Supporting Information

Stereospecific Suzuki Cross-Coupling of Alkyl α-Cyanohydrin Triflates

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General Procedures. All reactions were maintained under an argon atmosphere. Anhydrous solvents were freshly distilled from sodium benzophenone ketyl or from CaH_2. Unless otherwise noted, commercially available materials were used without further purification. Flash chromatography (FC) was performed using E. Merck silica gel 60 (240–400 mesh). Thin layer chromatography (TLC) was performed using pre-coated plates purchased from E. Merck (silica gel 60 PF254, 0.25 mm). spectra were recorded in $CDCl_3$. on Varian 300, 400 or 500 spectrometers at operating frequencies of 300/400/500 MHz (^{1}H) or 75/100/125 MHz (^{13}C) as showed in the parameter of each NMR spectrum. Chemical shifts (δ) are given in ppm relative to residual solvent (usually chloroform δ = 7.26 for ^{1}H NMR or δ = 77.23 for proton decoupled ^{13}C NMR and δ of ^{19}F NMR were relative to neat $CFCl_3$) and coupling constants (J) in Hz. Multiplicity is tabulated as s for singlet, d for doublet, t for triplet, q for quadruplet, and m for multiplet. Optical rotations were measured at room temperature and corrected to 20 ºC on a Rudolph Research Analytical Autopol® IV polarimeter. LC/MS spectra were obtained with an Agilent 1200 series LC/MSD spectrometer. The high-resolution mass spectral analyses were kindly provided by Professor Kasem Nithipatikom at the Medical College of Wisconsin Mass Spectroscopy Facility. The enantiomeric excesses, expressed as % ee, were determined using a Shimazu HPLC system with chiral columns as specified in the individual experimental descriptions and verified using appropriate racemic mixtures.

Racemic[1] and non-racemic[2] α-cyanohydrins were prepared according to literature procedures. 2-Hydroxy-2-phenylacetonitrile was purchased from Aldrich. All boronic acids, boronate esters, potassium trifluoroborate and MIDA boronates were purchased (Aldrich, Frontier Scientific, or Oakwood Products). Anhydrous solvents (THF, DME, benzene) were freshly distilled from sodium benzophenone ketyl; toluene was freshly distilled from CaH_2. All other chemicals were reagent-grade and used as received.

(1) (a) Watahiki, T.; Ohba, S.; Oriyama, T. *Org. Lett.* **2003**, *5*, 2679–2681. (b) Kulkarni, B. A.; Sharma, A.; Gamre, S.; Chattopadhyay, S. *Synthesis*, **2004**, 595–599.
(2) Hamashima, Y.; Sawada, D.; Kanai, M.; Shibasaki, M. *J. Am. Chem. Soc.* **1999**, *121*, 2641–2642.

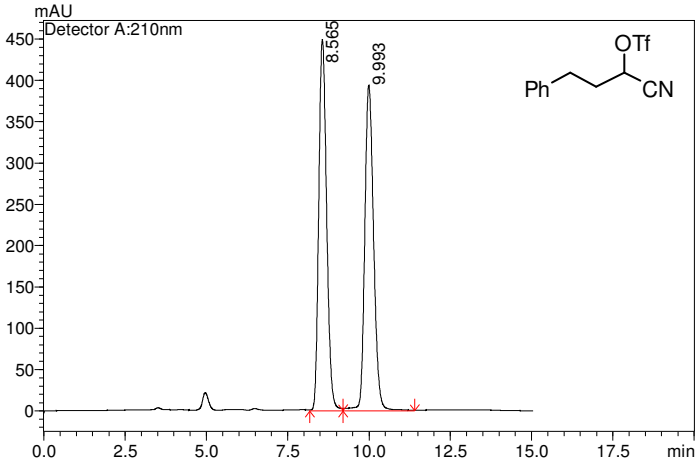
Experimental

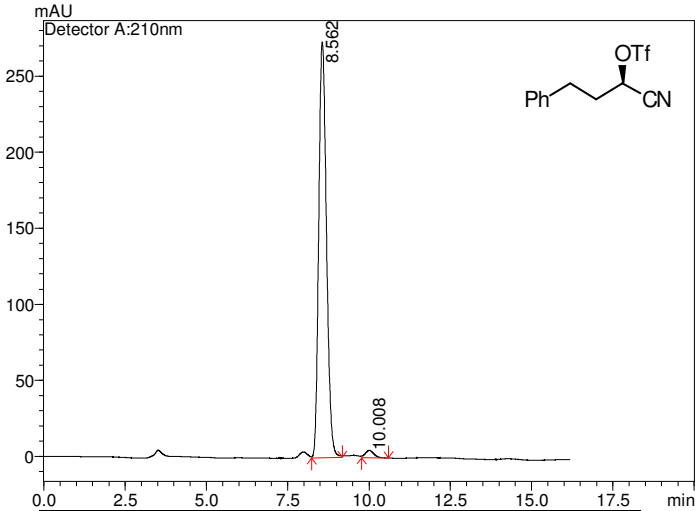
Preparation of α-cyanohydrin triflate/mesylate. To a ≤ −50 ºC solution of α-cyanohydrin (10 mmol) in CH_2Cl_2 (25 mL) in a 100 mL RBF was added 2,6-lutidine (12 mmol) dropwise followed by Tf_2O (or MsCl, 12 mmol). After stirring at 0 ºC for 1-2 h for Tf_2O or overnight for MsCl, the reaction was quenched with water, then extracted with CH_2Cl_2. The organic extracts were combined and washed with brine, dried over anhydrous Na_2SO_4, then concentrated on a rotavapor. The residue was purified by SiO_2 chromatography to give α-cyanohydrin triflate/mesylate (80-90% yield) which was stored neat under an inert atmosphere at −25 ºC until used.

Representative cross-coupling: (*S*)-4-Phenyl-2-*p*-tolylbutyronitrile 3 (Table 2, entry 1). A mixture of 4-tolylboronic acid (**2**) (37 mg, 0.3 mmol), KF (35 mg, 0.6 mmol), and palladium catalyst **A** (5.3 mg, 0.0075 mmol) in toluene (1 mL) and H_2O (10 μL, sparged with argon) were stirred at rt under an argon atmosphere for 5 min. To this was added a solution of (*S*)-1-cyano-3-phenylpropyl trifluoromethanesulfonate **1** (44 mg, 0.15 mmol, 99% e.e.) in toluene (1 mL) and then stirred at 40 ºC. After 20 h, the reaction mixture was filtered though a pad of silica gel and the silica gel pad was washed with EtOAc (100 mL). The combined filtrate was concentrated under reduced pressure and the residue was purified by SiO_2 chromatography to give (*S*)-4-phenyl-2-*p*-tolylbutyronitrile **3** (31 mg, 91%, 98% e.e.).

New Compound Characterization and HPLC Chromatograms

1-Cyano-3-phenylpropyl trifluoromethanesulfonate (1). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.19 (5H, m), 5.28 (1H, t, J = 6 Hz), 2.90 (2H, t, J = 6 Hz), 2.48-2.40 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.7, 129.2, 128.5, 127.4, 118.4 (q, $J_{C\text{-}F}$ = 320 Hz), 113.9, 71.4, 35.3, 30.2; ^{19}F NMR (282 MHz, $CDCl_3$) δ 74.5; LC/MS (ES) m/z 293 $[M]^+$.





Peak#	Retention time (min)	Area%
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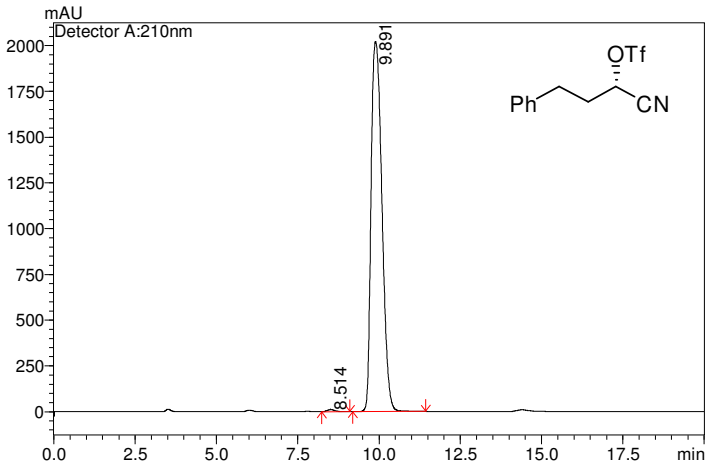
2	10.0	2.0



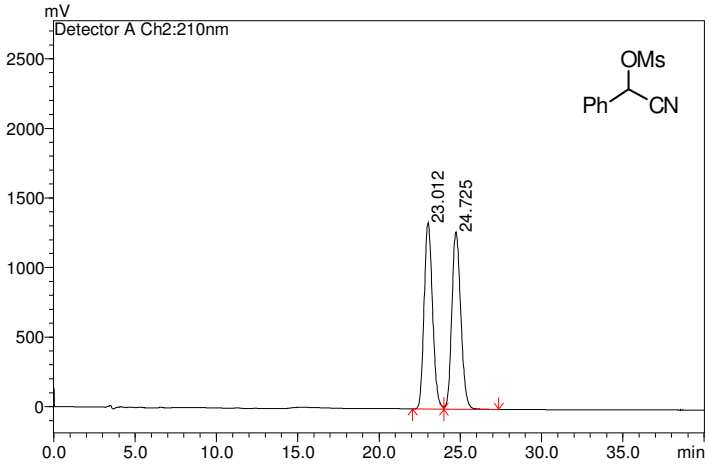
Peak#	Retention time (min)	Area%
1	8.5	0.4
2	9.9	99.6

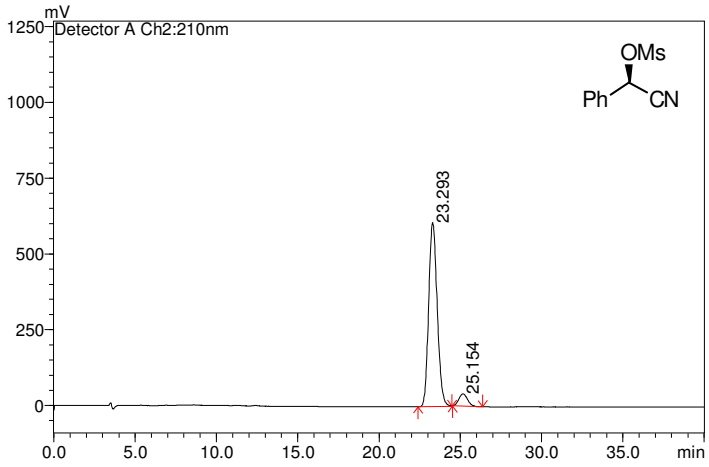
Chiralpak AD (4.6 × 250 mm), hexane/IPA 100:0.5, 1 mL/min, 210 nm

1-Cyano(cyclohexyl)methyl trifluoromethanesulfonate (19). ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.14 (1H, d, *J* ~ 6 Hz), 2.10-1.10 (11H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 118.4 (q, $J_{C\text{-}F}$ ~ 320 Hz), 113.4, 76.6, 41.4, 27.5, 25.4, 25.1, 25.05; ^{19}F NMR (282 MHz, $CDCl_3$) δ 74.5; LC/MS (APCI) *m/z* 271 $[M]^+$.

1-Cyano-2,2-dimethylpropyl trifluoromethanesulfonate (21). ^{1}H NMR (300 MHz, $CDCl_3$) δ 4.98 (1H, s), 1.19 (9H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ 118.5 (q, $J_{C\text{-}F}$ ~ 320 Hz), 113.3, 80.5, 36.3, 24.7; ^{19}F NMR (282 MHz, $CDCl_3$) δ 74.3; LC/MS (APCI) *m/z* 268 $[M+Na]^+$.

(*R*)-Cyano(phenyl)methyl methanesulfonate (27).[3] (87% e.e.) ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59-7.46 (5H. m), 6.22 (1H, s), 3.12 (3H, s).



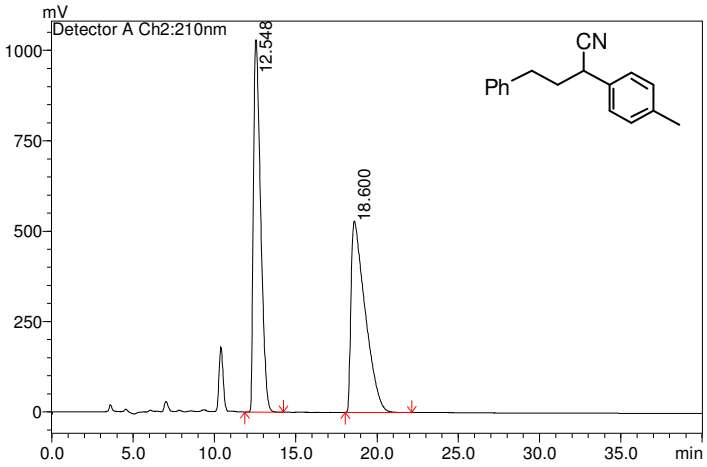


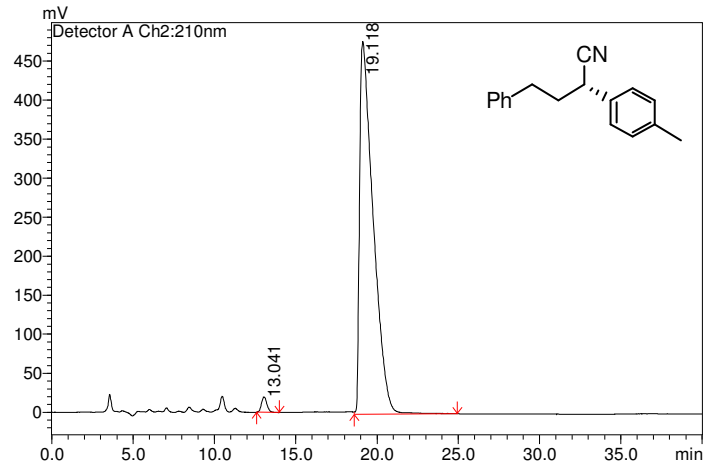
Peak#	Retention time (min)	Area%
1	23.3	93.6
2	25.2	6.4

Chiralpak AD (4.6 × 250 mm), hexane/IPA 100:5, 1 mL/min, 210 nm.

(3) Marco, J. L.; Ingate, S. T.; Jaime, C.; Bea, I. *Tetrahedron*, **2000**, *56*, 2523–2531.

(*S*)-4-Phenyl-2-p-tolylbutanenitrile 3[4] (Table 2, entry 1, 98% e.e.). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.21 (10H, m), 3.72 (1H, dd, *J* ~ 9, 6 Hz), 2.85-2.78 (2H, m), 2.37 (3H, s), 2.33-2.10 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.1, 138.1, 132.8, 129.9, 128.8, 128.6, 127.3, 126.6, 121.0, 37.5, 36.3, 33.2, 21.3.



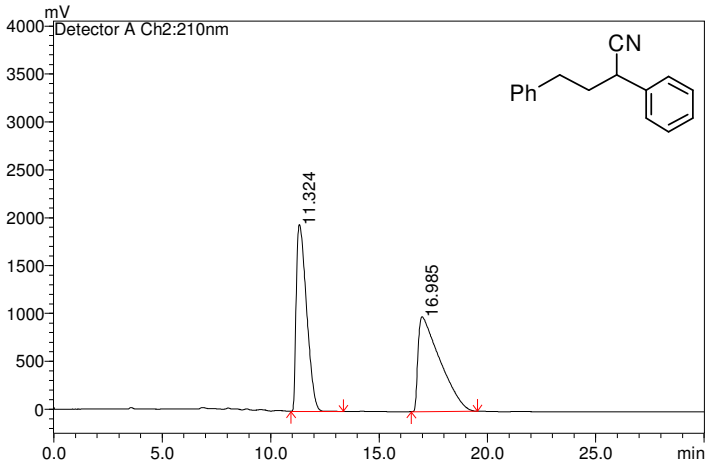


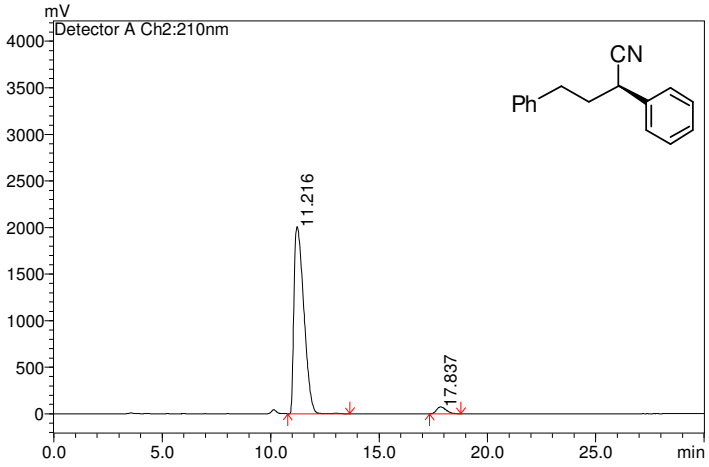
Peak#	Retention time (min)	Area%
1	13.0	1.6
2	19.1	98.4

Chiralpak AD (4.6 × 250 mm), hexane/IPA 100:1, 1 mL/min, 210 nm

(4) Hino, K.; Nagai, Y.; Uno, H.; Masuda, Y.; Oka, M.; Karasawa, T. *J. Med. Chem.* **1988**, *31*, 107–117.

(*R*)-2,4-diphenylbutanenitrile 6[5] (Table 2, entry 2, 94% e.e.). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42-7.19 (10H, m), 3.75 (1H, dd, *J* ~ 9, 6 Hz), 2.86-2.79 (2H, m), 2.34-2.11 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 135.8, 129.3, 128.9, 128.6, 128.3, 127.5, 126.7, 120.8, 37.6, 36.8, 33.2.





Peak#	Retention time (min)	Area%
1	11.2	96.8
2	17.8	3.2

Chiralpak AD (4.6 × 250 mm), hexane/IPA 100:1, 1 mL/min, 210 nm.

(5) Kozikowski, A. P.; Tueckmantel, W.; George, C. *J. Org. Chem.* **2000**, *65*, 5371–5381.

4-Phenyl-2-*o*-tolylbutanenitrile 8 (Table 2, entry 3). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.14 (9H, m), 3.86 (1H, dd, *J* ~ 9, 5 Hz), 2.94-2.76 (2H, m), 2.15 (3H, s), 2.25-2.03 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.0, 135.1, 134.2, 131.2, 128.9, 128.6, 128.3, 127.5, 127.1, 126.8, 121.1, 36.2, 33.5, 33.4, 19.0; HRMS Calcd. for $C_{17}H_{17}NNa$ $[M+Na]^+$ *m/z* 258.1253. Found: 258.1258.

2-(4-Methoxyphenyl)-4-phenylbutanenitrile 10[4] (Table 2, entry 4). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.18 (7H, m), 6.93-6.88 (2H, m), 3.81 (3H, s), 3.70 (1H, dd, *J* ~ 9, 6 Hz), 2.83-2.74 (2H, m), 2.32-2.08 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 140.0, 128.8, 128.61, 128.60, 127.7, 126.6, 121.1, 114.6, 55.5, 37.5, 35.9, 33.2.

2-(4-Acetylphenyl)-4-phenylbutanenitrile 12 (Table 2, entry 5). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (2H, d, *J* ~ 8 Hz), 7.28 (2H, d, *J* ~ 8 Hz), 7.33-7.18 (5H, m), 3.80 (1H, dd, *J* ~ 9, 6 Hz), 2.86-2.80 (2H, m), 2.61 (3H, s), 2.30-2.16 (2H, m); HRMS Calcd. for $C_{18}H_{17}NNaO$ $[M+Na]^+$ *m/z* 286.1202. Found: 286.1208.

2-(4-Fluorophenyl)-4-phenylbutanenitrile 14[4] (Table 2, entry 6). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.18 (7H, m), 6.93-6.88 (2H, m), 3.81 (3H, s), 3.70 (1H, dd, *J* ~ 9, 6 Hz), 2.83-2.74 (2H, m), 2.32-2.08 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.6 (d, J_{C-F} ~ 248 Hz), 139.8, 131.6, 129.2 (d, J_{C-F} ~ 8 Hz), 128.9, 128.6, 126.8, 120.6, 116.3 (d, J_{C-F} ~ 22 Hz), 37.6, 36.0, 33.1.

2-(2-Chlorophenyl)-4-phenylbutanenitrile 16[4] (Table 2, entry 7). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (1H, dd, *J* ~ 6, 3 Hz), 7.41-7.21 (8H, m), 4.25 (1H, dd, *J* ~ 9, 6 Hz), 2.99-2.78 (2H, m), 2.26-2.12 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.8, 133.7, 132.8, 130.3, 129.7, 129.1, 128.8, 128.7, 127.8, 126.7, 120.2, 35.8, 34.4, 33.5.

(*E*)-2-Phenethyl-4-phenylbut-3-enenitrile 18 (Table 2, entry 8). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.21 (9H, m), 6.72 (1H, d, *J* ~ 16 Hz), 6.03 (1H, dd, *J* ~ 16, 7 Hz), 3.40-3.36 (1H, m), 2.92-2.79 (2H, m), 2.15-2.02 (2H, m); ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.1, 135.9, 133.8, 128.8, 126.8, 123.0, 120.2, 35.1, 33.9, 33.1; HRMS Calcd. for $C_{18}H_{17}N$ $[M]^+$ *m/z* 248.1434. Found: 248.1440.

2-Cyclohexyl-2-p-tolylacetonitrile 20[6] (Table 2, entry 9). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17 (5H, s), 3.59 (1H, d, *J* ~ 9 Hz), 2.35 (3H, s), 1.90-1.10 (11H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.9, 131.8, 129.6, 128.0, 120.5, 44.1, 42.9, 31.4, 29.8, 26.1, 26.04, 26.00, 21.3.

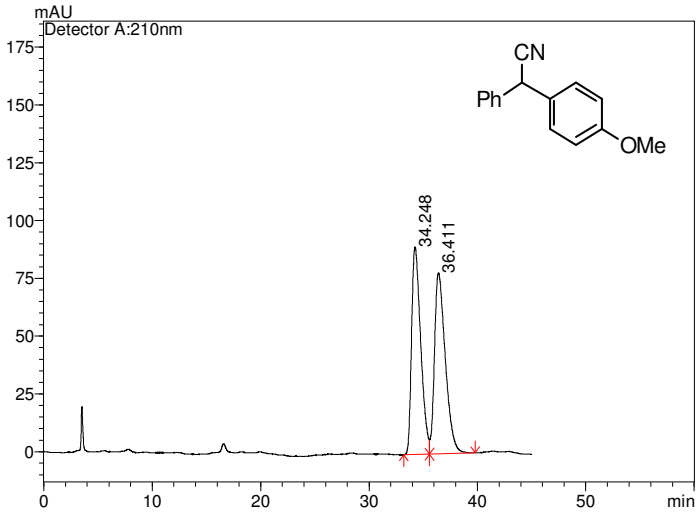
3,3-Dimethyl-2-p-tolylbutanenitrile (22)[7] (Table 2, entry 10). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.16 (5H, s), 3.52 (1H, s), 2.35 (3H, s), 1.04 (9H, s); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.0, 130.5, 129.4, 129.2, 120.8, 49.5, 35.2, 27.6, 21.3.

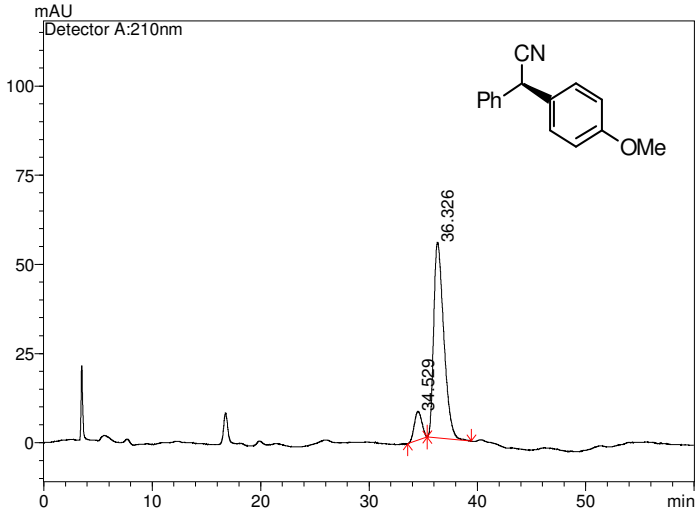
4-Phenyl-2-(thiophen-2-yl)butanenitrile (24) (Table 2, entry 11). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.20 (6H, m), 7.07 (1H, d, *J* ~ 4 Hz), 6.99 (1H, dd, *J* ~ 6, 4 Hz), 3.95 (1H, dd, *J* ~ 8, 7 Hz), 2.88-2.80 (2H, m), 2.39-2.24 (2H, m); ^{13}C NMR (75 MHz, $CDCl_3$) δ 139.7, 137.8, 129.0, 128.7, 127.3, 126.8, 126.5, 125.8, 119.9, 37.5, 33.0, 31.9; HRMS Calcd. for $C_{14}H_{13}NNaS$ $[M+Na]^+$ *m/z* 250.0661. Found: 250.0670.

4-Phenyl-2-(thiophen-3-yl)butanenitrile (26) (Table 2, entry 12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.19 (7H, m), 7.03 (1H, dd, *J* ~ 6, 3 Hz), 3.95 (1H, dd, *J* ~ 6, 3 Hz), 2.85-2.76 (2H, m), 2.32-2.15 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 135.7, 128.9, 128.7, 127.4, 126.7, 126.4, 122.8, 120.6, 36.4, 33.1, 32.0; HRMS Calcd. for $C_{14}H_{13}NNaS$ $[M+Na]^+$ *m/z* 250.0661. Found: 250.0680.

(6) Bordwell, F. G.; Bausch, M. J.; Cheng, J. P.; Cripe, T. H.; Lynch, T. Y.; Mueller, M. E. *J. Org. Chem.* **1990**, *55*, 58–63.
(7) Fischer, H.; Reindl, D.; Hofmann, J.; Troll, C. *J. Organomet. Chem.* **1994**, *472*, 163–174.

(*R*)-2-(4-Methoxyphenyl)-2-phenylacetonitrile (28)[8] (Table 2, entry 13, 80% e.e.). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.31 (5H, m), 7.28-7.25 (2H, m), 6.92-6.89 (2H, m), 5.11 (1H, s), 3.81 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 136.4, 129.4, 129.1, 128.4, 128.1, 127.8, 120.1, 114.7, 55.6, 42.0.



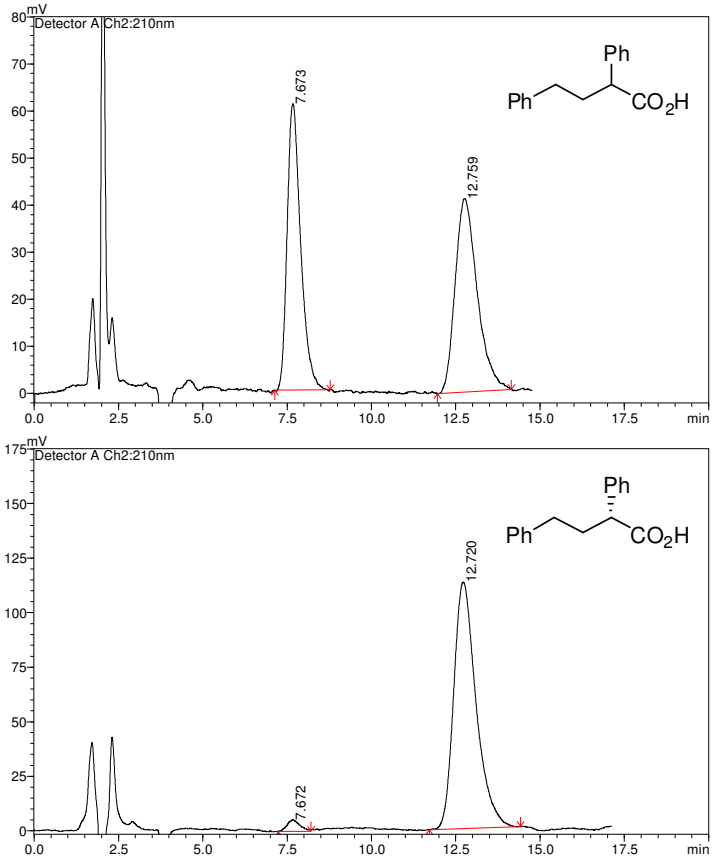


Peak#	Retention time (min)	Area%
1	34.5	9.9
2	36.3	90.1

Chiralpak AD (4.6 × 250 mm), hexane/IPA 100:0.5, 1 mL/min, 210 nm.

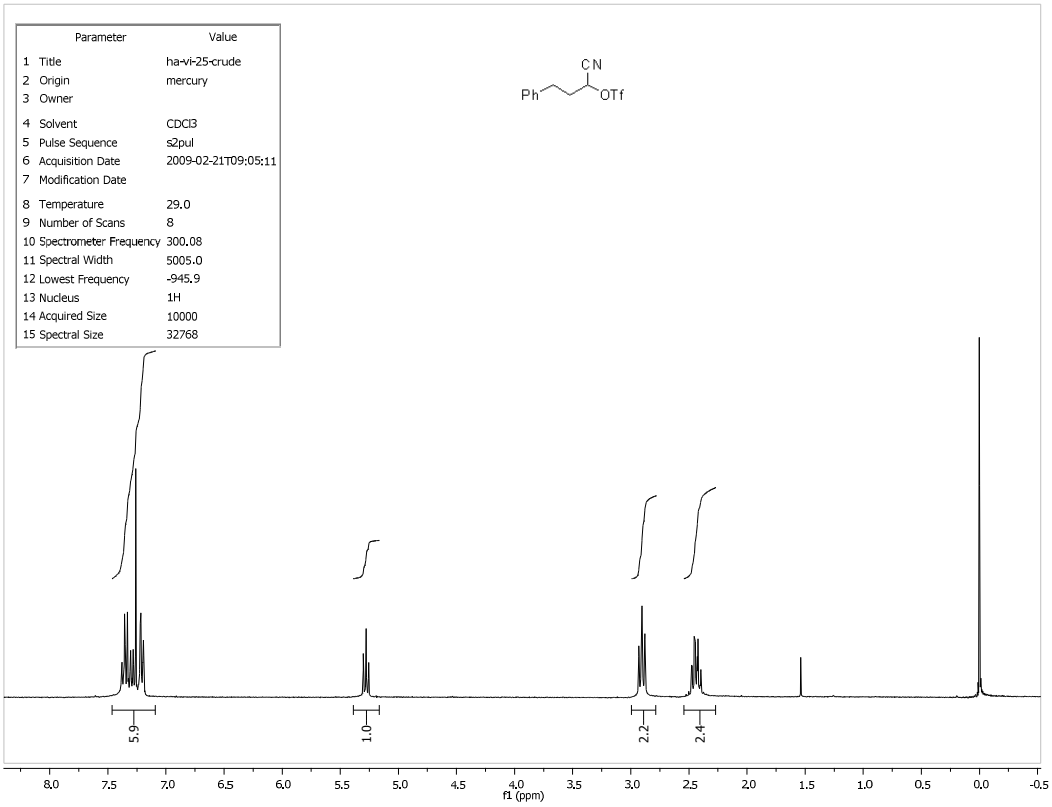
(8) Chen, G.; Wang, Z.; Wu, J.; Ding, K. *Org. Lett.* **2008**, 10, 4573–4576.

(*S*)-2,4-Diphenylbutanoic acid (29)[5] (94% e.e.). $[\alpha]_D^{20}$ = -48.0 (c 0.05, $CHCl_3$); literature[5] $[\alpha]_D$ = -56.8 (*c* 24.9, $CHCl_3$). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.13 (10H, m), 3.58 (1H, t, *J* ~ 9 Hz), 2.59 (2H, t, *J* ~ 9 Hz), 2.48-2.36 (1H, m), 2.18-2.06 (1H, m).



Peak#	Retention time (min)	Area%
1	7.7	2.6
2	12.7	97.3

Chiralcel OD, (4.6 × 250 mm), hexane/IPA/AcOH 100:2/0.2, 2 mL/min, 210 nm.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11 Spectral Width 5005.0
12 Lowest Frequency -945.9
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CN
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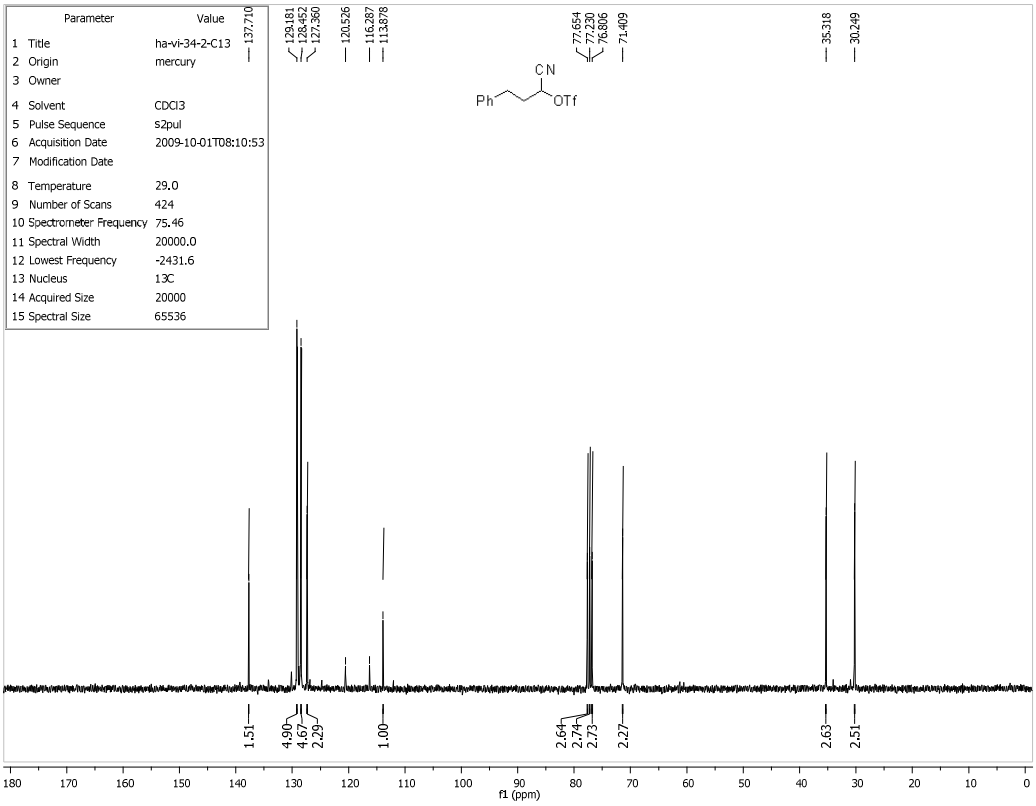
2.2
2.4
f1 (ppm)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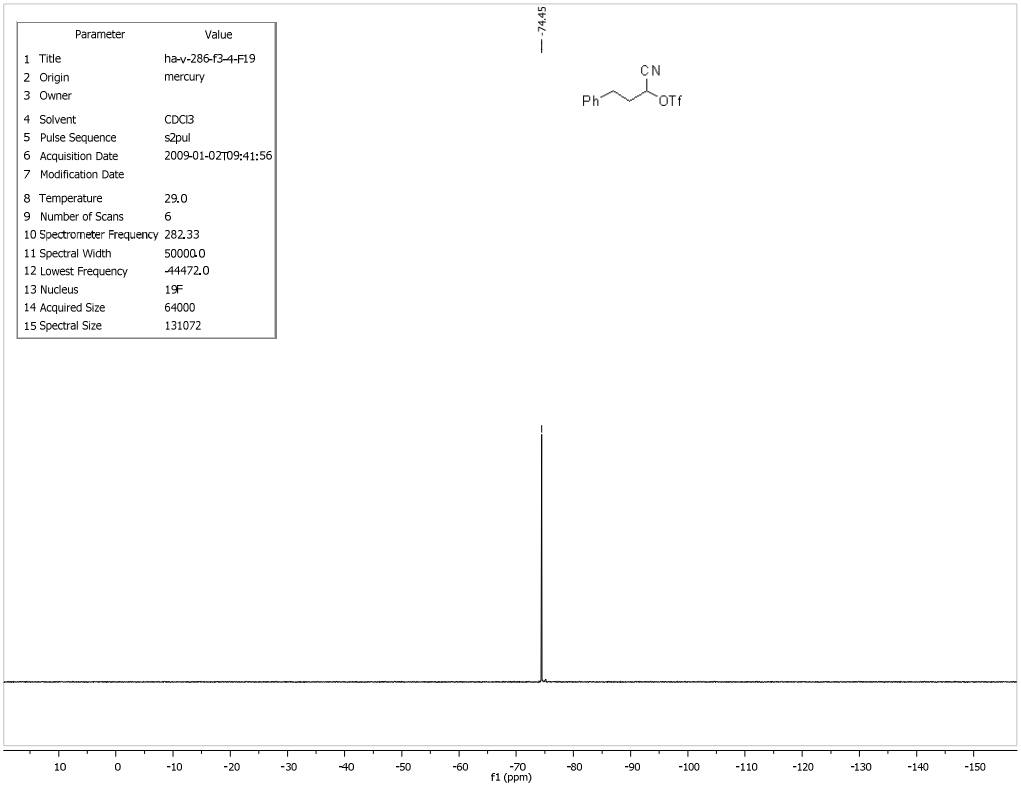
f1 (ppm)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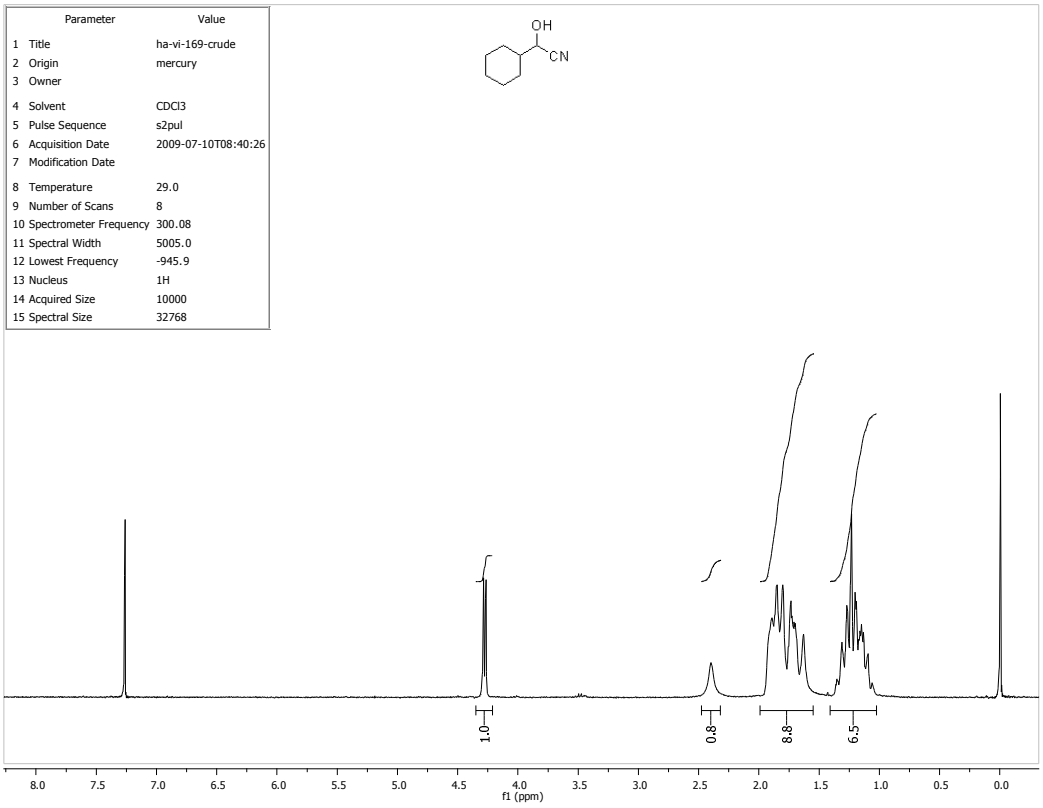
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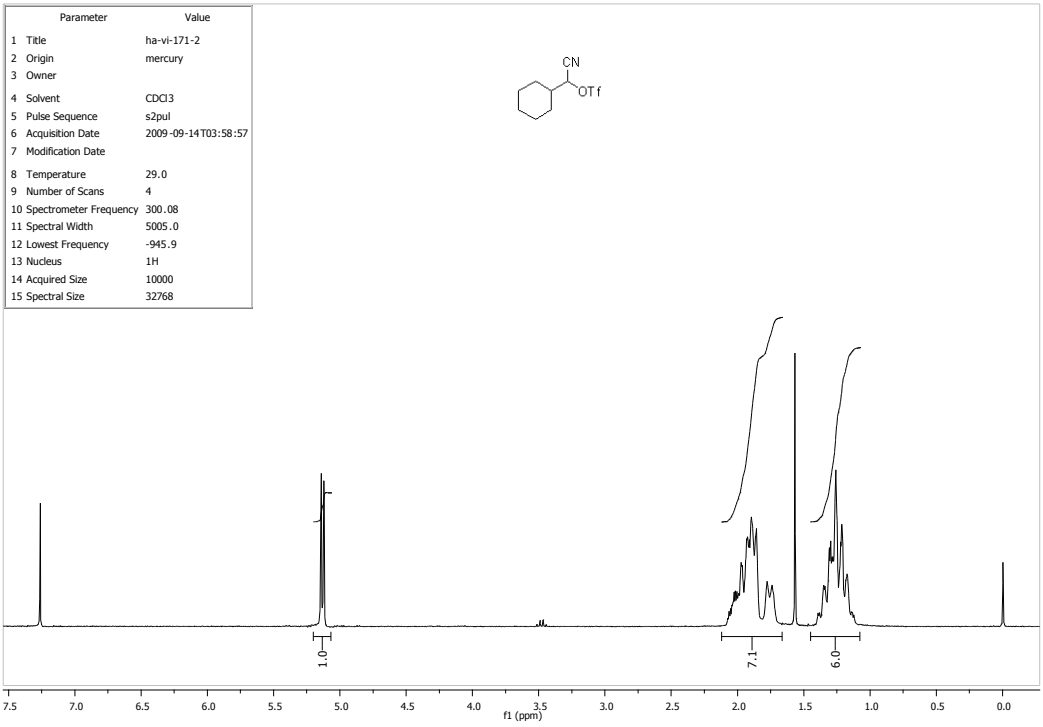
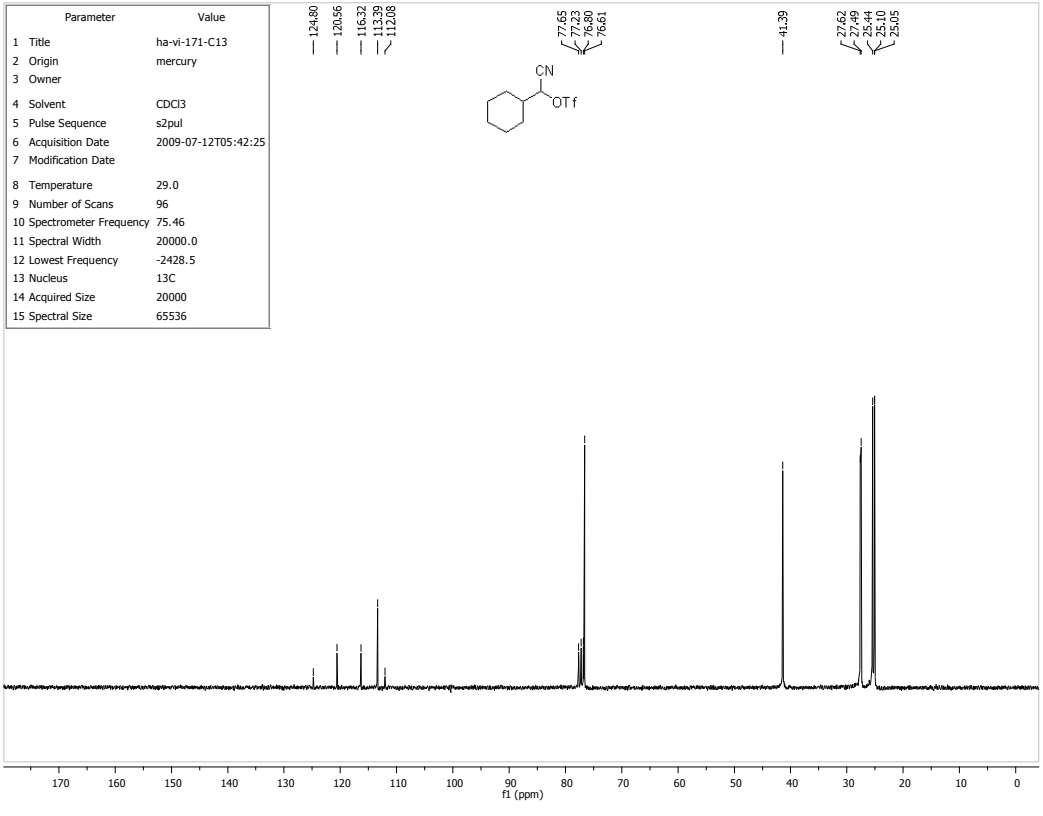
8.8
6.5
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

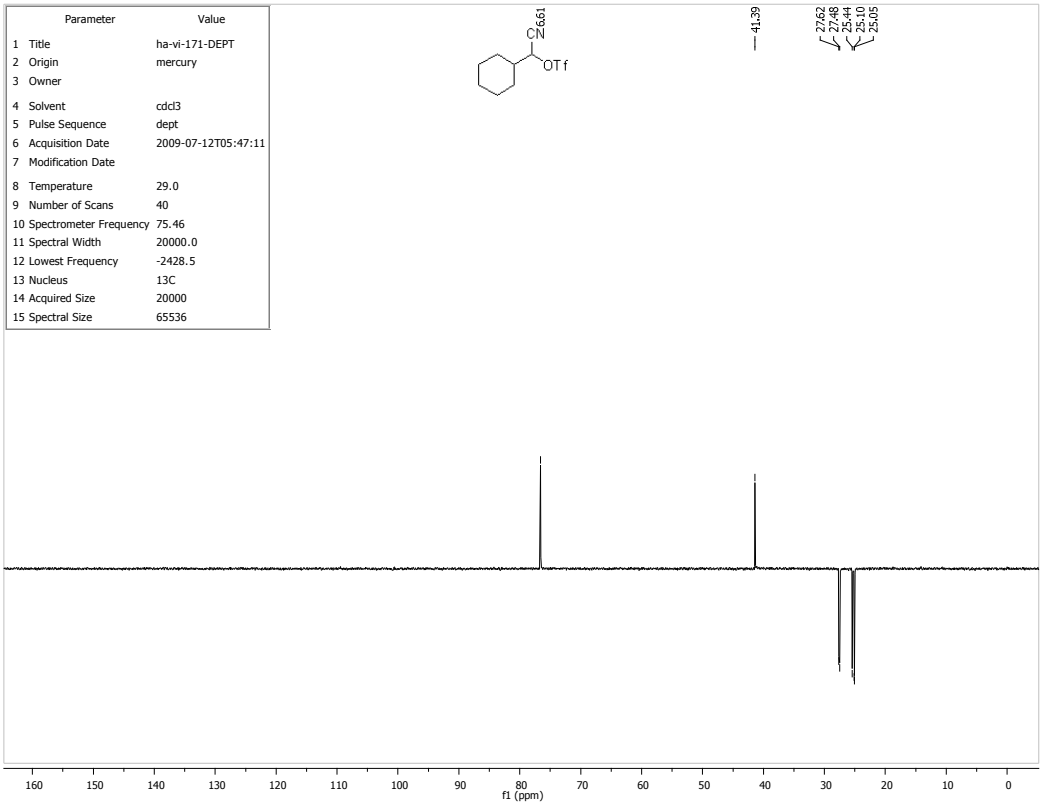
Parameter	Value
1 Title	ha-vi-171-2
2 Origin	mercury
3 Owner	
4 Solvent	CDCl3
5 Pulse Sequence	s2pul
6 Acquisition Date	2009-09-14T03:58:57
7 Modification Date	
8 Temperature	29.0
9 Number of Scans	4
10 Spectrometer Frequency	300.08
11 Spectral Width	5005.0
12 Lowest Frequency	-945.9
13 Nucleus	1H
14 Acquired Size	10000
15 Spectral Size	32768



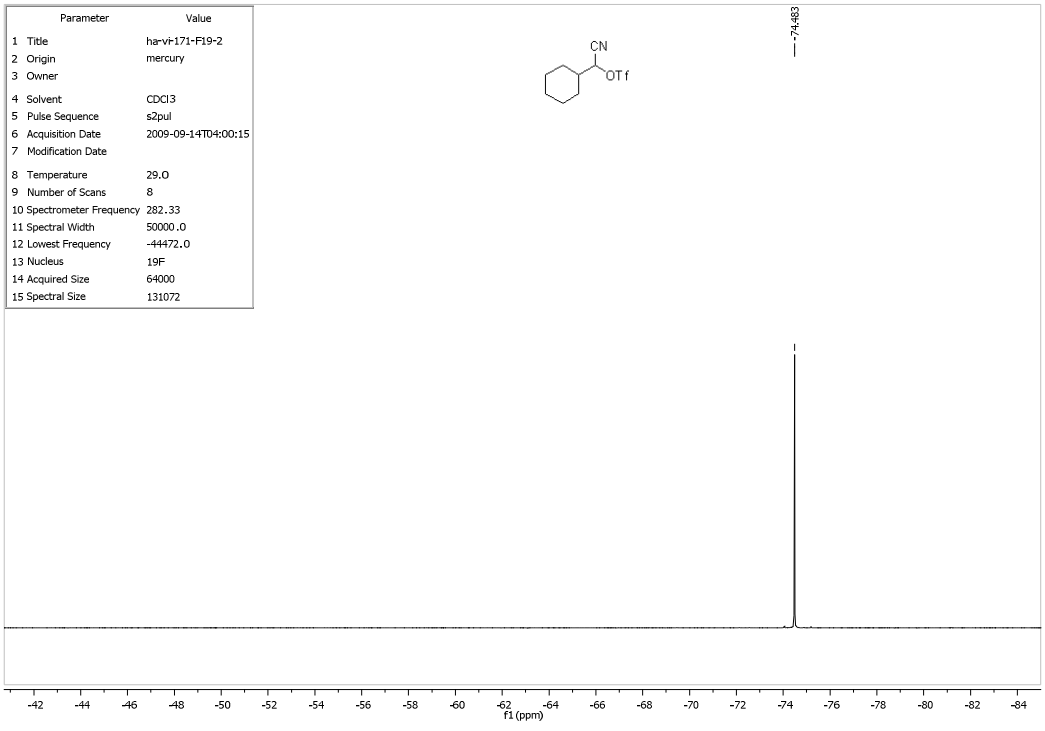
Parameter	Value
1 Title	ha-vi-171-C13
2 Origin	mercury
3 Owner	
4 Solvent	CDCl3
5 Pulse Sequence	s2pul
6 Acquisition Date	2009-07-12T05:42:25
7 Modification Date	
8 Temperature	29.0
9 Number of Scans	96
10 Spectrometer Frequency	75.46
11 Spectral Width	20000.0
12 Lowest Frequency	-2428.5
13 Nucleus	13C
14 Acquired Size	20000
15 Spectral Size	65536



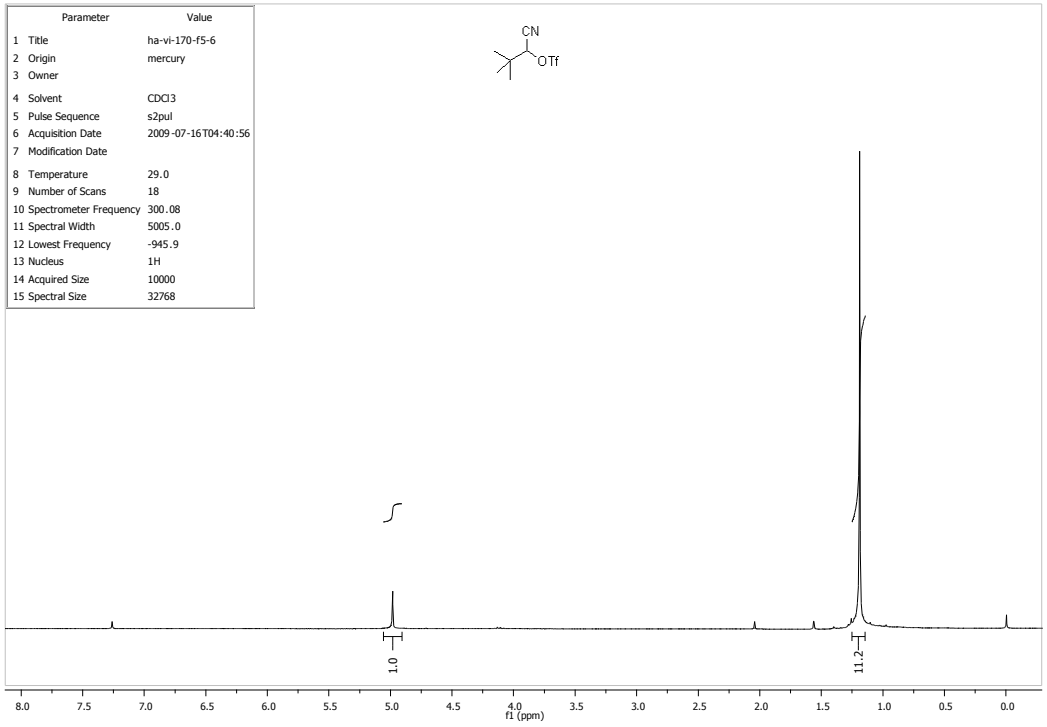
	Parameter	Value
1	Title	ha-vi-171-DEPT
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	dept
6	Acquisition Date	2009-07-12T05:47:11
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	40
10	Spectrometer Frequency	75.46
11	Spectral Width	20000.0
12	Lowest Frequency	-2428.5
13	Nucleus	13C
14	Acquired Size	20000
15	Spectral Size	65536



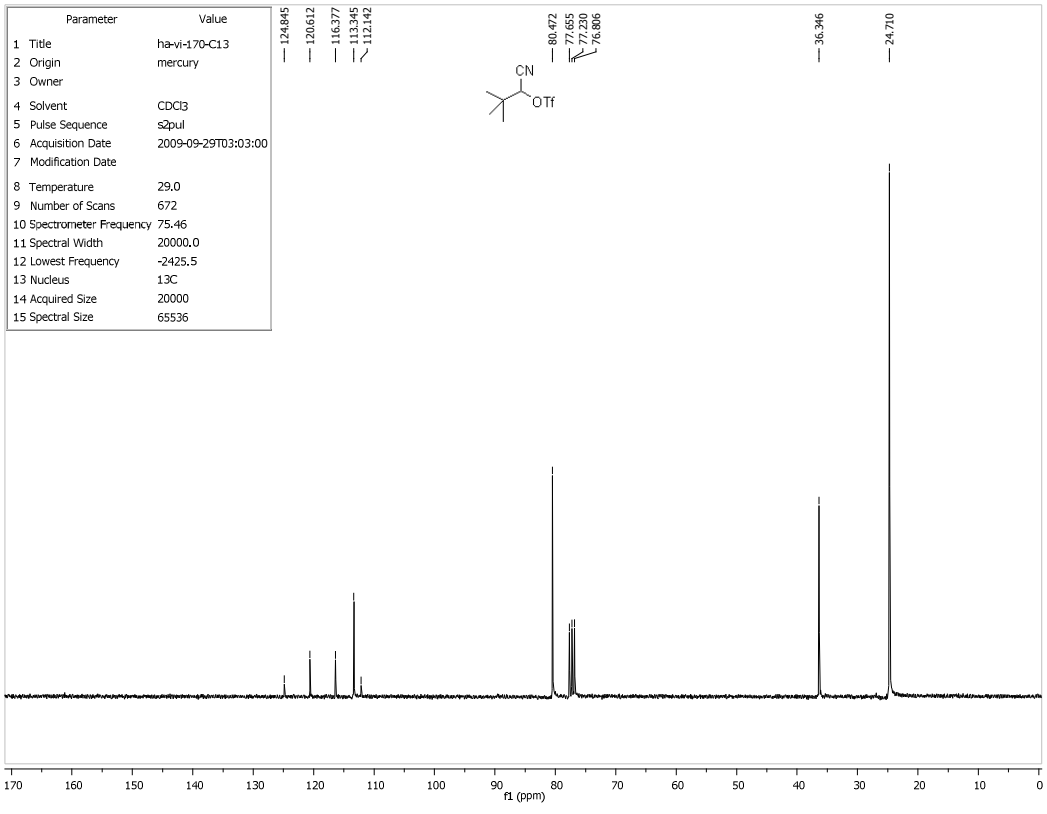
	Parameter	Value
1	Title	ha-vi-171-F19-2
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-09-14T04:00:15
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	8
10	Spectrometer Frequency	282.33
11	Spectral Width	50000.0
12	Lowest Frequency	-44472.0
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072



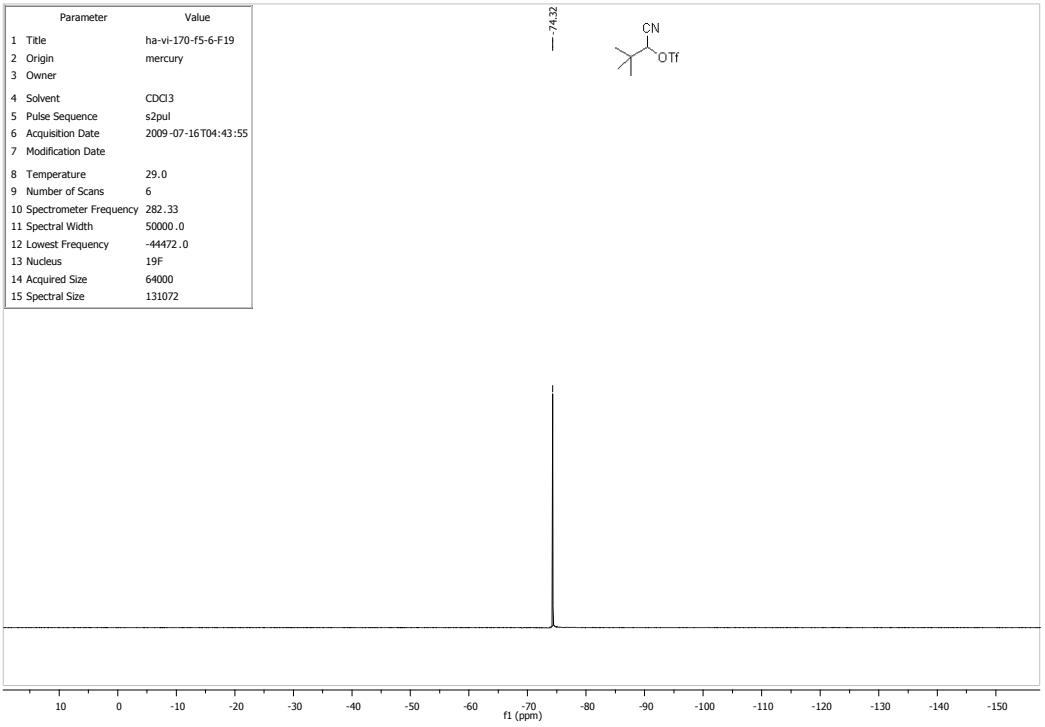
Parameter	Value
1 Title	ha-vi-170-f5-6
2 Origin	mercury
3 Owner	
4 Solvent	CDCl3
5 Pulse Sequence	s2pul
6 Acquisition Date	2009-07-16T04:40:56
7 Modification Date	
8 Temperature	29.0
9 Number of Scans	18
10 Spectrometer Frequency	300.08
11 Spectral Width	5005.0
12 Lowest Frequency	-945.9
13 Nucleus	1H
14 Acquired Size	10000
15 Spectral Size	32768



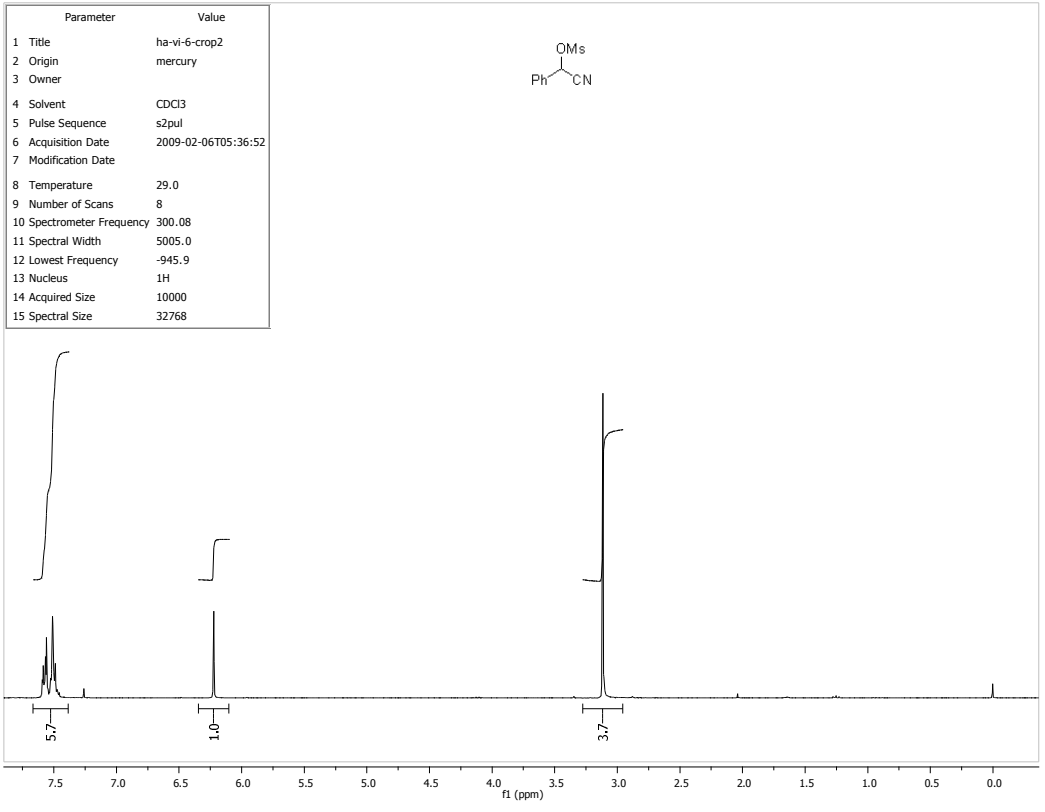
Parameter	Value
1 Title	ha-vi-170-C13
2 Origin	mercury
3 Owner	
4 Solvent	CDCl3
5 Pulse Sequence	s2pul
6 Acquisition Date	2009-09-29T03:03:00
7 Modification Date	
8 Temperature	29.0
9 Number of Scans	672
10 Spectrometer Frequency	75.46
11 Spectral Width	20000.0
12 Lowest Frequency	-2425.5
13 Nucleus	13C
14 Acquired Size	20000
15 Spectral Size	65536

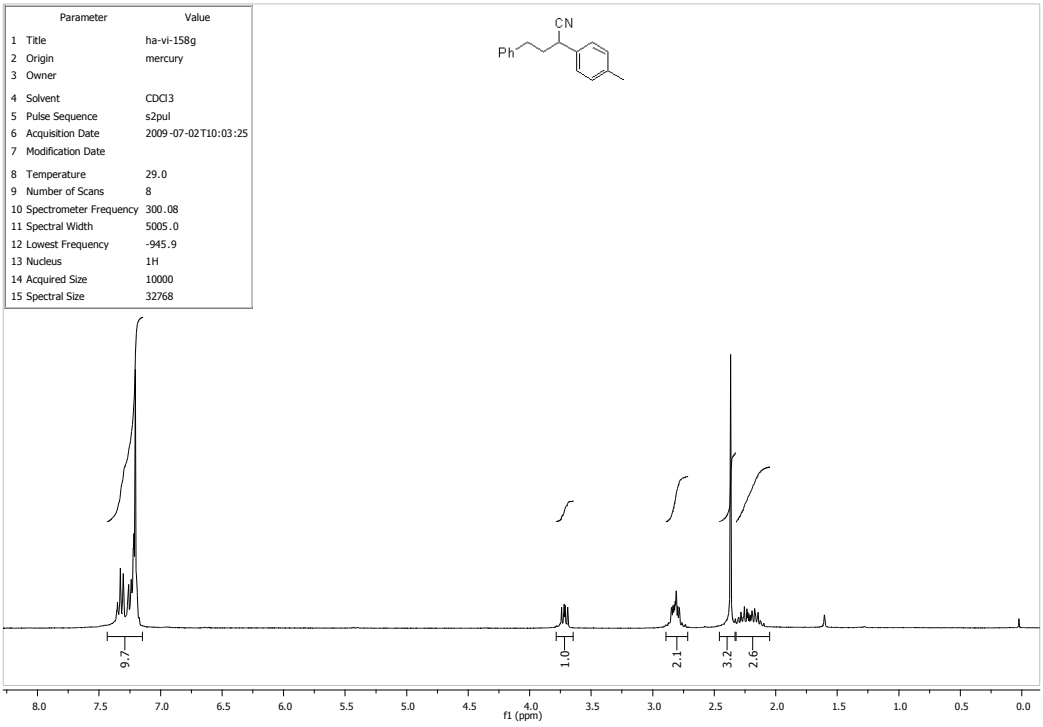


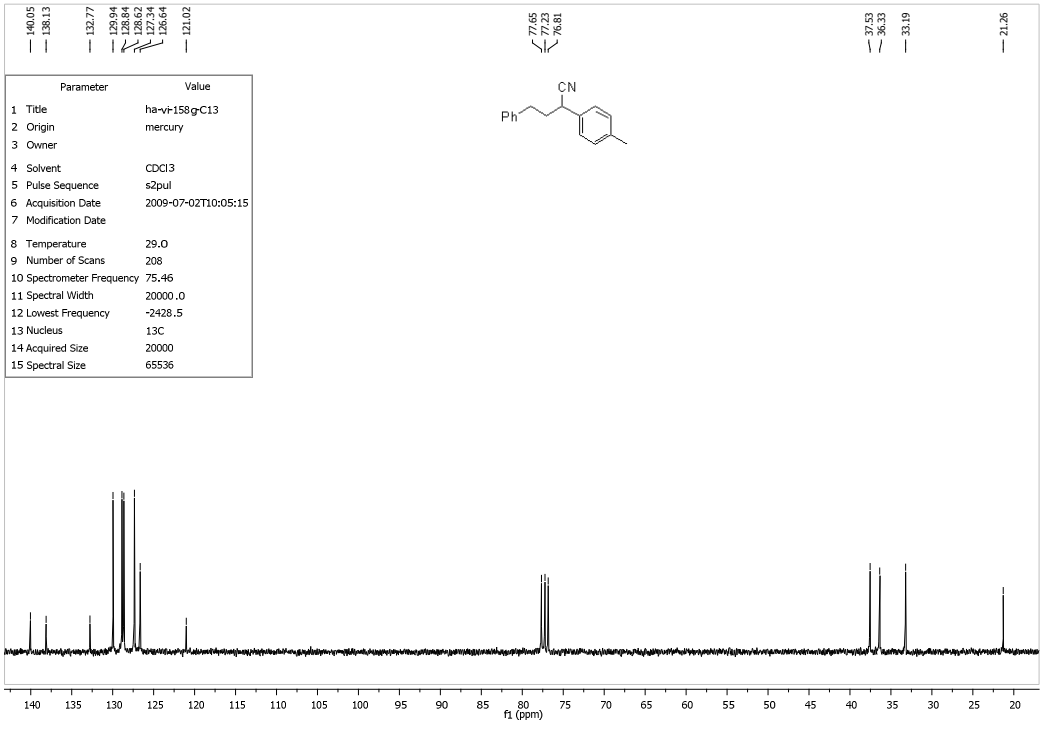
	Parameter	Value
1	Title	ha-vi-170-f5-6-F19
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-07-16T04:43:55
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	6
10	Spectrometer Frequency	282.33
11	Spectral Width	50000.0
12	Lowest Frequency	-44472.0
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072

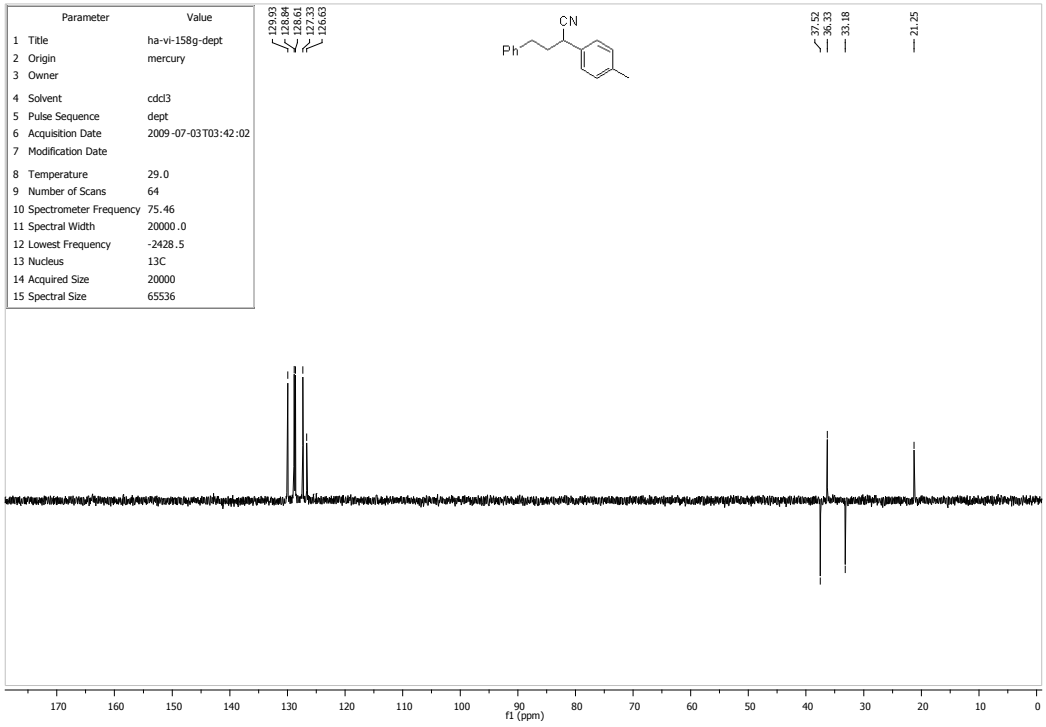


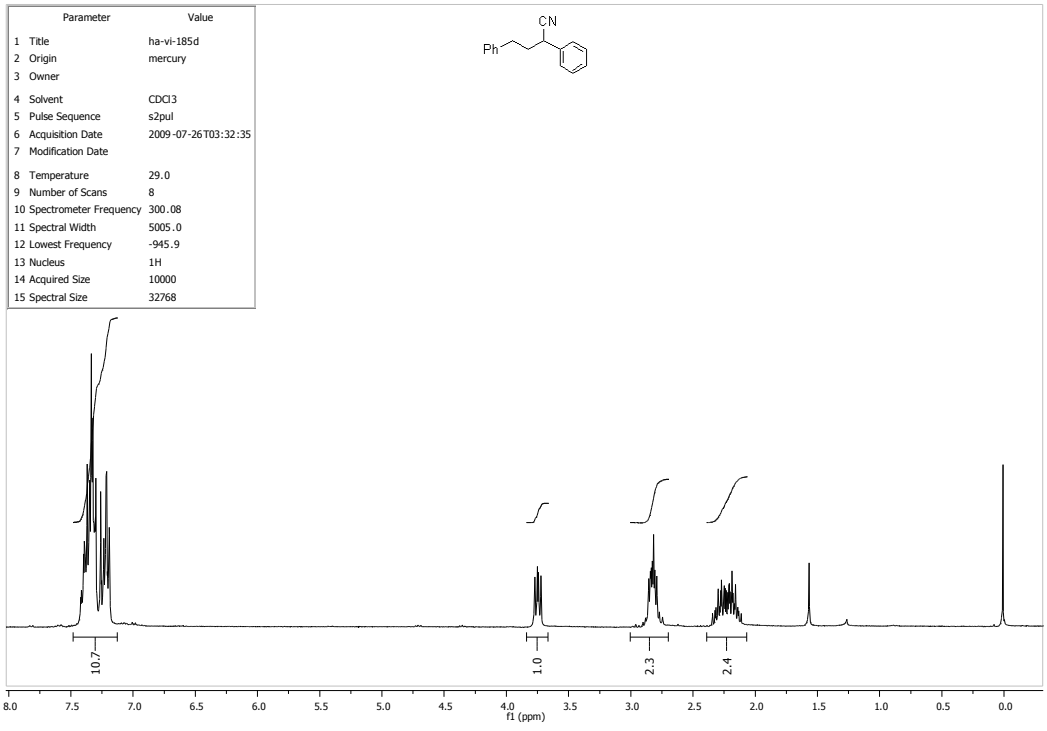
	Parameter	Value
1	Title	ha-vi-6-crop2
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-02-06T05:36:52
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	8
10	Spectrometer Frequency	300.08
11	Spectral Width	5005.0
12	Lowest Frequency	-945.9
13	Nucleus	1H
14	Acquired Size	10000
15	Spectral Size	32768

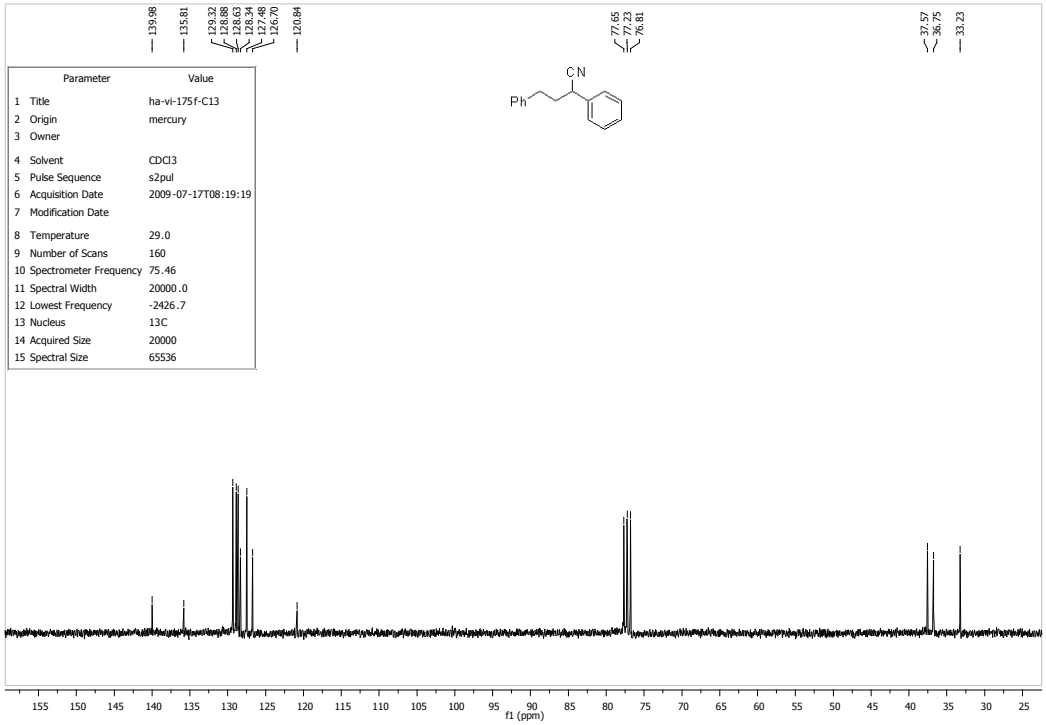


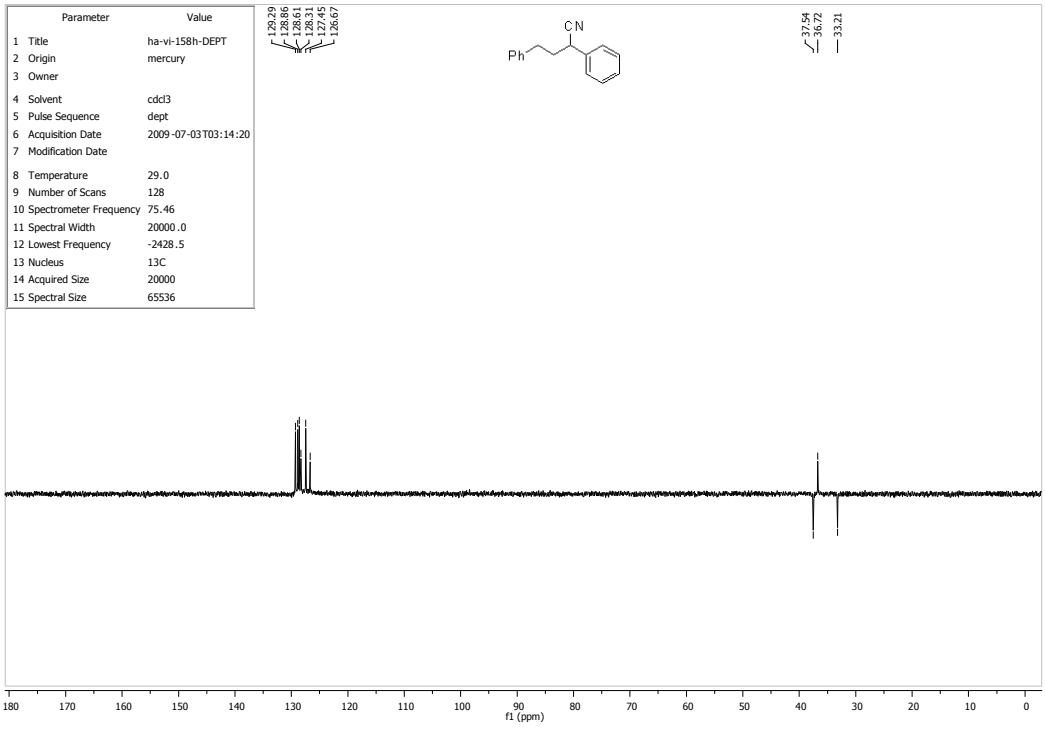

Parameter Value
1 Title ha-vi-158g
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-02T10:03:25
7 Modification Date
8 Temperature 29.0
9 Number of Scans 8
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -945.9
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
Ph
9.7
1.0
2.1
3.2
2.6
f1 (ppm)

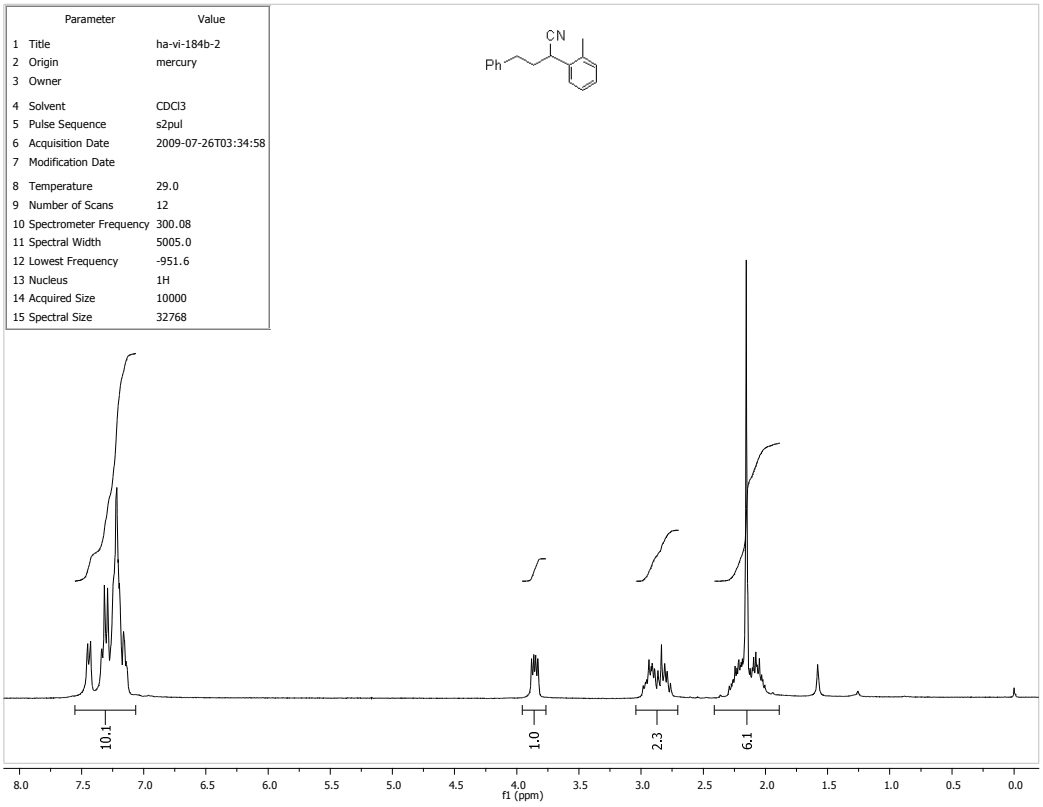

140.05
138.13
132.77
129.94
128.84
128.62
127.34
126.64
121.02
77.65
77.23
76.81
37.53
36.33
33.19
21.26
Parameter Value
1 Title ha-vi-158g-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-02T10:05:15
7 Modification Date
8 Temperature 29.0
9 Number of Scans 208
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2428.5
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
CN
Ph
f1 (ppm)

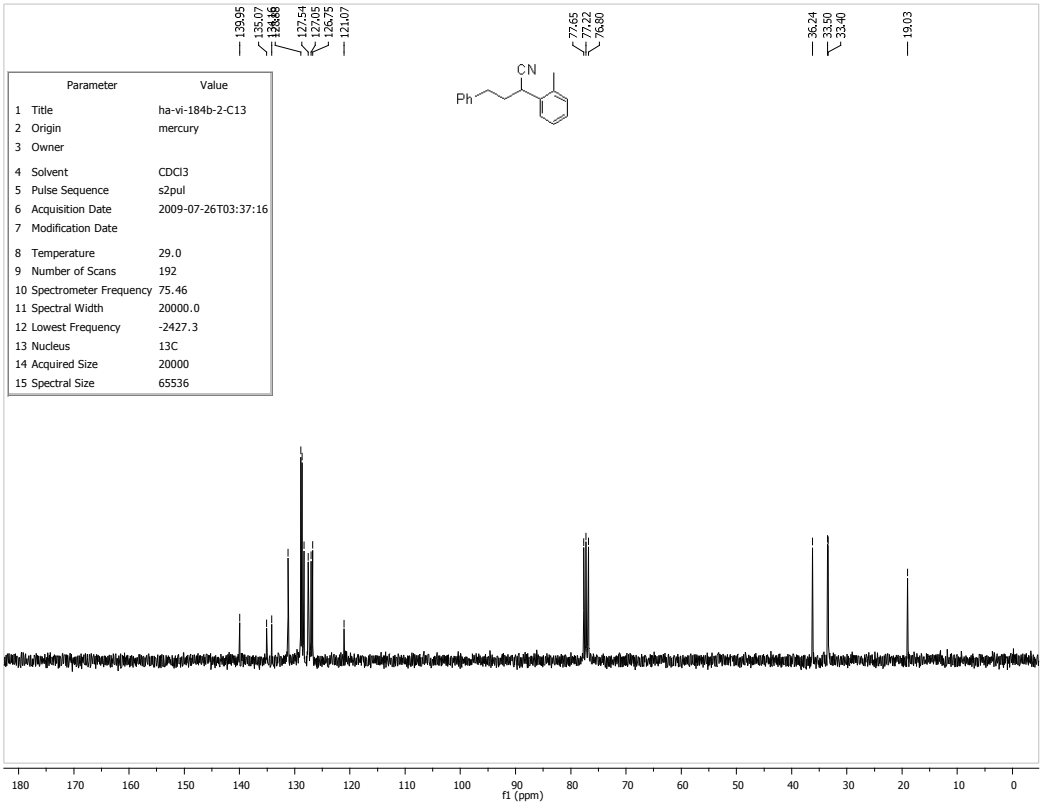

Parameter Value
1 Title ha-vi-158g-dept
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-03T03:42:02
7 Modification Date
8 Temperature 29.0
9 Number of Scans 64
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2428.5
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
129.93
128.84
128.61
127.33
126.63
37.52
36.33
33.18
21.25
CN
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

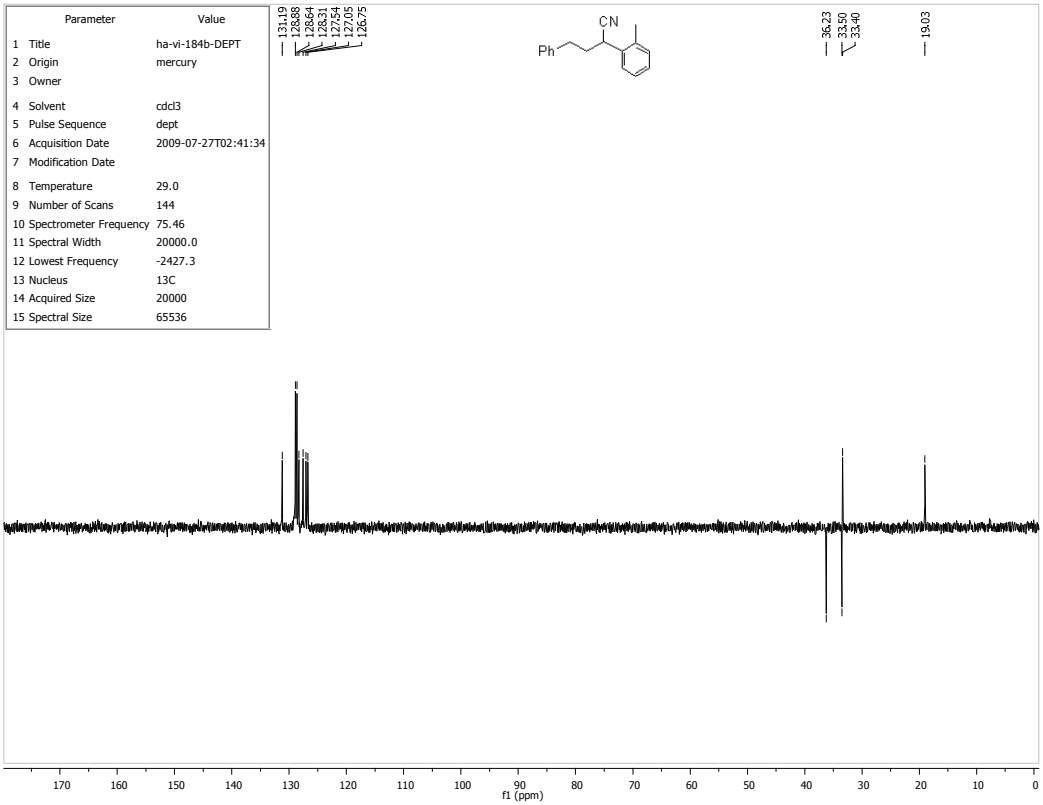

Parameter Value
1 Title ha-vi-185d
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-26T03:32:35
7 Modification Date
8 Temperature 29.0
9 Number of Scans 8
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -945.9
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
Ph
10.7
1.0
2.3
2.4
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

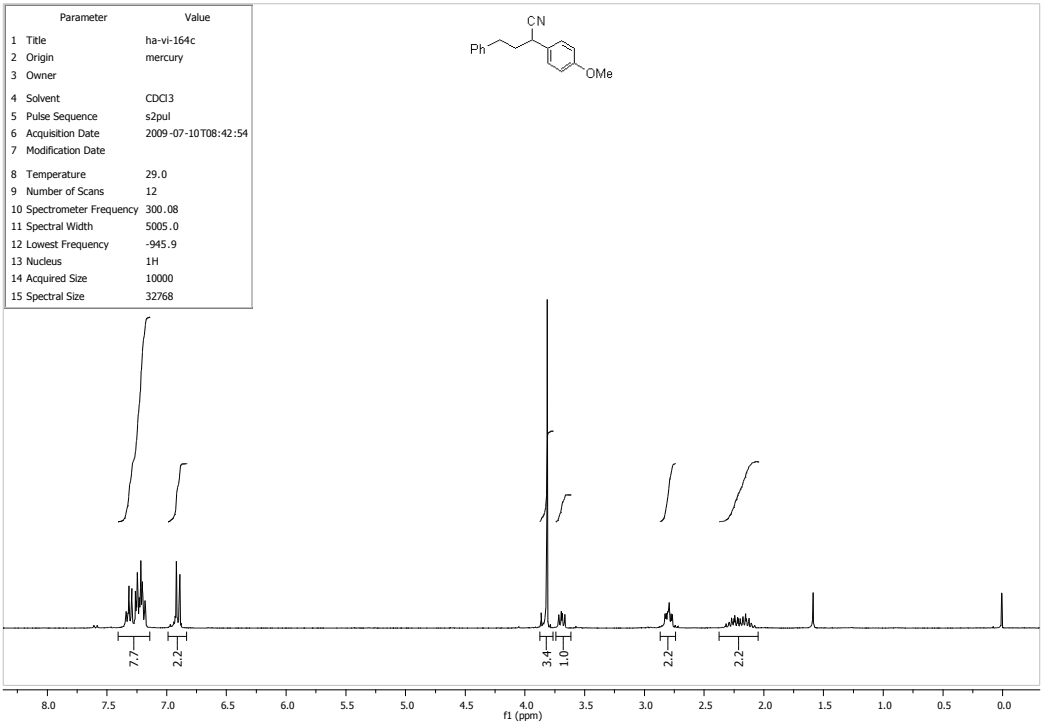

139.98
135.81
129.32
128.88
128.63
128.34
127.48
126.70
120.84
77.65
77.23
76.81
37.57
36.75
33.23
CN
Ph
Parameter Value
1 Title ha-vi-175f-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-17T08:19:19
7 Modification Date
8 Temperature 29.0
9 Number of Scans 160
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2426.7
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)

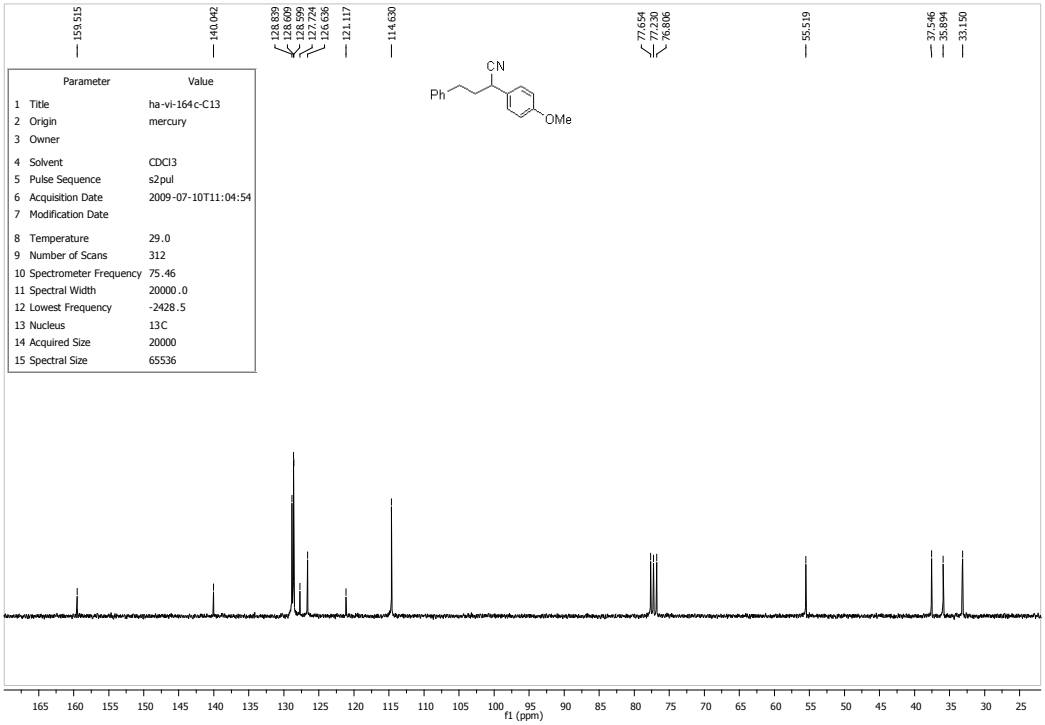

129.29
128.86
128.61
128.31
127.45
126.67
37.54
36.72
33.21
CN
Ph
Parameter Value
1 Title ha-vi-158h-DEPT
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-03T03:14:20
7 Modification Date
8 Temperature 29.0
9 Number of Scans 128
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2428.5
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

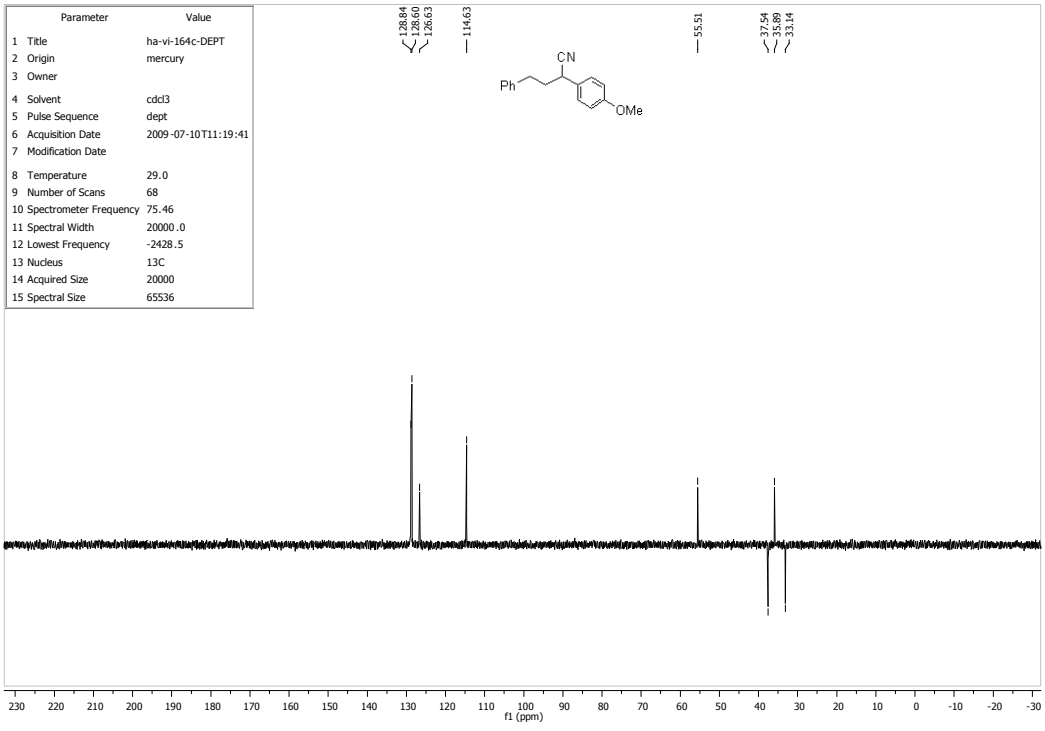

Parameter Value
1 Title ha-vi-184b-2
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-26T03:34:58
7 Modification Date
8 Temperature 29.0
9 Number of Scans 12
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -951.6
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
Ph
10.1
1.0
2.3
6.1
f1 (ppm)

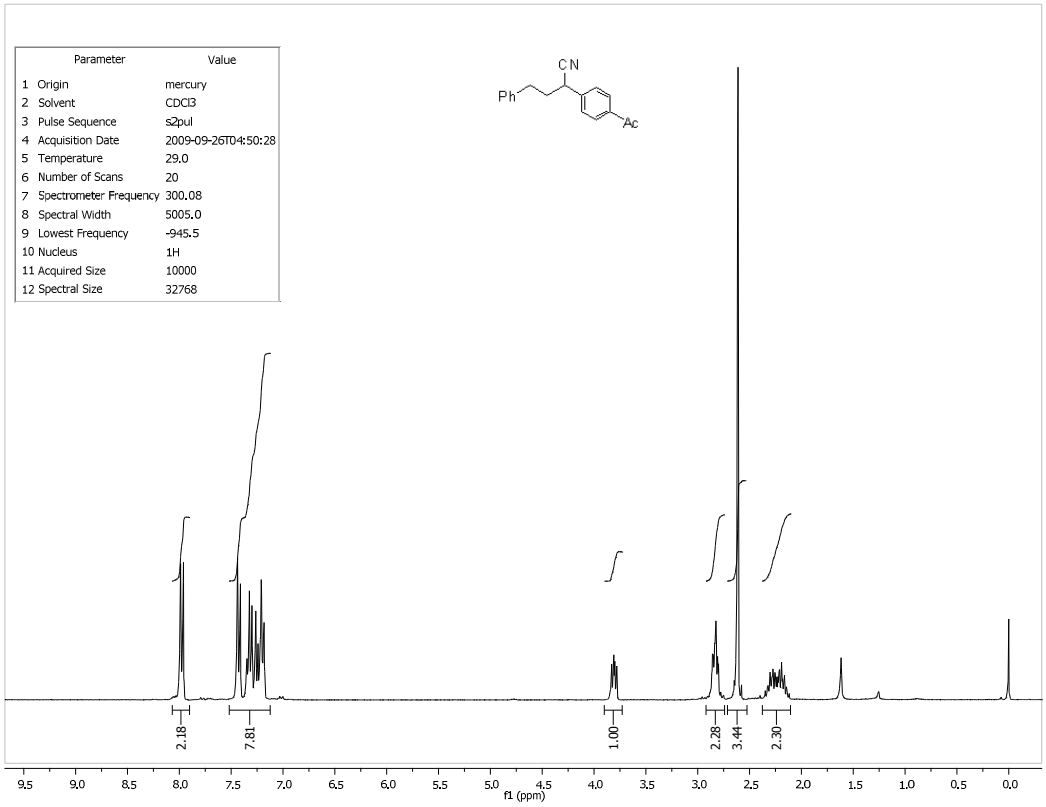

139.95
135.07
127.54
127.05
126.75
121.07
77.65
77.22
76.80
36.24
33.50
33.40
19.03
Parameter Value
1 Title ha-vi-184b-2-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-26T03:37:16
7 Modification Date
8 Temperature 29.0
9 Number of Scans 192
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2427.3
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
CN
Ph
f1 (ppm)

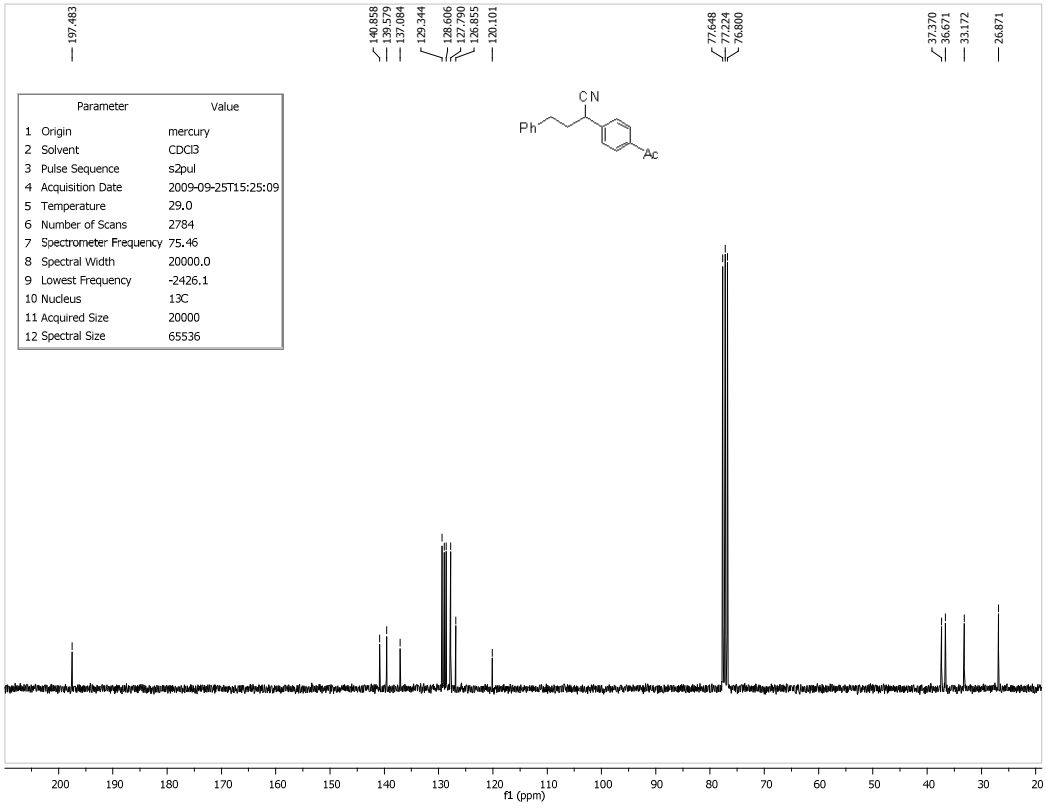

Parameter Value
1 Title ha-vi-184b-DEPT
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-27T02:41:34
7 Modification Date
8 Temperature 29.0
9 Number of Scans 144
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2427.3
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
131.19
128.88
128.64
128.31
127.54
127.05
126.75
CN
Ph
36.23
33.50
33.40
19.03
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Parameter Value
1 Title ha-vi-164c
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-10T08:42:54
7 Modification Date
8 Temperature 29.0
9 Number of Scans 12
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -945.9
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
Ph
OMe
7.7
2.2
3.4
1.0
2.2
2.2
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

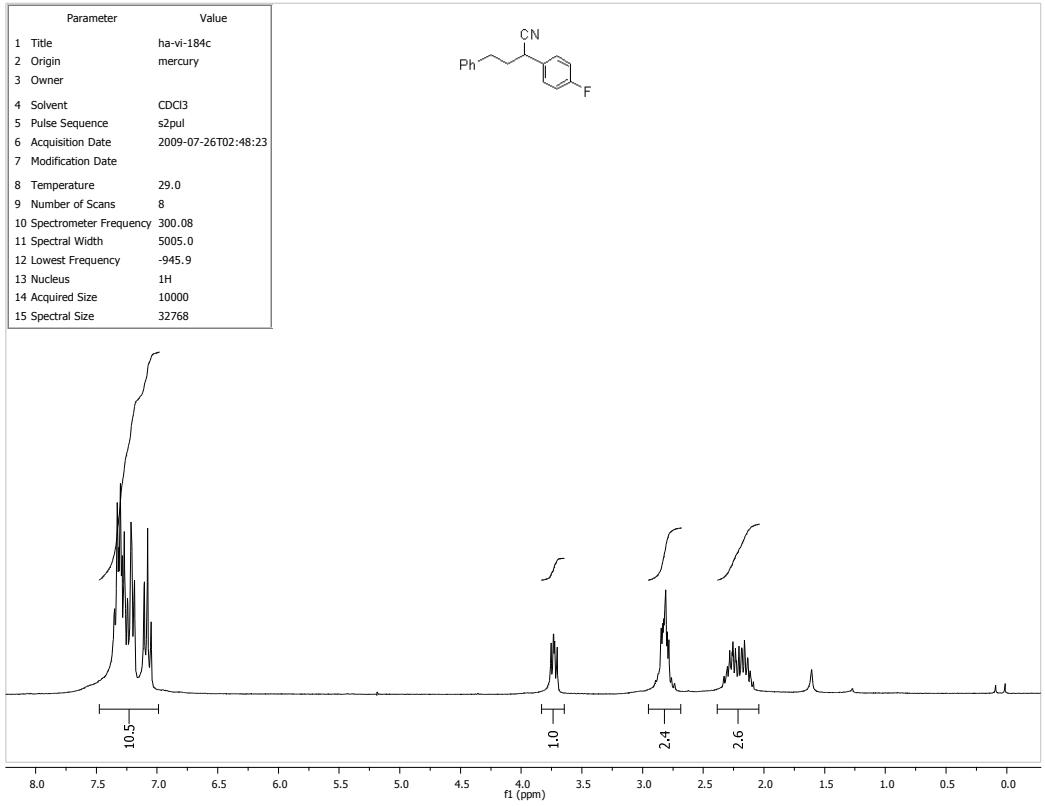

159.515
140.042
128.839
128.609
128.599
127.724
126.636
121.117
114.630
77.654
77.230
76.806
55.519
37.546
35.894
33.150
CN
Ph
OMe
Parameter Value
1 Title ha-vi-164c-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-10T11:04:54
7 Modification Date
8 Temperature 29.0
9 Number of Scans 312
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2428.5
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
f1 (ppm)

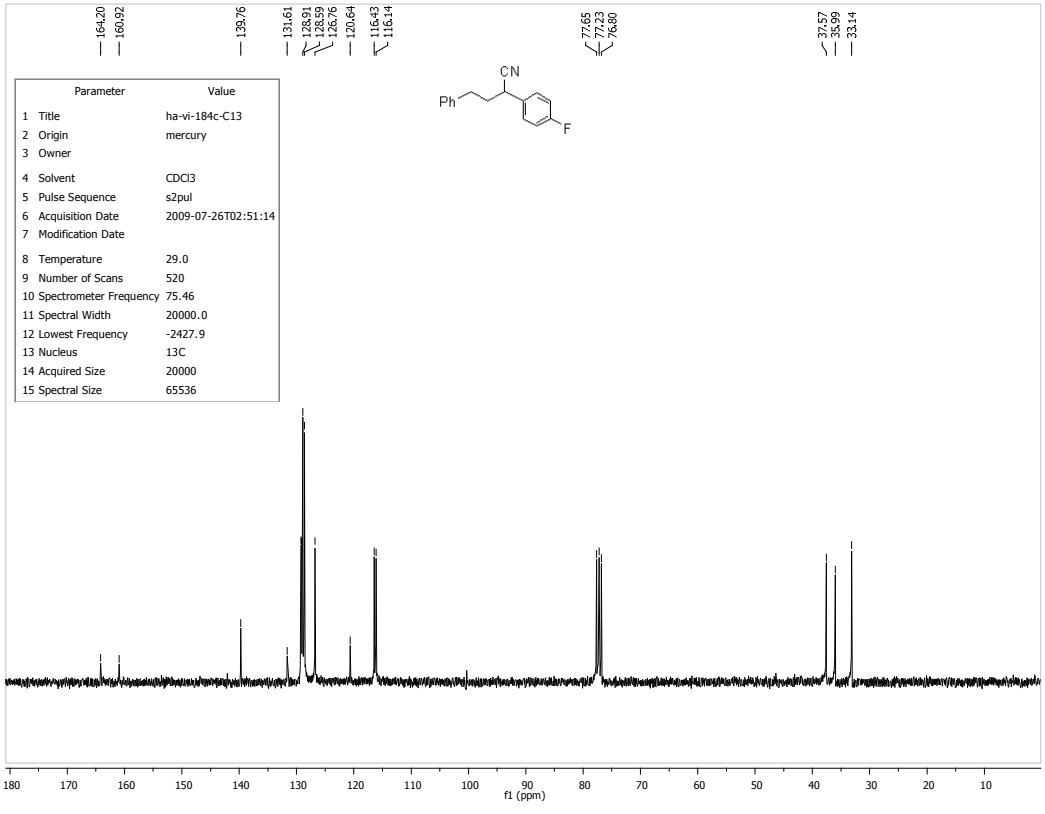

128.84
128.60
126.63
114.63
55.51
37.54
35.89
33.14
CN
Ph
OMe
Parameter Value
1 Title ha-vi-164c-DEPT
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-10T11:19:41
7 Modification Date
8 Temperature 29.0
9 Number of Scans 68
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2428.5
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
f1 (ppm)


Parameter Value
1 Origin mercury
2 Solvent CDCl3
3 Pulse Sequence s2pul
4 Acquisition Date 2009-09-26T04:50:28
5 Temperature 29.0
6 Number of Scans 20
7 Spectrometer Frequency 300.08
8 Spectral Width 5005.0
9 Lowest Frequency -945.5
10 Nucleus 1H
11 Acquired Size 10000
12 Spectral Size 32768
CN
Ph
Ac
2.18
7.81
1.00
2.28
3.44
2.30
f1 (ppm)

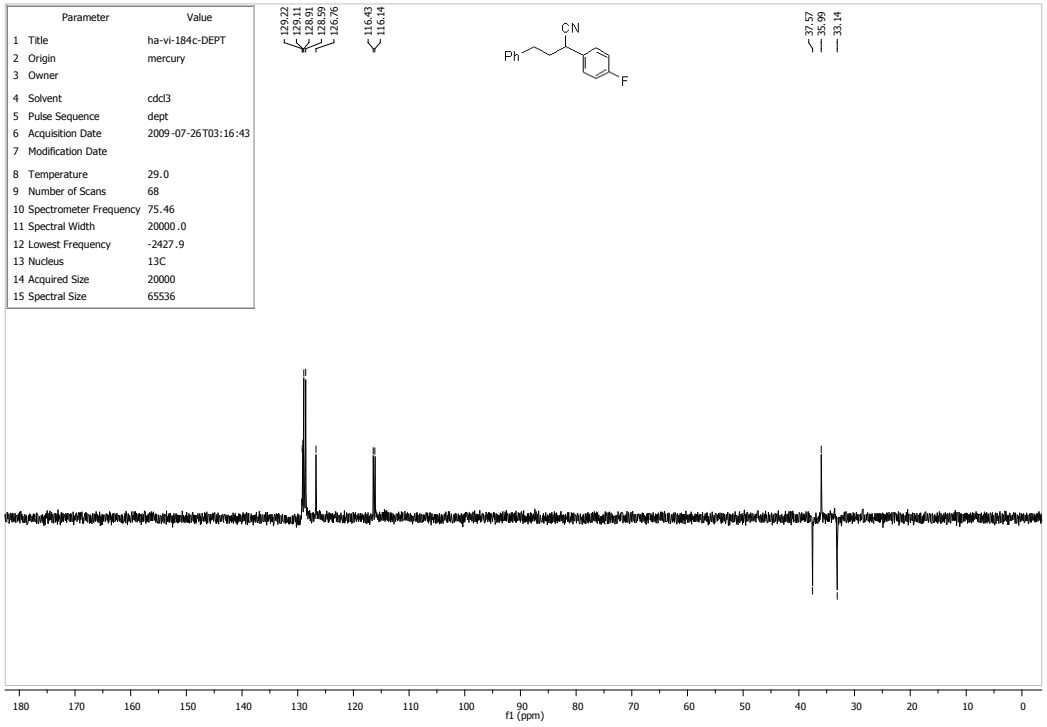

197.483
140.858
139.579
137.084
129.344
128.606
127.790
126.855
120.101
77.648
77.224
76.800
37.370
36.671
33.172
26.871
Parameter Value
1 Origin mercury
2 Solvent CDCl3
3 Pulse Sequence s2pul
4 Acquisition Date 2009-09-25T15:25:09
5 Temperature 29.0
6 Number of Scans 2784
7 Spectrometer Frequency 75.46
8 Spectral Width 20000.0
9 Lowest Frequency -2426.1
10 Nucleus 13C
11 Acquired Size 20000
12 Spectral Size 65536
CN
Ph
Ac
f1 (ppm)

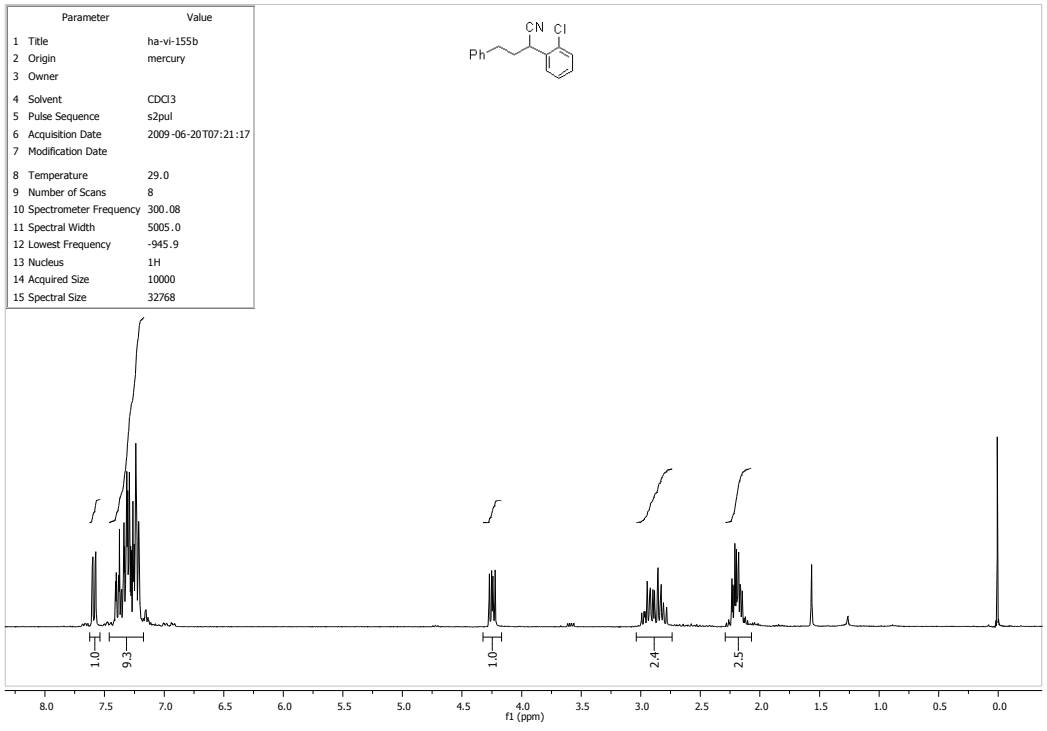
	Parameter	Value
1	Title	ha-vi-184c
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-07-26T02:48:23
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	8
10	Spectrometer Frequency	300.08
11	Spectral Width	5005.0
12	Lowest Frequency	-945.9
13	Nucleus	1H
14	Acquired Size	10000
15	Spectral Size	32768

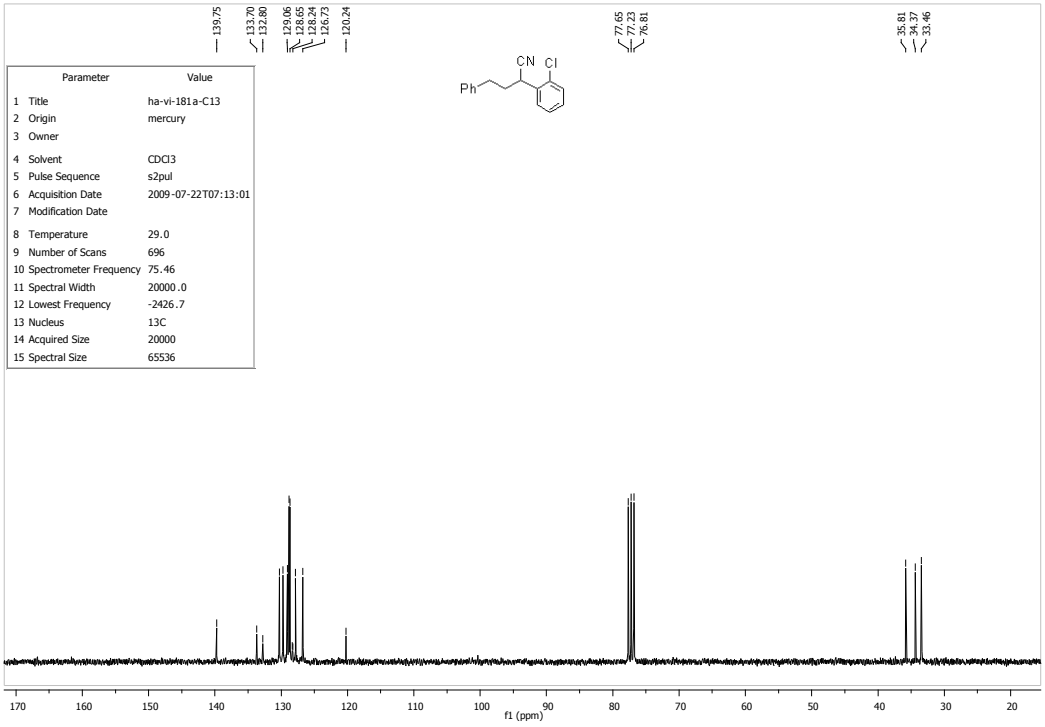


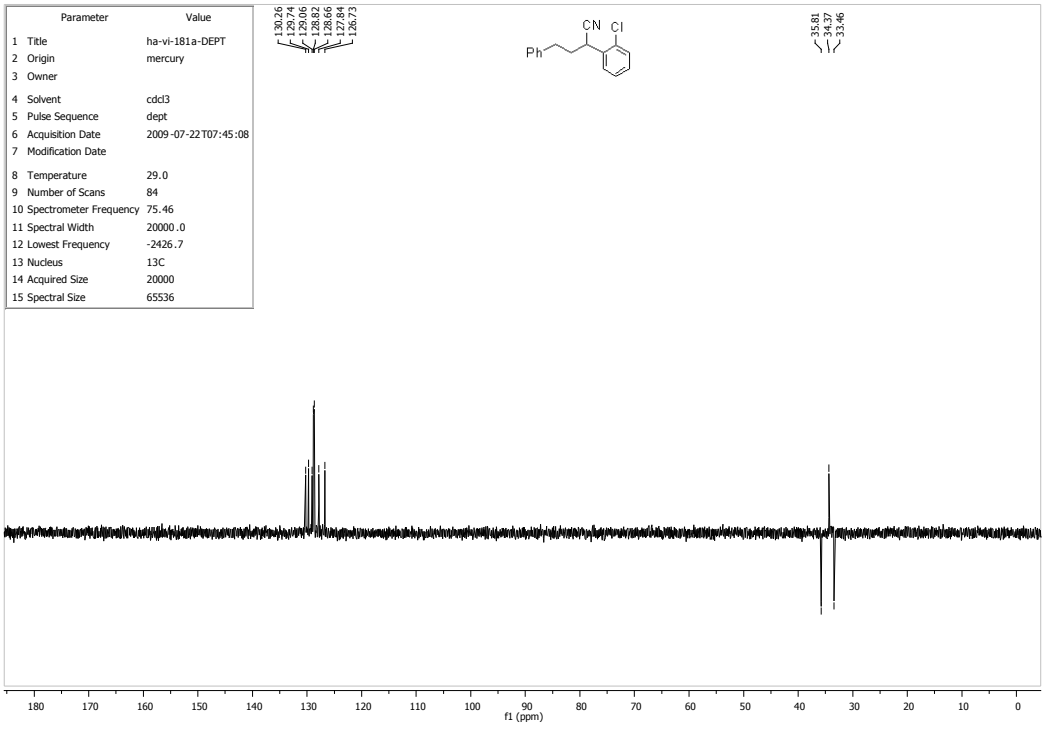


	Parameter	Value
1	Title	ha-vi-184c-C13
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-07-26T02:51:14
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	520
10	Spectrometer Frequency	75.46
11	Spectral Width	20000.0
12	Lowest Frequency	-2427.9
13	Nucleus	13C
14	Acquired Size	20000
15	Spectral Size	65536

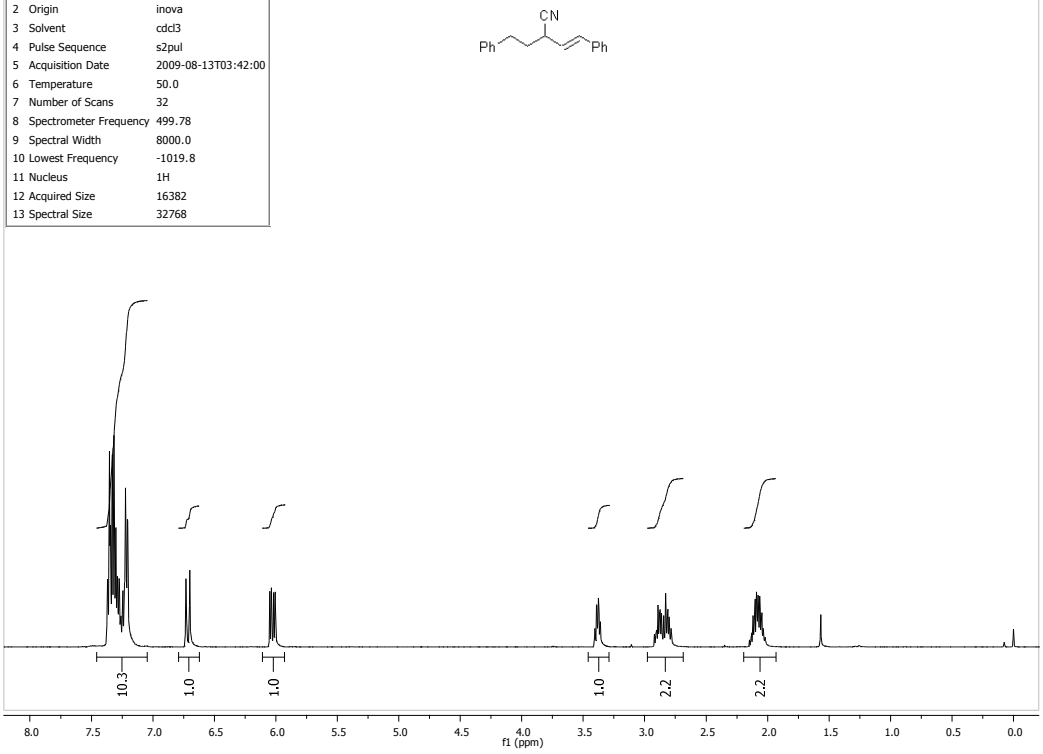

Parameter Value
1 Title ha-vi-184c-DEPT
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-26T03:16:43
7 Modification Date
8 Temperature 29.0
9 Number of Scans 68
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2427.9
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
129.22
129.11
128.91
128.59
126.76
116.43
116.14
37.57
35.99
33.14
CN
Ph
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

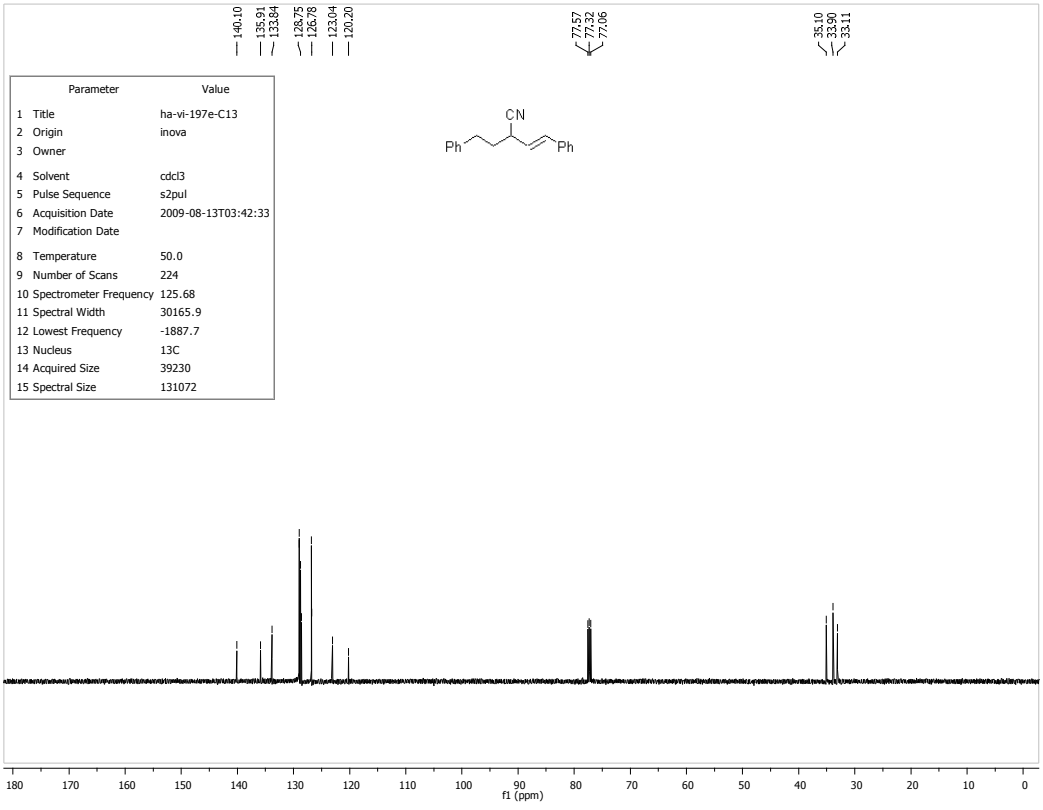

Parameter Value
1 Title ha-vi-155b
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-06-20T07:21:17
7 Modification Date
8 Temperature 29.0
9 Number of Scans 8
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -945.9
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
Cl
Ph
1.0
9.3
1.0
2.4
2.5
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


139.75
133.70
132.80
129.06
128.65
128.24
126.73
120.24
77.65
77.23
76.81
35.81
34.37
33.46
CN
Cl
Ph
Parameter Value
1 Title ha-vi-181a-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-22T07:13:01
7 Modification Date
8 Temperature 29.0
9 Number of Scans 696
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2426.7
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


130.26
129.74
129.06
128.82
128.66
127.84
126.73
35.81
34.37
33.46
CN
Cl
Ph
Parameter Value
1 Title ha-vi-181a-DEPT
2 Origin mercury
3 Owner
4 Solvent cdcl3
5 Pulse Sequence dept
6 Acquisition Date 2009-07-22T07:45:08
7 Modification Date
8 Temperature 29.0
9 Number of Scans 84
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2426.7
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

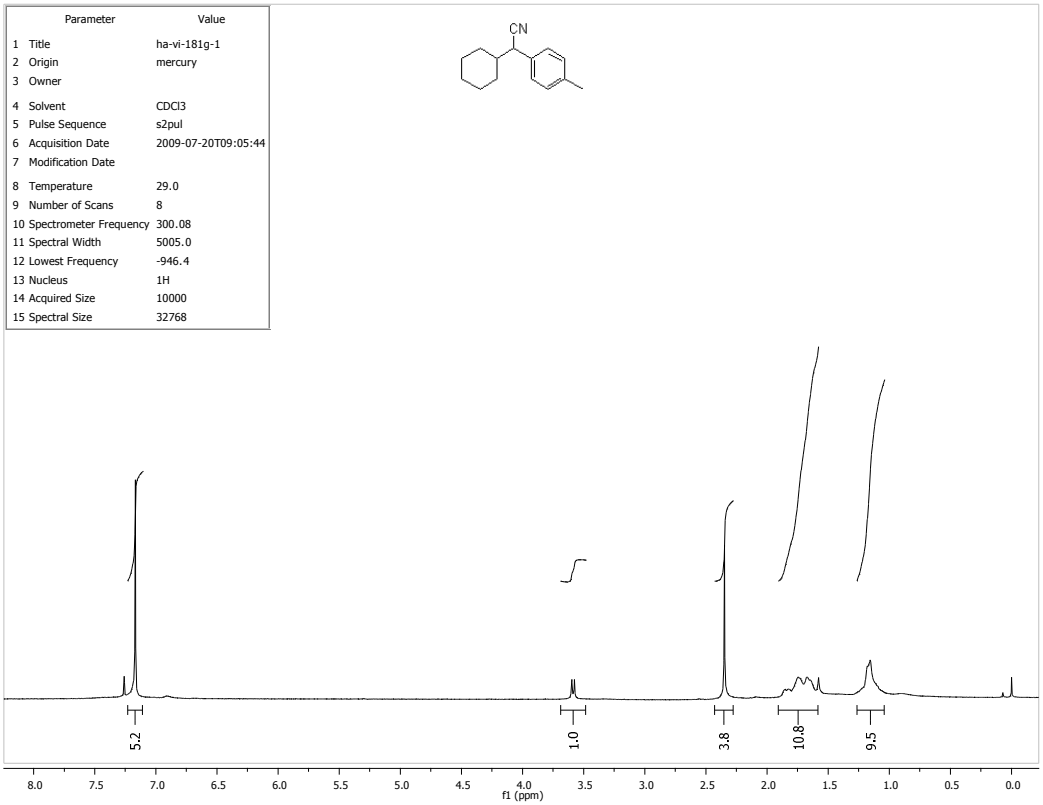
	Parameter	Value
1	Title	ha-vi-197e
2	Origin	inova
3	Solvent	cdcl3
4	Pulse Sequence	s2pul
5	Acquisition Date	2009-08-13T03:42:00
6	Temperature	50.0
7	Number of Scans	32
8	Spectrometer Frequency	499.78
9	Spectral Width	8000.0
10	Lowest Frequency	-1019.8
11	Nucleus	1H
12	Acquired Size	16382
13	Spectral Size	32768

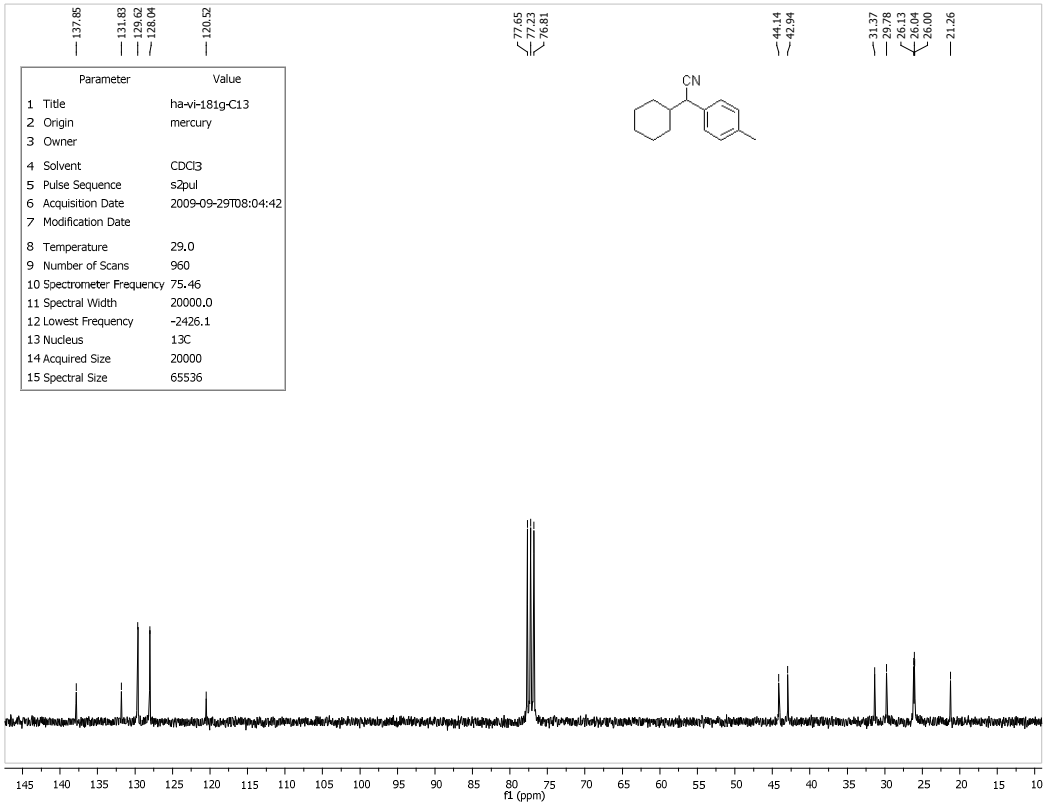




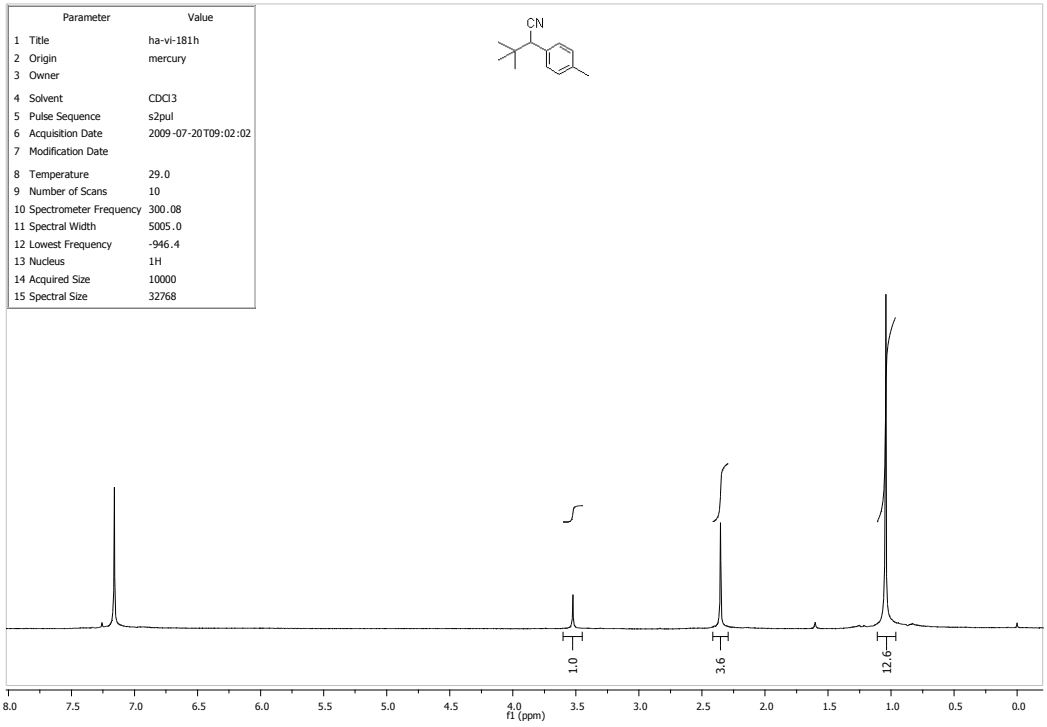
	Parameter	Value
1	Title	ha-vi-197e-C13
2	Origin	inova
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-08-13T03:42:33
7	Modification Date	
8	Temperature	50.0
9	Number of Scans	224
10	Spectrometer Frequency	125.68
11	Spectral Width	30165.9
12	Lowest Frequency	-1887.7
13	Nucleus	13C
14	Acquired Size	39230
15	Spectral Size	131072

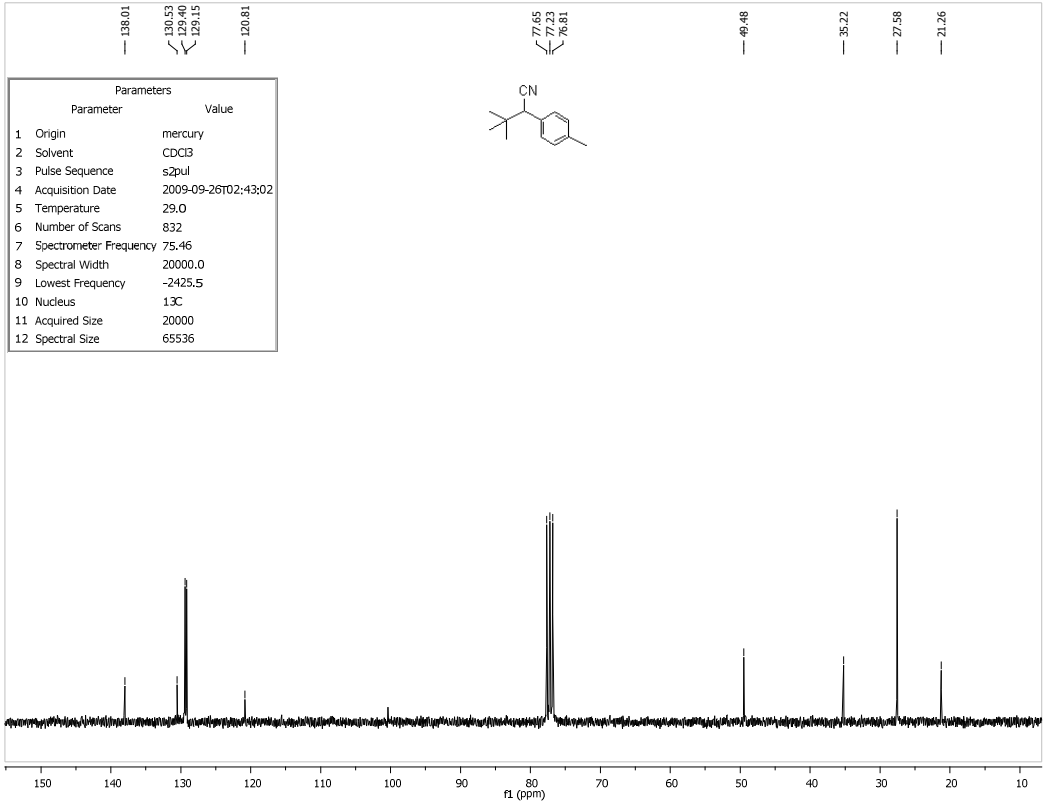
	Parameter	Value
1	Title	ha-vi-181g-1
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-07-20T09:05:44
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	8
10	Spectrometer Frequency	300.08
11	Spectral Width	5005.0
12	Lowest Frequency	-946.4
13	Nucleus	1H
14	Acquired Size	10000
15	Spectral Size	32768

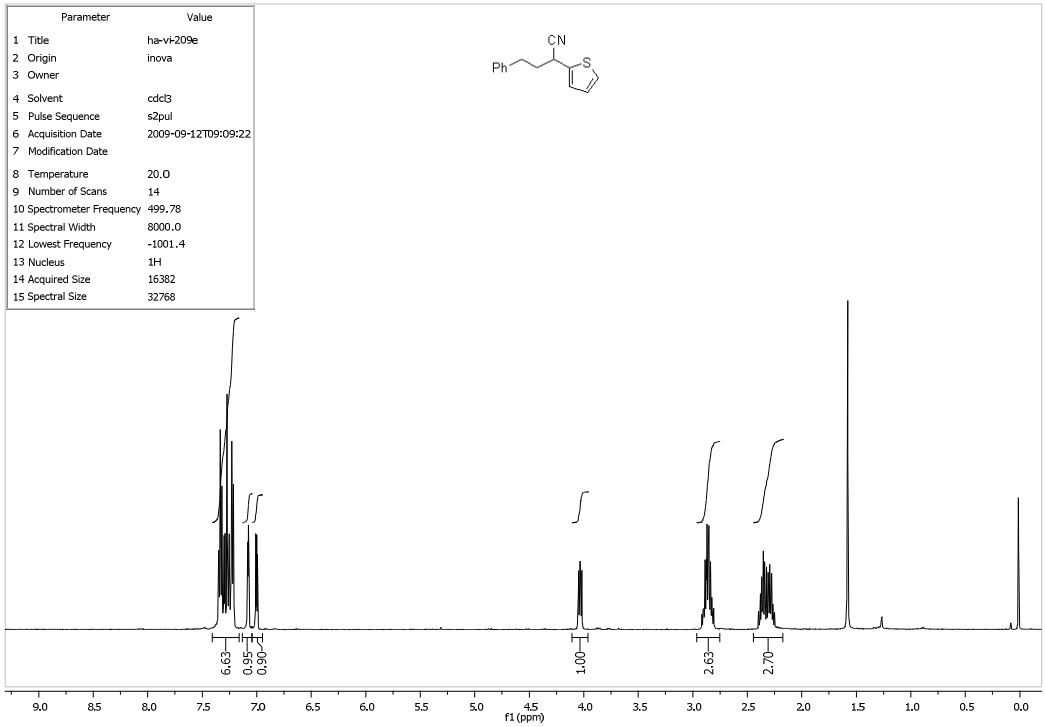


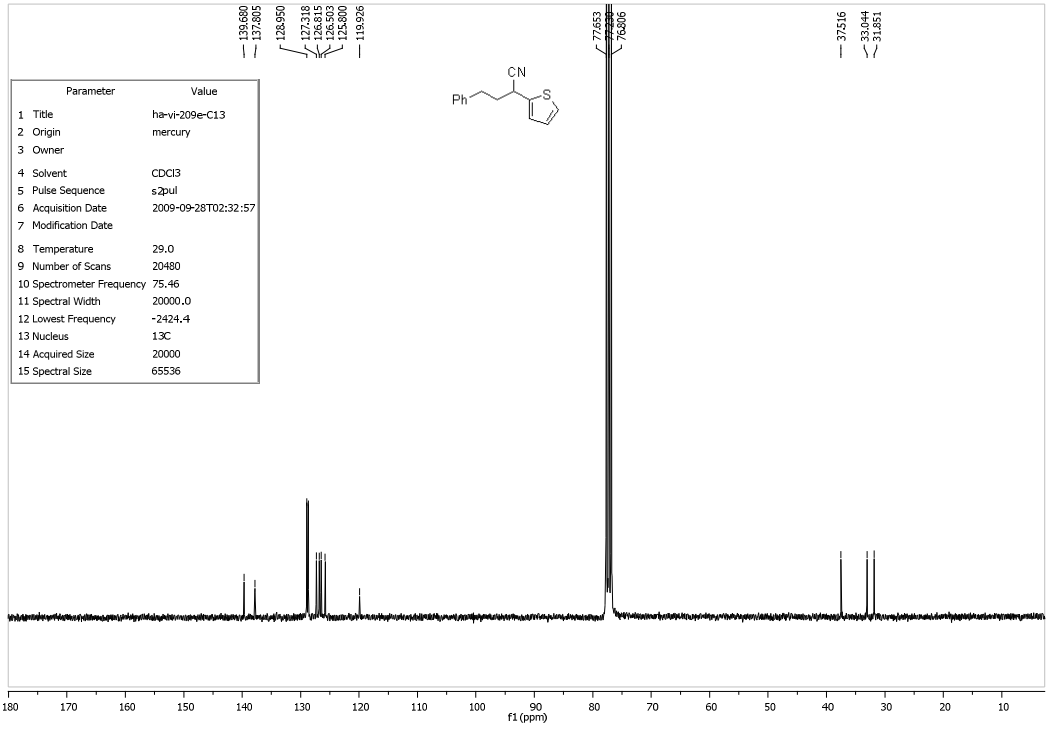


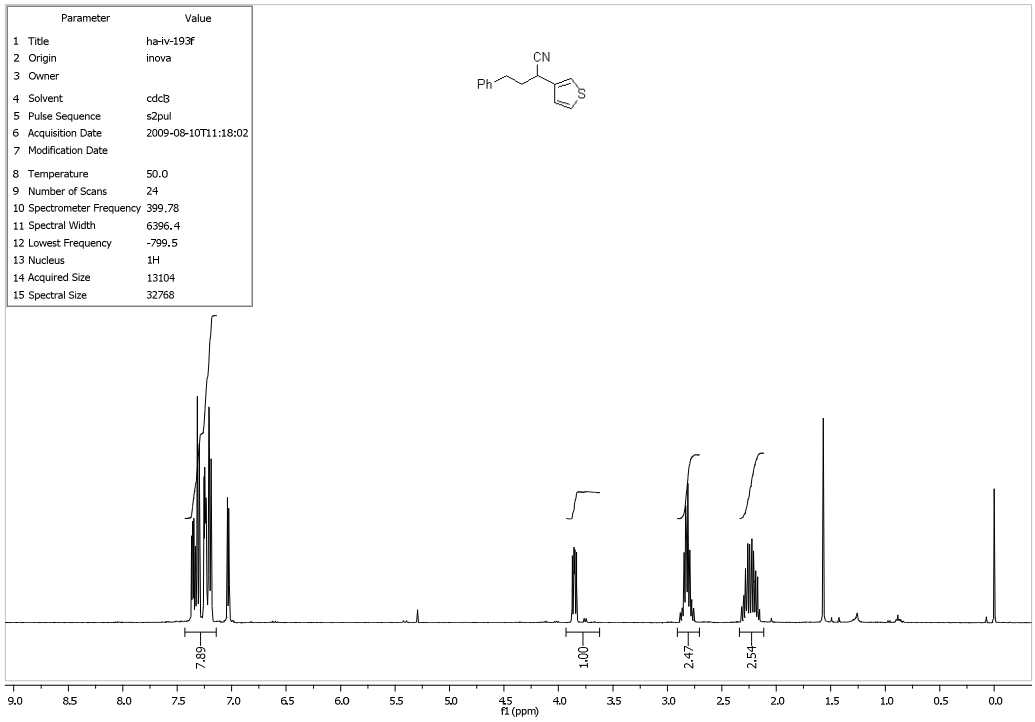
	Parameter	Value
1	Title	ha-vi-181g-C13
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2009-09-29T08:04:42
7	Modification Date	
8	Temperature	29.0
9	Number of Scans	960
10	Spectrometer Frequency	75.46
11	Spectral Width	20000.0
12	Lowest Frequency	-2426.1
13	Nucleus	13C
14	Acquired Size	20000
15	Spectral Size	65536

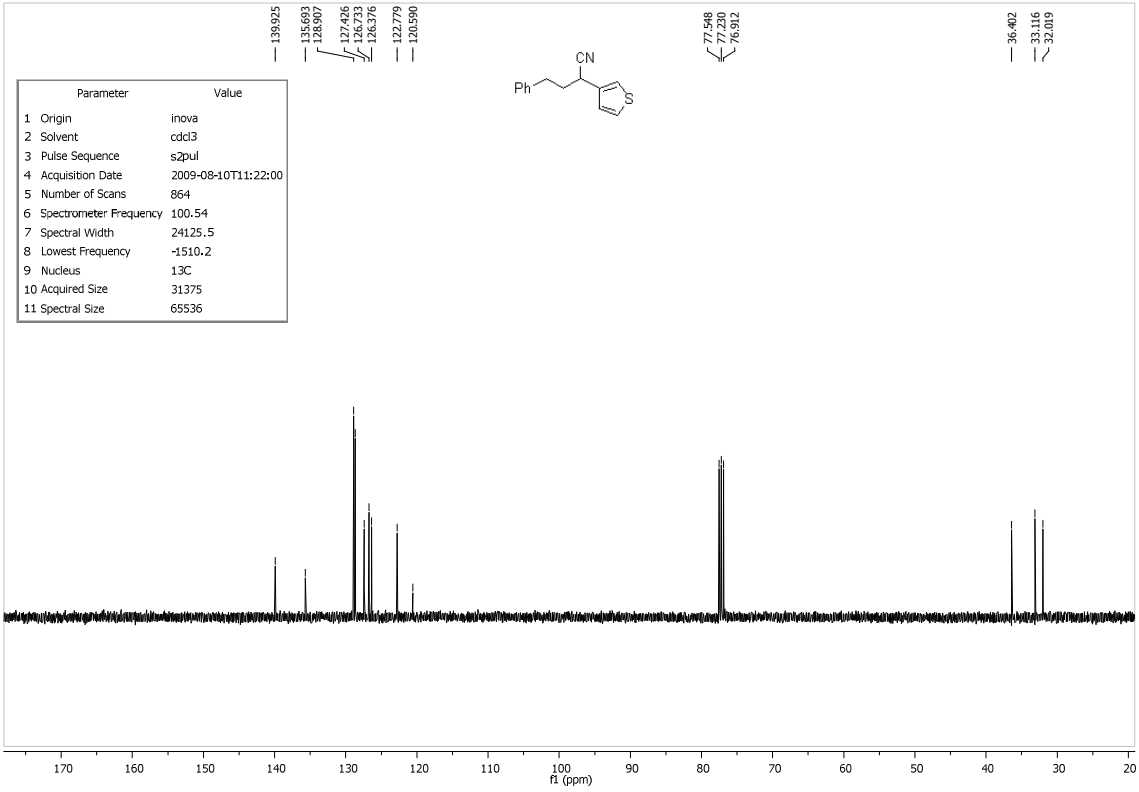

Parameter Value
1 Title ha-vi-181h
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-07-20T09:02:02
7 Modification Date
8 Temperature 29.0
9 Number of Scans 10
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -946.4
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
CN
1.0
3.6
12.6
f1 (ppm)

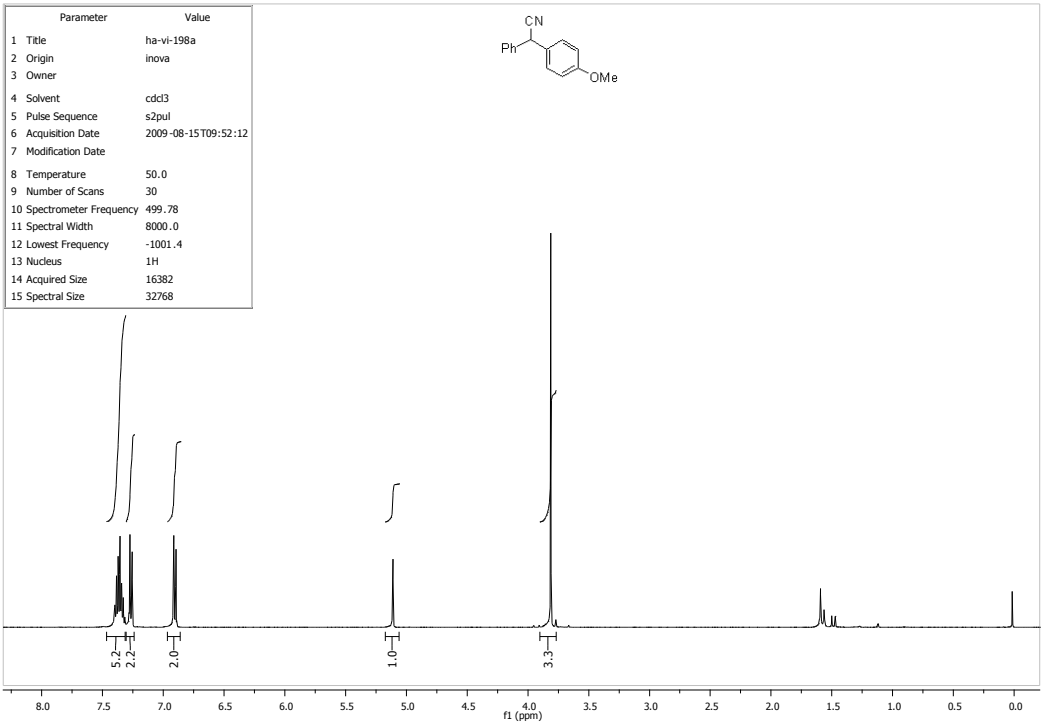

138.01
130.53
129.40
129.15
120.81
77.65
77.23
76.81
49.48
35.22
27.58
21.26
Parameters
Parameter Value
1 Origin mercury
2 Solvent CDCl3
3 Pulse Sequence s2pul
4 Acquisition Date 2009-09-26T02:43:02
5 Temperature 29.0
6 Number of Scans 832
7 Spectrometer Frequency 75.46
8 Spectral Width 20000.0
9 Lowest Frequency -2425.5
10 Nucleus 13C
11 Acquired Size 20000
12 Spectral Size 65536
CN
f1 (ppm)

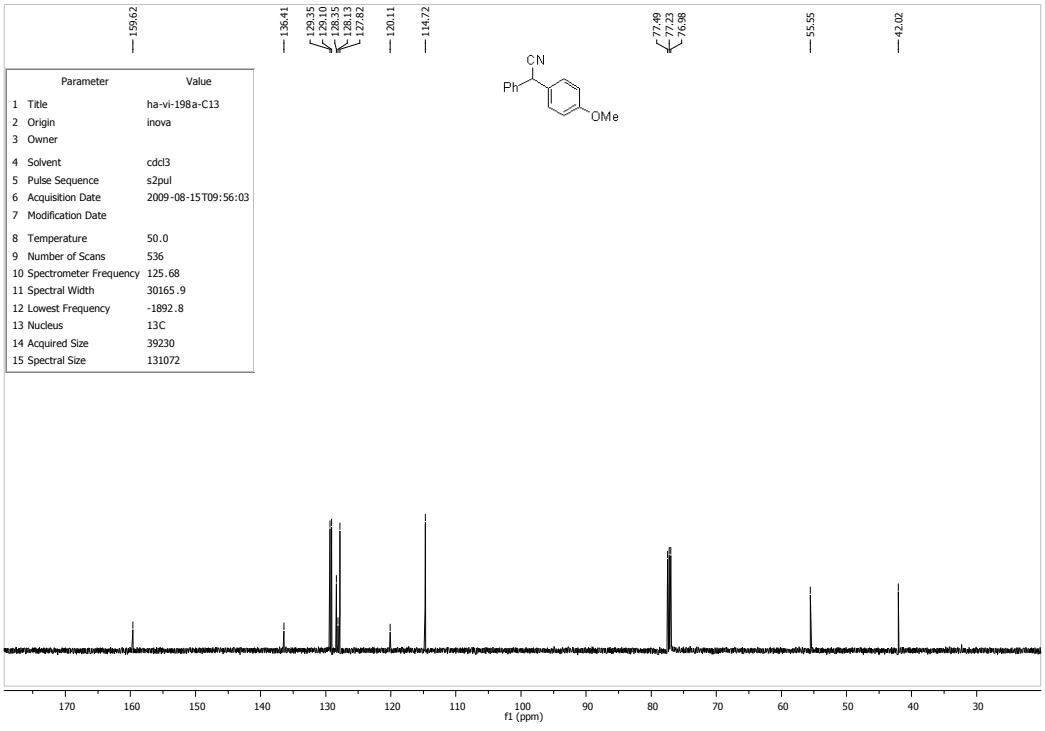

Parameter Value
1 Title ha-vi-209e
2 Origin inova
3 Owner
4 Solvent cdcl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-09-12T09:09:22
7 Modification Date
8 Temperature 20.0
9 Number of Scans 14
10 Spectrometer Frequency 499.78
11 Spectral Width 8000.0
12 Lowest Frequency -1001.4
13 Nucleus 1H
14 Acquired Size 16382
15 Spectral Size 32768
CN
Ph
S
6.63
0.95
0.90
1.00
2.63
2.70
f1 (ppm)

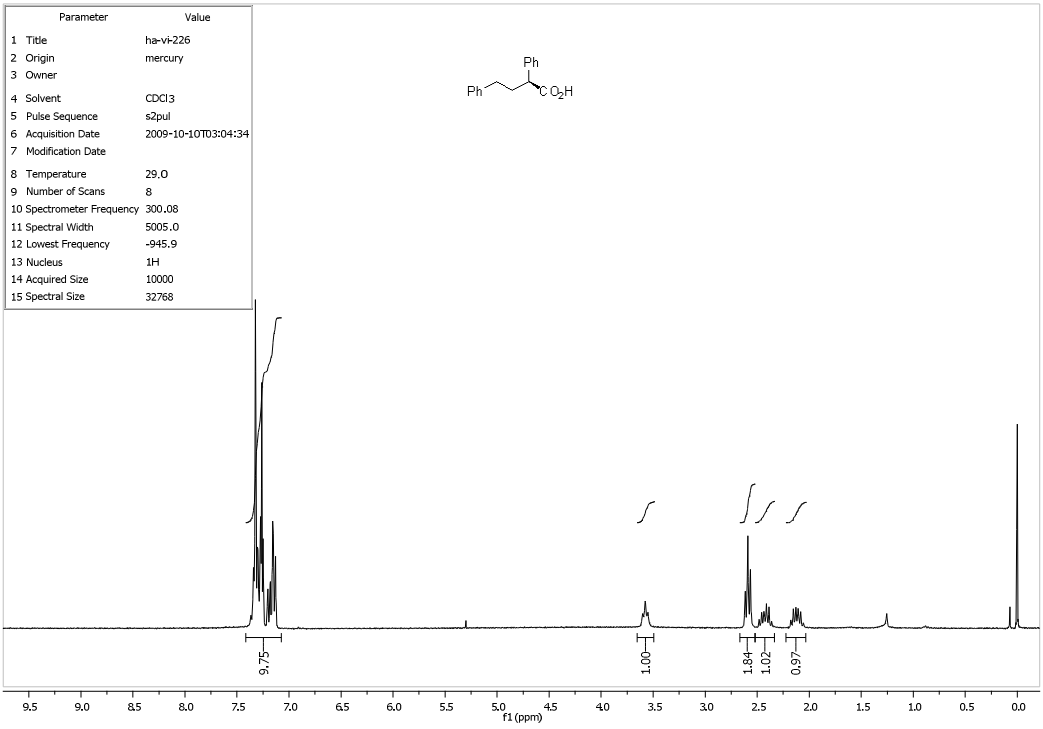

139.680
137.805
128.950
127.318
126.815
126.503
125.800
119.926
77.653
77.339
76.806
37.516
33.044
31.851
Parameter Value
1 Title ha-vi-209e-C13
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-09-28T02:32:57
7 Modification Date
8 Temperature 29.0
9 Number of Scans 20480
10 Spectrometer Frequency 75.46
11 Spectral Width 20000.0
12 Lowest Frequency -2424.4
13 Nucleus 13C
14 Acquired Size 20000
15 Spectral Size 65536
CN
Ph
S
f1 (ppm)


Parameter Value
1 Title ha-iv-193f
2 Origin inova
3 Owner
4 Solvent cdcl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-08-10T11:18:02
7 Modification Date
8 Temperature 50.0
9 Number of Scans 24
10 Spectrometer Frequency 399.78
11 Spectral Width 6396.4
12 Lowest Frequency -799.5
13 Nucleus 1H
14 Acquired Size 13104
15 Spectral Size 32768
CN
Ph
S
7.89
1.00
2.47
2.54
f1 (ppm)


139.925
135.693
128.907
127.426
126.733
126.376
122.779
120.590
77.548
77.230
76.912
36.402
33.116
32.019
Parameter Value
1 Origin inova
2 Solvent cdcl3
3 Pulse Sequence s2pul
4 Acquisition Date 2009-08-10T11:22:00
5 Number of Scans 864
6 Spectrometer Frequency 100.54
7 Spectral Width 24125.5
8 Lowest Frequency -1510.2
9 Nucleus 13C
10 Acquired Size 31375
11 Spectral Size 65536
CN
Ph
O
f1 (ppm)


Parameter Value
1 Title ha-vi-198a
2 Origin inova
3 Owner
4 Solvent cdcl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-08-15T09:52:12
7 Modification Date
8 Temperature 50.0
9 Number of Scans 30
10 Spectrometer Frequency 499.78
11 Spectral Width 8000.0
12 Lowest Frequency -1001.4
13 Nucleus 1H
14 Acquired Size 16382
15 Spectral Size 32768
CN
Ph
OMe
5.2
2.2
2.0
1.0
3.3
f1 (ppm)


159.62
136.41
129.35
129.10
128.35
128.13
127.82
120.11
114.72
77.49
77.23
76.98
55.55
42.02
Parameter Value
1 Title ha-vi-198a-C13
2 Origin inova
3 Owner
4 Solvent cdcl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-08-15T09:56:03
7 Modification Date
8 Temperature 50.0
9 Number of Scans 536
10 Spectrometer Frequency 125.68
11 Spectral Width 30165.9
12 Lowest Frequency -1892.8
13 Nucleus 13C
14 Acquired Size 39230
15 Spectral Size 131072
CN
Ph
OMe
f1 (ppm)


Parameter Value
1 Title ha-vi-226
2 Origin mercury
3 Owner
4 Solvent CDCl3
5 Pulse Sequence s2pul
6 Acquisition Date 2009-10-10T03:04:34
7 Modification Date
8 Temperature 29.0
9 Number of Scans 8
10 Spectrometer Frequency 300.08
11 Spectral Width 5005.0
12 Lowest Frequency -945.9
13 Nucleus 1H
14 Acquired Size 10000
15 Spectral Size 32768
Ph
Ph
CO2H
9.75
1.00
1.84
1.02
0.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)