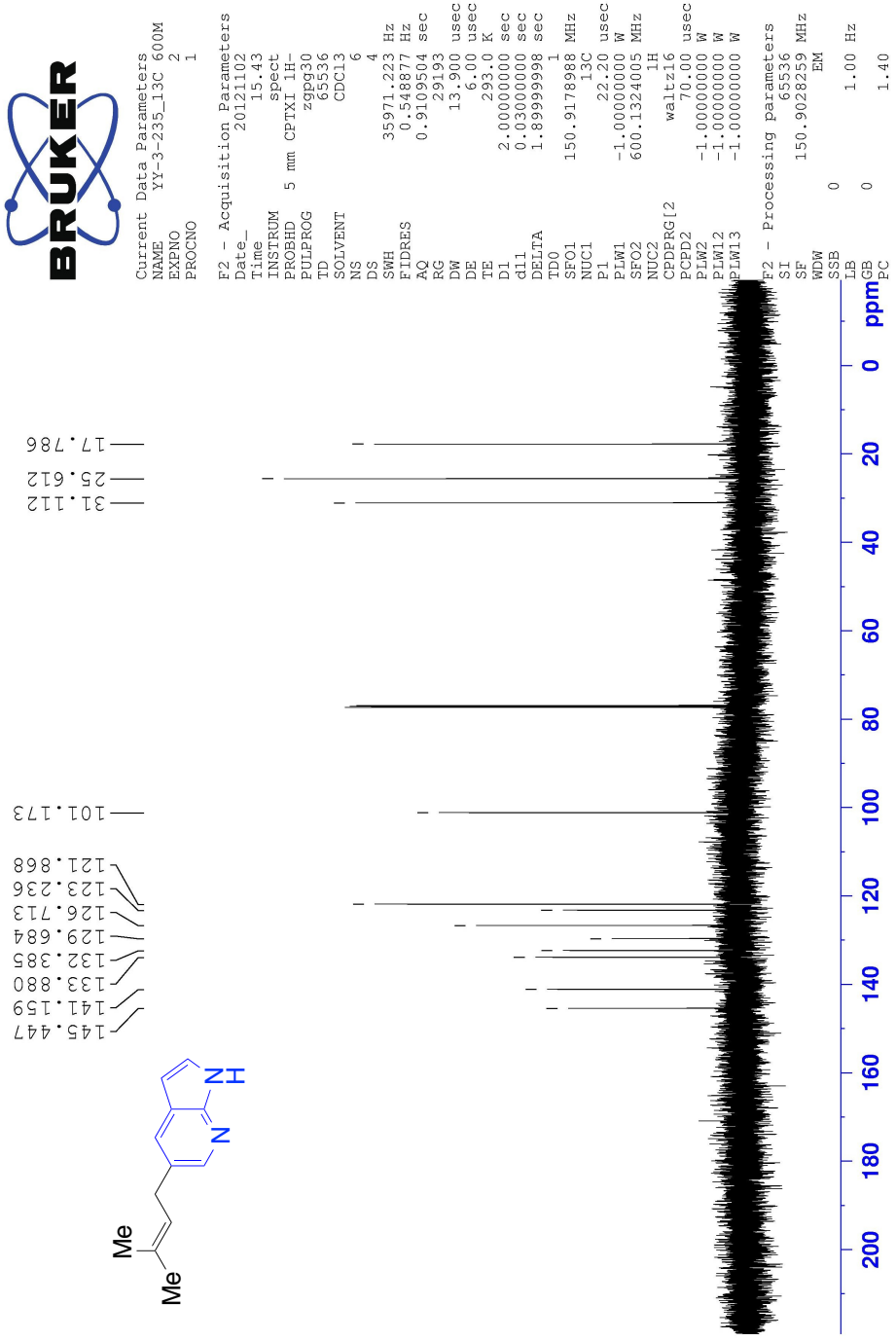
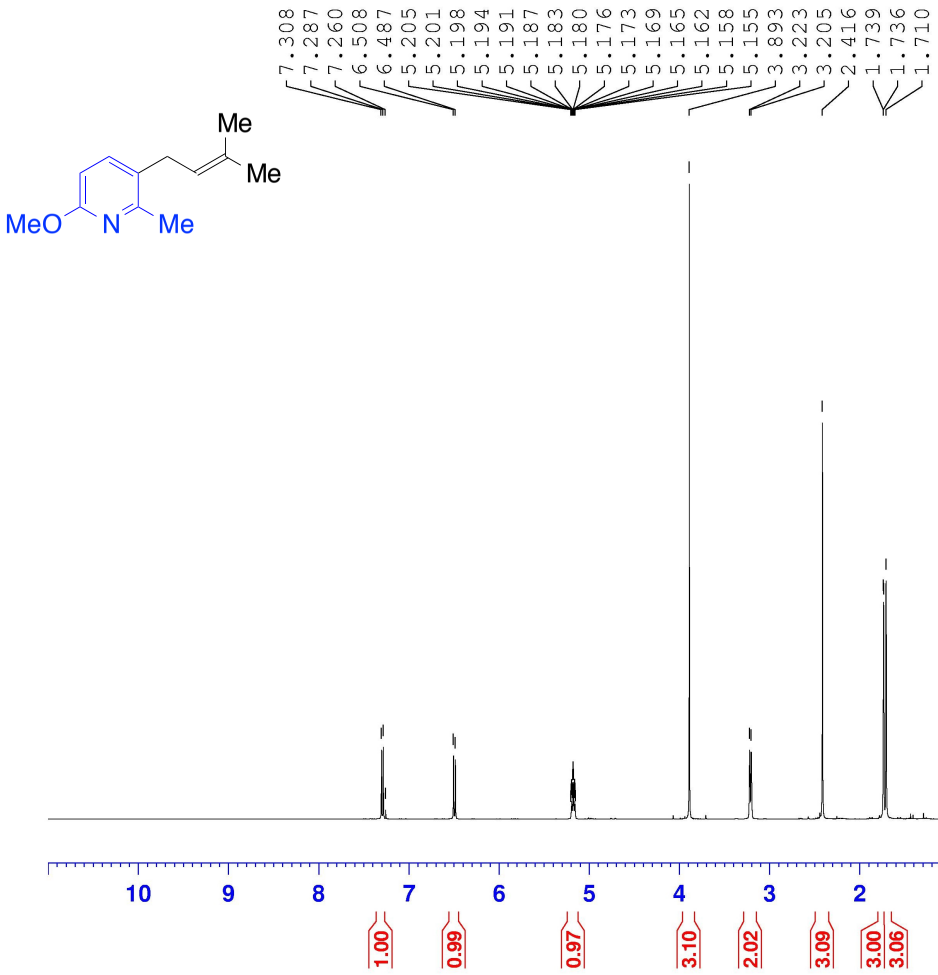
```
Current Data Parameters
NAME        YY-3-268 Fr2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20121109
Time              10.32
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    0
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ             1.3664256 sec
RG               18390.4
DW                20.850 usec
DE                 6.00 usec
TE                297.2 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                 8.75 usec
PLW1        -1.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        -1.00000000 W
PLW12       -1.00000000 W
PLW13       -1.00000000 W

F2 - Processing parameters
SI                65536
SF          100.6127684 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


Current Data Parameters
NAME YY-3-235
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121101
Time_ 0.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.07 usec
PL1 0 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10.730
8.014
8.011
7.920
7.386
7.378
7.371
6.513
6.508
6.505
6.500
5.221
5.203
5.185
3.373
3.355
1.699
1.645
2.78
2.87
1.97
1.00
1.07
1.14
0.97
1.00
0.98
Me
Me
NH
N
ppm


Current Data Parameters
NAME YY-3-235_13C 600M
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121102
Time 15.43
INSTRUM spect
PROBHD 5 mm CPTXI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9109504 sec
RG 29193
DW 13.900 usec
DE 6.00 usec
TE 293.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 22.20 usec
PLW1 -1.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 150.9028259 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.786
25.612
31.112
101.173
121.868
123.236
126.713
129.684
132.385
133.880
141.159
145.447
Me
Me
NH
N
200
180
160
140
120
100
80
60
40
20
0
ppm



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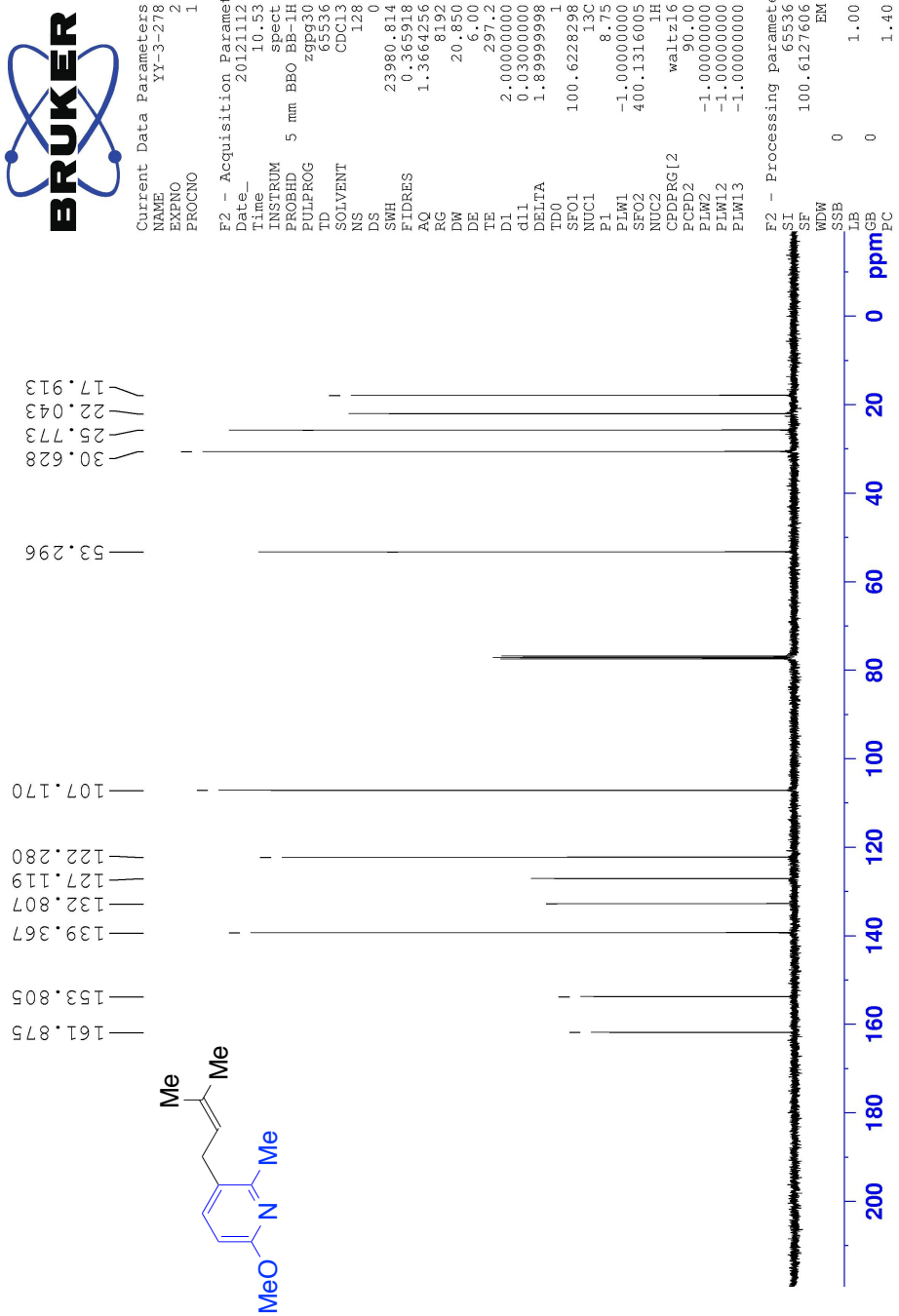
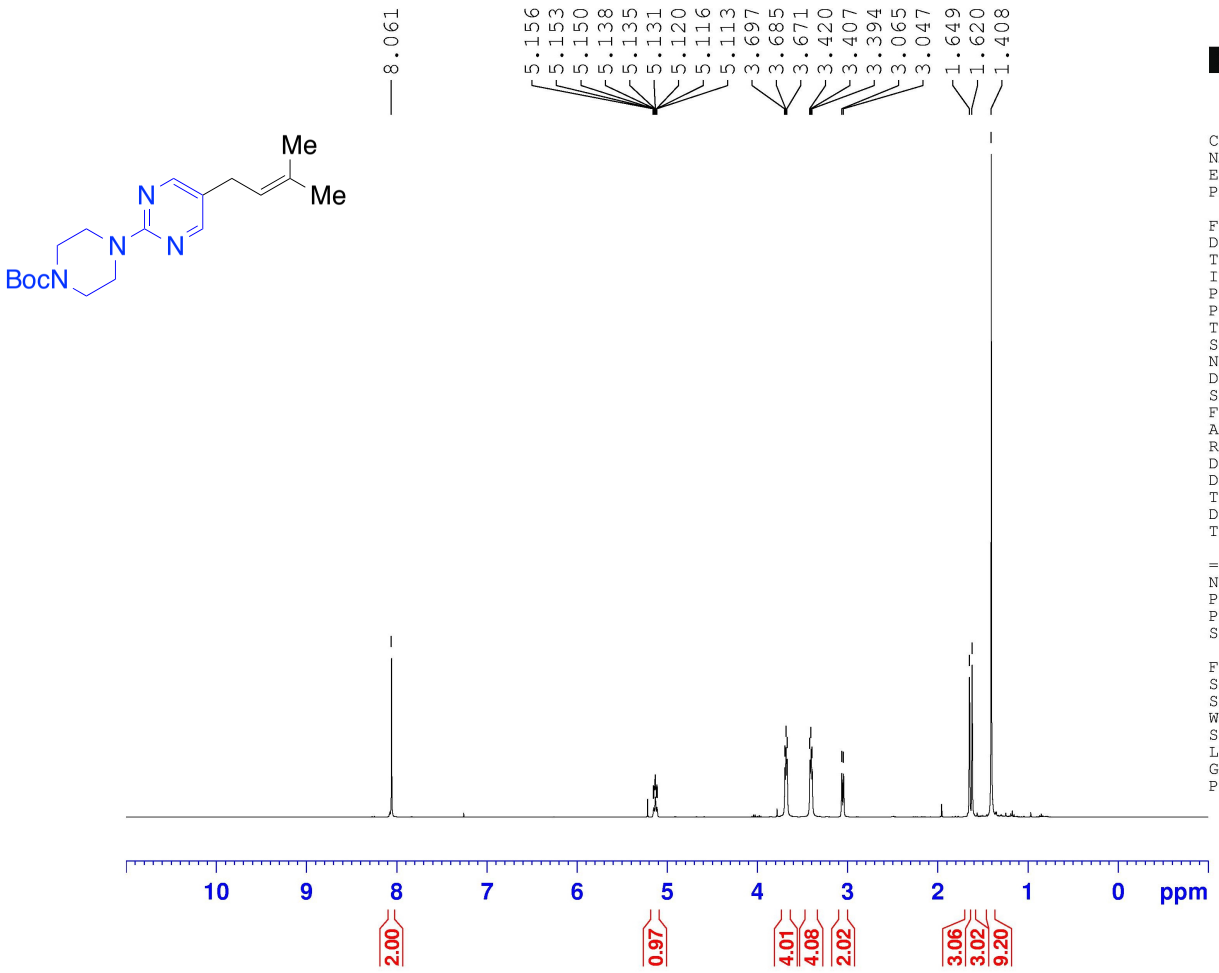
```
Current Data Parameters
NAME                  YY-3-278
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20121112
Time                    10.51
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          0
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9583745 sec
RG                       35.9
DW                     60.400 usec
DE                      6.00 usec
TE                     297.2 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1       0 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      65536
SF                400.1300094 MHz
WDW                        EM
SSB       0
LB                       0.30 Hz
GB        0
PC                       1.00
```


Current Data Parameters
NAME YY-3-278
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121112
Time 10.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127606 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
0
20
40
60
80
100
120
140
160
180
200
17.913
22.043
25.773
30.628
53.296
107.170
122.280
127.119
132.807
139.367
153.805
161.875
Me
Me
Me
N
MeO



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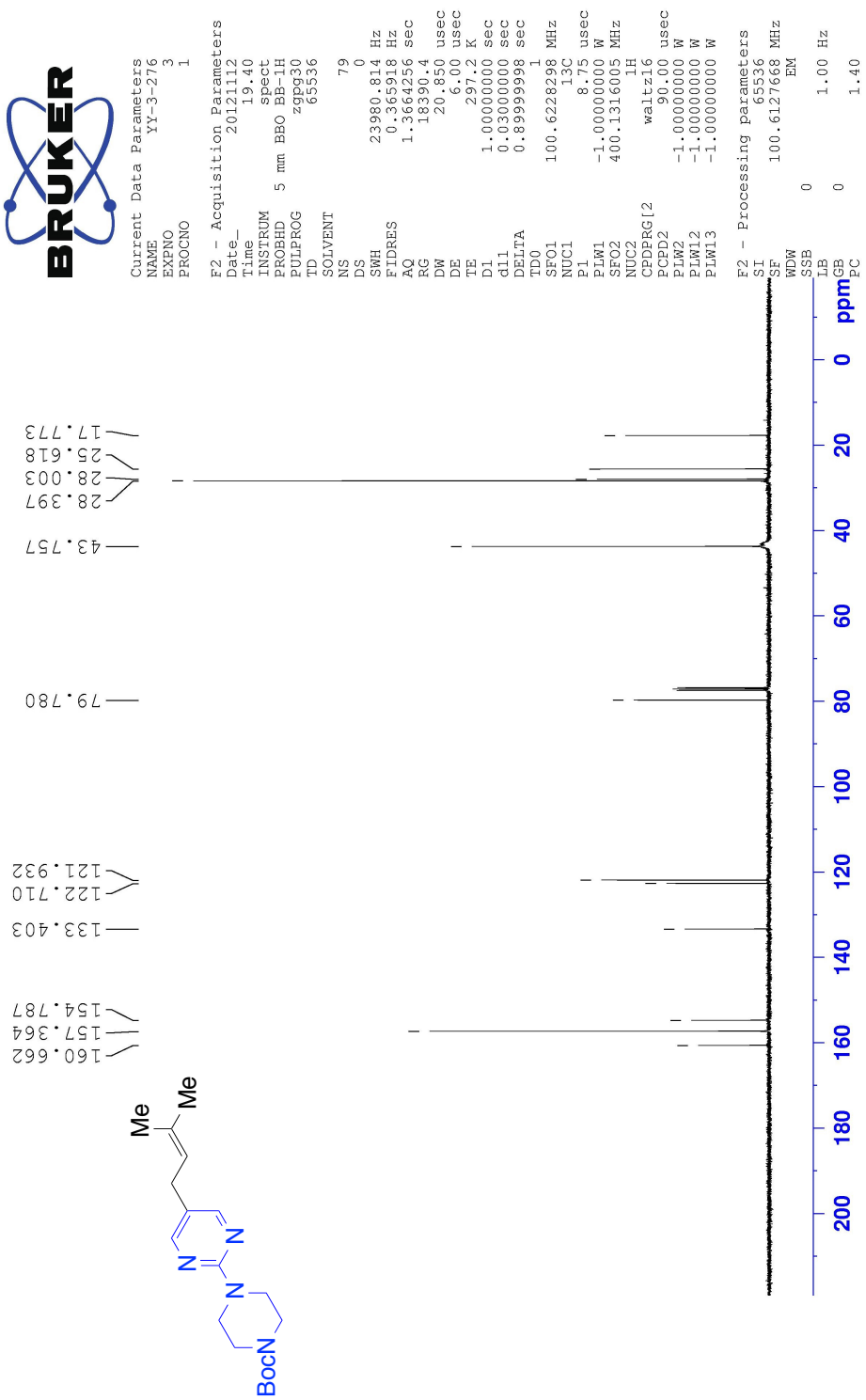
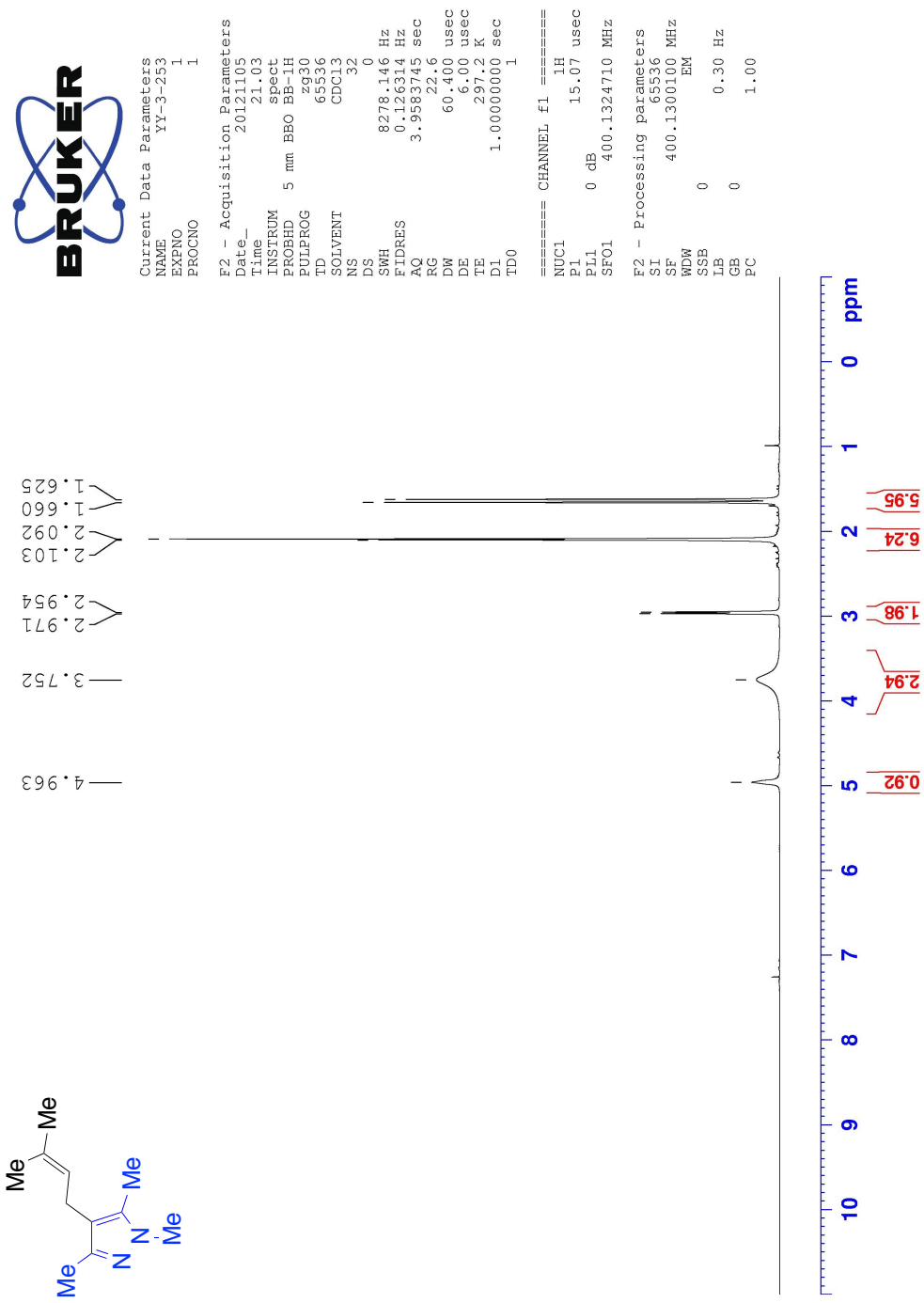
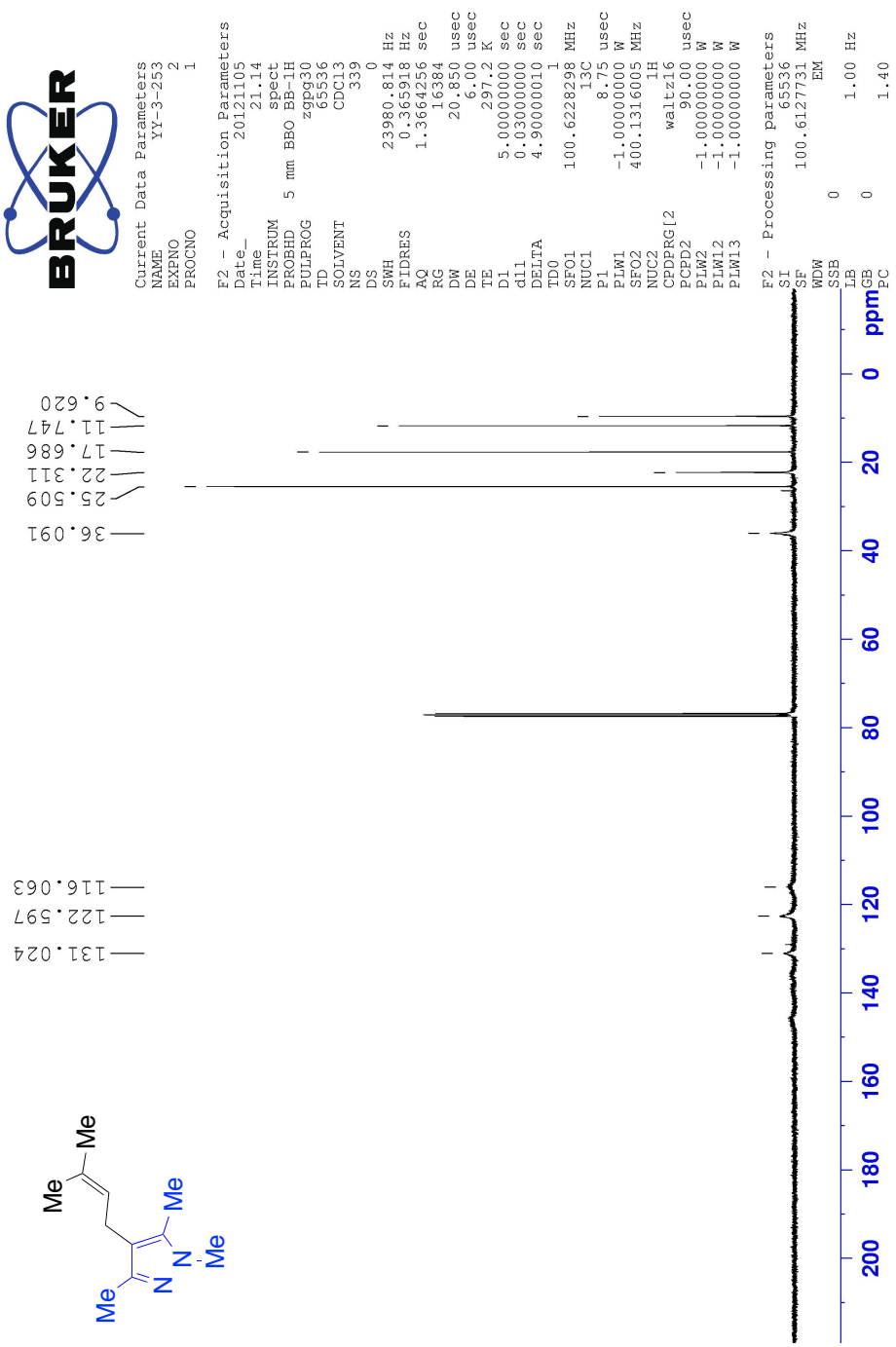
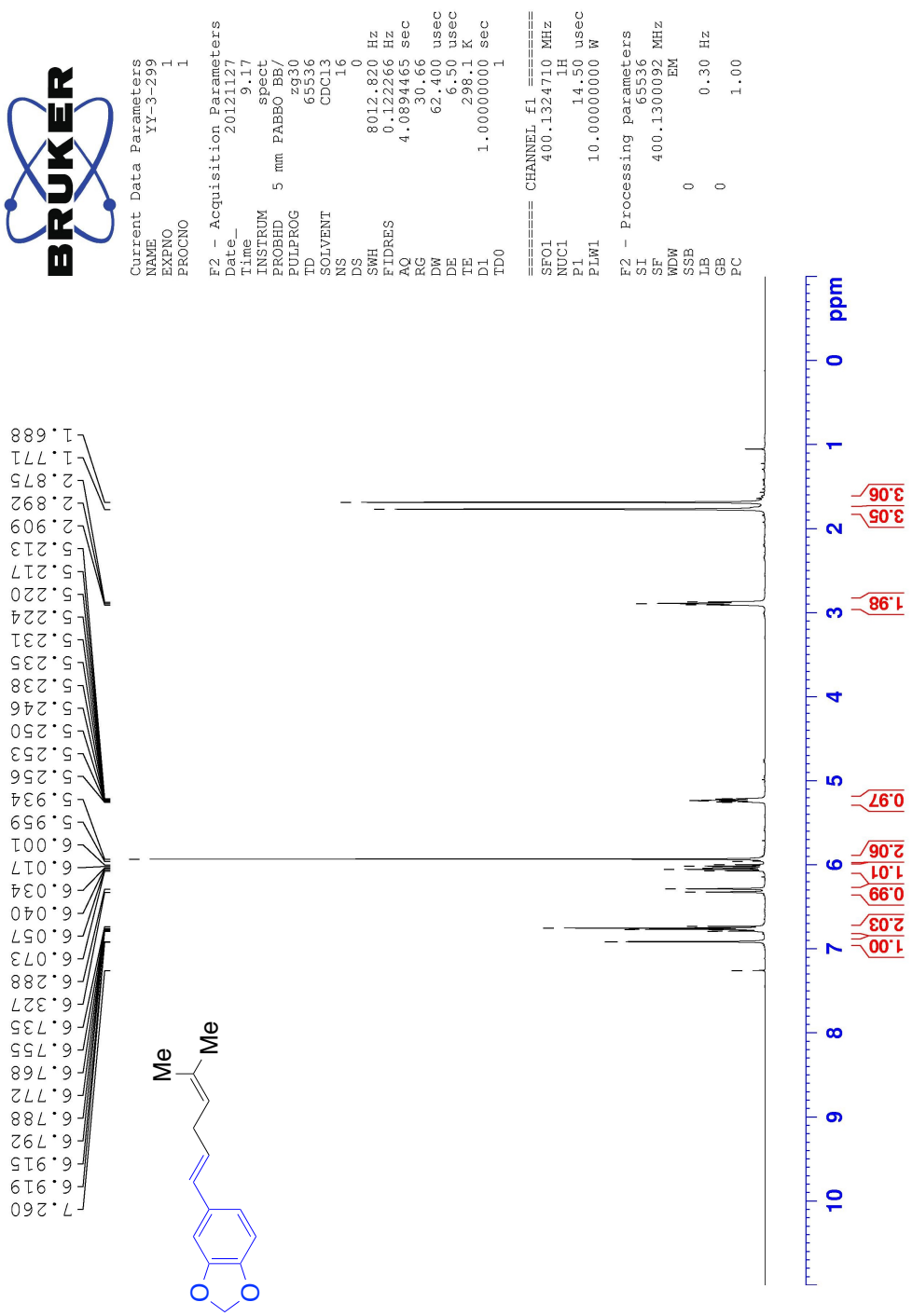
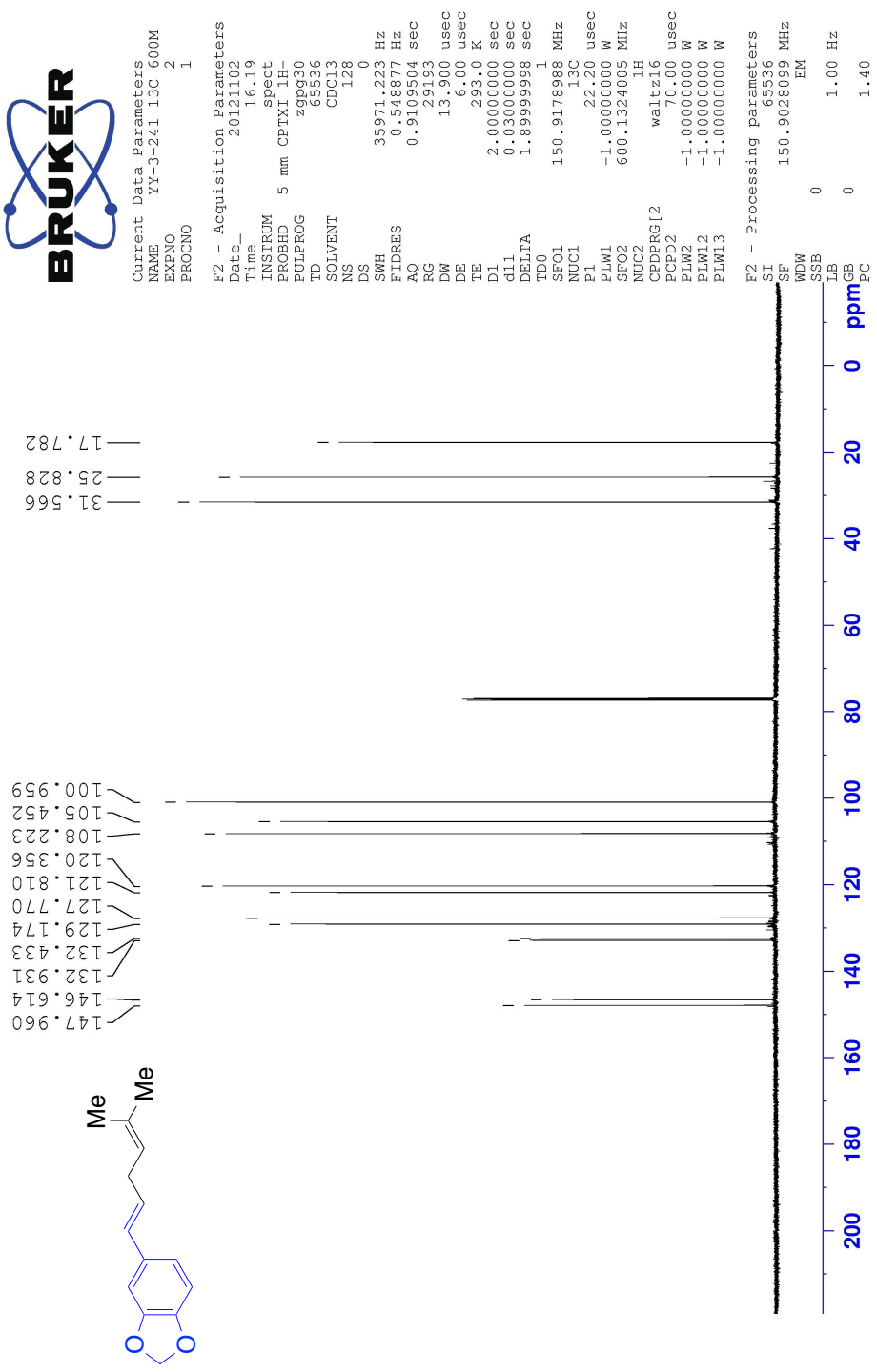
```
Current Data Parameters
NAME                  YY-3-276
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20121112
Time                     19.36
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9583745 sec
RG                          18
DW                       60.400 usec
DE                        6.00 usec
TE                       297.2 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.07 usec
PL1       0 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                 400.1300093 MHz
WDW                         EM
SSB       0
LB                        0.30 Hz
GB        0
PC                        1.00
```

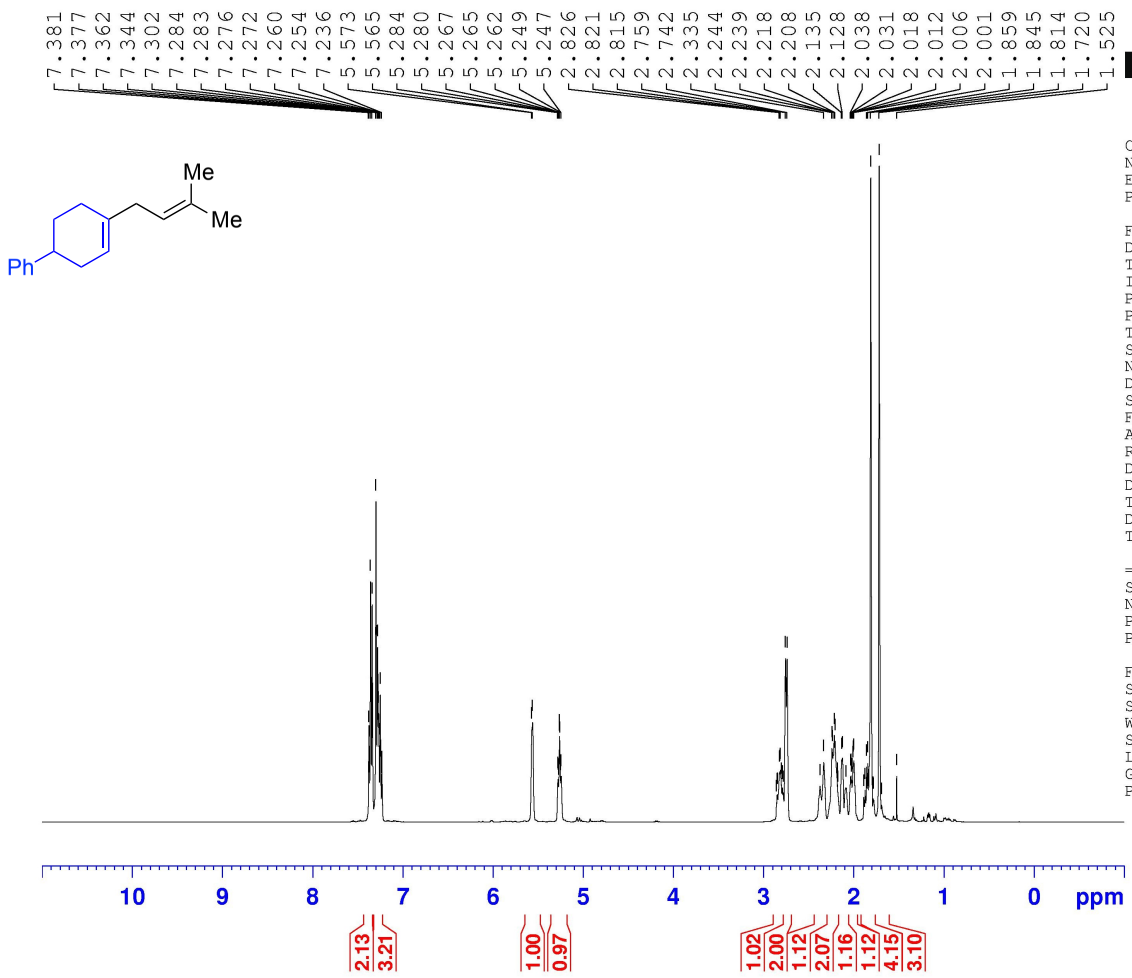

Current Data Parameters
NAME YY-3-276
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121112
Time 19.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT
NS 79
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127668 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.773
25.618
28.003
28.397
43.757
79.780
121.932
122.710
133.403
154.787
157.364
160.662
Me
Me
N
N
N
N
BocN
ppm
0
20
40
60
80
100
120
140
160
180
200


Current Data Parameters
NAME YY-3-253
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121105
Time 21.03
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 22.6
DW 60.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.07 usec
PL1 0 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4.963
3.752
2.971
2.954
2.103
2.092
1.660
1.625
0.92
2.94
1.98
6.24
5.95
ppm
Me
Me
Me
Me
N
N
Me

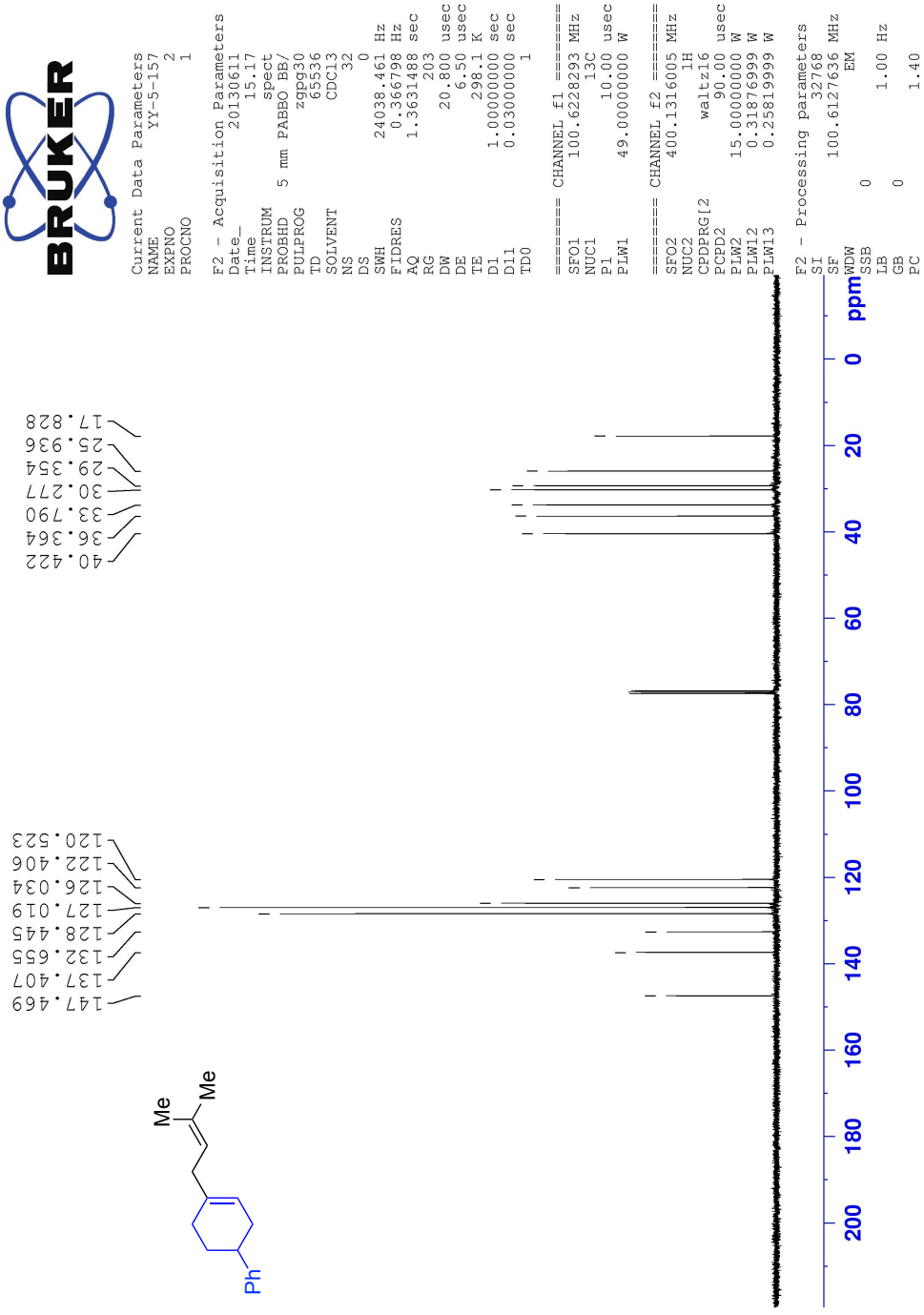

Current Data Parameters
NAME YY-3-253
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121105
Time 21.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 339
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 8.75 usec
PLW1 -1.00000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
9.620
11.747
17.686
22.311
25.509
36.091
116.063
122.597
131.024
ppm
0
20
40
60
80
100
120
140
160
180
200
Me
Me
Me
Me
N
N
Me

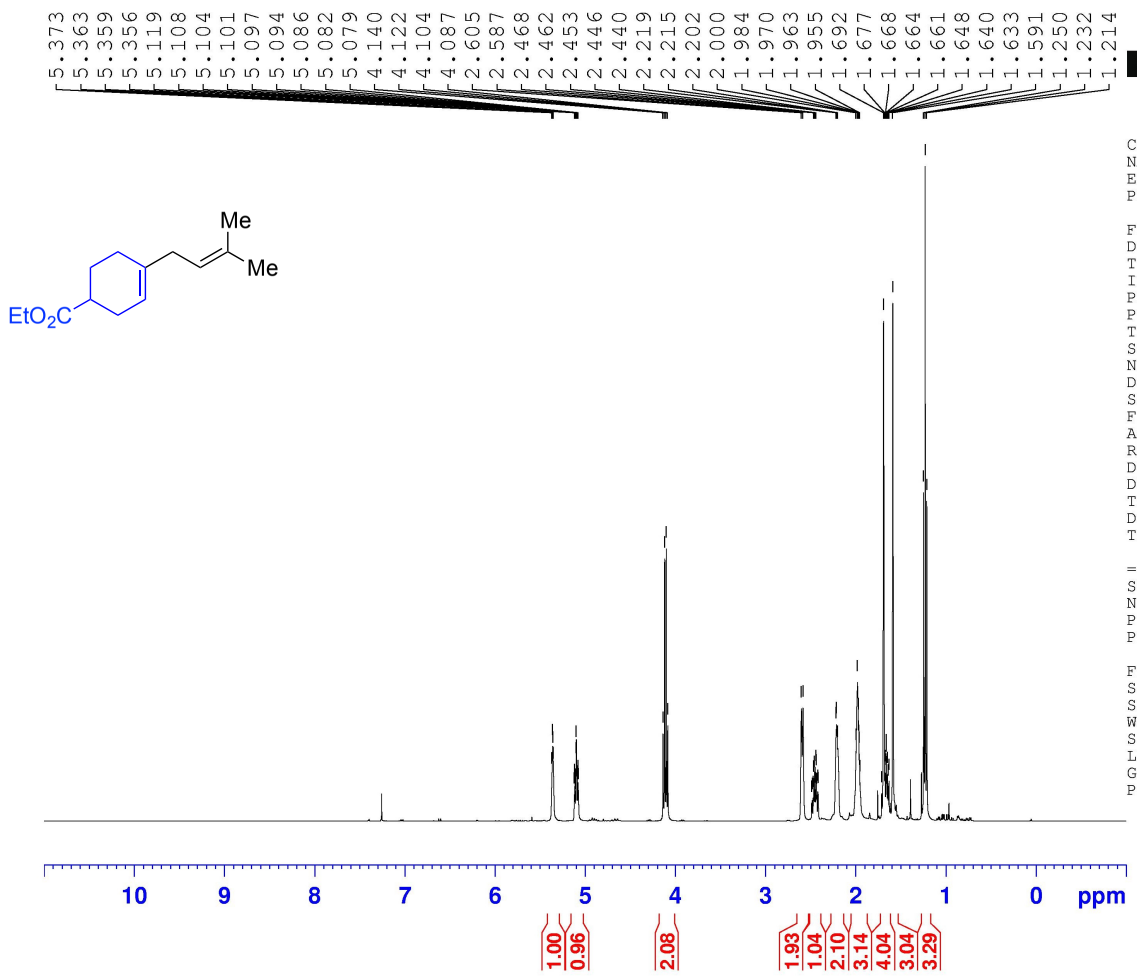

Current Data Parameters
NAME YY-3-299
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121127
Time 9.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 30.66
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.260
6.919
6.915
6.792
6.788
6.772
6.768
6.755
6.735
6.327
6.288
6.073
6.057
6.040
6.034
6.017
6.001
5.959
5.934
5.256
5.253
5.250
5.246
5.238
5.235
5.231
5.224
5.220
5.217
5.213
2.909
2.892
2.875
1.771
1.688
Me
Me
O
O
ppm
10
9
8
7
6
5
4
3
2
1
0
1.00
2.03
0.99
1.01
2.06
0.97
1.98
3.05
3.06

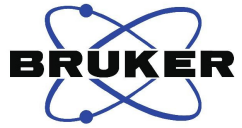

Current Data Parameters
NAME YY-3-241 13C 600M
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121102
Time 16.19
INSTRUM spect
PROBHD 5 mm CPTXI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.91109504 sec
RG 29193
DW 13.900 usec
DE 6.00 usec
TE 293.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 22.20 usec
PLW1 -1.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 65536
SF 150.9028099 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.782
25.828
31.566
100.959
105.452
108.223
120.356
121.810
127.770
129.174
132.433
132.931
146.614
147.960
Me
Me
O
O
ppm
200
180
160
140
120
100
80
60
40
20
0



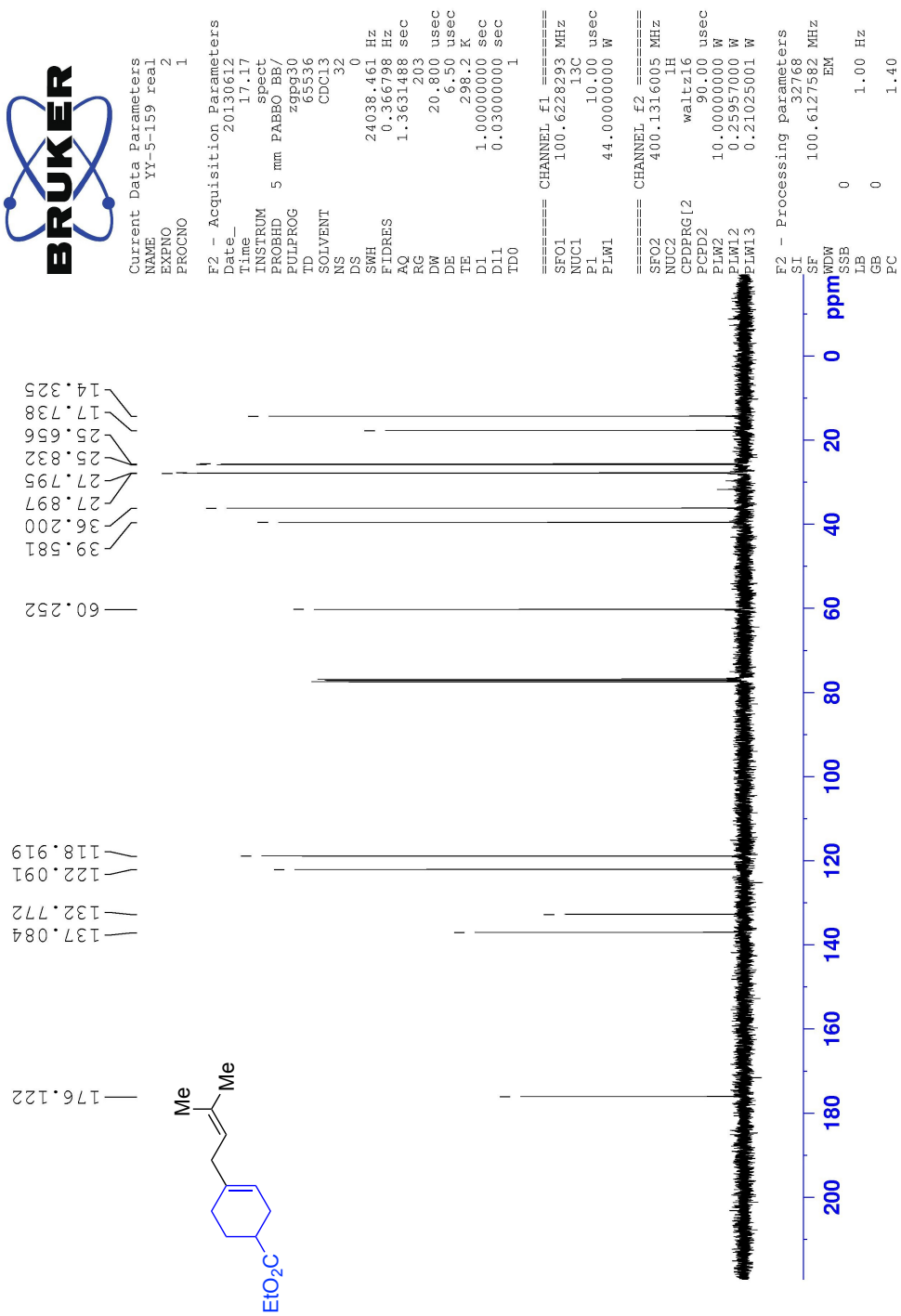

```
Current Data Parameters
NAME                  YY-5-157
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130611
Time                     15.14
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                          32
DW                       62.400 usec
DE                        6.50 usec
TE                       298.1 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       13.12 usec
PLW1               15.00000000 W

F2 - Processing parameters
SI                       65536
SF                  400.1300089 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

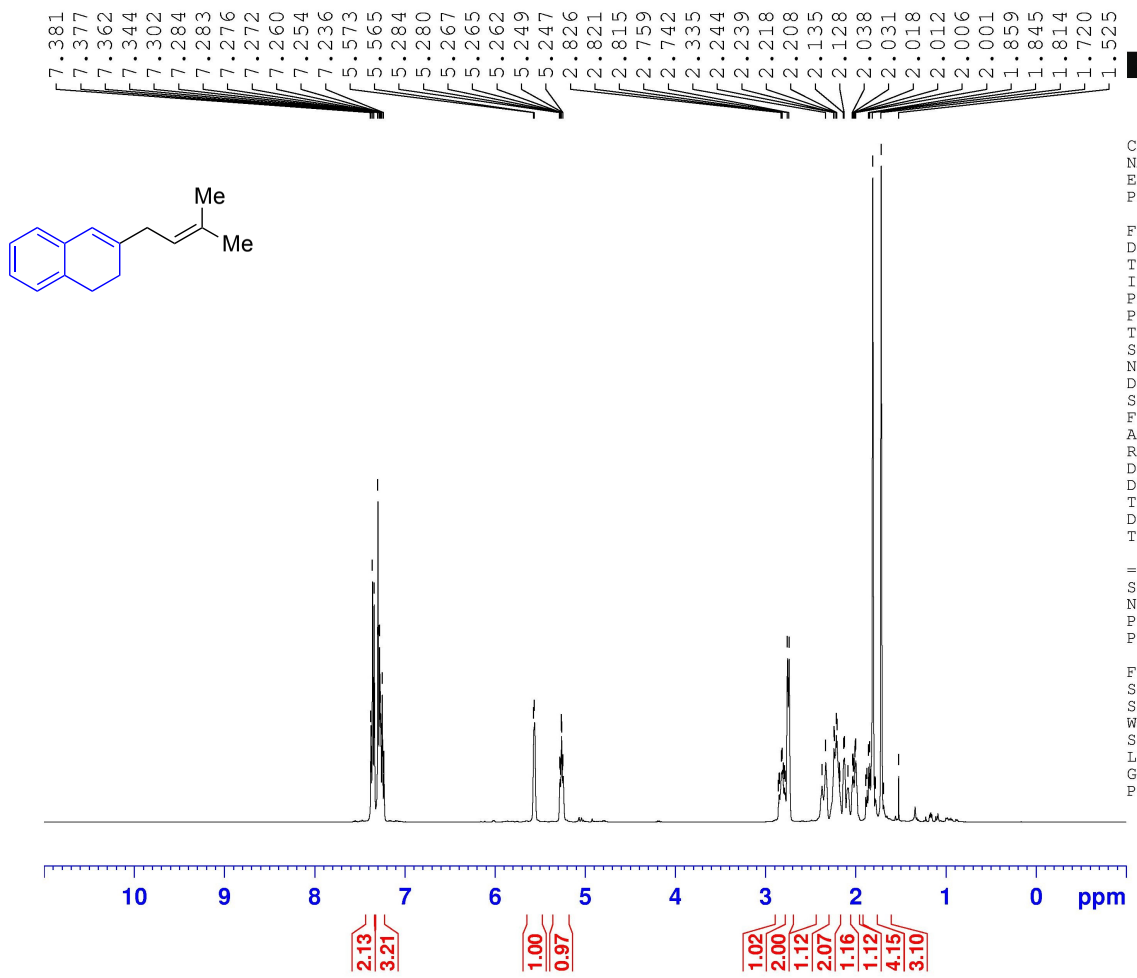

Current Data Parameters
NAME YY-5-157
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130611
Time 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127636 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
147.469
137.407
132.655
128.445
127.019
126.034
122.406
120.523
40.422
36.364
33.790
30.277
29.354
25.936
17.828
Me
Me
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm



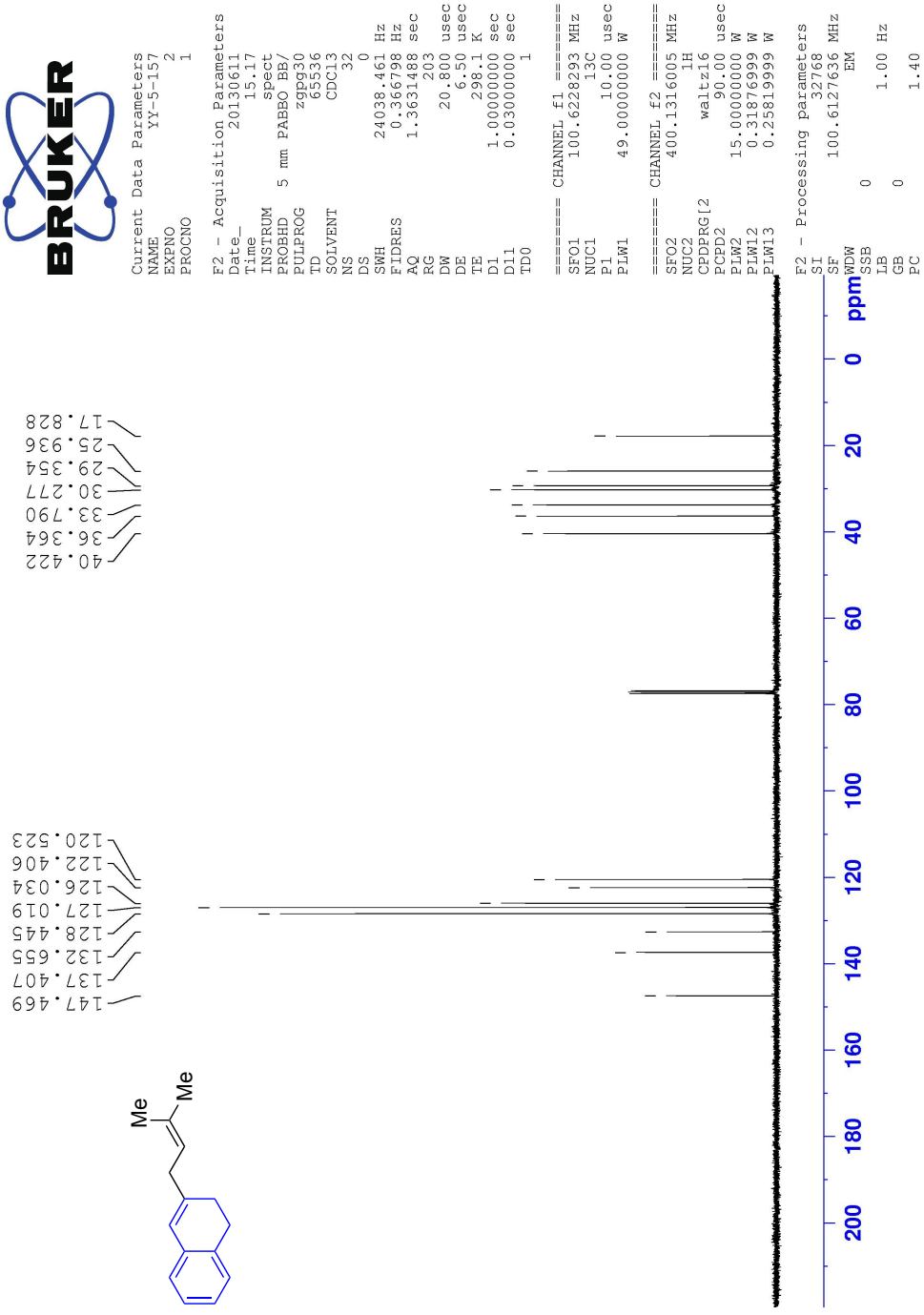


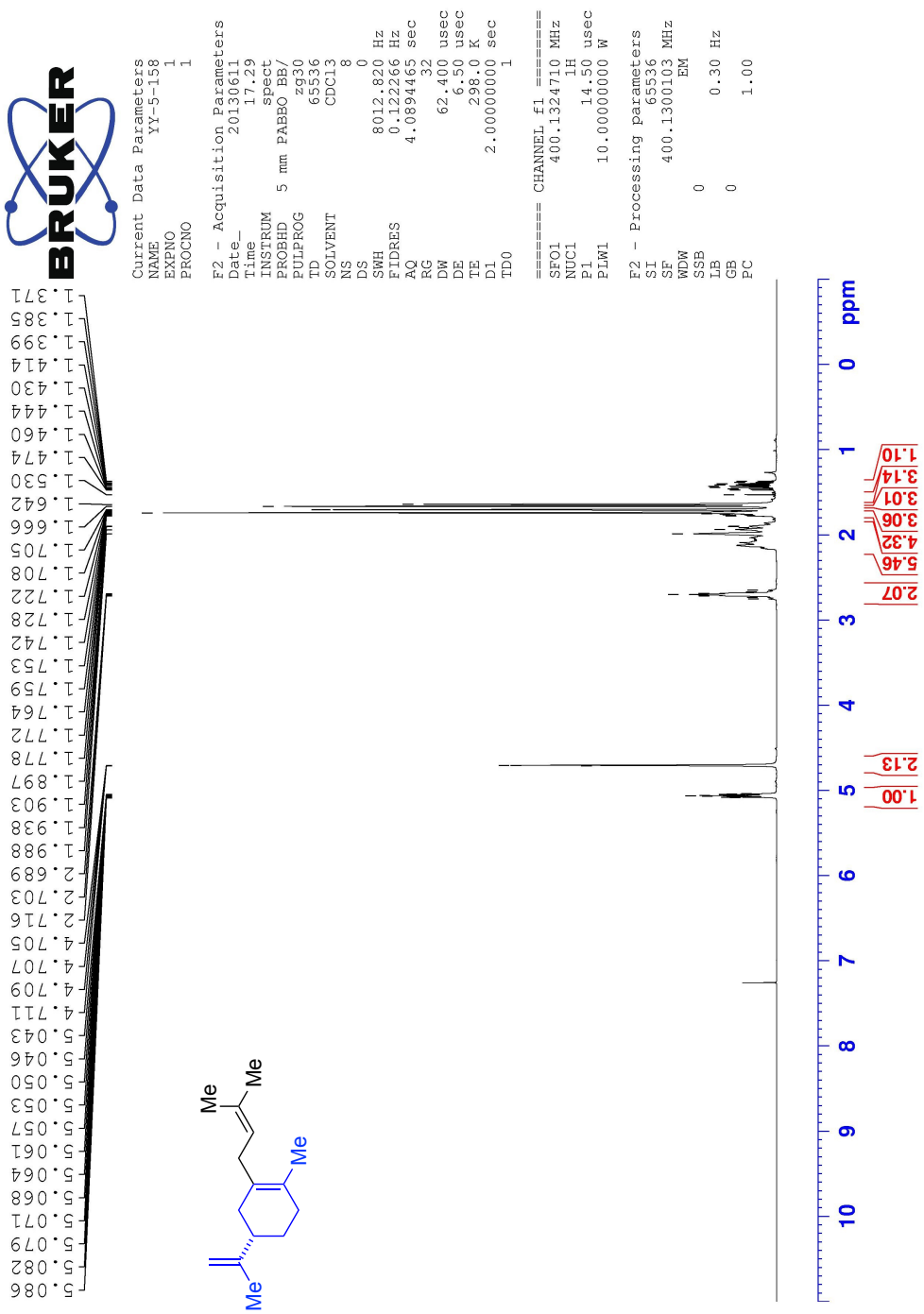

```
Current Data Parameters
NAME       YY-5-159 real
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20130612
Time              17.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                   32
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                14.50 usec
PLW1         10.00000000 W

F2 - Processing parameters
SI                65536
SF           400.1300100 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

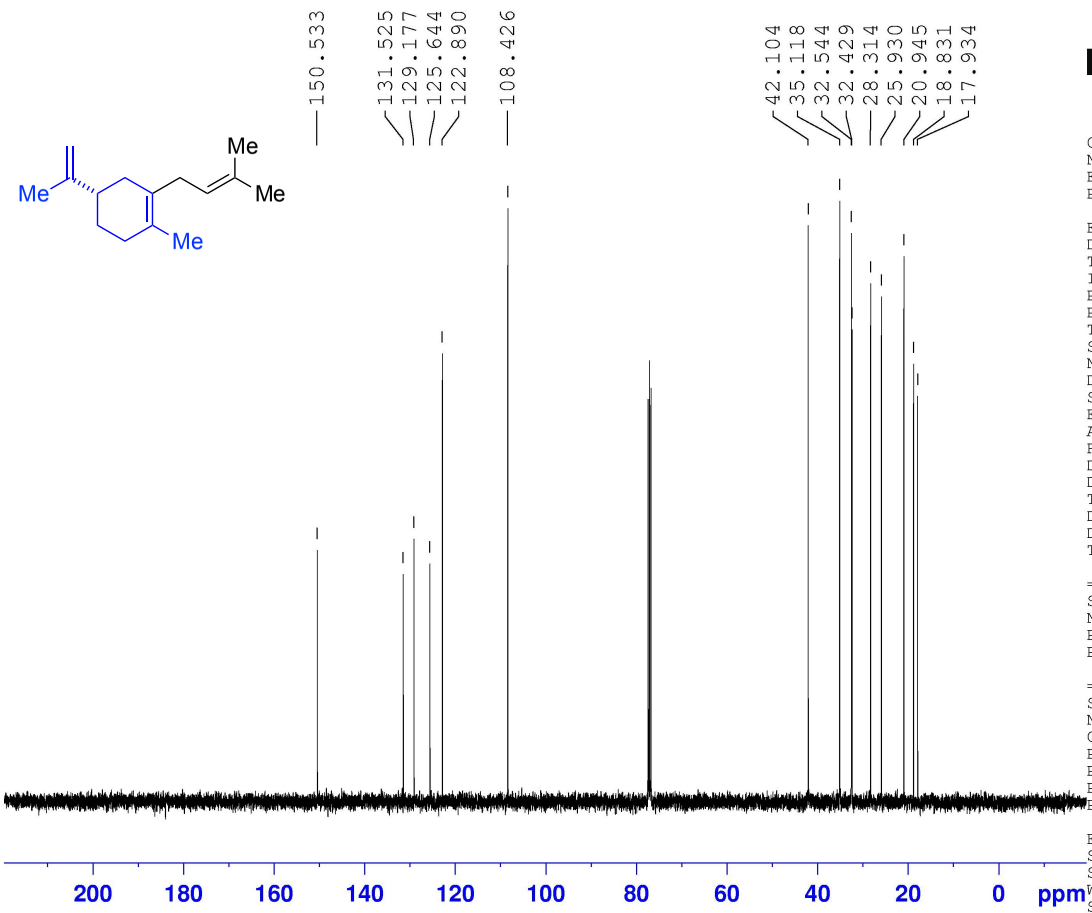

Current Data Parameters
NAME YY-5-159 real
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130612
Time_ 17.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 44.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.25957000 W
PLW13 0.21025001 W
F2 - Processing parameters
SI 32768
SF 100.6127582 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
14.325
17.738
25.656
25.832
27.795
27.897
36.200
39.581
60.252
118.919
122.091
132.772
137.084
176.122
Me
Me
EtO2C
ppm
0
20
40
60
80
100
120
140
160
180
200




```
Current Data Parameters
NAME                  YY-5-157
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130611
Time                     15.14
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                          32
DW                     62.400 usec
DE                      6.50 usec
TE                      298.1 K
D1                 2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                        1H
P1                      13.12 usec
PLW1           15.00000000 W

F2 - Processing parameters
SI                      65536
SF              400.1300089 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```


Current Data Parameters
NAME YY-5-157
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130611
Time 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127636 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
147.469
137.407
132.655
128.445
127.019
126.034
122.406
120.523
40.422
36.364
33.790
30.277
29.354
25.936
17.828
Me
Me
ppm
200
180
160
140
120
100
80
60
40
20
0


Current Data Parameters
NAME YY-5-158
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130611
Time 17.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
Me
Me
Me
ppm
1.00
2.13
2.07
5.46
4.32
3.06
3.01
3.14
1.10



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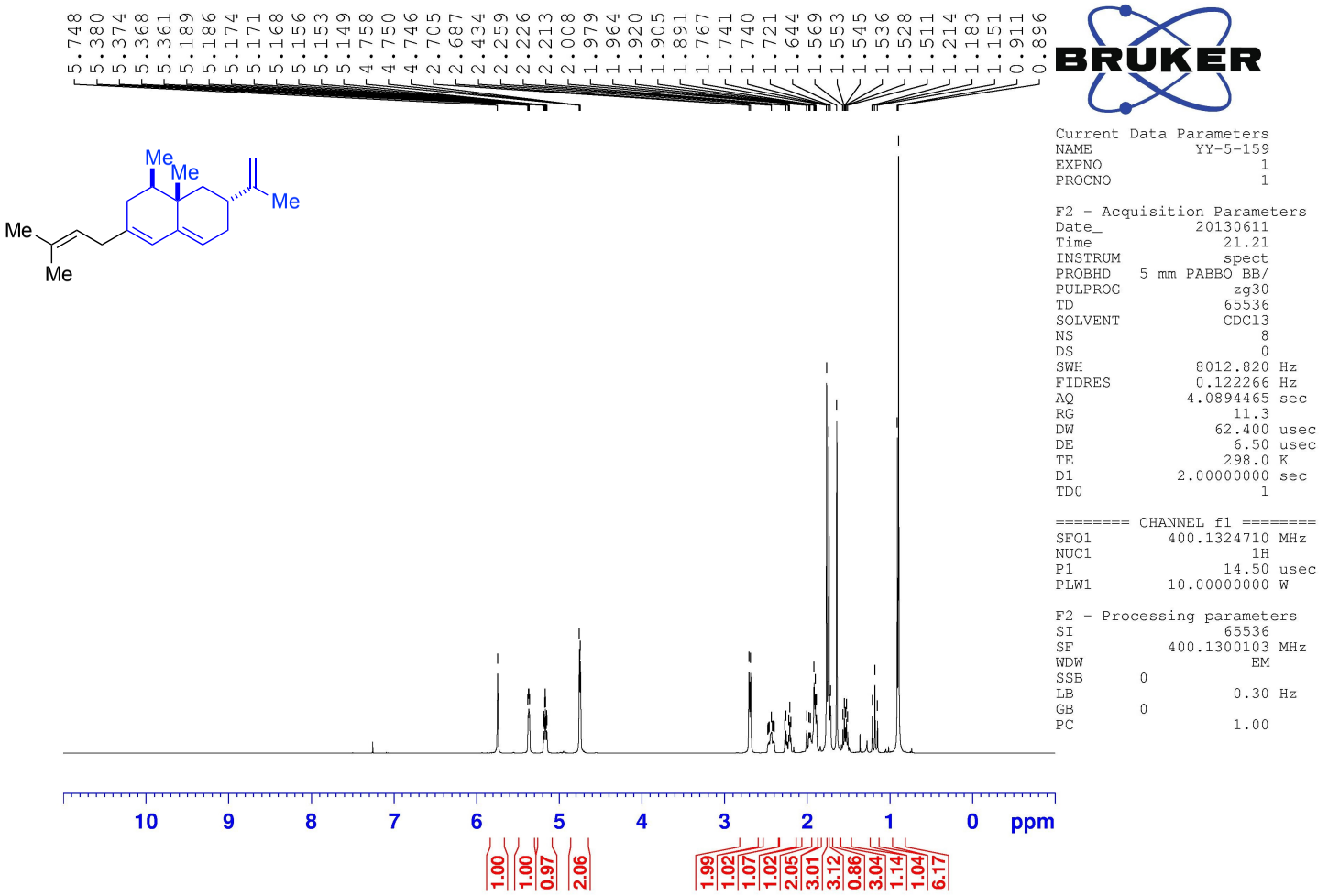
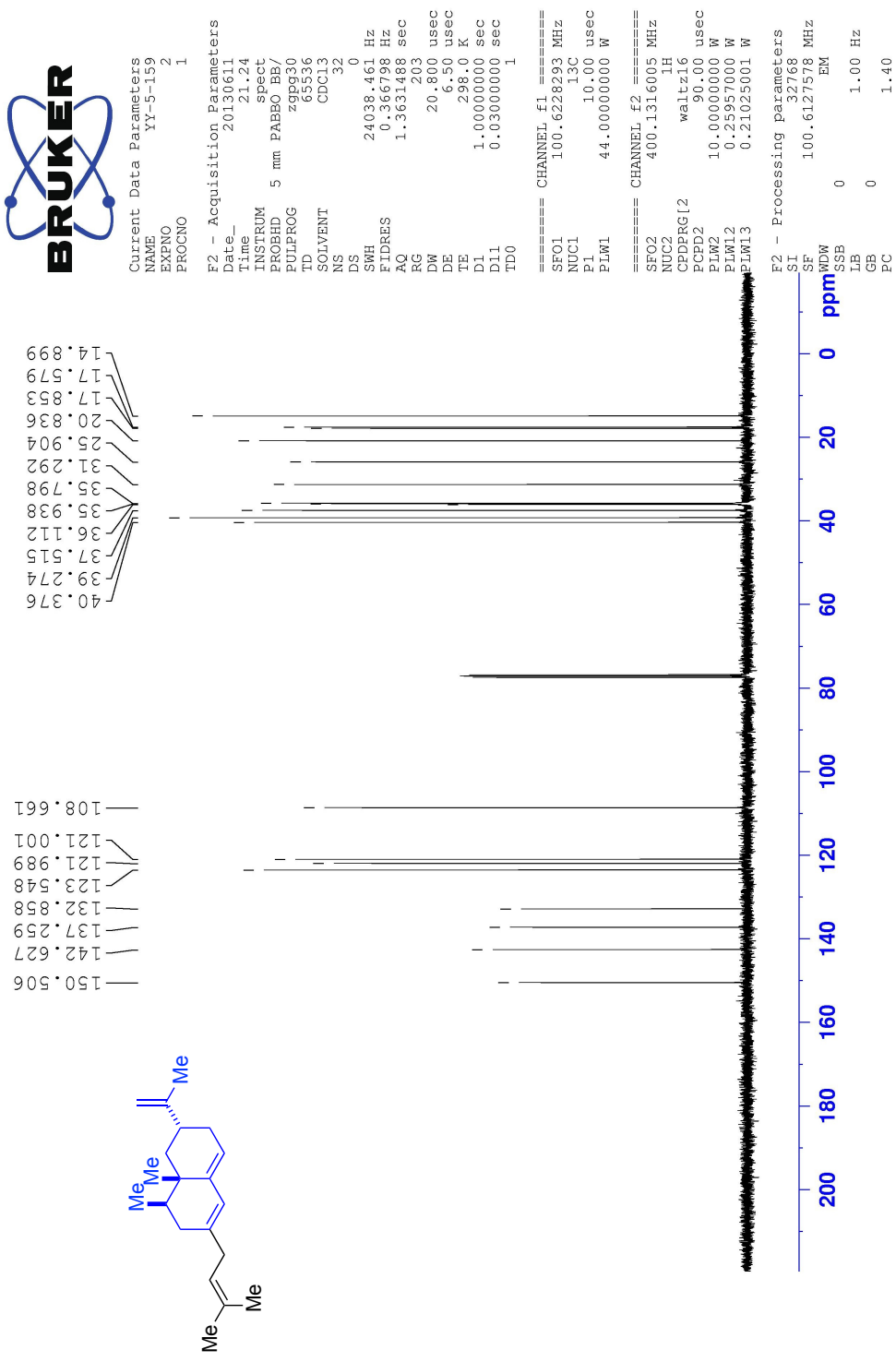
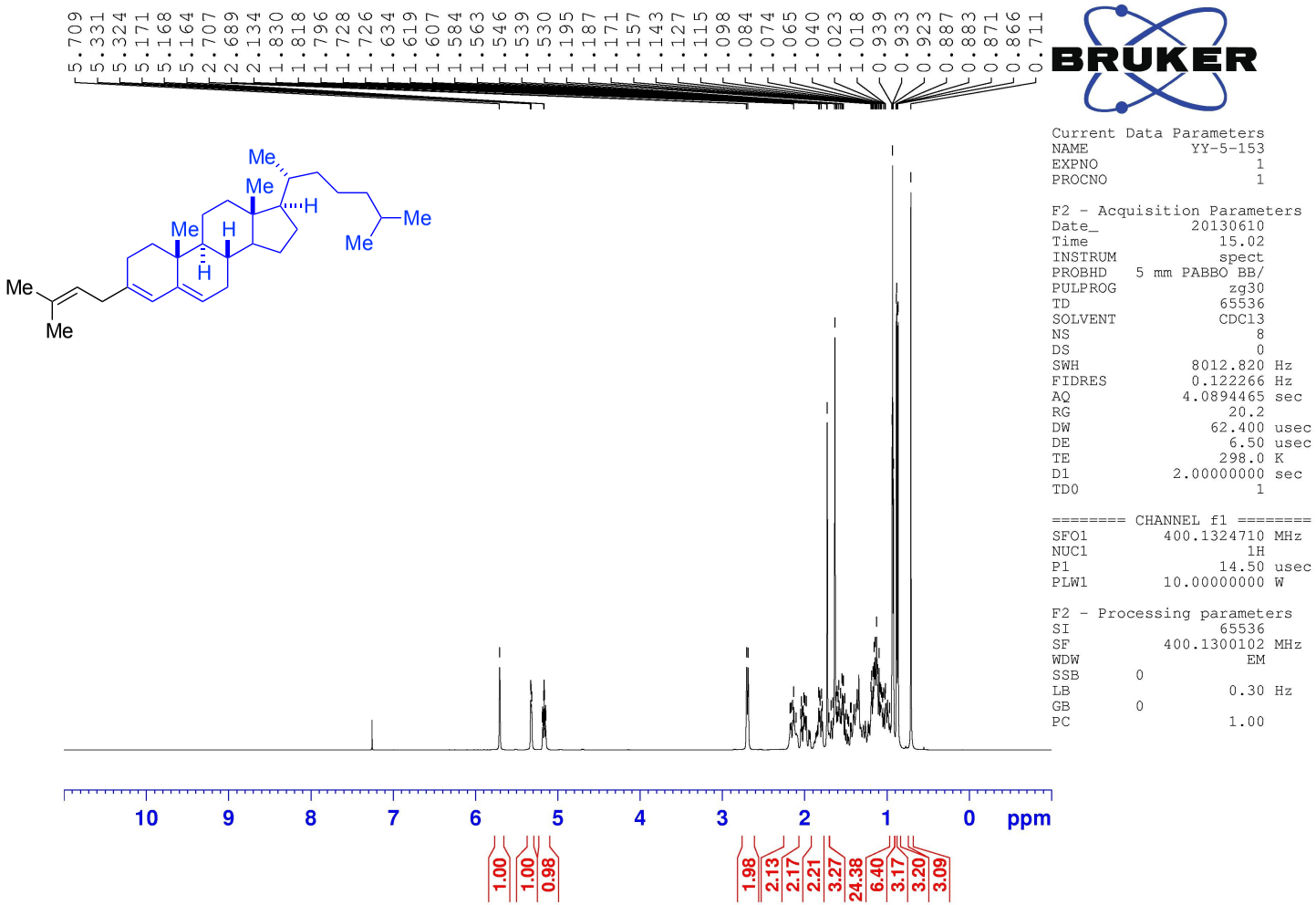
```
Current Data Parameters
NAME                  YY-5-158
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130611
Time                     17.30
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          32
DS                           0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                         203
DW                    20.800 usec
DE                     6.50 usec
TE                     298.1 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             100.6228293 MHz
NUC1                      13C
P1                      10.00 usec
PLW1             44.00000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                   90.00 usec
PLW2             10.00000000 W
PLW12             0.25957000 W
PLW13             0.21025001 W

F2 - Processing parameters
SI                       32768
SF               100.6127548 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

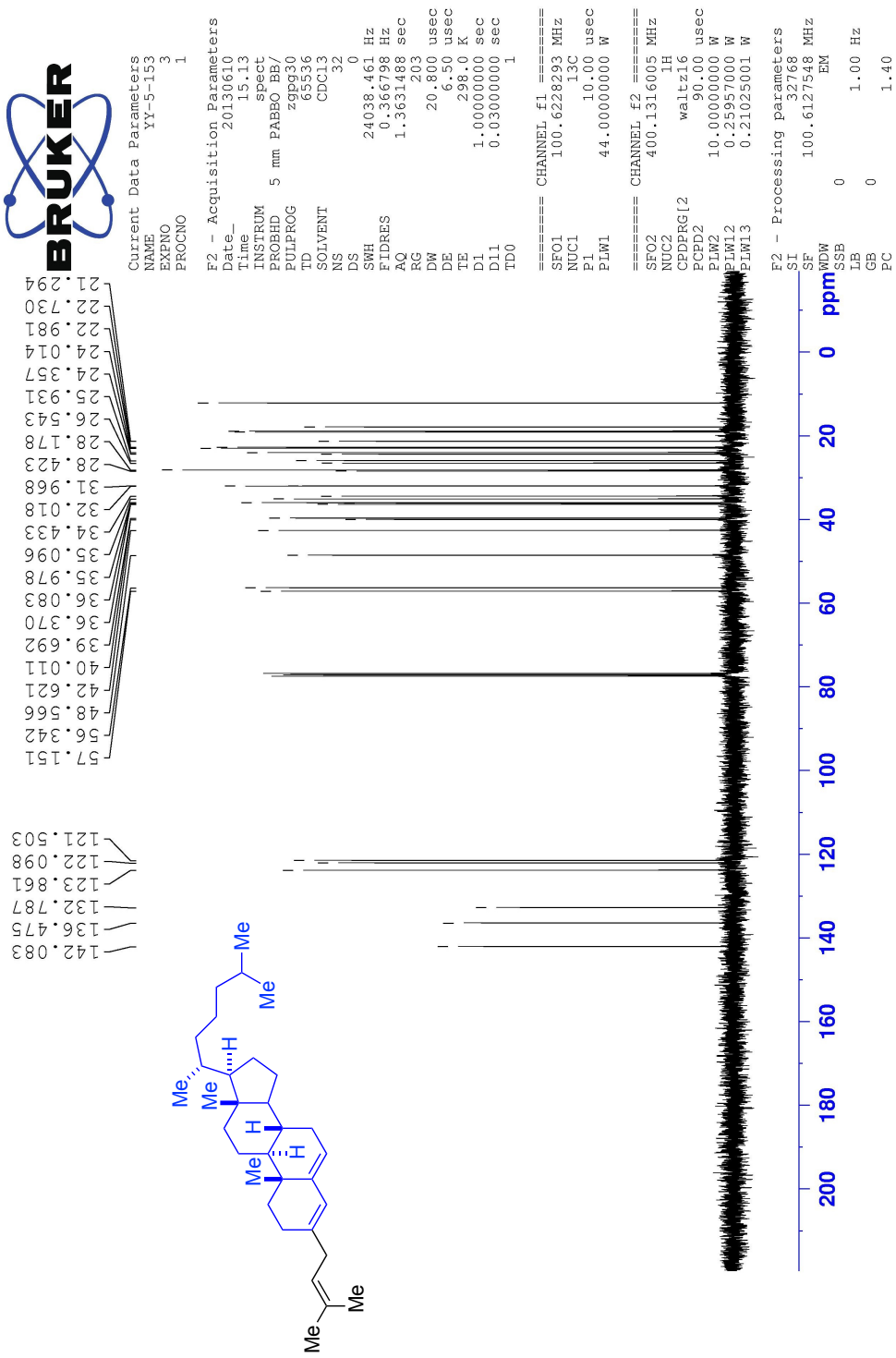


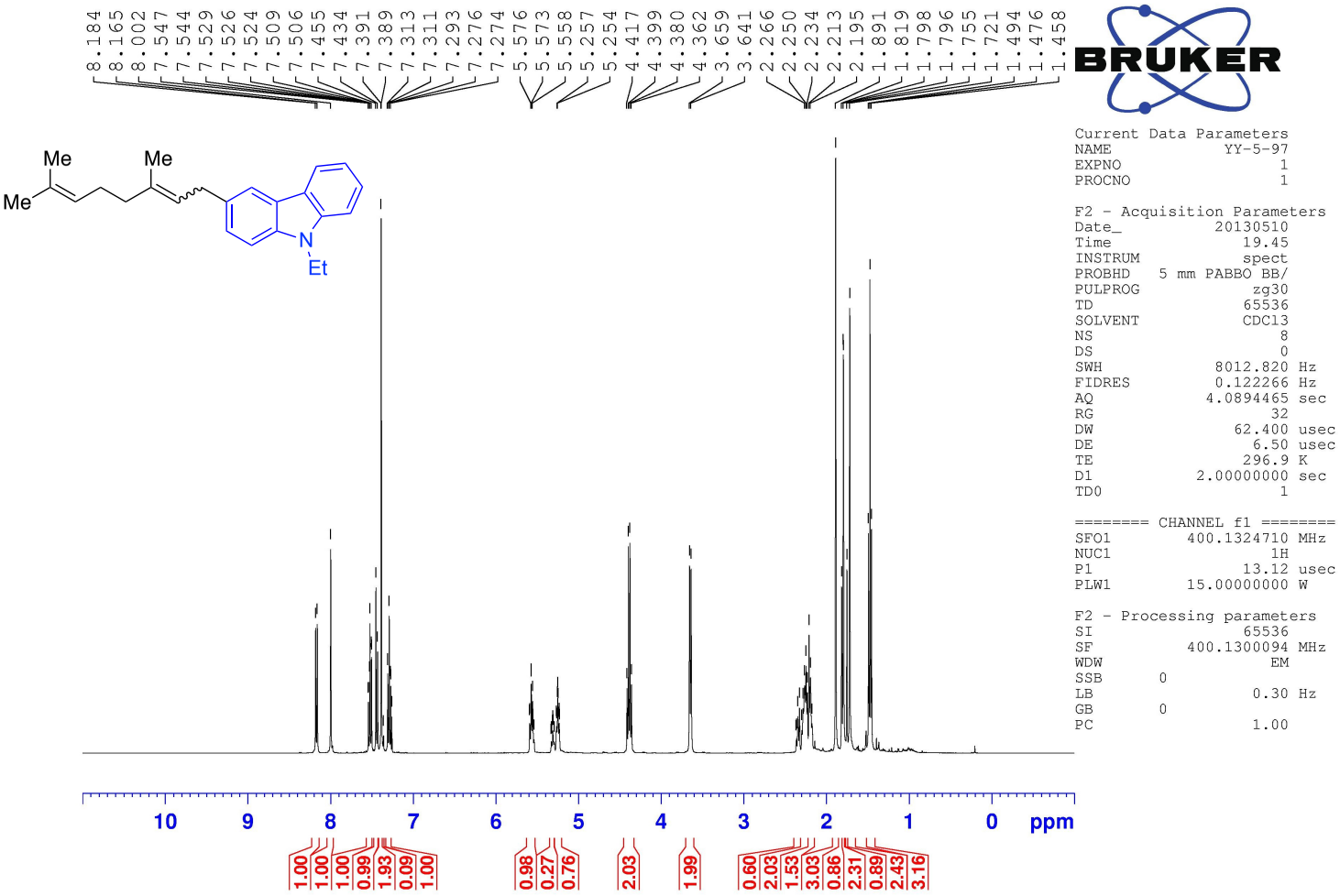

```
Current Data Parameters
NAME                  YY-5-159
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130611
Time                     21.21
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                        11.3
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1            10.00000000 W

F2 - Processing parameters
SI                      65536
SF               400.1300103 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```


Current Data Parameters
NAME YY-5-159
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130611
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 44.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.25957000 W
PLW13 0.21025001 W
F2 - Processing parameters
SI 32768
SF 100.6127578 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150.506
142.627
137.259
132.858
123.548
121.989
121.001
108.661
40.376
39.274
37.515
36.112
35.938
35.798
31.292
25.904
20.836
17.853
17.579
14.899
ppm
Me
Me
Me
Me
Me



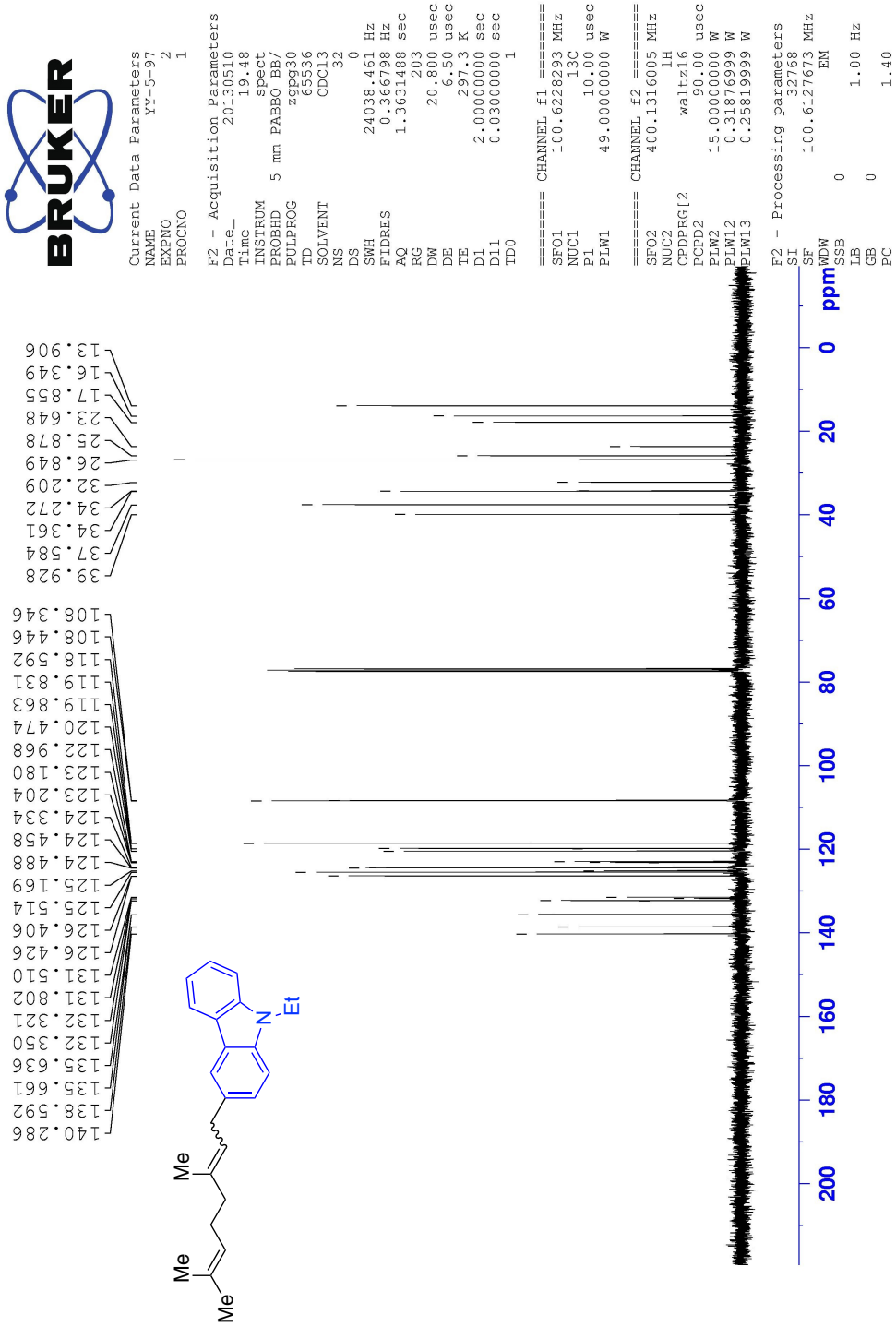

```
Current Data Parameters
NAME                  YY-5-153
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130610
Time                     15.02
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                        20.2
DW                      62.400 usec
DE                       6.50 usec
TE                      298.0 K
D1                  2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1            10.00000000 W

F2 - Processing parameters
SI                      65536
SF               400.1300102 MHz
WDW                        EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

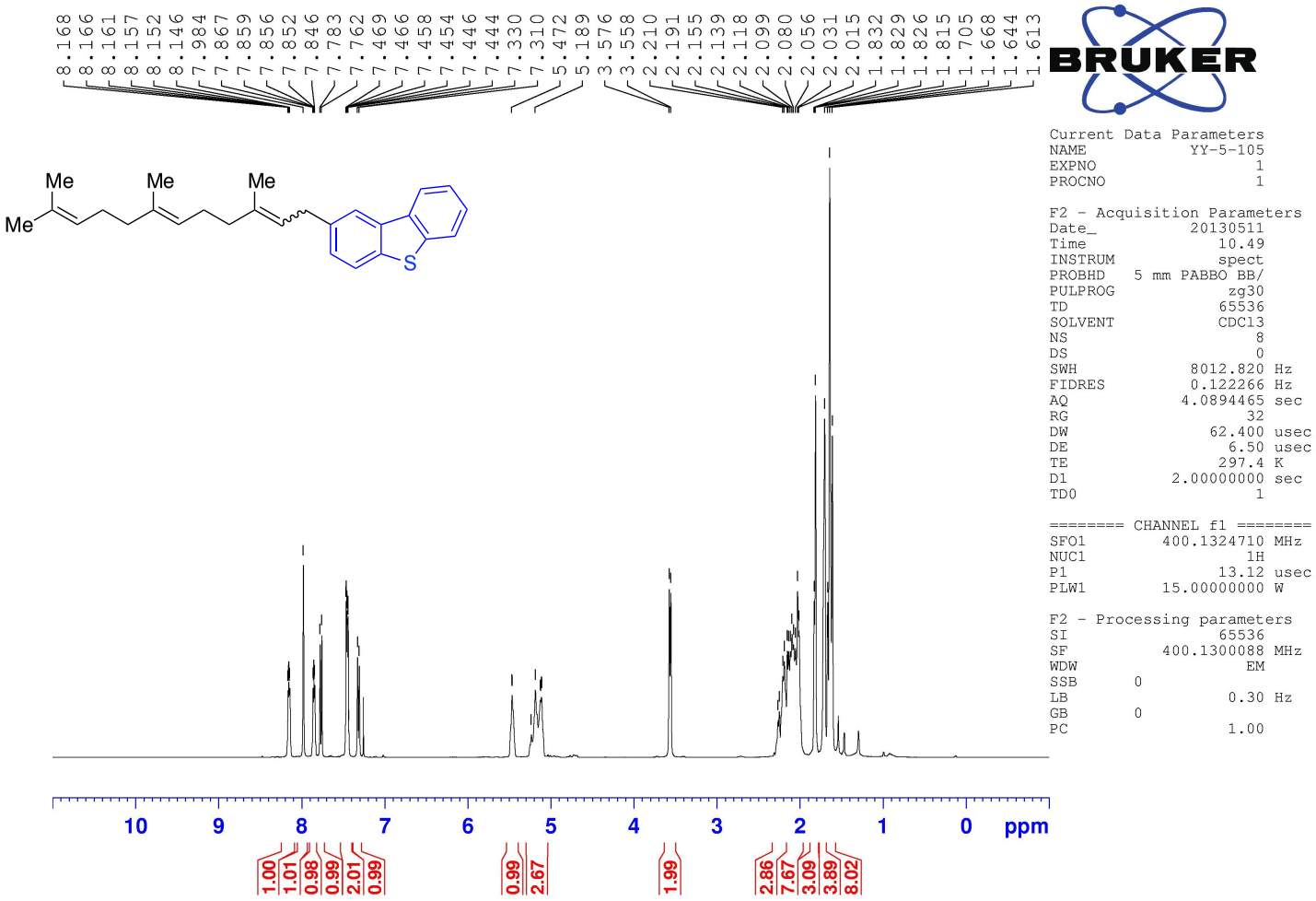

BRUKER
Current Data Parameters
NAME YY-5-153
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130610
Time 15.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 44.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.25957000 W
PLW13 0.21025001 W
F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
200
180
160
140
120
100
80
60
40
20
0
142.083
136.475
132.787
123.861
122.098
121.503
57.151
56.342
48.566
42.621
40.011
39.692
36.370
36.083
35.978
35.096
34.433
32.018
31.968
28.423
28.178
26.543
25.931
24.357
24.014
22.981
22.730
21.294
Me
Me
H
Me
Me
H
H
Me
Me
Me



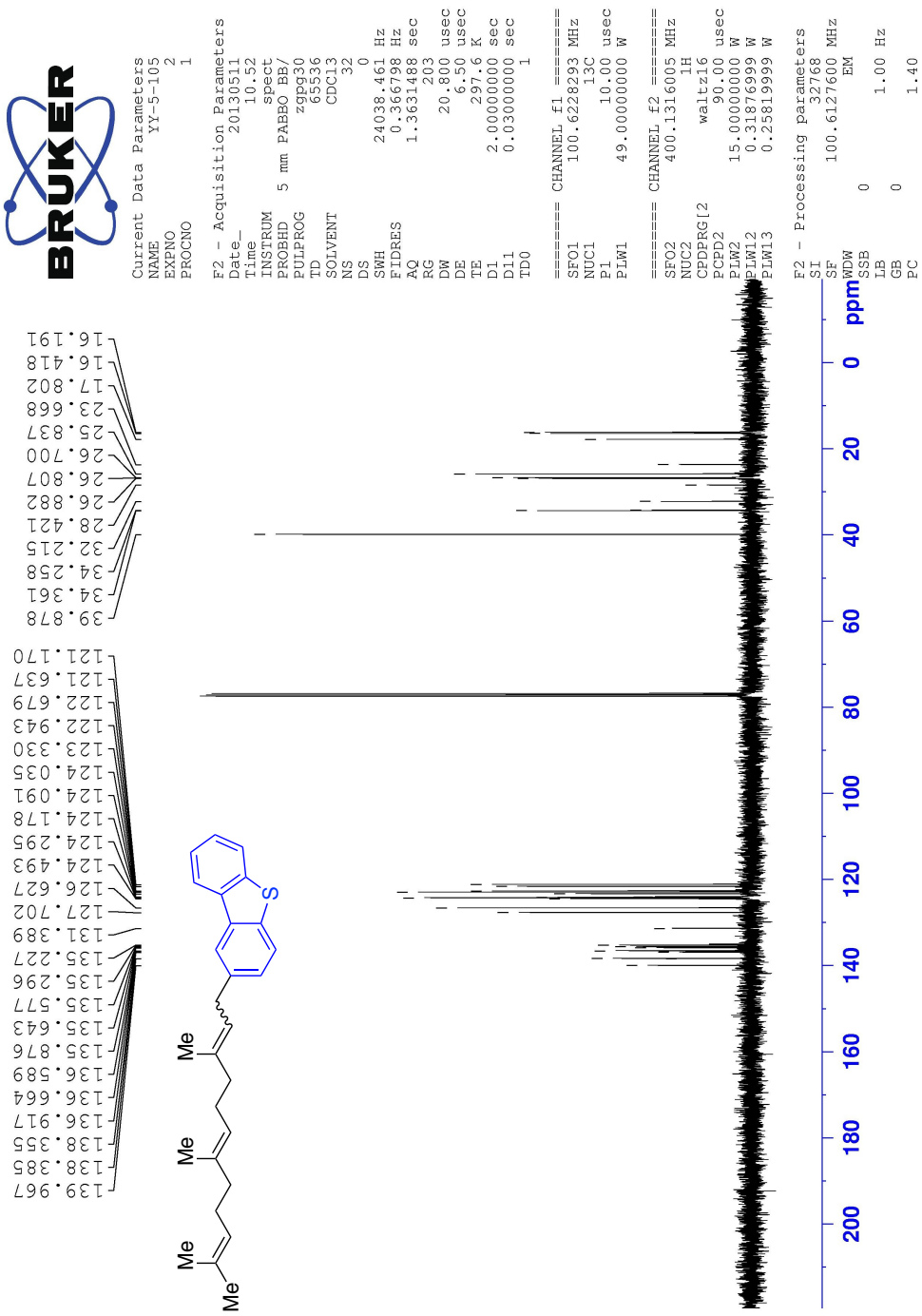
BRUKER

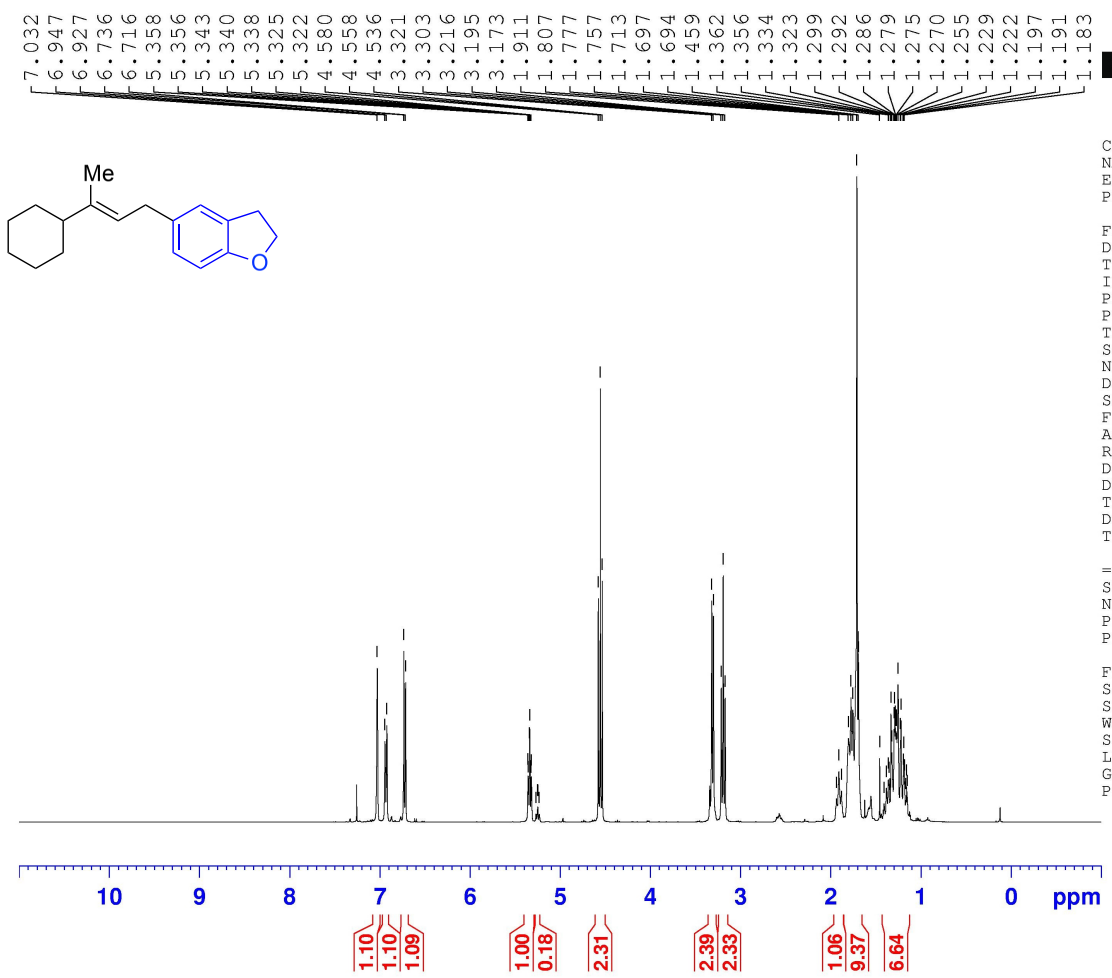
```
Current Data Parameters
NAME                  YY-5-97
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20130510
Time                  19.45
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                       32
DW                    62.400 usec
DE                     6.50 usec
TE                    296.9 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                    13.12 usec
PLW1           15.00000000 W

F2 - Processing parameters
SI                    65536
SF              400.1300094 MHz
WDW                     EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```


Current Data Parameters
NAME YY-5-97
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130510
Time_ 19.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127673 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
200
180
160
140
120
100
80
60
40
20
0
140.286
138.592
135.661
135.636
132.350
132.321
131.802
131.510
126.426
126.406
125.514
125.169
124.488
124.458
124.334
123.204
123.180
122.968
120.474
119.863
119.831
118.592
108.446
108.346
39.928
37.584
34.361
34.272
32.209
26.849
25.878
23.648
17.855
16.349
13.906
N
Et
Me
Me
Me



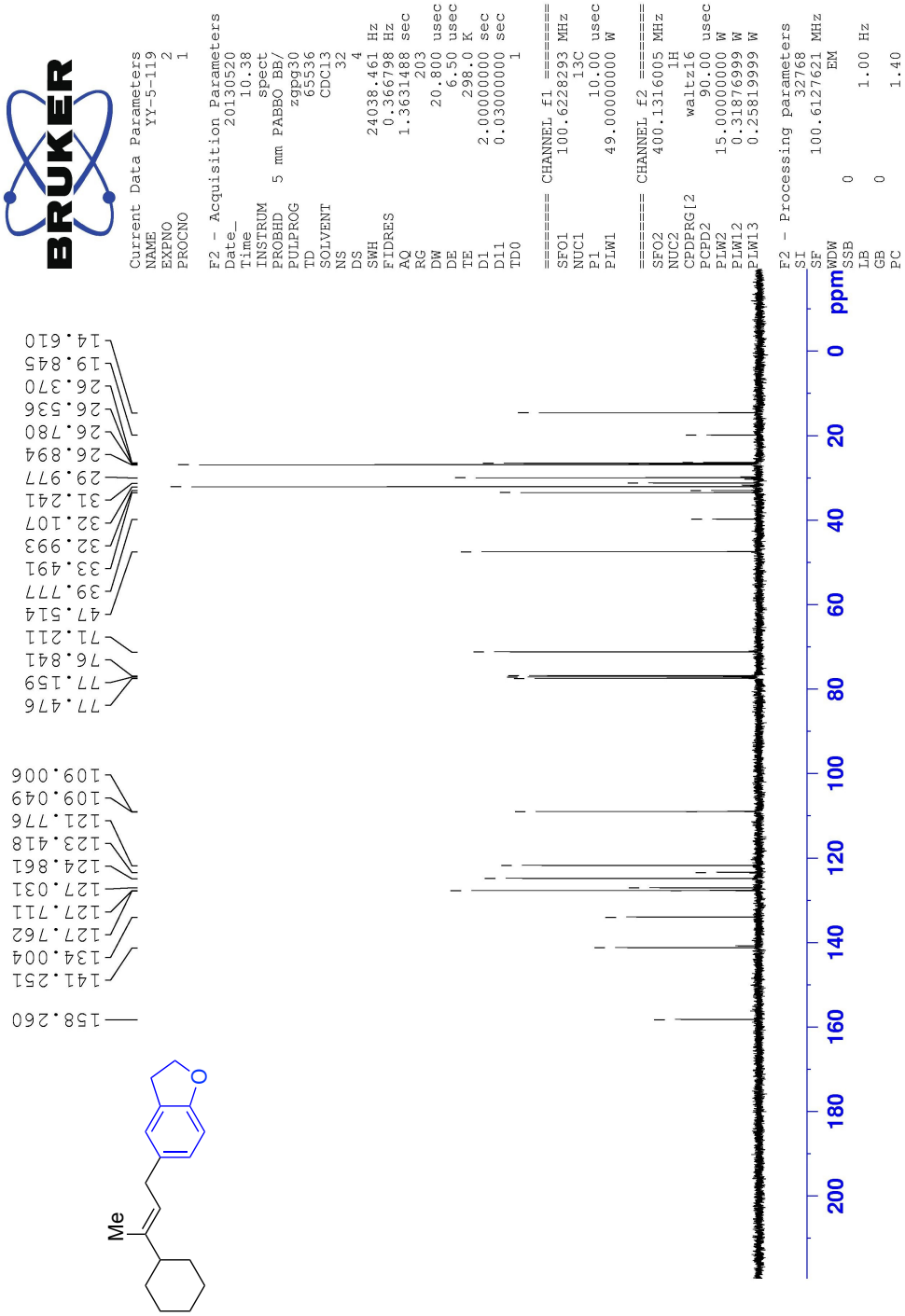

```
Current Data Parameters
NAME                  YY-5-105
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20130511
Time                     10.49
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                   8012.820 Hz
FIDRES                0.122266 Hz
AQ                    4.0894465 sec
RG                          32
DW                       62.400 usec
DE                        6.50 usec
TE                       297.4 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324710 MHz
NUC1                        1H
P1                       13.12 usec
PLW1               15.00000000 W

F2 - Processing parameters
SI                       65536
SF                  400.1300088 MHz
WDW                         EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
```

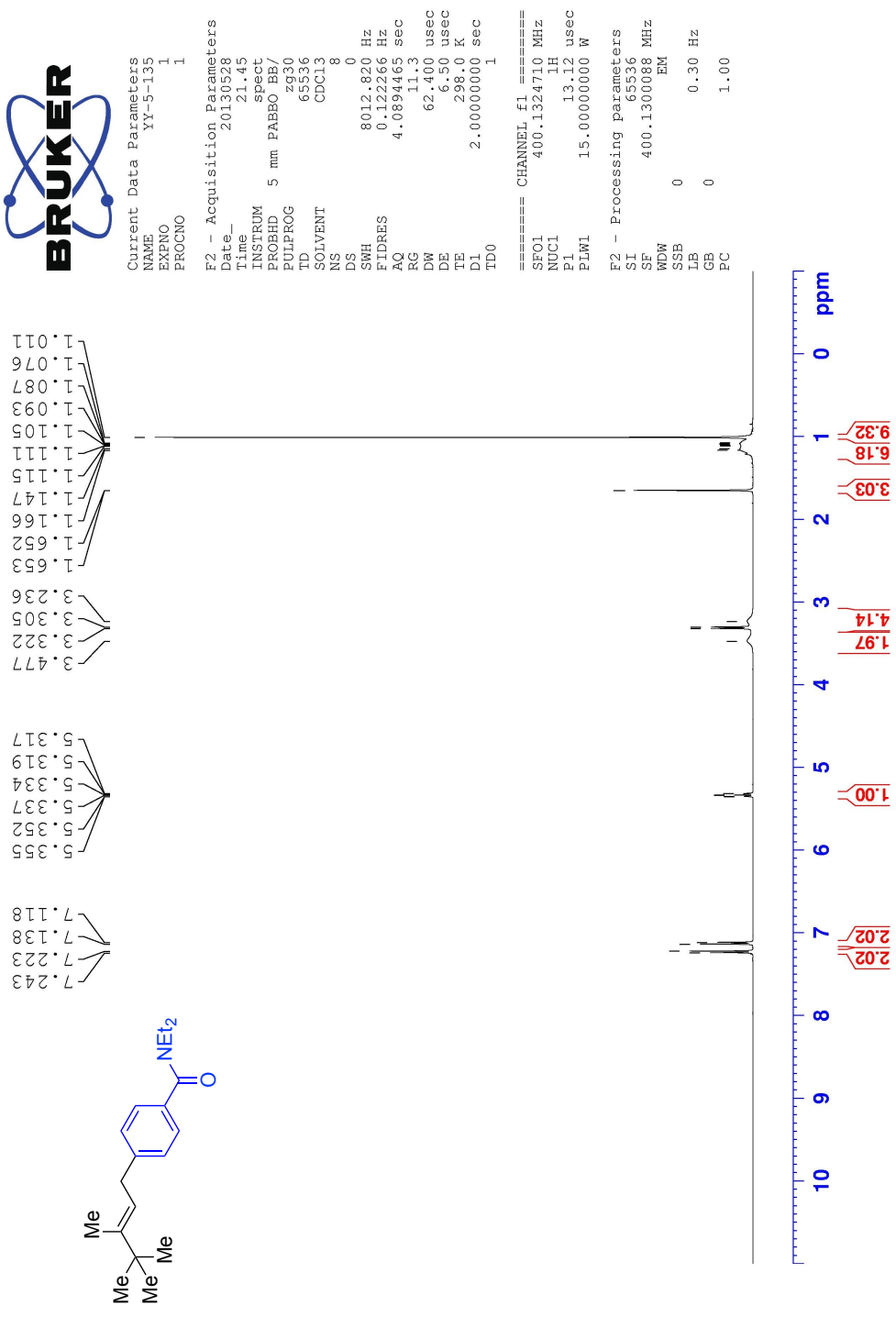

Current Data Parameters
NAME YY-5-105
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130511
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127600 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
200
180
160
140
120
100
80
60
40
20
0
139.967
138.385
138.355
136.917
136.664
136.589
135.876
135.643
135.577
135.296
135.227
131.389
127.702
126.627
124.493
124.295
124.178
124.091
124.035
123.330
122.943
122.679
121.637
121.170
39.878
34.361
34.258
32.215
28.421
26.882
26.807
26.700
25.837
23.668
17.802
16.418
16.191
S
Me
Me
Me
Me

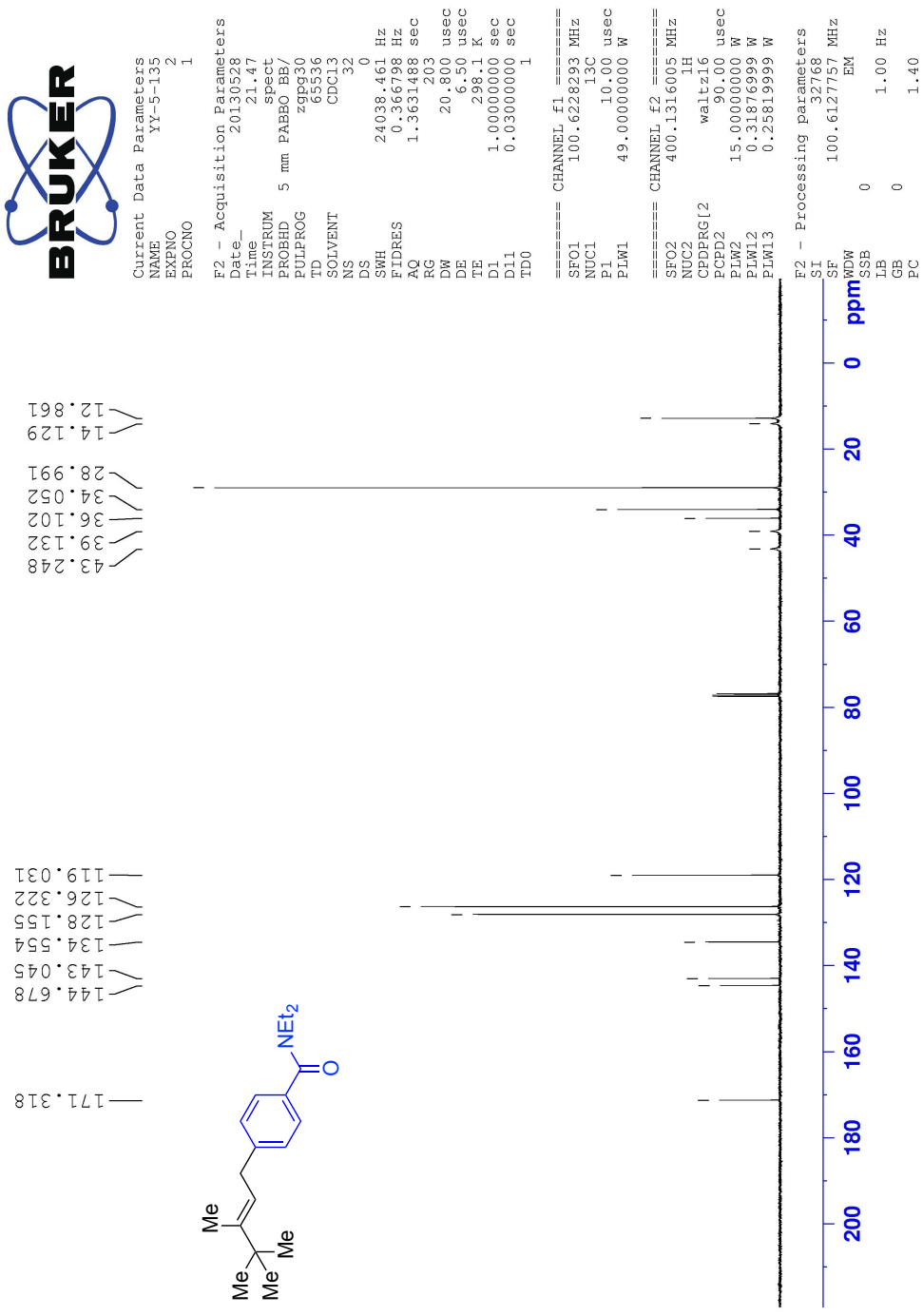


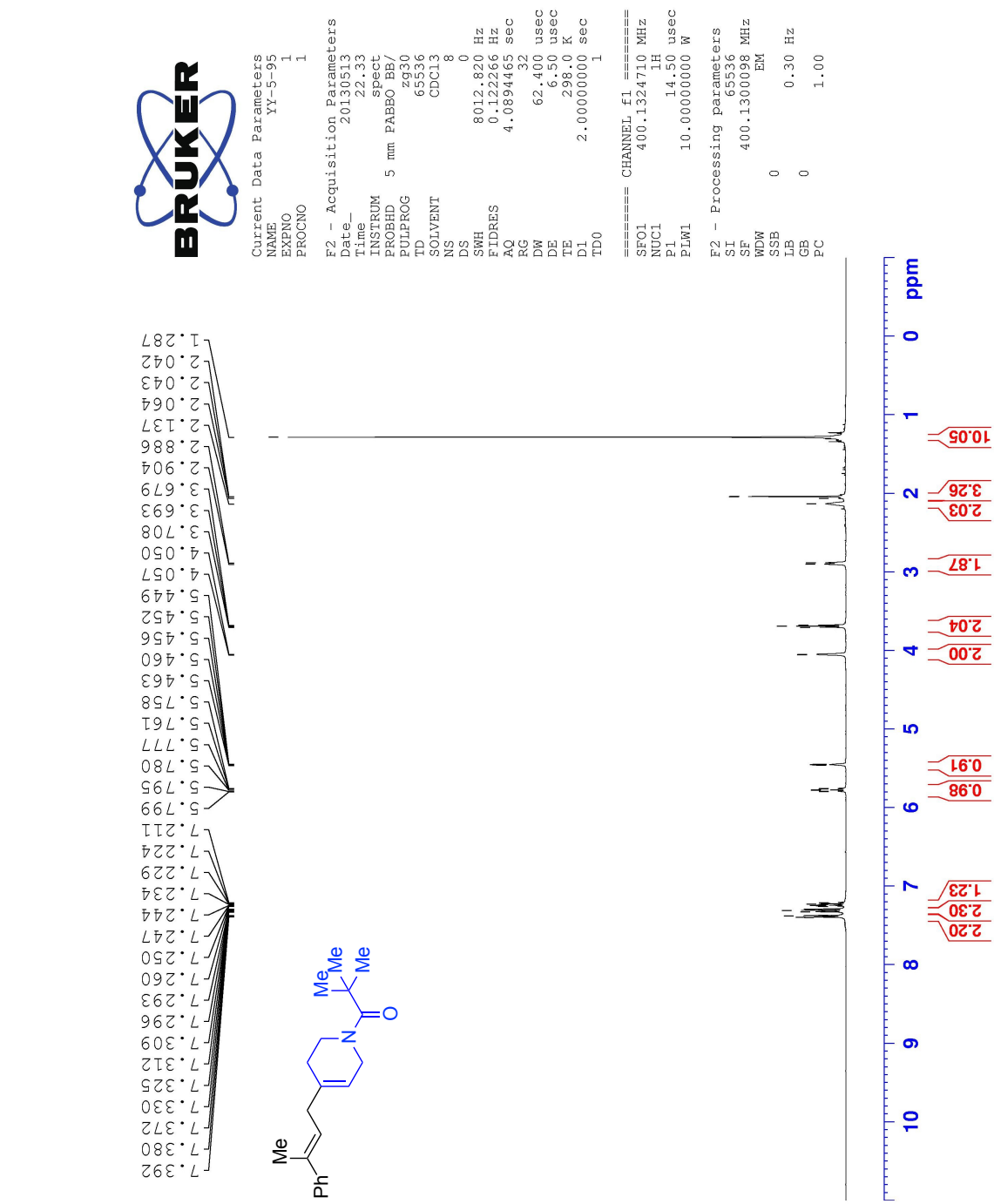
BRUKER

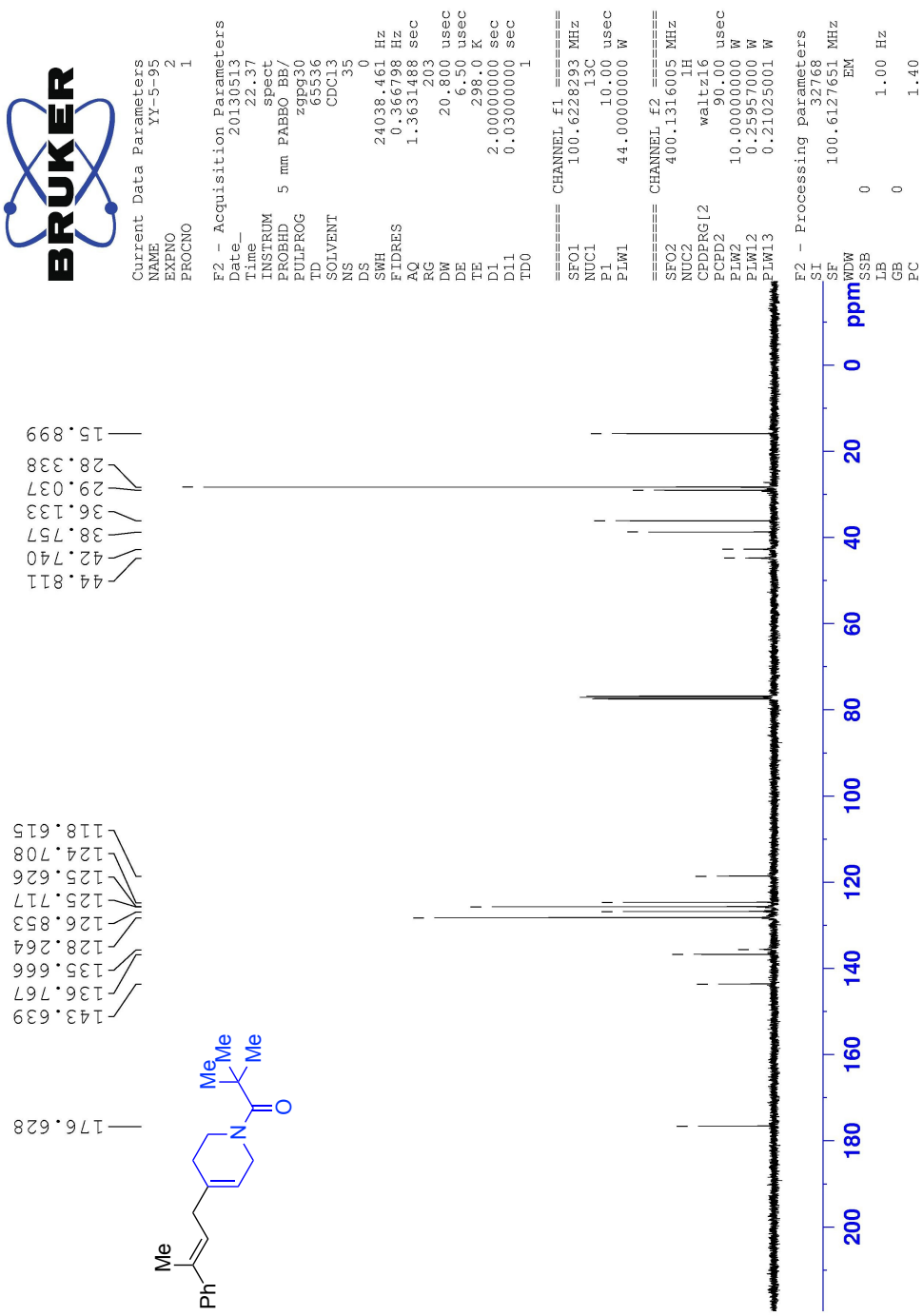
```
Current Data Parameters
NAME                  YY-5-119
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                20130520
Time                    10.36
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                          32
DW                     62.400 usec
DE                      6.50 usec
TE                     298.0 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                       1H
P1                      13.12 usec
PLW1               15.00000000 W

F2 - Processing parameters
SI                       65536
SF                 400.1300094 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

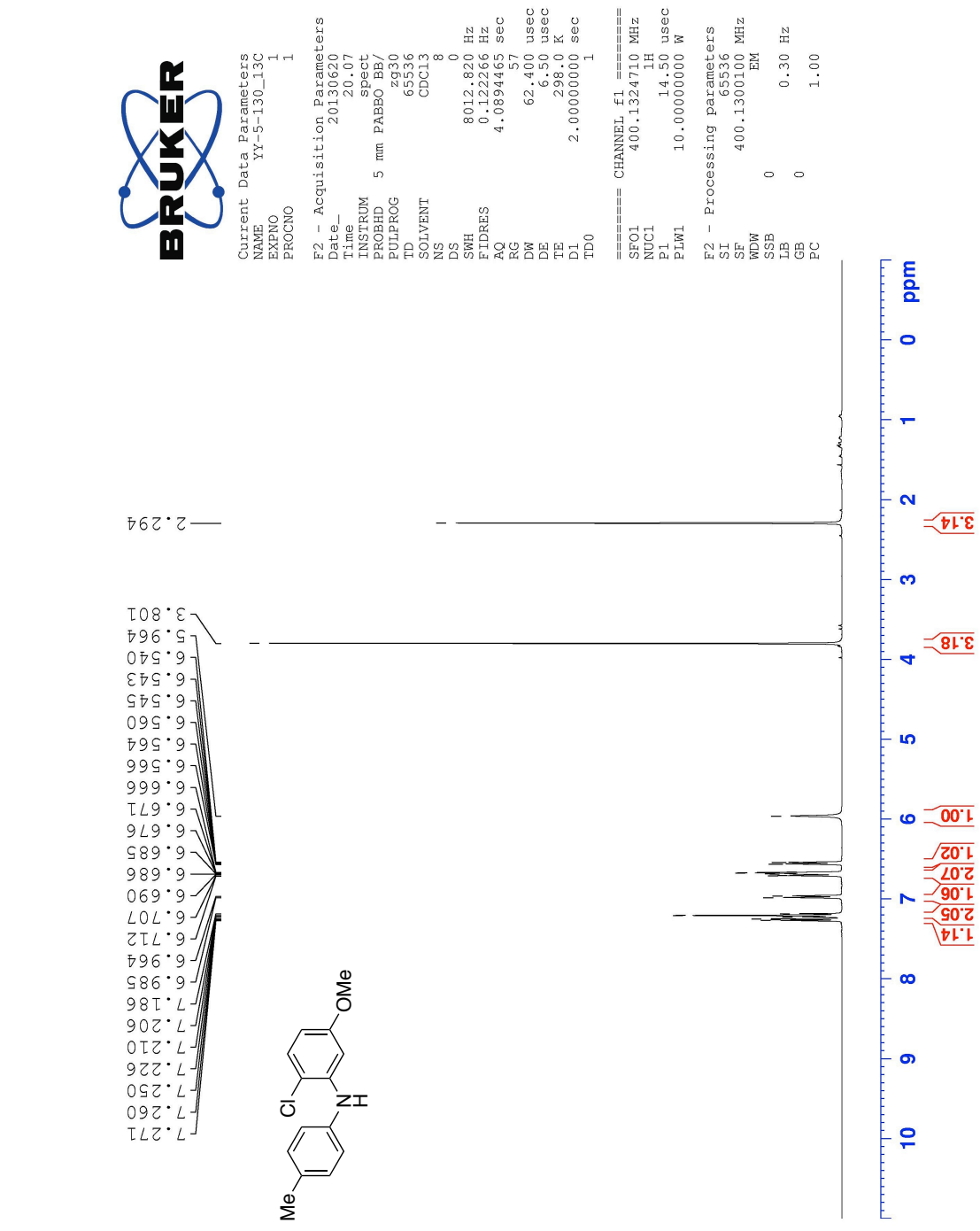

Current Data Parameters
NAME YY-5-119
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130520
Time_ 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127621 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm
200
180
160
140
120
100
80
60
40
20
0
158.260
141.251
134.004
127.762
127.711
127.031
124.861
123.418
121.776
109.049
109.006
77.476
77.159
76.841
71.211
47.514
39.777
33.491
32.993
32.107
31.241
29.977
26.894
26.780
26.536
26.370
19.845
14.610
Me
O

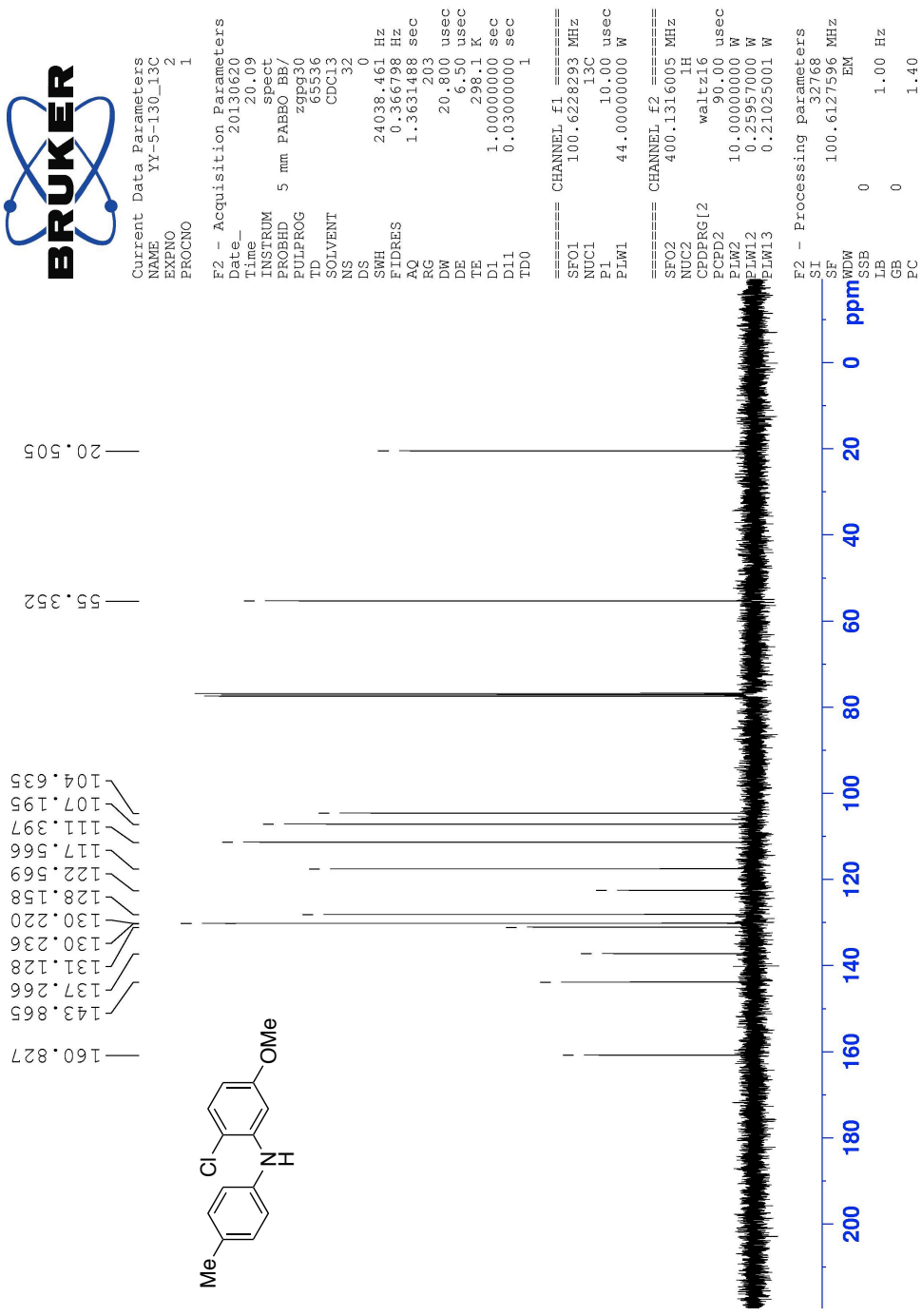

Current Data Parameters
NAME YY-5-135
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130528
Time_ 21.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 11.3
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 13.12 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.243
7.223
7.138
7.118
5.355
5.352
5.337
5.334
5.319
5.317
3.477
3.322
3.305
3.236
1.653
1.652
1.166
1.147
1.115
1.111
1.105
1.093
1.087
1.076
1.011
9.32
6.18
3.03
4.14
1.97
1.00
2.02
2.02
ppm
NEt2
O
Me
Me
Me
Me


Current Data Parameters
NAME YY-5-135
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130528
Time 21.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.31876999 W
PLW13 0.25819999 W
F2 - Processing parameters
SI 32768
SF 100.6127757 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
171.318
144.678
143.045
134.554
128.155
126.322
119.031
43.248
39.132
36.102
34.052
28.991
14.129
12.861
ppm
0
20
40
60
80
100
120
140
160
180
200
NEt2
O
Me
Me
Me
Me


Current Data Parameters
NAME YY-5-95
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130513
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.392
7.380
7.372
7.330
7.325
7.312
7.309
7.296
7.293
7.260
7.250
7.247
7.244
7.234
7.229
7.224
7.211
5.799
5.795
5.780
5.777
5.761
5.758
5.463
5.460
5.456
5.452
5.449
4.057
4.050
3.708
3.693
3.679
2.904
2.886
2.137
2.064
2.043
2.042
1.287
Me
Ph
Me
Me
Me
N
O
ppm
10.05
3.26
2.03
1.87
2.04
2.00
0.91
0.98
1.23
2.30
2.20


Current Data Parameters
NAME YY-5-95
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130513
Time 22.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 35
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 44.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.25957000 W
PLW13 0.21025001 W
F2 - Processing parameters
SI 32768
SF 100.6127651 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
176.628
143.639
136.767
135.666
128.264
126.853
125.717
125.626
124.708
118.615
44.811
42.740
38.757
36.133
29.037
28.338
15.899
ppm
200
180
160
140
120
100
80
60
40
20
0
Me
Ph
Me
Me
Me
N
O


Current Data Parameters
NAME YY-5-130_13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130620
Time 20.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 10.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.294
3.801
5.964
6.540
6.543
6.545
6.560
6.564
6.566
6.666
6.671
6.676
6.685
6.686
6.690
6.707
6.712
6.964
6.985
7.186
7.206
7.210
7.226
7.250
7.260
7.271
OMe
Cl
N
H
Me
3.14
3.18
1.00
1.02
2.07
1.06
2.05
1.14
ppm


Current Data Parameters
NAME YY-5-130_13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130620
Time 20.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 44.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.25957000 W
PLW13 0.21025001 W
F2 - Processing parameters
SI 32768
SF 100.6127596 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
20.505
55.352
104.635
107.195
111.397
117.566
122.569
128.158
130.220
130.236
131.128
137.266
143.865
160.827
ppm
200
180
160
140
120
100
80
60
40
20
0
Cl
N
H
OMe
Me