

Supporting Material

**Synthesis by Free Radical Polymerization and Properties of
BN-Polystyrene and BN-Poly(vinylbiphenyl)**

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1. General Methods.

All oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box.

The 499.9 MHz ^1H and 125.7 MHz ^{13}C NMR spectra were recorded on a Varian Unity/INOVA 500 spectrometer. The 160.4 MHz ^{11}B NMR spectra were recorded with a boron-free probe using boron-free quartz NMR tubes. The ^1H and ^{13}C NMR spectra were referenced internally to the solvent peaks and the ^{11}B NMR spectra externally to $\text{BF}_3 \cdot \text{Et}_2\text{O}$ ($\delta = 0$). IR spectra were recorded on a Bruker FTIP Alpha (ATR mode) spectrometer. High-resolution mass spectrometry (DART) was performed at the Mass Spectrometry Facility, Boston College, Chestnut Hill, MA.

GPC-RI analyses were performed in THF (1.0 mL/min, 35 °C) using a Viscotek GPCmax with a VE 2001 GPC solvent/sample module, a 2600 UV-PDA detector, and a TDA 305 triple detector array. A set of three columns, including one PLgel 5 mm mixed-D and two PLgel 5 mm mixed-C columns was used for separation and polystyrene standards (Polymer Laboratories, Varian Inc.) for calibration. Differential scanning calorimetry (DSC) measurements were performed on a Perkin Elmer Pyris 1 system at a scan rate of 20 °C / min. The results reported are from the second heating cycle. UV-vis absorption spectra were acquired on a Varian Cary 500 UV-Vis / NIR spectrophotometer. The fluorescence data was measured using an Horiba Fluorolog-3 spectrofluorometer equipped with a FluoroHub R-928 detector. Absolute quantum yields (Φ_{F}) were measured with a pre-calibrated Quanta- ϕ integrating sphere attached to the Fluorolog-3 instrument. Light from the sample compartment is directed into the sphere via a fiber-optic cable and the F-3000 Fiber-Optic Adapter and then returned to the sample compartment (and ultimately the emission monochromator) via a second fiber-optic cable and the F-3000.

2. Materials

THF, Et₂O, pentane, and hexanes were purified by passing through a neutral alumina column under argon or distilled from Na/benzophenone. Chlorinated solvents were distilled from CaH₂. DMF was dried over molecular sieves and then freshly distilled under high vacuum to remove amine impurities. All other solvents were purchased and used as received. Azobisisobutyronitrile (AIBN) and 1,1'-azobis(cyclohexanecarbonitrile) (ACHN) initiator were recrystallized in methanol. The chain transfer agent (CTA) (2-(dodecylthiocarbonothioylthio)-2-methyl-propionic acid (DMP) was synthesized according to a literature procedure.¹ All other solvents and chemicals were purchased from commercial sources and used without further purification unless noted otherwise.

3. Syntheses

1-Hydro-2-vinyl-1,2-azaborinine (BN-St). BN-St (0.65 g, 29%) was synthesized as a strongly odorous light yellow oil from 1-hydro-2-*n*-butoxy-1,2-azaborinine (**1**)² (3.2 g, 21 mmol), vinylmagnesium bromide (53 mL 1.0M THF solution, 53 mmol), and hydrogen chloride (27 mL 2.0 M Et₂O solution, 53 mmol). Inside a nitrogen atmosphere dry box, **1** and 30 mL THF were added to a round bottom flask equipped with a stir bar. The flask was fitted with a rubber septum and transferred to a fume hood. The contents of the flask were cooled to 0 °C on an ice/water bath and put under nitrogen. The vinylmagnesium bromide solution was added dropwise over 40 minutes via syringe to the stirred contents of the flask. The reaction mixture was stirred at 0 °C for 30 minutes and then allowed to warm to room temperature. After stirring at room temperature for 1 hour the progress of the reaction was checked by performing a mini-workup: A sealed NMR tube was evacuated and backfilled with nitrogen, and 0.5 mL 2M HCl/Et₂O was added to the tube. This NMR tube was left attached to a nitrogen outlet and a 0.1 mL aliquot of the

¹ a) J. T. Lai, D. Filla and R. Shea, *Macromolecules*, 2002, **35**, 6754-6756; b) W. M. Wan and C. Y. Pan, *Chem. Commun.*, 2008, 5639-5641.

² E. A. Abbey, A. N. Lamm, A. W. Baggett, L. N. Zakharov and S.-Y. Liu, *J. Am. Chem. Soc.* 2013, **135**, 12908-12913.

reaction was added, resulting in a small amount of bubbling. When the evolution of gas was observed to cease, the NMR tube was detached from the nitrogen outlet and a ^{11}B spectrum was recorded. This spectrum revealed complete conversion of **1** and production of **BN-St** as the major product. The reaction mixture was cooled to 0 °C again and the HCl/Et₂O solution was added dropwise over 40 minutes. The reaction mixture was allowed to warm to room temperature and taken back into a dry box. 200 mL pentane was added to precipitate inorganic salts, which were removed by filtration through a fritted glass funnel under mild vacuum. The salts were washed with an additional 50 mL pentane. The combined organic fractions were taken back into a fume hood, and solvent was removed using a diaphragm pump connected to a dry ice trap. The resulting crude material was purified by chromatography on neutral alumina using 3:97 Et₂O:pentane as eluent to yield **BN-St** as a light yellow oil.

^1H NMR (500 MHz, CD₂Cl₂): δ 8.04 (br t, 1H), 7.75 (dd, $^3J_{\text{HH}} = 11.5, 7.0$ Hz, 1H), 7.31 (t, $^3J_{\text{HH}} = 7.0$ Hz, 1H), 7.06 (d, $^3J_{\text{HH}} = 11.5$ Hz, 1H), 6.50 (dd, $^3J_{\text{HH}} = 19.5, 12.5$ Hz, 1H), 6.38 (m, 1H), 6.15 (d, $^3J_{\text{HH}} = 19.5$ Hz, 1H), 5.98 (d, $^3J_{\text{HH}} = 12.5$ Hz, 1H); ^{13}C NMR (125 MHz, CD₂Cl₂): δ 144.7, 138.6 (br), 134.3, 130.2, 128.4 (br), 111.3; ^{11}B NMR (160 MHz, CD₂Cl₂): δ 32.4; FTIR (ATR): $\nu = 3378, 3054, 3020, 2948, 1612, 1533, 1460, 1423, 1353, 1290, 1232, 1213, 1200, 1155, 1140, 1113, 1079, 1063, 1011, 986, 943, 838, 783, 729, 557, 501, 411$; HRMS (DART) calcd for C₆H₉BN [$M + \text{H}$]⁺ 106.08280, 106.08311 found.

1-Tert-butyldimethylsilyl-2-(*p*-vinylstyryl)-1,2-azaborinine (2a). **2a** (0.44 g, 44%) was synthesized as a white crystalline solid from 1-*tert*-butyldimethylsilyl-2-chloro-1,2-azaborinine (**2**)³ (0.78 g, 3.4 mmol), *p*-(trimethylstannyl)styrene (1.0 g, 3.8 mmol), chlorobis(ethylene)rhodium(I) dimer (0.053 g, 0.14 mmol), and 2,2'-bis(diphenylphosphino)-1,1'-biphenyl (BIPHEP) (0.14 g, 0.27 mmol). The rhodium catalyst and BIPHEP ligand were dissolved in 5 mL THF and aged for 10 minutes. This solution was then added to **2** and the *p*-(trimethylstannyl)styrene in a thick-walled glass pressure vessel, and 25 mL THF was added. The reaction mixture was sealed and heated at 80 °C for 16 hours. After

³ G. E. Rudebusch, L. N. Zakharov and S.-Y. Liu, *Angew. Chem. Int. Ed.*, 2013, **52**, 9316-9319.

cooling to room temperature, volatiles were removed under reduced pressure, and the crude residue was purified by silica gel chromatography using pentane as eluent to yield **2a** as a white crystalline solid.

^1H NMR (500 MHz, CD_2Cl_2): δ 7.59 (dd, $^3J_{\text{HH}} = 10.5, 6.5$ Hz, 1H), 7.43 (d, $^3J_{\text{HH}} = 7.0$ Hz, 1H), 7.34 (m, 2H), 6.74 (dd, $^3J_{\text{HH}} = 17.5, 11.5$ Hz, 1H), 6.61 (d, $^3J_{\text{HH}} = 10.5$ Hz, 1H), 6.43 (t, $^3J_{\text{HH}} = 6.5$ Hz, 1H), 5.78 (d, $^3J_{\text{HH}} = 17.5$ Hz, 1H), 5.21 (d, $^3J_{\text{HH}} = 11.5$ Hz, 1H), 0.89 (s, 9H), 0.07 (s, 6H); ^{13}C NMR (125 MHz, CD_2Cl_2): δ 146.2 (br), 143.5, 138.9, 137.9, 136.4, 132.9, 132.8 (br), 125.2, 113.3, 112.5, 27.3, 19.5, -1.5; ^{11}B NMR (160 MHz, CD_2Cl_2): δ 38.6; FTIR (ATR): $\hat{\nu} = 3021, 3001, 2982, 2957, 2928, 2900, 2884, 2855, 1628, 1602, 1499, 1463, 1450, 1386, 1360, 1284, 1271, 1262, 1237, 1203, 1174, 1150, 1095, 1031, 1014, 997, 956, 938, 898, 833, 820, 808, 782, 740, 707, 676, 6345, 620, 574, 511, 471, 414$; HRMS (DART) calcd for $\text{C}_{18}\text{H}_{27}\text{BNSi}$ [$M + \text{H}$] $^+$ 296.20058, 296.20110 found.

1-Hydro-2-(4-vinylstyryl)-1,2-azaborinine (BN-VBP). **BN-VBP** (0.26 g, 72%) was synthesized as a white crystalline solid from **2a** (0.44 g, 1.5 mmol) and tetra-*n*-butylammonium fluoride (TBAF) (1.6 mL 1.0 M THF solution, 1.6 mmol). **2a** was dissolved in 6 mL THF and TBAF was added dropwise over one minute. The reaction was determined to be complete after less than 5 minutes by TLC. The THF solution was poured into 20 mL water and extracted with 3 x 15 mL Et_2O . The combined organic layers were washed with brine, dried with MgSO_4 , and concentrated under reduced pressure. The nonvolatile residue was purified by silica gel chromatography using 1:9 Et_2O :pentane as eluent to yield **BN-VBP** as a crystalline white solid.

^1H NMR (500 MHz, CD_2Cl_2): δ 8.38 (s, 1H), 7.82 (m, 3H), 7.54 (d, $^3J_{\text{HH}} = 9.0$ Hz, 2H), 7.42 (t, $^3J_{\text{HH}} = 7.5$ Hz, 1H), 7.25 (d, $^3J_{\text{HH}} = 11.0$ Hz, 1H), 6.83 (dd, $^3J_{\text{HH}} = 17.5, 11.5$ Hz, 1H), 6.44 (t, $^3J_{\text{HH}} = 6.5$ Hz, 1H), 5.88 (d, $^3J_{\text{HH}} = 17.5$ Hz, 1H), 5.31 (d, $^3J_{\text{HH}} = 11.5$ Hz, 1H); ^{13}C NMR (126 MHz, CD_2Cl_2): δ 145.2, 138.7, 137.5, 134.7, 133.0, 129.0 (br), 128.7 (br), 126.5, 114.3, 111.5; ^{11}B NMR (160 MHz, THF- d_8): δ 32.3; FTIR (ATR): $\hat{\nu} = 3374, 3069, 2998, 2981, 1611, 1599, 1531, 1457, 1415, 1396, 1355, 1320, 1233, 1188, 1160, 1115, 1090, 1076, 1033, 993, 978, 904, 845, 827, 757, 712, 690, 677, 662, 637, 557, 506, 437$; HRMS (DART) calcd for $\text{C}_{12}\text{H}_{13}\text{BN}$ [$M + \text{H}$] $^+$

182,11410, 182.11347 found.

Conventional Free Radical Polymerization of BN-St. In a glove box BN-St monomer (52.5 mg, 500 μmol), ACHN (6.1 mg, 25 μmol) or AIBN (4.1 mg, 25 μmol), and 0.1 mL of THF or DMF ($[\text{BN-St}]/[\text{ACHN}]$ or $[\text{BN-St}]/[\text{AIBN}] = 20/1$) were loaded into a Schlenk tube. After 3 freeze-pump-thaw cycles, the tube was immersed in a 70 or 90 $^{\circ}\text{C}$ oil bath and kept stirring for a pre-determined period of time. The tube was placed in liquid nitrogen to terminate the reaction. Then 1 drop of polymerization solution was taken for ^1H NMR measurement to determine the monomer conversion. No polymer was observed for the polymerization in THF, while 48% conversion was achieved in DMF at 90 $^{\circ}\text{C}$ over 48 hours. The polymer was then precipitated in a 10-fold volume of cold hexanes, redissolved in THF, precipitated in a 10-fold volume of cold hexanes again, and freeze-dried in benzene. After drying in high vacuum, the polymer BN-PS was obtained as a white powder, which was stored under N_2 atmosphere (in air the polymer slowly turned brown). Yield: 21 mg (40%). GPC-RI: $M_{n,\text{GPC}} = 1900 \text{ g mol}^{-1}$, $M_{w,\text{GPC}} = 3900 \text{ g mol}^{-1}$, $D = 2.07$, $X_{n,\text{GPC}} = 18$. Similar results were obtained when performing the polymerization in the presence of a small amount of benzene (20 vol%) or in bulk for periods of 48 to 96 h at 90 $^{\circ}\text{C}$ (see Table S2).

RAFT Polymerization of BN-St. In a glove box BN-St monomer (52.5 mg, 500 μmol), DMP (4.6 mg, 13 μmol), ACHN (3.1 mg, 13 μmol , taken from stock solution), and 0.1 mL of THF or DMF ($[\text{BN-St}]/[\text{DMP}]/[\text{ACHN}] = 40/1/1$) were loaded into a Schlenk tube. After 3 freeze-pump-thaw cycles, the tube was immersed in a 90 $^{\circ}\text{C}$ oil bath and kept stirring for 20 h. The tube was placed in liquid nitrogen to terminate the reaction. Then 1 drop of polymerization solution was taken for ^1H NMR measurement to determine the monomer conversion. No polymer was observed for polymerization in THF, while 27% conversion was achieved in DMF. The polymer was then precipitated in a 10-fold volume of cold hexanes, redissolved in THF, precipitated in a 10-fold volume of cold hexanes again, and freeze-dried from benzene. After drying in high vacuum, the polymer BN-PS was obtained as a light yellow powder, which was stored under N_2 atmosphere (in air the polymer slowly turned brown). Yield: 9.2 mg (18%).

GPC-RI: $M_{n,\text{GPC}} = 1100 \text{ g mol}^{-1}$, $M_{w,\text{GPC}} = 1500 \text{ g mol}^{-1}$, $D = 1.38$, $X_{n,\text{GPC}} = 10$.

Conventional Free Radical Polymerization of BN-VBP. In a glove box BN-VBP monomer (36.2 mg, 200 μmol), AIBN (1.6 mg, 10 μmol), and 0.1 mL of THF ($[\text{BN-VBP}]/[\text{AIBN}] = 20/1$) were loaded into a Schlenk tube. After 3 freeze-pump-thaw cycles, the tube was immersed in a 70 °C oil bath and kept stirring for 24 h. The tube was placed in liquid nitrogen to terminate the reaction. Then 1 drop of polymerization solution was taken for ^1H NMR measurement to determine the monomer conversion (96%). The polymer was then precipitated in a 10-fold volume of cold hexanes, redissolved in THF, precipitated in a 10-fold volume of cold hexanes again, and freeze-dried in benzene. After drying in high vacuum, the polymer BN-PVBP was obtained as a white powder, which was stored under N_2 atmosphere. Yield: 33 mg (91%). GPC-RI: $M_{n,\text{GPC}} = 19200 \text{ g mol}^{-1}$, $M_{w,\text{GPC}} = 86000 \text{ g mol}^{-1}$, $D = 4.48$, $X_{n,\text{GPC}} = 106$.

RAFT Polymerization of BN-VBP. In a glove box BN-VBP monomer (36.2 mg, 200 μmol), DMP (0.73 mg, 2.0 μmol), AIBN (0.033 mg, 0.20 μmol , taken from stock solution), and 0.1 mL of THF ($[\text{BN-VBP}]/[\text{DMP}]/[\text{AIBN}] = 100/1/0.1$) were loaded into a Schlenk tube. After 3 freeze-pump-thaw cycles, the tube was immersed in a 70 °C oil bath and the mixture kept stirring for 24 h. The tube was placed in liquid nitrogen to terminate the reaction. Then 1 drop of polymerization solution was taken for ^1H NMR measurement to determine the monomer conversion (90%). The polymer was then precipitated in a 10-fold volume of cold hexanes, redissolved in THF, precipitated in a 10-fold volume of cold hexanes again, and freeze-dried in benzene. After drying in high vacuum, the polymer BN-PVBP was obtained as a light yellow powder, which was stored under N_2 atmosphere. Yield: 28 mg (77%). GPC-RI: $M_{n,\text{GPC}} = 1400 \text{ g mol}^{-1}$, $M_{w,\text{GPC}} = 1650 \text{ g mol}^{-1}$, $D = 1.18$, $X_{n,\text{GPC}} = 8$.

Table S1. Polymerization data for BN-St and BN-VBP without (**Entries 1-4**) and with DMP as a chain transfer agent (CTA) (**Entries 5-7**).

Entry	Monomer	Feed ratio ^a	Initiator	T / t (°C / h)	Solvent	Conv (%) ^b	M _n	X _n	M _n	M _w	<i>D</i>	X _n
							NMR ^c	NMR ^c	GPC ^d	GPC ^d	GPC ^d	GPC ^d
1	BN-St	20:0:1	AIBN	70 / 24	THF	0						
2	BN-St	20:0:1	ACHN	70 / 24	THF	0						
3	BN-St	20:0:1	ACHN	90 / 48	DMF	48	^e	^e	1900	3900	2.07	18
4	BN-VBP	20:0:1	AIBN	70 / 24	THF	96	^e	^e	19200 ^f	86000 ^f	4.48	106 ^f
5	BN-VBP	40:0:1	AIBN	70 / 20	THF	>99	^e	^e	38500 ^f	150000 ^f	3.91	212 ^f
6	BN-St	40:1:1	ACHN	90 / 20	DMF	27	1500	11	1100	1500	1.38	10
7	BN-VBP	100:1:0.1	AIBN	70 / 24	THF	90	15800	85	1400 ^f	1650 ^f	1.18	8 ^f
8 ^g	BN-VBP	400:1:0.1	AIBN	70 / 24	THF	85	64800	356	3400 ^f	5100 ^f	1.49	19 ^f

[a] Feed ratio of [Monomer]:[CTA]:[Initiator]; CTA = (2-(dodecylthiocarbonothioylthio)-2-methylpropionic acid (DMP)). [b] Conversion estimated based on ¹H NMR integration of residual monomer and polymer before purification. [c] Calculated based on ¹H NMR integration of the end group (δ at 3.7 ppm for BN-PS and 3.2 ppm for BN-PVBP) and the aromatic moieties of the polymer repeat units (δ from 6.4 to 5.6 ppm for BN-PS and 6.5 to 6.1 ppm for BN-PVBP) after purification. [d] Based on GPC analysis in THF relative to PS standards. [e] Not measured. [f] The molecular weight is likely to be underestimated due to the larger side group in comparison to polystyrene. [g] Chain extension of polymeric product from Entry 7 with additional monomer BN-VBP (see Figure S1).

Table S2. Polymerization data for BN-St with ACHN as an initiator under different conditions.

Entry	Feed ratio ^a	T / t (°C / h)	Solvent	Conv (%) ^b	M _n	M _w	<i>D</i>	M _n	M _w	<i>D</i>
					THF ^c	THF ^c	THF ^c	DMF ^c	DMF ^c	DMF ^c
1	100:1	90 / 72	C ₆ D ₆	50	1600	2120	1.33	1570	2550	1.62
2	200:1	90 / 72	C ₆ D ₆	40	1630	2190	1.35	1740	2830	1.63
3	150:1	90 / 96	neat	60	1070	1990	1.86	1700	2960	1.74

[a] Feed ratio of [BN-St]:[ACHN]. [b] Conversion estimated based on ¹H NMR integration of residual monomer and polymer before purification. [c] Based on GPC analysis of crude product in THF relative to PS standards. [d] Based on GPC analysis of crude product in DMF/1%LiBr relative to PMMA standards.

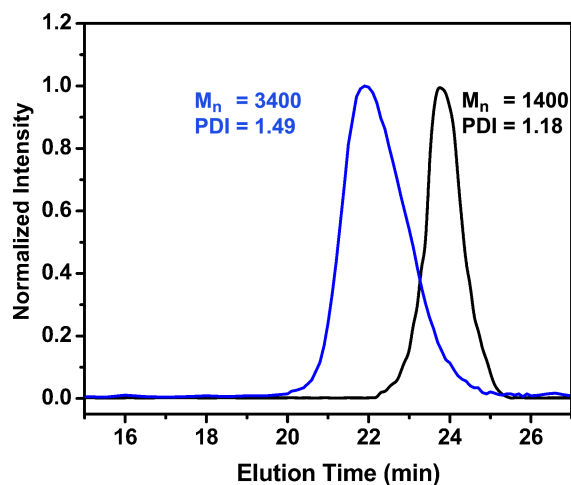


Figure S1. GPC traces for the chain extension of BN-VBP with additional monomer according to Entry 8, Table S1 (THF, 1 mL min⁻¹).

Table S3. Comparison of solubility characteristics of BN-PS, BN-PVBP and PS.

Solvent	Cyclohexane	Toluene	THF	DMF	DMSO	Methanol	H ₂ O
δ / MPa ^{1/2} ^a	16.8	18.2	18.6	24.8	29.7	29.7	47.9
PS	Soluble >35 °C	Soluble	Soluble	Soluble	Soluble >150 °C	Insoluble	Insoluble
BN-PS ^b	Insoluble	Soluble	Soluble	Soluble	Soluble	Soluble	Dispersible
BN-PVBP ^c	Insoluble	Soluble	Soluble	Soluble	Soluble	Dispersible	Insoluble

[a] Solubility parameter, values from ref. 4. [b] Sample from Entry 6 in Table S1. [c] Sample from Entry 8 in Table S1.

⁴ J. Bandrup, E. H. Immergut and E. A. Grulke, eds., *Polymer Handbook*, 4th edn., John Wiley & Sons, Inc., New York, 1999.

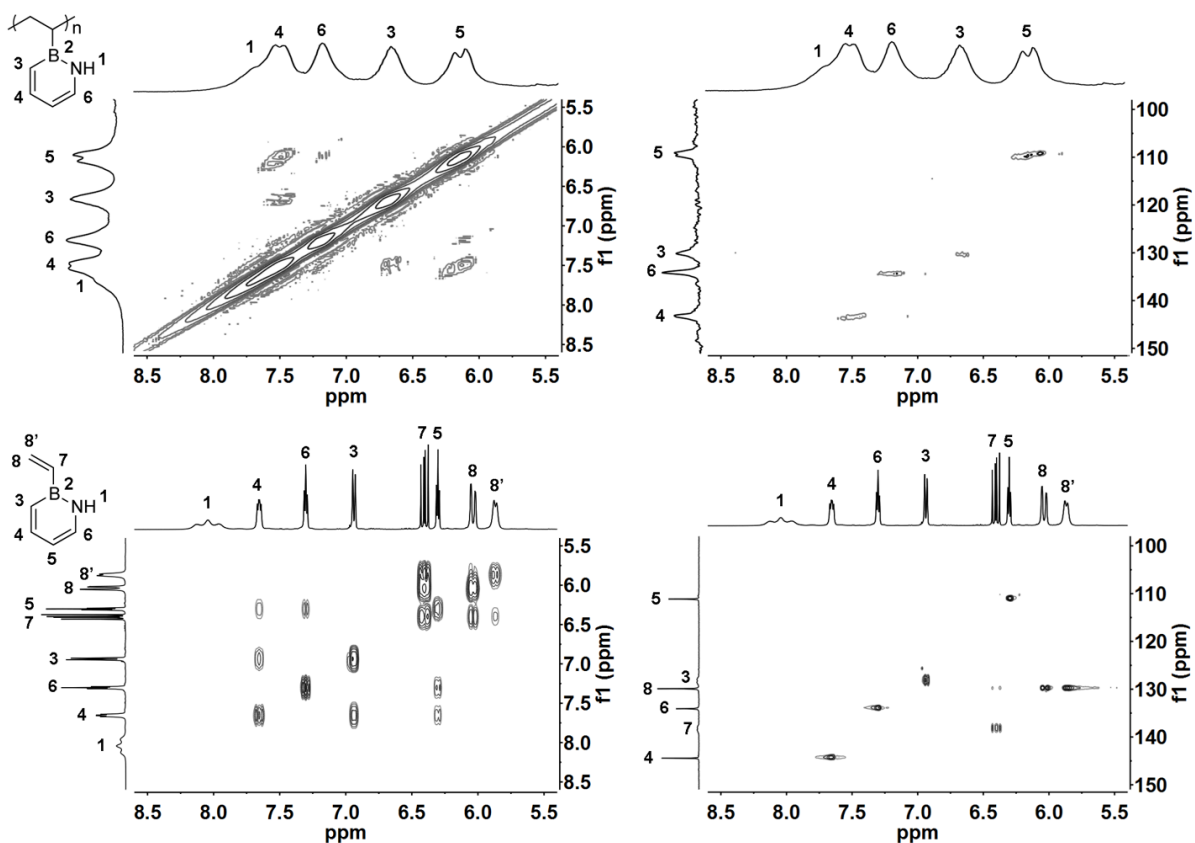


Figure S2. Aromatic and olefinic regions of the ^1H , ^1H -COSY and ^1H , ^{13}C -HSQC NMR spectra of BN-St monomer and BN-PS polymer in CD_2Cl_2 .

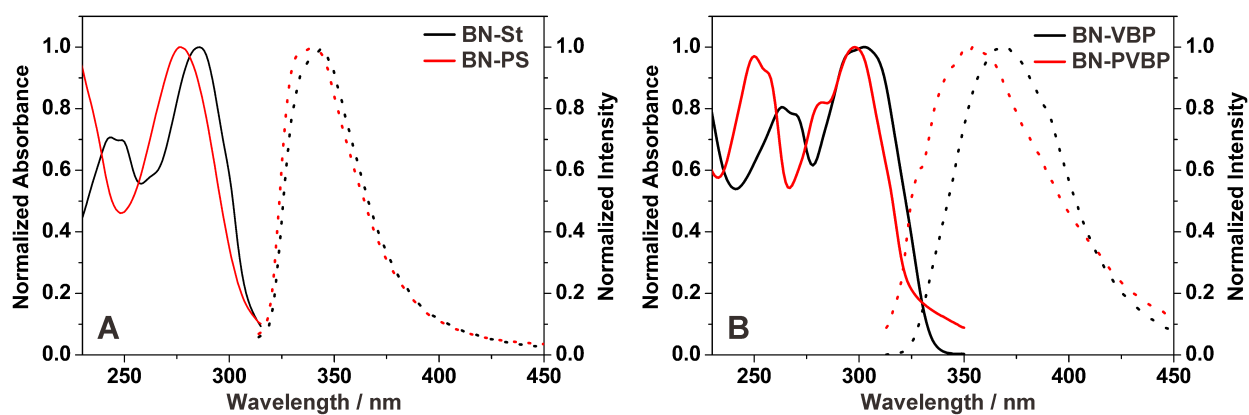
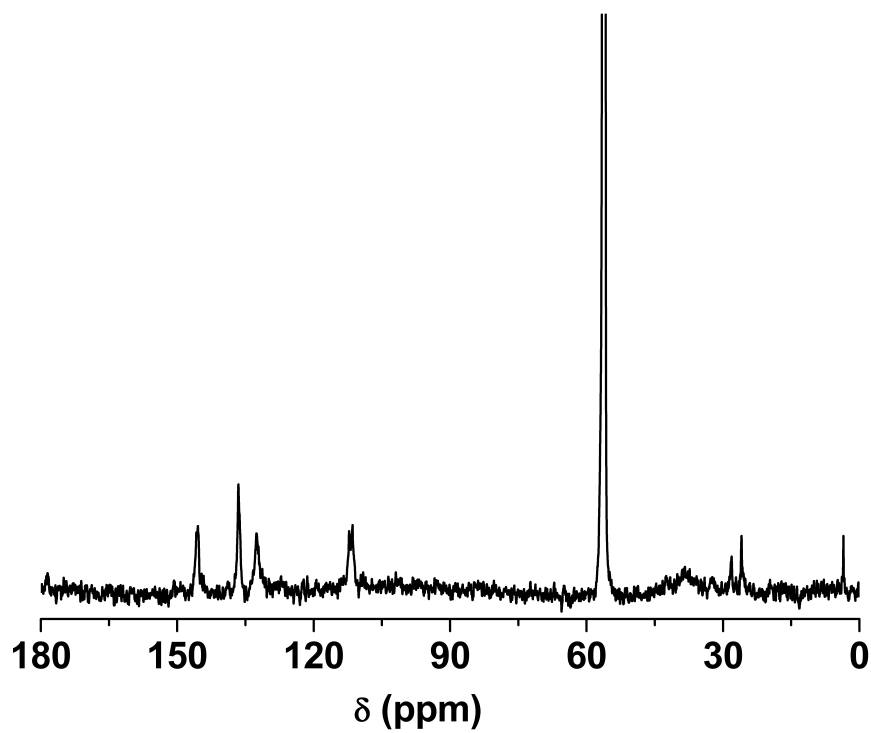
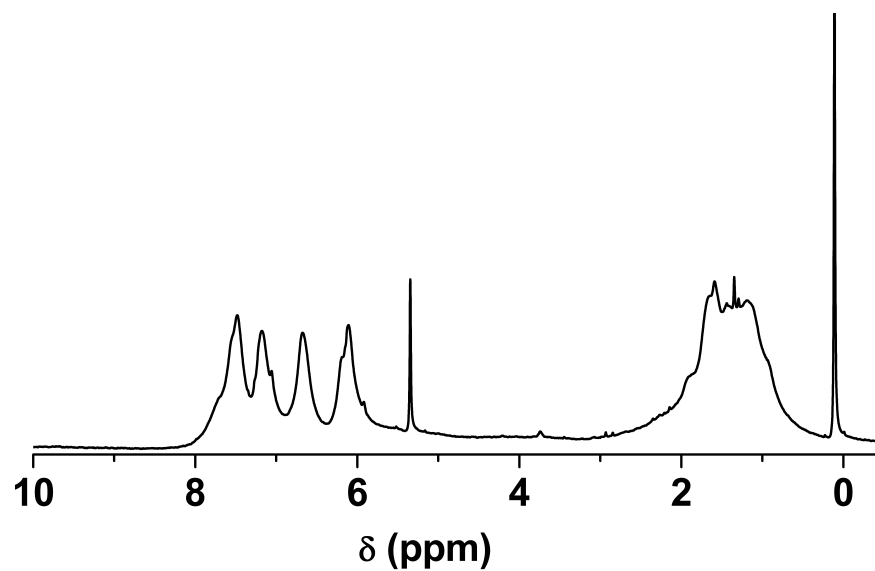
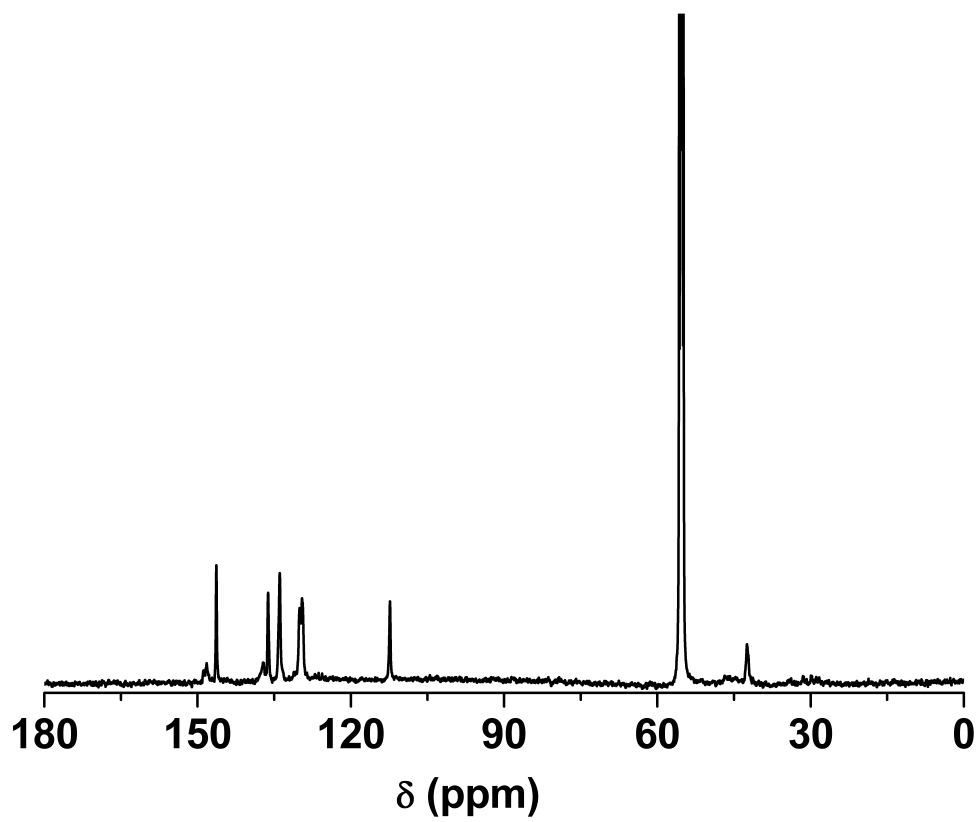
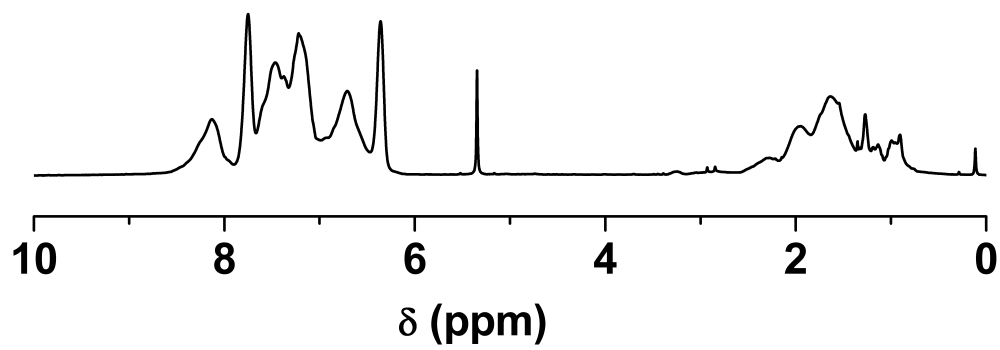


Figure S3. Absorption (solid lines) and emission (dotted lines) spectra of (A) BN-St and BN-PS and (B) BN-VBP and BN-PVBP in THF. Excited at longest wavelength absorption maxima.

Additional Spectral Data for Polymers



Full ^1H and ^{13}C NMR spectra of polymer BN-PS in CD_2Cl_2



Full ^1H and ^{13}C NMR spectra of polymer BN-PVBP in CD_2Cl_2

AWB-VI-83A

Sample Name:

Data Collected on:
nmr18-vnmr5500
Archive directory:

Sample directory:

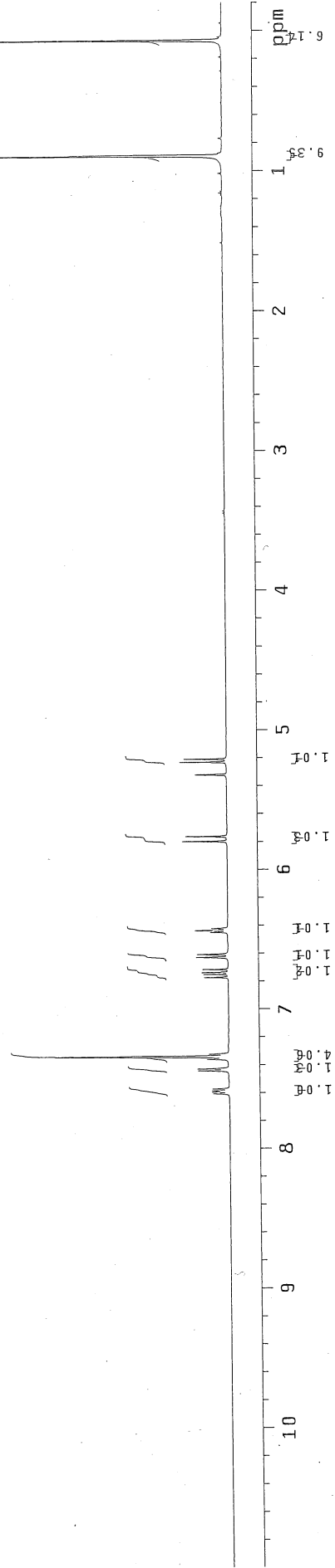
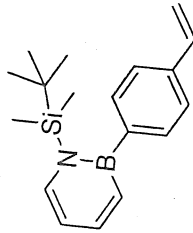
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Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: May 8 2014

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 12.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions

OBSERVE H1 499.8817682 MHZ
DATA PROCESSING
FT size 32768
Total time 20420 hr, 29 min



AWB-VI-83C

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

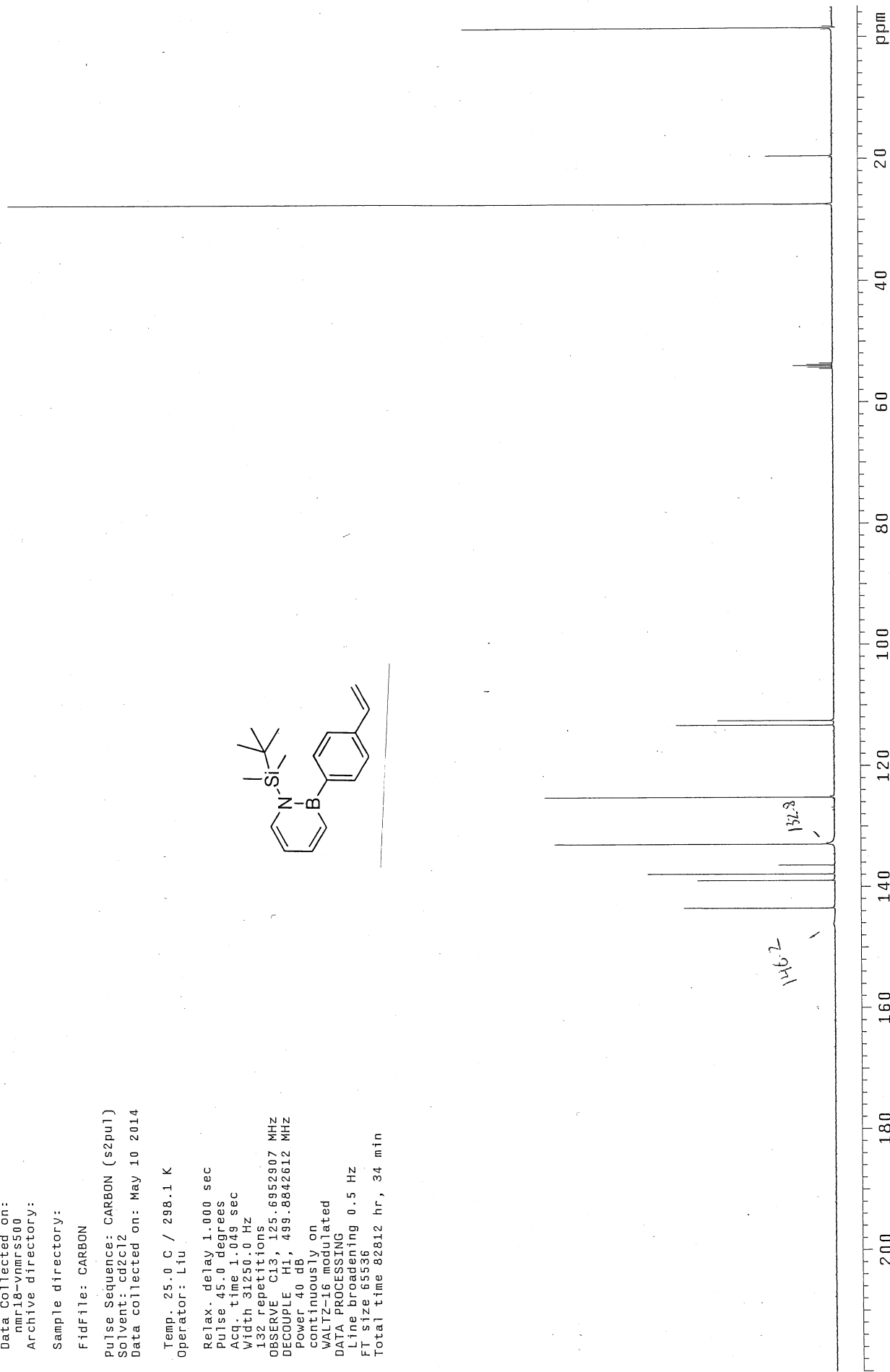
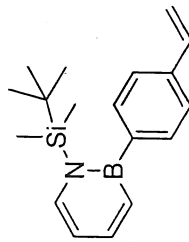
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: May 10 2014

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
132 repetitions

OBSERVE C13, 125.6952907 MHZ
DECOUPLE H1, 499.8842612 MHZ
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 82812 hr, 34 min



AWB-VI-83B

Sample Name:

Data Collected on:
nmr18-vnmrs500

Archive directory:

Sample directory:

FidFile: AWB-VI-83B

Pulse Sequence: s2pul

Solvent: cd2cl2

Data collected on: May 8 2014

Temp. 25.0 C / 298.1 K

Operator: Liu

Relax. delay 0.100 sec

Pulse 88.9 degrees

Acq. time 0.100 sec

Width 35714.3 Hz

44 repetitions

OBSERVE B11, 160.3816809 MHz

DECOUPLE H1, 499.8842612 MHz

Power 40 dB,

on during acquisition

off during delay

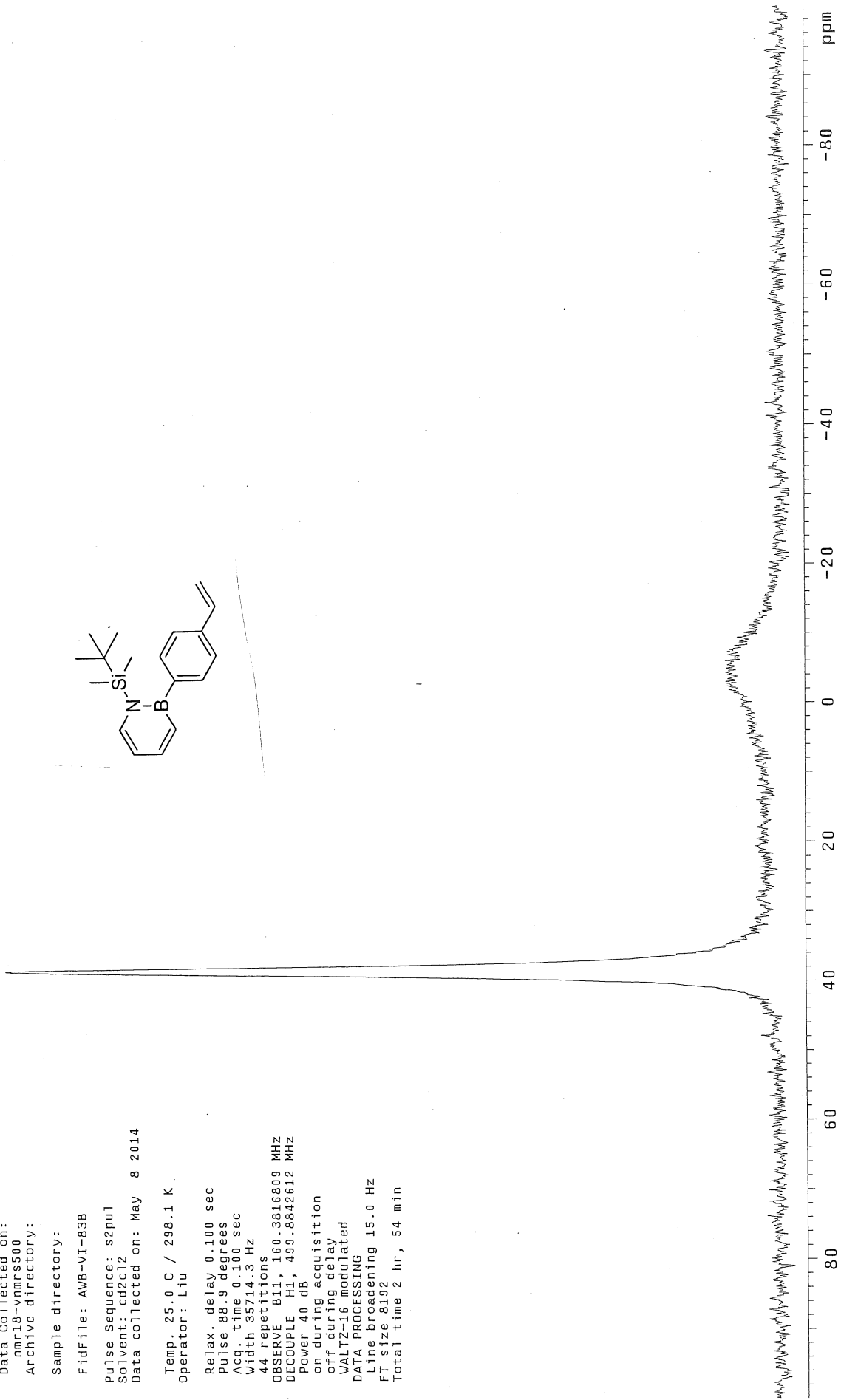
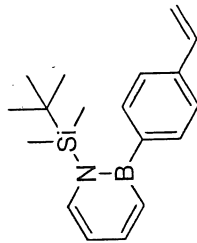
WALTZ-16 modulated

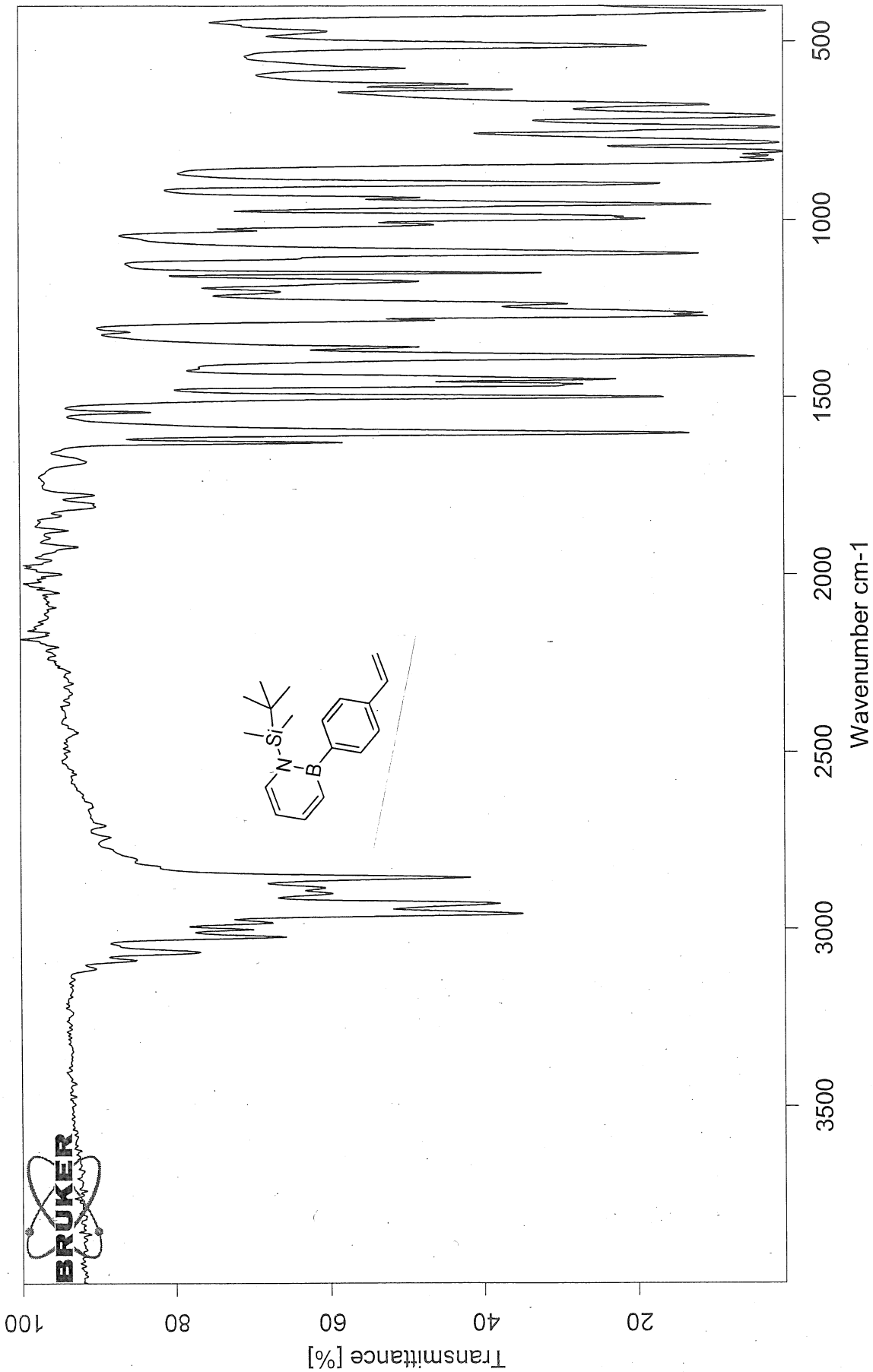
DATA PROCESSING

Line broadening 15.0 Hz

FT size 8192

Total time 2 hr, 54 min





C:\OPUS_7.2.139.1294\MEAS\Sample description.9	Instrument type and / or accessory	5/9/2014
AwB-01-83D		

AWB-VI-93A

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

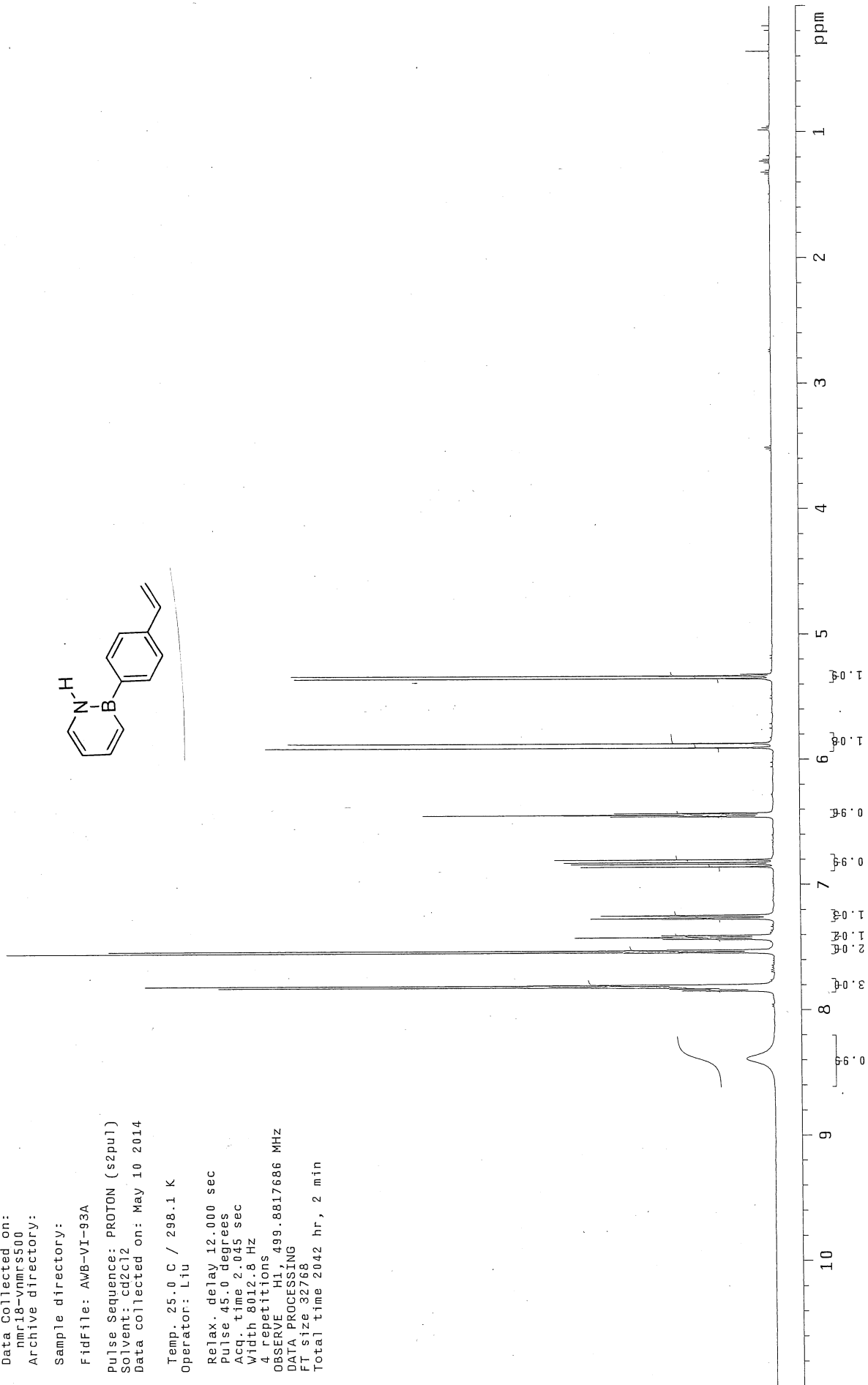
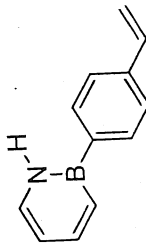
Fidfile: AWB-VI-93A

Pulse Sequence: PROTON (szpul)
Solvent: cd2cl2
Data collected on: May 10 2014

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 12.000 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
4 repetitions

OBSERVE H1 499.8817686 MHZ
DATA PROCESSING
FT size 32768
Total time 2042 hr, 2 min



AWB-VI-93C

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

Fidfile: AWB-VI-93C

Pulse Sequence: CARBON (szpu1)
Solvent: cd2cl2
Data collected on: May 10 2014

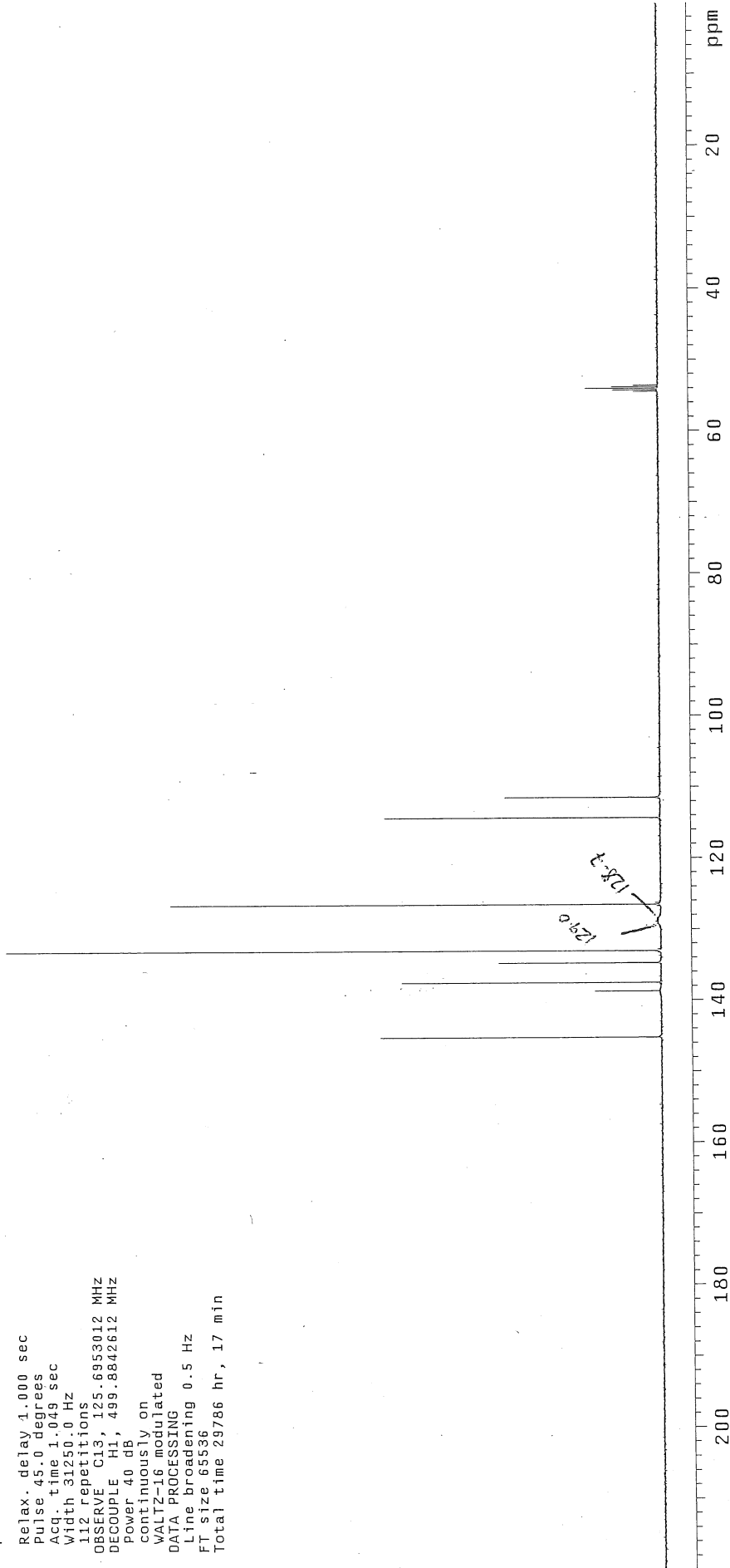
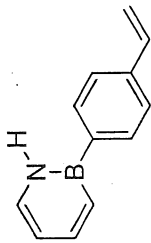
Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz

112 repetitions
OBSERVE C13, 125.6953012 MHZ
DECOUPLE H1, 499.8842612 MHZ
Power 40 dB

continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536

Total time 29786 hr, 17 min



AVB-VI-938

Sample Name:

Data Collected on:
nmr18-vnmr500
Archive directory:

Sample directory:

FidFile: AVB-VI-938

Pulse Sequence: s2pu1

Solvent: cd2cl2

Data collected on: May 10 2014

Temp. 25.0 C / 298.1 K

Operator: Liu

Relax. delay 0.100 sec

Pulse 88.9 degrees

Acq. time 0.100 sec

Width 35714.3 Hz

52 repetitions

OBSERVE B11, 160.3819948 MHz

DECOUPLE H1, 499.8842612 MHz

Power 40 dB

on during acquisition

off during delay

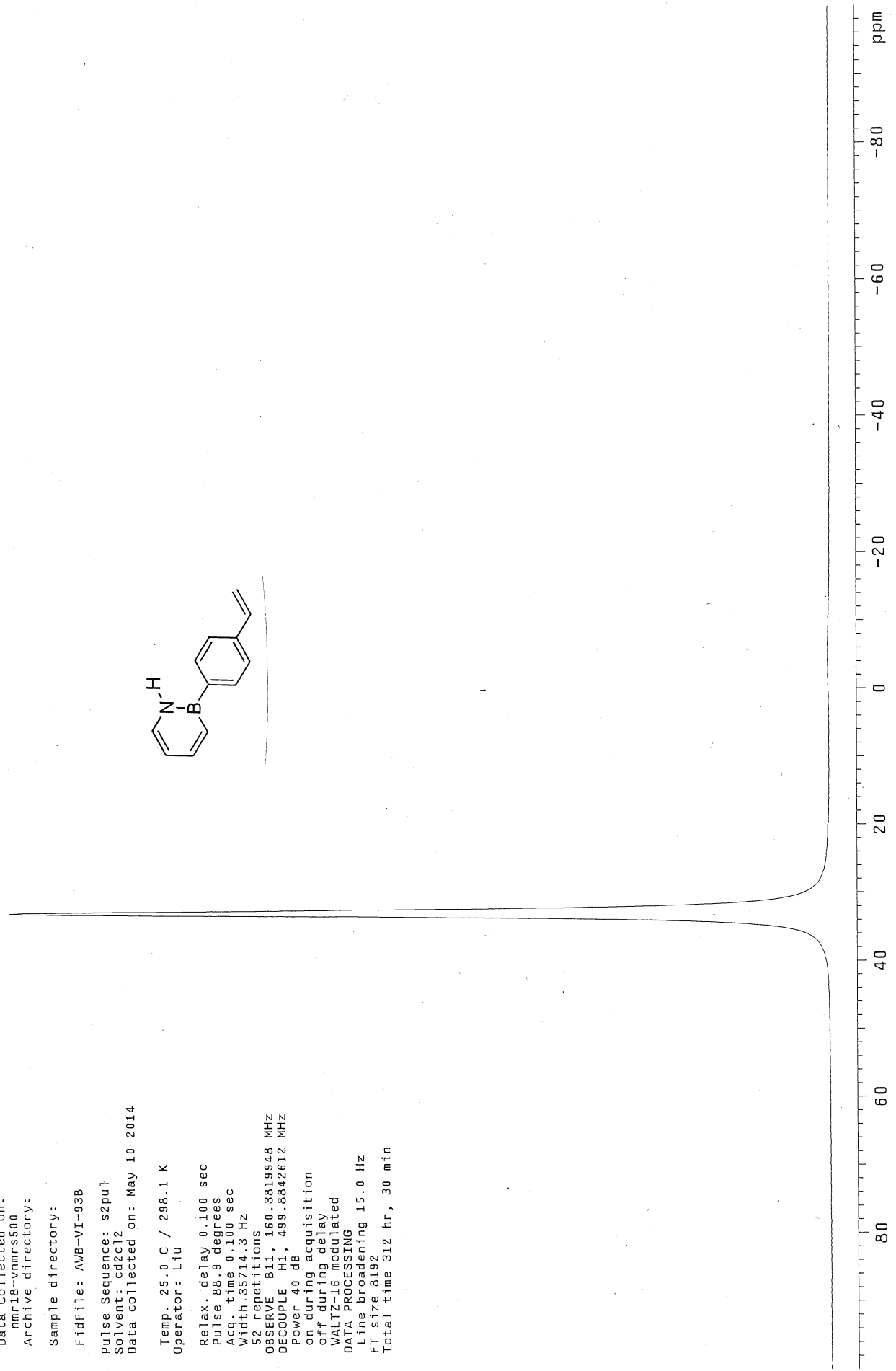
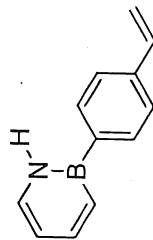
WALTZ-16 modulated

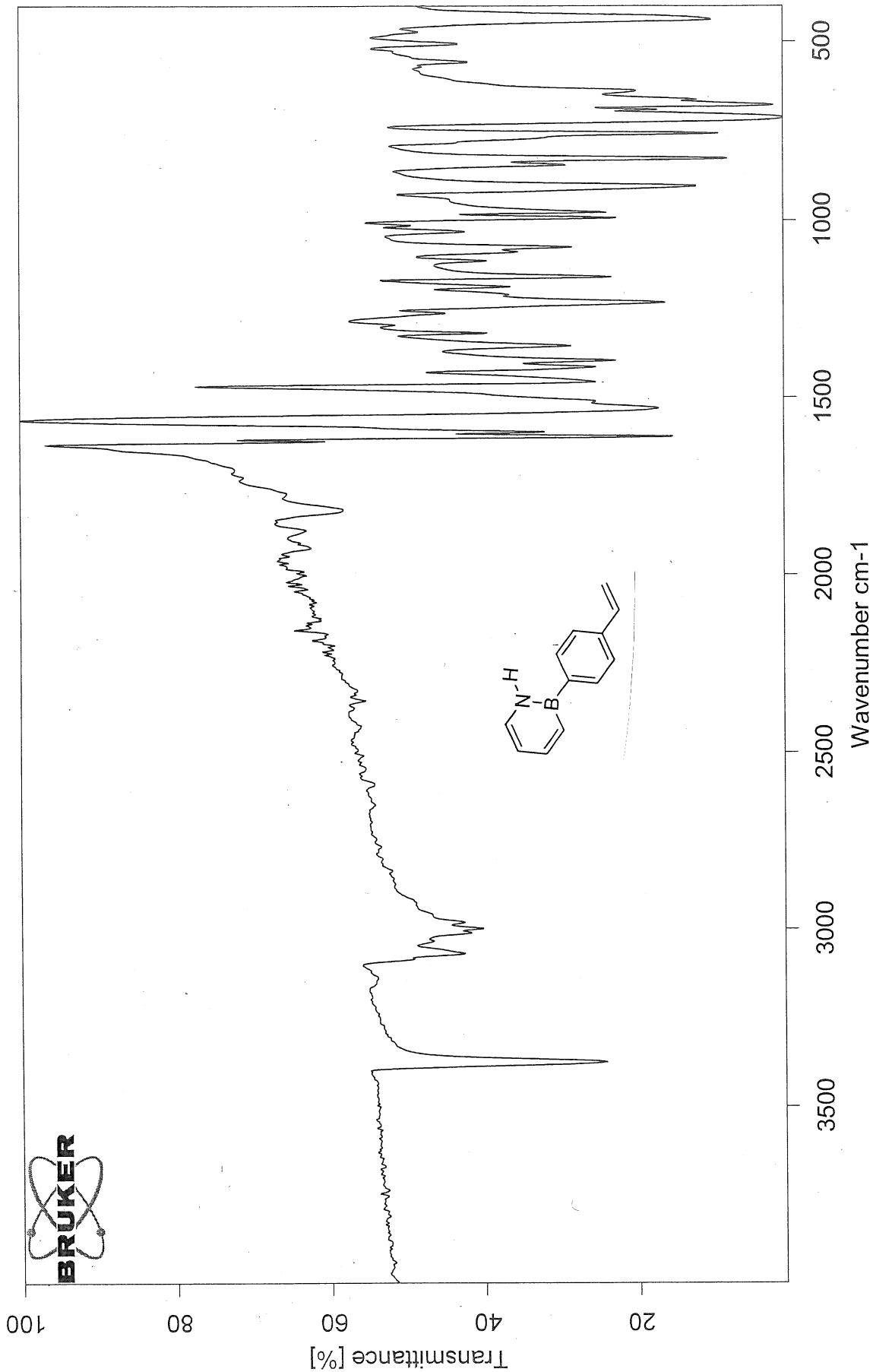
DATA PROCESSING

Line broadening 15.0 Hz

FT size 8192

Total time 312 hr, 30 min





C:\OPUS_7.2.139\1MEAS\Sample description.10	Sample description	Instrument type and / or accessory	5/10/2014
AWS-VI-93D			

AWB-VI-117J

Sample Name:

Data Collected on:
nmr11-inova500
Archive directory:

Sample directory:

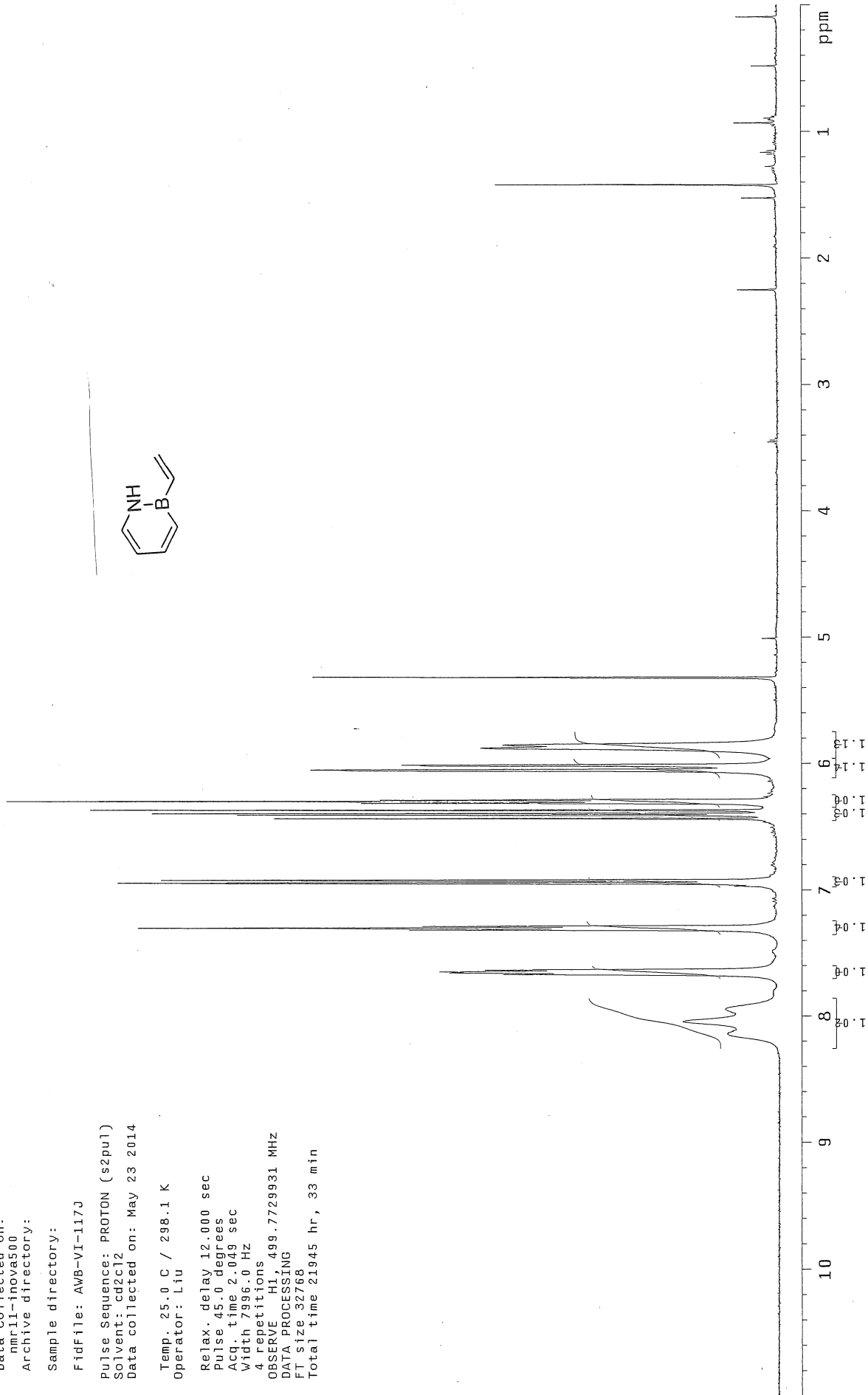
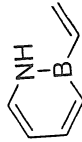
FidFile: AWB-VI-117J

Pulse Sequence: PROTON (s2pul)
Solvent: cd2c12
Data collected on: May 23 2014

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 12.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 7996.0 Hz
4 repetitions

ORSERVE H1, 499.7729931 MHZ
DATA PROCESSING
F1 size 32768
Total time 21945 hr, 33 min



AWB-V-109D

Sample Name:

Data Collected on:
nmr18-vnmrs500
Archive directory:

Sample directory:

Fidfile: AWB-V-109D

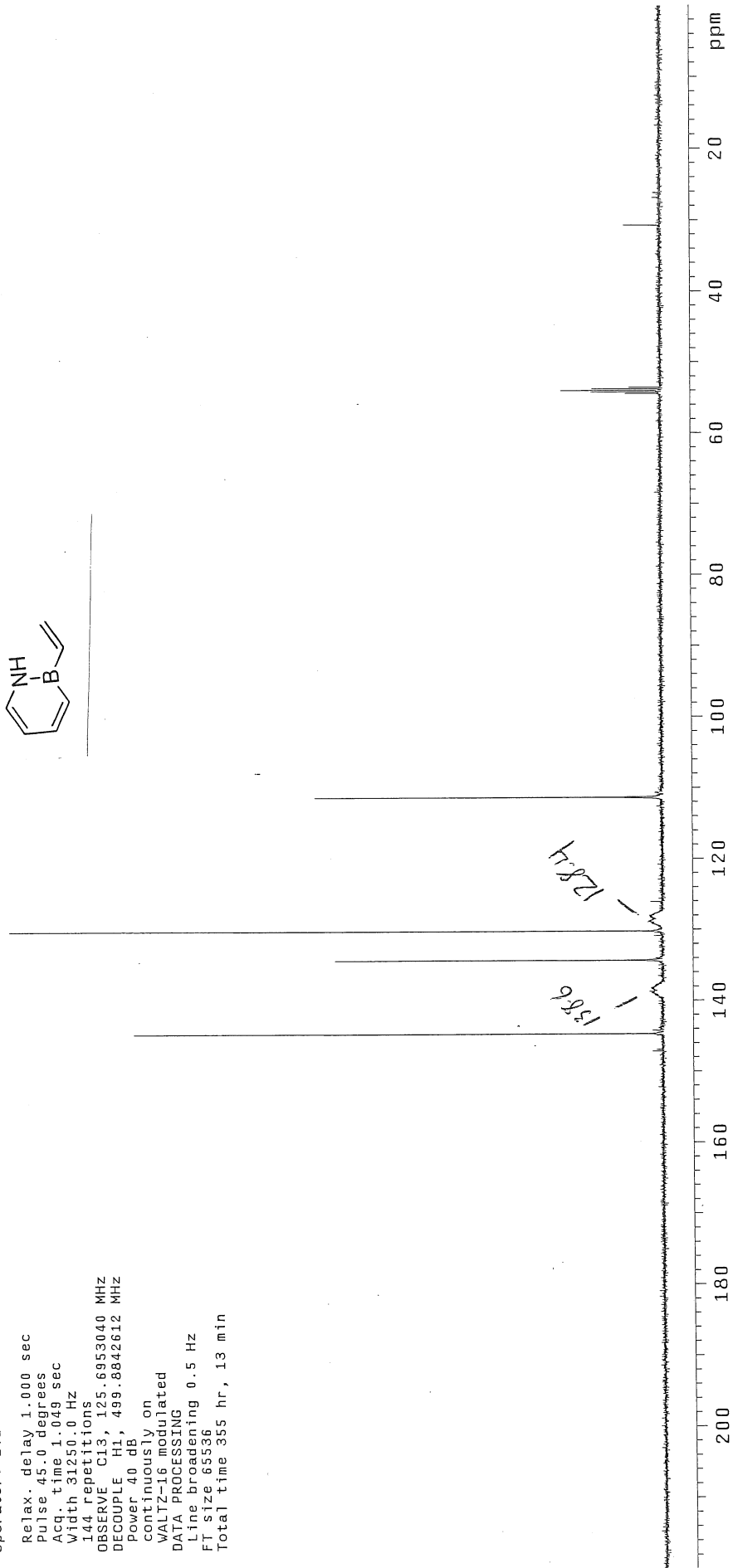
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Oct 26 2013

Temp. 25.0 C / 298.1 K
Operator: Liu

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.049 sec
Width 31250.0 Hz
144 repetitions

ORSERVE C13, 125.6953040 MHZ
DECOUPLE H1, 499.8842612 MHZ

Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 355 hr, 13 min



AVB-V-109C

Sample Name:

Data Collected on:
nmr18-vnmrs500

Archive directory:

Sample directory:

FidFile: AVB-V-109C

Pulse Sequence: s2pul

Solvent: cd2c12

Data collected on: Oct 26 2013

Temp. 25.0 C / 298.1 K

Operator: Liu

Relax. delay 0.100 sec

Pulse 37.8 degrees

Acq. time 0.100 sec

Width 32051.3 Hz

20 repetitions

OBSERVE B11, 160.3819345 MHz

DECOUPLE H1, 499.8842612 MHz

Power 40 dB

on during acquisition

off during delay

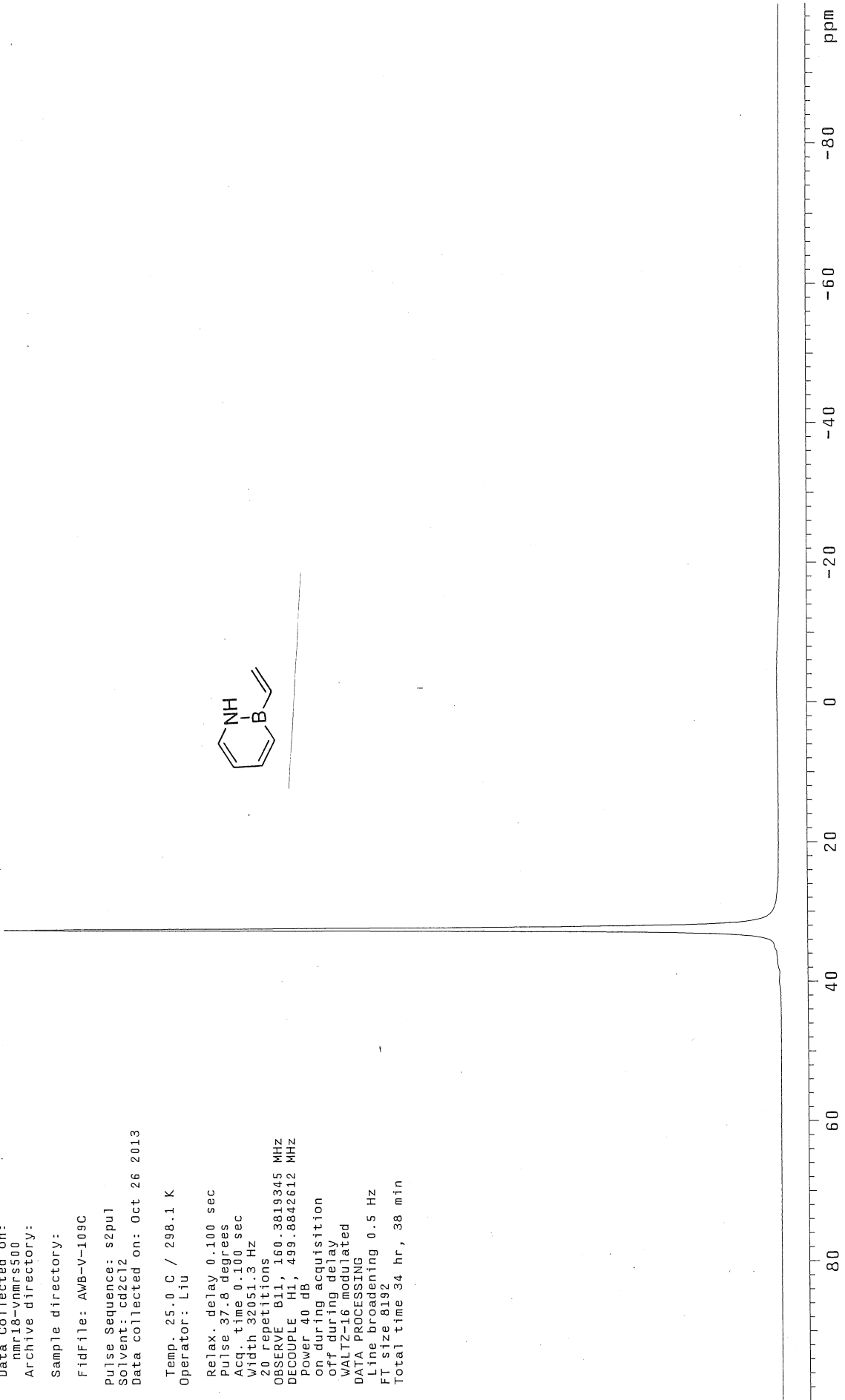
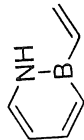
WALTZ-16 modulated

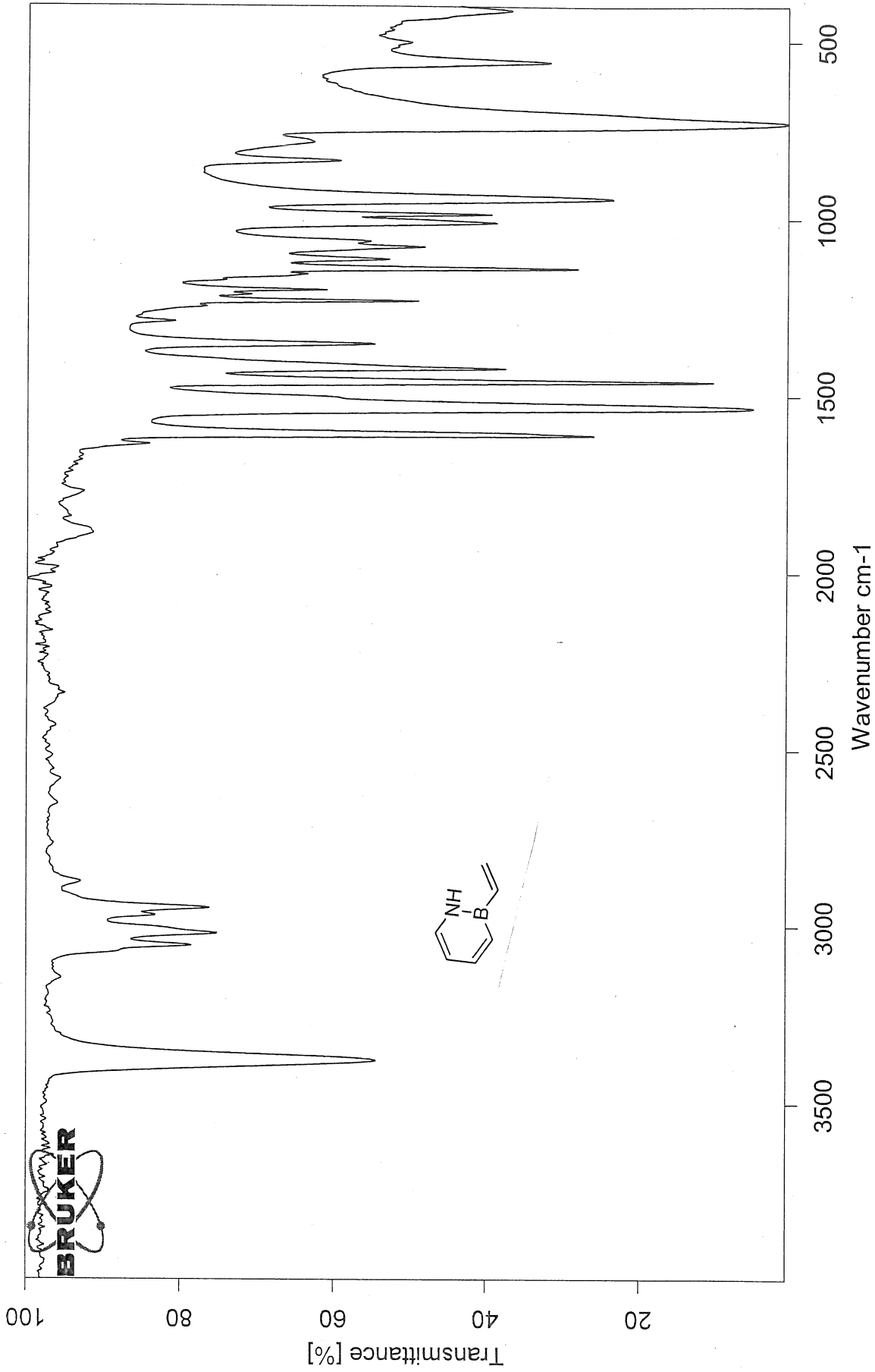
DATA PROCESSING

Line broadening 0.5 Hz

FT size 8192

Total time 34 hr, 38 min





C:\OPUS_7.2.139\MEAS\Sample description.11

Sample description Instrument type and / or accessory

5/16/2014