Practical and Broadly Applicable Synthesis of Readily Differentiable Vicinal Diboronate Compounds by Catalytic Three-Component Reactions

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SUPPORTING INFORMATION

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1. Reagents

Allylic phosphates: prepared from the corresponding allylic alcohols based on an established method.[1]

Bis(pinacolato)diboron [$B_2(pin)_2$]: purchased from Frontier Scientific, Inc., recrystallized from pentane and dried under vacuum prior to use.

Buffer solution pH 7.0 (20 ºC): purchased from Aldrich and used as received.

***Z*-1-Bromo-2-fluoroethene:** purchased from Synquest and used as received.

***N*-Bromosuccinimide:** purchased from Aldrich, recrystallized from water and dried under vacuum prior to use.

***tert*-Butyldimethylsilyl chloride:** purchased from Oakwood and used as received.

***n*-Butyllithium (1.6 M in hexanes):** purchased from Aldrich and used as received.

Copper(I) chloride: purchased from Strem and used as received.

***Z*-1,2-Dichloroethene:** purchased from Aldrich and used as received.

Diethyl allyl phosphate: purchased from Aldrich and used as received.

Furan: purchased from Aldrich and purified by washing with aqueous 5% KOH, dried with Na_2SO_4, then distilled over KOH under reduced pressure prior to use.

Isopropenylboronic acid pinacol ester (2): purchased from Aldrich and used as received.

Imidazole: purchased from Aldrich and used as received.

Imidazolinium salt imid-1: purchased from Aldrich and used as received.

Lithium *tert*-butoxide: purchased from Strem and used as received.

Mo-1: prepared according to a previously reported procedure.[2]

Pinacol: purchased from Aldrich and used as received.

Phosphine ligands (PPh_3, $P(n\text{-}Bu)_3$, PCy_3, rac-binap, and phos-1–6): purchased from Strem and used as received.

Potassium *tert*-butoxide: purchased from Strem and used as received.

***trans*-1-Propenylboronic acid pinacol ester (4):** purchased from Aldrich and used as received.

Sodium *tert*-butoxide: purchased from Strem and used as received.

Sodium perborate tetrahydrate ($NaBO_3 \bullet 4H_2O$): purchased from Aldrich and used as received.

2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-2,3-dihydro-1H-naphtho[1,8-de][1,3,2]diazaborinine [(dan)B–B(pin)]: purchased from AKSci and used as received.

Vinylboronic acid pinacol ester [vinyl–B(pin)]: purchased from Combi-Blocks and distilled over CaH_2 prior to used.

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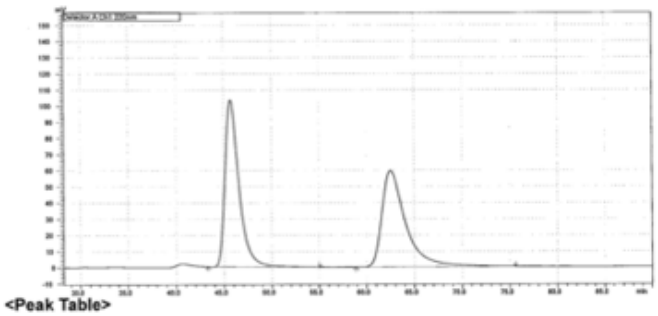
(1) Kacprzynski, M. A.; May, T. L.; Kazane, S. A.; Hoveyda, A. H. *Angew. Chem., Int. Ed.* **2007**, *46*, 4554–4558.

(2) Koh, M. J.; Nguyen, T. T.; Zhang, H.; Schrock, R. R.; Hoveyda, A. H. *Nature* **2016**, 531, 459–465.

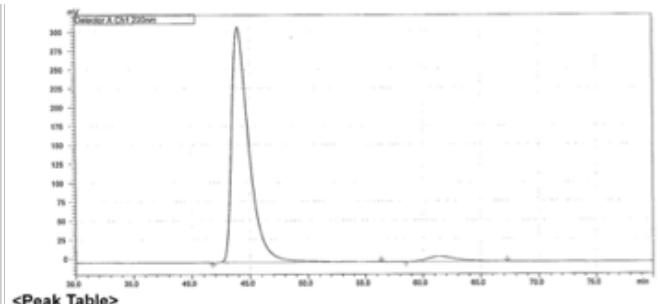
Vinyl–B(dan): prepared from vinyl–B(pin) according to a previously reported procedure.[3]

2-(2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-1-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (1a): Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (96:4 er. shown; Chiralcel OJ–H column, 98% hexanes, 0.3 mL/min, 220 nm).



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area%
1	45.697	10483479	103209	50.477
2	62.530	10285406	59512	49.523
Total		20768886	162721	100.000

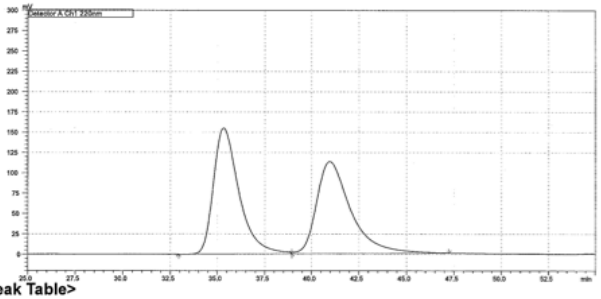


<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area%
1	44.009	31784319	311203	96.280
2	61.401	1228102	7055	3.720
Total		33012420	318258	100.000

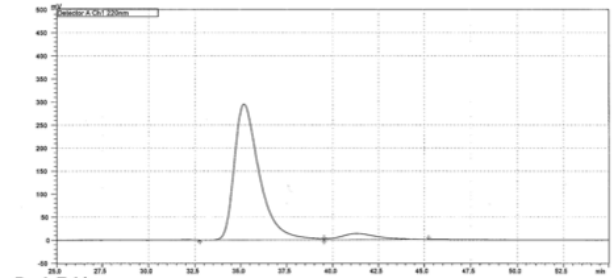
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	45.697	50.477	1	44.009	96.280
2	62.530	49.523	2	61.401	3.720

2-(4-Methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-1-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (1b): Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (94:6 er. shown; Chiralcel OJ–H column, 98% hexanes, 0.3 mL/min, 220 nm).



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	35.330	14529014	154924	50.568	50.568
2	40.964	14202824	113070	49.432	49.432
Total		28731838	267994		100.000



<Peak Table>
Detector A Channel 1 220nm

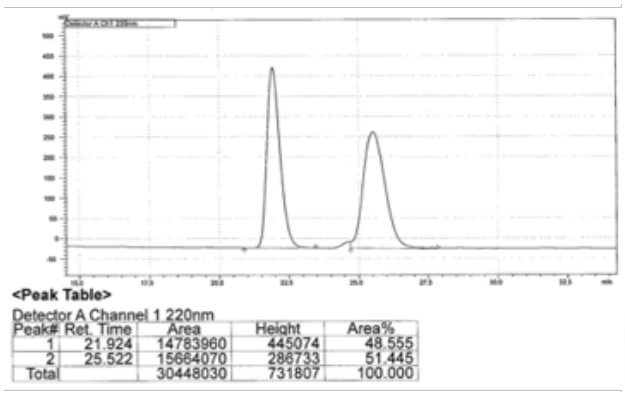
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	35.173	27844516	295094	93.911	93.911
2	41.330	1805348	13249	6.089	6.089
Total		29649864	308344		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	35.330	50.568	1	35.173	93.911
2	40.946	49.432	2	41.330	6.089

2-(4-(((*tert*-Butyldimethylsilyl)oxy)methyl)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-1-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (1c): Enantiomeric

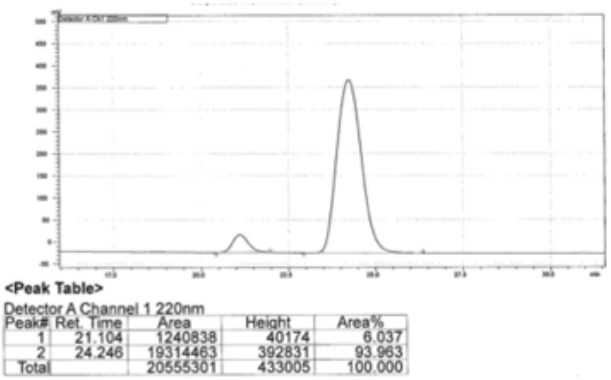
(3) Iannazzo, L.; Vollhardt, K. P. C.; Malacria, M.; Aubert, C.; Gandon, V. *Eur. J. Org. Chem.* **2011**, 3238–3292.

purity was determined by HPLC analysis in comparison with authentic racemic material (94:6 er. shown; Chiralpak AD–H column, 99% hexanes, 0.3 mL/min, 220 nm)



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area%
1	21.924	14783960	445074	48.555
2	25.522	15664070	286733	51.445
Total		30448030	731807	100.000

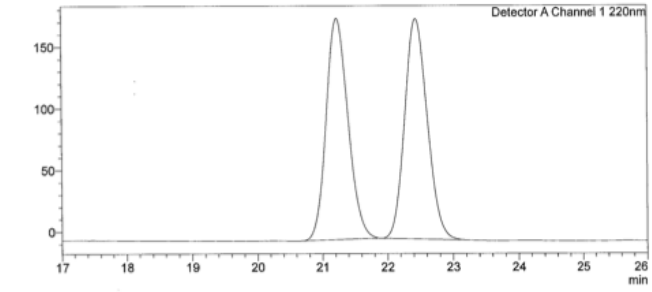


<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area%
1	21.104	1240838	40174	6.037
2	24.246	19314463	392831	93.963
Total		20555301	433005	100.000

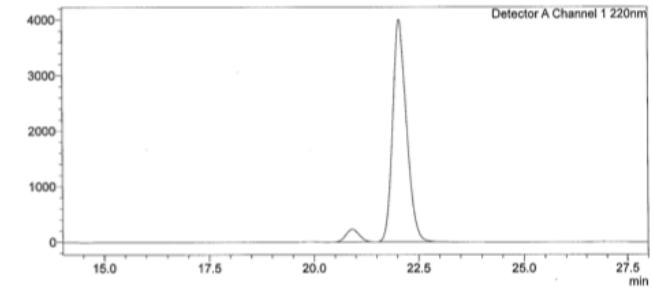
Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	21.924	48.555	1	21.104	6.037
2	25.522	51.445	2	24.246	93.963

2-(4-Phenyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-1-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (1d): Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (95:5 er. shown; Chiralcel AZ–H column, 98% hexanes, 0.3 mL/min, 220 nm).



<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.
1	21.226	4223120	179472	49.654
2	22.438	4282020	178674	50.346
Total		8505140	358146	

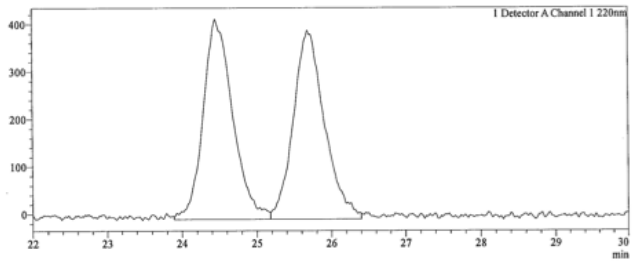


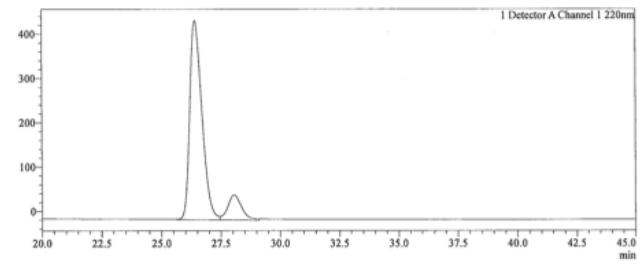
<Peak Table>
Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	20.911	5125681	230050	5.292	5.292
2	22.046	91727249	3997526	94.708	94.708
Total		96852930	4227576		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	21.226	49.654	1	20.911	5.292
2	22.438	50.346	2	22.046	94.708

2-(2-Methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-1-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (3): Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (87:13 er. shown; Chiralcel OD–H column, 99% hexanes, 0.3 mL/min, 220 nm).





<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	24.454	11631584	421378	50.223	50.223
2	25.688	11528194	397274	49.777	49.777
Total		23159778	818652		100.000

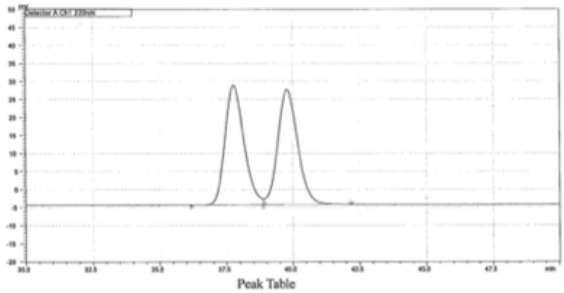
<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	26.421	16081177	449962	87.377	87.377
2	28.054	2323107	56856	12.623	12.623
Total		18404284	506818		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	24.454	50.223	1	26.421	87.377
2	25.688	49.777	2	28.054	12.623

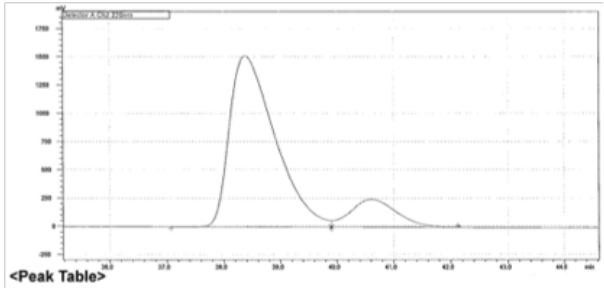
2-(1-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)pent-4-en-2-yl)-2,3-dihydro-1*H*-naphtho[1,8-*de*][1,3,2]diazaborinine (6): Enantiomeric purity was determined by HPLC analysis in comparison with authentic racemic material (86:14 er shown; Chiralcel OD–H column, 99% hexanes, 0.3 mL/min, 220 nm).



Peak Table

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Area%
1	37.769	1643565	33186	49.487
2	39.785	1677664	31993	50.513
Total		3321229	65179	100.000



<Peak Table>

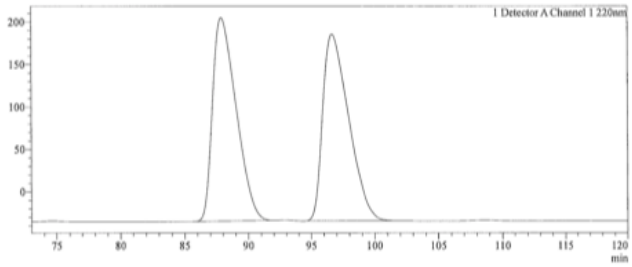
Detector A Channel 2 220nm

Peak#	Ret. Time	Area	Height	Area%
1	38.379	84381751	1514059	85.794
2	40.607	13972307	247695	14.206
Total		98354058	1761754	100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	37.769	49.487	1	38.379	85.794
2	39.785	50.513	2	40.607	14.206

2,2'-(2-Methylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (15): Enantiomeric purity was determined by HPLC analysis of 1-phenylpent-4-en-2-ol, the product after cross-coupling of **15** with PhBr[4] and oxidation with $NaBO_3$ in comparison with authentic racemic material (68:32 er shown; Chiralcel OJ–H column, 99% hexanes, 0.3 mL/min, 220 nm).

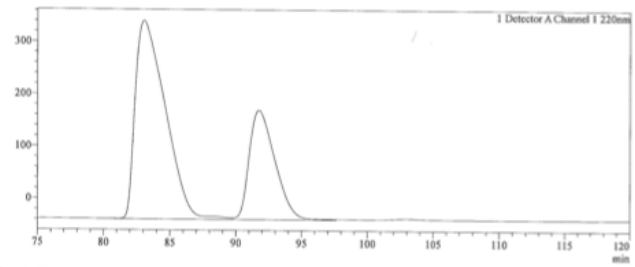
(4) Mlynarski, S. N.; Schuster, C. H.; Morken, J. P. *Nature* **2014**, *505*, 386–390.



<Peak Table>

Detector A Channel 1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Area%
1	87.903	31057175	239707	49.614	49.614
2	96.660	31539975	220074	50.386	50.386
Total		62597150	459781		100.000



<Peak Table>

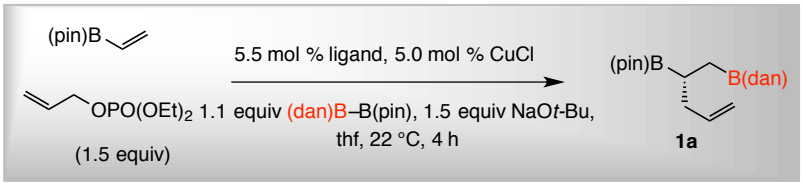
Detector A Channel 1 220nm

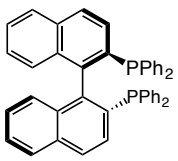
Peak#	Ret. Time	Area	Height	Conc.	Area%
1	83.028	59795957	380030	67.697	67.697
2	91.727	28532698	209480	32.303	32.303
Total		88328655	589510		100.000

Peak #	Time (min)	Area (%)	Peak #	Time (min)	Area (%)
1	87.903	49.614	1	83.028	67.697
2	96.660	50.386	2	91.727	32.303

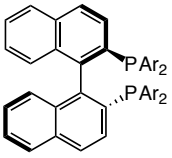
2. Examination of Different Types of Chiral Cu Complexes on Catalytic Enantioselective Variants

Scheme S1. Ligand screen for reactions of vinyl–B(pin) and (dan)B–B(pin).[a]

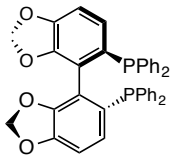




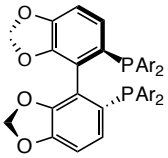
phos-6
>98% conv, 69% yield
92:8 er



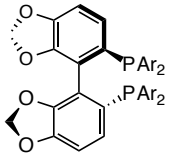
Ar = 3,5-$(Me)_2C_6H_3$
L1
>98% conv, 45% yield
92:8 er



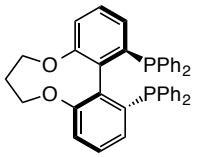
L2
>98 % conv, 82% yield
92:8 er



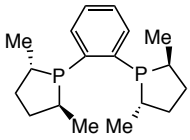
Ar = 3,5-$(t\text{-}Bu)_2$-4-$OMeC_6H_2$
L3
>98% conv, 20% yield
90:10 er



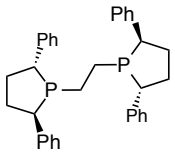
Ar = 3,5-$(Me)_2C_6H_3$
phos-3
>98% conv, 67% yield
96:4 er



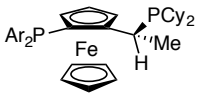
L4
>98% conv, 71% yield
95:5 er



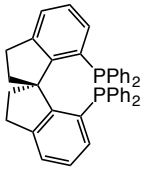
L5
>98% conv
60:40 er



phos-4
>98% conv
86:14 er



Ar = 3,5-$(t\text{-}Bu)_2$-4-$OMeC_6H_2$
L6
>98% conv, 34% yield
84:16 er

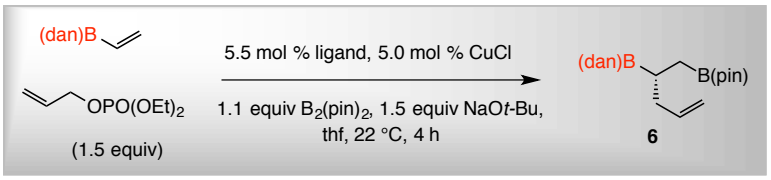


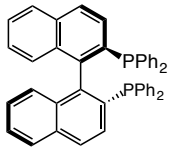
L7
48% conv, 22% yield
52:48 er

[a]Reactions were carried out under N_2 atm. Conversion determined by analysis of the ^1H NMR spectra of the unpurified mixtures; conv. (±2%) refer to disappearance of a limiting reagent [vinyl–B(pin)]. Yields are for purified products (±5%).

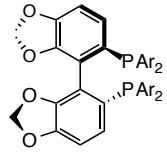
A three-component process with vinyl–B(pin), allylphosphate and (dan)B–B(pin) was examined with various types of chiral Cu complexes as shown in Scheme S1. Reaction with **phos-6** is efficient and enantioselective (69% yield, 92:8 er). Enantioselectivities obtained from binap and segphos type ligands were high with **phos-3** as the optimal ligand (67% yield, 96:4 er). Reaction with **L4** are similarly efficient and enantioselective; however, **phos-3** is available in a lower price.

Scheme S2. Ligand screen for reactions of vinyl–B(dan) and $B_2(pin)_2$.[a]



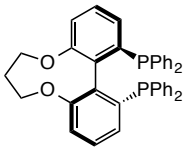


phos-6
>98% conv, 56% yield
65:35 er

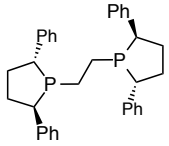


Ar = 3,5-$(Me)_2C_6H_3$

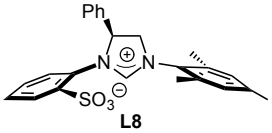
phos-3
27% yield, 60:40 er



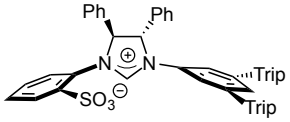
L4
42% yield
53:47 er



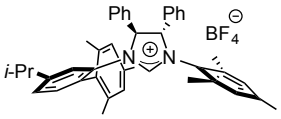
phos-4
67% yield, 86:14 er



L8
26% conv
39:61 er



L9
8% conv



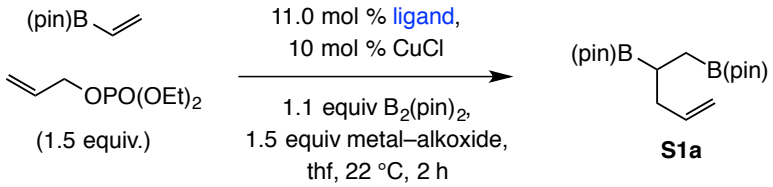
L10
9% conv

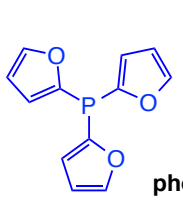
[a]Reactions were carried out under N_2 atm. Conversion determined by analysis of the ^{1}H NMR spectra of the unpurified mixtures; conv. (±2%) refer to disappearance of a limiting reagent [vinyl–B(dan)]. Yields are for purified products (±5%).

Examination of reactions with vinyl–B(dan), allylphosphate and $B_2(pin)_2$ with various types of chiral Cu complexes is shown in Scheme S2. Reaction with **phos-4** showed the most promising result (67% yield, 86:14 er). Reactions with an NHC as a ligand were not efficient nor enantioselective likely due to a competitive boron allylic substitution reaction.

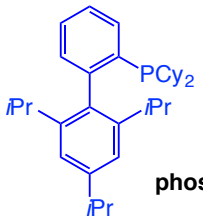
3. Results of Reactions Affording Vicinal Di–B(pin) Compounds

Table S1. Examination of different Cu complexes.[a]

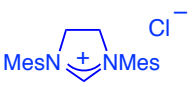




phos-1



phos-2



imid-1

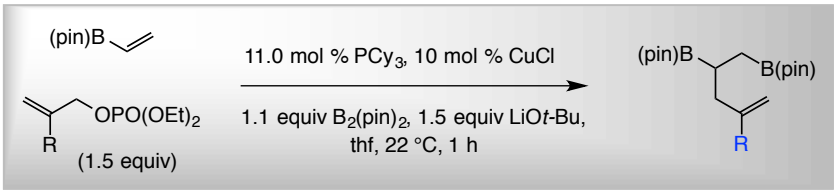
entry	ligand	alkoxide	conv (%)[b]	yield (%)[c]
1	none	NaO*t*-Bu	90	13
2	PPh_3	NaO*t*-Bu	>98	81
3	PPh_3	LiO*t*-Bu	>98	92 (85)
4	PPh_3	KO*t*-Bu	>98	72
5	$P(n\text{-}Bu)_3$	LiO*t*-Bu	>98	16
6	PCy_3	LiO*t*-Bu	>98	91(92)
7	**phos-1**	LiO*t*-Bu	91	47
8	**phos-2**	LiO*t*-Bu	91	53
9	*rac*-binap	LiO*t*-Bu	96	58
10	**imid-1**	LiO*t*-Bu	83	17

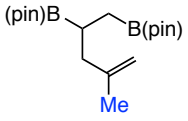
[a]Reactions were carried out under N_2 atm. [b]Determined by analysis of the ^{1}H NMR spectra of the unpurified mixtures; conv. (±2%) refer to disappearance of a limiting reagent [vinyl–B(pin)]. Yields are for purified products (±5%); yields in parenthesis were obtained from reactions quenched after 1 h.

A three-component process with vinyl–B(pin), allylphosphate and $B_2(pin)_2$ was investigated as shown in Table S1. With NaO*t*-Bu as the base but in the absence of a ligand there was 90% conv of the limiting reagent [(vinyl–B(pin)] but **S1a** was obtained in 13% yield (entry 1). Addition of 11.0 mol % PPh_3 resulted in substantially improved efficiency affording **S1a** in 81% yield (entry 2). Subsequent evaluation of several mono- and bidentate phosphines including N-heterocyclic carbene (NHC) as a ligand (entries 5–10) indicated that the combination of PCy_3 and LiO*t*-Bu is optimal affording **S1a** in 92% yield after 1 h (entry 6, Table S1).

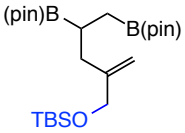
Various 2-substituted allylic phosphates were used as suitable substrates. Products (**S1b–i**) were obtained in 56–88% yield as shown in Scheme S3.

Scheme S3. Reactions with 2-substituted allylic phosphates that afford products with vicinal B(pin) groups.[a]

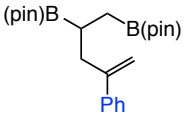




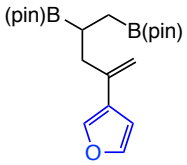
S1b
>98% conv, 88% yield



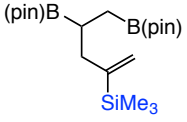
S1c
>98% conv, 88% yield



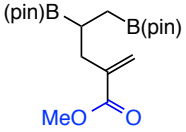
S1d
89% conv, 61% yield



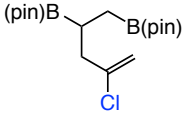
S1e
91% conv, 72% yield



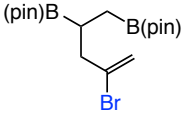
S1f
>98% conv, 84% yield



S1g
90% conv, 56% yield



S1h
>98% conv, 85% yield



S1i
90% conv, 78% yield

[a]See Table S1.

Representative Procedure for Reactions that Afford Vicinal Di–B(pin) Compounds

In a N_2-filled glove box, an oven-dried 1 dram vial equipped with a stir bar was charged with PCy_3 (3.1 mg, 0.011 mmol), LiO*t*-Bu (12 mg, 0.15 mmol), and CuCl (1.0 mg, 0.010 mmol), and thf (1.0 mL). The mixture was allowed to stir for 15 min at 22 °C; during this time the solution turned light-yellow. $B_2(pin)_2$ (27.9 mg, 0.11 mmol) was added to the mixture, causing the solution to turn dark brown immediately. Vinyl–B(pin) (15.4 mg, 0.10 mmol), allylphosphate (29.1 mg, 0.15 mmol), and thf (0.50 mL) were added. The vial was sealed with a cap and electrical tape before removal from the glove box. The resulting mixture was allowed to stir at 22 °C for 1 h. The mixture was then passed through a short plug of silica gel (4 x 1 cm) and eluted with Et_2O. The organic layer was concentrated under reduced pressure, affording yellow oil, which was purified by silica gel chromatography (100% hexanes→hexanes:Et_2O = 50:1) to afford S**1a** as colorless oil (29.6 mg, 0.092 mmol, 92% yield).

2,2'-(Pent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1a): IR (neat): 2978 (m), 2927 (w), 1371 (s), 1314 (s), 1143 (s), 968 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.84–5.74 (1H, m), 5.00–4.90 (2H, m), 2.25–2.18 (1H, m), 2.11–2.04 (1H, m), 1.22 (12H, s), 1.21 (12H, s), 1.27–1.21 (1H, m), 0.90–0.78 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.8, 115.1, 83.0, 82.96, 38.0, 25.0, 24.99, 24.93, 24.91; HRMS (DART): Calcd for $C_{17}H_{33}B_2O_4$ [M+H]+: 323.2565, Found: 323.2575.

2,2'-(4-Methylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1b): IR (neat): 2978 (m), 2928 (w), 1370 (s), 1314 (s), 1143 (s), 968 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 4.68 (1H, d, *J* = 1.6 Hz), 4.66 (1H, d, *J* = 0.8 Hz), 2.20 (1H, dd, *J* = 14.0, 7.2 Hz), 2.00 (1H, dd, *J* = 14.2, 8.6 Hz), 1.58 (3H, s), 1.35–1.27 (1H, m), 1.22 (12H, s), 1.217 (12H, s), 0.85–0.74 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.2, 117.2, 83.3, 83.1, 44.6, 25.0, 24.97, 24.9; HRMS (DART): Calcd for $C_{18}H_{35}B_2O_4$ $[M+H]^+$: 337.2721, Found: 337.2722.

***tert*-Butyldimethyl((2-methylene-4,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentyl)oxy)silane (S1c)**: IR (neat): 2977 (w), 2929 (w), 2856 (w), 1370 (s), 1313 (s), 1252 (m), 1142 (s), 1101 (m), 968 (m), 836 (s), 776 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.05–5.04 (1H, m), 4.83–4.81 (1H, m), 4.05 (2H, s), 2.19 (1H, dd, *J* = 14.6, 7.4 Hz), 1.98 (1H, dd, *J* = 14.4, 8.4 Hz), 1.33–1.19 (1H, m), 1.22 (12H, s), 1.21 (12H, s), 0.90 (9H, s), 0.88–0.74 (2H, m), 0.05 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 108.9, 83.0, 82.99, 65.7, 36.7, 26.1, 25.0, 24.97, 24.9, 18.6, –5.2; HRMS (DART): Calcd for $C_{24}H_{52}B_2N_1O_5Si_1$ $[M+NH_4]^+$: 484.3801, Found: 484.3795.

2,2'-(4-Phenylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1d): IR (neat): 2977 (m), 2927 (w), 1370 (s), 1313 (s), 1142 (s), 968 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.43–7.41 (2H, m), 7.30–7.22 (3H, m), 5.25 (1H, d, *J* = 2.0 Hz), 5.06 (1H, d, *J* = 1.2 Hz), 2.73 (1H, dd, *J* = 13.6, 7.6 Hz), 2.48 (1H, dd, *J* = 14.6, 7.8 Hz), 1.34–1.27 (1H, m), 1.22 (12H, s), 1.21 (12H, s), 0.88–0.79 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 141.6, 128.2, 127.2, 126.5, 113.2, 83.0, 82.99, 39.0, 25.0, 24.99, 24.96, 24.92; HRMS (DART): Calcd for $C_{23}H_{40}B_2N_1O_4$ $[M+NH_4]^+$: 416.3143, Found: 416.3127.

2,2'-(4-(Furan-3-yl)pent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1e): IR (neat): 2977 (m), 2928 (w), 1369 (s), 1312 (s), 1140 (s), 968 (m), 872 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.54 (1H, s), 7.32 (1H, t, *J* = 1.6 Hz), 6.51 (1H, dd, *J* = 1.8, 1.0 Hz), 5.20 (1H, d, *J* = 1.2 Hz), 4.93 (1H, d, *J* = 1.6 Hz), 2.54 (1H, ddd, *J* = 14.1, 7.9, 0.9 Hz), 2.30 (1H, dd, *J* = 14.0, 7.6 Hz), 1.46–1.37 (1H, m), 1.23 (12H, s), 1.21 (12H, s), 0.90–0.81 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.9, 139.5, 139.3, 126.8, 110.9, 108.5, 83.1, 83.0, 38.7, 25.03, 25.01, 24.96, 24.94; HRMS (DART): Calcd for $C_{21}H_{35}B_2O_5$ $[M+H]^+$: 389.2671, Found: 389.2667.

(4,5-Bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-1-en-2-yl)trimethylsilane (S1f): IR (neat): 2977 (m), 1370 (s), 1313 (s), 1247 (m), 1142 (s), 968 (m), 836 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.57–5.56 (1H, m), 5.31–5.30 (1H, m), 2.38–2.32 (1H, m), 2.08 (1H, dd, *J* = 14.6, 8.2 Hz), 1.37–1.29 (1H, m), 1.22 (12H, s), 1.20 (12H, s), 0.86–0.73 (2H, m), 0.07 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 124.4, 82.9, 82.87, 39.7, 25.0, 24.96, 24.9, –1.2; HRMS (DART): Calcd for $C_{20}H_{44}B_2N_1O_4Si_1$ $[M+NH_4]^+$: 412.3226, Found: 412.3222.

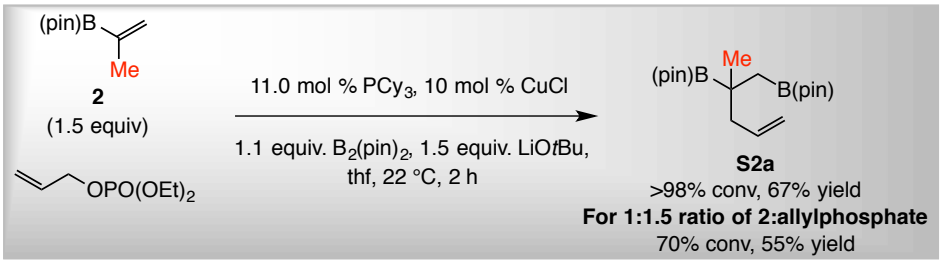
Methyl 2-methylene-4,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanoate (S1g): IR (neat): 2978 (m), 2928 (w), 1722 (m), 1629 (w), 1370 (s), 1315 (s), 1141 (s), 968 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 6.14 (1H, d, *J* = 1.2 Hz), 5.53 (1H, dd, *J* = 2.8, 1.2 Hz), 3.72 (3H, s), 2.54 (1H, ddd, *J* = 14.6, 7.4, 0.8 Hz), 2.26 (1H, dd, *J* = 14.5, 7.7 Hz), 1.40–1.33 (1H, m), 1.22 (24H, s), 0.83 (2H, d, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 140.4, 125.5, 83.1,

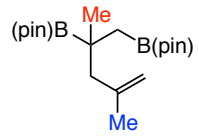
83.06, 51.8, 35.4, 30.5, 25.0, 24.98, 24.9; HRMS (DART): Calcd for $C_{19}H_{35}B_2O_6$ $[M+H]^+$: 381.2620, Found: 381.2635.

2,2'-(4-Chloropent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1h): IR (neat): 2979 (m), 2929 (w), 1633 (w), 1371 (s), 1317 (s), 1142 (s), 968 (w) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.13 (1H, d, J = 0.8 Hz), 5.10 (1H, d, J = 1.2 Hz), 2.52 (1H, ddd, J = 14.7, 6.5, 0.9 Hz), 2.35 (1H, ddd, J = 14.8, 8.8, 0.4 Hz), 1.53–1.42 (1H, m), 1.22 (24H, s), 0.90–0.79 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.0, 112.7, 83.3, 83.1, 42.4, 25.0, 24.97, 24.93, 24.92; HRMS (DART): Calcd for $C_{17}H_{32}B_2Cl_1O_4$ $[M+H]^+$: 357.2175, Found: 357.2179.

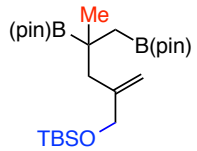
2,2'-(4-Bromopent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S1i): IR (neat): 2977 (m), 2928 (w), 1627 (w), 1369 (s), 1313 (s), 1139 (s), 967 (m), 882 (m), 856 (m), 844 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.54 (1H, d, J = 1.2 Hz), 5.38 (1H, d, J = 1.2 Hz), 2.61 (1H, dd, J = 14.2, 5.8 Hz), 2.43 (1H, dd, J = 15.0, 9.0 Hz), 1.54–1.46 (1H, m), 1.23 (24H, s), 0.91–0.78 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.2, 117.2, 83.3, 83.1, 44.6, 25.0, 24.97, 24.9; HRMS (DART): Calcd for $C_{17}H_{32}B_2Br_1O_4$ $[M+H]^+$: 401.1670, Found: 401.1684.

Scheme S4. Reactions with 2-propenyl–B(pin) that afford products containing a tertiary C–B(pin).[a]

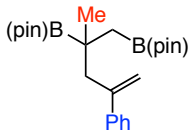




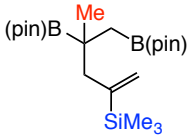
S2b
>98% conv, 79% yield



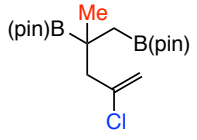
S2c
>98% conv, 95% yield



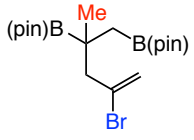
S2d
>98% conv, 54% yield



S2e
>98% conv, 68% yield



S2f
79% conv, 62% yield



S2g
77% conv, 48% yield

[a]See Table S1.

A three-component process with isopropenyl–B(pin) (**2**), allylphosphate and $B_2(pin)_2$ was also examined as shown in Scheme S4. Use of slightly excess of 2 is required for optimal efficiency. Several 2-substituted allylic phosphates can be used as substrates. Products (**S2a–g**) were obtained in 48–95% yield as shown in Scheme S4.

Representative Procedure for Reactions with 2-Propenyl–B(pin)

In a N_2-filled glove box, an oven-dried 1 dram vial equipped with a stir bar was charged with PCy_3 (3.1 mg, 0.011 mmol), Li*O*t-Bu (12 mg, 0.15 mmol), and CuCl (1.0 mg, 0.010 mmol), and thf (1.0 mL). The mixture was allowed to stir for 15 min at 22 °C; during this time the solution turned light-yellow. $B_2(pin)_2$ (27.9 mg, 0.11 mmol) was added to the mixture, causing the solution to turn dark brown immediately. 2-Propenyl–B(pin) (25.2 mg, 0.15 mmol), allylphosphate (19.4 mg, 0.10 mmol), and thf (0.50 mL) were added. The vial was sealed with a cap and electrical tape before removal from the glove box. The resulting mixture was allowed to stir at 22 °C for 2 h. The mixture was then passed through a short plug of silica gel (4 x 1 cm) and eluted with Et_2O. The organic layer was concentrated under reduced pressure, affording yellow oil, which was purified by silica gel chromatography (100% hexanes→hexanes:Et_2O = 50:1) to afford S**2a** as colorless oil (22.5 mg, 0.067 mmol, 67% yield).

2,2'-(2-Methylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S2a): IR (neat): 2977 (m), 2930 (w), 1360 (s), 1307 (s), 1139 (s), 969 (m), 845 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.82 (1H, ddt, *J* = 17.0, 10.2, 7.4 Hz), 2.13 (1H, dd, *J* = 14.2, 7.2 Hz), 2.05 (1H, dd, *J* = 14.2, 7.0 Hz), 1.23 (12H, s), 1.21 (12H, s), 0.96 (3H, s), 0.94 (1H, d, *J* = 15.2 Hz), 0.70 (1H, d, *J* = 16.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.9, 116.2, 83.1, 82.9, 46.0, 25.1, 25.0, 24.9, 24.89, 24.0; HRMS (DART): Calcd for $C_{18}H_{35}B_2O_4$ $[M+H]^+$: 337.2721, Found: 337.2738.

2,2'-(2,4-Dimethylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S2b): IR (neat): 2977 (m), 2929 (w), 1461 (m), 1370 (s), 1359 (s), 1307 (s), 1213 (m), 1142 (s), 969 (m), 848 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 4.74–4.72 (1H, m), 4.66 (1H, s), 2.18 (1H, d, *J* = 13.6 Hz), 2.06 (1H, d, *J* = 13.6 Hz), 1.72, (3H, s), 1.23 (12H, s), 1.22 (12H, s), 0.99 (3H, s), 0.96 (1H, d, *J* = 16.0 Hz), 0.73 (1H, d, *J* = 15.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.8, 112.8, 83.2, 82.9, 49.1, 25.1, 25.06, 24.9, 24.7, 24.3; HRMS (DART): Calcd for $C_{19}H_{37}B_2O_4$ $[M+H]^+$: 351.2878, Found: 351.2892.

***tert*-Butyldimethyl((4-methyl-2-methylene-4,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentyl)oxy)silane (S2c)**: IR (neat): 2977 (m), 2929 (m), 2857 (m), 1462 (m), 1370 (s), 1360 (s), 1309 (s), 1253 (m), 1213 (m), 1142 (s), 1109 (s), 970 (m), 836 (s), 775 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.14–5.12 (1H, m), 4.86 (1H, s), 4.03 (2H, s), 2.13 (1H, d, *J* = 14.0 Hz), 2.02 (1H, d, *J* = 14.4 Hz), 1.23 (12H, s), 1.22 (12H, s), 0.98 (3H, s), 0.94 (1H, d, *J* = 15.6 Hz), 0.90 (9H, s), 0.75 (1H, d, *J* = 15.6 Hz), 0.04 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.9, 110.6, 83.2, 82.9, 66.9, 43.7, 26.1, 25.1, 25.07, 25.0, 24.9, 24.4, 18.5, –5.2; HRMS (DART): Calcd for $C_{25}H_{54}B_2N_1O_5Si_1$ $[M+NH_4]^+$: 498.3967, Found: 498.3969.

2,2'-(2-Methyl-4-phenylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S2d): IR (neat): 2977 (m), 2928 (w), 1463 (w), 1369 (s), 1359 (s), 1310 (s), 1213 (m), 1143 (s), 970 (m), 700 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 7.40–7.38 (2H, m), 7.28–7.18 (3H, m), 5.20 (1H, d, *J* = 2.0 Hz), 5.07 (1H, s), 2.72 (1H, d, *J* = 14.0 Hz), 2.57 (1H, d, *J* = 14.0 Hz), 1.21 (6H, s), 1.207 (6H, s), 1.14 (12H, s), 0.95 (1H, d, *J* = 15.6 Hz), 0.86 (3H, s), 0.72 (1H, d, *J* = 15.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.8, 143.9, 128.1, 127.0, 126.9, 116.1, 83.1, 82.9, 45.7,

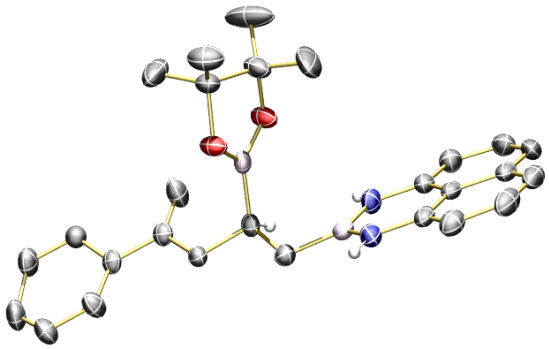
25.1, 25.05, 24.94, 24.9; HRMS (DART): Calcd for $C_{24}H_{42}B_2N_1O_4$ $[M+NH_4]^+$: 430.3300, Found: 430.3287.

Trimethyl(4-methyl-4,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pent-1-en-2-yl)silane (S2e): IR (neat): 2977 (m), 1465 (w), 1378 (s), 1370 (s), 1359 (s), 1310 (s), 1248 (m), 1143 (s), 970 (m), 837 (s) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.67–5.65 (1H, m), 5.41–5.40 (1H, m), 2.32 (1H, dt, *J* = 15.6, 1.4 Hz), 2.12 (1H, dd, *J* = 15.6, 1.2 Hz), 1.23 (24H, s), 1.01 (3H, s), 0.99 (1H, d, *J* = 14.4 Hz), 0.74 (1H, d, *J* = 15.2 Hz), 0.06 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.8, 125.4, 83.1, 82.9, 45.5, 25.2, 25.1, 24.9, 24.0, –1.1; HRMS (DART): Calcd for $C_{121}H_{43}B_2O_4Si_1$ $[M+H]^+$: 409.3117, Found: 409.3119.

2,2'-(4-Chloro-2-methylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S2f): IR (neat): 2977 (m), 2929 (w), 1629 (w), 1461 (w), 1369 (s), 1311 (s), 1138 (s), 969 (m), 845 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.17 (1H, d, *J* = 1.2 Hz), 5.11 (1H, d, *J* = 1.2 Hz), 2.54 (1H, d, *J* = 14.4 Hz), 2.45 (1H, d, *J* = 14.8 Hz), 1.24 (12H, s), 1.22 (12H, s), 1.05 (3H, s), 1.02 (1H, d, *J* = 15.6 Hz), 0.80 (1H, d, *J* = 16.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.5, 114.4, 83.4, 83.0, 49.4, 25.1, 25.03, 25.0, 24.9, 23.8; HRMS (DART): Calcd for $C_{18}H_{34}B_2Cl_1O_4$ $[M+H]^+$: 371.2332, Found: 371.2323.

2,2'-(4-Bromo-2-methylpent-4-ene-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (S2g): IR (neat): 2977 (m), 2929 (w), 1623 (w), 1462 (m), 1369 (s), 1313 (s), 1140 (s), 969 (m), 845 (m) cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 5.57 (1H, d, *J* = 1.2 Hz), 5.45 (1H, d, *J* = 1.6 Hz), 2.67 (1H, d, *J* = 14.8 Hz), 2.58 (1H, d, *J* = 14.8 Hz), 1.25 (12H, s), 1.23 (12H, s), 1.07 (3H, s), 1.04 (1H, d, *J* = 16.0 Hz), 0.83 (1H, d, *J* = 15.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.4, 119.0, 83.4, 83.0, 51.2, 25.1, 25.0, 24.97, 23.8; HRMS (DART): Calcd for $C_{18}H_{34}B_2Br_1O_4$ $[M+H]^+$: 415.1827, Found: 415.1843.

4. X-ray Crystallography Data



X-ray structure of 1d

Table S1. **Crystal data and structure refinement for $C_{27}H_{32}B_2N_2O_2$.**

Identification code	C27H32B2N2O2	
Empirical formula	C27 H32 B2 N2 O2	
Formula weight	438.16	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.7928(4) Å	α = 90°.
	b = 9.8354(4) Å	β = 95.934(3)°.
	c = 20.6121(8) Å	γ = 90°.
Volume	2377.92(16) Å^3	
Z	4	
Density (calculated)	1.224 Mg/m^3	
Absorption coefficient	0.586 mm^{-1}	
F(000)	936	
Crystal size	0.200 x 0.200 x 0.080 mm^3	
Theta range for data collection	4.144 to 69.789°.	
Index ranges	-14<=h<=13, -11<=k<=9, -24<=l<=24	
Reflections collected	11807	
Independent reflections	4197 [R(int) = 0.0410]	
Completeness to theta = 66.500∞	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.6540	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4197 / 0 / 324
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1220
R indices (all data)	R1 = 0.0724, wR2 = 0.1361
Extinction coefficient	n/a
Largest diff. peak and hole	0.247 and -0.222 e. $Å^{-3}$

Table S2. **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $C_{27}H_{32}B_2N_2O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U(eq)
O(1)	3349(1)	5792(2)	5712(1)	38(1)
O(2)	3952(1)	6823(2)	6673(1)	42(1)
N(1)	6786(1)	6903(2)	6488(1)	34(1)
N(2)	7137(1)	5288(2)	5663(1)	32(1)
B(1)	6521(2)	6431(2)	5838(1)	30(1)
B(2)	3961(2)	6847(2)	6011(1)	28(1)
C(1)	2750(2)	9637(3)	5920(1)	45(1)
C(2)	2890(2)	9456(2)	5294(1)	30(1)
C(3)	3844(2)	8597(2)	5078(1)	28(1)
C(4)	4623(2)	7894(2)	5624(1)	28(1)
C(5)	5605(2)	7140(2)	5333(1)	31(1)
C(6)	7666(2)	6371(2)	6922(1)	32(1)
C(7)	7965(2)	6926(2)	7531(1)	39(1)
C(8)	8870(2)	6368(3)	7939(1)	43(1)
C(9)	9453(2)	5258(2)	7757(1)	42(1)
C(10)	9162(2)	4641(2)	7139(1)	35(1)
C(11)	9725(2)	3477(2)	6932(1)	43(1)
C(12)	9441(2)	2955(2)	6323(1)	45(1)
C(13)	8590(2)	3552(2)	5887(1)	40(1)
C(14)	7999(2)	4668(2)	6075(1)	32(1)
C(15)	8268(2)	5229(2)	6711(1)	30(1)
C(16)	2104(2)	10109(2)	4775(1)	30(1)
C(17)	2199(2)	9898(2)	4118(1)	40(1)

C(18)	1470(2)	10514(2)	3633(1)	40(1)
C(19)	635(2)	11367(3)	3788(1)	47(1)
C(20)	655(8)	11816(12)	4419(4)	53(2)
C(21)	1355(7)	11184(11)	4901(2)	43(2)
C(20X)	348(11)	11257(16)	4447(5)	43(3)
C(21X)	1095(7)	10655(12)	4933(3)	32(2)
C(22)	2708(2)	5148(2)	6207(1)	37(1)
C(23)	3464(2)	5513(2)	6838(1)	44(1)
C(24)	1552(2)	5821(3)	6140(2)	65(1)
C(25)	2588(2)	3658(3)	6065(1)	57(1)
C(26)	4463(2)	4551(4)	6987(2)	86(1)
C(27)	2815(3)	5711(4)	7429(1)	90(1)

***Table S3*. Bond lengths [Å] and angles [°] for $C_{27}H_{32}B_2N_2O_2$.**

O(1)-B(2)	1.373(3)
O(1)-C(22)	1.474(2)
O(2)-B(2)	1.365(2)
O(2)-C(23)	1.466(3)
N(1)-C(6)	1.400(2)
N(1)-B(1)	1.422(3)
N(1)-H(1N)	0.87(2)
N(2)-C(14)	1.396(2)
N(2)-B(1)	1.406(3)
N(2)-H(2N)	0.87(2)
B(1)-C(5)	1.582(3)
B(2)-C(4)	1.560(3)
C(1)-C(2)	1.331(3)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(16)	1.487(3)
C(2)-C(3)	1.510(3)
C(3)-C(4)	1.541(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900

C(4)-C(5)	1.548(2)
C(4)-H(4)	1.0000
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.379(3)
C(6)-C(15)	1.421(3)
C(7)-C(8)	1.402(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.364(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.421(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.411(3)
C(10)-C(15)	1.426(3)
C(11)-C(12)	1.365(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.405(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.377(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.427(3)
C(16)-C(21X)	1.375(7)
C(16)-C(17)	1.386(3)
C(16)-C(21)	1.418(5)
C(17)-C(18)	1.389(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.357(3)
C(18)-H(18)	0.9500
C(19)-C(20)	1.372(8)
C(19)-C(20X)	1.438(11)
C(19)-H(19)	0.9500
C(20)-C(21)	1.373(8)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(20X)-C(21X)	1.395(12)
C(20X)-H(20X)	0.9500

C(21X)-H(21X)	0.9500
C(22)-C(25)	1.499(3)
C(22)-C(24)	1.509(3)
C(22)-C(23)	1.540(3)
C(23)-C(26)	1.518(4)
C(23)-C(27)	1.518(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800

B(2)-O(1)-C(22)	107.35(15)
B(2)-O(2)-C(23)	106.93(16)
C(6)-N(1)-B(1)	123.84(18)
C(6)-N(1)-H(1N)	113.8(16)
B(1)-N(1)-H(1N)	122.2(16)
C(14)-N(2)-B(1)	123.80(18)
C(14)-N(2)-H(2N)	117.4(16)
B(1)-N(2)-H(2N)	118.8(16)
N(2)-B(1)-N(1)	115.72(18)
N(2)-B(1)-C(5)	121.32(18)
N(1)-B(1)-C(5)	122.96(19)
O(2)-B(2)-O(1)	112.13(17)
O(2)-B(2)-C(4)	125.32(18)
O(1)-B(2)-C(4)	122.50(16)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0

C(1)-C(2)-C(16)	120.56(18)
C(1)-C(2)-C(3)	122.15(18)
C(16)-C(2)-C(3)	117.29(15)
C(2)-C(3)-C(4)	116.20(15)
C(2)-C(3)-H(3A)	108.2
C(4)-C(3)-H(3A)	108.2
C(2)-C(3)-H(3B)	108.2
C(4)-C(3)-H(3B)	108.2
H(3A)-C(3)-H(3B)	107.4
C(3)-C(4)-C(5)	110.19(14)
C(3)-C(4)-B(2)	112.20(15)
C(5)-C(4)-B(2)	108.40(16)
C(3)-C(4)-H(4)	108.7
C(5)-C(4)-H(4)	108.7
B(2)-C(4)-H(4)	108.7
C(4)-C(5)-B(1)	116.36(15)
C(4)-C(5)-H(5A)	108.2
B(1)-C(5)-H(5A)	108.2
C(4)-C(5)-H(5B)	108.2
B(1)-C(5)-H(5B)	108.2
H(5A)-C(5)-H(5B)	107.4
C(7)-C(6)-N(1)	122.42(19)
C(7)-C(6)-C(15)	120.20(18)
N(1)-C(6)-C(15)	117.38(18)
C(6)-C(7)-C(8)	119.9(2)
C(6)-C(7)-H(7)	120.0
C(8)-C(7)-H(7)	120.0
C(9)-C(8)-C(7)	121.5(2)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	120.47(19)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(11)-C(10)-C(9)	122.72(19)
C(11)-C(10)-C(15)	118.8(2)
C(9)-C(10)-C(15)	118.47(19)

C(12)-C(11)-C(10)	120.4(2)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	121.5(2)
C(11)-C(12)-H(12)	119.3
C(13)-C(12)-H(12)	119.3
C(14)-C(13)-C(12)	120.1(2)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-N(2)	122.34(19)
C(13)-C(14)-C(15)	119.70(18)
N(2)-C(14)-C(15)	117.96(18)
C(6)-C(15)-C(10)	119.43(18)
C(6)-C(15)-C(14)	121.10(17)
C(10)-C(15)-C(14)	119.47(18)
C(21X)-C(16)-C(17)	116.7(3)
C(17)-C(16)-C(21)	113.9(3)
C(21X)-C(16)-C(2)	119.3(3)
C(17)-C(16)-C(2)	122.01(17)
C(21)-C(16)-C(2)	123.0(2)
C(16)-C(17)-C(18)	122.1(2)
C(16)-C(17)-H(17)	118.9
C(18)-C(17)-H(17)	118.9
C(19)-C(18)-C(17)	120.6(2)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	118.8(4)
C(18)-C(19)-C(20X)	115.1(5)
C(18)-C(19)-H(19)	120.6
C(20)-C(19)-H(19)	120.6
C(19)-C(20)-C(21)	119.4(6)
C(19)-C(20)-H(20)	120.3
C(21)-C(20)-H(20)	120.3
C(20)-C(21)-C(16)	123.0(4)
C(20)-C(21)-H(21)	118.5
C(16)-C(21)-H(21)	118.5

C(21X)-C(20X)-C(19)	121.1(8)
C(21X)-C(20X)-H(20X)	119.4
C(19)-C(20X)-H(20X)	119.4
C(16)-C(21X)-C(20X)	119.6(6)
C(16)-C(21X)-H(21X)	120.2
C(20X)-C(21X)-H(21X)	120.2
O(1)-C(22)-C(25)	109.28(17)
O(1)-C(22)-C(24)	105.79(17)
C(25)-C(22)-C(24)	110.2(2)
O(1)-C(22)-C(23)	100.97(16)
C(25)-C(22)-C(23)	115.30(19)
C(24)-C(22)-C(23)	114.4(2)
O(2)-C(23)-C(26)	106.24(19)
O(2)-C(23)-C(27)	108.5(2)
C(26)-C(23)-C(27)	111.2(2)
O(2)-C(23)-C(22)	102.45(15)
C(26)-C(23)-C(22)	113.3(2)
C(27)-C(23)-C(22)	114.3(2)
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(23)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. **Anisotropic displacement parameters ($Å^2$ x 10^3) for $C_{27}H_{32}B_2N_2O_2$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	48(1)	40(1)	27(1)	3(1)	9(1)	-11(1)
O(2)	53(1)	49(1)	24(1)	3(1)	3(1)	-14(1)
N(1)	28(1)	36(1)	37(1)	1(1)	3(1)	7(1)
N(2)	31(1)	32(1)	31(1)	2(1)	2(1)	-1(1)
B(1)	25(1)	32(1)	34(1)	4(1)	5(1)	-5(1)
B(2)	22(1)	36(1)	27(1)	0(1)	-1(1)	4(1)
C(1)	48(1)	56(2)	31(1)	-2(1)	0(1)	20(1)
C(2)	30(1)	30(1)	28(1)	-4(1)	-1(1)	-2(1)
C(3)	27(1)	31(1)	25(1)	2(1)	0(1)	-2(1)
C(4)	27(1)	31(1)	25(1)	-2(1)	-1(1)	2(1)
C(5)	29(1)	34(1)	29(1)	1(1)	4(1)	-2(1)
C(6)	26(1)	37(1)	32(1)	9(1)	6(1)	0(1)
C(7)	35(1)	48(1)	35(1)	4(1)	6(1)	3(1)
C(8)	38(1)	62(2)	30(1)	7(1)	6(1)	-3(1)
C(9)	30(1)	61(2)	36(1)	23(1)	1(1)	1(1)
C(10)	25(1)	39(1)	43(1)	17(1)	8(1)	-2(1)
C(11)	29(1)	40(1)	61(1)	22(1)	8(1)	4(1)
C(12)	34(1)	32(1)	70(2)	10(1)	13(1)	5(1)
C(13)	35(1)	33(1)	51(1)	1(1)	9(1)	-2(1)
C(14)	24(1)	31(1)	40(1)	9(1)	5(1)	-4(1)
C(15)	24(1)	31(1)	35(1)	11(1)	8(1)	-2(1)
C(16)	29(1)	29(1)	30(1)	-4(1)	-3(1)	-2(1)

C(17)	46(1)	41(1)	32(1)	4(1)	4(1)	14(1)
C(18)	49(1)	39(1)	32(1)	5(1)	-3(1)	5(1)
C(19)	37(1)	58(2)	44(1)	2(1)	-9(1)	10(1)
C(20)	43(4)	53(5)	61(3)	-3(4)	-6(3)	20(3)
C(21)	47(3)	40(4)	39(2)	-11(2)	-3(2)	10(3)
C(20X)	34(4)	52(7)	43(4)	0(4)	-1(3)	12(4)
C(22)	38(1)	41(1)	32(1)	9(1)	9(1)	-4(1)
C(23)	56(1)	49(2)	28(1)	10(1)	3(1)	-13(1)
C(24)	33(1)	62(2)	99(2)	33(2)	11(1)	-2(1)
C(25)	78(2)	46(2)	50(1)	0(1)	21(1)	-16(1)
C(26)	62(2)	92(2)	99(2)	65(2)	-20(2)	-5(2)
C(27)	144(3)	91(2)	42(2)	-11(2)	45(2)	-58(2)

Table S5. **Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^2 x10^3) for $C_{27}H_{32}B_2N_2O_2$.**

	x	y	z	U(eq)
H(1N)	6450(20)	7600(30)	6640(11)	45(7)
H(2N)	6986(19)	4950(20)	5276(12)	44(7)
H(1A)	2143	10188	6039	54
H(1B)	3256	9216	6248	54
H(3A)	4324	9181	4827	34
H(3B)	3504	7887	4778	34
H(4)	4958	8604	5934	34
H(5A)	6005	7800	5075	37
H(5B)	5267	6437	5028	37
H(7)	7557	7686	7672	47
H(8)	9082	6773	8353	52
H(9)	10057	4894	8046	51
H(11)	10304	3055	7217	52
H(12)	9828	2171	6191	54
H(13)	8423	3186	5461	47
H(17)	2782	9313	3996	47

H(18)	1557	10336	3187	48
H(19)	47	11647	3466	57
H(20)	190	12558	4522	64
H(21)	1337	11480	5339	51
H(20X)	-363	11600	4554	52
H(21X)	907	10623	5370	38
H(24A)	1643	6800	6219	97
H(24B)	1084	5430	6460	97
H(24C)	1178	5670	5699	97
H(25A)	2138	3528	5643	85
H(25B)	2201	3218	6408	85
H(25C)	3345	3254	6052	85
H(26A)	4864	4441	6598	129
H(26B)	4182	3665	7119	129
H(26C)	4987	4926	7343	129
H(27A)	3353	5922	7811	135
H(27B)	2400	4875	7511	135
H(27C)	2273	6462	7348	135

Table S6. **Torsion angles [°] for $C_{27}H_{32}B_2N_2O_2$.**

C(14)-N(2)-B(1)-N(1)	-3.0(3)
C(14)-N(2)-B(1)-C(5)	176.25(17)
C(6)-N(1)-B(1)-N(2)	5.5(3)
C(6)-N(1)-B(1)-C(5)	-173.80(17)
C(23)-O(2)-B(2)-O(1)	10.6(2)
C(23)-O(2)-B(2)-C(4)	-166.82(19)
C(22)-O(1)-B(2)-O(2)	10.8(2)
C(22)-O(1)-B(2)-C(4)	-171.68(17)
C(1)-C(2)-C(3)-C(4)	2.2(3)
C(16)-C(2)-C(3)-C(4)	-178.09(16)
C(2)-C(3)-C(4)-C(5)	-175.95(16)
C(2)-C(3)-C(4)-B(2)	63.2(2)
O(2)-B(2)-C(4)-C(3)	-126.9(2)

O(1)-B(2)-C(4)-C(3)	55.9(2)
O(2)-B(2)-C(4)-C(5)	111.2(2)
O(1)-B(2)-C(4)-C(5)	-66.0(2)
C(3)-C(4)-C(5)-B(1)	176.79(16)
B(2)-C(4)-C(5)-B(1)	-60.1(2)
N(2)-B(1)-C(5)-C(4)	152.57(18)
N(1)-B(1)-C(5)-C(4)	-28.2(3)
B(1)-N(1)-C(6)-C(7)	174.35(19)
B(1)-N(1)-C(6)-C(15)	-4.6(3)
N(1)-C(6)-C(7)-C(8)	-178.55(18)
C(15)-C(6)-C(7)-C(8)	0.4(3)
C(6)-C(7)-C(8)-C(9)	-1.6(3)
C(7)-C(8)-C(9)-C(10)	0.7(3)
C(8)-C(9)-C(10)-C(11)	-178.87(19)
C(8)-C(9)-C(10)-C(15)	1.4(3)
C(9)-C(10)-C(11)-C(12)	-177.49(19)
C(15)-C(10)-C(11)-C(12)	2.2(3)
C(10)-C(11)-C(12)-C(13)	0.0(3)
C(11)-C(12)-C(13)-C(14)	-1.8(3)
C(12)-C(13)-C(14)-N(2)	-179.24(18)
C(12)-C(13)-C(14)-C(15)	1.1(3)
B(1)-N(2)-C(14)-C(13)	-179.67(18)
B(1)-N(2)-C(14)-C(15)	0.0(3)
C(7)-C(6)-C(15)-C(10)	1.8(3)
N(1)-C(6)-C(15)-C(10)	-179.25(16)
C(7)-C(6)-C(15)-C(14)	-177.83(18)
N(1)-C(6)-C(15)-C(14)	1.1(3)
C(11)-C(10)-C(15)-C(6)	177.64(17)
C(9)-C(10)-C(15)-C(6)	-2.7(3)
C(11)-C(10)-C(15)-C(14)	-2.7(3)
C(9)-C(10)-C(15)-C(14)	176.96(17)
C(13)-C(14)-C(15)-C(6)	-179.30(17)
N(2)-C(14)-C(15)-C(6)	1.1(3)
C(13)-C(14)-C(15)-C(10)	1.1(3)
N(2)-C(14)-C(15)-C(10)	-178.54(16)
C(1)-C(2)-C(16)-C(21X)	-14.0(7)

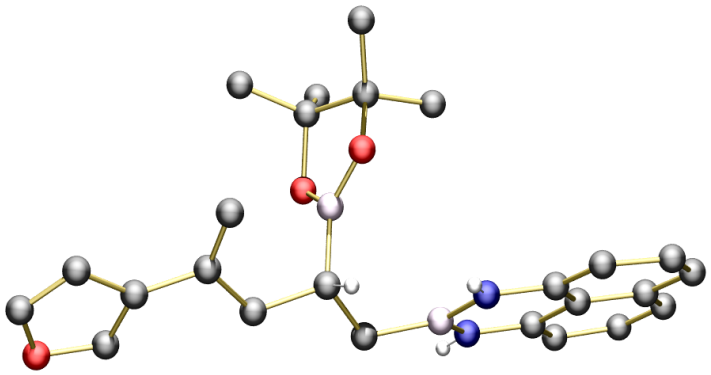
C(3)-C(2)-C(16)-C(21X)	166.4(6)
C(1)-C(2)-C(16)-C(17)	-177.4(2)
C(3)-C(2)-C(16)-C(17)	2.9(3)
C(1)-C(2)-C(16)-C(21)	15.3(7)
C(3)-C(2)-C(16)-C(21)	-164.4(6)
C(21X)-C(16)-C(17)-C(18)	16.6(7)
C(21)-C(16)-C(17)-C(18)	-11.2(6)
C(2)-C(16)-C(17)-C(18)	-179.6(2)
C(16)-C(17)-C(18)-C(19)	0.7(4)
C(17)-C(18)-C(19)-C(20)	12.4(7)
C(17)-C(18)-C(19)-C(20X)	-18.0(8)
C(18)-C(19)-C(20)-C(21)	-13.9(9)
C(19)-C(20)-C(21)-C(16)	2.6(8)
C(17)-C(16)-C(21)-C(20)	9.6(8)
C(2)-C(16)-C(21)-C(20)	177.9(4)
C(18)-C(19)-C(20X)-C(21X)	19.2(12)
C(17)-C(16)-C(21X)-C(20X)	-15.0(8)
C(2)-C(16)-C(21X)-C(20X)	-179.3(5)
C(19)-C(20X)-C(21X)-C(16)	-2.6(11)
B(2)-O(1)-C(22)-C(25)	-147.90(19)
B(2)-O(1)-C(22)-C(24)	93.5(2)
B(2)-O(1)-C(22)-C(23)	-26.0(2)
B(2)-O(2)-C(23)-C(26)	92.9(2)
B(2)-O(2)-C(23)-C(27)	-147.5(2)
B(2)-O(2)-C(23)-C(22)	-26.2(2)
O(1)-C(22)-C(23)-O(2)	31.0(2)
C(25)-C(22)-C(23)-O(2)	148.64(18)
C(24)-C(22)-C(23)-O(2)	-82.1(2)
O(1)-C(22)-C(23)-C(26)	-83.0(2)
C(25)-C(22)-C(23)-C(26)	34.6(3)
C(24)-C(22)-C(23)-C(26)	163.9(2)
O(1)-C(22)-C(23)-C(27)	148.2(2)
C(25)-C(22)-C(23)-C(27)	-94.2(3)
C(24)-C(22)-C(23)-C(27)	35.1(3)

Symmetry transformations used to generate equivalent atoms:

Table S7. **Hydrogen bonds for $C_{27}H_{32}B_2N_2O_2$ [Å and º].**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...O(1)#1	0.87(2)	2.16(3)	3.026(2)	177(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1



X-ray structure of 1f

Table S8. **Crystal data and structure refinement for $C_{25}H_{30}B_2N_2O_3$.**

Identification code	C25H30B2N2O3	
Empirical formula	C25 H30 B2 N2 O3	
Formula weight	428.13	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.4630(2) Å	α = 90º.
	b = 9.8897(2) Å	β = 98.190(2)º.
	c = 20.2832(4) Å	γ = 90º.
Volume	2275.97(8) Å^3	
Z	4	
Density (calculated)	1.249 Mg/m^3	

Absorption coefficient	0.634 mm^{-1}
F(000)	912
Crystal size	0.180 x 0.120 x 0.110 mm^3
Theta range for data collection	4.194 to 70.315∞.
Index ranges	-13<=h<=13, -11<=k<=11, -24<=l<=18
Reflections collected	9224
Independent reflections	4102 [R(int) = 0.0431]
Completeness to theta = 67.679∞	97.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.6406
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4102 / 2 / 299
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1142
R indices (all data)	R1 = 0.0620, wR2 = 0.1228
Extinction coefficient	n/a
Largest diff. peak and hole	0.243 and -0.272 e. $Å^{-3}$

Table S9. **Atomic coordinates (x10^4) and equivalent isotropic displacement parameters ($Å^2$ x10^3) for $C_{25}H_{30}B_2N_2O_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U(eq)
O(1)	8811(1)	-457(1)	6521(1)	32(1)
O(2)	6287(1)	2950(1)	3410(1)	26(1)
O(3)	6699(1)	4158(1)	4371(1)	24(1)
N(1)	3143(1)	2780(2)	3502(1)	23(1)
N(2)	2878(1)	4569(1)	4269(1)	22(1)
B(1)	3473(2)	3365(2)	4143(1)	21(1)
B(2)	6169(2)	3030(2)	4066(1)	21(1)
C(1)	7503(2)	212(2)	4259(1)	29(1)
C(2)	7284(1)	472(2)	4873(1)	23(1)
C(3)	6252(1)	1315(2)	5031(1)	22(1)
C(4)	5472(1)	1979(2)	4443(1)	20(1)
C(5)	4420(1)	2716(2)	4691(1)	21(1)

C(6)	1990(1)	5153(2)	3817(1)	21(1)
C(7)	1424(2)	6325(2)	3958(1)	25(1)
C(8)	544(2)	6888(2)	3483(1)	30(1)
C(9)	207(2)	6277(2)	2885(1)	29(1)
C(10)	746(1)	5052(2)	2723(1)	24(1)
C(11)	400(2)	4350(2)	2116(1)	29(1)
C(12)	958(2)	3176(2)	1983(1)	31(1)
C(13)	1887(2)	2642(2)	2434(1)	28(1)
C(14)	2241(1)	3286(2)	3029(1)	22(1)
C(15)	1664(1)	4493(2)	3193(1)	21(1)
C(16)	8043(1)	-71(2)	5458(1)	24(1)
C(17)	9014(2)	-1007(2)	5481(1)	38(1)
C(18)	9422(2)	-1190(2)	6124(1)	38(1)
C(19)	7973(2)	207(2)	6100(1)	27(1)
C(20)	6760(2)	4247(2)	3226(1)	26(1)
C(21)	5699(2)	5102(2)	2951(1)	44(1)
C(22)	7541(2)	3997(2)	2693(1)	42(1)
C(23)	7412(2)	4762(2)	3899(1)	23(1)
C(24)	7432(2)	6286(2)	3983(1)	37(1)
C(25)	8645(2)	4176(2)	4078(1)	34(1)

Table S10. **Bond lengths [Å] and angles [º] for $C_{25}H_{30}B_2N_2O_3$.**

O(1)-C(18)	1.350(2)
O(1)-C(19)	1.360(2)
O(2)-B(2)	1.359(2)
O(2)-C(20)	1.463(2)
O(3)-B(2)	1.374(2)
O(3)-C(23)	1.471(2)
N(1)-C(14)	1.398(2)
N(1)-B(1)	1.424(3)
N(1)-H(1N)	0.890(15)
N(2)-C(6)	1.395(2)
N(2)-B(1)	1.414(2)

N(2)-H(2N)	0.863(15)
B(1)-C(5)	1.575(2)
B(2)-C(4)	1.573(2)
C(1)-C(2)	1.330(3)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(16)	1.469(3)
C(2)-C(3)	1.517(2)
C(3)-C(4)	1.533(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.553(2)
C(4)-H(4)	1.0000
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.379(2)
C(6)-C(15)	1.425(3)
C(7)-C(8)	1.406(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.362(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.420(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.418(3)
C(10)-C(15)	1.426(2)
C(11)-C(12)	1.371(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.404(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.375(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.427(2)
C(16)-C(19)	1.345(3)
C(16)-C(17)	1.443(2)
C(17)-C(18)	1.334(3)
C(17)-H(17)	0.9500

C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(22)	1.519(3)
C(20)-C(21)	1.520(3)
C(20)-C(23)	1.546(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.517(2)
C(23)-C(25)	1.523(2)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(18)-O(1)-C(19)	105.42(15)
B(2)-O(2)-C(20)	106.95(13)
B(2)-O(3)-C(23)	106.76(13)
C(14)-N(1)-B(1)	123.73(15)
C(14)-N(1)-H(1N)	113.6(14)
B(1)-N(1)-H(1N)	122.4(14)
C(6)-N(2)-B(1)	123.72(15)
C(6)-N(2)-H(2N)	115.4(14)
B(1)-N(2)-H(2N)	120.9(14)
N(2)-B(1)-N(1)	115.77(16)
N(2)-B(1)-C(5)	121.10(16)
N(1)-B(1)-C(5)	123.12(15)
O(2)-B(2)-O(3)	112.85(15)
O(2)-B(2)-C(4)	124.37(15)
O(3)-B(2)-C(4)	122.75(16)
C(2)-C(1)-H(1A)	120.0

C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(16)	121.04(16)
C(1)-C(2)-C(3)	124.08(16)
C(16)-C(2)-C(3)	114.88(15)
C(2)-C(3)-C(4)	117.20(15)
C(2)-C(3)-H(3A)	108.0
C(4)-C(3)-H(3A)	108.0
C(2)-C(3)-H(3B)	108.0
C(4)-C(3)-H(3B)	108.0
H(3A)-C(3)-H(3B)	107.2
C(3)-C(4)-C(5)	110.03(14)
C(3)-C(4)-B(2)	112.32(13)
C(5)-C(4)-B(2)	108.59(13)
C(3)-C(4)-H(4)	108.6
C(5)-C(4)-H(4)	108.6
B(2)-C(4)-H(4)	108.6
C(4)-C(5)-B(1)	116.76(14)
C(4)-C(5)-H(5A)	108.1
B(1)-C(5)-H(5A)	108.1
C(4)-C(5)-H(5B)	108.1
B(1)-C(5)-H(5B)	108.1
H(5A)-C(5)-H(5B)	107.3
C(7)-C(6)-N(2)	122.13(16)
C(7)-C(6)-C(15)	119.88(16)
N(2)-C(6)-C(15)	117.99(15)
C(6)-C(7)-C(8)	120.16(17)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(9)-C(8)-C(7)	121.37(17)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	120.44(16)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(11)-C(10)-C(9)	122.75(16)

C(11)-C(10)-C(15)	118.57(16)
C(9)-C(10)-C(15)	118.68(16)
C(12)-C(11)-C(10)	120.31(16)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	121.50(17)
C(11)-C(12)-H(12)	119.2
C(13)-C(12)-H(12)	119.2
C(14)-C(13)-C(12)	119.94(17)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-N(1)	122.25(16)
C(13)-C(14)-C(15)	120.21(16)
N(1)-C(14)-C(15)	117.52(15)
C(6)-C(15)-C(10)	119.43(15)
C(6)-C(15)-C(14)	121.16(15)
C(10)-C(15)-C(14)	119.41(16)
C(19)-C(16)-C(17)	104.53(17)
C(19)-C(16)-C(2)	126.63(16)
C(17)-C(16)-C(2)	128.84(18)
C(18)-C(17)-C(16)	106.36(18)
C(18)-C(17)-H(17)	126.8
C(16)-C(17)-H(17)	126.8
C(17)-C(18)-O(1)	111.69(17)
C(17)-C(18)-H(18)	124.2
O(1)-C(18)-H(18)	124.2
C(16)-C(19)-O(1)	111.99(16)
C(16)-C(19)-H(19)	124.0
O(1)-C(19)-H(19)	124.0
O(2)-C(20)-C(22)	108.47(15)
O(2)-C(20)-C(21)	105.99(14)
C(22)-C(20)-C(21)	110.59(18)
O(2)-C(20)-C(23)	102.30(13)
C(22)-C(20)-C(23)	114.99(15)
C(21)-C(20)-C(23)	113.64(17)
C(20)-C(21)-H(21A)	109.5

C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(3)-C(23)-C(24)	109.37(15)
O(3)-C(23)-C(25)	105.89(14)
C(24)-C(23)-C(25)	110.69(16)
O(3)-C(23)-C(20)	101.39(13)
C(24)-C(23)-C(20)	115.07(16)
C(25)-C(23)-C(20)	113.54(15)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S11. **Anisotropic displacement parameters ($Å^2x10^3$) for $C_{25}H_{30}B_2N_2O_3$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	31(1)	30(1)	31(1)	6(1)	-4(1)	2(1)
O(2)	29(1)	27(1)	21(1)	-1(1)	2(1)	-8(1)
O(3)	28(1)	26(1)	19(1)	0(1)	5(1)	-7(1)
N(1)	21(1)	24(1)	25(1)	0(1)	2(1)	4(1)
N(2)	21(1)	23(1)	19(1)	0(1)	-2(1)	0(1)
B(1)	18(1)	22(1)	24(1)	3(1)	4(1)	-4(1)
B(2)	16(1)	23(1)	22(1)	-1(1)	-2(1)	2(1)
C(1)	27(1)	29(1)	30(1)	0(1)	2(1)	2(1)
C(2)	21(1)	20(1)	29(1)	1(1)	1(1)	-3(1)
C(3)	20(1)	23(1)	23(1)	2(1)	1(1)	-2(1)
C(4)	19(1)	20(1)	20(1)	-2(1)	-1(1)	0(1)
C(5)	19(1)	23(1)	22(1)	1(1)	3(1)	-1(1)
C(6)	17(1)	21(1)	25(1)	7(1)	2(1)	-3(1)
C(7)	25(1)	20(1)	30(1)	2(1)	1(1)	-3(1)
C(8)	24(1)	20(1)	44(1)	7(1)	3(1)	1(1)
C(9)	21(1)	29(1)	35(1)	14(1)	0(1)	0(1)
C(10)	18(1)	29(1)	25(1)	11(1)	2(1)	-4(1)
C(11)	21(1)	42(1)	23(1)	11(1)	-2(1)	-3(1)
C(12)	29(1)	44(1)	19(1)	0(1)	2(1)	-7(1)
C(13)	26(1)	33(1)	24(1)	-2(1)	5(1)	0(1)
C(14)	18(1)	27(1)	21(1)	5(1)	4(1)	-2(1)
C(15)	18(1)	23(1)	22(1)	7(1)	3(1)	-4(1)
C(16)	20(1)	21(1)	31(1)	2(1)	3(1)	-1(1)
C(17)	33(1)	42(1)	39(1)	2(1)	6(1)	14(1)
C(18)	29(1)	42(1)	42(1)	8(1)	2(1)	14(1)
C(19)	25(1)	23(1)	31(1)	2(1)	-2(1)	2(1)
C(20)	29(1)	25(1)	22(1)	3(1)	2(1)	-6(1)
C(21)	37(1)	44(1)	46(1)	22(1)	-7(1)	-3(1)
C(22)	54(1)	46(1)	26(1)	-6(1)	14(1)	-18(1)
C(23)	26(1)	24(1)	21(1)	1(1)	5(1)	-5(1)

C(24)	48(1)	26(1)	39(1)	-2(1)	18(1)	-9(1)
C(25)	22(1)	40(1)	39(1)	10(1)	1(1)	-7(1)

Table S12. **Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^2 x 10^3) for $C_{25}H_{30}B_2N_2O_3$.**

	x	y	z	U(eq)
H(1N)	3456(18)	2014(17)	3379(10)	28
H(2N)	3036(18)	4980(20)	4646(8)	26
H(1A)	8160	-332	4193	35
H(1B)	7003	571	3886	35
H(3A)	6566	2038	5344	26
H(3B)	5746	730	5267	26
H(4)	5154	1257	4121	24
H(5A)	4741	3441	5002	26
H(5B)	4013	2062	4949	26
H(7)	1628	6754	4378	30
H(8)	178	7711	3582	36
H(9)	-393	6674	2573	34
H(11)	-220	4696	1801	35
H(12)	710	2713	1577	37
H(13)	2271	1836	2327	34
H(17)	9305	-1411	5112	45
H(18)	10064	-1767	6284	45
H(19)	7405	797	6243	32
H(21A)	5229	4620	2583	66
H(21B)	5969	5965	2789	66
H(21C)	5216	5272	3304	66
H(22A)	8138	3317	2852	62
H(22B)	7931	4842	2598	62
H(22C)	7059	3670	2287	62
H(24A)	6622	6630	3931	55
H(24B)	7850	6696	3644	55
H(24C)	7836	6519	4427	55

H(25A)	8962	4431	4535	52
H(25B)	9158	4531	3771	52
H(25C)	8608	3188	4041	52

Table S13. **Torsion angles [°] for $C_{25}H_{30}B_2N_2O_3$.**

C(6)-N(2)-B(1)-N(1)	2.2(2)
C(6)-N(2)-B(1)-C(5)	-176.55(14)
C(14)-N(1)-B(1)-N(2)	-3.9(2)
C(14)-N(1)-B(1)-C(5)	174.82(15)
C(20)-O(2)-B(2)-O(3)	-10.43(18)
C(20)-O(2)-B(2)-C(4)	167.82(15)
C(23)-O(3)-B(2)-O(2)	-10.59(18)
C(23)-O(3)-B(2)-C(4)	171.13(14)
C(1)-C(2)-C(3)-C(4)	-4.2(2)
C(16)-C(2)-C(3)-C(4)	176.43(14)
C(2)-C(3)-C(4)-C(5)	176.25(13)
C(2)-C(3)-C(4)-B(2)	-62.66(19)
O(2)-B(2)-C(4)-C(3)	121.06(17)
O(3)-B(2)-C(4)-C(3)	-60.9(2)
O(2)-B(2)-C(4)-C(5)	-117.02(17)
O(3)-B(2)-C(4)-C(5)	61.1(2)
C(3)-C(4)-C(5)-B(1)	-175.56(14)
B(2)-C(4)-C(5)-B(1)	61.14(18)
N(2)-B(1)-C(5)-C(4)	-146.63(15)
N(1)-B(1)-C(5)-C(4)	34.7(2)
B(1)-N(2)-C(6)-C(7)	179.63(15)
B(1)-N(2)-C(6)-C(15)	0.1(2)
N(2)-C(6)-C(7)-C(8)	179.08(15)
C(15)-C(6)-C(7)-C(8)	-1.4(2)
C(6)-C(7)-C(8)-C(9)	1.9(3)
C(7)-C(8)-C(9)-C(10)	-0.4(3)
C(8)-C(9)-C(10)-C(11)	177.80(17)
C(8)-C(9)-C(10)-C(15)	-1.5(2)
C(9)-C(10)-C(11)-C(12)	179.44(16)
C(15)-C(10)-C(11)-C(12)	-1.3(2)

C(10)-C(11)-C(12)-C(13)	-0.7(3)
C(11)-C(12)-C(13)-C(14)	1.2(3)
C(12)-C(13)-C(14)-N(1)	178.53(15)
C(12)-C(13)-C(14)-C(15)	0.3(3)
B(1)-N(1)-C(14)-C(13)	-175.20(16)
B(1)-N(1)-C(14)-C(15)	3.1(2)
C(7)-C(6)-C(15)-C(10)	-0.5(2)
N(2)-C(6)-C(15)-C(10)	179.03(14)
C(7)-C(6)-C(15)-C(14)	179.42(15)
N(2)-C(6)-C(15)-C(14)	-1.1(2)
C(11)-C(10)-C(15)-C(6)	-177.40(15)
C(9)-C(10)-C(15)-C(6)	1.9(2)
C(11)-C(10)-C(15)-C(14)	2.7(2)
C(9)-C(10)-C(15)-C(14)	-177.98(14)
C(13)-C(14)-C(15)-C(6)	177.88(16)
N(1)-C(14)-C(15)-C(6)	-0.5(2)
C(13)-C(14)-C(15)-C(10)	-2.2(2)
N(1)-C(14)-C(15)-C(10)	179.42(14)
C(1)-C(2)-C(16)-C(19)	174.13(18)
C(3)-C(2)-C(16)-C(19)	-6.5(2)
C(1)-C(2)-C(16)-C(17)	-6.0(3)
C(3)-C(2)-C(16)-C(17)	173.32(18)
C(19)-C(16)-C(17)-C(18)	-0.1(2)
C(2)-C(16)-C(17)-C(18)	-179.95(18)
C(16)-C(17)-C(18)-O(1)	-0.3(2)
C(19)-O(1)-C(18)-C(17)	0.6(2)
C(17)-C(16)-C(19)-O(1)	0.4(2)
C(2)-C(16)-C(19)-O(1)	-179.68(15)
C(18)-O(1)-C(19)-C(16)	-0.6(2)
B(2)-O(2)-C(20)-C(22)	147.47(15)
B(2)-O(2)-C(20)-C(21)	-93.75(17)
B(2)-O(2)-C(20)-C(23)	25.56(16)
B(2)-O(3)-C(23)-C(24)	147.31(16)
B(2)-O(3)-C(23)-C(25)	-93.38(16)
B(2)-O(3)-C(23)-C(20)	25.37(16)
O(2)-C(20)-C(23)-O(3)	-30.45(16)

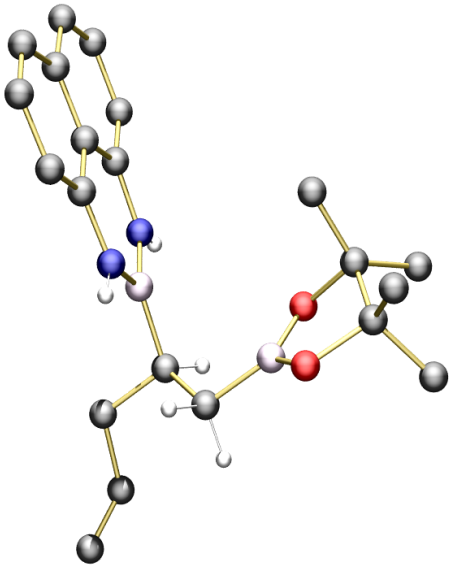
C(22)-C(20)-C(23)-O(3)	-147.80(16)
C(21)-C(20)-C(23)-O(3)	83.32(17)
O(2)-C(20)-C(23)-C(24)	-148.35(15)
C(22)-C(20)-C(23)-C(24)	94.3(2)
C(21)-C(20)-C(23)-C(24)	-34.6(2)
O(2)-C(20)-C(23)-C(25)	82.65(17)
C(22)-C(20)-C(23)-C(25)	-34.7(2)
C(21)-C(20)-C(23)-C(25)	-163.58(16)

Symmetry transformations used to generate equivalent atoms:

Table S14. **Hydrogen bonds for $C_{25}H_{30}B_2N_2O_3$ [Å and º].**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...O(3)#1	0.863(15)	2.150(16)	3.0082(19)	173.5(19)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1



X-ray structure of 6

Table S15. **Crystal data and structure refinement for $C_{21}H_{28}B_2N_2O_2$.**

Identification code	C21H28B2N2O2	
Empirical formula	C21 H28 B2 N2 O2	
Formula weight	362.07	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9787(12) Å	α = 100.956(8)°.
	b = 10.6797(13) Å	β = 114.093(7)°.
	c = 11.8681(15) Å	γ = 100.609(8)°.
Volume	1084.2(2) $Å^3$	
Z	2	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.543 mm^{-1}	
F(000)	388	
Crystal size	0.250 x 0.170 x 0.120 mm^3	
Theta range for data collection	4.271 to 66.697∞.	
Index ranges	-10<=h<=11, -12<=k<=12, -14<=l<=14	
Reflections collected	9561	
Independent reflections	3784 [R(int) = 0.0269]	
Completeness to theta = 66.697∞	98.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6548
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3784 / 339 / 339
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0521, wR2 = 0.1394
R indices (all data)	R1 = 0.0794, wR2 = 0.1586
Extinction coefficient	n/a
Largest diff. peak and hole	0.155 and -0.158 e. $Å^{-3}$

Table S16. **Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) for $C_{21}H_{28}B_2N_2O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U(eq)
O(1)	3515(2)	1845(1)	5296(1)	68(1)
N(1)	7339(2)	1370(2)	5886(2)	60(1)
N(2)	7489(2)	3651(2)	5950(2)	61(1)
B(1)	6735(3)	2284(2)	5258(2)	56(1)
B(2)	3587(2)	2765(2)	4654(2)	56(1)
C(1)	4721(8)	1701(8)	609(5)	163(3)
C(2)	4792(6)	1117(6)	1472(4)	102(2)
C(3)	5989(4)	1731(3)	2882(3)	61(1)
C(1X)	3370(40)	70(50)	90(30)	330(20)
C(2X)	3810(30)	130(30)	1250(20)	160(8)
C(3X)	5330(30)	1300(30)	2250(20)	145(8)
C(4)	5349(2)	1803(2)	3858(2)	62(1)
C(5)	8599(2)	1749(2)	7107(2)	63(1)
C(6)	9126(3)	830(3)	7711(2)	82(1)
C(7)	10415(3)	1256(3)	8918(3)	101(1)
C(8)	11169(3)	2566(4)	9520(3)	98(1)
C(9)	10672(3)	3551(3)	8943(2)	79(1)
C(10)	11408(3)	4933(3)	9528(3)	97(1)
C(11)	10857(3)	5842(3)	8968(3)	96(1)
C(12)	9538(3)	5440(2)	7776(2)	78(1)

C(13)	8795(2)	4102(2)	7151(2)	62(1)
C(14)	9346(2)	3131(2)	7724(2)	62(1)
C(15)	4243(2)	2675(2)	3673(2)	64(1)
O(2)	2962(3)	3729(3)	4934(3)	70(1)
C(16)	3122(4)	2406(4)	6314(5)	70(1)
C(17)	2251(4)	3333(3)	5724(4)	76(1)
C(18)	2264(6)	1316(5)	6612(5)	95(2)
C(19)	4657(4)	3174(5)	7521(3)	117(2)
C(20)	2329(6)	4555(3)	6625(5)	111(1)
C(21)	536(3)	2562(5)	4773(4)	108(1)
O(2X)	3610(20)	4020(20)	5420(20)	70(5)
C(16X)	3130(30)	2280(20)	6250(40)	86(5)
C(17X)	2930(30)	3640(20)	6220(20)	98(5)
C(18X)	1850(30)	1140(30)	6070(30)	73(7)
C(19X)	4640(30)	2320(40)	7410(30)	122(9)
C(20X)	3540(50)	4700(20)	7430(30)	127(8)
C(21X)	1170(30)	3520(30)	5430(30)	111(1)

Table S17. **Bond lengths [Å] and angles [°] for $C_{21}H_{28}B_2N_2O_2$.**

O(1)-B(2)	1.362(2)
O(1)-C(16)	1.473(5)
N(1)-C(5)	1.395(3)
N(1)-B(1)	1.412(3)
N(1)-H(1N)	0.86(2)
N(2)-C(13)	1.398(3)
N(2)-B(1)	1.417(3)
N(2)-H(2N)	0.83(2)
B(1)-C(4)	1.574(3)
B(2)-O(2)	1.355(3)
B(2)-C(15)	1.548(3)
C(1)-C(2)	1.281(6)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(3)	1.523(5)

C(2)-H(2)	0.9500
C(3)-C(4)	1.530(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(15)	1.547(3)
C(4)-H(4)	1.03(2)
C(5)-C(6)	1.379(3)
C(5)-C(14)	1.418(3)
C(6)-C(7)	1.395(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.352(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.417(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.412(4)
C(9)-C(14)	1.420(3)
C(10)-C(11)	1.354(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.400(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.379(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.418(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
O(2)-C(17)	1.465(3)
C(16)-C(18)	1.500(4)
C(16)-C(17)	1.520(4)
C(16)-C(19)	1.539(4)
C(17)-C(20)	1.488(4)
C(17)-C(21)	1.559(4)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800

C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

B(2)-O(1)-C(16)	107.19(19)
C(5)-N(1)-B(1)	123.82(19)
C(5)-N(1)-H(1N)	116.4(14)
B(1)-N(1)-H(1N)	119.8(14)
C(13)-N(2)-B(1)	123.44(18)
C(13)-N(2)-H(2N)	115.6(16)
B(1)-N(2)-H(2N)	120.5(15)
N(1)-B(1)-N(2)	115.8(2)
N(1)-B(1)-C(4)	121.72(19)
N(2)-B(1)-C(4)	122.44(19)
O(2)-B(2)-O(1)	112.2(2)
O(2)-B(2)-C(15)	124.2(2)
O(1)-B(2)-C(15)	123.54(18)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(3)	122.3(5)
C(1)-C(2)-H(2)	118.9
C(3)-C(2)-H(2)	118.9
C(2)-C(3)-C(4)	115.1(3)
C(2)-C(3)-H(3A)	108.5
C(4)-C(3)-H(3A)	108.5
C(2)-C(3)-H(3B)	108.5
C(4)-C(3)-H(3B)	108.5
H(3A)-C(3)-H(3B)	107.5
C(3)-C(4)-C(15)	112.61(19)
C(3)-C(4)-B(1)	108.52(19)
C(15)-C(4)-B(1)	112.89(17)

C(3)-C(4)-H(4)	101.5(12)
C(15)-C(4)-H(4)	109.4(12)
B(1)-C(4)-H(4)	111.3(11)
C(6)-C(5)-N(1)	122.3(2)
C(6)-C(5)-C(14)	120.1(2)
N(1)-C(5)-C(14)	117.64(18)
C(5)-C(6)-C(7)	120.2(3)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	121.1(3)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(7)-C(8)-C(9)	121.0(3)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	123.4(3)
C(10)-C(9)-C(14)	118.1(2)
C(8)-C(9)-C(14)	118.5(2)
C(11)-C(10)-C(9)	121.5(3)
C(11)-C(10)-H(10)	119.2
C(9)-C(10)-H(10)	119.2
C(10)-C(11)-C(12)	120.8(3)
C(10)-C(11)-H(11)	119.6
C(12)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	119.9(2)
C(13)-C(12)-H(12)	120.1
C(11)-C(12)-H(12)	120.1
C(12)-C(13)-N(2)	122.0(2)
C(12)-C(13)-C(14)	120.2(2)
N(2)-C(13)-C(14)	117.76(18)
C(5)-C(14)-C(13)	121.42(19)
C(5)-C(14)-C(9)	119.2(2)
C(13)-C(14)-C(9)	119.4(2)
C(4)-C(15)-B(2)	113.40(16)
C(4)-C(15)-H(15A)	108.9
B(2)-C(15)-H(15A)	108.9

C(4)-C(15)-H(15B)	108.9
B(2)-C(15)-H(15B)	108.9
H(15A)-C(15)-H(15B)	107.7
B(2)-O(2)-C(17)	107.1(2)
O(1)-C(16)-C(18)	110.7(3)
O(1)-C(16)-C(17)	101.0(3)
C(18)-C(16)-C(17)	116.7(3)
O(1)-C(16)-C(19)	106.2(3)
C(18)-C(16)-C(19)	109.3(3)
C(17)-C(16)-C(19)	112.2(3)
O(2)-C(17)-C(20)	108.9(2)
O(2)-C(17)-C(16)	102.9(2)
C(20)-C(17)-C(16)	117.5(3)
O(2)-C(17)-C(21)	106.4(2)
C(20)-C(17)-C(21)	109.2(3)
C(16)-C(17)-C(21)	111.2(3)
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(17)-C(21)-H(21A)	109.5
C(17)-C(21)-H(21B)	109.5

H(21A)-C(21)-H(21B)	109.5
C(17)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S18. **Anisotropic displacement parameters ($Å^2x10^3$) for $C_{21}H_{28}B_2N_2O_2$. The anisotropic displacement factor exponent takes the form: $-2p^2$ [$h^2 a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	81(1)	58(1)	81(1)	28(1)	48(1)	29(1)
N(1)	62(1)	55(1)	67(1)	22(1)	31(1)	19(1)
N(2)	67(1)	57(1)	69(1)	24(1)	35(1)	25(1)
B(1)	57(1)	58(1)	69(1)	24(1)	40(1)	22(1)
B(2)	48(1)	54(1)	68(1)	23(1)	25(1)	17(1)
C(1)	190(6)	250(7)	83(3)	51(4)	67(3)	125(5)
C(2)	111(3)	141(4)	49(2)	13(2)	33(2)	48(3)
C(3)	70(2)	67(2)	54(2)	17(1)	30(2)	32(1)
C(1X)	280(30)	490(50)	178(13)	66(15)	87(14)	80(30)
C(2X)	152(15)	209(19)	144(11)	20(11)	79(10)	112(13)
C(3X)	165(16)	206(18)	119(9)	54(9)	85(10)	126(13)
C(4)	63(1)	61(1)	71(1)	24(1)	35(1)	26(1)
C(5)	63(1)	73(1)	66(1)	29(1)	37(1)	26(1)
C(6)	88(2)	88(2)	84(2)	45(1)	40(1)	36(1)
C(7)	106(2)	123(2)	89(2)	57(2)	40(2)	54(2)
C(8)	90(2)	134(2)	70(2)	36(2)	28(1)	44(2)
C(9)	73(1)	100(2)	62(1)	18(1)	31(1)	25(1)
C(10)	82(2)	112(2)	72(2)	5(2)	28(1)	16(2)
C(11)	95(2)	85(2)	86(2)	-4(1)	44(2)	6(2)
C(12)	87(2)	67(1)	82(2)	11(1)	47(1)	17(1)
C(13)	65(1)	65(1)	64(1)	16(1)	39(1)	19(1)

C(14)	62(1)	74(1)	61(1)	21(1)	36(1)	23(1)
C(15)	63(1)	69(1)	71(1)	29(1)	34(1)	29(1)
O(2)	80(2)	65(1)	107(2)	45(1)	64(2)	39(1)
C(16)	84(2)	65(2)	76(2)	24(2)	49(2)	23(2)
C(17)	89(2)	70(2)	113(2)	43(2)	74(2)	40(2)
C(18)	133(4)	81(2)	106(4)	45(2)	78(3)	34(2)
C(19)	101(2)	147(4)	76(2)	15(2)	31(2)	21(2)
C(20)	158(4)	74(2)	164(4)	40(2)	125(3)	48(2)
C(21)	62(2)	152(4)	135(3)	68(3)	56(2)	38(2)
O(2X)	83(12)	58(6)	90(9)	28(5)	55(9)	26(6)
C(16X)	124(12)	64(9)	102(8)	27(7)	81(8)	27(8)
C(17X)	149(10)	74(9)	129(9)	43(6)	108(7)	42(7)
C(18X)	89(12)	75(11)	96(18)	53(11)	63(11)	43(8)
C(19X)	135(13)	140(20)	104(10)	38(11)	69(9)	43(12)
C(20X)	210(20)	71(11)	133(10)	29(8)	113(10)	40(12)
C(21X)	158(4)	74(2)	164(4)	40(2)	125(3)	48(2)

Table S19. **Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^{2}x10^3) for $C_{21}H_{28}B_2N_2O_2$.**

	x	y	z	U(eq)
H(1N)	6940(20)	530(20)	5500(20)	72
H(2N)	7240(20)	4240(20)	5610(20)	73
H(1A)	5429	2546	840	196
H(1B)	3959	1288	-262	196
H(2)	4075	272	1223	123
H(3A)	6560	2645	2994	74
H(3B)	6730	1205	3085	74
H(1X1)	3924	703	-143	398
H(1X2)	2471	-605	-553	398
H(2X)	3285	-489	1513	192
H(3X1)	5385	2078	1918	174
H(3X2)	6244	997	2357	174
H(4)	4740(20)	820(20)	3622(19)	74

H(6)	8609	-95	7304	98
H(7)	10770	614	9324	121
H(8)	12044	2831	10341	118
H(10)	12311	5231	10334	116
H(11)	11373	6766	9389	115
H(12)	9155	6088	7397	94
H(15A)	3380	2303	2787	77
H(15B)	4795	3586	3757	77
H(18A)	2014	1708	7290	143
H(18B)	1315	792	5831	143
H(18C)	2903	735	6909	143
H(19A)	4458	3570	8231	175
H(19B)	5265	2560	7772	175
H(19C)	5225	3882	7327	175
H(20A)	1855	4300	7159	166
H(20B)	3404	5077	7183	166
H(20C)	1778	5092	6127	166
H(21A)	9	2275	5260	162
H(21B)	41	3147	4309	162
H(21C)	480	1779	4152	162
H(18D)	1524	1391	6737	109
H(18E)	987	939	5216	109
H(18F)	2215	355	6153	109
H(19D)	4586	2616	8219	182
H(19E)	4778	1425	7308	182
H(19F)	5512	2939	7430	182
H(20D)	3064	4419	7957	191
H(20E)	4656	4866	7907	191
H(20F)	3317	5514	7254	191
H(21D)	629	3268	5913	166
H(21E)	1067	4382	5290	166
H(21F)	736	2841	4591	166

Table S20. **Torsion angles [°] for $C_{21}H_{28}B_2N_2O_2$.**

C(5)-N(1)-B(1)-N(2)	-0.3(3)
C(5)-N(1)-B(1)-C(4)	177.63(17)
C(13)-N(2)-B(1)-N(1)	3.0(3)
C(13)-N(2)-B(1)-C(4)	-174.87(17)
C(16)-O(1)-B(2)-O(2)	-13.7(3)
C(16)-O(1)-B(2)-C(15)	168.9(2)
C(1)-C(2)-C(3)-C(4)	128.2(4)
C(2)-C(3)-C(4)-C(15)	-61.5(3)
C(2)-C(3)-C(4)-B(1)	172.8(3)
N(1)-B(1)-C(4)-C(3)	-91.1(2)
N(2)-B(1)-C(4)-C(3)	86.7(2)
N(1)-B(1)-C(4)-C(15)	143.38(19)
N(2)-B(1)-C(4)-C(15)	-38.8(3)
B(1)-N(1)-C(5)-C(6)	177.7(2)
B(1)-N(1)-C(5)-C(14)	-2.5(3)
N(1)-C(5)-C(6)-C(7)	178.3(2)
C(14)-C(5)-C(6)-C(7)	-1.4(3)
C(5)-C(6)-C(7)-C(8)	0.2(4)
C(6)-C(7)-C(8)-C(9)	0.0(4)
C(7)-C(8)-C(9)-C(10)	179.7(3)
C(7)-C(8)-C(9)-C(14)	0.9(4)
C(8)-C(9)-C(10)-C(11)	-177.2(3)
C(14)-C(9)-C(10)-C(11)	1.5(4)
C(9)-C(10)-C(11)-C(12)	-0.6(4)
C(10)-C(11)-C(12)-C(13)	-0.8(4)
C(11)-C(12)-C(13)-N(2)	-178.90(19)
C(11)-C(12)-C(13)-C(14)	1.2(3)
B(1)-N(2)-C(13)-C(12)	177.31(19)
B(1)-N(2)-C(13)-C(14)	-2.7(3)
C(6)-C(5)-C(14)-C(13)	-177.37(19)
N(1)-C(5)-C(14)-C(13)	2.8(3)
C(6)-C(5)-C(14)-C(9)	2.4(3)
N(1)-C(5)-C(14)-C(9)	-177.38(17)

C(12)-C(13)-C(14)-C(5)	179.62(18)
N(2)-C(13)-C(14)-C(5)	-0.3(3)
C(12)-C(13)-C(14)-C(9)	-0.2(3)
N(2)-C(13)-C(14)-C(9)	179.89(17)
C(10)-C(9)-C(14)-C(5)	179.1(2)
C(8)-C(9)-C(14)-C(5)	-2.1(3)
C(10)-C(9)-C(14)-C(13)	-1.2(3)
C(8)-C(9)-C(14)-C(13)	177.6(2)
C(3)-C(4)-C(15)-B(2)	-179.8(2)
B(1)-C(4)-C(15)-B(2)	-56.5(2)
O(2)-B(2)-C(15)-C(4)	160.7(2)
O(1)-B(2)-C(15)-C(4)	-22.2(3)
O(1)-B(2)-O(2)-C(17)	-6.9(3)
C(15)-B(2)-O(2)-C(17)	170.5(2)
B(2)-O(1)-C(16)-C(18)	151.4(3)
B(2)-O(1)-C(16)-C(17)	27.1(3)
B(2)-O(1)-C(16)-C(19)	-90.1(3)
B(2)-O(2)-C(17)-C(20)	149.0(3)
B(2)-O(2)-C(17)-C(16)	23.6(3)
B(2)-O(2)-C(17)-C(21)	-93.4(3)
O(1)-C(16)-C(17)-O(2)	-30.0(3)
C(18)-C(16)-C(17)-O(2)	-150.0(4)
C(19)-C(16)-C(17)-O(2)	82.7(4)
O(1)-C(16)-C(17)-C(20)	-149.6(3)
C(18)-C(16)-C(17)-C(20)	90.3(4)
C(19)-C(16)-C(17)-C(20)	-36.9(5)
O(1)-C(16)-C(17)-C(21)	83.6(3)
C(18)-C(16)-C(17)-C(21)	-36.4(5)
C(19)-C(16)-C(17)-C(21)	-163.7(3)

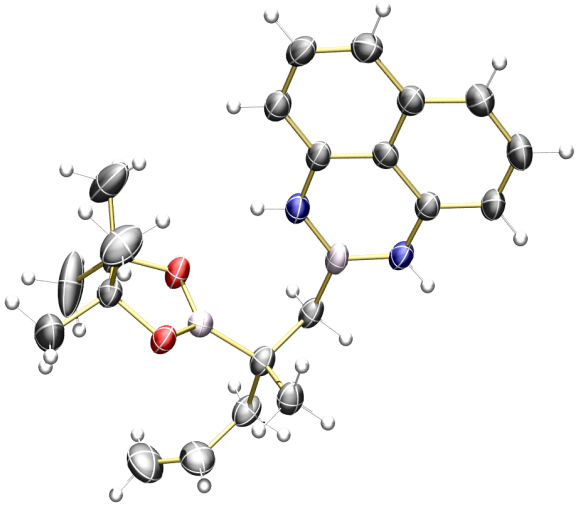
Symmetry transformations used to generate equivalent atoms:

Table S21. **Hydrogen bonds for $C_{21}H_{28}B_2N_2O_2$ [Å and º].**

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

N(1)-H(1N)...O(1)#1	0.86(2)	2.42(2)	3.256(2)	165.4(19)
N(2)-H(2N)...O(2)#2	0.83(2)	2.40(2)	3.213(3)	167(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x+1,-y+1,-z+1



X-ray structure of 3

Table S22. **Crystal data and structure refinement for $C_{22}H_{30}B_2N_2O_2$.**

Identification code	C22H30B2N2O2	
Empirical formula	C22 H30 B2 N2 O2	
Formula weight	376.10	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.0973(9) Å	α= 90°.
	b = 9.1634(10) Å	β= 90°.
	c = 51.260(6) Å	γ= 90°.
Volume	4273.1(8) $Å^3$	
Z	8	
Density (calculated)	1.169 Mg/m^3	
Absorption coefficient	0.568 mm^{-1}	
F(000)	1616	
Crystal size	0.220 x 0.180 x 0.090 mm^3	

Theta range for data collection	1.724 to 69.481°.
Index ranges	-10<=h<=8, -9<=k<=10, -60<=l<=60
Reflections collected	28850
Independent reflections	7512 [R(int) = 0.0507]
Completeness to theta = 67.679∞	97.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6258
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7512 / 8 / 564
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0539, wR2 = 0.1256
R indices (all data)	R1 = 0.0609, wR2 = 0.1325
Absolute structure parameter	0.06(11)
Extinction coefficient	0.00081(13)
Largest diff. peak and hole	0.320 and -0.208 e. $Å^{-3}$

Table S23. **Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x10^3) for $C_{22}H_{30}B_2N_2O_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.**

	x	y	z	U(eq)
O(1)	1137(3)	5934(3)	2024(1)	37(1)
O(2)	2732(3)	7758(3)	2122(1)	34(1)
N(1)	2932(4)	6746(3)	2710(1)	34(1)
N(2)	4479(4)	4820(4)	2870(1)	34(1)
B(1)	2527(5)	6289(5)	2100(1)	31(1)
B(2)	4057(5)	5704(5)	2656(1)	33(1)
C(1)	3947(15)	3510(13)	1528(2)	98(5)
C(1X)	3782(19)	5275(19)	1436(3)	85(6)
C(2)	3889(6)	4631(7)	1654(1)	64(1)

C(3)	4721(5)	4984(5)	1899(1)	43(1)
C(4)	3766(4)	5113(4)	2149(1)	32(1)
C(5)	4784(4)	5562(4)	2378(1)	33(1)
C(6)	2268(4)	6922(4)	2955(1)	32(1)
C(7)	1199(4)	7946(4)	3001(1)	39(1)
C(8)	566(5)	8068(5)	3249(1)	44(1)
C(9)	1006(5)	7204(5)	3450(1)	46(1)
C(10)	2117(5)	6150(4)	3413(1)	37(1)
C(11)	2621(5)	5222(5)	3616(1)	44(1)
C(12)	3696(5)	4224(5)	3570(1)	44(1)
C(13)	4326(5)	4069(4)	3324(1)	40(1)
C(14)	3873(4)	4940(4)	3120(1)	32(1)
C(15)	2764(4)	5993(4)	3161(1)	33(1)
C(16)	264(4)	7257(4)	1993(1)	35(1)
C(17)	1404(4)	8515(4)	2031(1)	36(1)
C(18)	-448(7)	7199(6)	1730(1)	75(2)
C(19)	-892(6)	7208(6)	2207(1)	76(2)
C(20)	1819(6)	9282(6)	1778(1)	67(2)
C(21)	1033(6)	9651(6)	2234(1)	70(2)
C(22)	3080(5)	3621(4)	2207(1)	40(1)
O(3)	6676(3)	6395(3)	5478(1)	35(1)
O(4)	4863(3)	4738(3)	5411(1)	37(1)
N(3)	5830(4)	4485(3)	4820(1)	36(1)
N(4)	7787(4)	2974(4)	4660(1)	36(1)
B(3)	6351(4)	4995(4)	5421(1)	29(1)
B(4)	6888(5)	3383(5)	4874(1)	35(1)
C(23)	7332(11)	3944(10)	6077(1)	75(3)
C(23X)	9460(20)	3760(20)	5958(3)	80(7)
C(24)	8143(6)	3806(6)	5863(1)	56(1)
C(25)	7759(5)	2895(4)	5630(1)	43(1)
C(26)	7552(4)	3769(4)	5373(1)	34(1)
C(27)	7065(4)	2689(4)	5155(1)	35(1)
C(28)	5643(4)	5144(4)	4576(1)	34(1)
C(29)	4601(4)	6192(4)	4531(1)	39(1)
C(30)	4462(5)	6830(4)	4283(1)	44(1)
C(31)	5339(5)	6404(5)	4081(1)	44(1)

C(32)	6421(4)	5311(4)	4119(1)	39(1)
C(33)	7363(5)	4846(5)	3916(1)	49(1)
C(34)	8409(5)	3802(5)	3961(1)	49(1)
C(35)	8567(5)	3165(4)	4206(1)	41(1)
C(36)	7668(4)	3586(4)	4411(1)	34(1)
C(37)	6580(4)	4676(4)	4370(1)	34(1)
C(38)	5322(4)	7229(4)	5502(1)	35(1)
C(39)	4090(4)	6048(4)	5505(1)	40(1)
C(40)	5440(6)	8184(6)	5738(1)	66(2)
C(41)	5272(6)	8195(6)	5261(1)	66(1)
C(42)	3555(8)	5712(6)	5781(1)	92(2)
C(43)	2816(6)	6316(6)	5329(1)	81(2)
C(44)	9013(4)	4464(4)	5297(1)	39(1)

Table S24. **Bond lengths [Å] and angles [°] for $C_{22}H_{30}B_2N_2O_2$.**

O(1)-B(1)	1.363(5)
O(1)-C(16)	1.458(4)
O(2)-B(1)	1.363(5)
O(2)-C(17)	1.469(4)
N(1)-C(6)	1.404(5)
N(1)-B(2)	1.427(5)
N(1)-H(1N)	0.89(5)
N(2)-C(14)	1.397(5)
N(2)-B(2)	1.417(5)
N(2)-H(2N)	0.86(4)
B(1)-C(4)	1.579(6)
B(2)-C(5)	1.574(6)
C(1)-C(2)	1.216(11)
C(1)-H(1A)	0.9500
C(1)-H(1B)	0.9500
C(2)-C(3)	1.501(6)
C(2)-H(2)	1.04(6)
C(3)-C(4)	1.550(5)

C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(22)	1.533(5)
C(4)-C(5)	1.553(5)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.372(5)
C(6)-C(15)	1.430(5)
C(7)-C(8)	1.399(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.358(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.411(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.421(5)
C(10)-C(15)	1.424(5)
C(11)-C(12)	1.359(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.394(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.380(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.413(5)
C(16)-C(18)	1.498(6)
C(16)-C(19)	1.521(6)
C(16)-C(17)	1.562(5)
C(17)-C(21)	1.511(6)
C(17)-C(20)	1.519(6)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800

C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
O(3)-B(3)	1.348(5)
O(3)-C(38)	1.455(5)
O(4)-B(3)	1.375(5)
O(4)-C(39)	1.472(4)
N(3)-C(28)	1.403(5)
N(3)-B(4)	1.422(5)
N(3)-H(3N)	0.89(5)
N(4)-C(36)	1.399(5)
N(4)-B(4)	1.421(5)
N(4)-H(4N)	0.86(5)
B(3)-C(26)	1.587(5)
B(4)-C(27)	1.582(6)
C(23)-C(24)	1.329(9)
C(23)-H(23A)	0.9500
C(23)-H(23B)	0.9500
C(24)-C(25)	1.499(6)
C(24)-H(24)	1.04(6)
C(25)-C(26)	1.553(5)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(44)	1.525(5)
C(26)-C(27)	1.556(5)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.369(5)
C(28)-C(37)	1.424(5)
C(29)-C(30)	1.406(6)
C(29)-H(29)	0.9500
C(30)-C(31)	1.361(6)

C(30)-H(30)	0.9500
C(31)-C(32)	1.417(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.413(6)
C(32)-C(37)	1.419(5)
C(33)-C(34)	1.369(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.393(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.383(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.422(5)
C(38)-C(40)	1.497(6)
C(38)-C(41)	1.524(6)
C(38)-C(39)	1.558(6)
C(39)-C(43)	1.488(7)
C(39)-C(42)	1.529(6)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800

B(1)-O(1)-C(16)	109.7(3)
B(1)-O(2)-C(17)	109.1(3)
C(6)-N(1)-B(2)	124.0(3)

C(6)-N(1)-H(1N)	117(3)
B(2)-N(1)-H(1N)	119(3)
C(14)-N(2)-B(2)	123.9(3)
C(14)-N(2)-H(2N)	114(3)
B(2)-N(2)-H(2N)	122(3)
O(1)-B(1)-O(2)	112.7(3)
O(1)-B(1)-C(4)	123.0(3)
O(2)-B(1)-C(4)	124.2(3)
N(2)-B(2)-N(1)	115.2(4)
N(2)-B(2)-C(5)	122.6(4)
N(1)-B(2)-C(5)	122.2(3)
C(2)-C(1)-H(1A)	120.0
C(2)-C(1)-H(1B)	120.0
H(1A)-C(1)-H(1B)	120.0
C(1)-C(2)-C(3)	127.4(7)
C(1)-C(2)-H(2)	120(7)
C(3)-C(2)-H(2)	113(7)
C(2)-C(3)-C(4)	115.1(4)
C(2)-C(3)-H(3A)	108.5
C(4)-C(3)-H(3A)	108.5
C(2)-C(3)-H(3B)	108.5
C(4)-C(3)-H(3B)	108.5
H(3A)-C(3)-H(3B)	107.5
C(22)-C(4)-C(3)	108.8(3)
C(22)-C(4)-C(5)	109.3(3)
C(3)-C(4)-C(5)	108.1(3)
C(22)-C(4)-B(1)	110.4(3)
C(3)-C(4)-B(1)	108.7(3)
C(5)-C(4)-B(1)	111.5(3)
C(4)-C(5)-B(2)	117.1(3)
C(4)-C(5)-H(5A)	108.0
B(2)-C(5)-H(5A)	108.0
C(4)-C(5)-H(5B)	108.0
B(2)-C(5)-H(5B)	108.0
H(5A)-C(5)-H(5B)	107.3
C(7)-C(6)-N(1)	122.6(3)

C(7)-C(6)-C(15)	120.2(3)
N(1)-C(6)-C(15)	117.2(3)
C(6)-C(7)-C(8)	120.2(4)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(9)-C(8)-C(7)	121.3(4)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(10)	120.5(4)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(9)-C(10)-C(11)	122.8(4)
C(9)-C(10)-C(15)	119.2(4)
C(11)-C(10)-C(15)	118.0(4)
C(12)-C(11)-C(10)	120.5(4)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(11)-C(12)-C(13)	121.4(4)
C(11)-C(12)-H(12)	119.3
C(13)-C(12)-H(12)	119.3
C(14)-C(13)-C(12)	120.4(4)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(13)-C(14)-N(2)	122.1(3)
C(13)-C(14)-C(15)	119.6(3)
N(2)-C(14)-C(15)	118.3(3)
C(14)-C(15)-C(10)	120.1(3)
C(14)-C(15)-C(6)	121.4(3)
C(10)-C(15)-C(6)	118.6(3)
O(1)-C(16)-C(18)	107.6(4)
O(1)-C(16)-C(19)	105.9(3)
C(18)-C(16)-C(19)	110.5(4)
O(1)-C(16)-C(17)	103.8(3)
C(18)-C(16)-C(17)	115.1(3)
C(19)-C(16)-C(17)	113.0(4)
O(2)-C(17)-C(21)	106.9(3)

O(2)-C(17)-C(20)	106.5(3)
C(21)-C(17)-C(20)	108.9(4)
O(2)-C(17)-C(16)	103.7(3)
C(21)-C(17)-C(16)	116.5(4)
C(20)-C(17)-C(16)	113.6(3)
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(17)-C(21)-H(21A)	109.5
C(17)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(17)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(4)-C(22)-H(22A)	109.5
C(4)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(4)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
B(3)-O(3)-C(38)	109.5(3)

B(3)-O(4)-C(39)	108.6(3)
C(28)-N(3)-B(4)	124.1(3)
C(28)-N(3)-H(3N)	118(3)
B(4)-N(3)-H(3N)	118(3)
C(36)-N(4)-B(4)	123.8(3)
C(36)-N(4)-H(4N)	114(3)
B(4)-N(4)-H(4N)	122(3)
O(3)-B(3)-O(4)	112.7(3)
O(3)-B(3)-C(26)	123.8(3)
O(4)-B(3)-C(26)	123.4(3)
N(4)-B(4)-N(3)	115.3(4)
N(4)-B(4)-C(27)	122.7(4)
N(3)-B(4)-C(27)	122.0(3)
C(24)-C(23)-H(23A)	120.0
C(24)-C(23)-H(23B)	120.0
H(23A)-C(23)-H(23B)	120.0
C(23)-C(24)-C(25)	125.6(6)
C(23)-C(24)-H(24)	120(5)
C(25)-C(24)-H(24)	114(5)
C(24)-C(25)-C(26)	114.6(3)
C(24)-C(25)-H(25A)	108.6
C(26)-C(25)-H(25A)	108.6
C(24)-C(25)-H(25B)	108.6
C(26)-C(25)-H(25B)	108.6
H(25A)-C(25)-H(25B)	107.6
C(44)-C(26)-C(25)	109.1(3)
C(44)-C(26)-C(27)	109.3(3)
C(25)-C(26)-C(27)	108.4(3)
C(44)-C(26)-B(3)	110.1(3)
C(25)-C(26)-B(3)	108.4(3)
C(27)-C(26)-B(3)	111.5(3)
C(26)-C(27)-B(4)	115.2(3)
C(26)-C(27)-H(27A)	108.5
B(4)-C(27)-H(27A)	108.5
C(26)-C(27)-H(27B)	108.5
B(4)-C(27)-H(27B)	108.5

H(27A)-C(27)-H(27B)	107.5
C(29)-C(28)-N(3)	122.4(3)
C(29)-C(28)-C(37)	120.1(4)
N(3)-C(28)-C(37)	117.5(3)
C(28)-C(29)-C(30)	120.4(4)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(31)-C(30)-C(29)	120.9(4)
C(31)-C(30)-H(30)	119.6
C(29)-C(30)-H(30)	119.6
C(30)-C(31)-C(32)	120.5(4)
C(30)-C(31)-H(31)	119.7
C(32)-C(31)-H(31)	119.7
C(33)-C(32)-C(31)	122.4(4)
C(33)-C(32)-C(37)	118.8(4)
C(31)-C(32)-C(37)	118.9(4)
C(34)-C(33)-C(32)	120.4(4)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	121.3(4)
C(33)-C(34)-H(34)	119.4
C(35)-C(34)-H(34)	119.4
C(36)-C(35)-C(34)	120.3(4)
C(36)-C(35)-H(35)	119.9
C(34)-C(35)-H(35)	119.9
C(35)-C(36)-N(4)	122.2(3)
C(35)-C(36)-C(37)	119.7(4)
N(4)-C(36)-C(37)	118.1(3)
C(32)-C(37)-C(36)	119.6(3)
C(32)-C(37)-C(28)	119.2(3)
C(36)-C(37)-C(28)	121.2(3)
O(3)-C(38)-C(40)	108.5(3)
O(3)-C(38)-C(41)	105.1(3)
C(40)-C(38)-C(41)	108.7(4)
O(3)-C(38)-C(39)	104.1(3)
C(40)-C(38)-C(39)	116.9(4)

C(41)-C(38)-C(39)	112.8(4)
O(4)-C(39)-C(43)	108.0(4)
O(4)-C(39)-C(42)	106.9(3)
C(43)-C(39)-C(42)	110.2(5)
O(4)-C(39)-C(38)	102.8(3)
C(43)-C(39)-C(38)	116.2(4)
C(42)-C(39)-C(38)	112.1(4)
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(38)-C(41)-H(41A)	109.5
C(38)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(38)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(39)-C(43)-H(43A)	109.5
C(39)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(39)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(26)-C(44)-H(44A)	109.5
C(26)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(26)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5

H(44B)-C(44)-H(44C) 109.5

Symmetry transformations used to generate equivalent atoms:

Table S25. **Anisotropic displacement parameters ($Å^2x10^3$) for $C_{22}H_{30}B_2N_2O_2$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	30(1)	29(1)	52(2)	-1(1)	-7(1)	3(1)
O(2)	33(1)	27(1)	43(1)	5(1)	-6(1)	1(1)
N(1)	37(2)	29(2)	35(2)	3(1)	-3(1)	1(1)
N(2)	34(2)	29(2)	39(2)	-1(1)	-6(1)	6(2)
B(1)	32(2)	36(2)	25(2)	-1(2)	1(2)	0(2)
B(2)	31(2)	29(2)	39(2)	0(2)	-10(2)	-4(2)
C(1)	127(11)	106(9)	61(6)	-40(6)	-24(6)	53(8)
C(1X)	100(12)	108(13)	47(8)	-8(8)	0(8)	-3(10)
C(2)	61(3)	91(4)	39(3)	-5(3)	2(2)	20(3)
C(3)	41(2)	45(2)	43(2)	4(2)	3(2)	13(2)
C(4)	34(2)	29(2)	34(2)	1(2)	-4(2)	0(2)
C(5)	25(2)	31(2)	44(2)	4(2)	-4(2)	3(2)
C(6)	33(2)	24(2)	38(2)	-2(1)	-6(2)	-2(2)
C(7)	42(2)	32(2)	43(2)	0(2)	-4(2)	4(2)
C(8)	41(2)	40(2)	50(2)	-7(2)	0(2)	9(2)
C(9)	51(3)	46(2)	41(2)	-10(2)	2(2)	1(2)
C(10)	42(2)	31(2)	38(2)	-7(2)	-5(2)	-2(2)
C(11)	53(3)	47(2)	34(2)	-2(2)	-5(2)	-5(2)
C(12)	53(3)	41(2)	36(2)	3(2)	-14(2)	-3(2)
C(13)	43(2)	37(2)	41(2)	2(2)	-11(2)	2(2)
C(14)	35(2)	27(2)	34(2)	0(2)	-8(2)	-5(2)
C(15)	31(2)	28(2)	39(2)	-3(2)	-8(2)	-5(2)
C(16)	32(2)	32(2)	40(2)	7(2)	-2(2)	3(2)
C(17)	37(2)	31(2)	39(2)	4(2)	-5(2)	6(2)
C(18)	96(4)	51(3)	79(3)	11(3)	-51(3)	-11(3)
C(19)	62(3)	51(3)	113(4)	14(3)	40(3)	5(3)

C(20)	52(3)	73(3)	77(3)	42(3)	-15(3)	-14(3)
C(21)	59(3)	63(3)	88(4)	-30(3)	-17(3)	18(3)
C(22)	45(2)	30(2)	47(2)	3(2)	-8(2)	1(2)
O(3)	27(1)	30(1)	49(2)	-7(1)	-2(1)	3(1)
O(4)	27(1)	27(1)	58(2)	-7(1)	8(1)	-2(1)
N(3)	32(2)	34(2)	41(2)	-8(1)	3(2)	2(1)
N(4)	30(2)	33(2)	45(2)	-7(1)	-1(1)	8(2)
B(3)	29(2)	28(2)	31(2)	1(2)	2(2)	-2(2)
B(4)	27(2)	28(2)	51(3)	-14(2)	3(2)	-2(2)
C(23)	100(7)	81(6)	44(4)	3(4)	-5(4)	10(5)
C(23X)	116(18)	73(13)	52(10)	10(9)	-38(11)	7(12)
C(24)	71(3)	53(3)	45(3)	11(2)	-7(2)	8(3)
C(25)	40(2)	37(2)	52(2)	11(2)	3(2)	9(2)
C(26)	31(2)	28(2)	44(2)	0(2)	4(2)	2(2)
C(27)	27(2)	26(2)	53(2)	-4(2)	4(2)	1(2)
C(28)	26(2)	30(2)	46(2)	-12(2)	-1(2)	-2(2)
C(29)	30(2)	38(2)	50(2)	-11(2)	-2(2)	2(2)
C(30)	35(2)	38(2)	58(3)	-12(2)	-11(2)	10(2)
C(31)	43(2)	44(2)	44(2)	-7(2)	-10(2)	5(2)
C(32)	34(2)	40(2)	43(2)	-14(2)	-6(2)	1(2)
C(33)	52(3)	56(3)	39(2)	-13(2)	-5(2)	12(2)
C(34)	51(3)	53(3)	42(2)	-18(2)	3(2)	8(2)
C(35)	38(2)	41(2)	43(2)	-15(2)	-1(2)	10(2)
C(36)	29(2)	32(2)	42(2)	-11(2)	-2(2)	0(2)
C(37)	31(2)	32(2)	38(2)	-13(2)	-7(2)	-2(2)
C(38)	34(2)	31(2)	42(2)	-5(2)	-2(2)	6(2)
C(39)	28(2)	33(2)	60(2)	-7(2)	9(2)	7(2)
C(40)	55(3)	69(3)	75(3)	-32(3)	-5(3)	10(3)
C(41)	56(3)	61(3)	82(4)	27(3)	6(3)	8(3)
C(42)	122(5)	50(3)	105(4)	7(3)	83(4)	15(3)
C(43)	41(3)	53(3)	148(6)	-25(3)	-20(3)	10(2)
C(44)	32(2)	38(2)	47(2)	-5(2)	7(2)	-3(2)

Table S26. **Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^2 x10^3) for $C_{22}H_{30}B_2N_2O_2$.**

	x	y	z	U(eq)
H(1N)	2700(60)	7390(60)	2588(10)	66(16)
H(2N)	5150(40)	4160(50)	2856(7)	34(11)
H(1A)	4574	2737	1581	117
H(1B)	3365	3408	1375	117
H(2)	3190(120)	5470(100)	1600(30)	117
H(1X1)	4297	6162	1407	102
H(1X2)	3187	4871	1302	102
H(2X)	3420(170)	3630(110)	1700(30)	102
H(3A)	5247	5918	1873	52
H(3B)	5469	4217	1928	52
H(5A)	5240	6512	2334	40
H(5B)	5587	4835	2390	40
H(7)	889	8575	2865	47
H(8)	-187	8769	3277	53
H(9)	562	7311	3617	55
H(11)	2204	5300	3785	53
H(12)	4025	3620	3709	52
H(13)	5072	3360	3297	48
H(18A)	306	7051	1596	113
H(18B)	-965	8118	1696	113
H(18C)	-1151	6389	1724	113
H(19A)	-1522	6352	2182	113
H(19B)	-1492	8095	2200	113
H(19C)	-406	7145	2377	113
H(20A)	2636	9954	1811	101
H(20B)	972	9831	1713	101
H(20C)	2118	8556	1649	101
H(21A)	771	9166	2398	105
H(21B)	201	10240	2173	105
H(21C)	1887	10283	2262	105
H(22A)	3860	2891	2226	61
H(22B)	2427	3341	2064	61
H(22C)	2514	3677	2369	61

H(3N)	5230(60)	4750(60)	4949(10)	67(16)
H(4N)	8500(50)	2360(50)	4677(9)	53(14)
H(23A)	6424	3438	6091	90
H(23B)	7661	4547	6216	90
H(24)	9050(80)	4470(90)	5837(17)	90
H(23C)	10183	3152	5880	96
H(23D)	9707	4339	6106	96
H(24X)	7220(150)	4400(200)	5920(40)	96
H(25A)	6839	2358	5667	52
H(25B)	8546	2164	5603	52
H(27A)	6114	2250	5206	42
H(27B)	7796	1890	5145	42
H(29)	3969	6491	4668	47
H(30)	3746	7569	4255	53
H(31)	5224	6842	3915	52
H(33)	7271	5260	3747	59
H(34)	9038	3507	3823	59
H(35)	9296	2438	4234	49
H(40A)	5618	7579	5893	99
H(40B)	4521	8729	5761	99
H(40C)	6256	8870	5716	99
H(41A)	6144	8822	5257	99
H(41B)	4386	8803	5266	99
H(41C)	5253	7582	5104	99
H(42A)	2820	4931	5774	138
H(42B)	3113	6590	5857	138
H(42C)	4388	5400	5888	138
H(43A)	3170	6502	5151	121
H(43B)	2263	7165	5391	121
H(43C)	2174	5457	5328	121
H(44A)	9328	5137	5434	58
H(44B)	8894	5002	5133	58
H(44C)	9756	3700	5274	58

Table S27. **Torsion angles [°] for $C_{22}H_{30}B_2N_2O_2$.**

C(16)-O(1)-B(1)-O(2)	-1.1(4)
C(16)-O(1)-B(1)-C(4)	-179.5(3)
C(17)-O(2)-B(1)-O(1)	-5.4(4)
C(17)-O(2)-B(1)-C(4)	173.0(3)
C(14)-N(2)-B(2)-N(1)	-0.6(5)
C(14)-N(2)-B(2)-C(5)	178.7(3)
C(6)-N(1)-B(2)-N(2)	0.2(5)
C(6)-N(1)-B(2)-C(5)	-179.1(3)
C(1)-C(2)-C(3)-C(4)	-112.2(11)
C(2)-C(3)-C(4)-C(22)	64.4(5)
C(2)-C(3)-C(4)-C(5)	-177.0(4)
C(2)-C(3)-C(4)-B(1)	-55.9(5)
O(1)-B(1)-C(4)-C(22)	-22.7(5)
O(2)-B(1)-C(4)-C(22)	159.1(3)
O(1)-B(1)-C(4)-C(3)	96.6(4)
O(2)-B(1)-C(4)-C(3)	-81.7(4)
O(1)-B(1)-C(4)-C(5)	-144.4(3)
O(2)-B(1)-C(4)-C(5)	37.4(5)
C(22)-C(4)-C(5)-B(2)	-59.6(4)
C(3)-C(4)-C(5)-B(2)	-177.9(3)
B(1)-C(4)-C(5)-B(2)	62.7(4)
N(2)-B(2)-C(5)-C(4)	118.0(4)
N(1)-B(2)-C(5)-C(4)	-62.7(5)
B(2)-N(1)-C(6)-C(7)	179.3(4)
B(2)-N(1)-C(6)-C(15)	0.2(5)
N(1)-C(6)-C(7)-C(8)	179.5(4)
C(15)-C(6)-C(7)-C(8)	-1.4(6)
C(6)-C(7)-C(8)-C(9)	1.3(6)
C(7)-C(8)-C(9)-C(10)	-0.3(7)
C(8)-C(9)-C(10)-C(11)	179.8(4)
C(8)-C(9)-C(10)-C(15)	-0.5(6)
C(9)-C(10)-C(11)-C(12)	-179.9(4)
C(15)-C(10)-C(11)-C(12)	0.4(6)
C(10)-C(11)-C(12)-C(13)	-0.6(6)
C(11)-C(12)-C(13)-C(14)	0.4(6)

C(12)-C(13)-C(14)-N(2)	179.9(4)
C(12)-C(13)-C(14)-C(15)	0.0(6)
B(2)-N(2)-C(14)-C(13)	-179.2(4)
B(2)-N(2)-C(14)-C(15)	0.6(5)
C(13)-C(14)-C(15)-C(10)	-0.2(5)
N(2)-C(14)-C(15)-C(10)	180.0(3)
C(13)-C(14)-C(15)-C(6)	179.7(3)
N(2)-C(14)-C(15)-C(6)	-0.2(5)
C(9)-C(10)-C(15)-C(14)	-179.7(3)
C(11)-C(10)-C(15)-C(14)	0.0(5)
C(9)-C(10)-C(15)-C(6)	0.4(5)
C(11)-C(10)-C(15)-C(6)	-179.9(3)
C(7)-C(6)-C(15)-C(14)	-179.3(3)
N(1)-C(6)-C(15)-C(14)	-0.2(5)
C(7)-C(6)-C(15)-C(10)	0.5(5)
N(1)-C(6)-C(15)-C(10)	179.7(3)
B(1)-O(1)-C(16)-C(18)	129.1(4)
B(1)-O(1)-C(16)-C(19)	-112.7(4)
B(1)-O(1)-C(16)-C(17)	6.5(4)
B(1)-O(2)-C(17)-C(21)	132.6(4)
B(1)-O(2)-C(17)-C(20)	-111.2(4)
B(1)-O(2)-C(17)-C(16)	9.0(4)
O(1)-C(16)-C(17)-O(2)	-9.2(3)
C(18)-C(16)-C(17)-O(2)	-126.6(4)
C(19)-C(16)-C(17)-O(2)	105.1(4)
O(1)-C(16)-C(17)-C(21)	-126.2(4)
C(18)-C(16)-C(17)-C(21)	116.4(5)
C(19)-C(16)-C(17)-C(21)	-11.9(5)
O(1)-C(16)-C(17)-C(20)	106.0(4)
C(18)-C(16)-C(17)-C(20)	-11.4(5)
C(19)-C(16)-C(17)-C(20)	-139.7(4)
C(38)-O(3)-B(3)-O(4)	-2.0(4)
C(38)-O(3)-B(3)-C(26)	178.4(3)
C(39)-O(4)-B(3)-O(3)	-8.3(4)
C(39)-O(4)-B(3)-C(26)	171.3(3)
C(36)-N(4)-B(4)-N(3)	-0.1(5)

C(36)-N(4)-B(4)-C(27)	-179.1(3)
C(28)-N(3)-B(4)-N(4)	0.4(5)
C(28)-N(3)-B(4)-C(27)	179.3(3)
C(23)-C(24)-C(25)-C(26)	117.6(7)
C(24)-C(25)-C(26)-C(44)	64.6(5)
C(24)-C(25)-C(26)-C(27)	-176.5(4)
C(24)-C(25)-C(26)-B(3)	-55.3(5)
O(3)-B(3)-C(26)-C(44)	-21.7(5)
O(4)-B(3)-C(26)-C(44)	158.7(3)
O(3)-B(3)-C(26)-C(25)	97.6(4)
O(4)-B(3)-C(26)-C(25)	-82.0(4)
O(3)-B(3)-C(26)-C(27)	-143.2(4)
O(4)-B(3)-C(26)-C(27)	37.2(5)
C(44)-C(26)-C(27)-B(4)	-57.9(4)
C(25)-C(26)-C(27)-B(4)	-176.7(3)
B(3)-C(26)-C(27)-B(4)	64.0(4)
N(4)-B(4)-C(27)-C(26)	115.6(4)
N(3)-B(4)-C(27)-C(26)	-63.2(5)
B(4)-N(3)-C(28)-C(29)	179.4(4)
B(4)-N(3)-C(28)-C(37)	-0.2(5)
N(3)-C(28)-C(29)-C(30)	179.5(4)
C(37)-C(28)-C(29)-C(30)	-0.9(6)
C(28)-C(29)-C(30)-C(31)	1.1(6)
C(29)-C(30)-C(31)-C(32)	-0.4(6)
C(30)-C(31)-C(32)-C(33)	-179.4(4)
C(30)-C(31)-C(32)-C(37)	-0.3(6)
C(31)-C(32)-C(33)-C(34)	179.0(4)
C(37)-C(32)-C(33)-C(34)	0.0(6)
C(32)-C(33)-C(34)-C(35)	0.5(7)
C(33)-C(34)-C(35)-C(36)	-0.4(7)
C(34)-C(35)-C(36)-N(4)	179.9(4)
C(34)-C(35)-C(36)-C(37)	-0.1(6)
B(4)-N(4)-C(36)-C(35)	179.7(4)
B(4)-N(4)-C(36)-C(37)	-0.3(5)
C(33)-C(32)-C(37)-C(36)	-0.4(6)
C(31)-C(32)-C(37)-C(36)	-179.5(3)

C(33)-C(32)-C(37)-C(28)	179.6(4)
C(31)-C(32)-C(37)-C(28)	0.5(5)
C(35)-C(36)-C(37)-C(32)	0.5(5)
N(4)-C(36)-C(37)-C(32)	-179.5(3)
C(35)-C(36)-C(37)-C(28)	-179.5(4)
N(4)-C(36)-C(37)-C(28)	0.5(5)
C(29)-C(28)-C(37)-C(32)	0.2(5)
N(3)-C(28)-C(37)-C(32)	179.8(3)
C(29)-C(28)-C(37)-C(36)	-179.9(3)
N(3)-C(28)-C(37)-C(36)	-0.3(5)
B(3)-O(3)-C(38)-C(40)	135.8(4)
B(3)-O(3)-C(38)-C(41)	-108.1(4)
B(3)-O(3)-C(38)-C(39)	10.7(4)
B(3)-O(4)-C(39)-C(43)	137.4(4)
B(3)-O(4)-C(39)-C(42)	-104.1(4)
B(3)-O(4)-C(39)-C(38)	14.0(4)
O(3)-C(38)-C(39)-O(4)	-14.6(4)
C(40)-C(38)-C(39)-O(4)	-134.2(4)
C(41)-C(38)-C(39)-O(4)	98.8(4)
O(3)-C(38)-C(39)-C(43)	-132.3(4)
C(40)-C(38)-C(39)-C(43)	108.1(5)
C(41)-C(38)-C(39)-C(43)	-18.9(5)
O(3)-C(38)-C(39)-C(42)	99.7(4)
C(40)-C(38)-C(39)-C(42)	-19.8(5)
C(41)-C(38)-C(39)-C(42)	-146.8(4)

Symmetry transformations used to generate equivalent atoms:

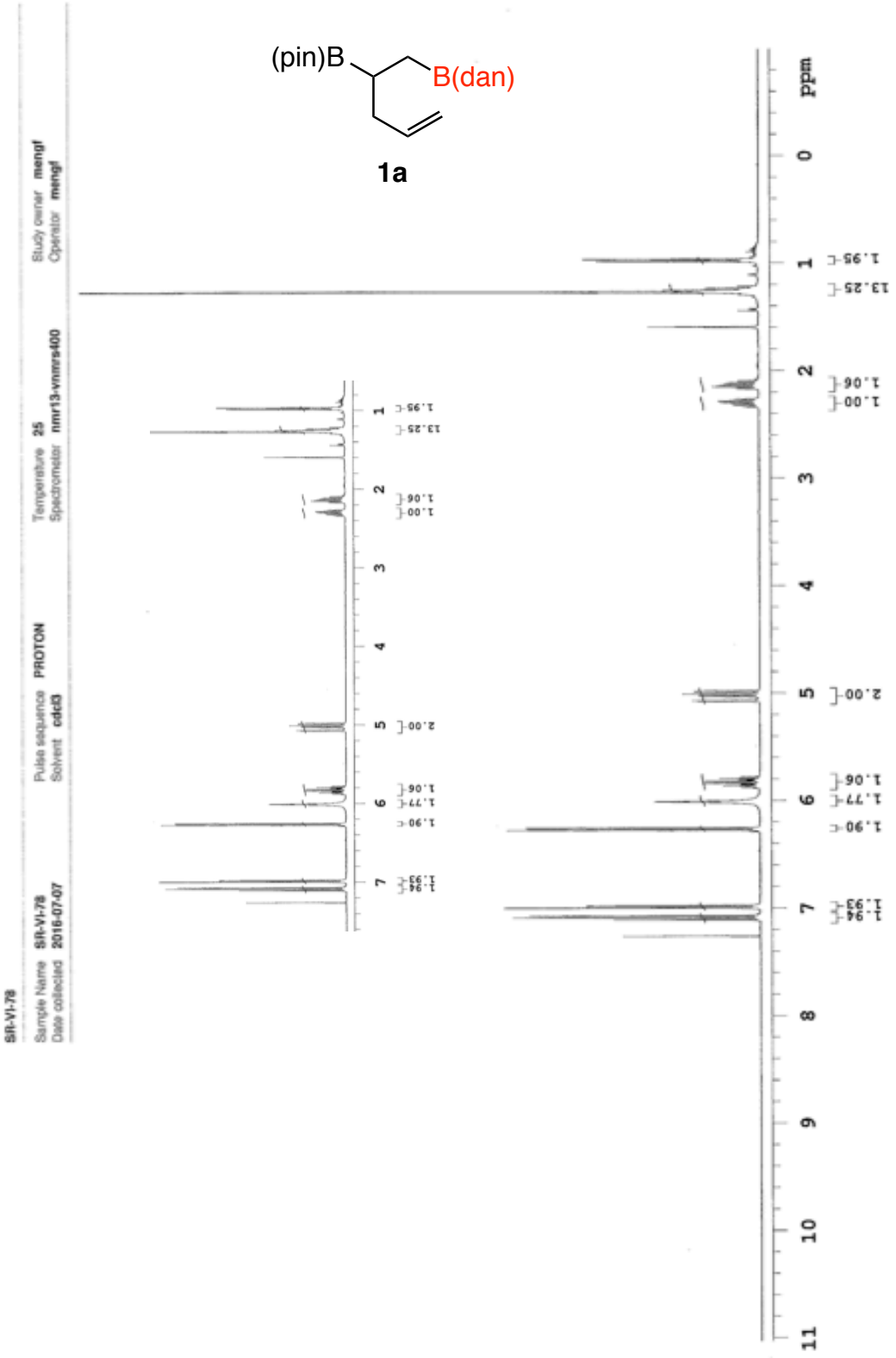
Table S28. **Hydrogen bonds for $C_{22}H_{30}B_2N_2O_2$ [Å and º].**

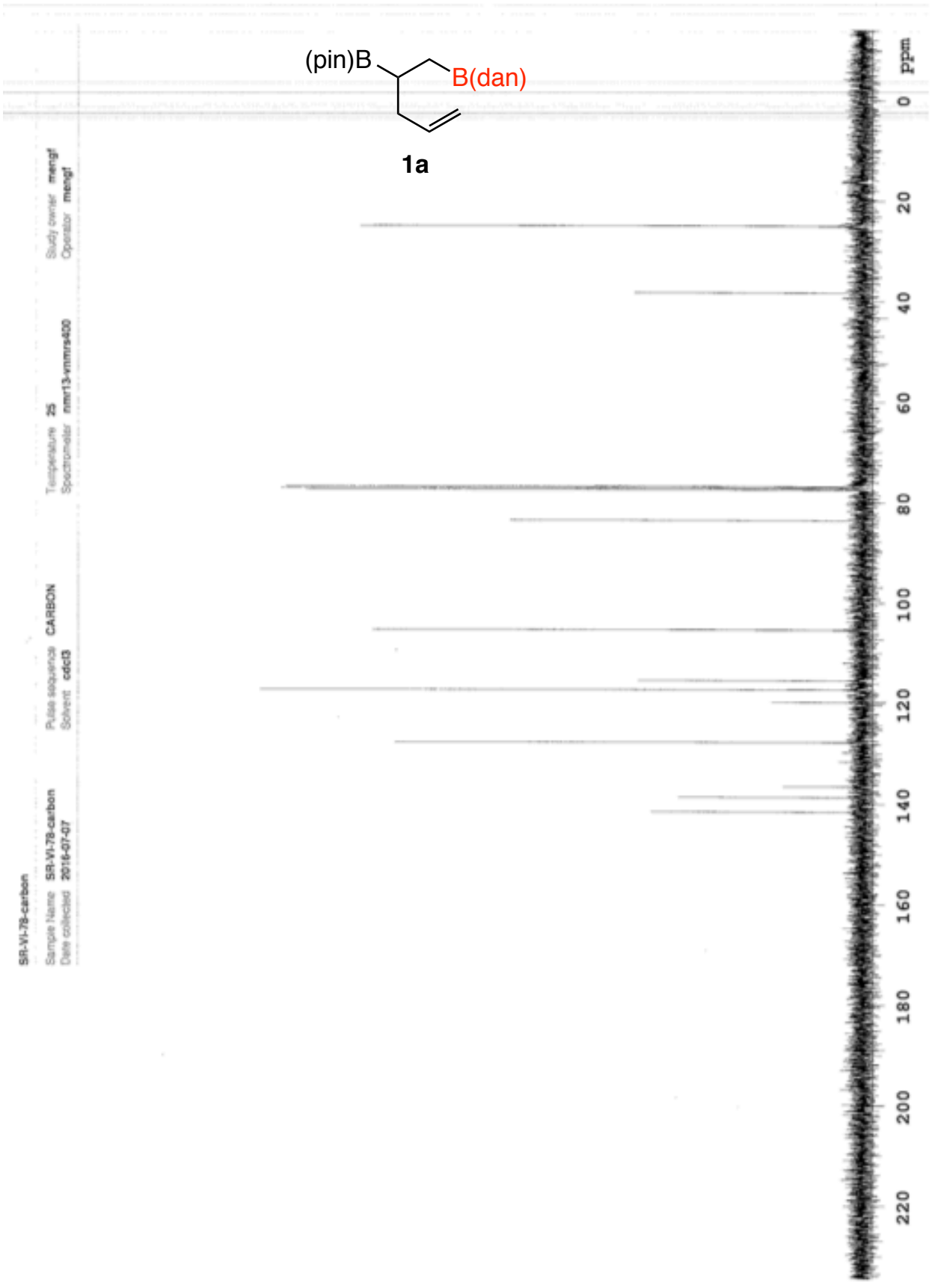
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...O(2)	0.89(5)	2.41(5)	3.159(4)	142(4)
N(2)-H(2N)...O(2)#1	0.86(4)	2.32(4)	3.165(4)	166(4)
N(3)-H(3N)...O(4)	0.89(5)	2.39(5)	3.160(4)	145(4)
N(4)-H(4N)...O(4)#2	0.86(5)	2.33(5)	3.142(4)	157(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z+1/2 #2 x+1/2,-y+1/2,-z+1

5. NMR Spectra

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Operator mengf
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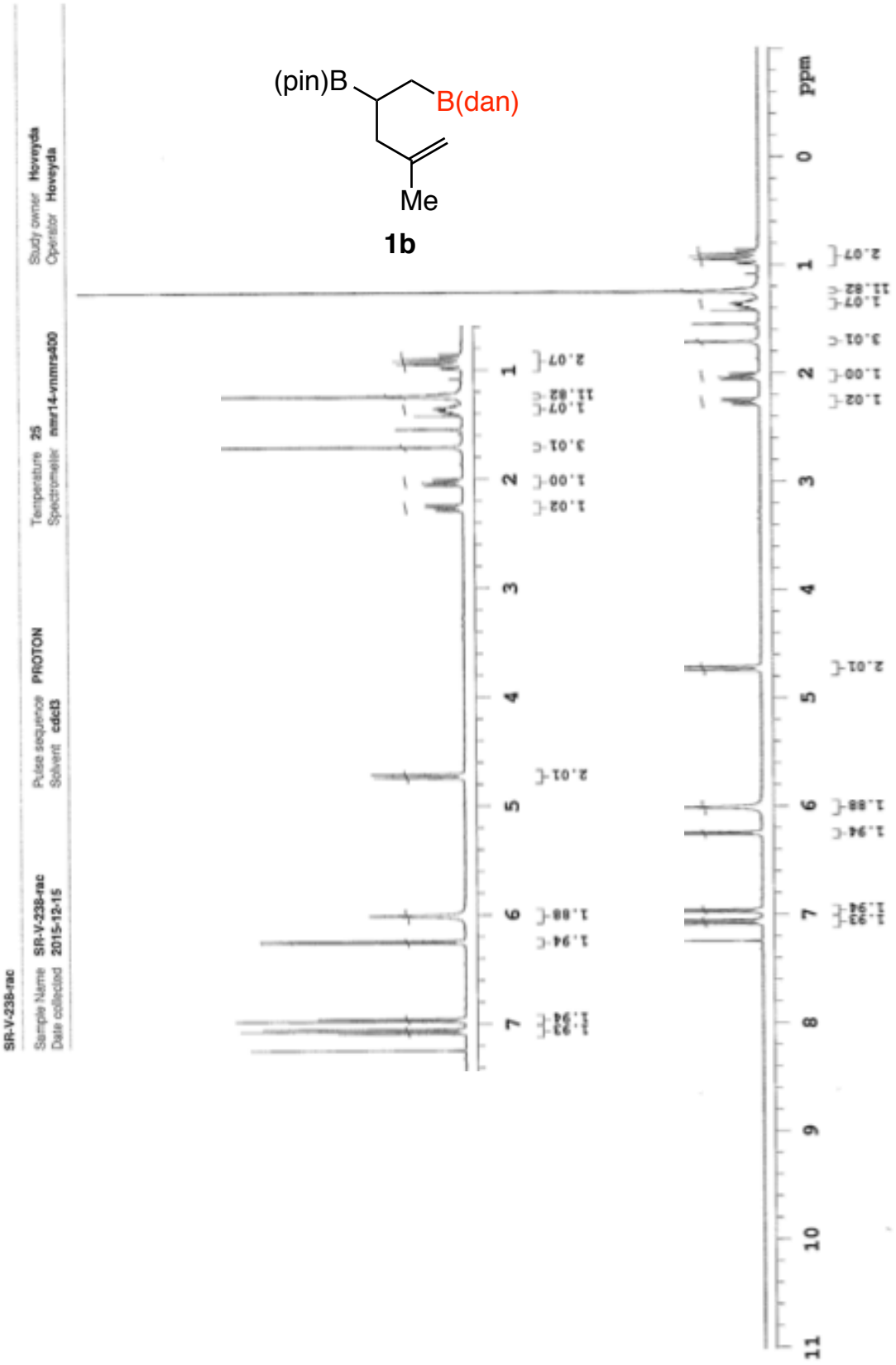
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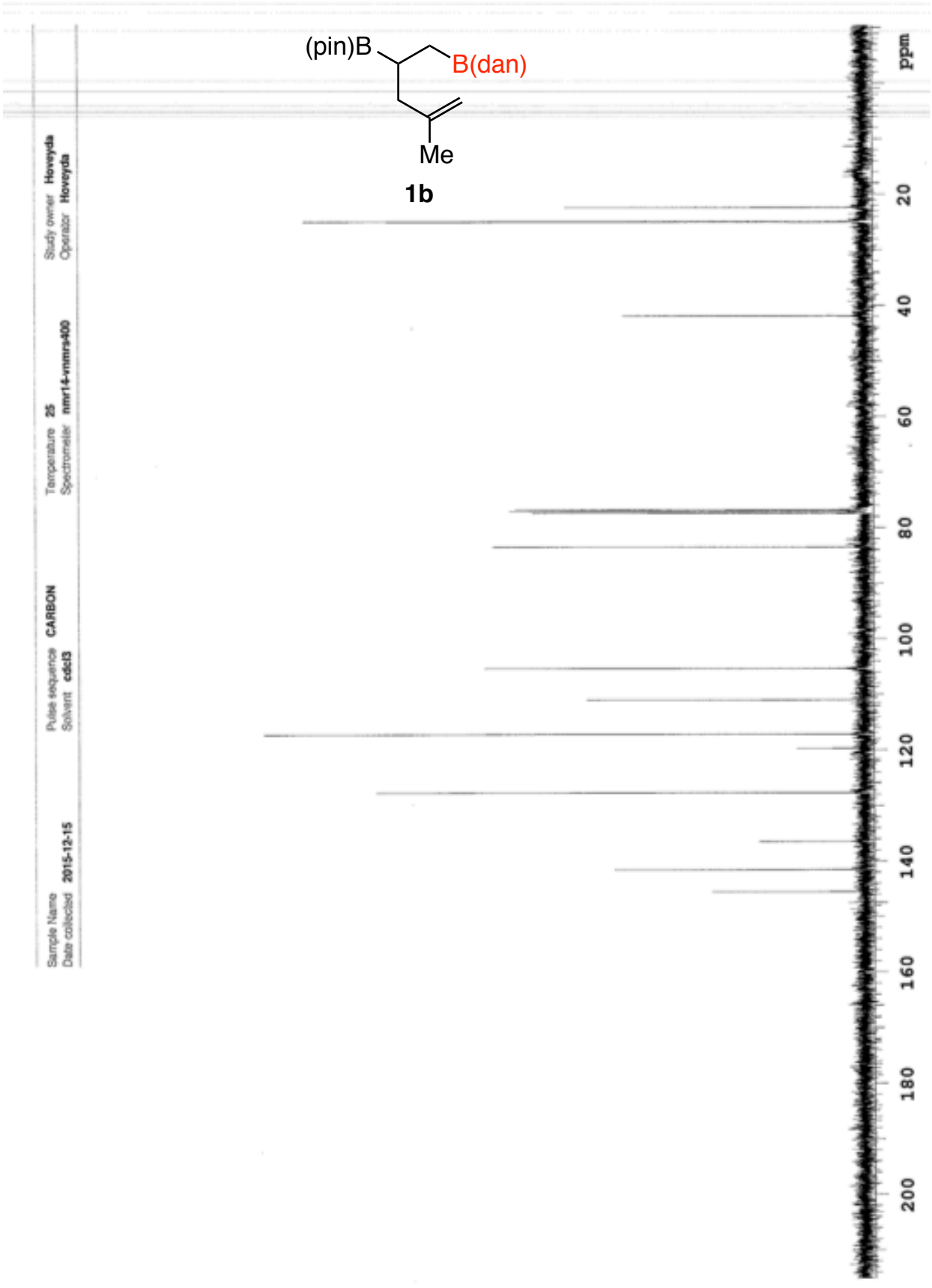
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Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs400
Study owner Hoveyda
Operator Hoveyda
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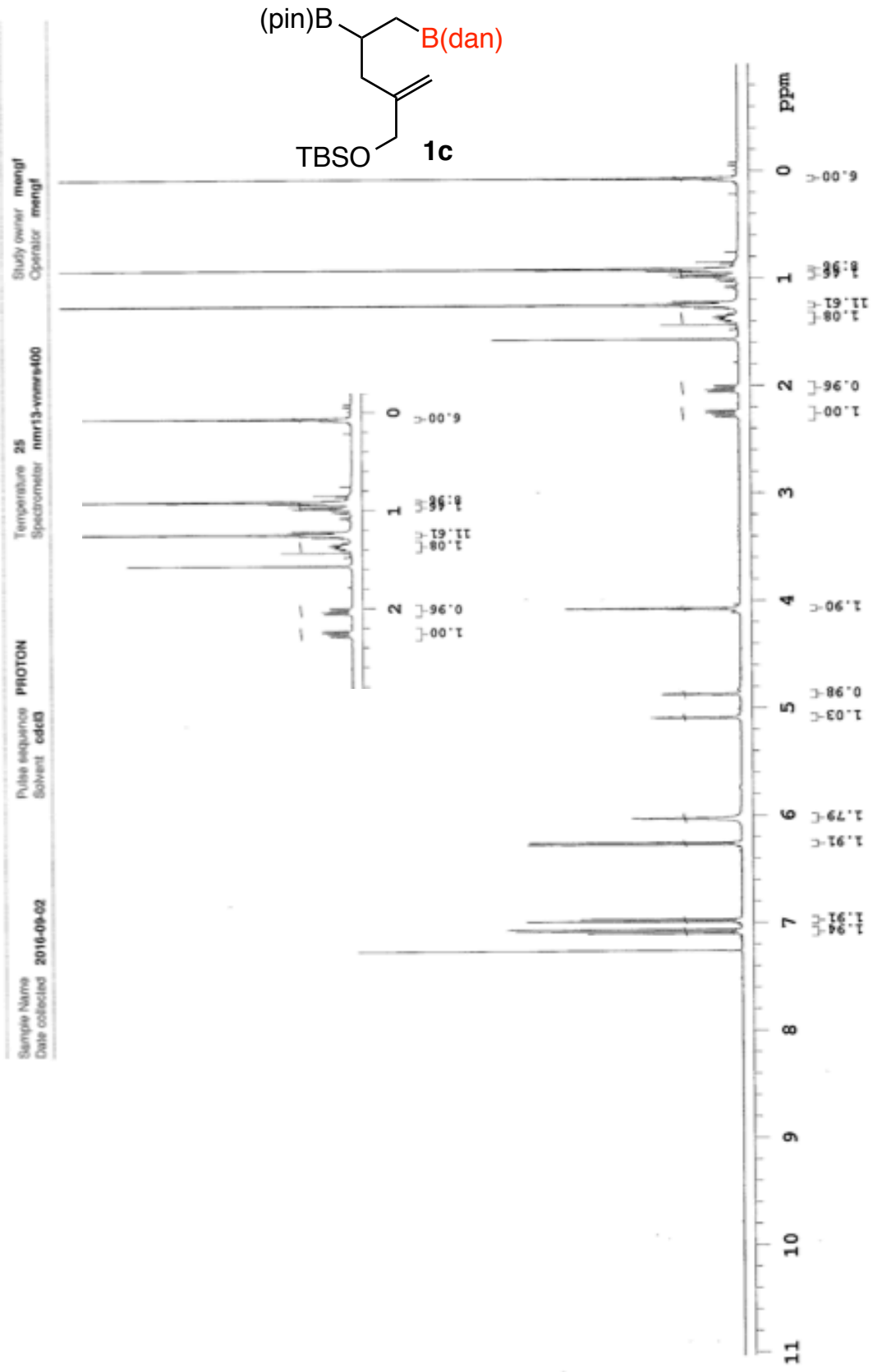
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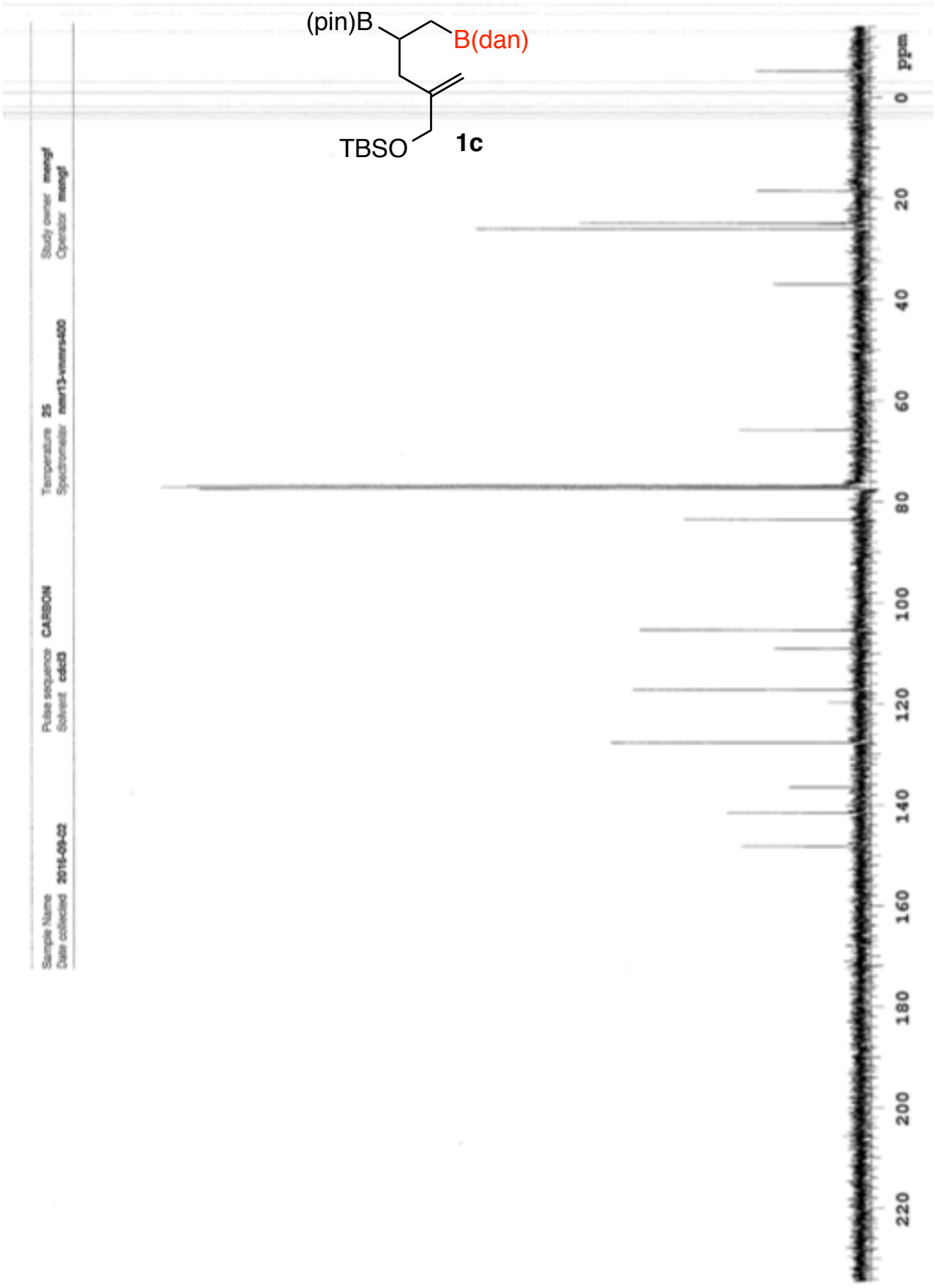
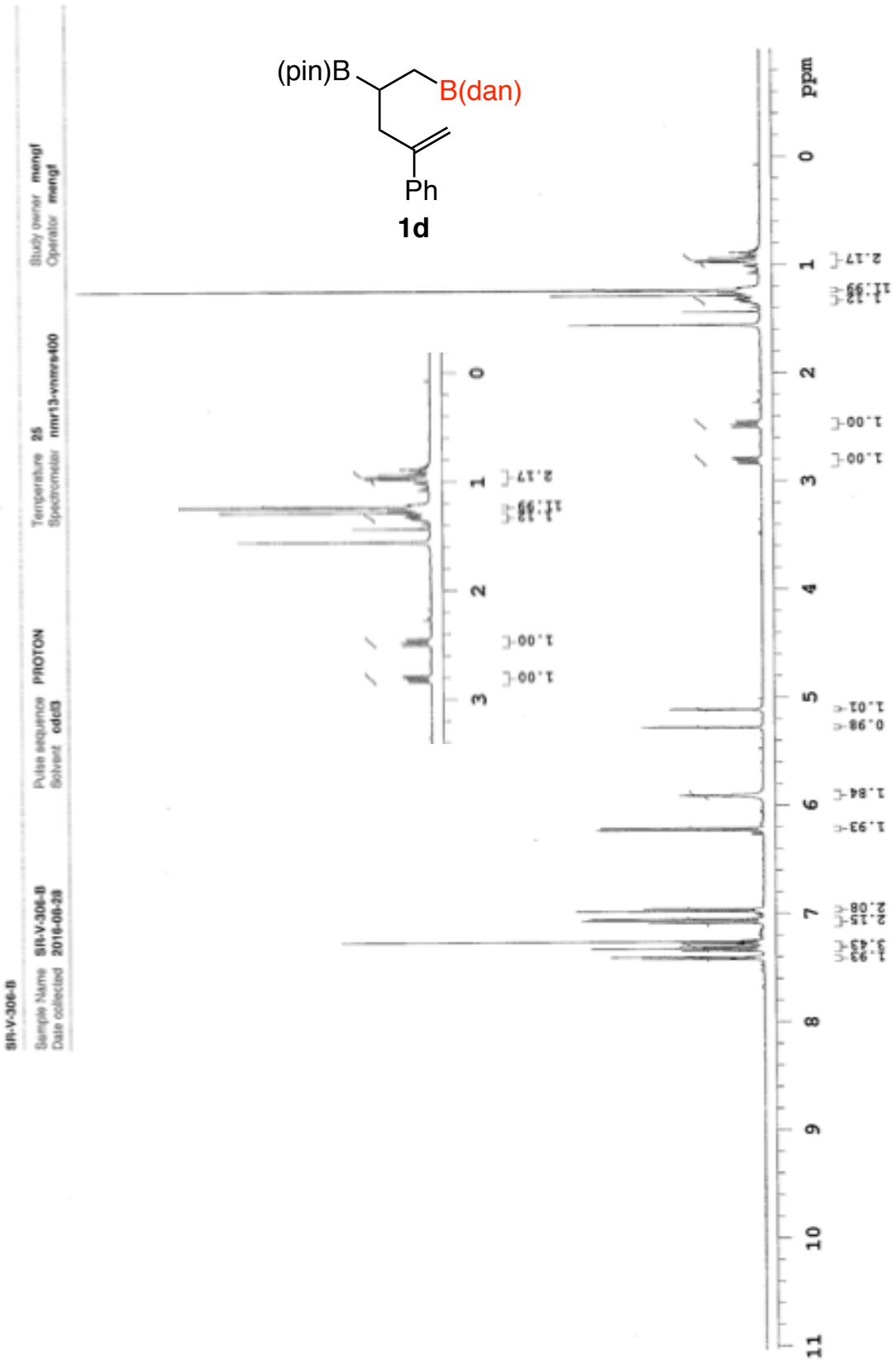
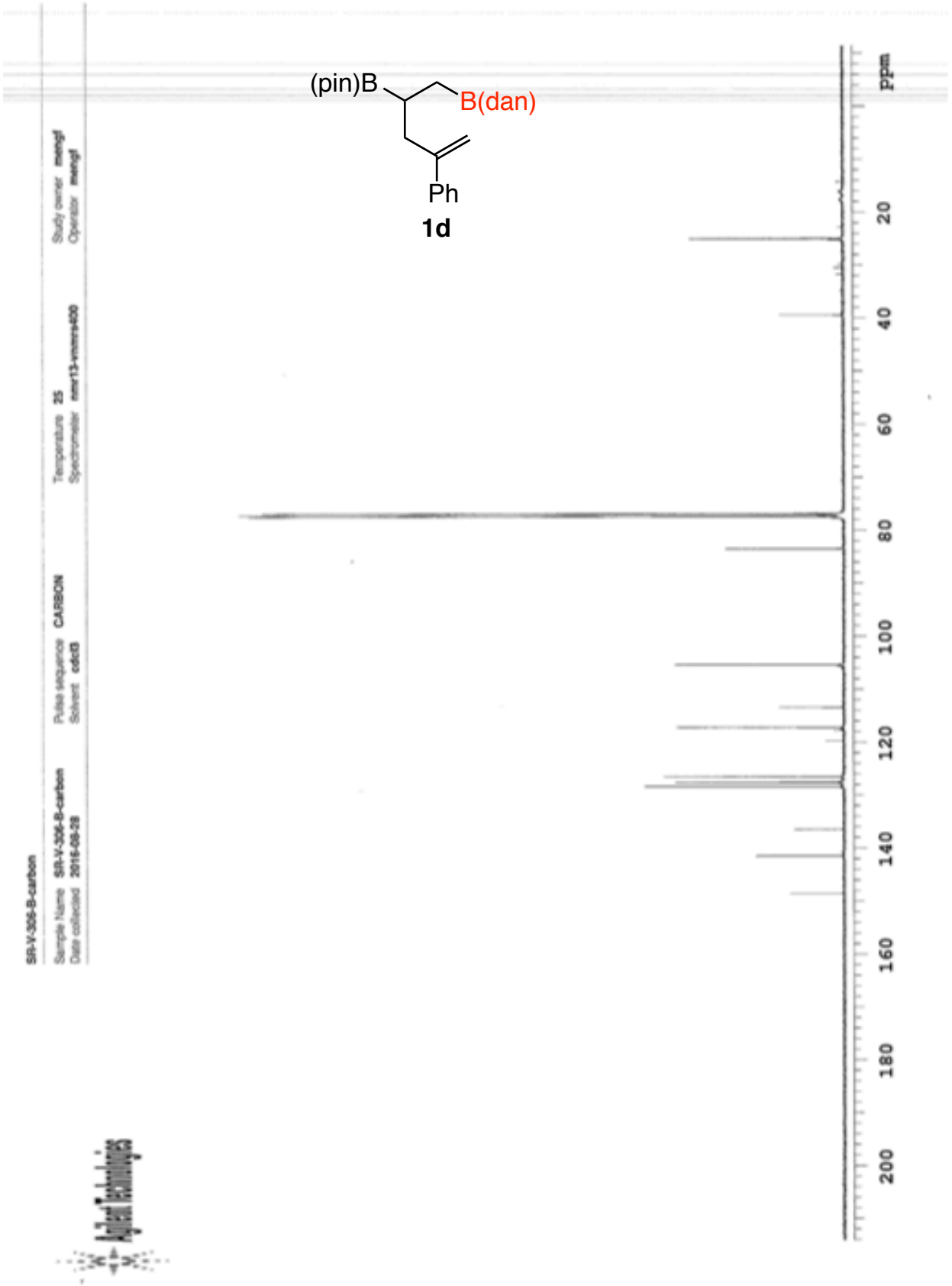
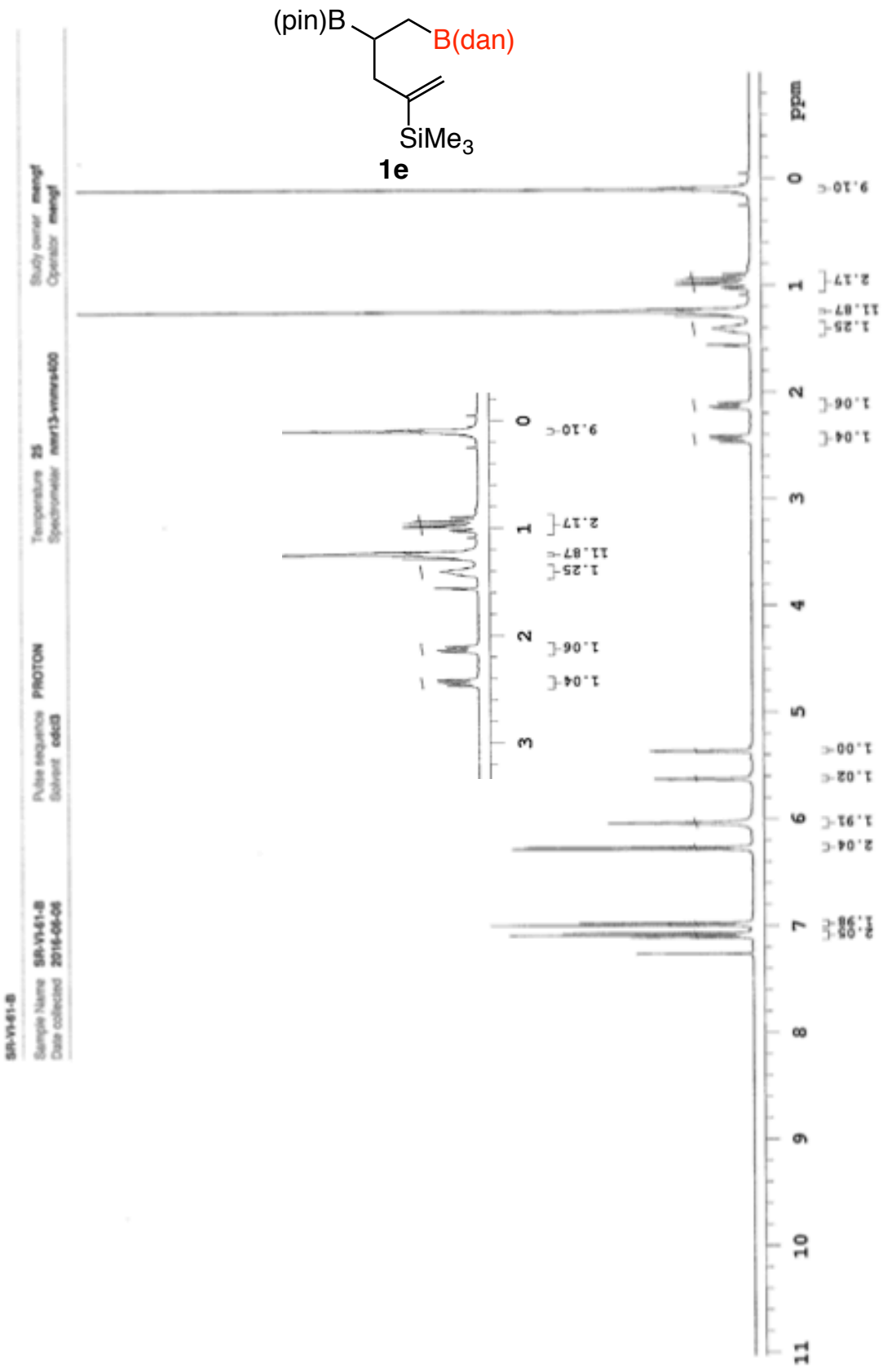
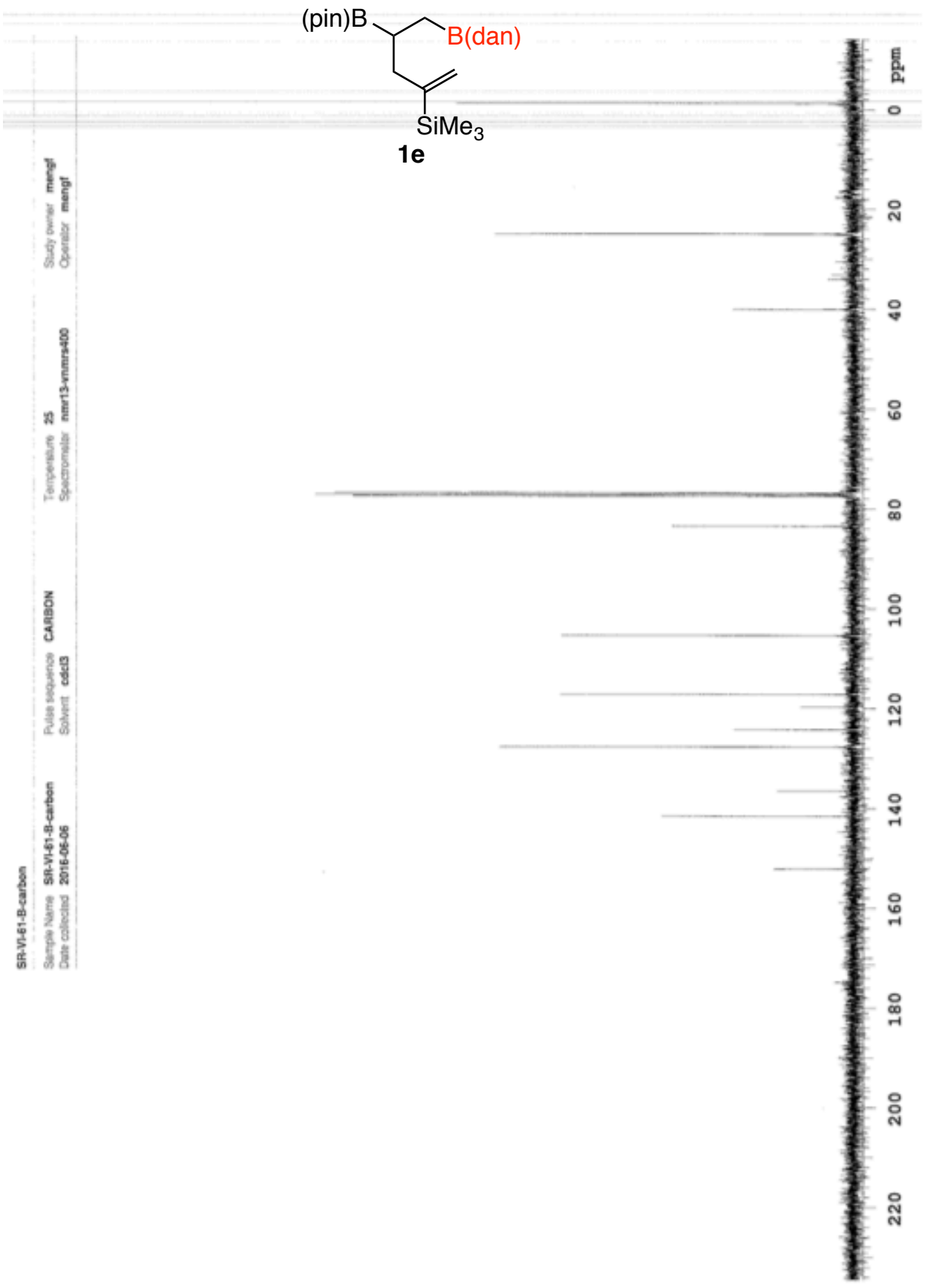
Operator mengf
ppm

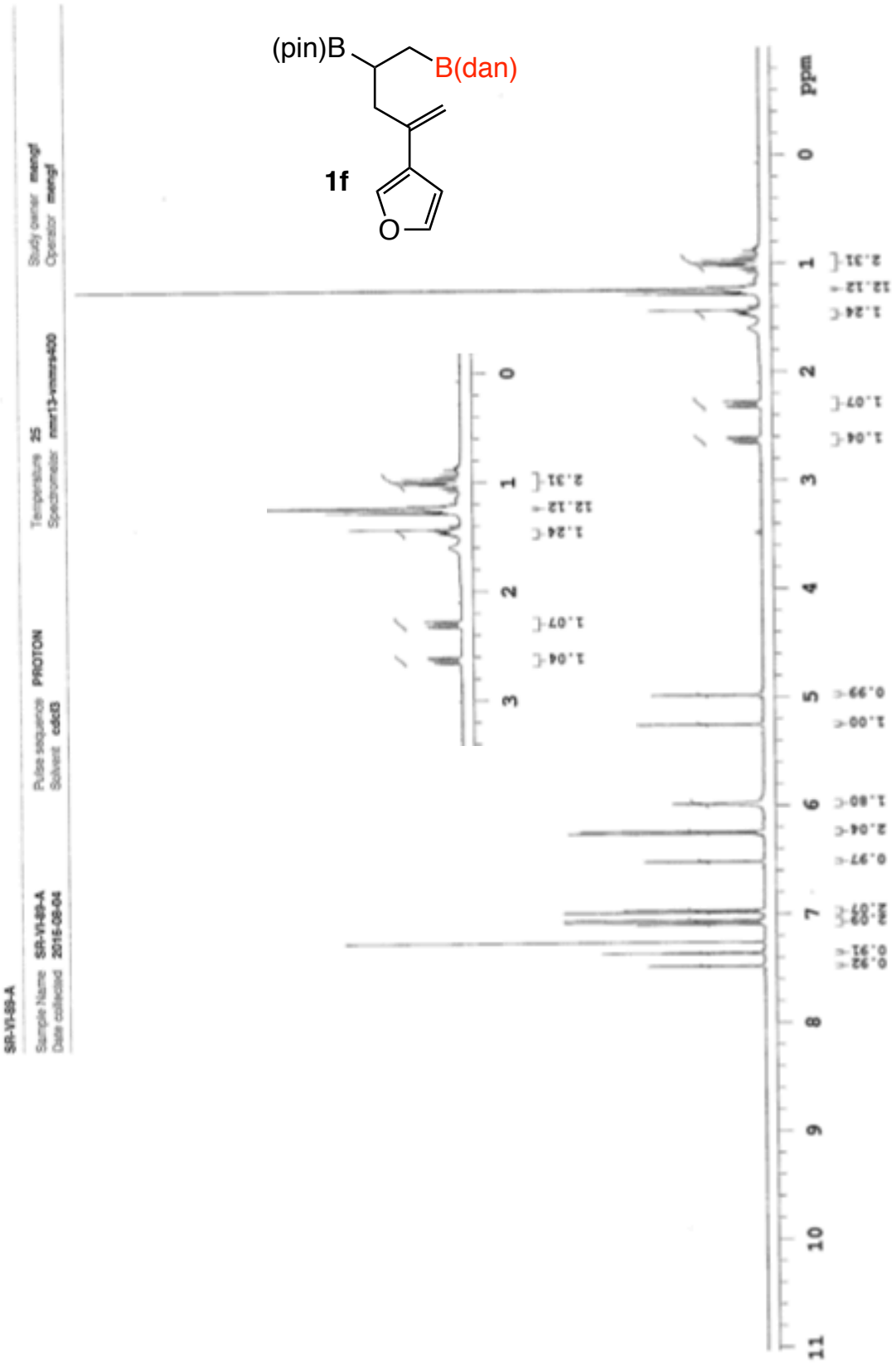

(pin)B
B(dan)
TBSO
1c
Sample Name
Date collected 2016-09-02
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

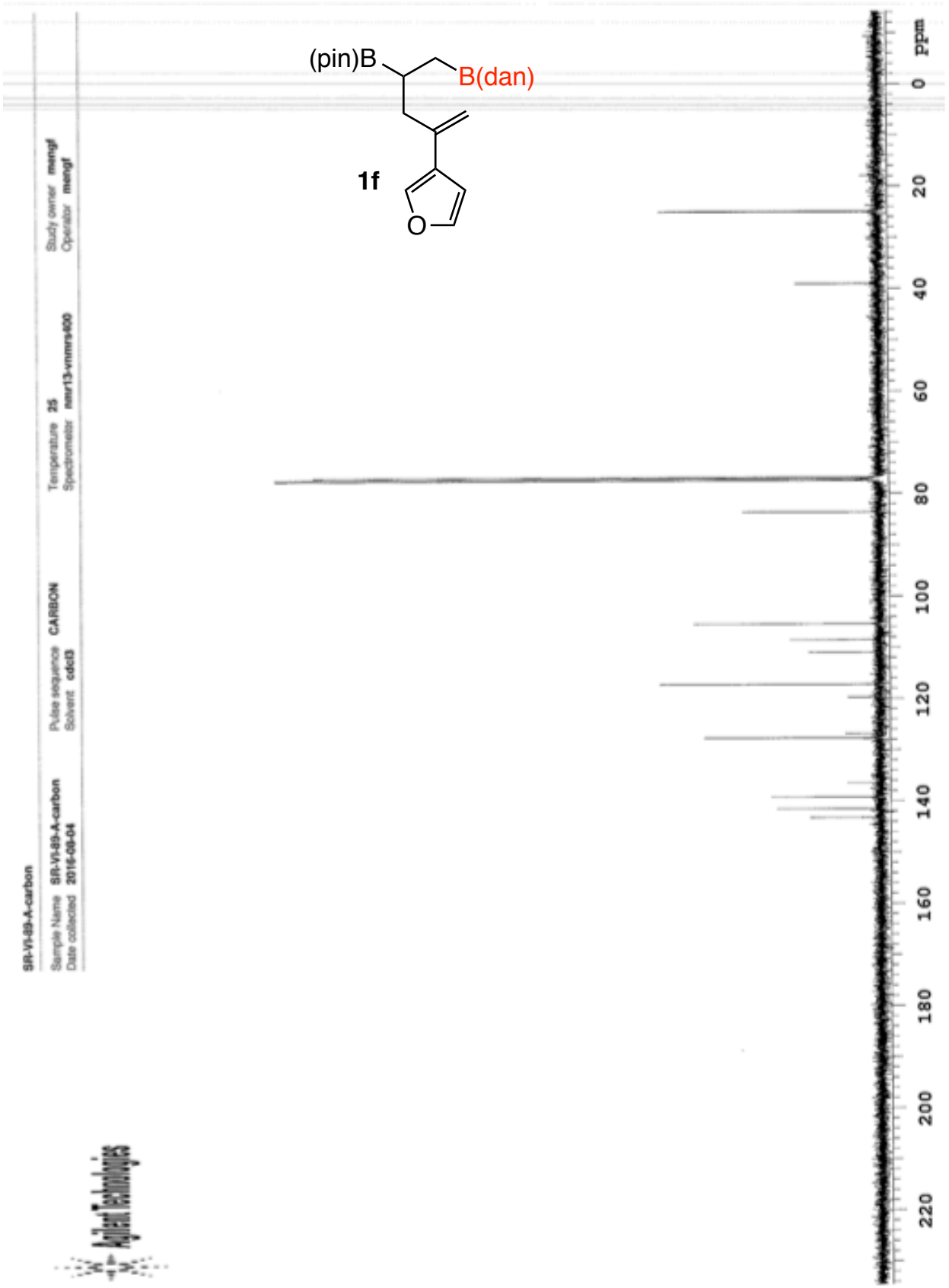

(pin)B
B(dan)
Ph
1d
BR-V-306-B
Sample Name BR-V-306-B
Date collected 2016-08-29
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

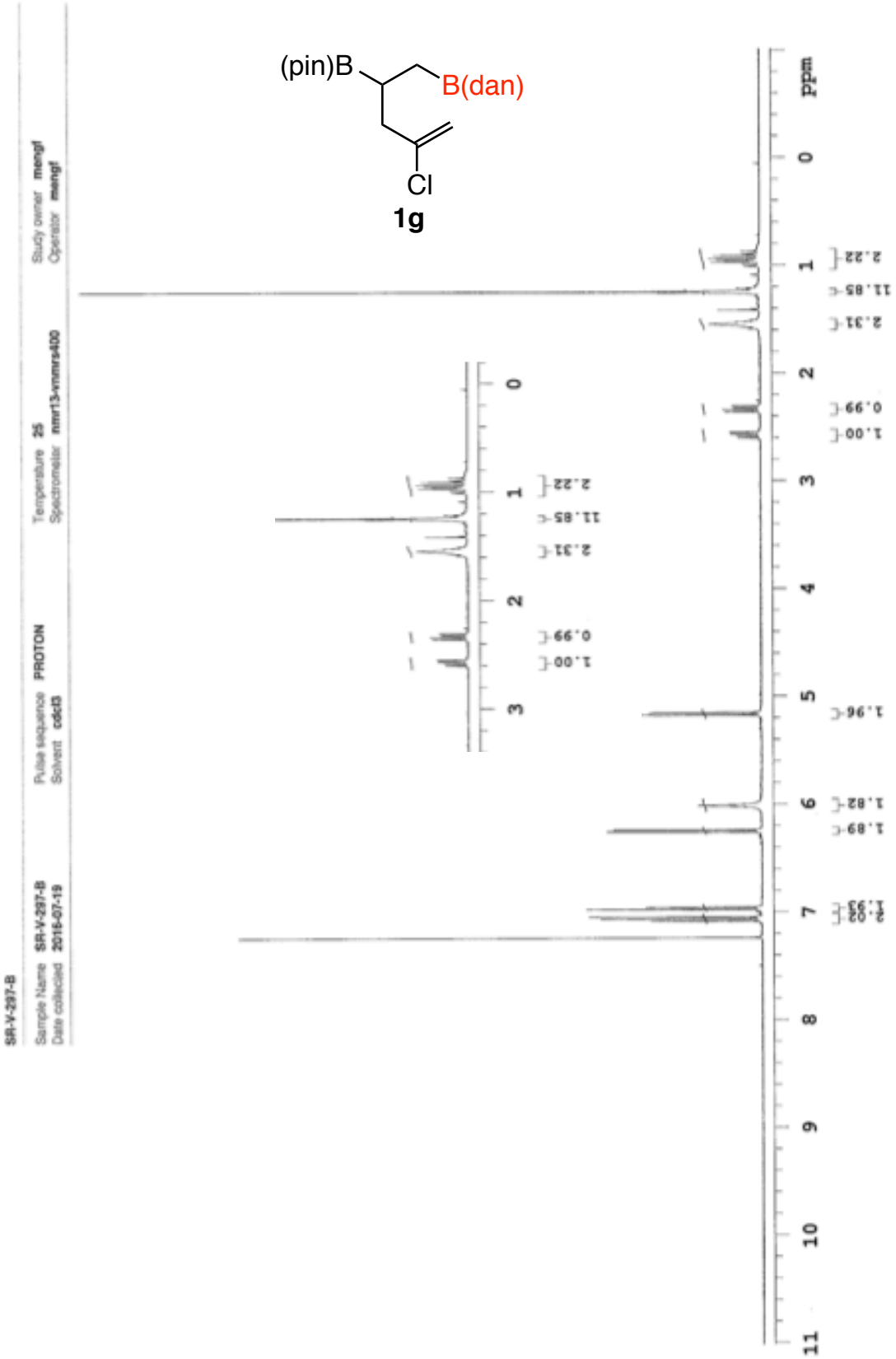

(pin)B
B(dan)
Ph
1d
SR-V-306-B-carbon
Sample Name SR-V-306-B-carbon
Date collected 2016-08-28
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
20
40
60
80
100
120
140
160
180
200

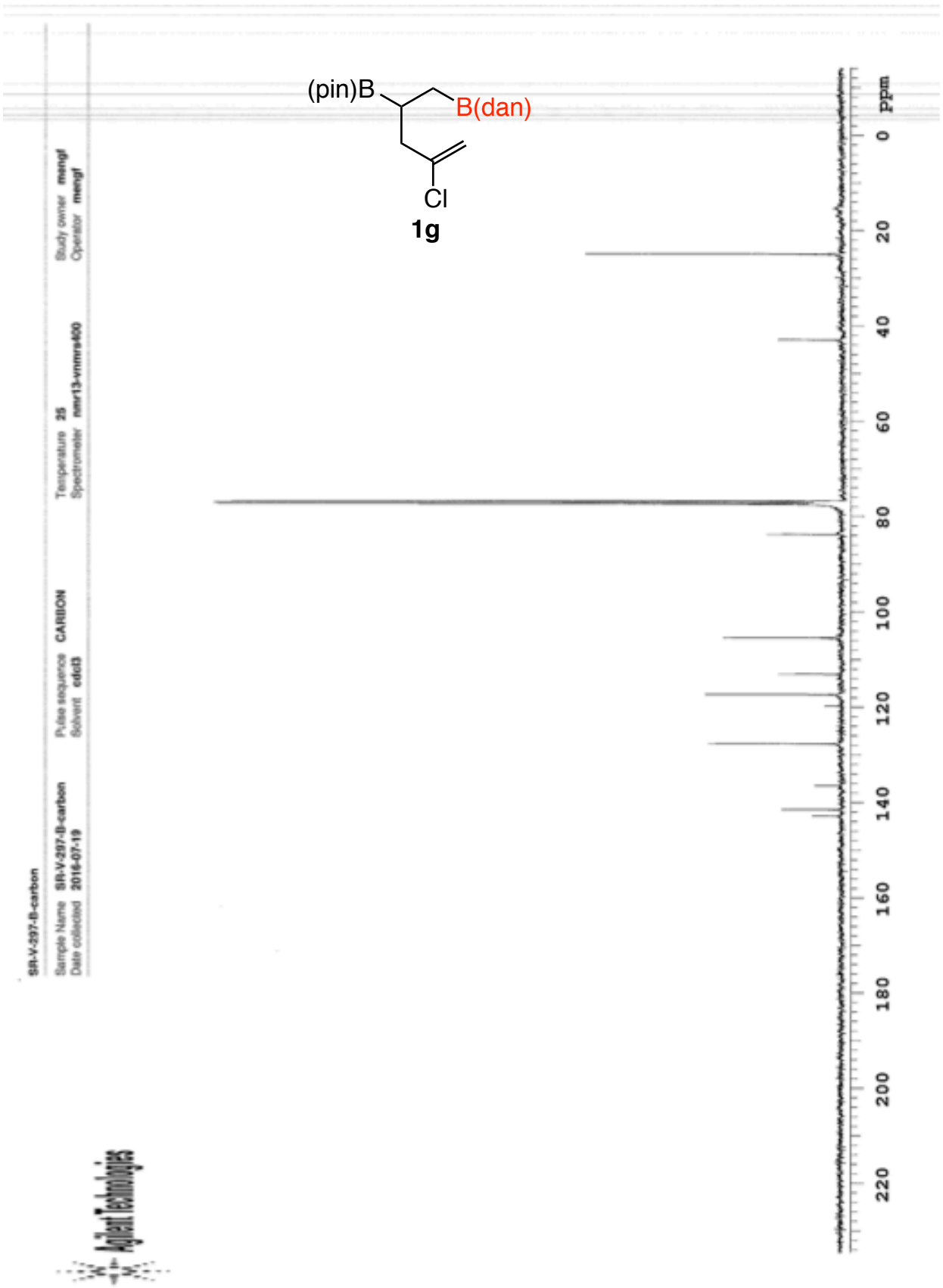

(pin)B
B(dan)
SiMe3
1e
SR-VI-61-B
Sample Name SR-VI-61-B
Date collected 2016-06-06
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mangf
Operator mangf
ppm

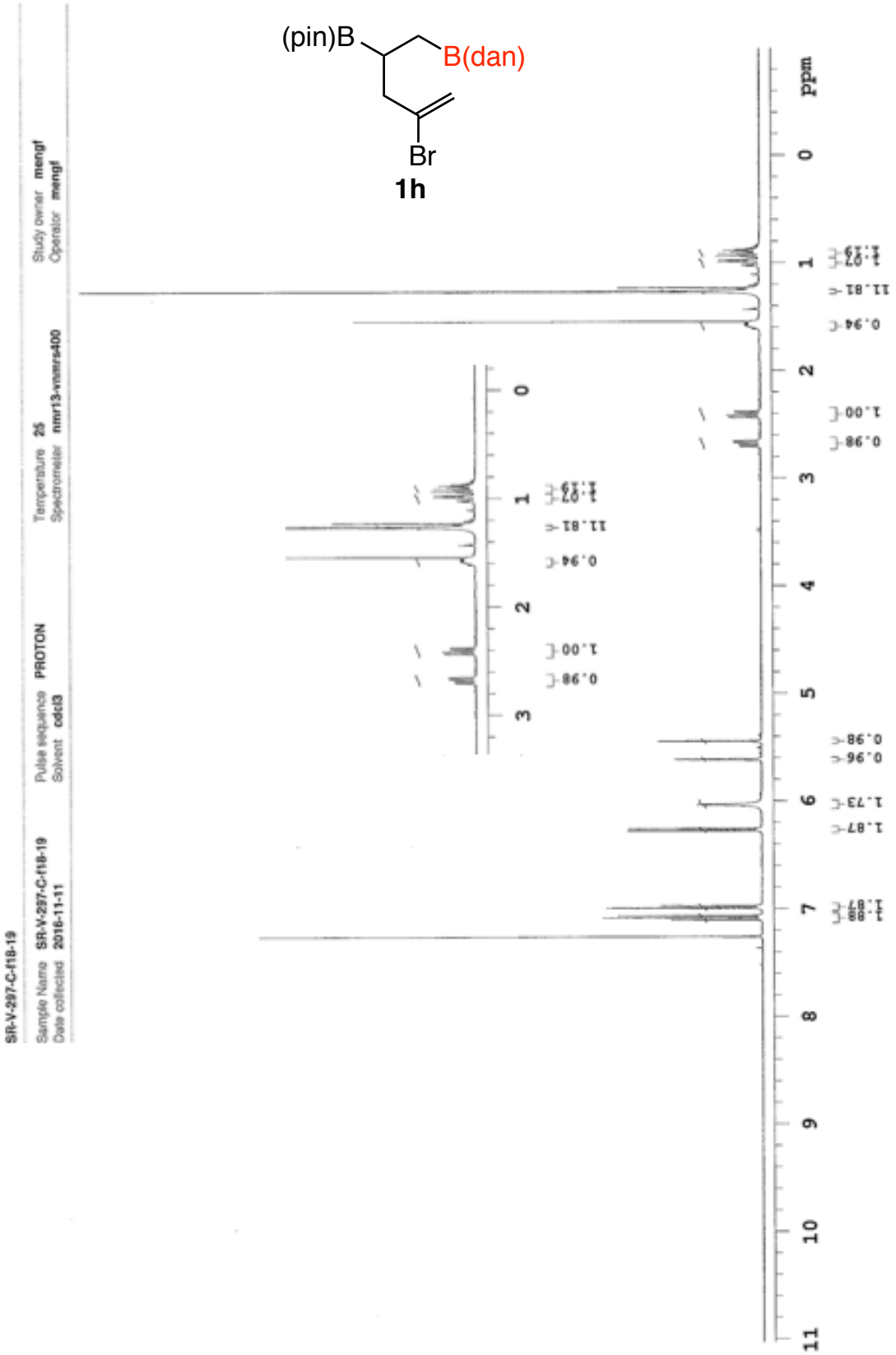

(pin)B
B(dan)
SiMe3
1e
SR-VI-61-B-carbon
Sample Name SR-VI-61-B-carbon
Date collected 2016-06-06
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

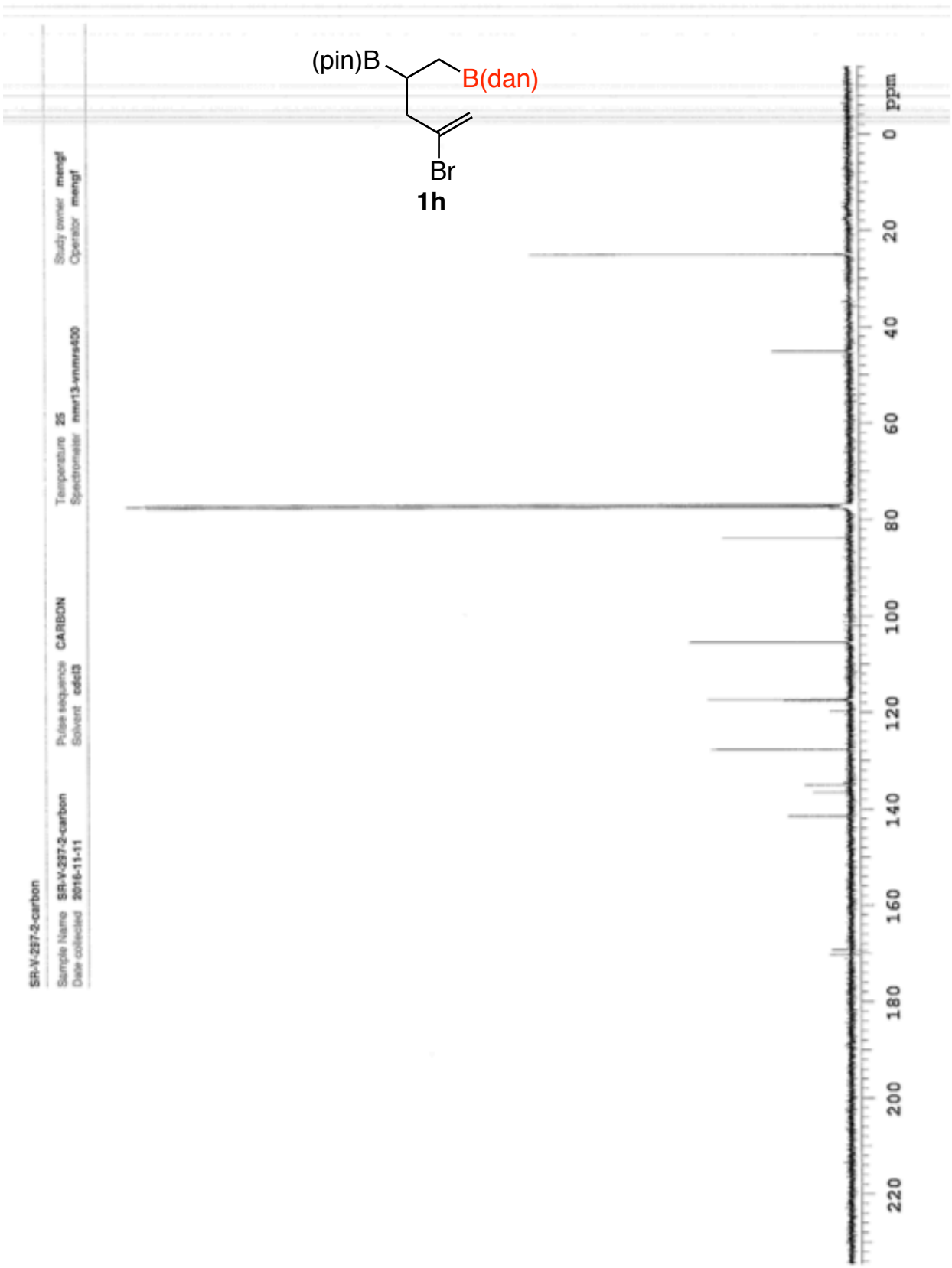

(pin)B
B(dan)
1f
O
SR-VI-89-A
Sample Name SR-VI-89-A
Date collected 2015-08-04
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

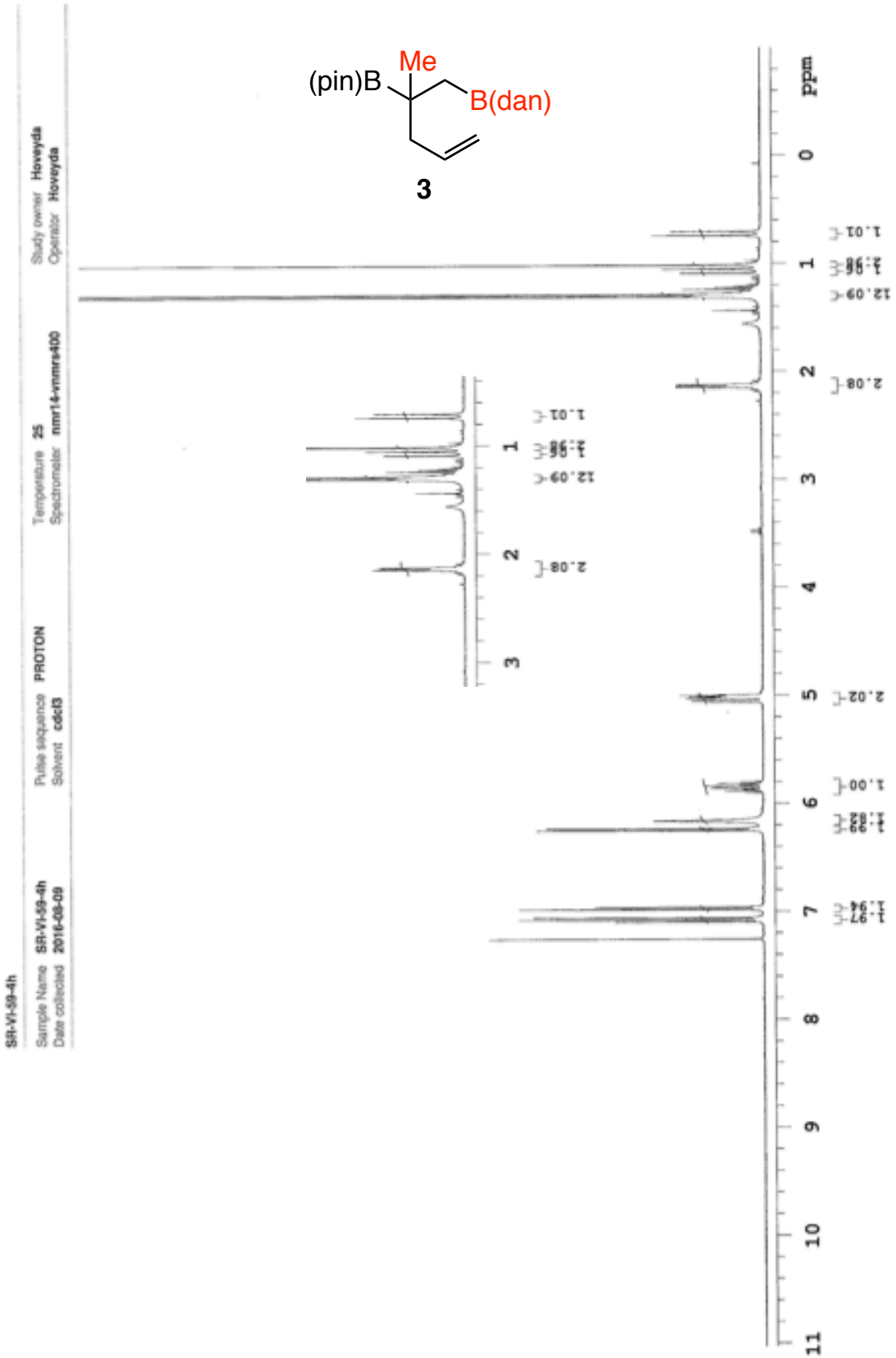

(pin)B
B(dan)
1f
O
SR-VI-89-A-carbon
Sample Name SR-VI-89-A-carbon
Date collected 2016-08-04
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

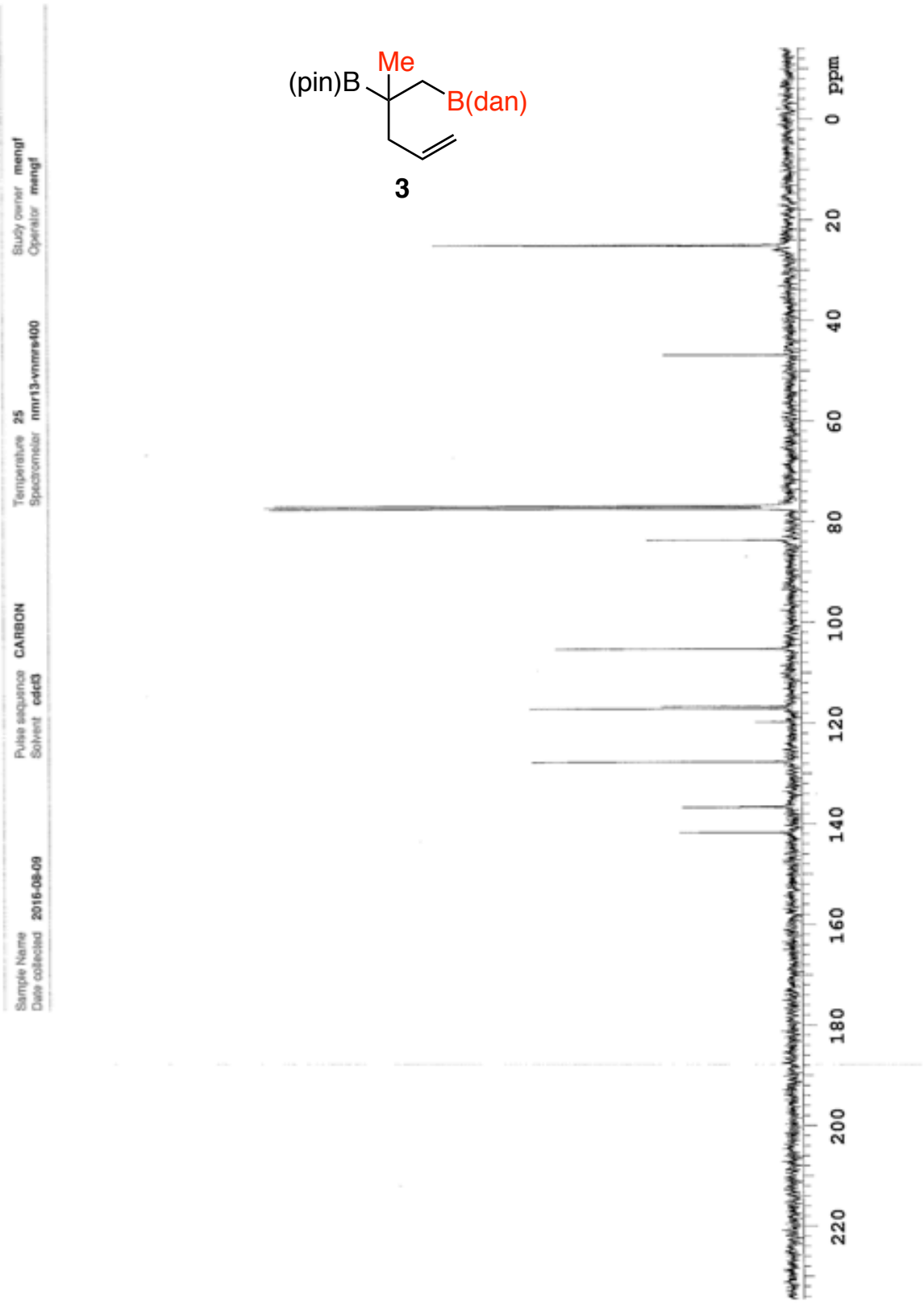

(pin)B
B(dan)
Cl
1g
SR-V-297-B
Sample Name SR-V-297-B
Date collected 2016-07-19
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.22
11.85
2.31
0.99
1.00
1.96
1.82
1.89
1.00

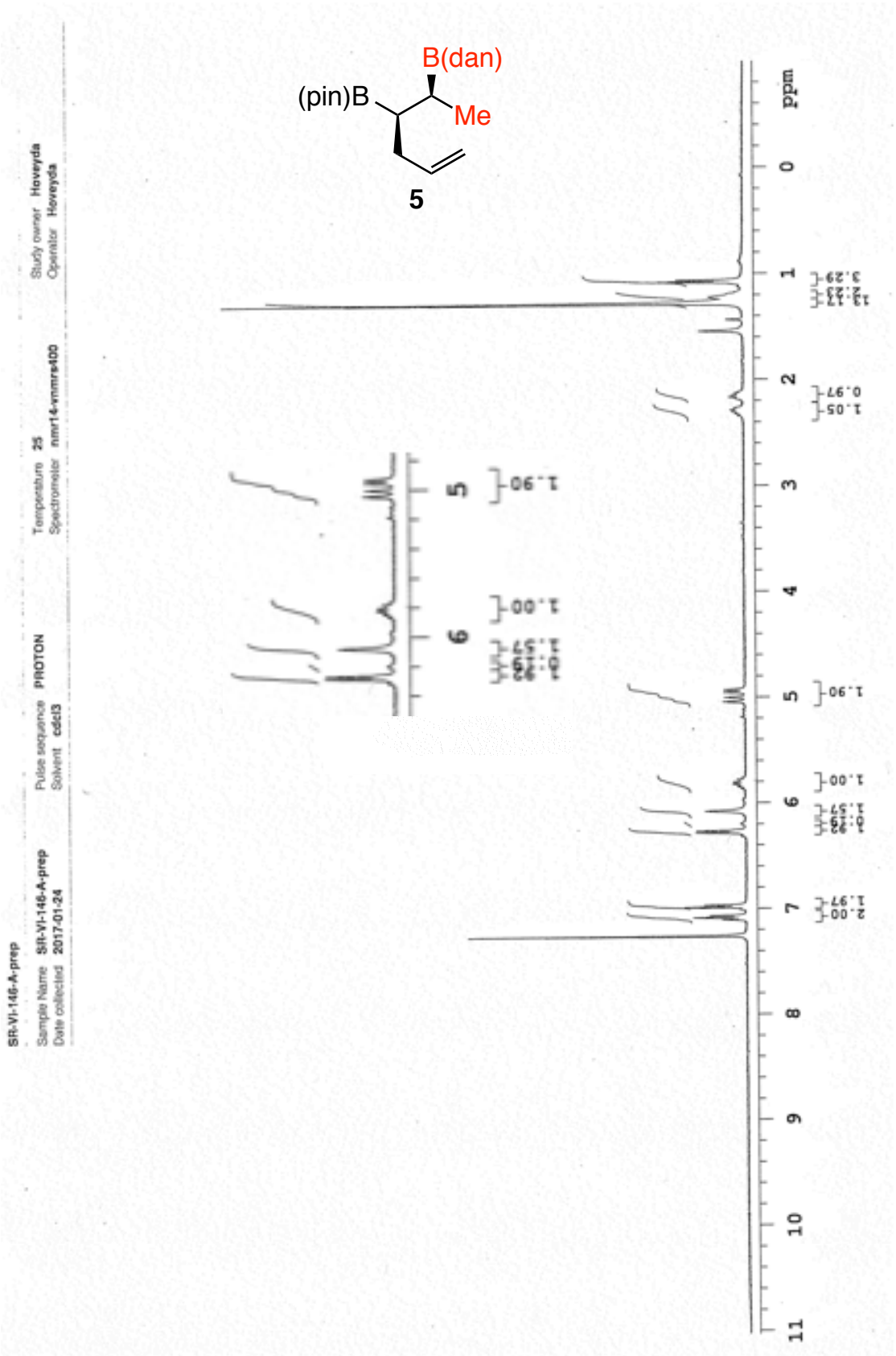

(pin)B
B(dan)
Cl
1g
SR-V-297-B-carbon
Sample Name SR-V-297-B-carbon
Date collected 2016-07-19
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengl
Operator mengl
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Agilent Technologies

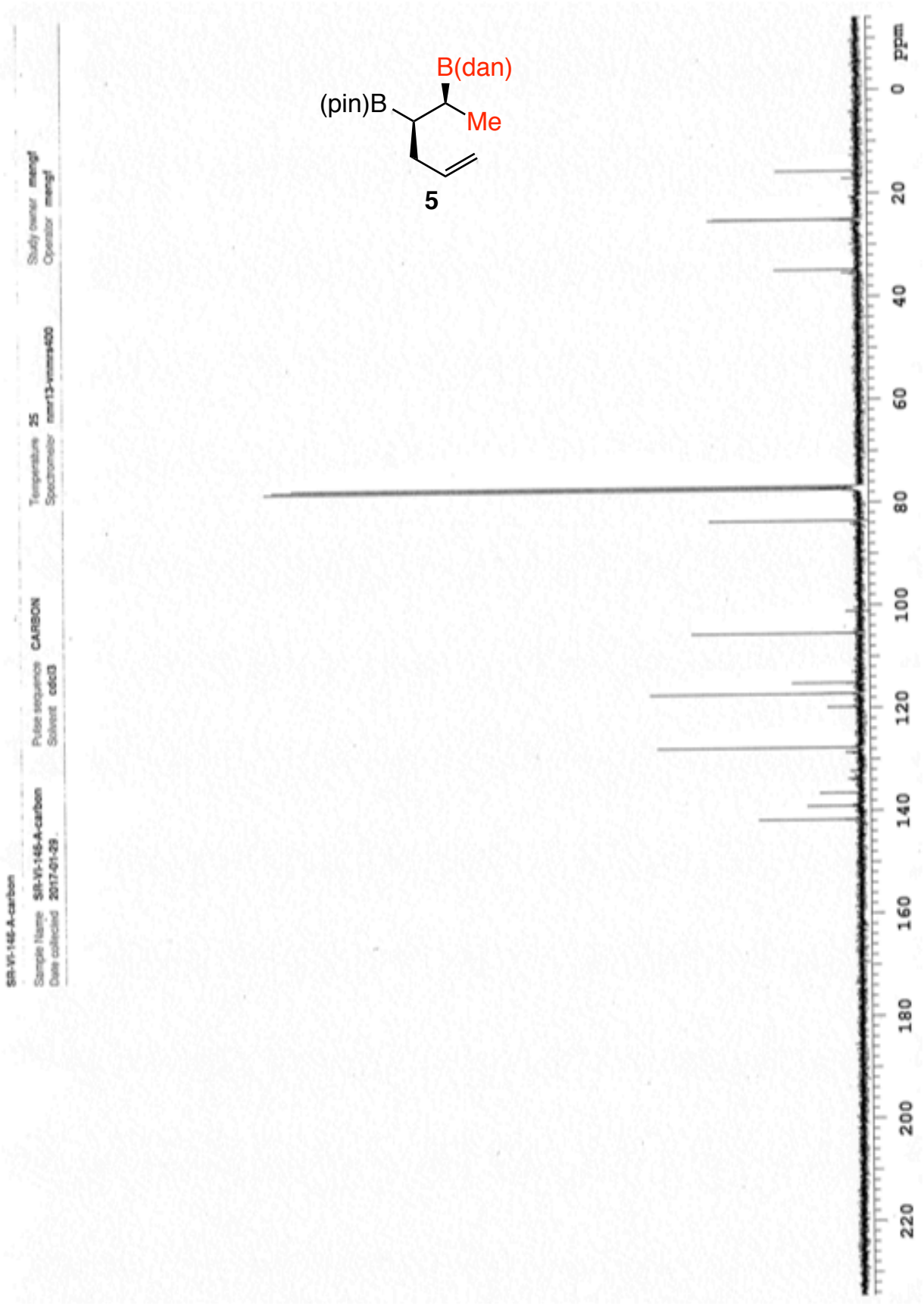

(pin)B
B(dan)
Br
1h
SR-V-297-C-f18-19
Sample Name SR-V-297-C-f18-19
Date collected 2016-11-11
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

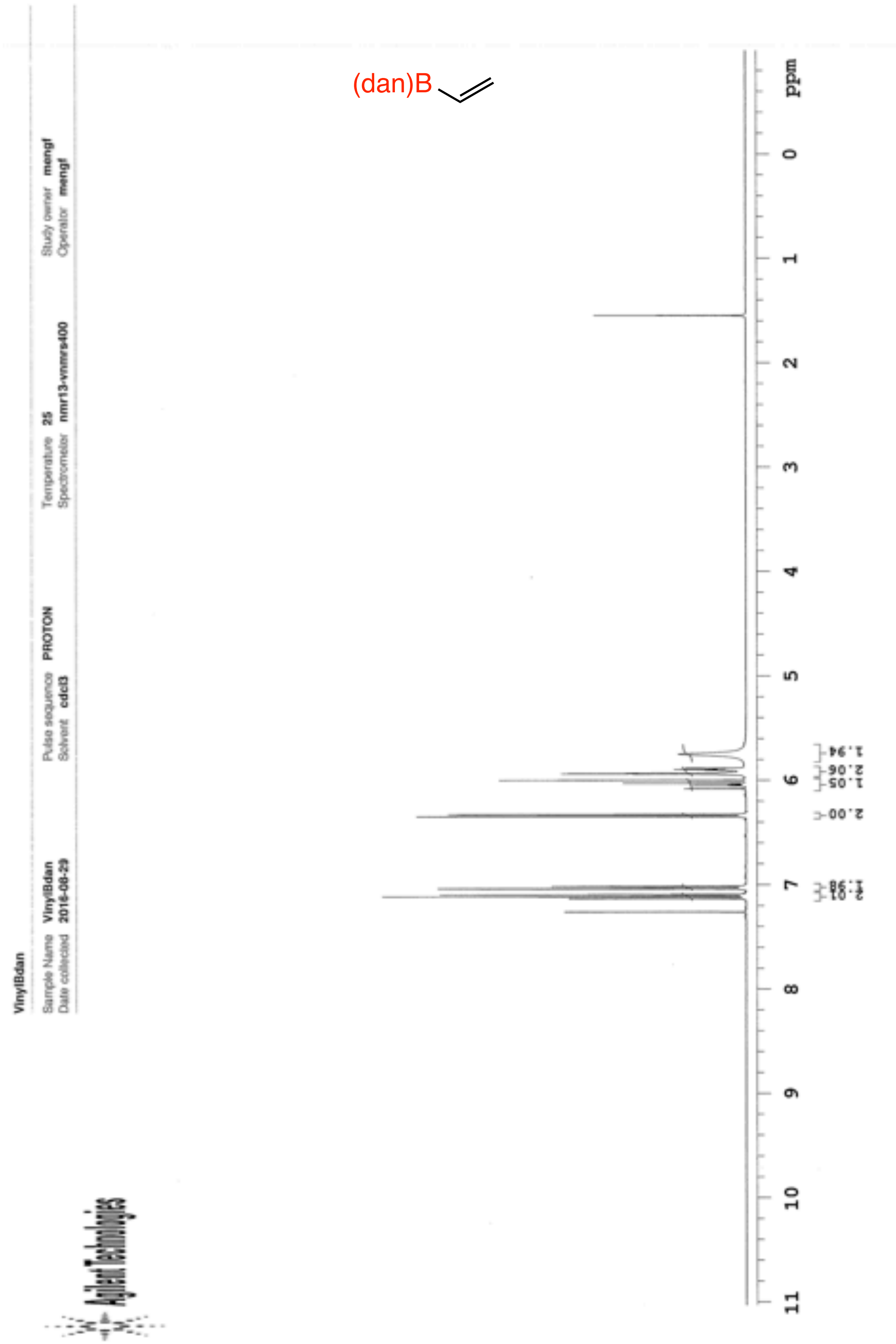

(pin)B
B(dan)
Br
1h
SR-V-297-2-carbon
Sample Name SR-V-297-2-carbon
Date collected 2016-11-11
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

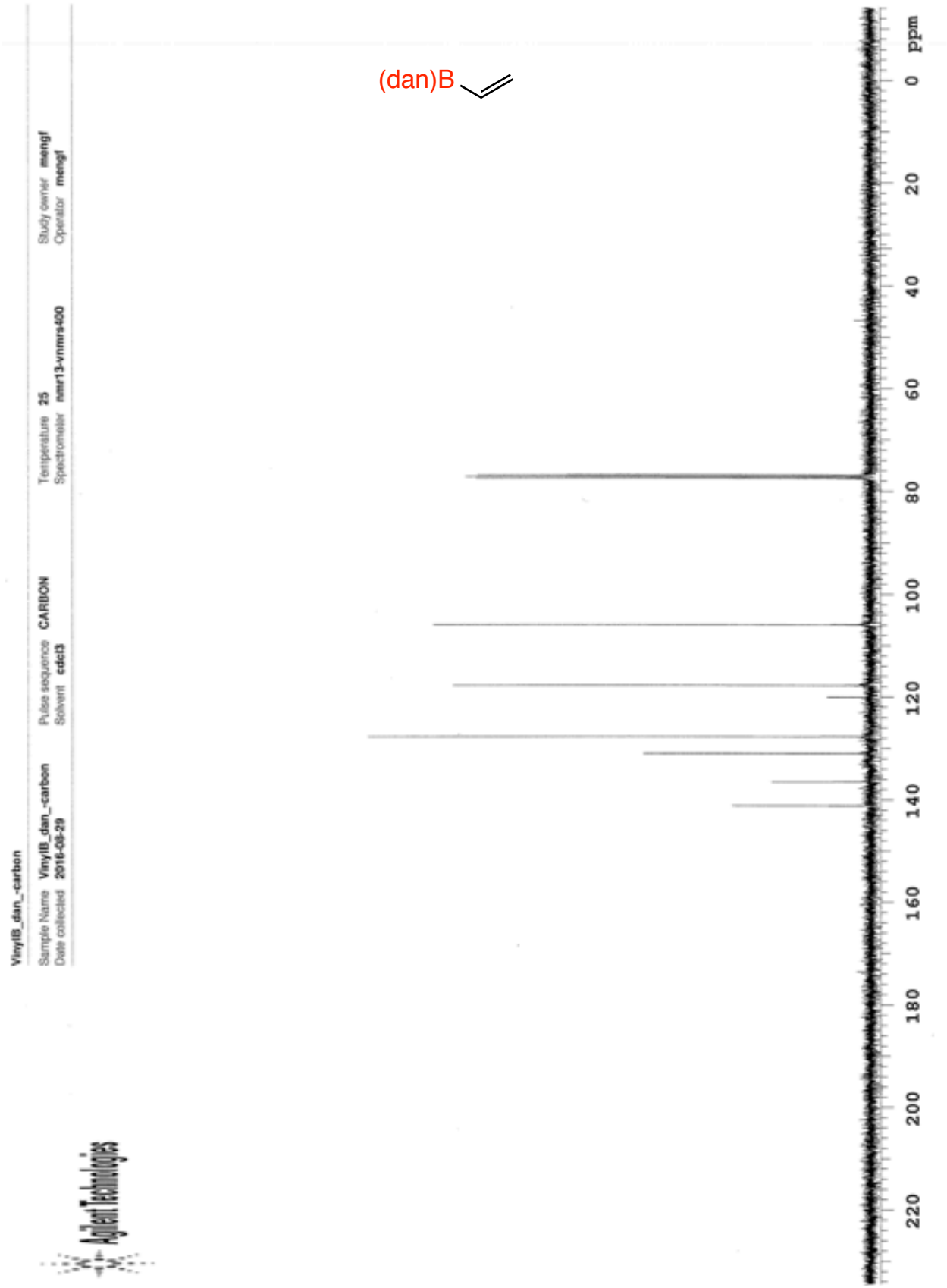

SR-VI-59-4h
Sample Name SR-VI-59-4h
Date collected 2016-08-09
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs400
Study owner Hoveyda
Operator Hoveyda
(pin)B
Me
B(dan)
3
ppm
1.01
2.98
12.09
2.08
2.02
1.00
1.89
1.97

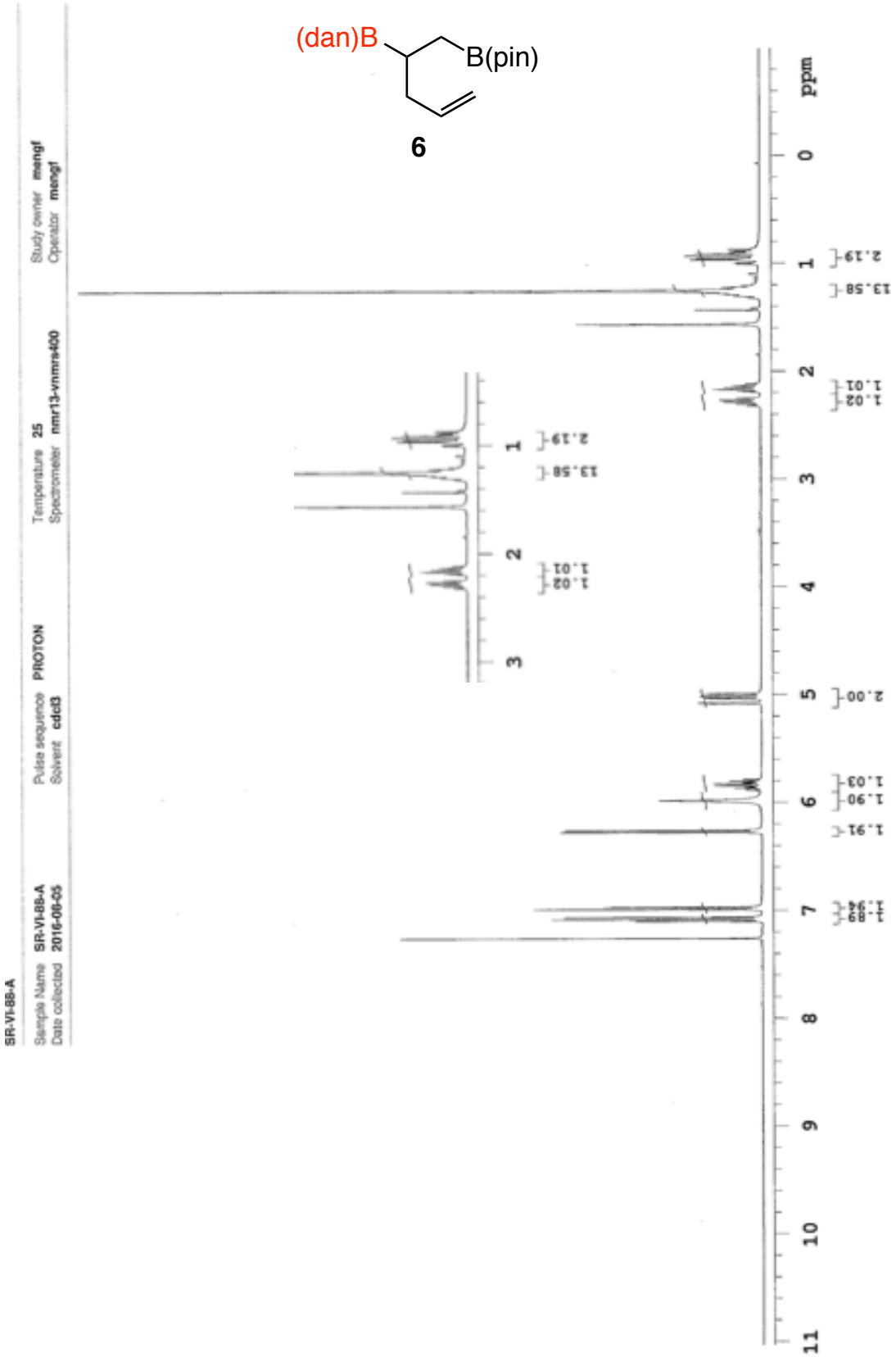

Sample Name
Date collected 2016-08-09
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
(pin)B
Me
B(dan)
3
0 ppm
20
40
60
80
100
120
140
160
180
200
220

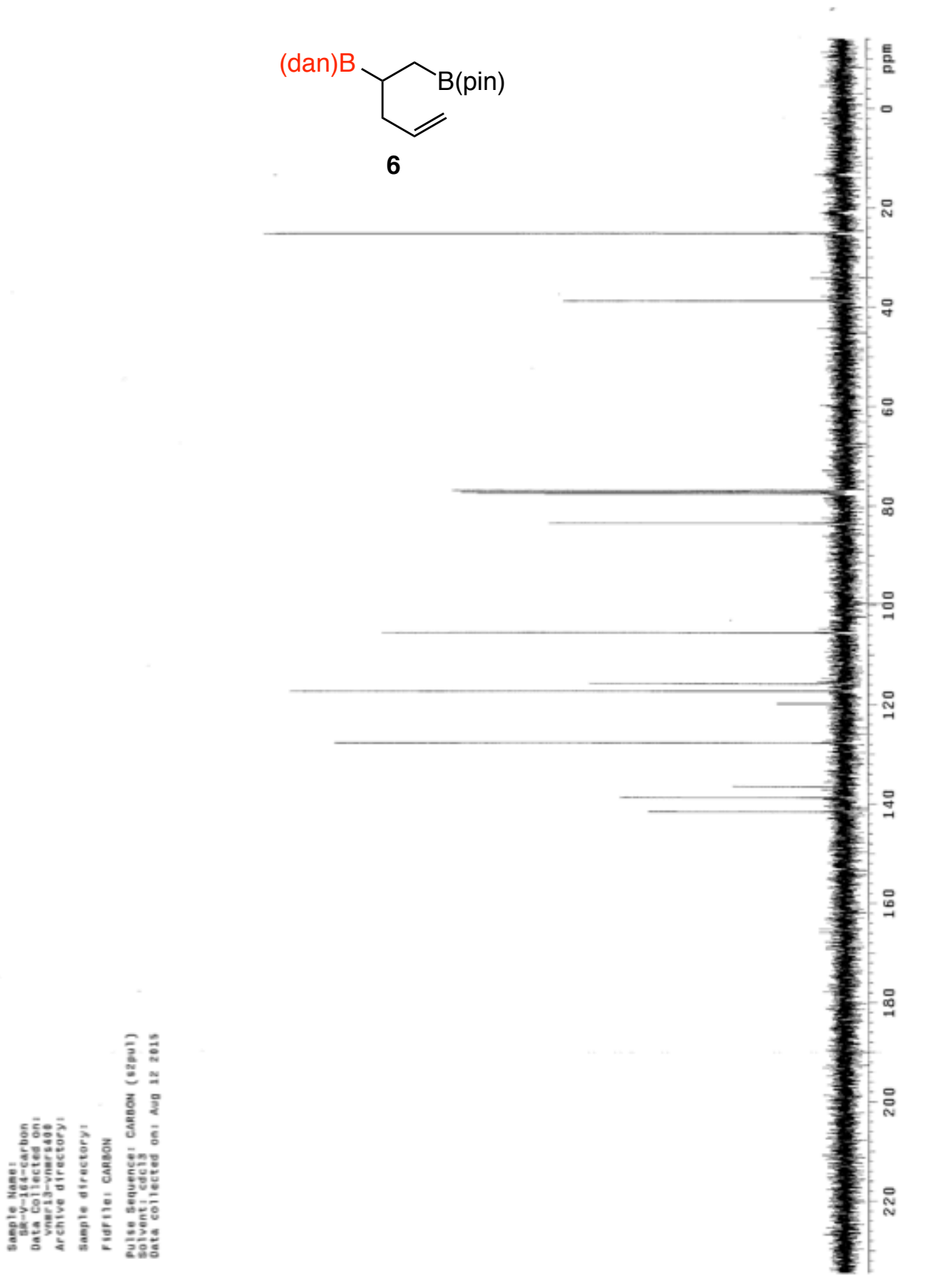

SR-VI-146-A-prep
Sample Name SR-VI-146-A-prep
Date collected 2017-01-24
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vmmrs400
Study owner Hoveyda
Operator Hoveyda
B(dan)
(pin)B
Me
5
ppm

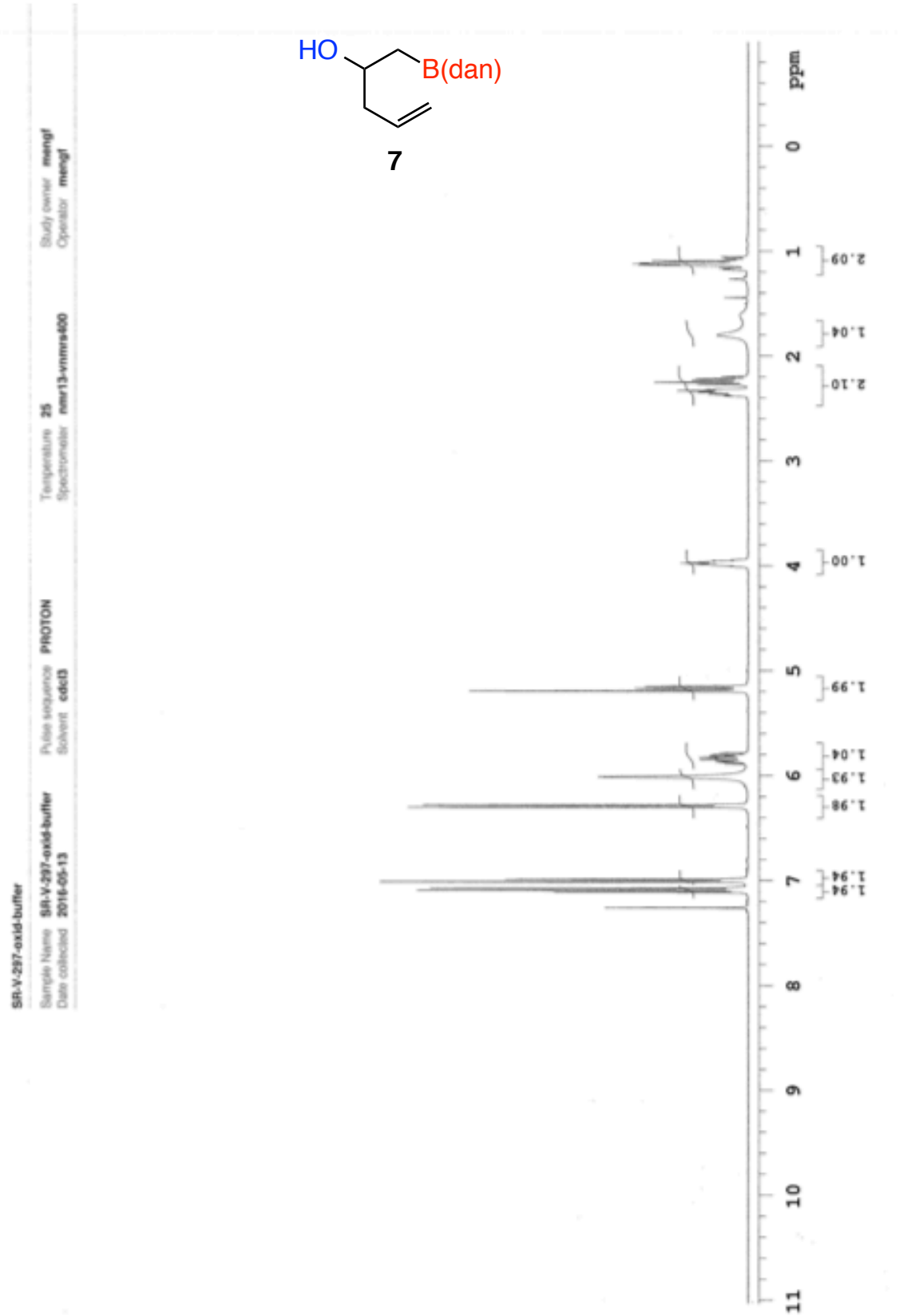

B(dan)
(pin)B
Me
5
SR-VI-146-A-carbon
Sample Name SR-VI-146-A-carbon
Date collected 2017-01-29
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

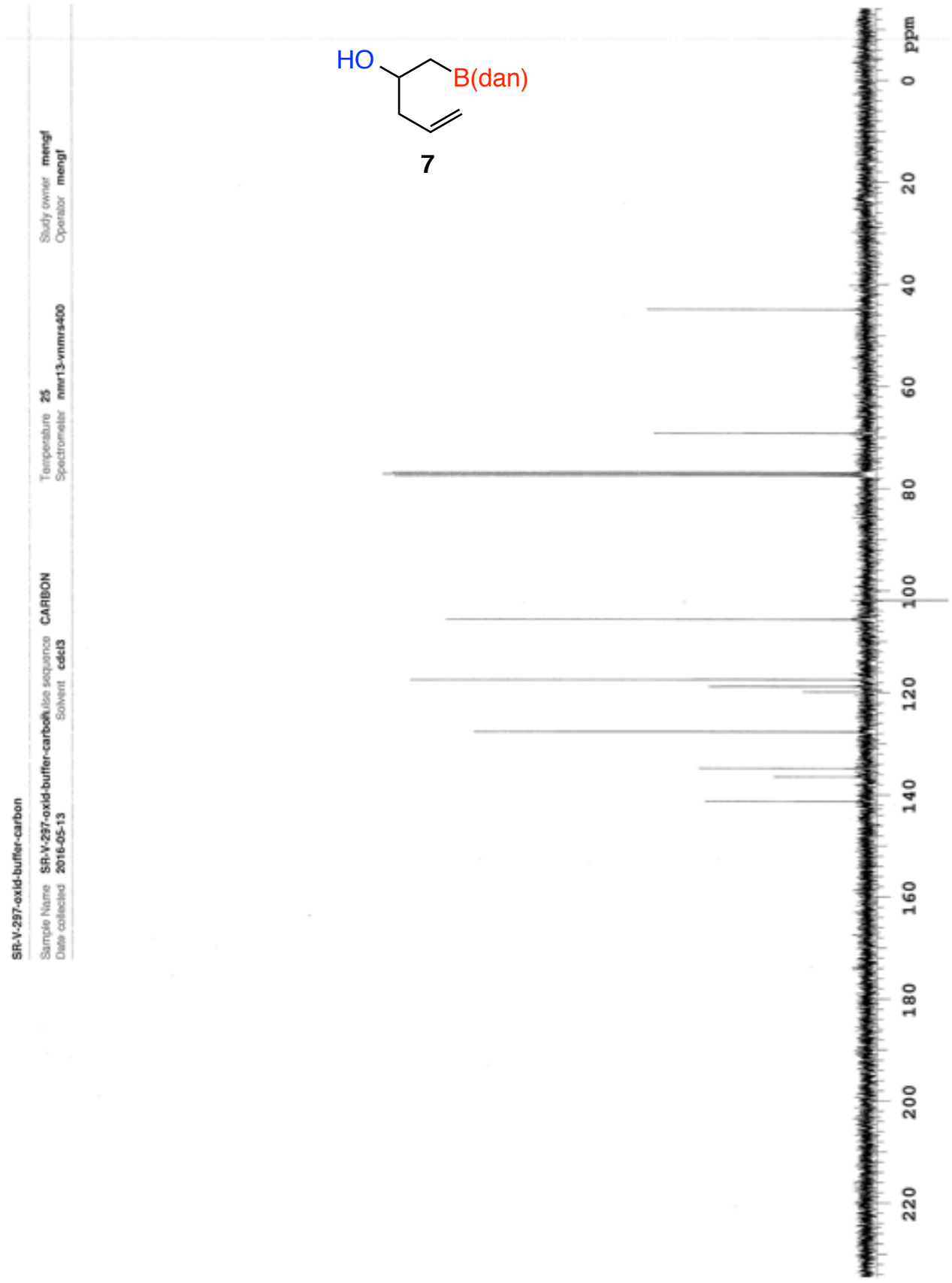

VinylBdan
Sample Name VinylBdan
Date collected 2016-08-29
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
(dan)B
ppm
0
1
2
3
4
5
6
7
8
9
10
11
1.94
2.06
1.05
2.00
1.98
2.01

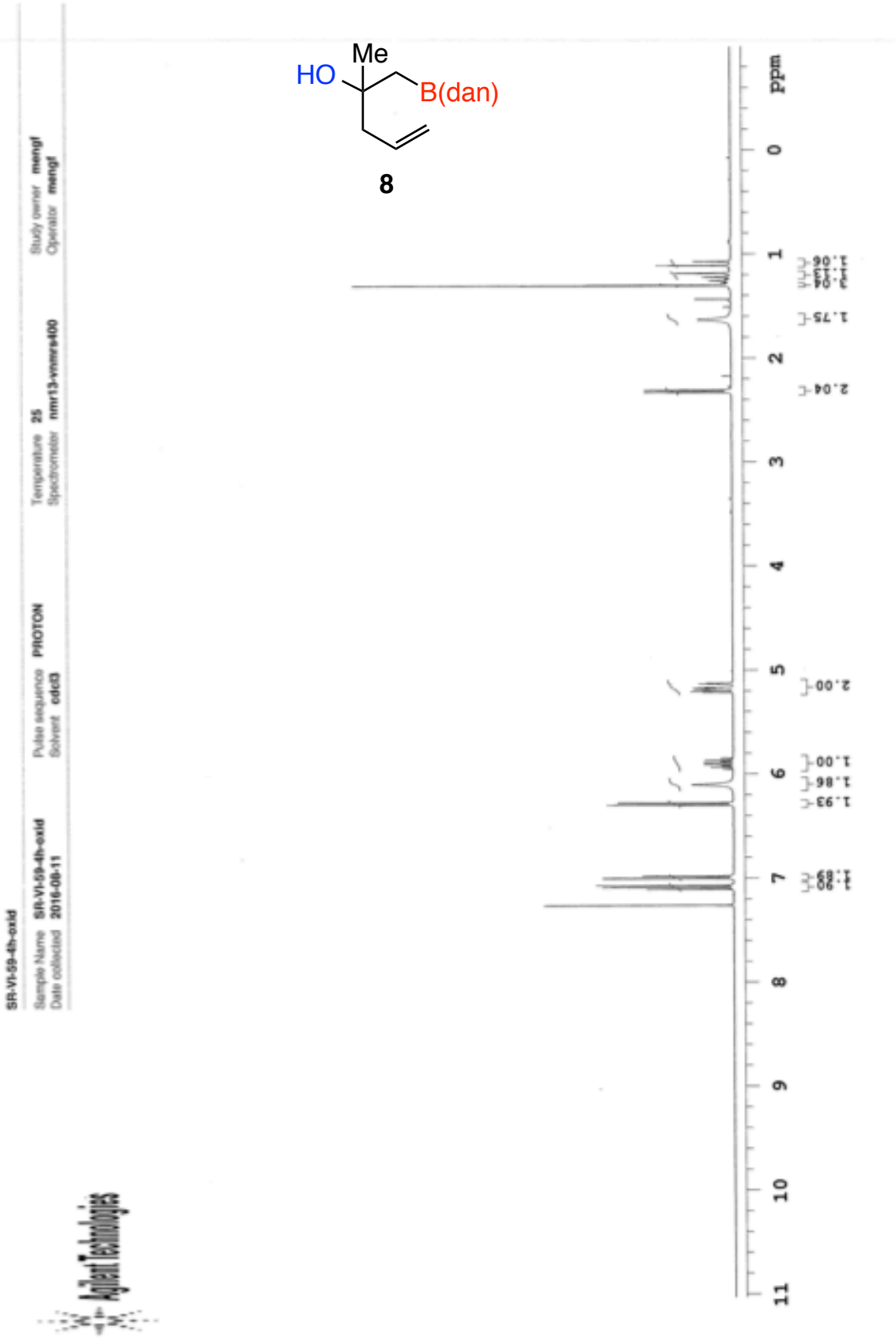

VinylB_dan_-carbon
Sample Name VinylB_dan_-carbon
Date collected 2016-08-29
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
(dan)B
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Agilent Technologies

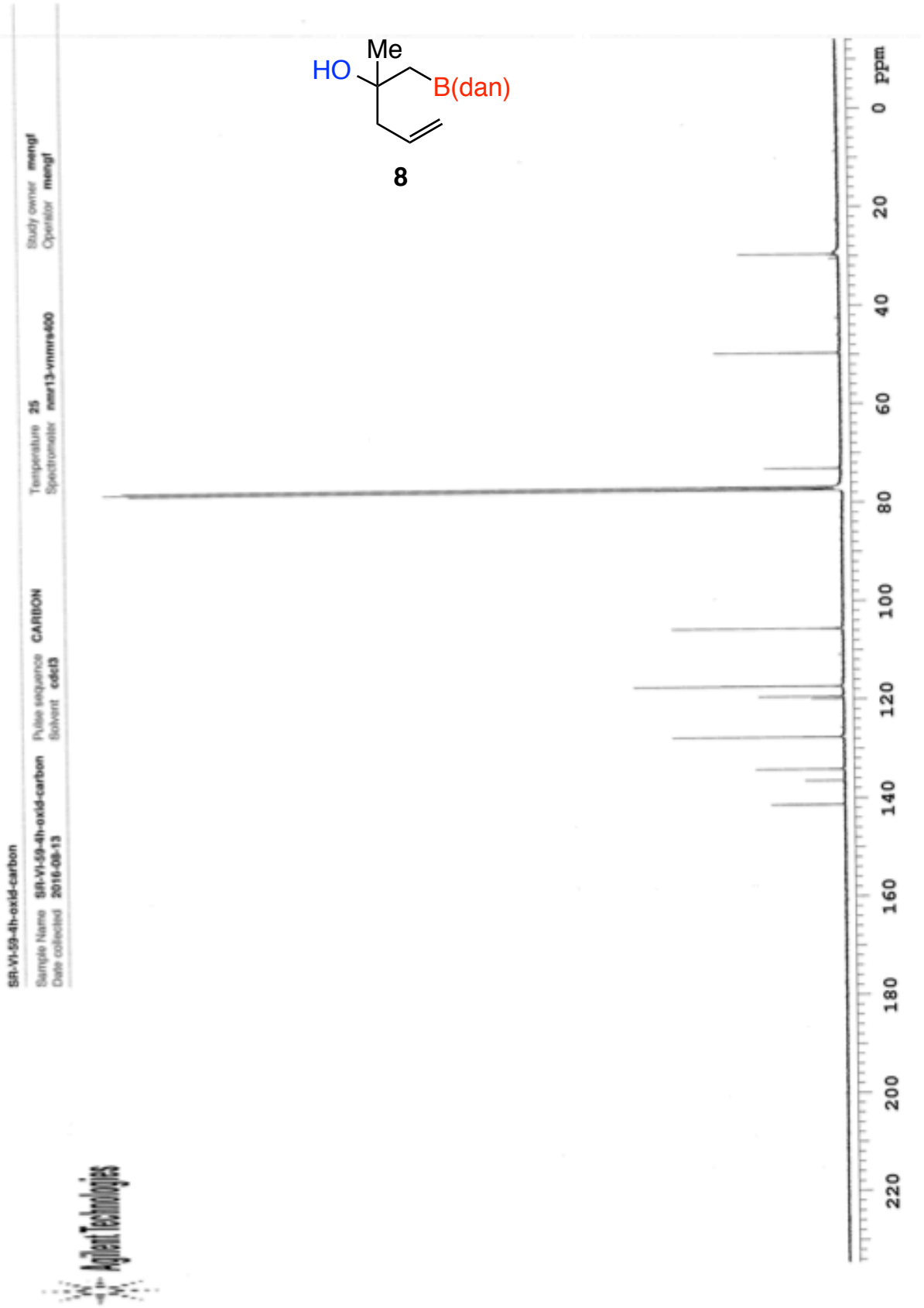

(dan)B
B(pin)
6
SR-VI-88-A
Sample Name SR-VI-88-A
Date collected 2016-06-05
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.19
13.58
1.01
1.02
2.00
1.03
1.90
1.91
1.89
1.96

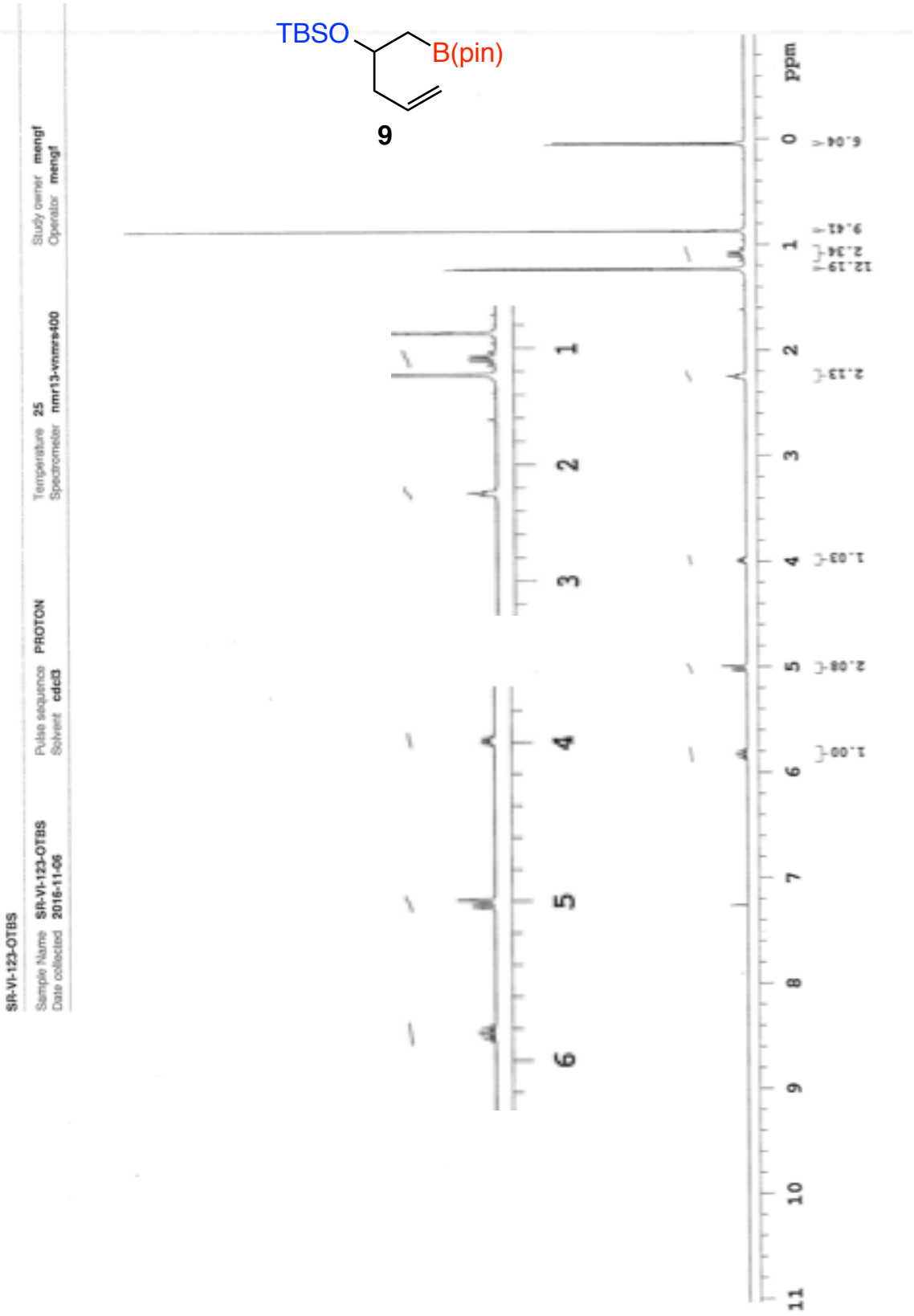

(dan)B
B(pin)
6
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Sample Name:
SR-V-164-carbon
Data Collected on:
vnmr13-vnmr400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 12 2015

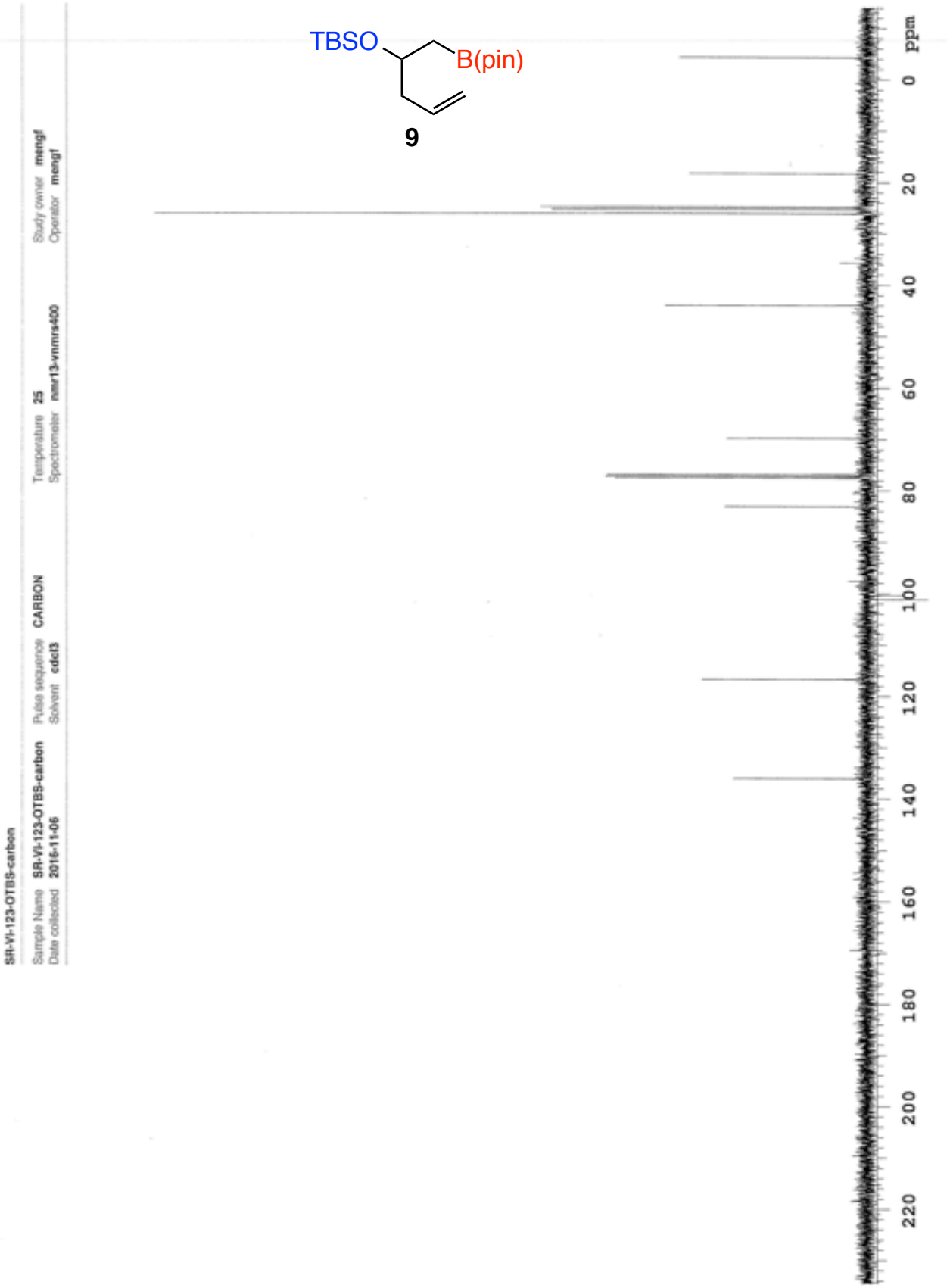

SR-V-297-oxid-buffer
Sample Name SR-V-297-oxid-buffer
Date collected 2016-05-13
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
HO
B(dan)
7
ppm
0
1
2
3
4
5
6
7
8
9
10
11
2.09
1.04
2.10
1.00
1.99
1.04
1.93
1.98
1.94
1.94

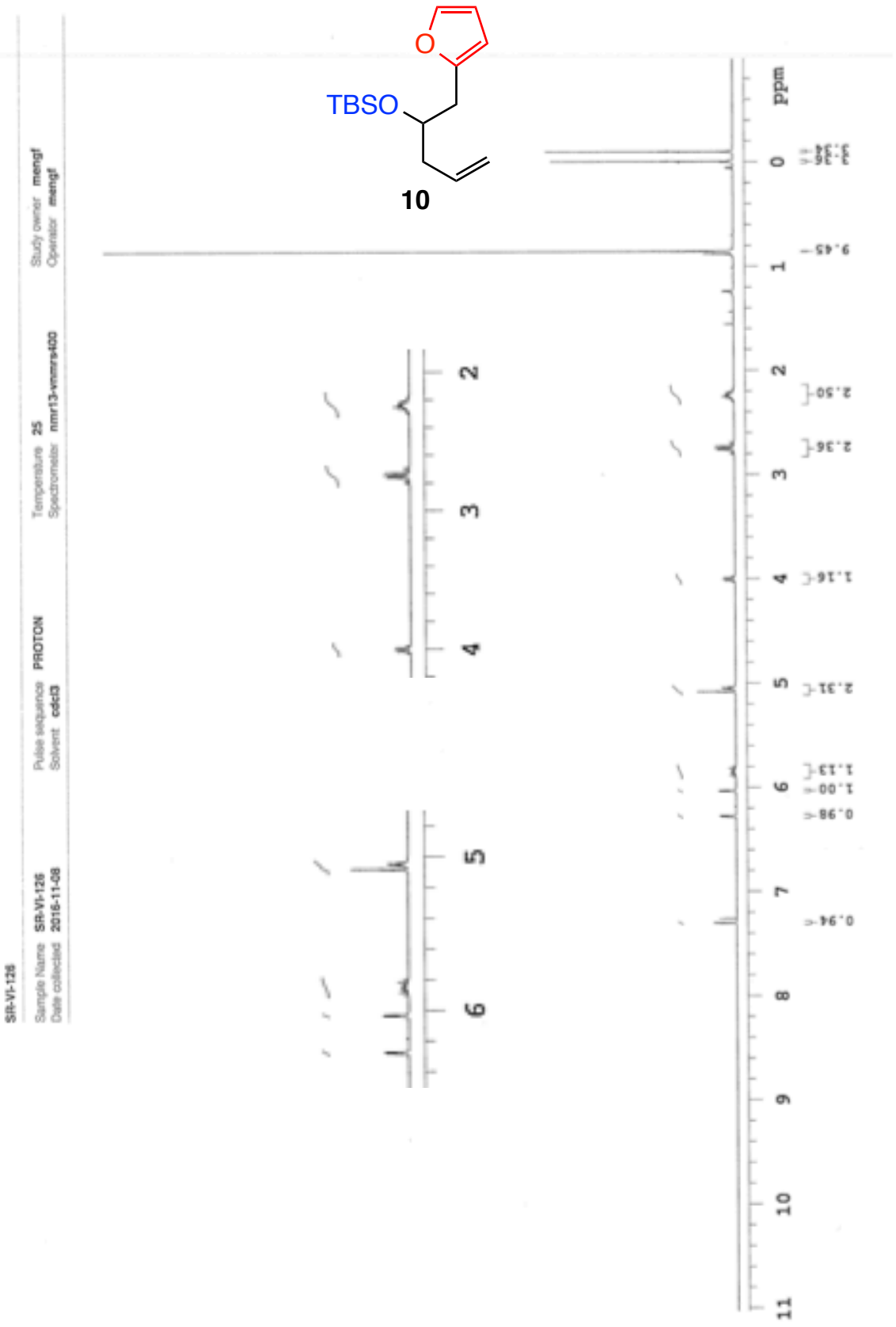

HO
B(dan)
7
SR-V-297-oxid-buffer-carbon
Sample Name SR-V-297-oxid-buffer-carbon
Date collected 2016-05-13
Use sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

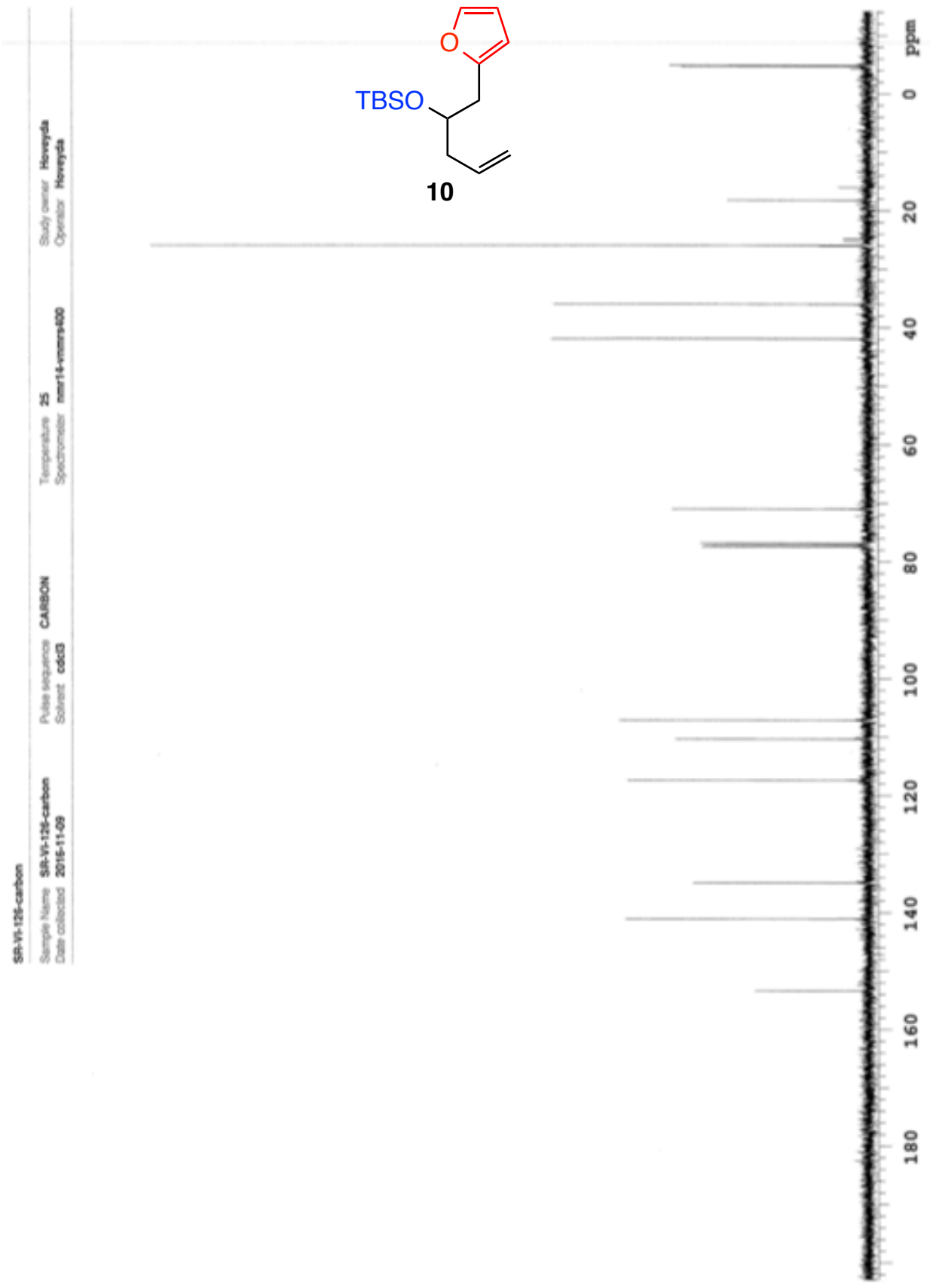

Me
HO
B(dan)
8
SR-VI-59-4h-exid
Sample Name SR-VI-59-4h-exid
Date collected 2016-08-11
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
1.06
1.75
2.04
2.00
1.00
1.86
1.93
1.00
Agilent Technologies

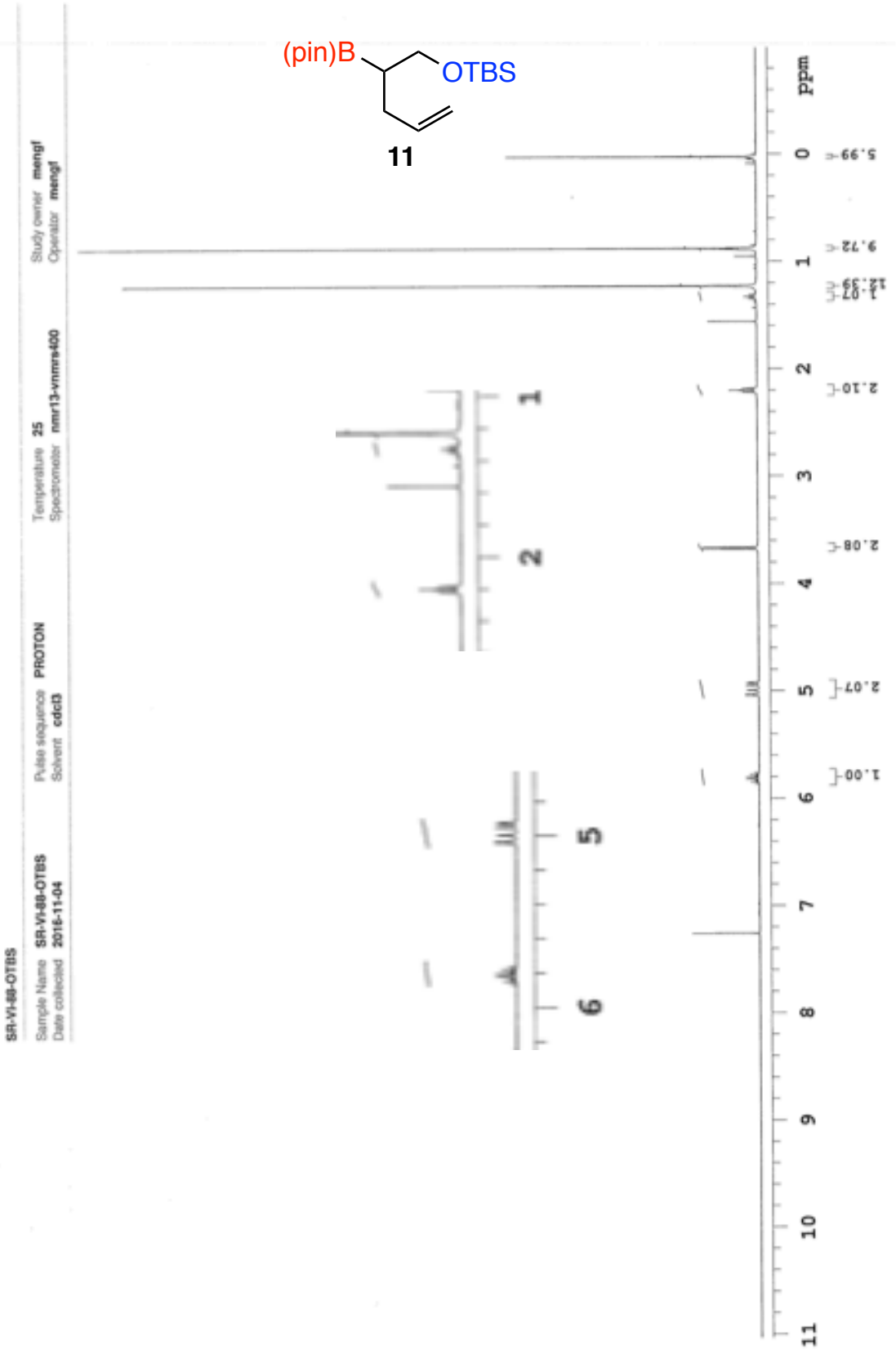

Me
HO
B(dan)
8
SR-VI-59-4h-oxid-carbon
Sample Name SR-VI-59-4h-oxid-carbon
Date collected 2016-08-13
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
220
200
180
160
140
120
100
80
60
40
20
0 ppm

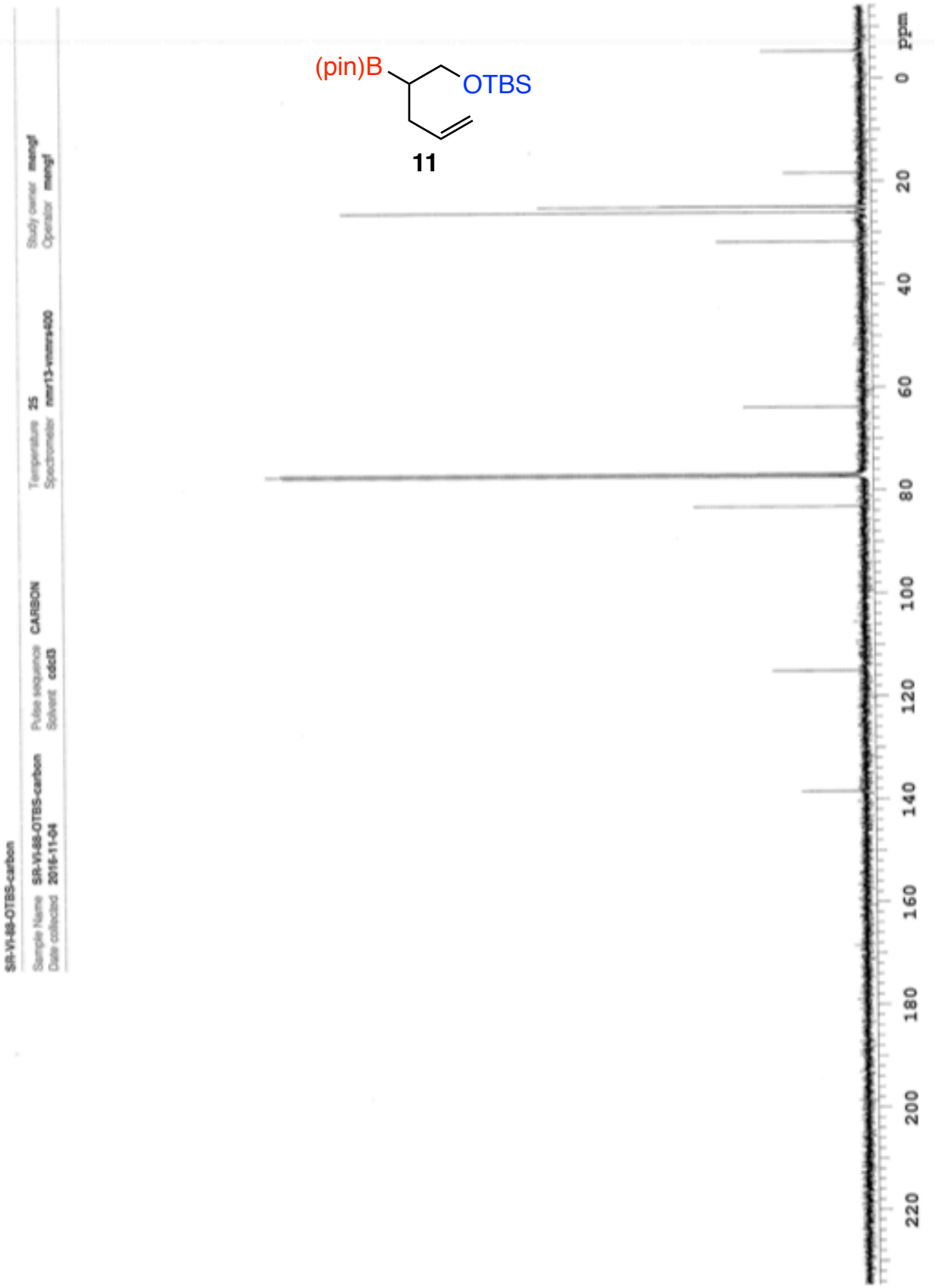

TBSO
B(pin)
9
SR-VI-123-OTBS
Sample Name SR-VI-123-OTBS
Date collected 2016-11-06
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
6.04
9.41
2.34
12.19
2.13
1.03
2.08
1.00

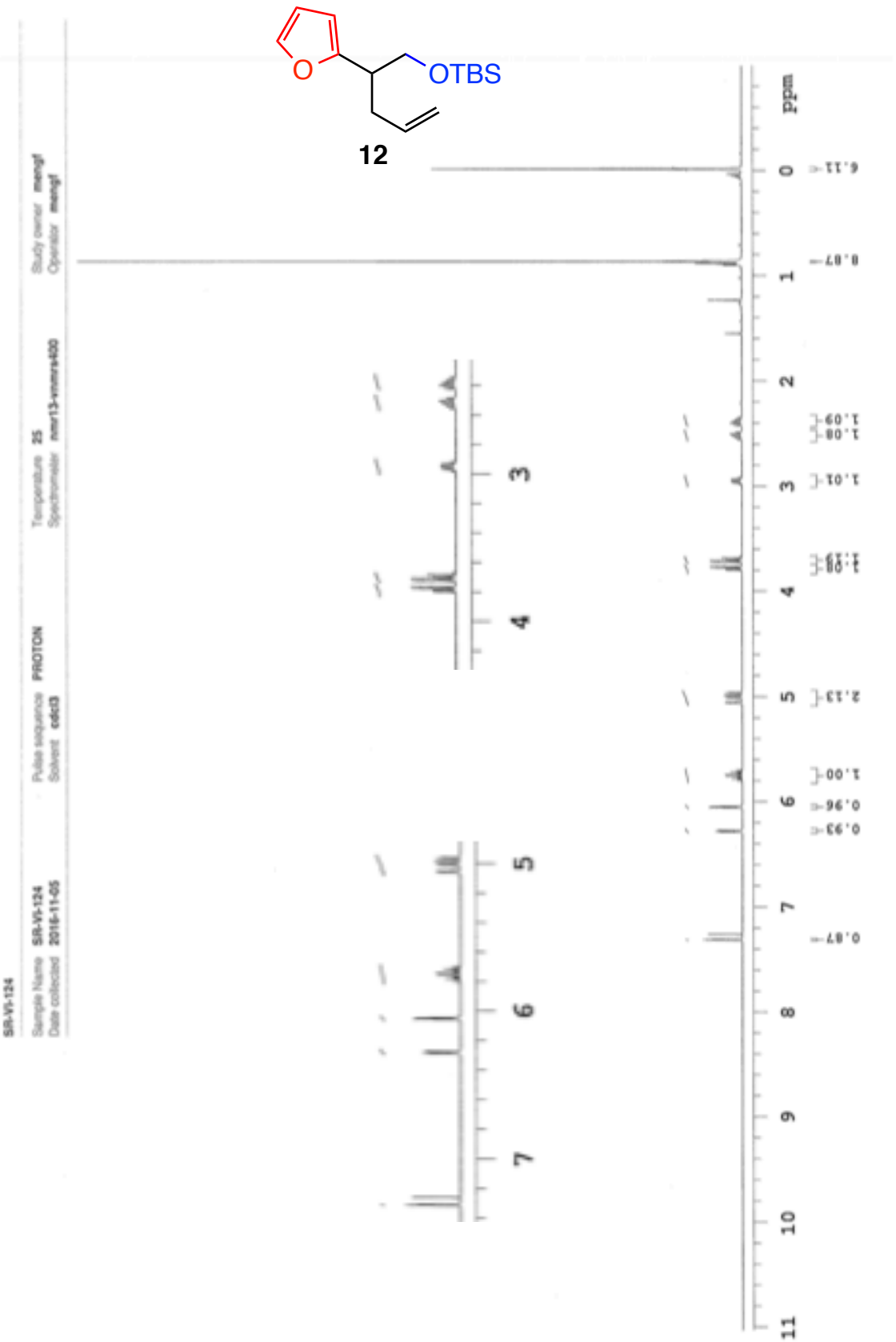

SR-VI-123-OTBS-carbon
Sample Name SR-VI-123-OTBS-carbon
Date collected 2016-11-06
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
TBSO
B(pin)
9
ppm
0
20
40
60
80
100
120
140
160
180
200
220

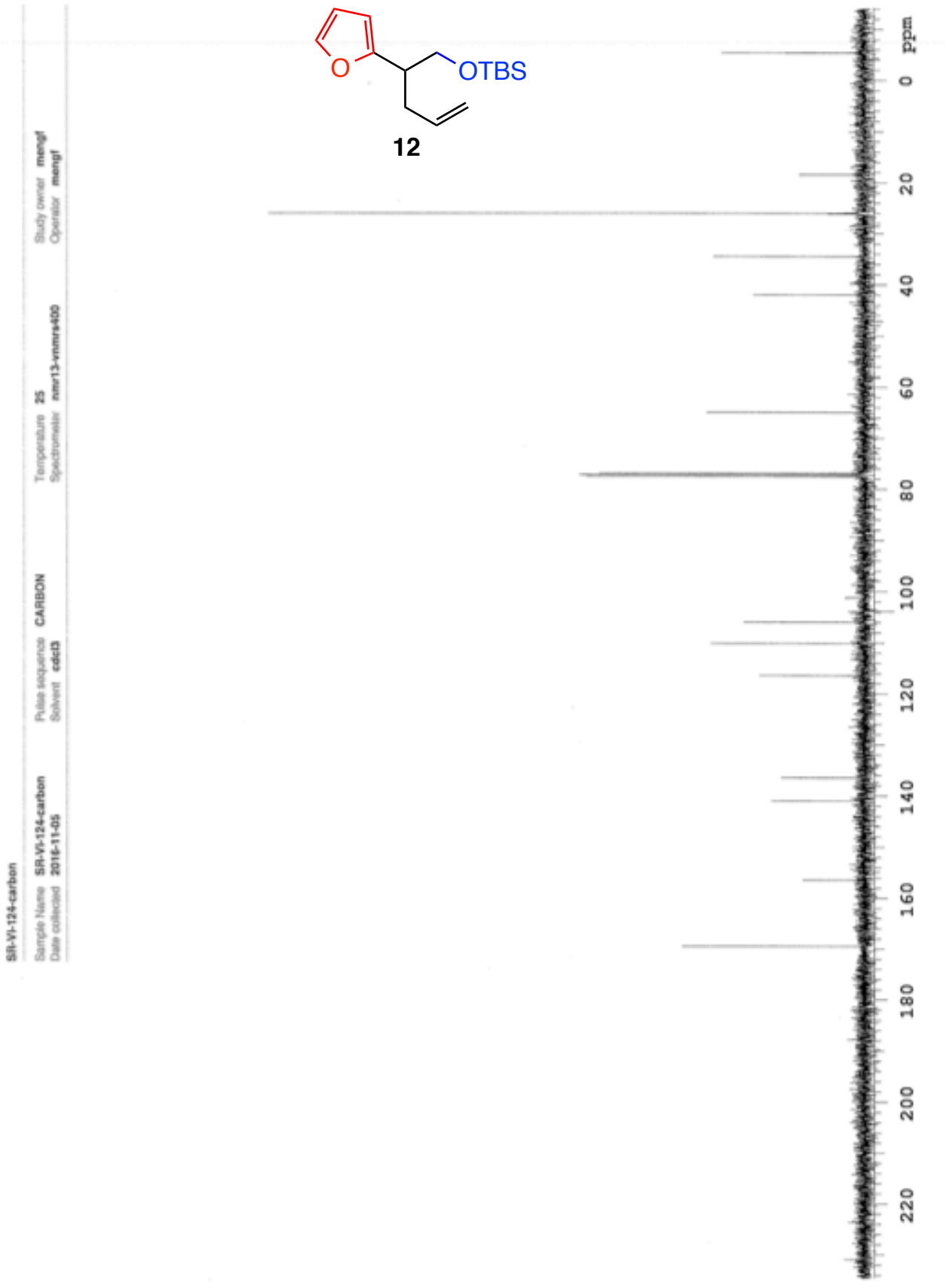

TBSO
O
10
SR-VI-126
Sample Name SR-VI-126
Date collected 2016-11-08
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

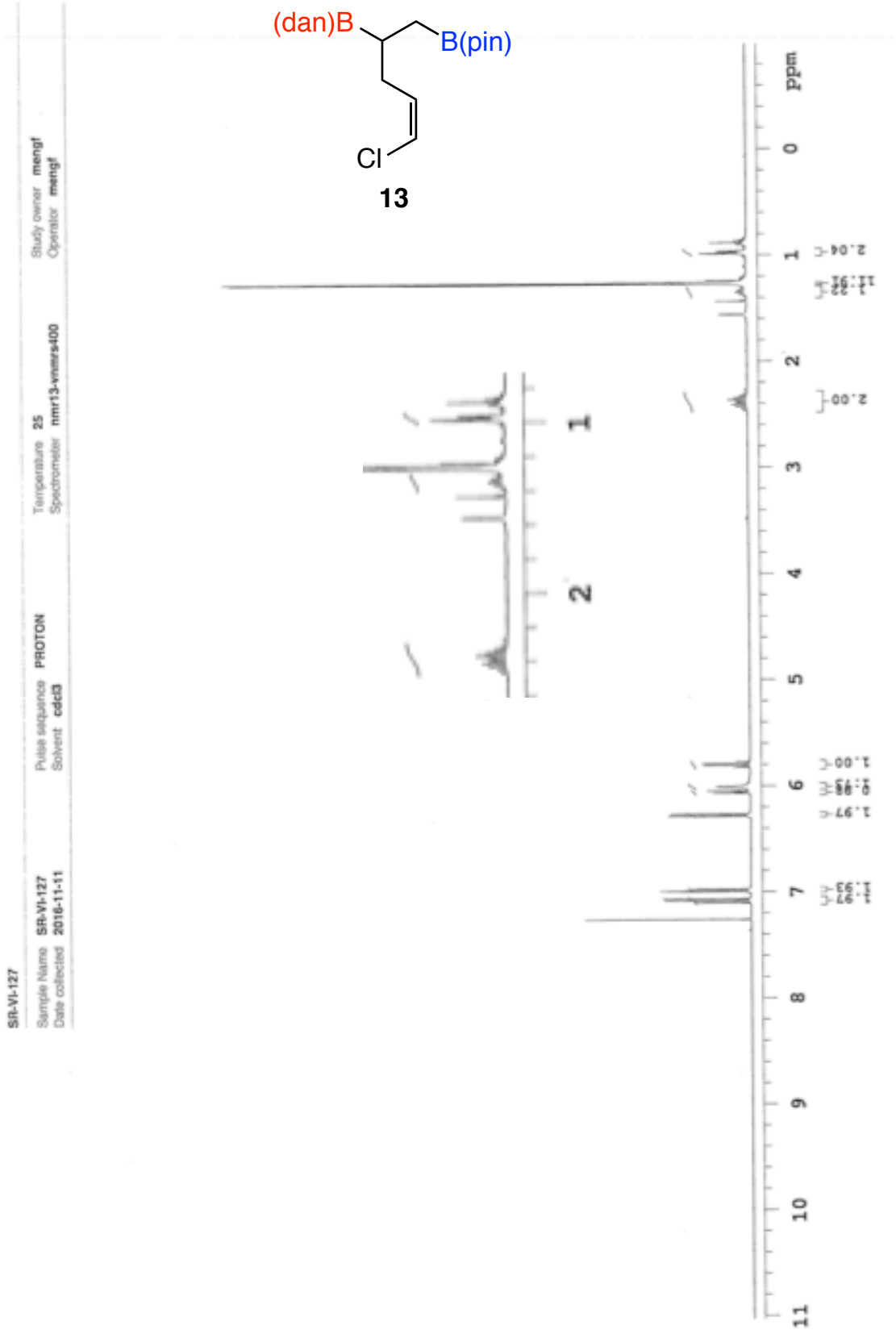

SR-VI-126-carbon
Sample Name SR-VI-126-carbon
Date collected 2016-11-09
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs600
Study owner Hoveyda
Operator Hoveyda
O
TBSO
10
ppm
0
20
40
60
80
100
120
140
160
180

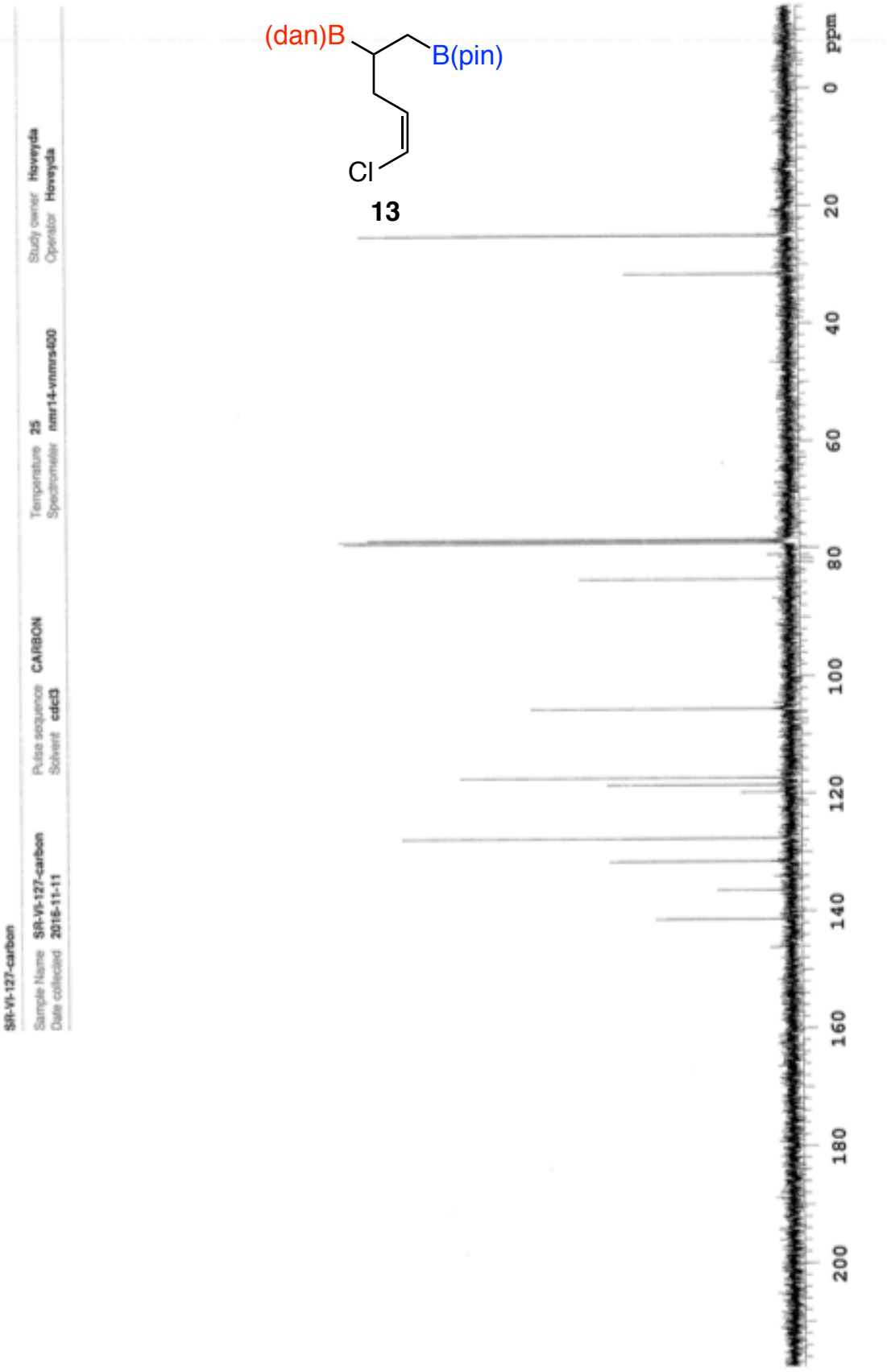

(pin)B
OTBS
11
SR-VI-88-OTBS
Sample Name SR-VI-88-OTBS
Date collected 2016-11-04
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
5.99
9.72
12.39
1.07
2.10
2.08
2.07
1.00

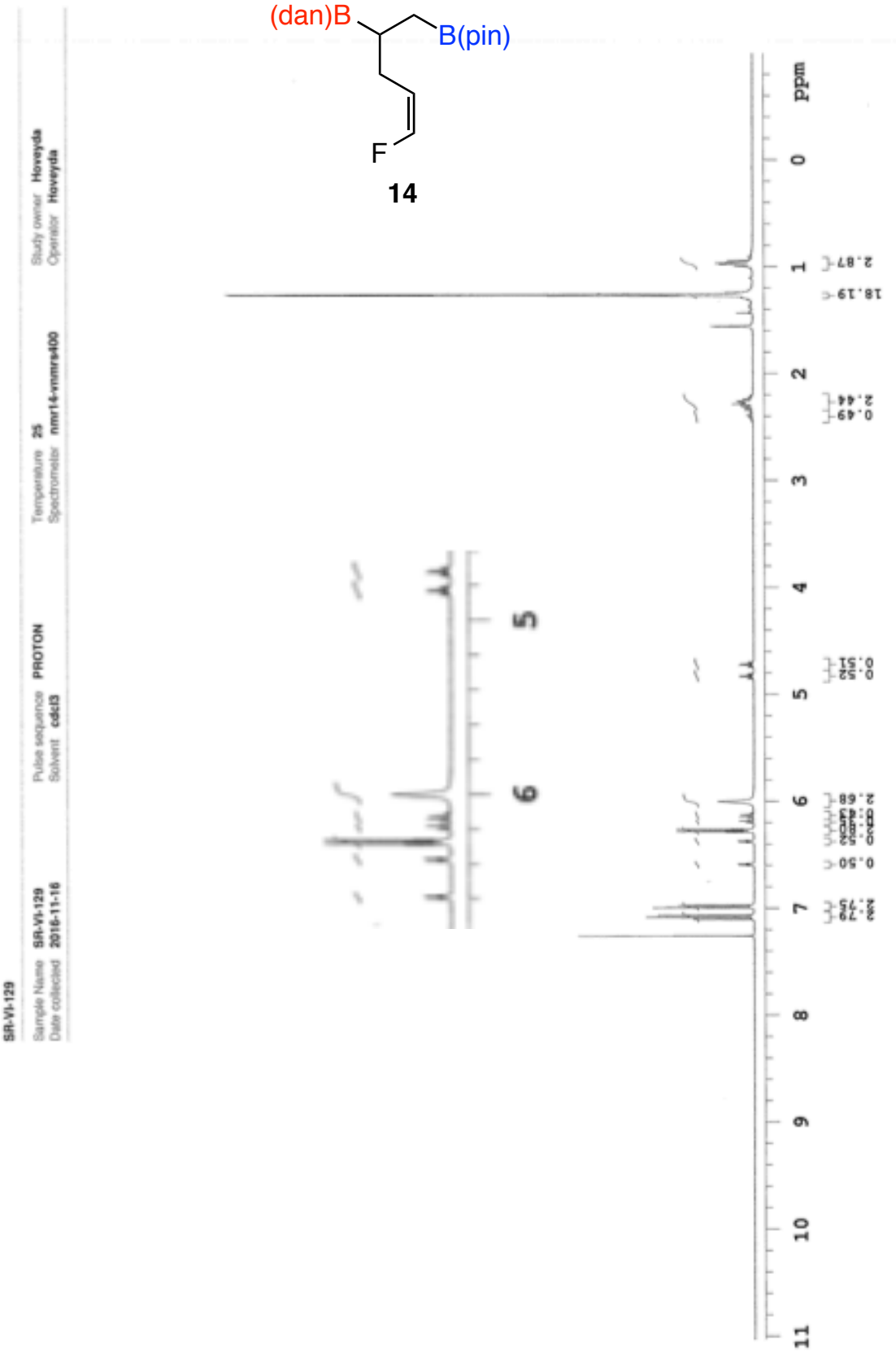

(pin)B
OTBS
11
$R-VI-88-OTBS-carbon
Sample Name SR-VI-88-OTBS-carbon
Date collected 2016-11-04
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

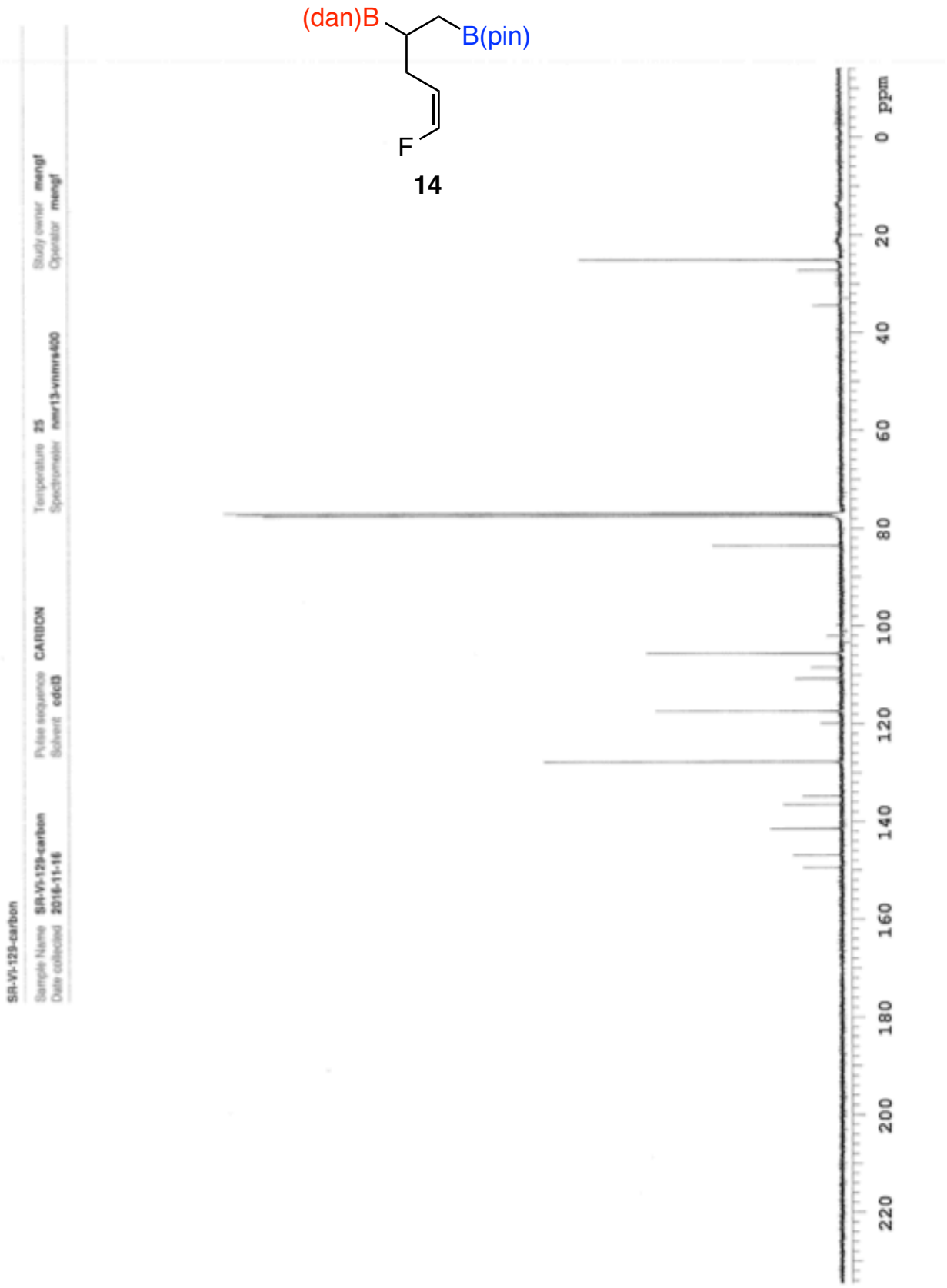

O
OTBS
12
SR-VI-124
Sample Name SR-VI-124
Date collected 2016-11-05
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mangf
Operator mangf
ppm
6.11
8.87
1.09
1.08
1.01
1.29
1.28
2.13
1.00
0.96
0.93
0.87

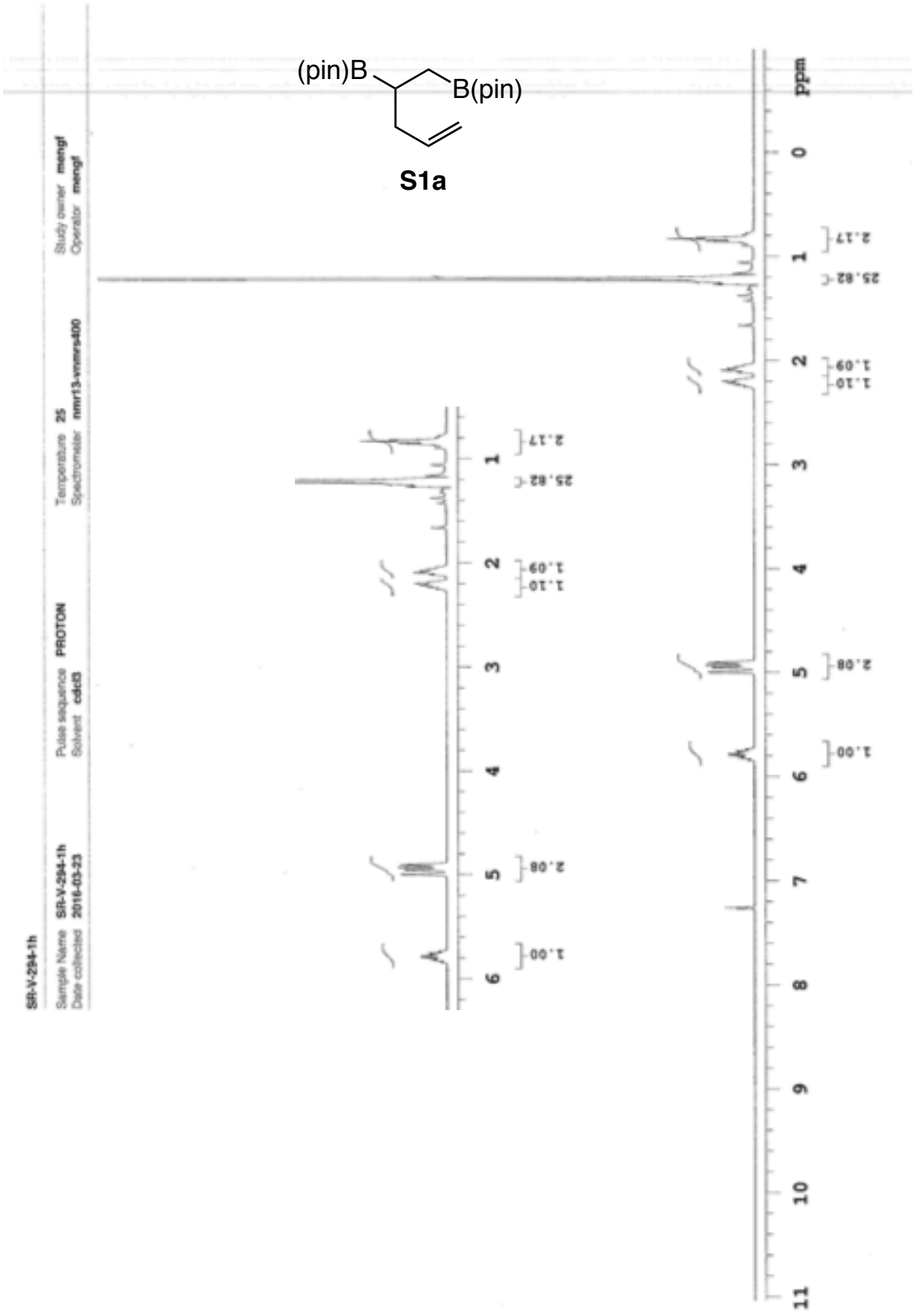

SR-VI-124-carbon
Sample Name SR-VI-124-carbon
Date collected 2016-11-05
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
O
OTBS
12
ppm
0
20
40
60
80
100
120
140
160
180
200
220

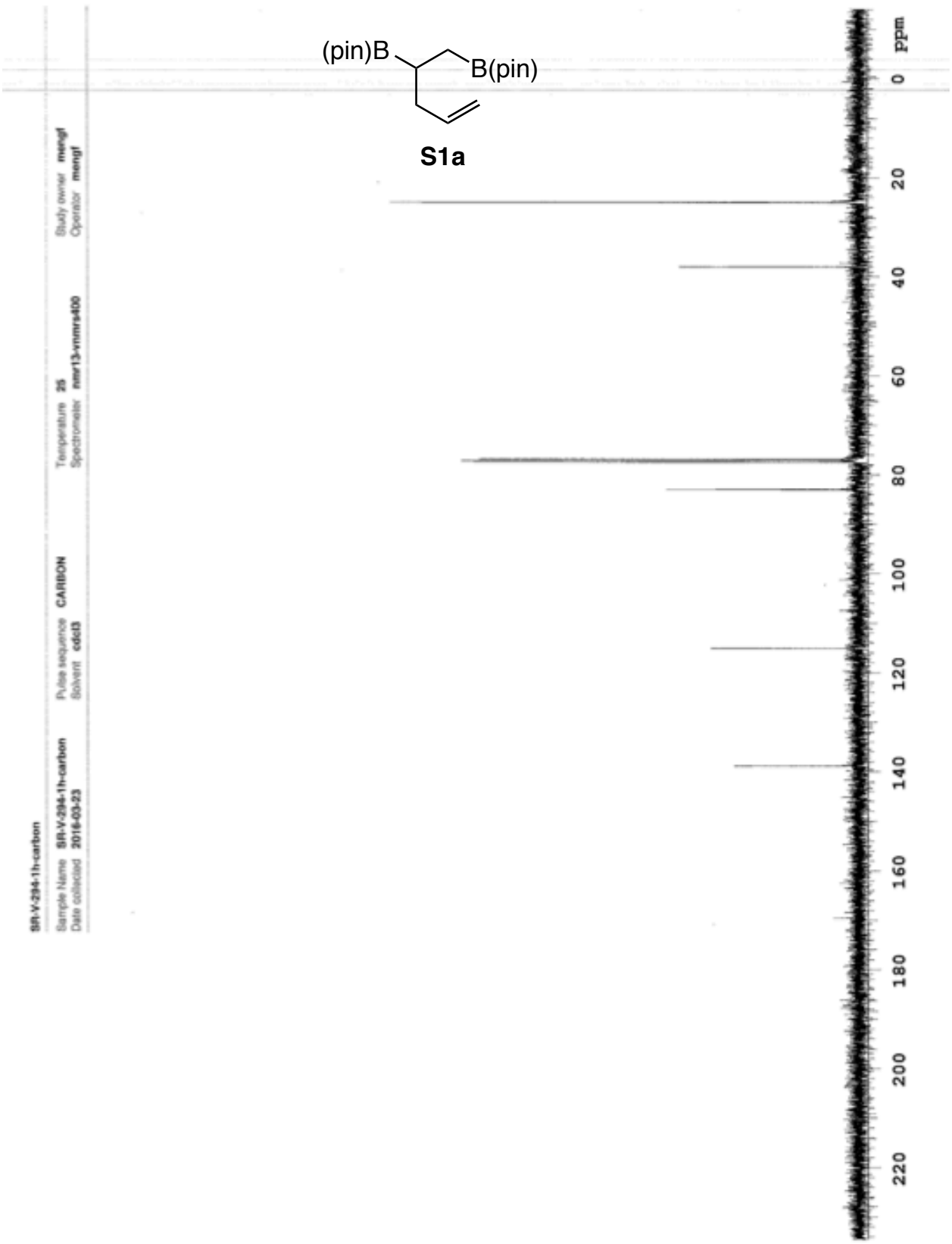

(dan)B
B(pin)
Cl
13
SR-VI-127
Sample Name SR-VI-127
Date collected 2016-11-11
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

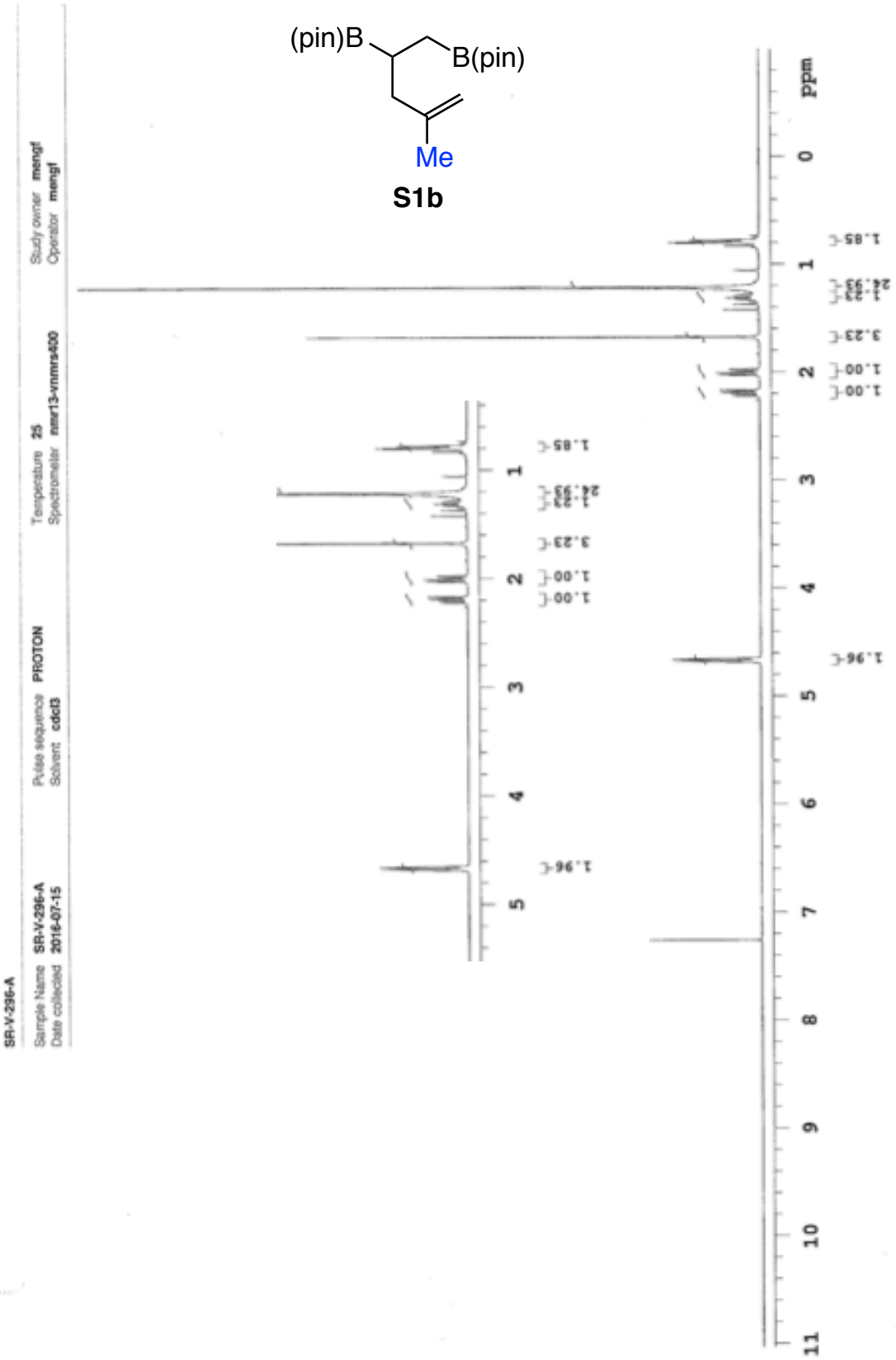

SR-VI-127-carbon
Sample Name SR-VI-127-carbon
Date collected 2016-11-11
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs400
Study owner Hoveyda
Operator Hoveyda
(dan)B
B(pin)
Cl
13
ppm
0
20
40
60
80
100
120
140
160
180
200

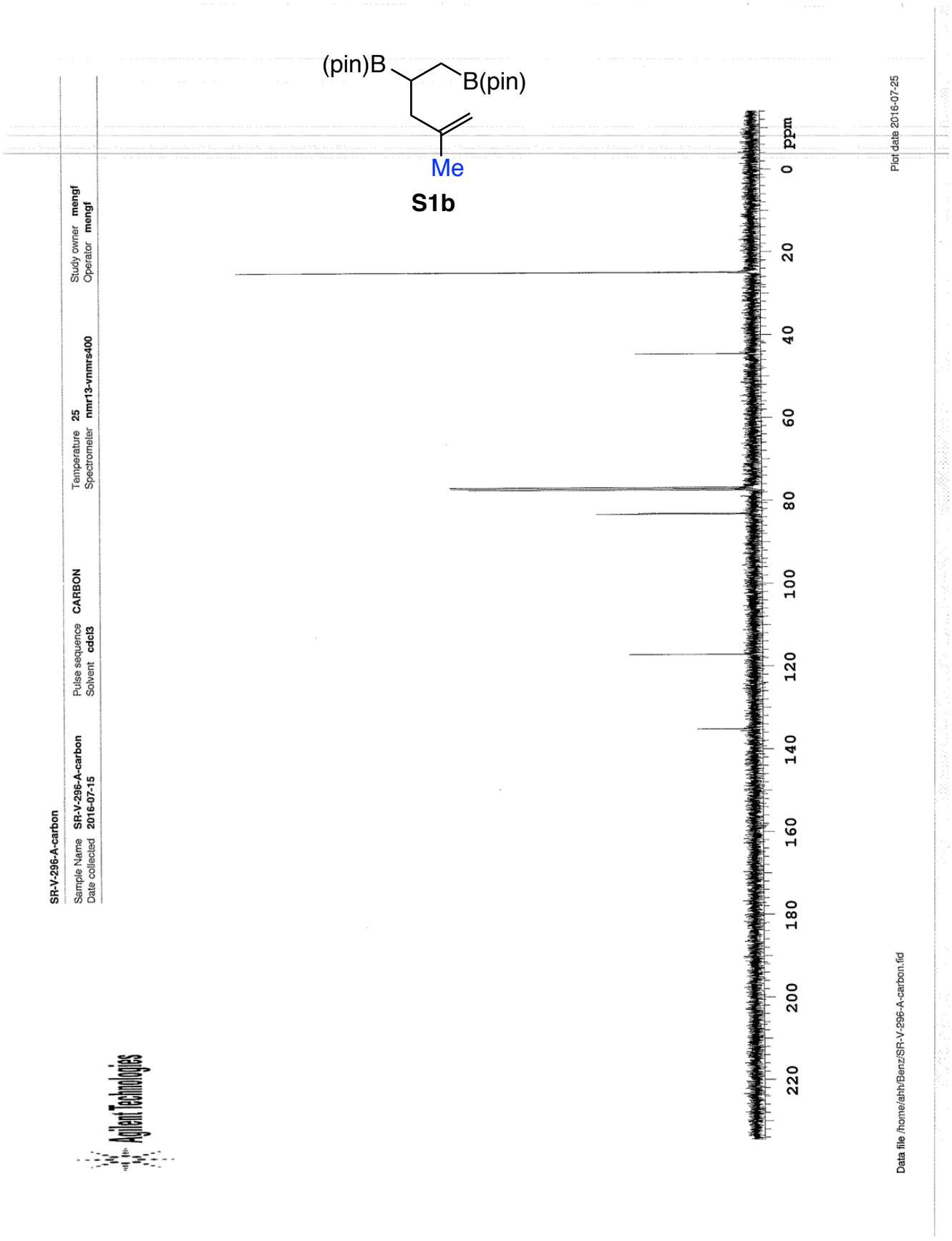

(dan)B
B(pin)
F
14
SR-VI-129
Sample Name SR-VI-129
Date collected 2016-11-16
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr14-vnmrs400
Study owner Hoveyda
Operator Hoveyda
ppm

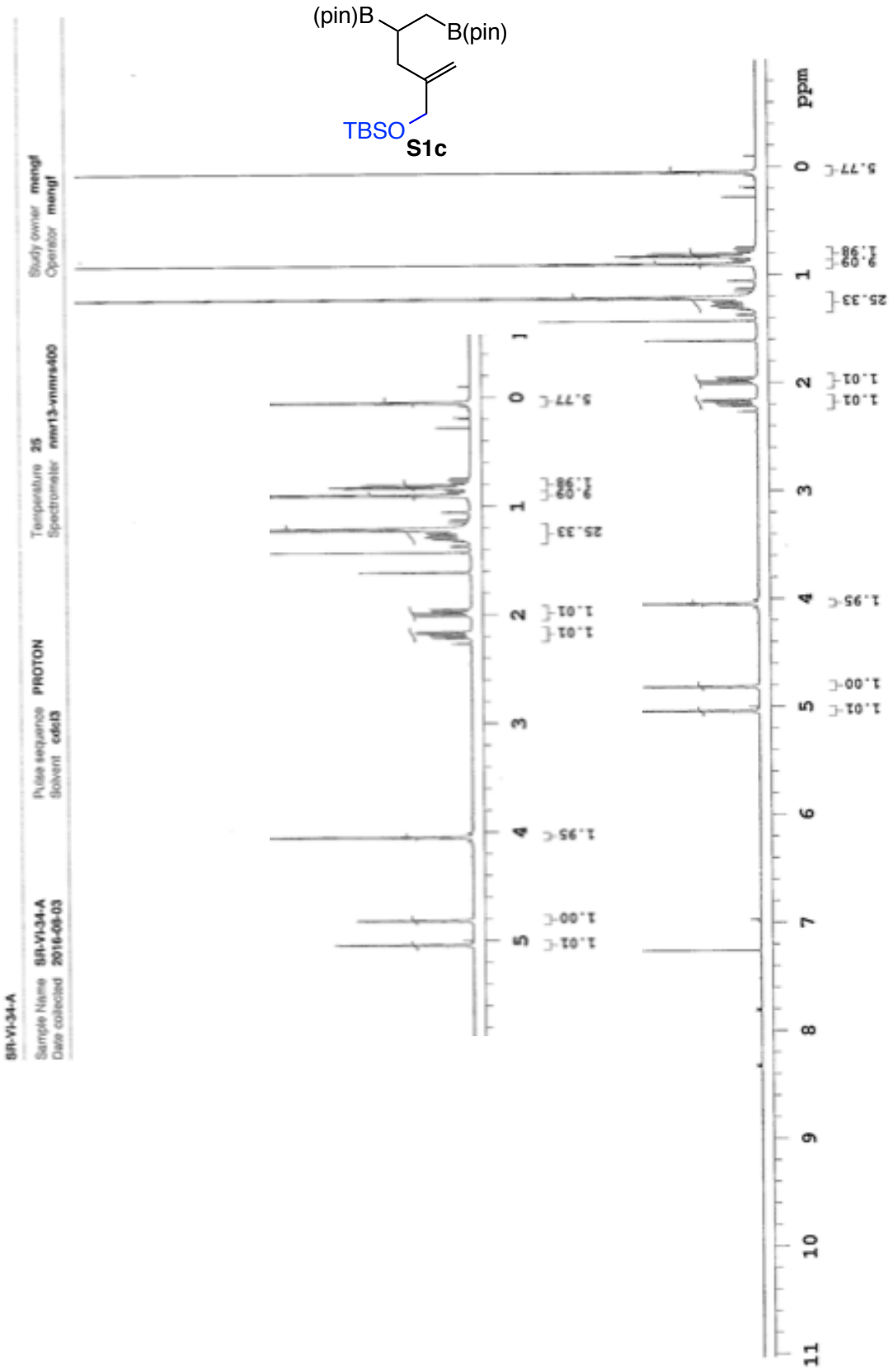

(dan)B
B(pin)
F
14
SR-VI-129-carbon
Sample Name SR-VI-129-carbon
Date collected 2016-11-16
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
0 ppm
20
40
60
80
100
120
140
160
180
200
220

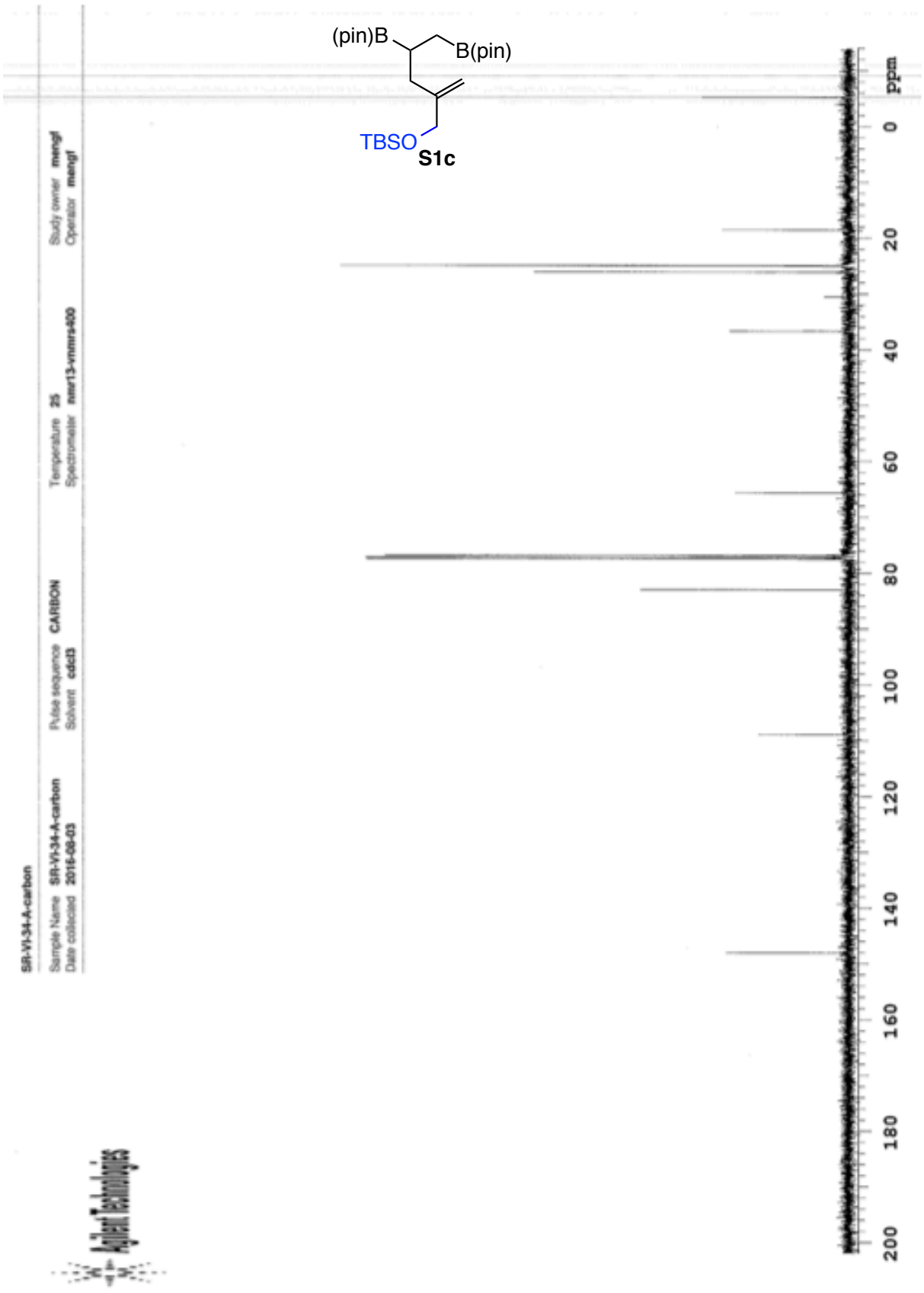

(pin)B
B(pin)
S1a
SR-V-294-1h
Sample Name SR-V-294-1h
Date collected 2016-03-23
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.17
25.82
1.09
1.10
2.08
1.00

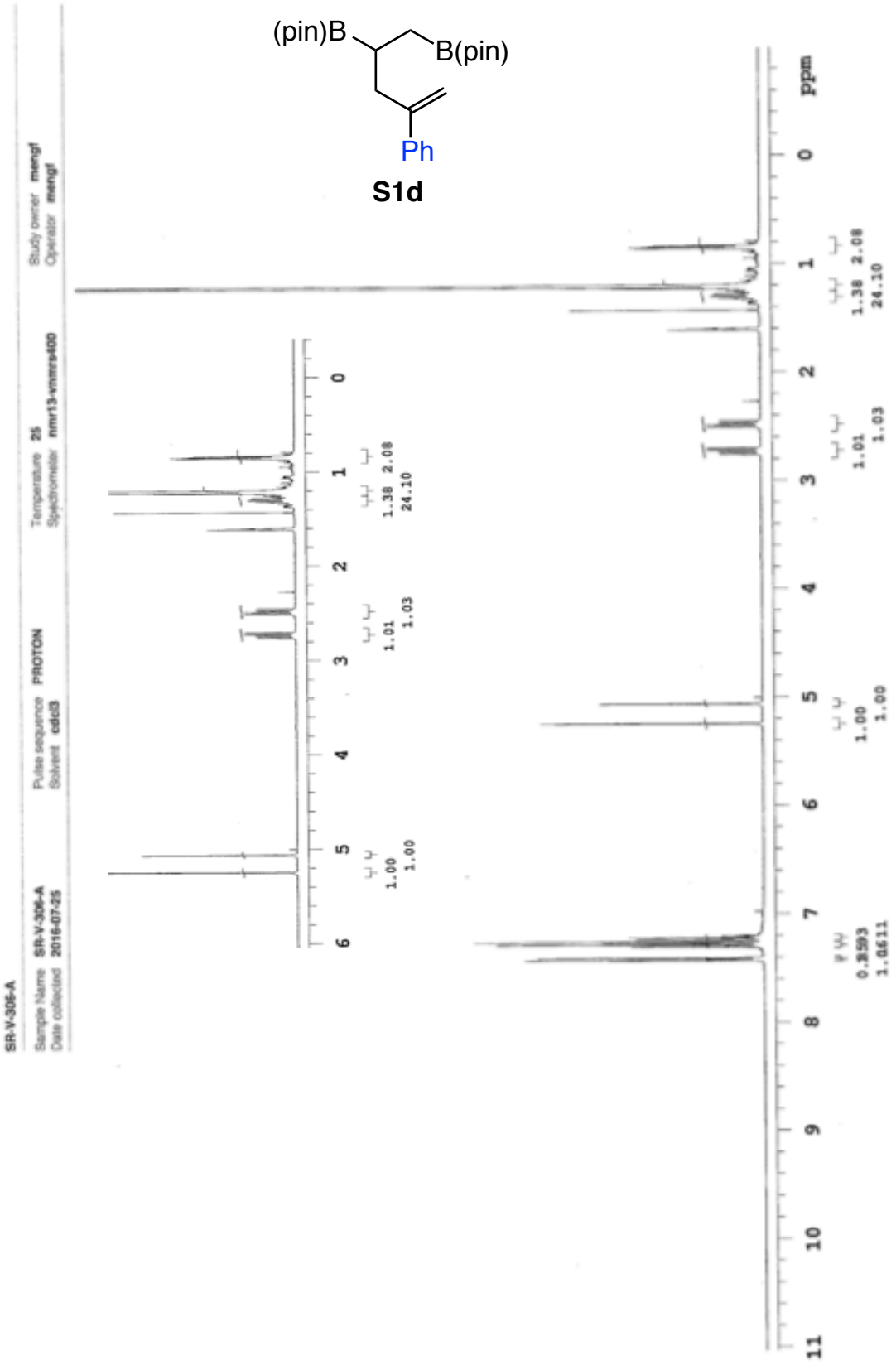

(pin)B
B(pin)
S1a
SR-V-294-1h-carbon
Sample Name SR-V-294-1h-carbon
Date collected 2018-03-23
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

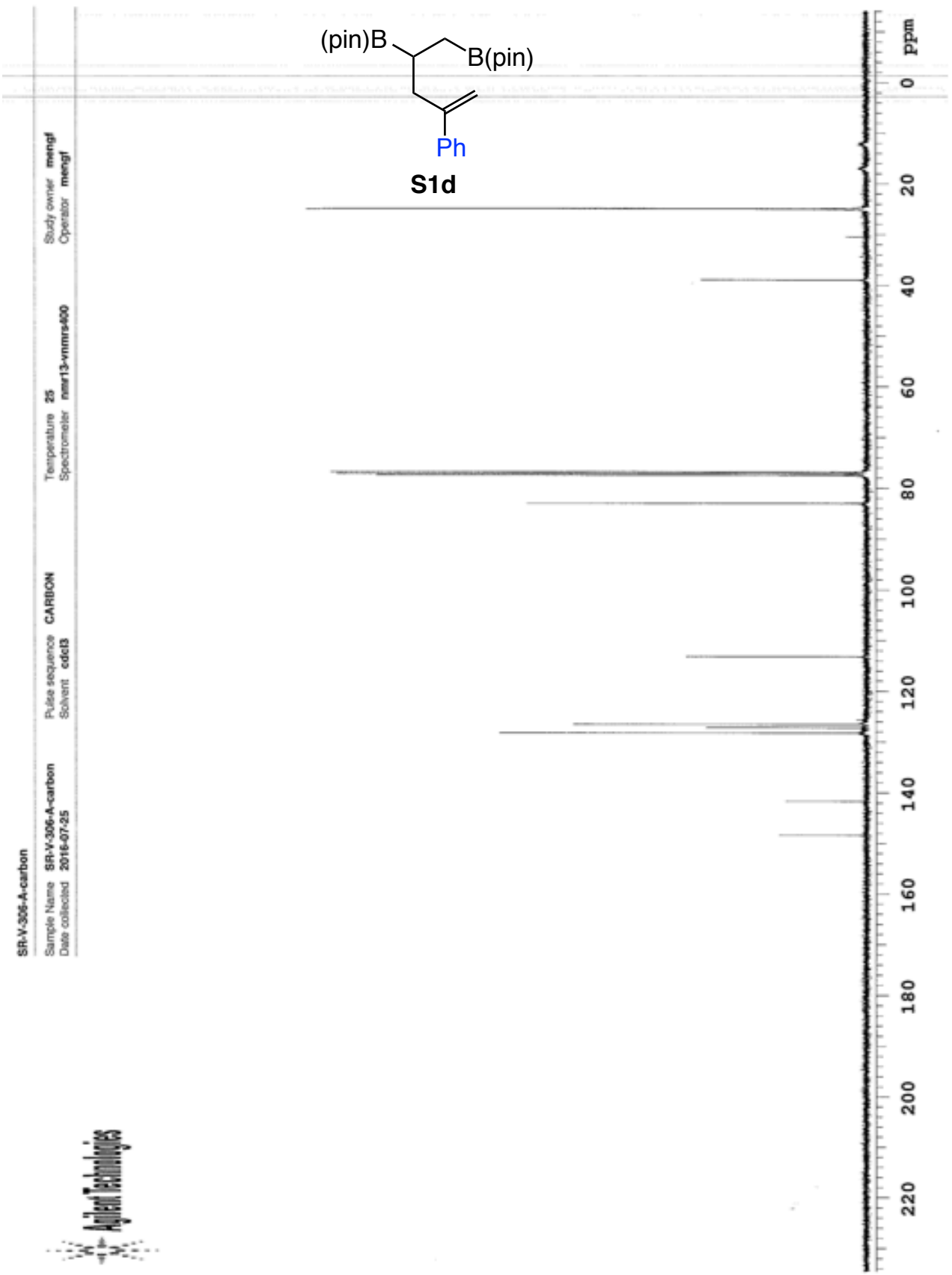

(pin)B
B(pin)
Me
S1b
SR-V-296-A
Sample Name SR-V-296-A
Date collected 2016-07-15
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
1.85
1.00
3.23
1.96
ppm

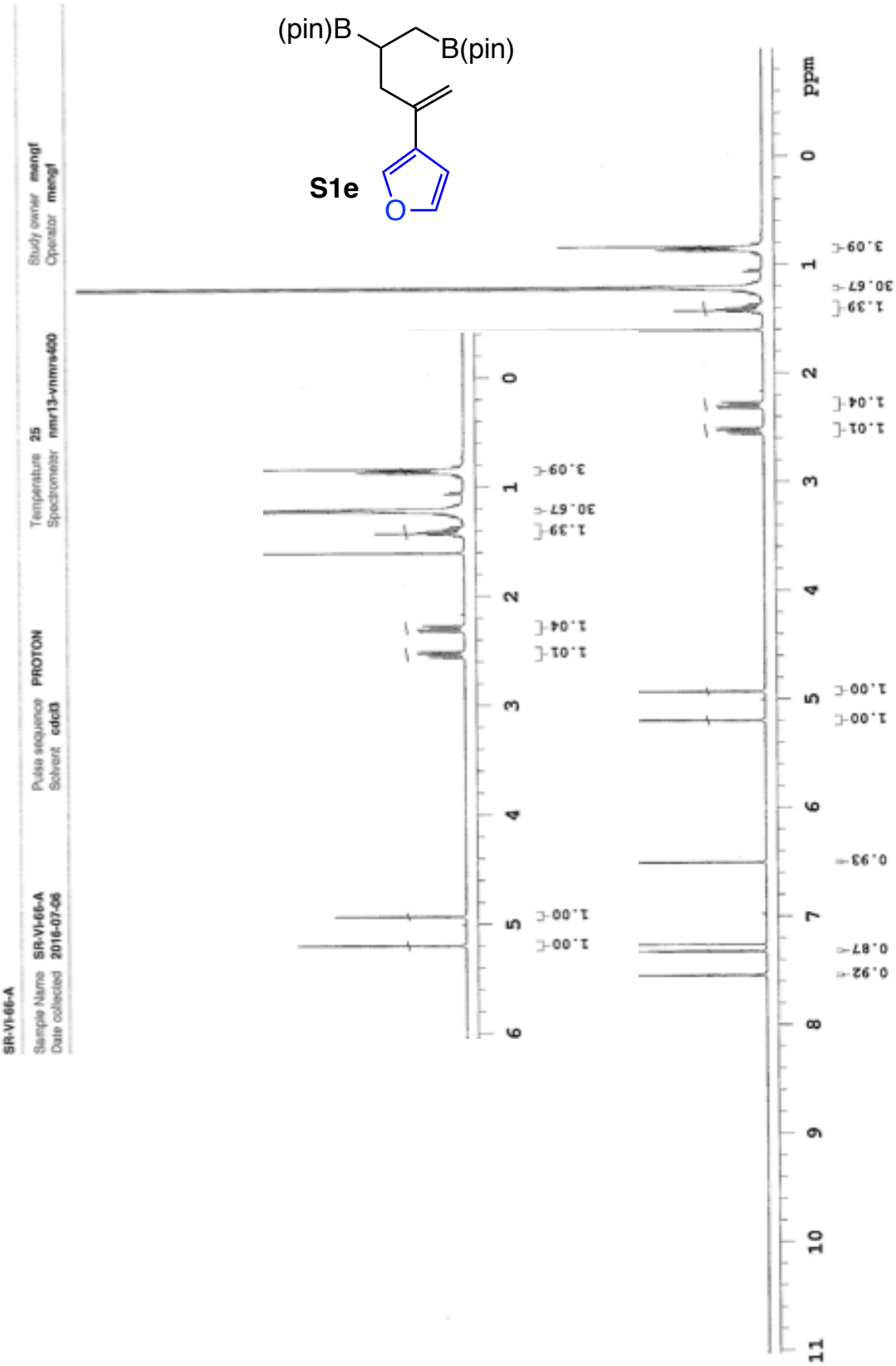

(pin)B
B(pin)
Me
S1b
SR-V-296-A-carbon
Sample Name SR-V-296-A-carbon
Date collected 2016-07-15
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Plot date 2016-07-25
Data file /home/ahh/Benz/SR-V-296-A-carbon.fid
Agilent Technologies

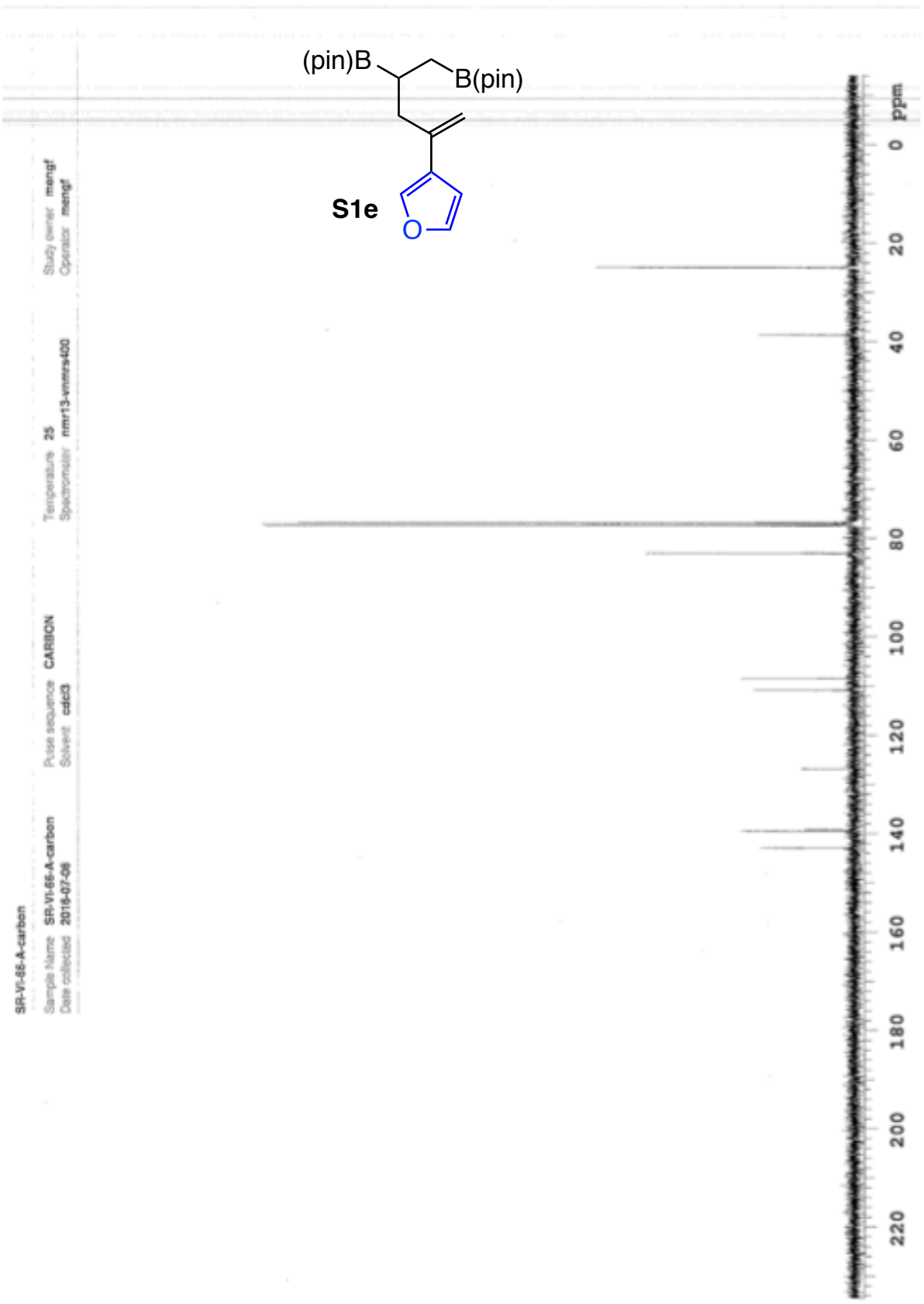

(pin)B
B(pin)
TBSO
S1c
BR-VI-34-A
Sample Name BR-VI-34-A
Date collected 2016-09-03
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
5.77
1.98
1.96
25.33
1.01
1.01
1.95
1.00
1.01

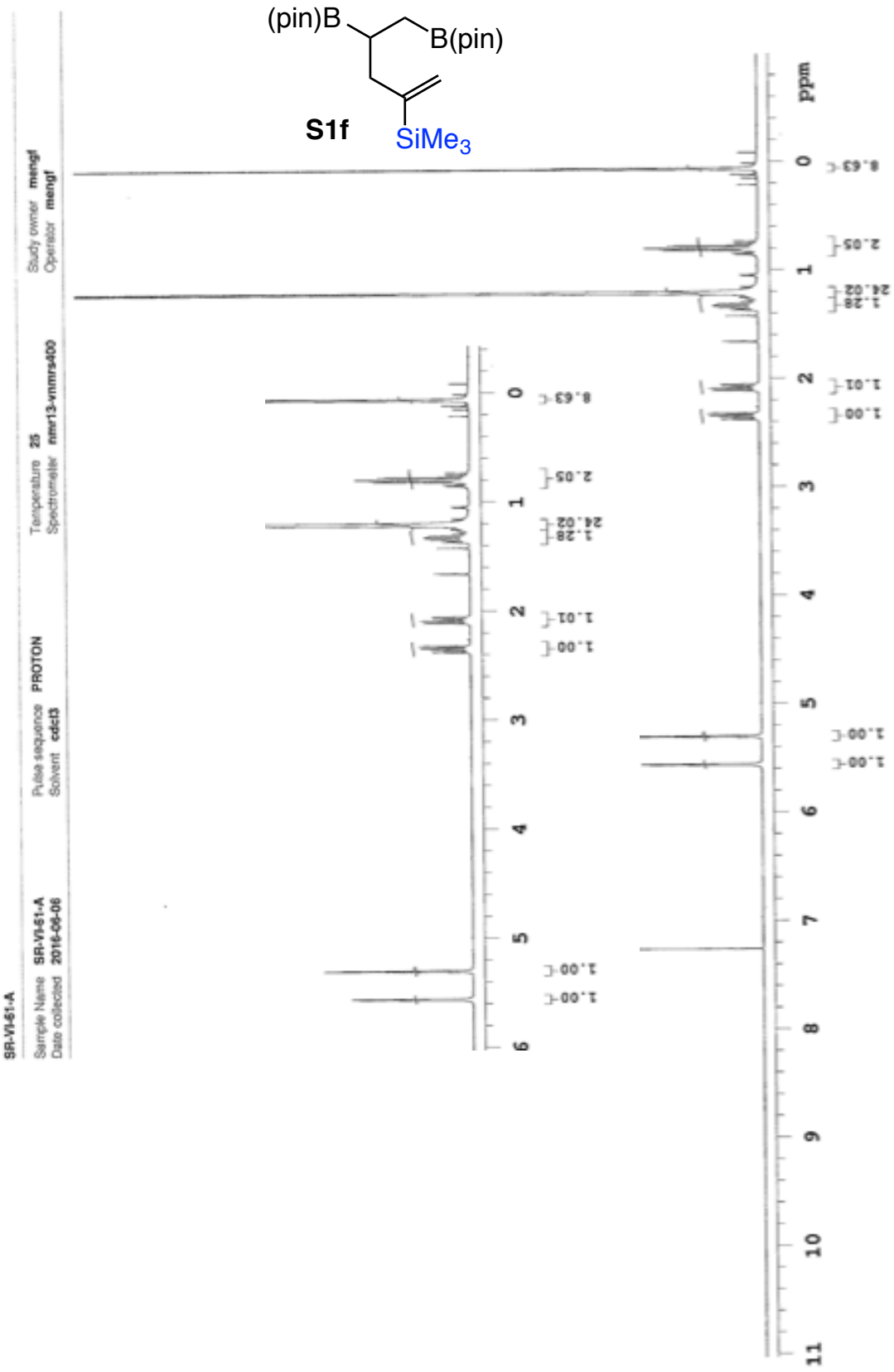

(pin)B
B(pin)
TBSO
S1c
SR-VI-34-A-carbon
Sample Name SR-VI-34-A-carbon
Date collected 2016-08-03
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200

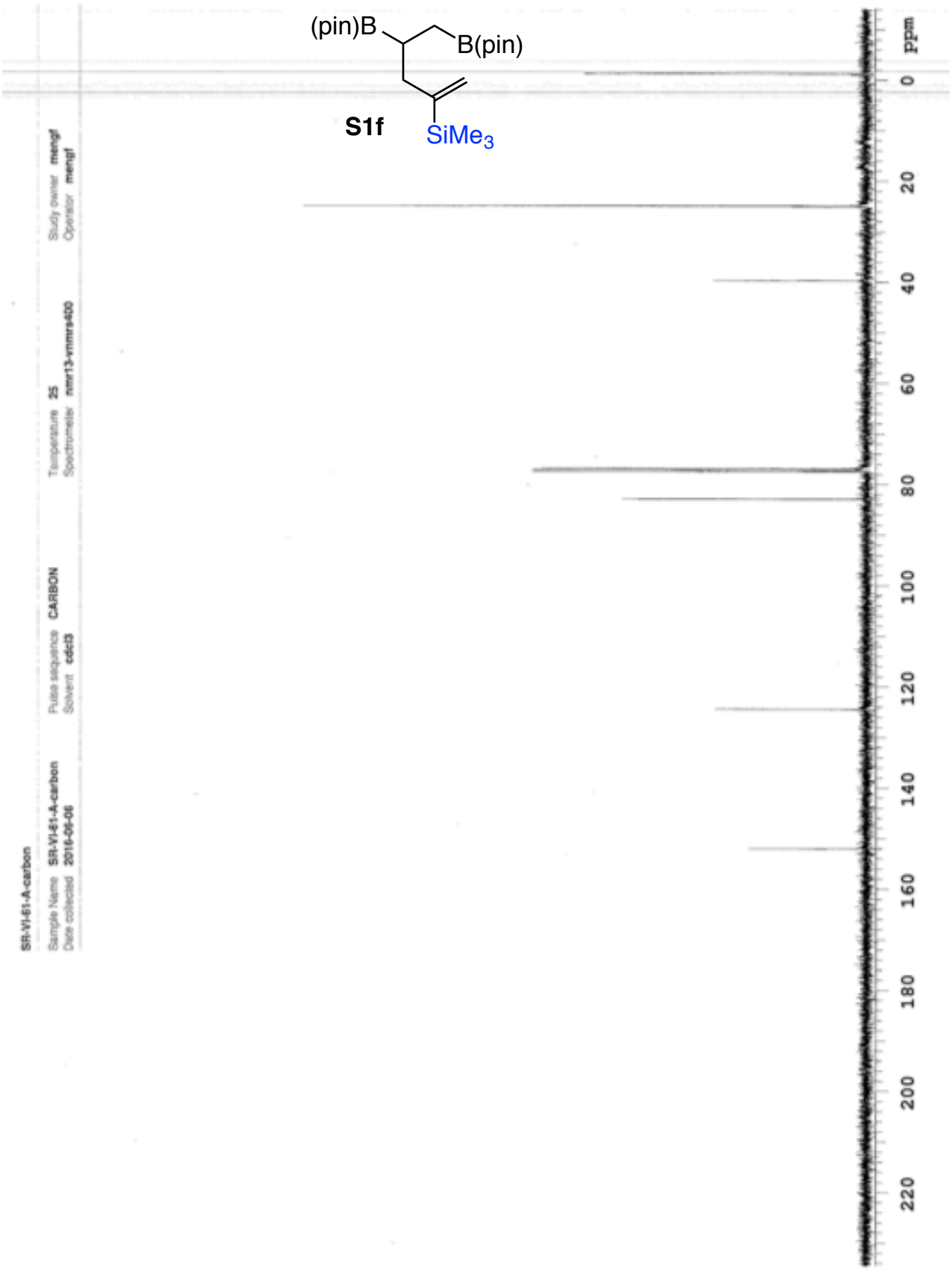

(pin)B
B(pin)
Ph
S1d
SR-V-306-A
Sample Name SR-V-306-A
Date collected 2016-07-25
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

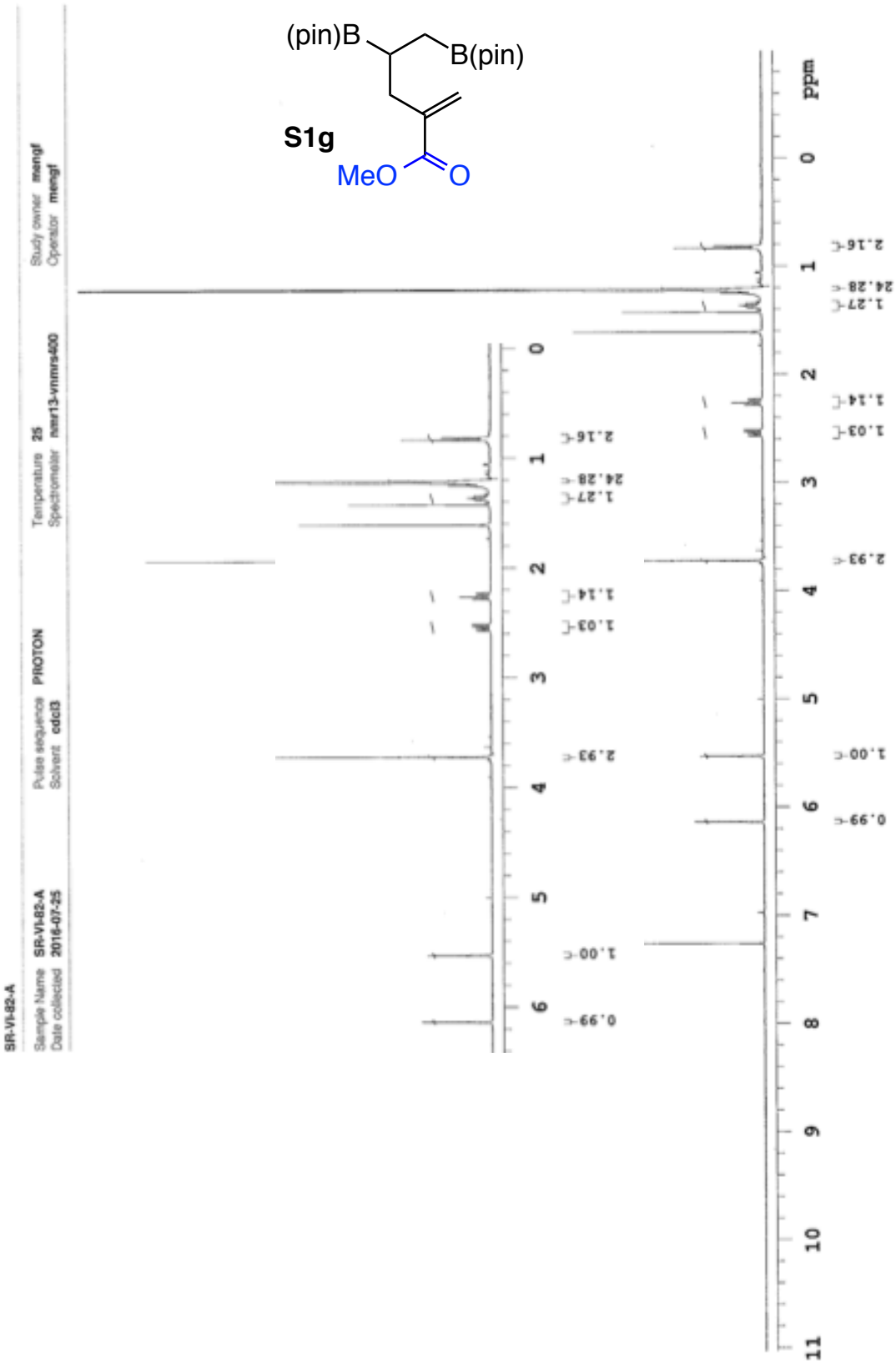

(pin)B
B(pin)
Ph
S1d
SR-V-306-A-carbon
Sample Name SR-V-306-A-carbon
Date collected 2016-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs600
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

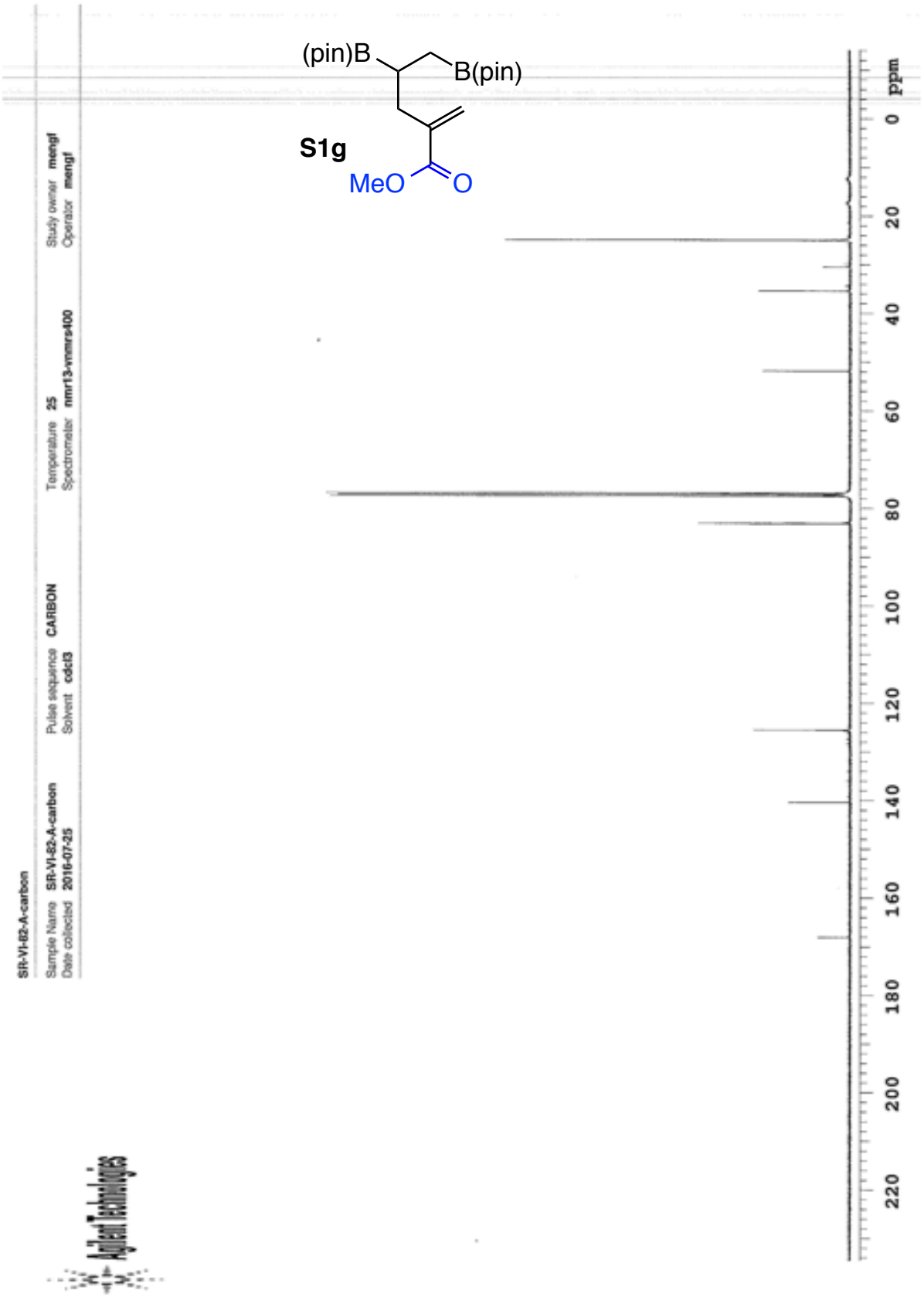

(pin)B
B(pin)
S1e
O
SR-VI-66-A
Sample Name SR-VI-66-A
Date collected 2016-07-06
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
3.09
30.67
1.39
1.04
1.01
1.00
1.00
0.93
0.87
0.92

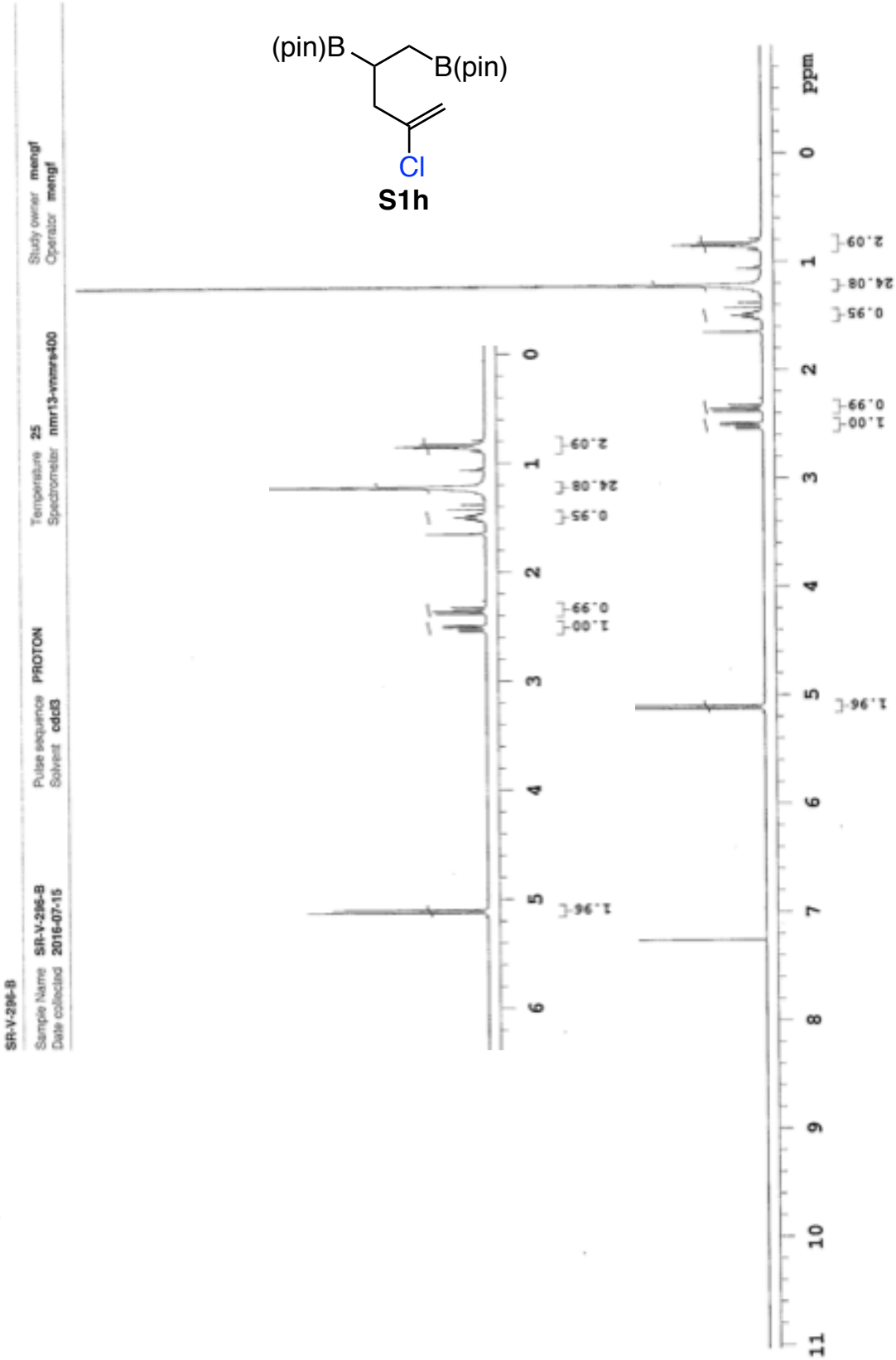

(pin)B
B(pin)
S1e
SR-VI-66-A-carbon
Sample Name SR-VI-66-A-carbon
Date collected 2016-07-06
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

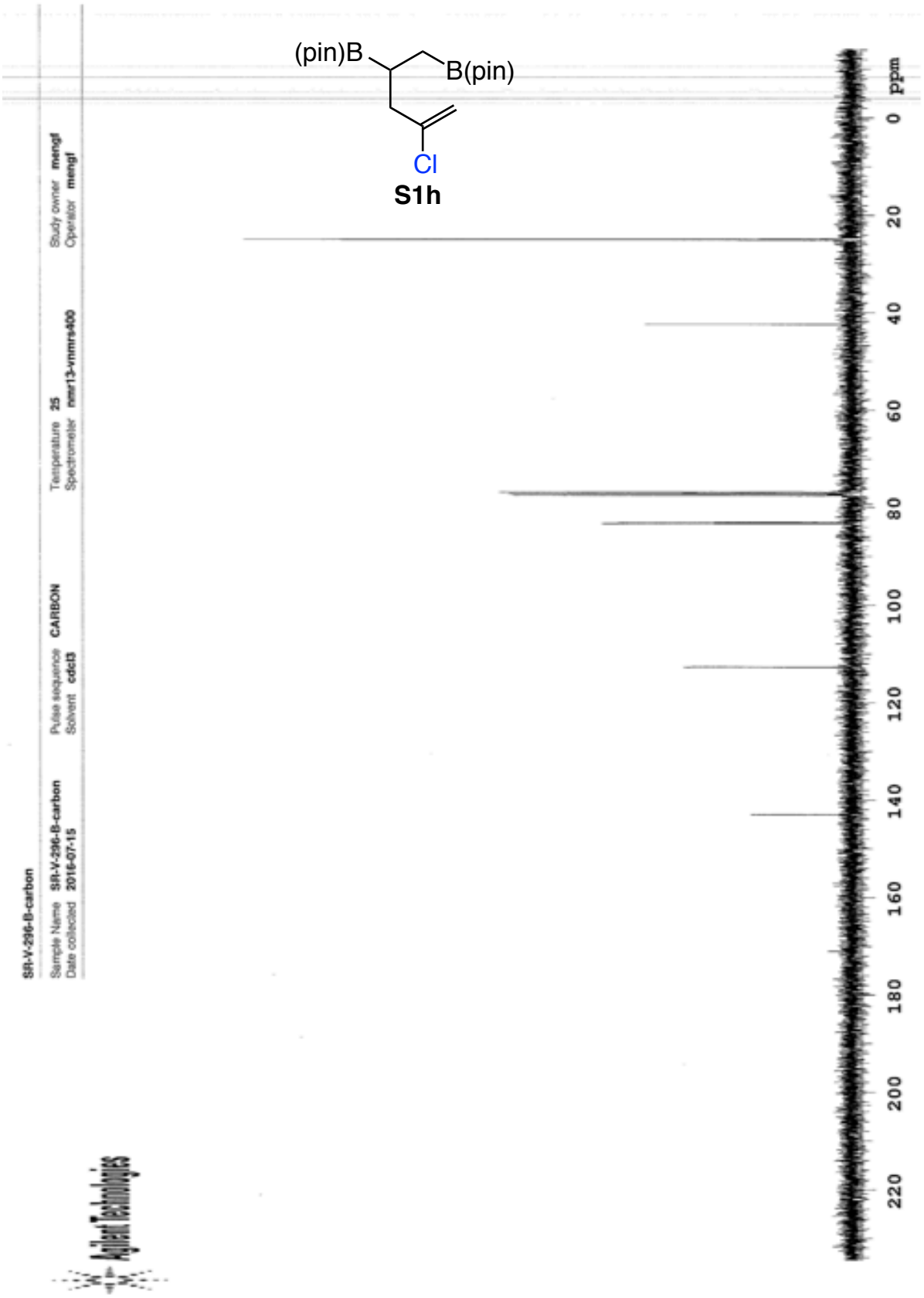

(pin)B
B(pin)
S1f
SiMe3
SR-VI-61-A
Sample Name SR-VI-61-A
Date collected 2016-06-06
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

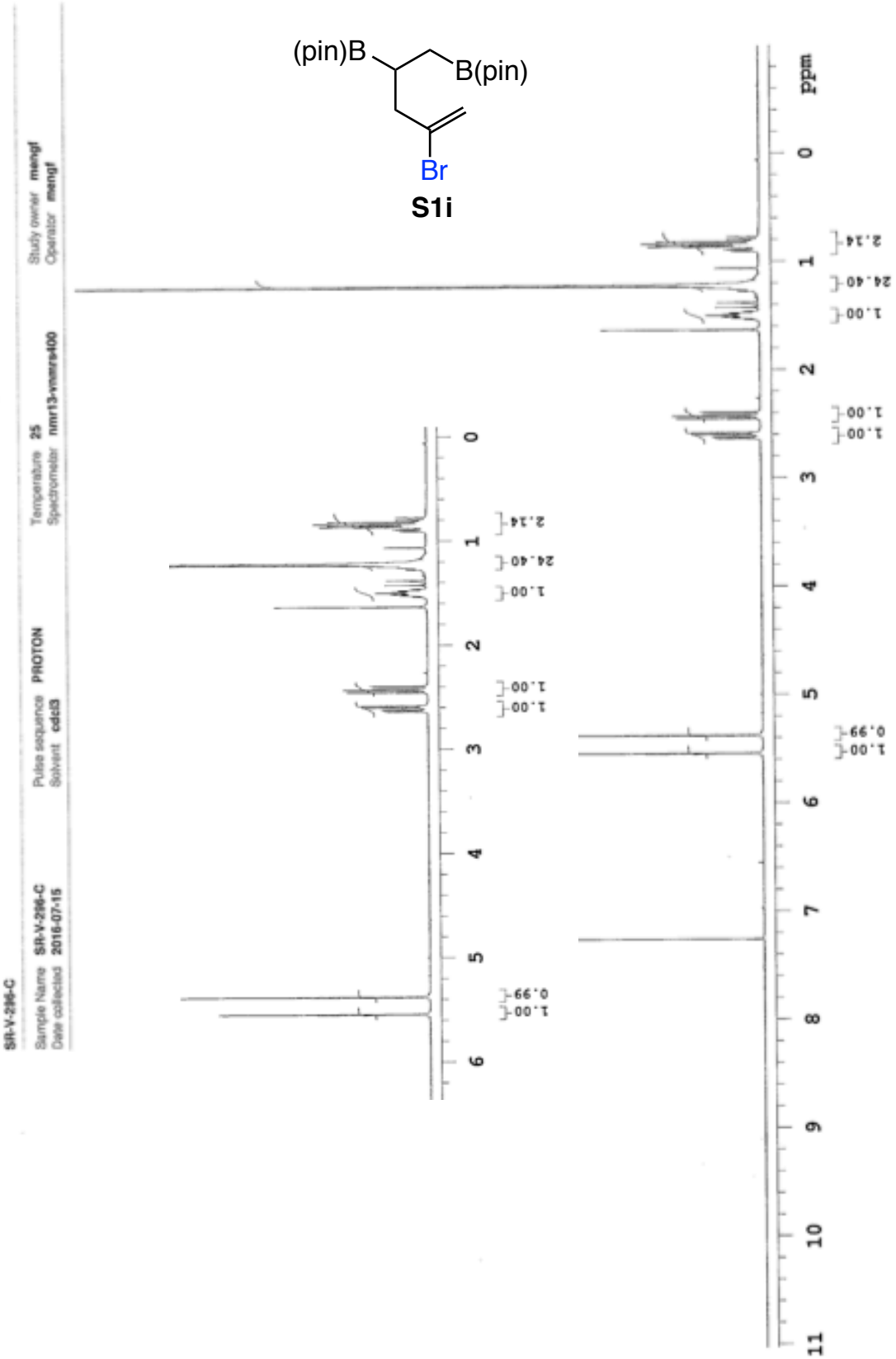

(pin)B
B(pin)
S1f
SiMe3
SR-VI-61-A-carbon
Sample Name SR-VI-61-A-carbon
Date collected 2016-06-06
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

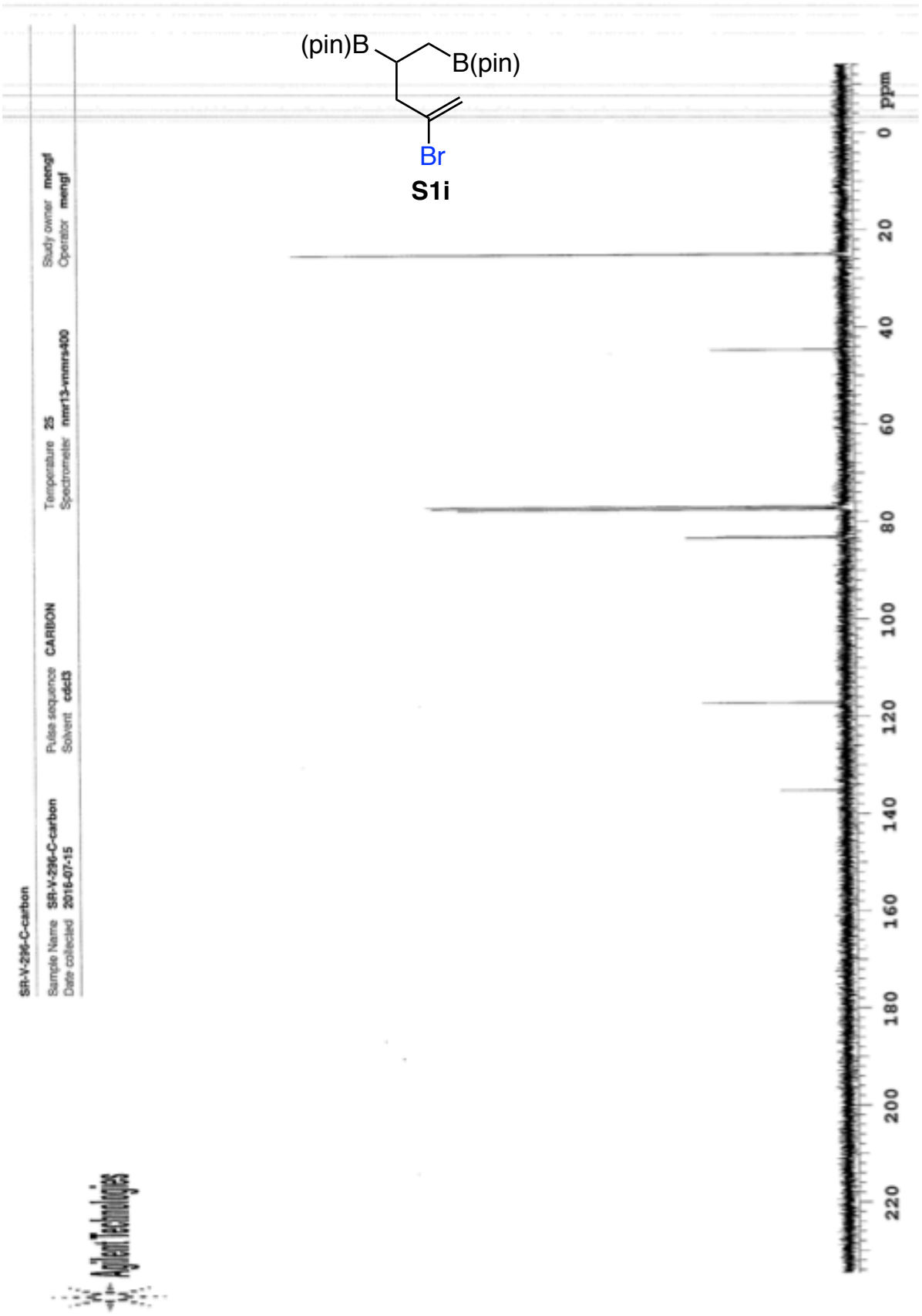

(pin)B
B(pin)
S1g
MeO
O
SR-VI-82-A
Sample Name SR-VI-82-A
Date collected 2016-07-25
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.16
24.28
1.27
1.14
1.03
2.93
1.00
0.99

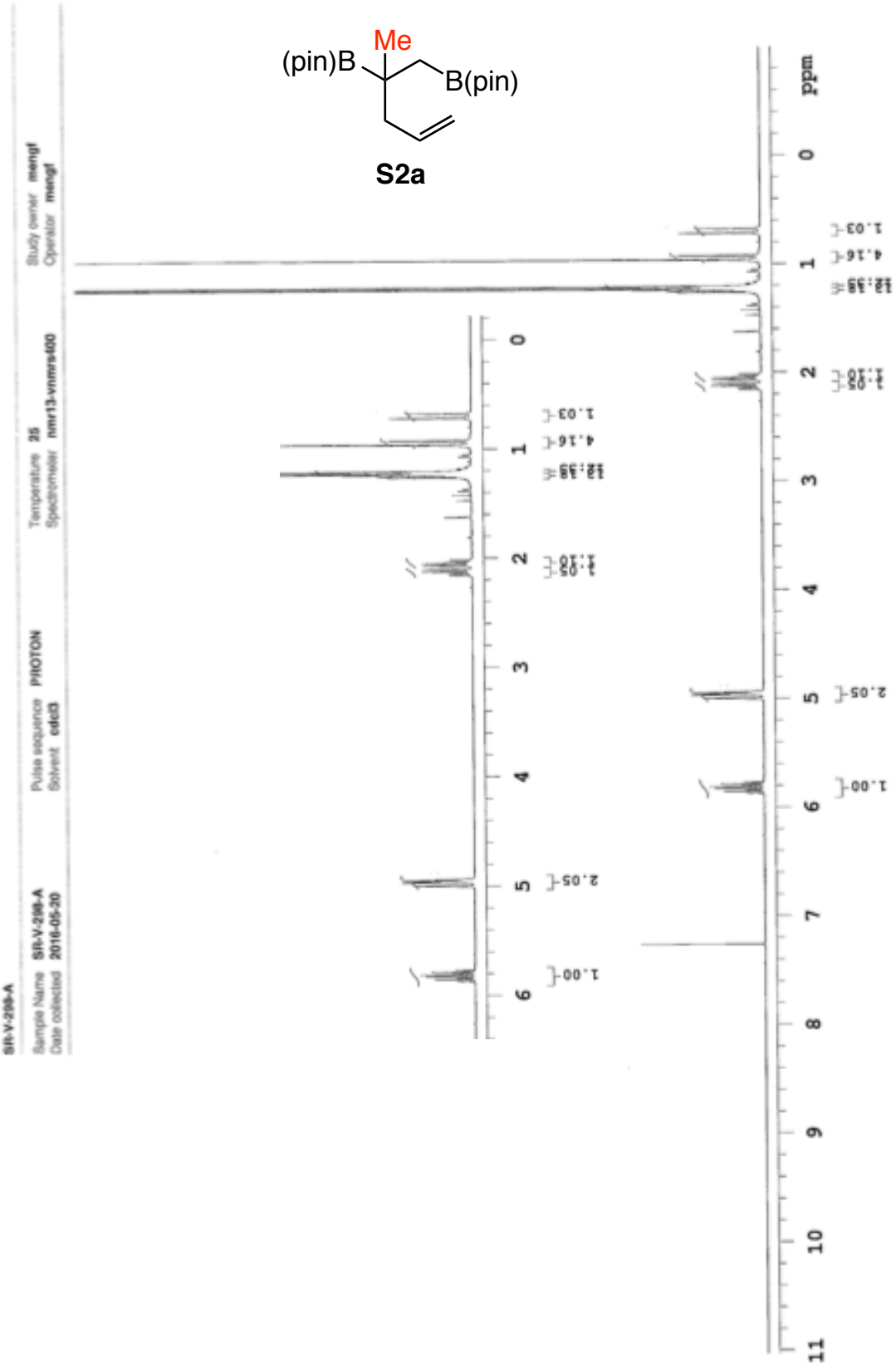

(pin)B
B(pin)
S1g
MeO
O
SR-VI-82-A-carbon
Sample Name SR-VI-82-A-carbon
Date collected 2016-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

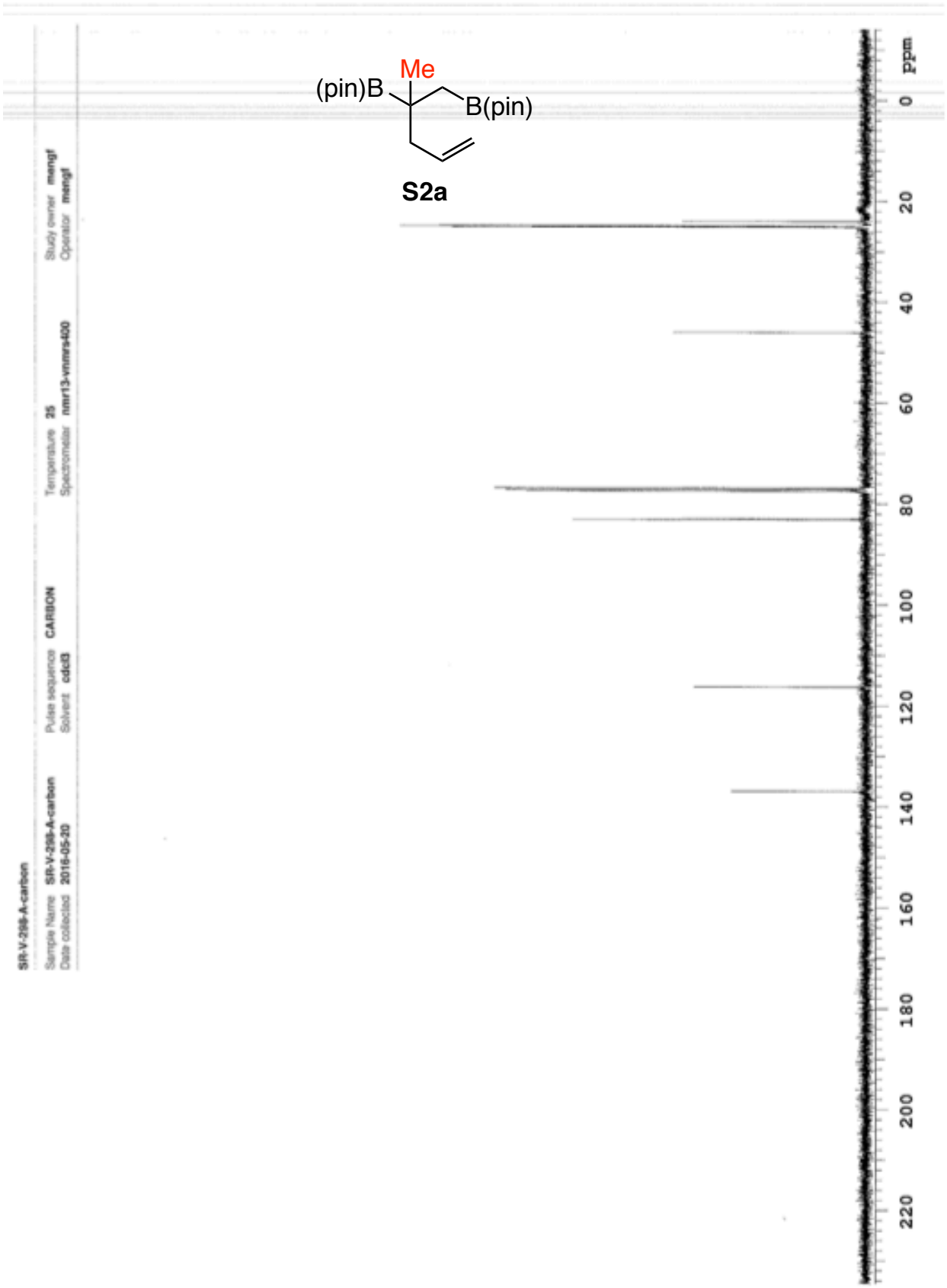

(pin)B
B(pin)
Cl
S1h
SR-V-296-B
Sample Name SR-V-296-B
Date collected 2016-07-15
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.09
24.08
0.95
0.99
1.00
1.96

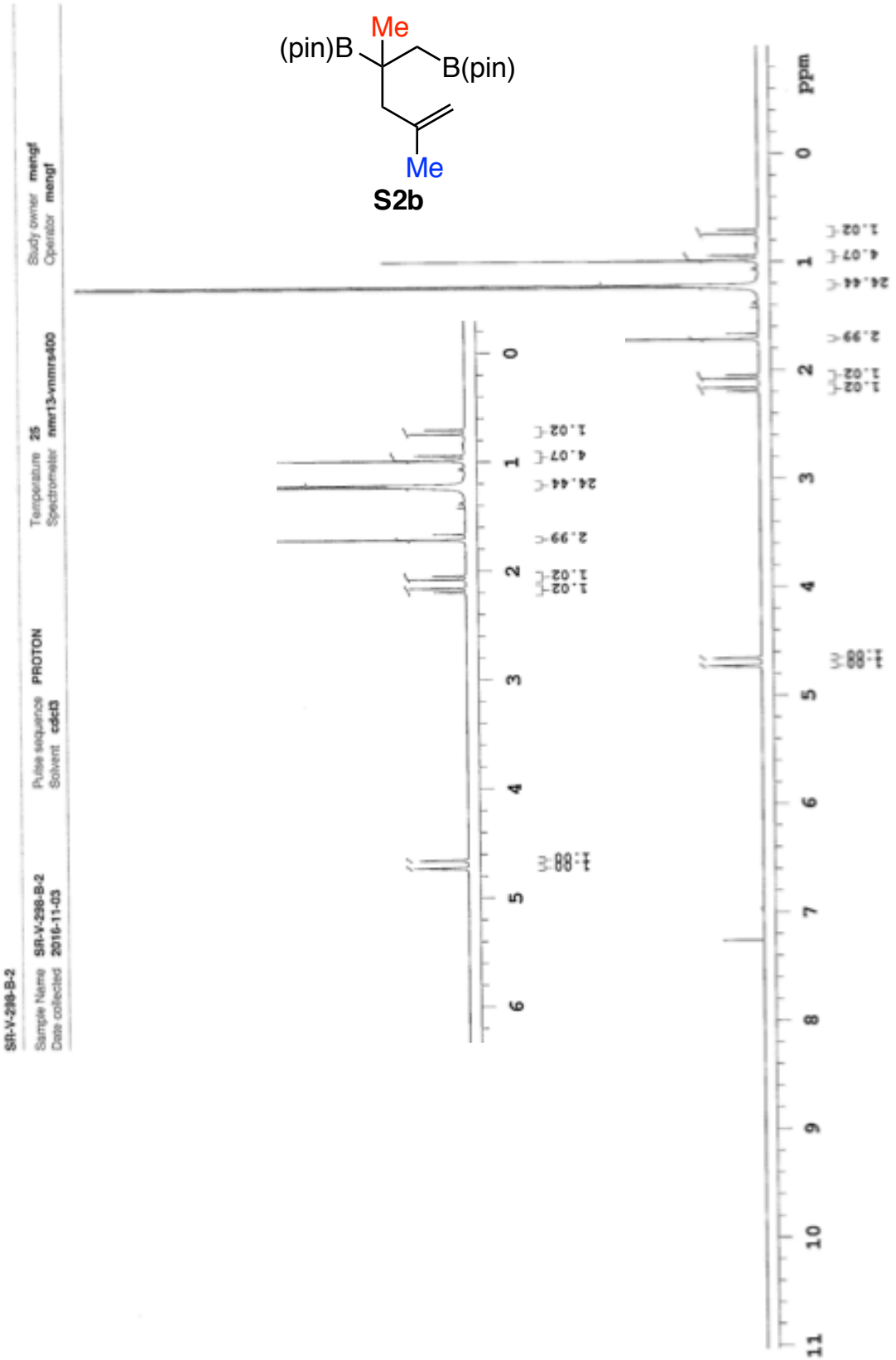

(pin)B
B(pin)
Cl
S1h
SR-V-296-B-carbon
Sample Name SR-V-296-B-carbon
Date collected 2016-07-15
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Agilent Technologies

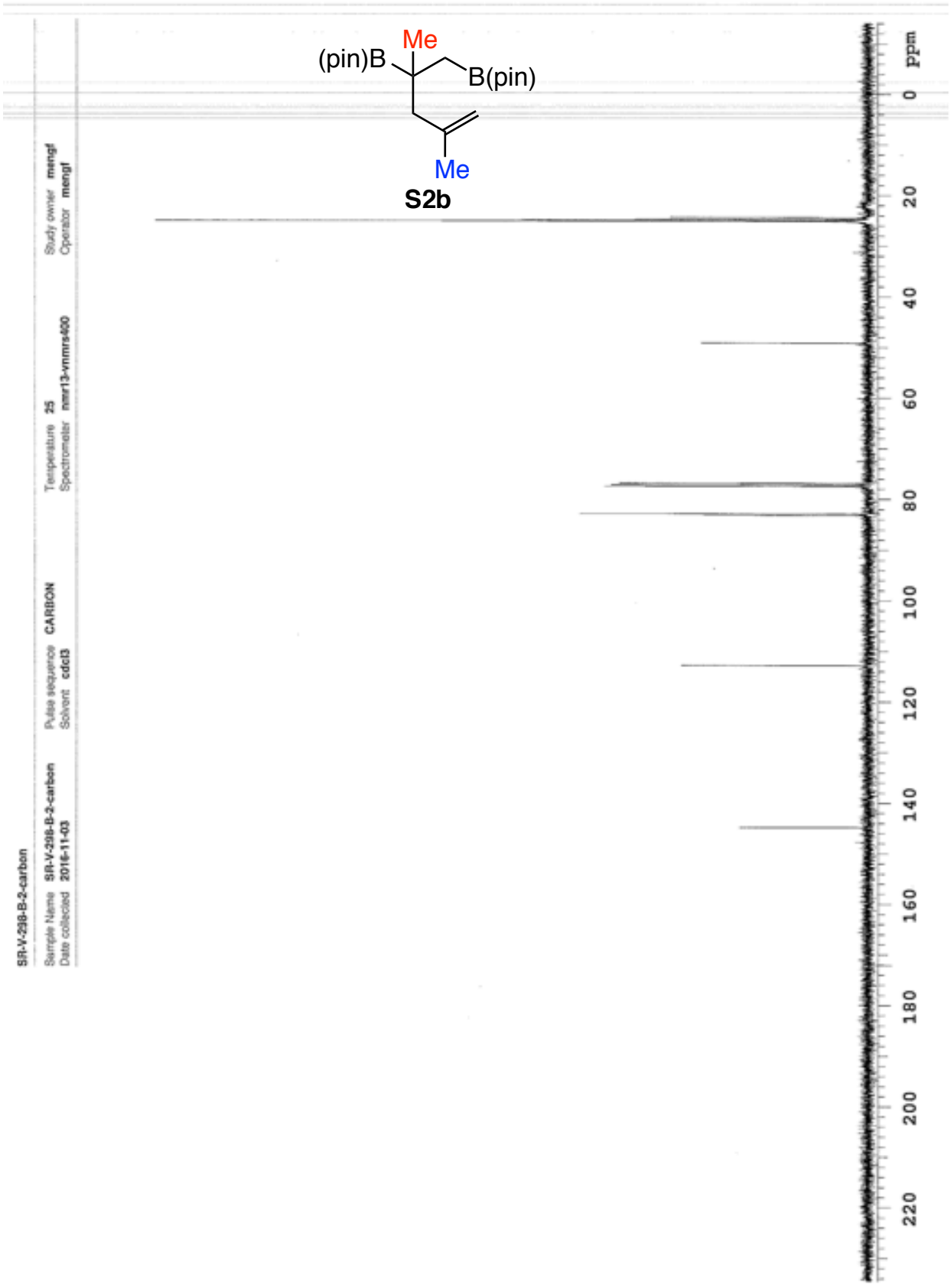

(pin)B
B(pin)
Br
S1i
SR-V-296-C
Sample Name SR-V-296-C
Date collected 2016-07-15
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
2.14
24.40
1.00
1.00
1.00
0.99
1.00

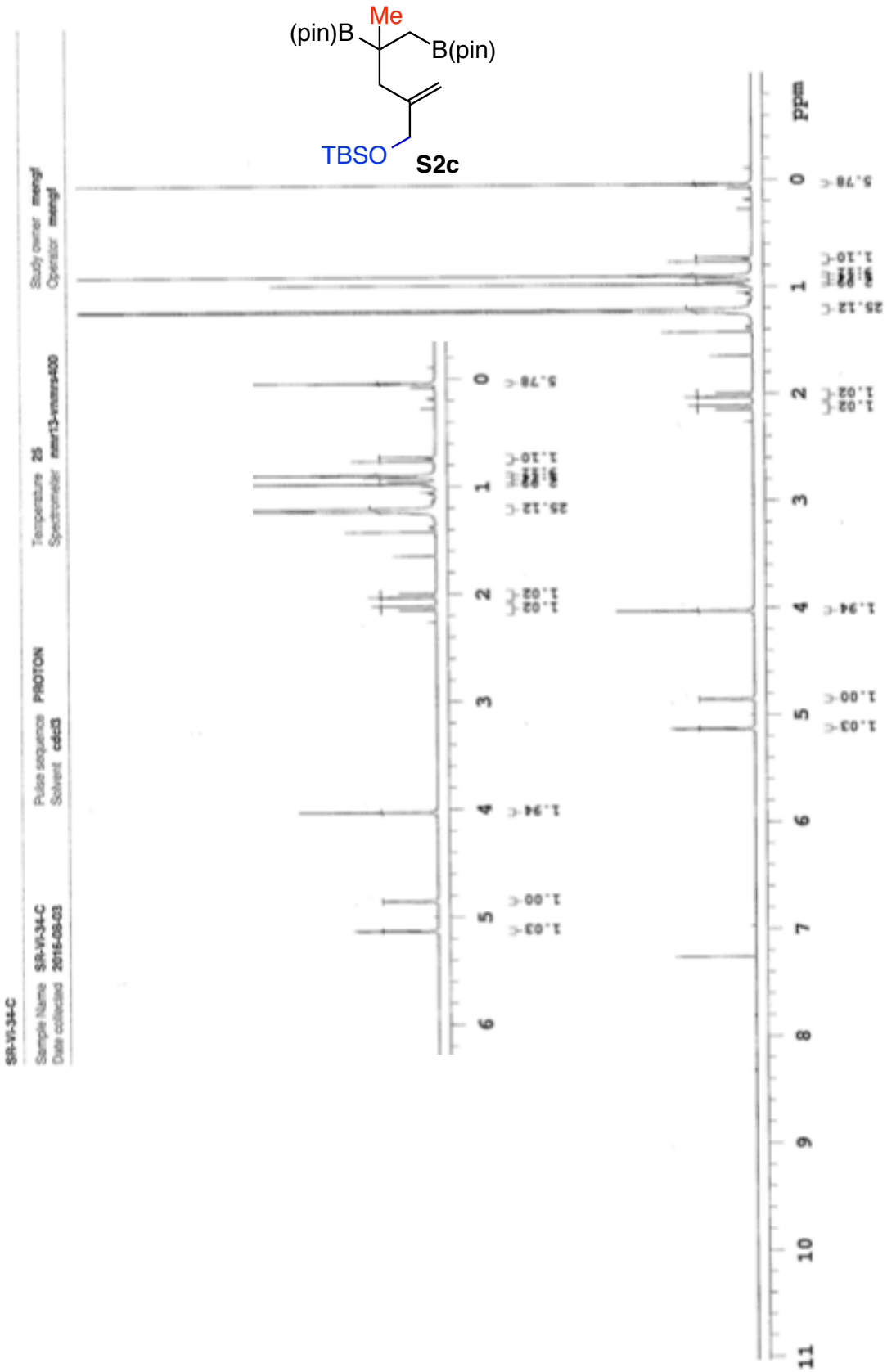

(pin)B
B(pin)
Br
S1i
SR-V-236-C-carbon
Sample Name SR-V-236-C-carbon
Date collected 2016-07-15
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

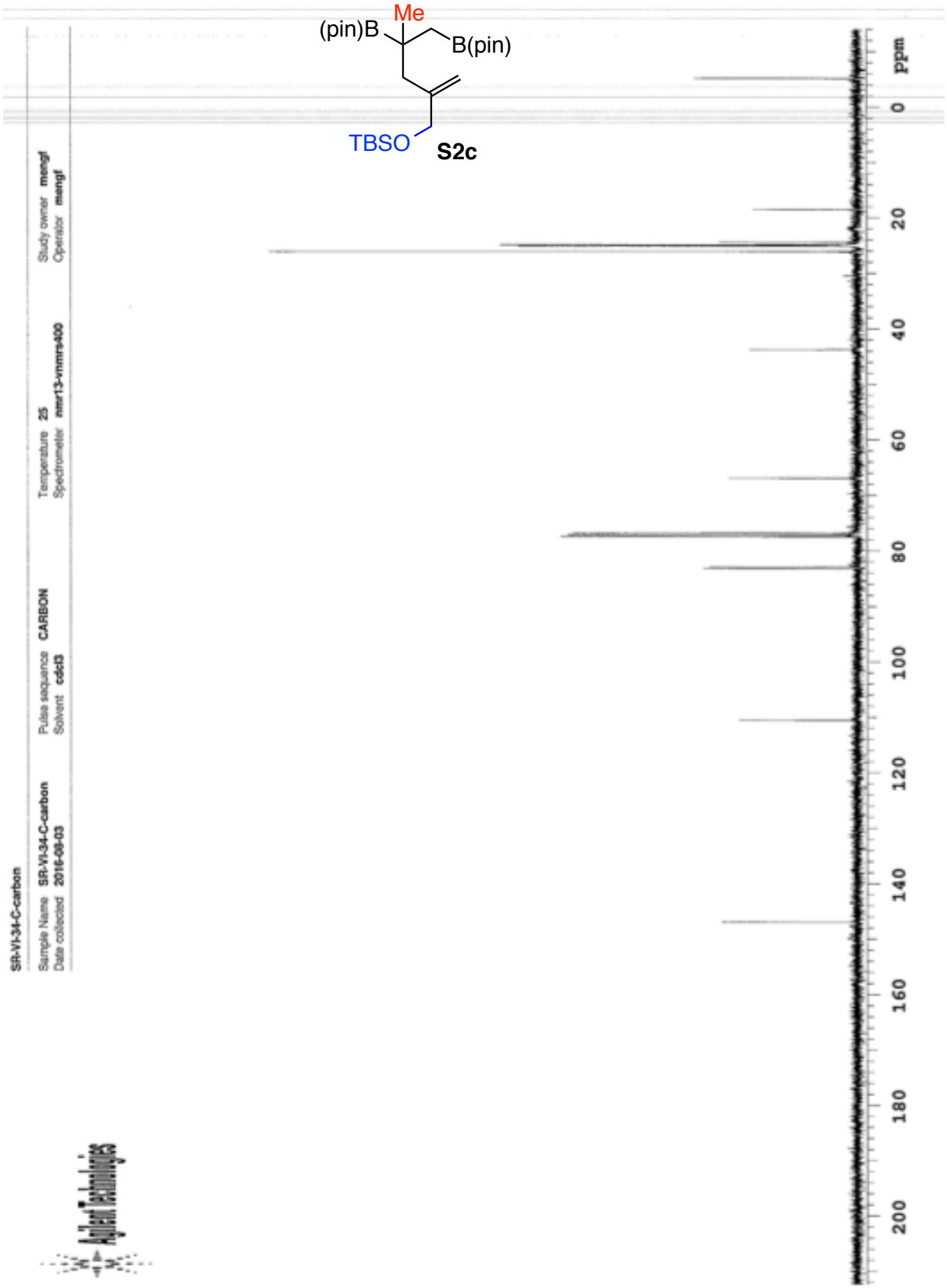

Me
(pin)B
B(pin)
S2a
SR-V-298-A
Sample Name SR-V-298-A
Date collected 2016-05-20
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
1.03
4.16
12.38
2.05
1.00

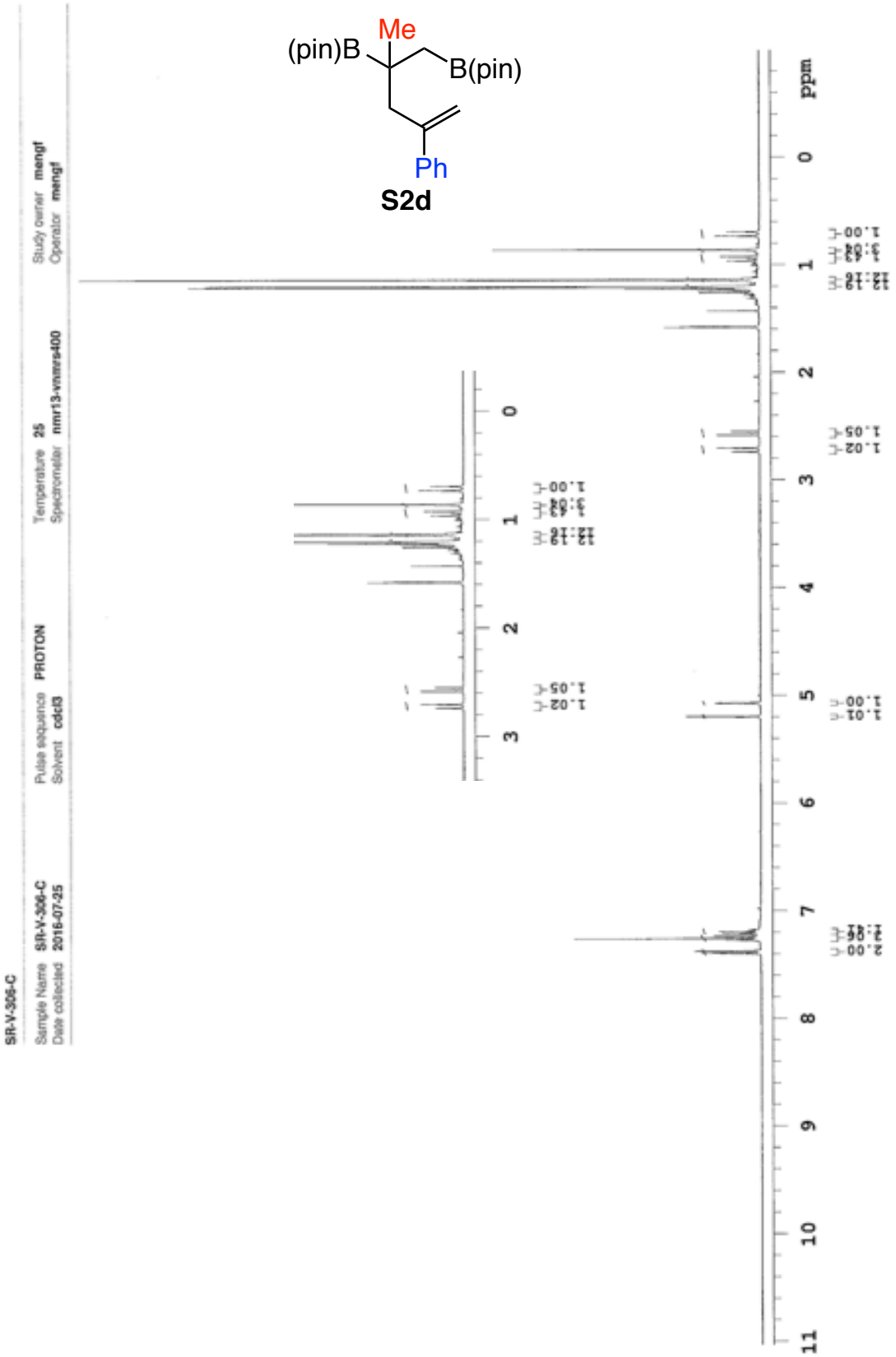

Me
(pin)B
B(pin)
S2a
SR-V-298-A-carbon
Sample Name SR-V-298-A-carbon
Date collected 2016-05-20
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

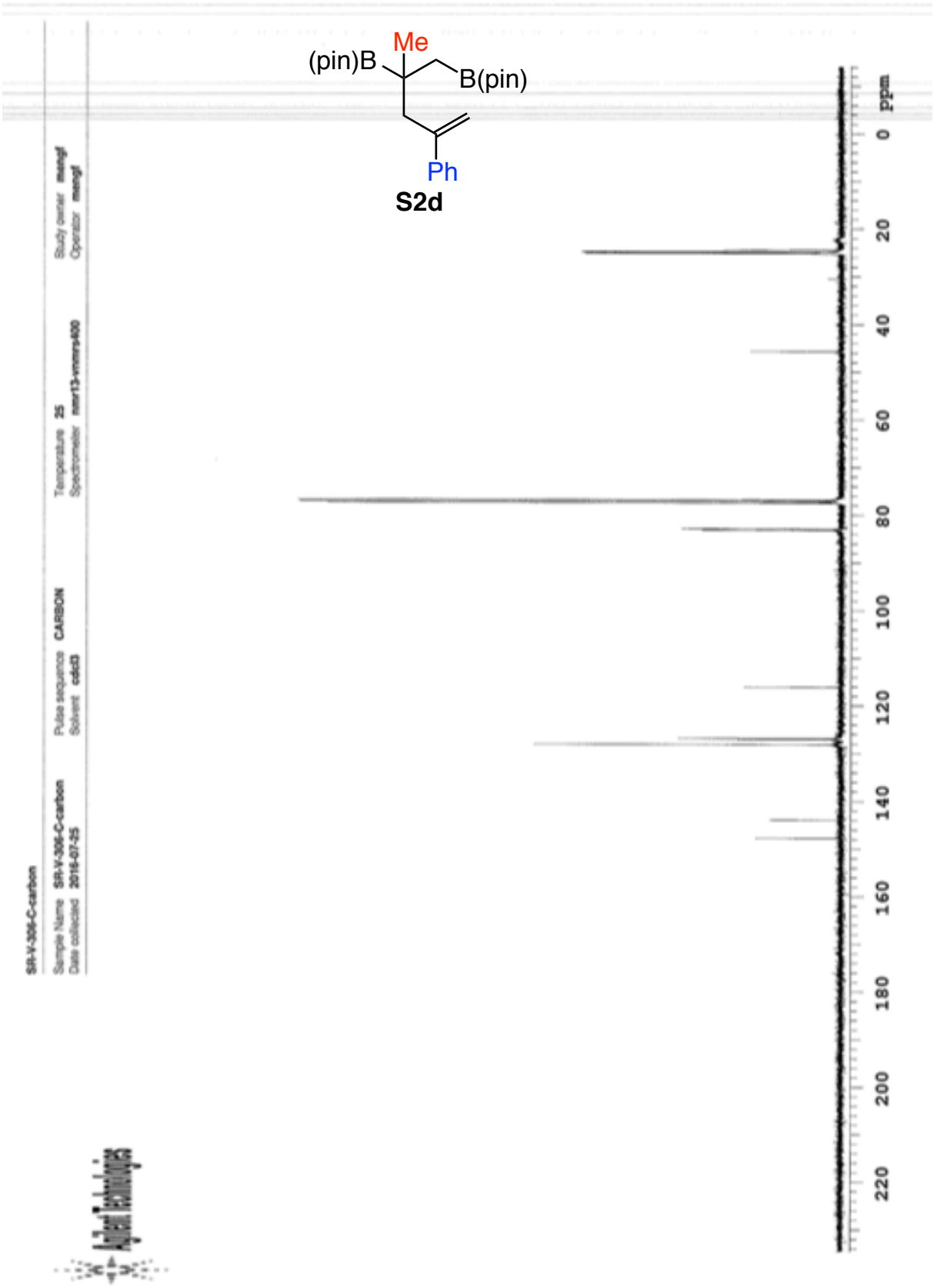

Me
(pin)B
B(pin)
Me
S2b
SR-V-298-B-2
Sample Name SR-V-298-B-2
Date collected 2016-11-03
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vmrrs400
Study owner mengf
Operator mengf
ppm
1.02
4.07
24.44
2.99
1.02
1.02
1.88
1.88
1.02
4.07
24.44
2.99
1.02
1.02

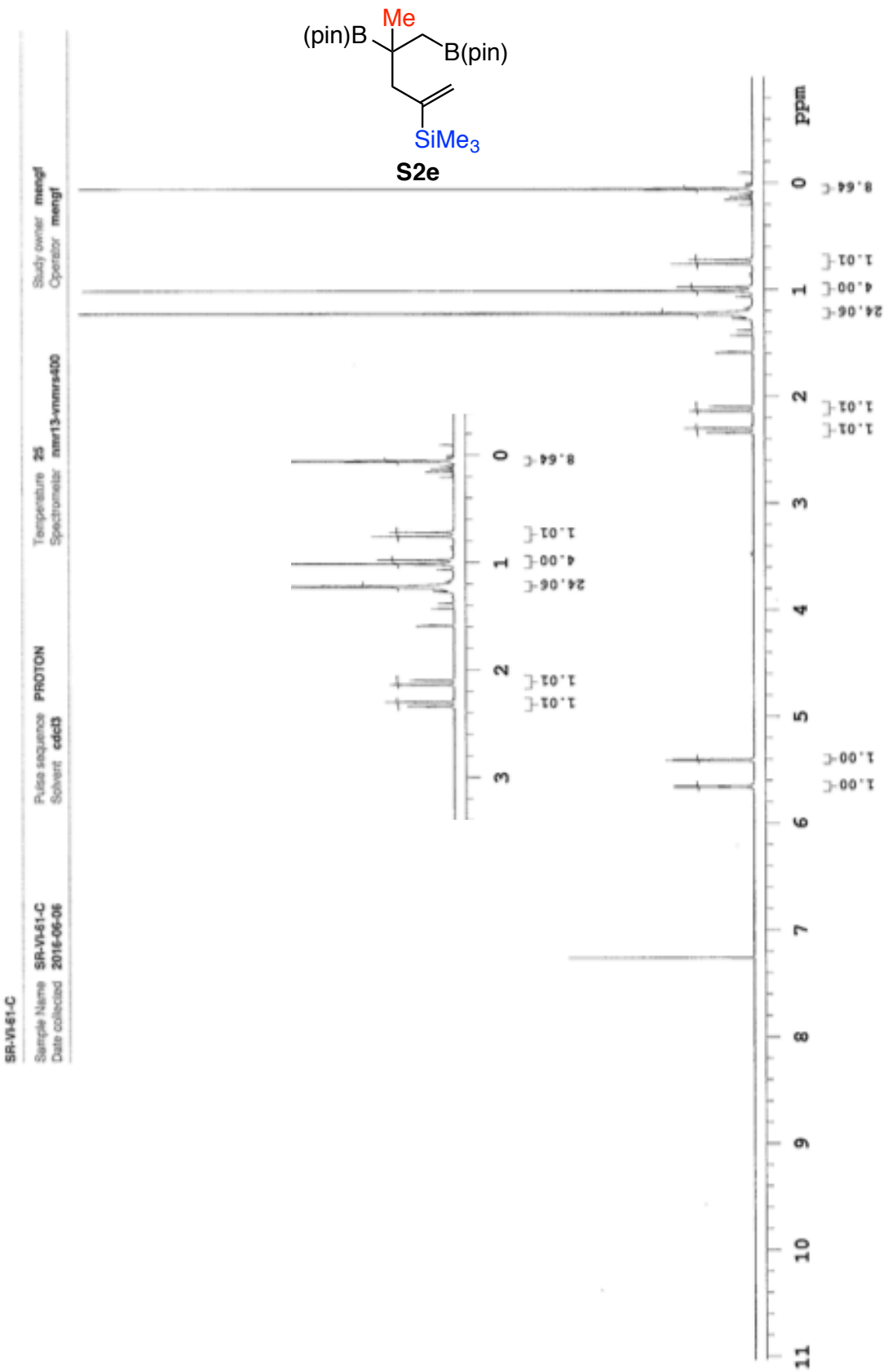

Me
(pin)B
B(pin)
Me
S2b
SR-V-298-B-2-carbon
Sample Name SR-V-298-B-2-carbon
Date collected 2016-11-03
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

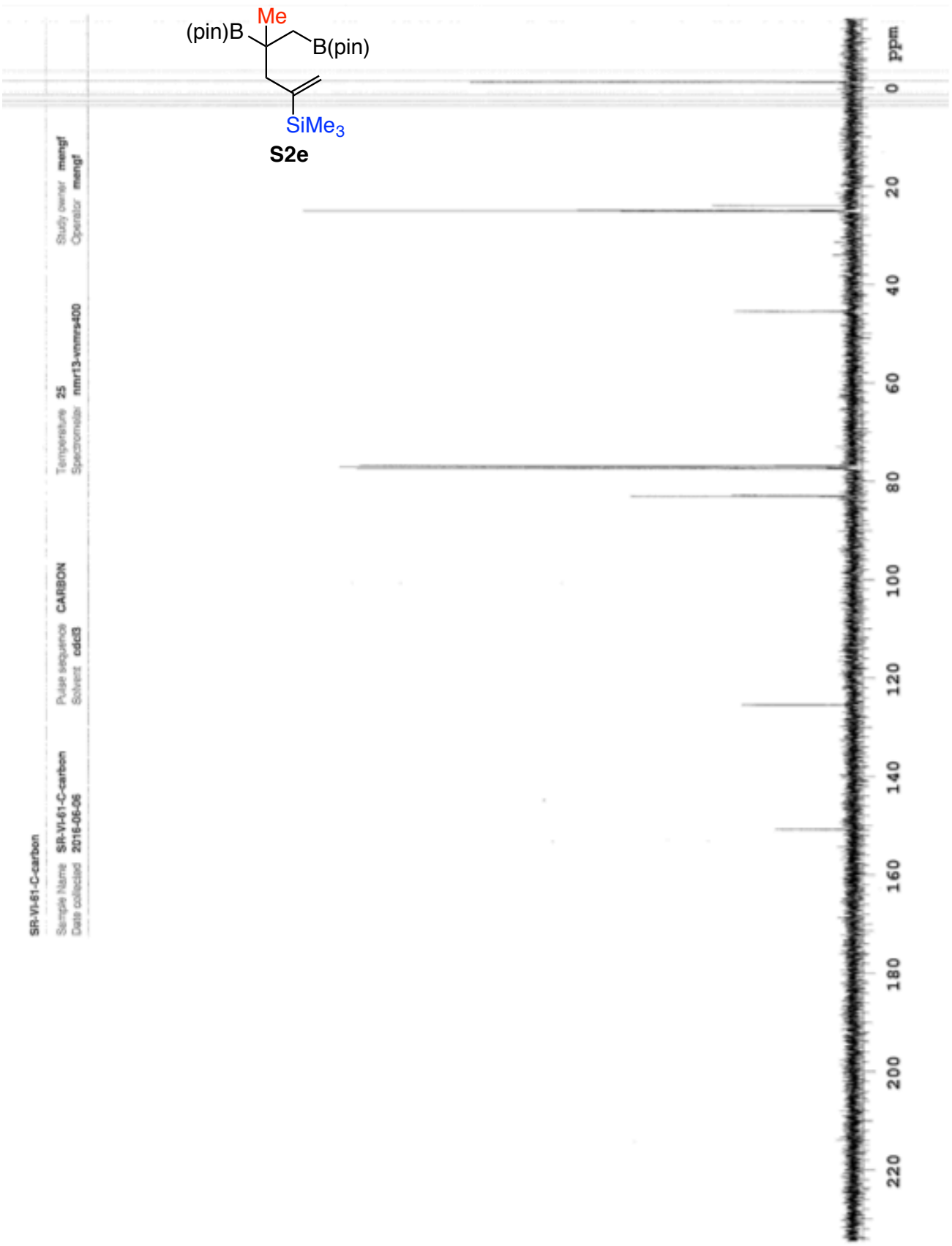

Me
(pin)B
B(pin)
TBSO
S2c
SR-VI-34-C
Sample Name SR-VI-34-C
Date collected 2016-08-03
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

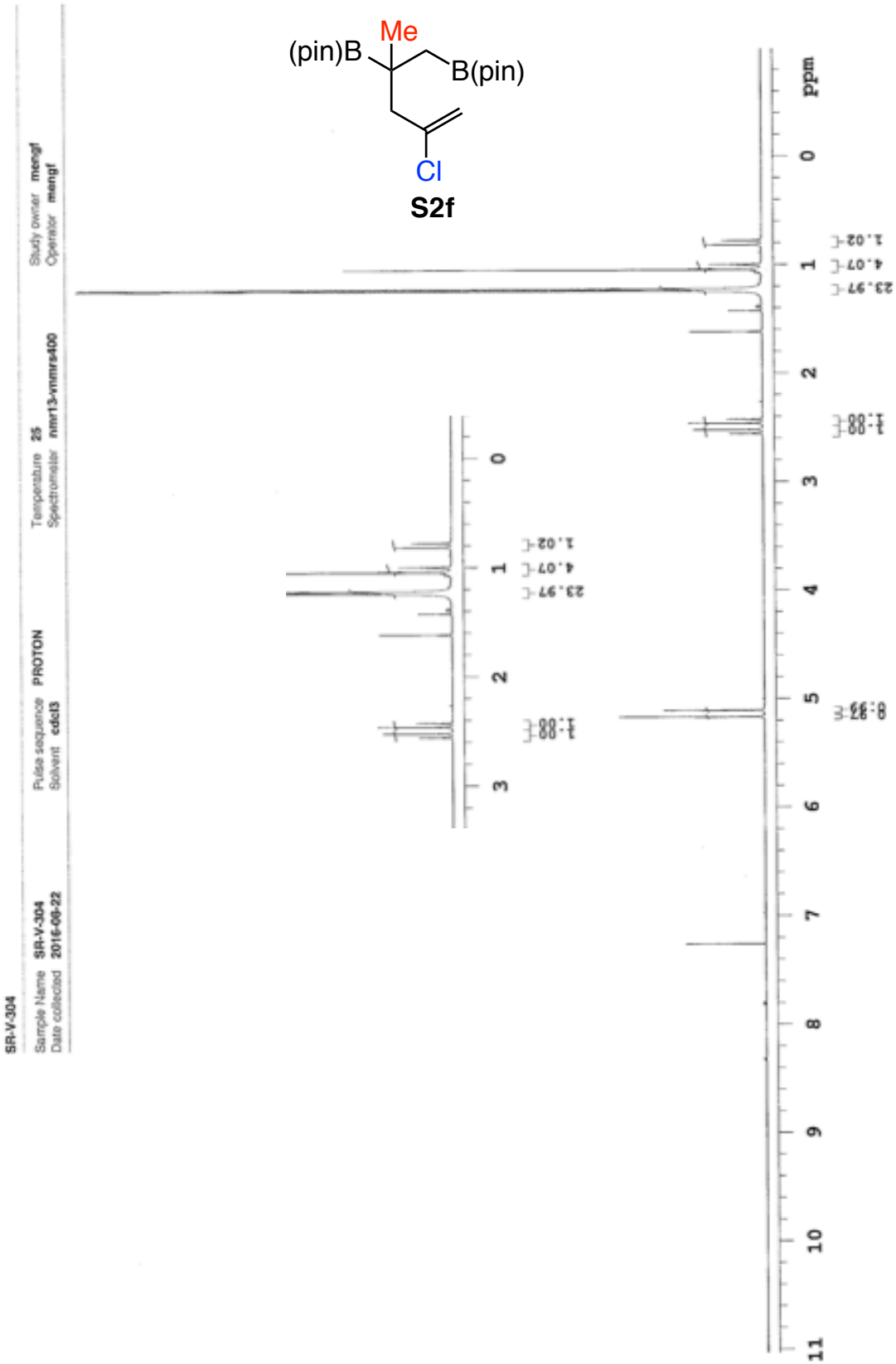

Me
(pin)B
B(pin)
TBSO
S2c
SR-VI-34-C-carbon
Sample Name SR-VI-34-C-carbon
Date collected 2016-08-03
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200

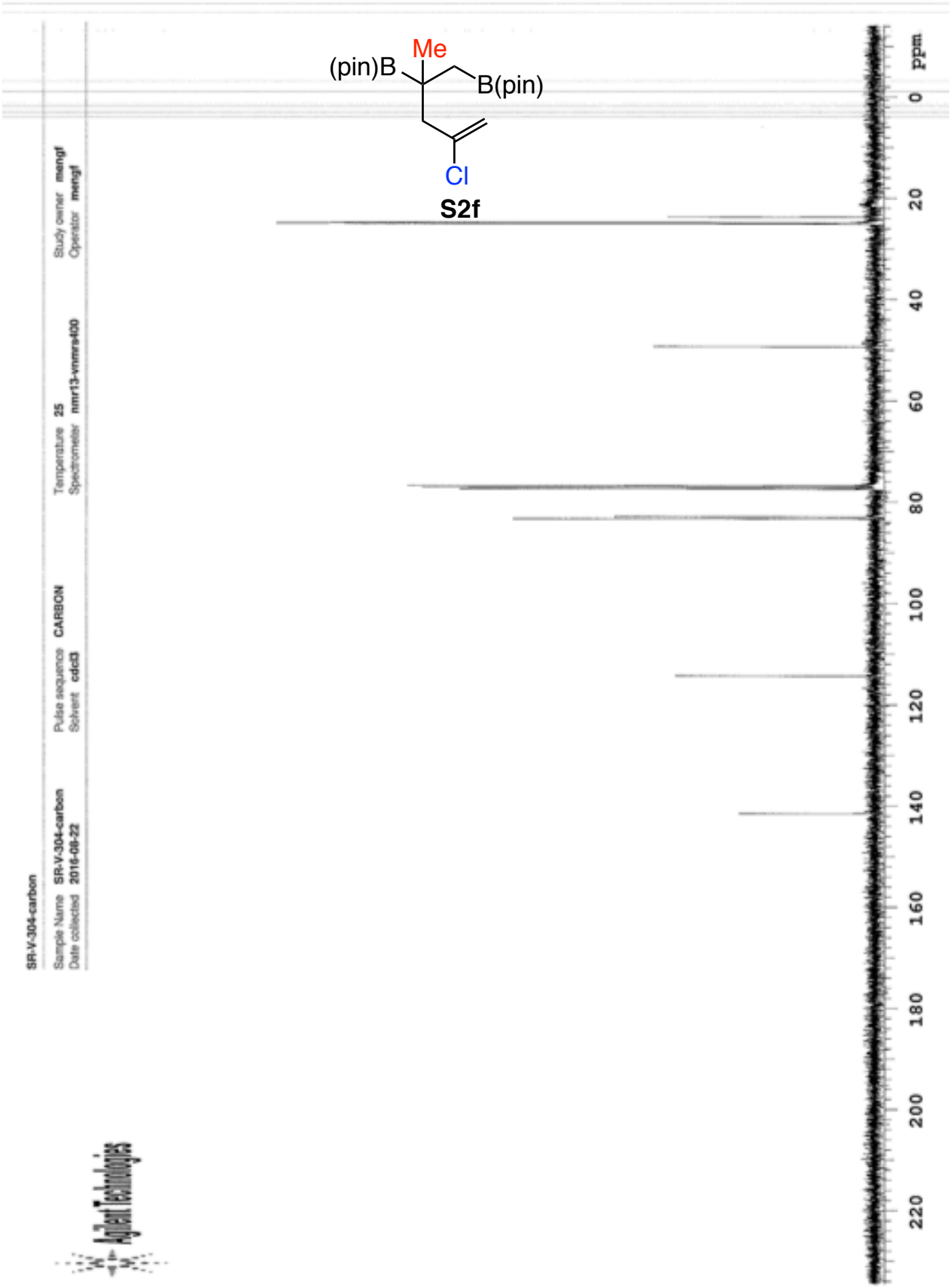

Me
(pin)B
B(pin)
Ph
S2d
SR-V-306-C
Sample Name SR-V-306-C
Date collected 2016-07-25
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm

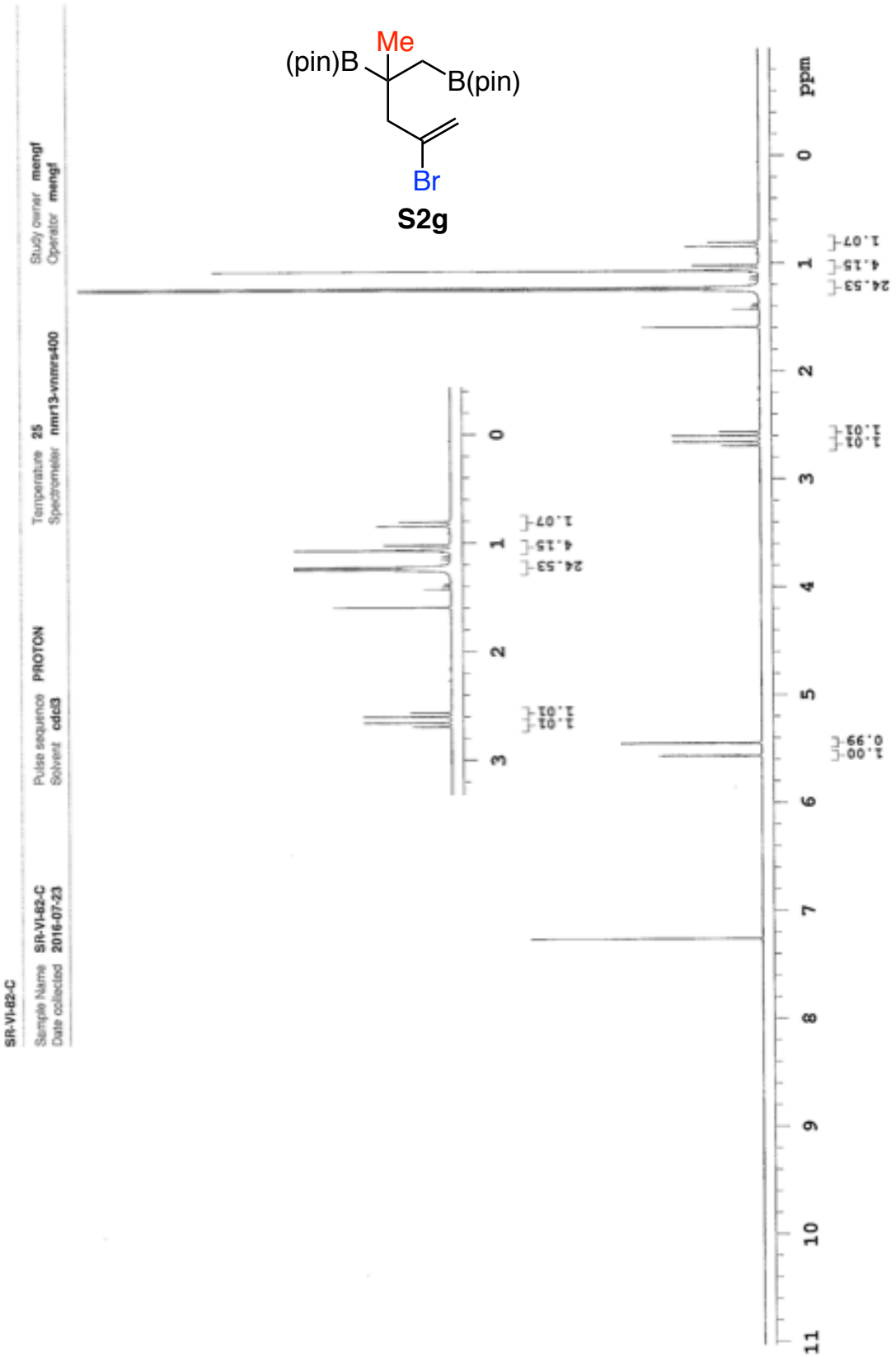

Me
(pin)B
B(pin)
Ph
S2d
SR-V-306-C-carbon
Sample Name SR-V-306-C-carbon
Date collected 2016-07-25
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220

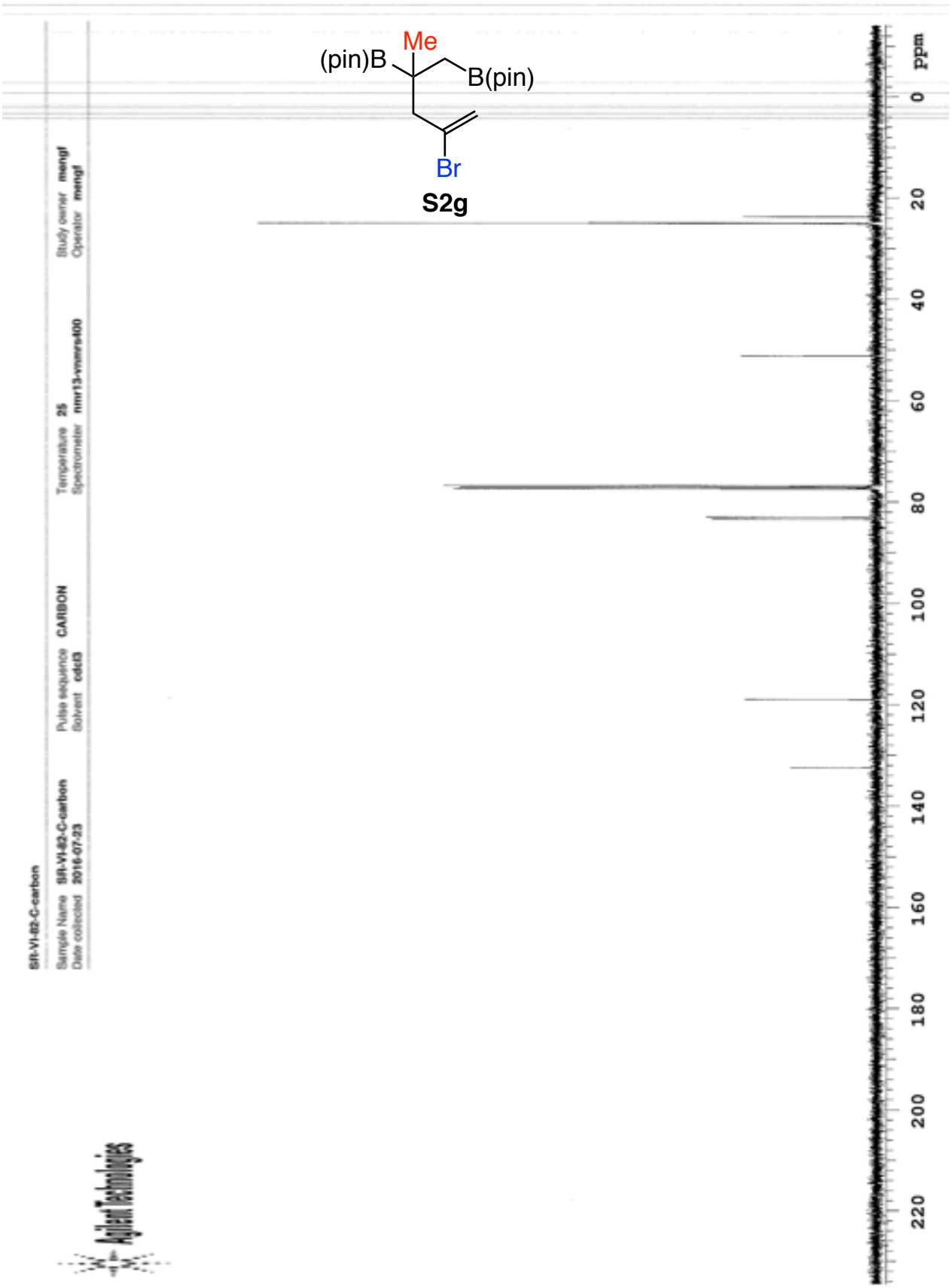

(pin)B
Me
B(pin)
SiMe3
S2e
SR-VI-61-C
Sample Name SR-VI-61-C
Date collected 2016-06-06
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
8.64
1.01
4.00
24.06
1.01
1.01
1.00
1.00


Me
(pin)B
B(pin)
SiMe3
S2e
SR-VI-61-C-carbon
Sample Name SR-VI-61-C-carbon
Date collected 2016-06-06
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220


Me
(pin)B
B(pin)
Cl
S2f
SR-V-304
Sample Name SR-V-304
Date collected 2016-08-22
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
1.02
4.07
23.97
1.88
8.93


Me
(pin)B
B(pin)
Cl
S2f
SR-V-304-carbon
Sample Name SR-V-304-carbon
Date collected 2016-08-22
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220


Me
(pin)B
B(pin)
Br
S2g
SR-VI-82-C
Sample Name SR-VI-82-C
Date collected 2016-07-23
Pulse sequence PROTON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
1.07
4.15
24.53
1.01
1.01
0.99
1.00


Me
(pin)B
B(pin)
Br
S2g
Efi-VI-82-C-carbon
Sample Name SR-VI-82-C-carbon
Date collected 2016-07-23
Pulse sequence CARBON
Solvent cdcl3
Temperature 25
Spectrometer nmr13-vnmrs400
Study owner mengf
Operator mengf
ppm
0
20
40
60
80
100
120
140
160
180
200
220